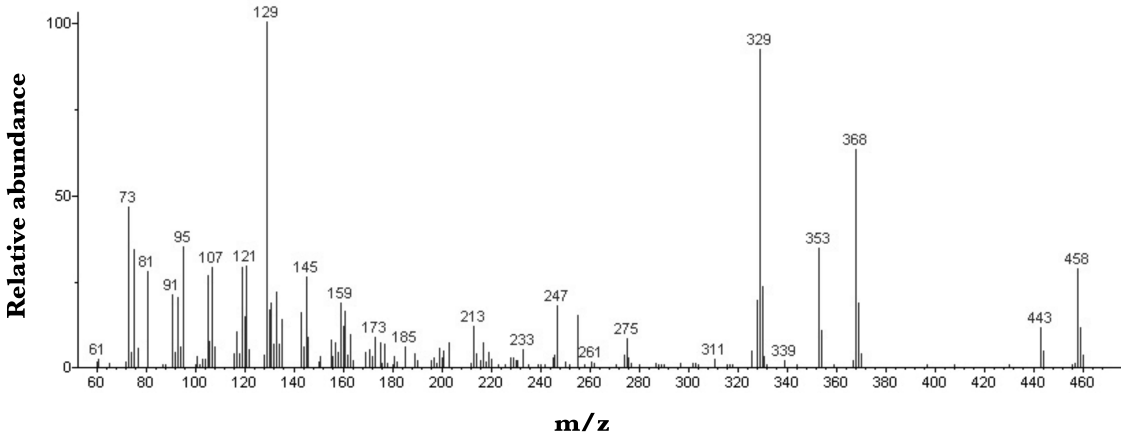
Appendix list

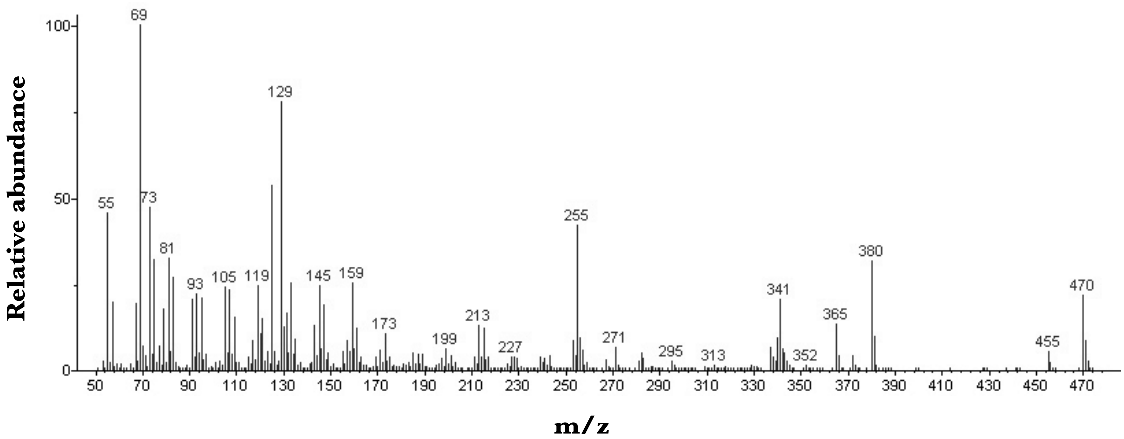
Appendix 3.1. Sterol TMS derivative mass spectra

Sterol 1TMS ethers were verified by comparison of mass spectra with entries in a library of MEOX/TMS-derivatised plant metabolites (Kopka et al., 2005) and with published mass isotopomer distributions. The following are those mass spectra found in BY-2 hexane extracts that were identified as sterols.

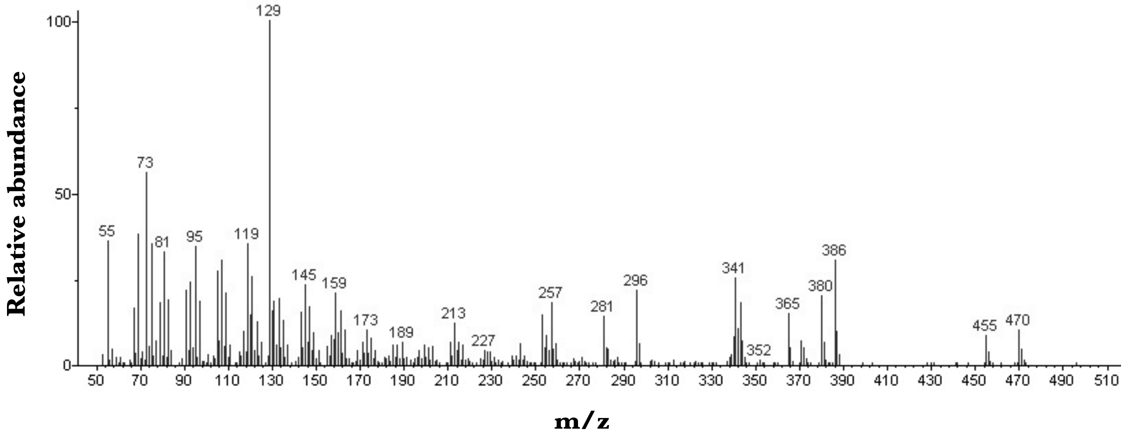
Cholesterol (1TMS): 52.86 min



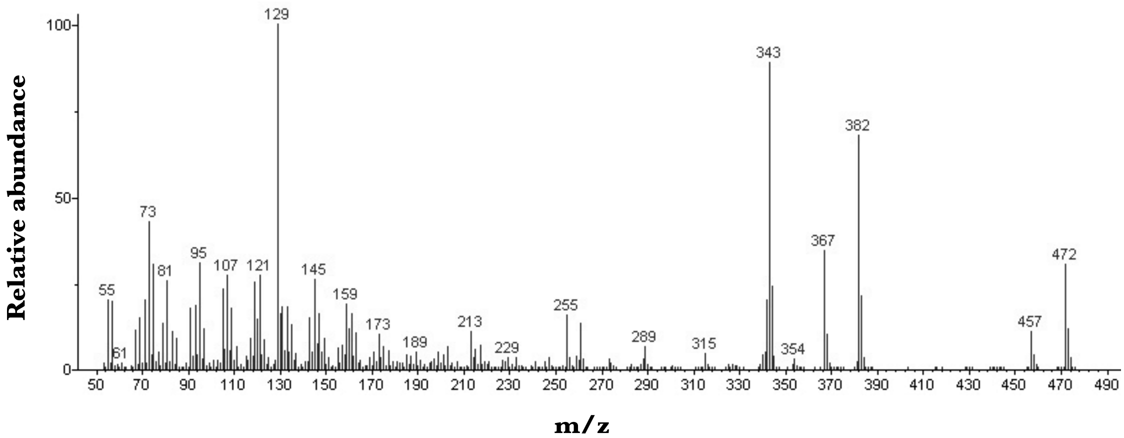
Brassicasterol (1TMS): 53.98 min



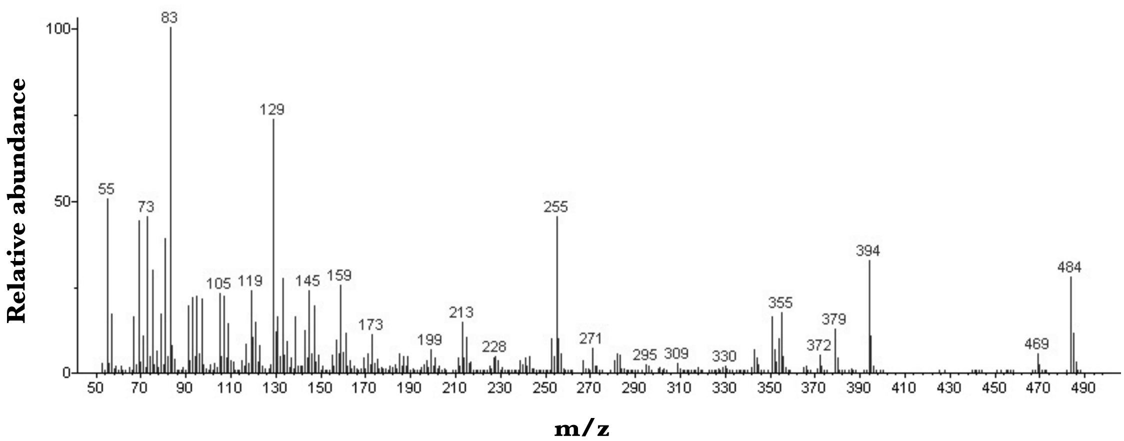
24-methylene cholesterol (1TMS) (Weete and Gandhi, 1997): 54.11 min



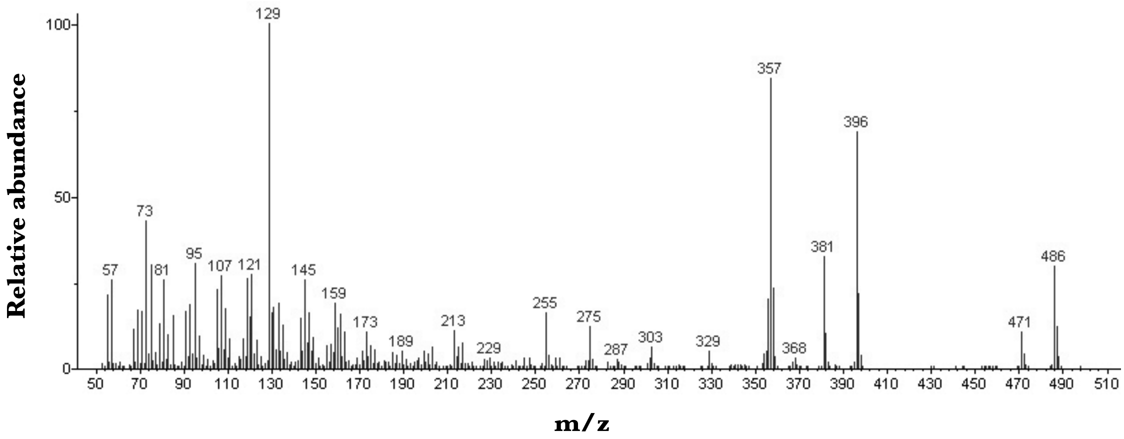
Campesterol (1TMS): 54.22 min



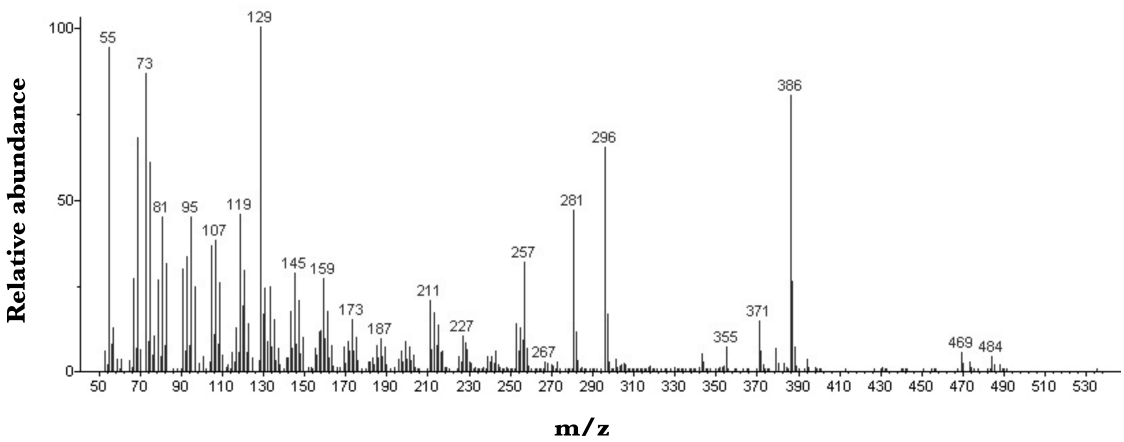
Stigmasterol (1TMS): 54.50 min



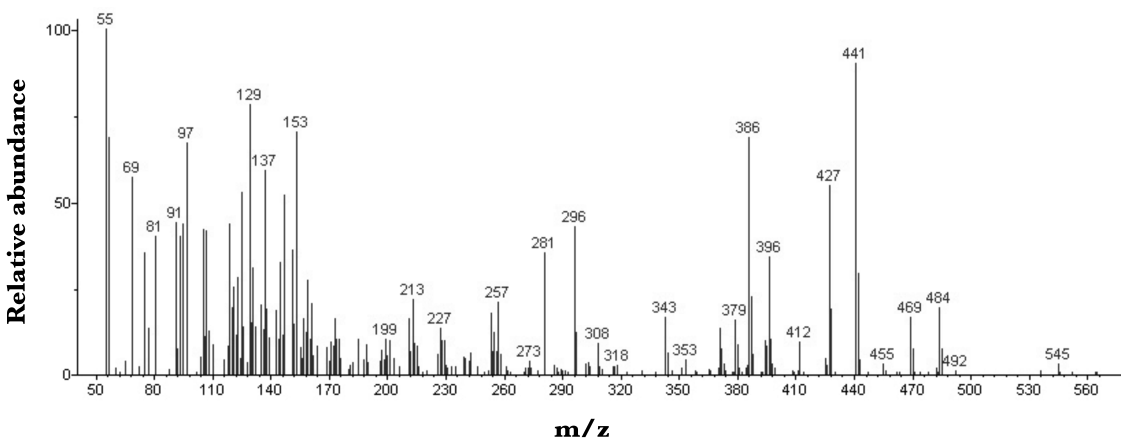
Sitosterol (1TMS): 55.25 min



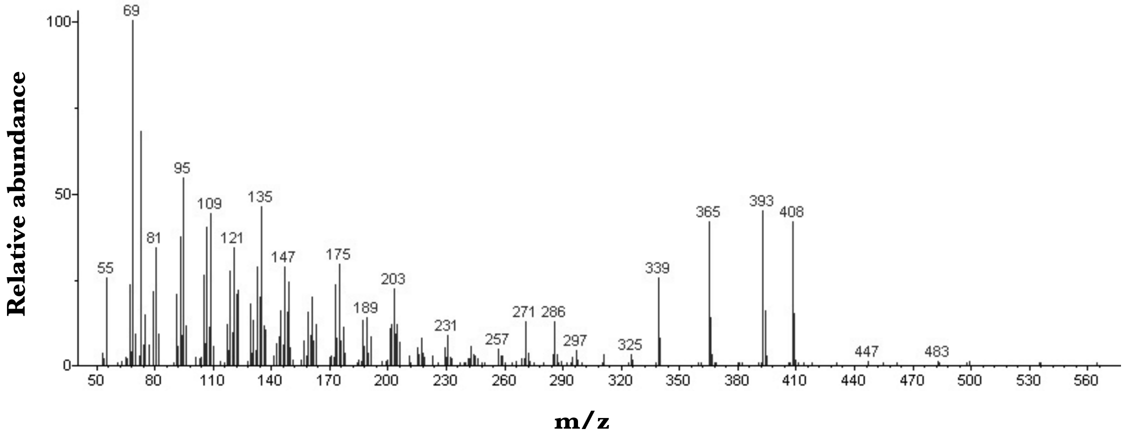
Fucosterol (1TMS): 55.42 min



Δ⁵-avenasterol (1TMS) (Kamal-Eldin et al., 1998; Xu et al., 2012): 55.71 min

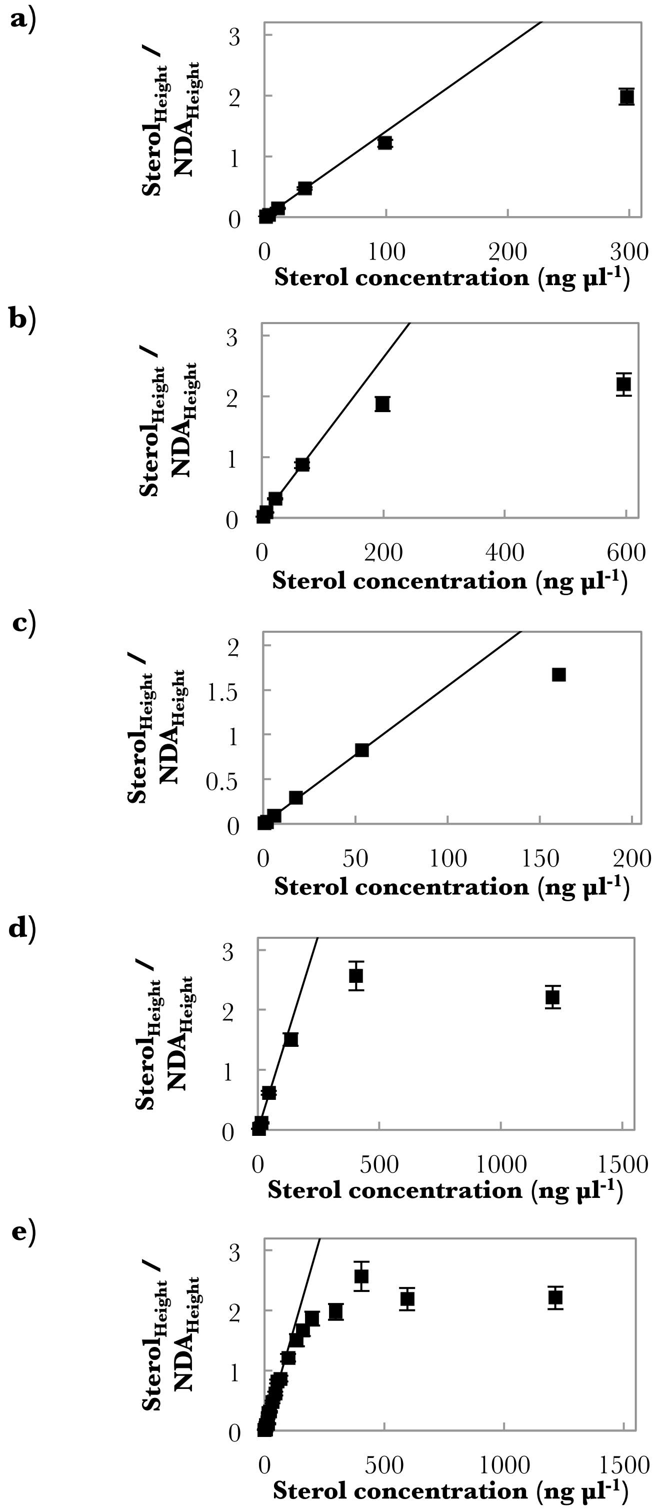


Cycloartenol (1TMS): 56.12 min



Appendix 3.2. GC-MS calibration to sterol concentrations (peak heights)

GC-MS detector response to sterols when peak heights were measured (and normalised to nonadecanoic acid peak height) was unfavourable compared to the response to peak areas. The following are the results of peak height measurements.



Linear regression formulae for injected concentrations up to 66 ng μl^{-1} for 1TMS sterol derivatives was **(a)** y = 0.0141x for brassicasterol, **(b)** y = 0.0132x for campesterol, **(c)** y = 0.0154x for stigmasterol, and **(d)** y = 0.0130x or sitosterol. **(e)** The linear regression formula for all sterols was y = 0.0139x. Data points = mean ± standard error, n = 5.

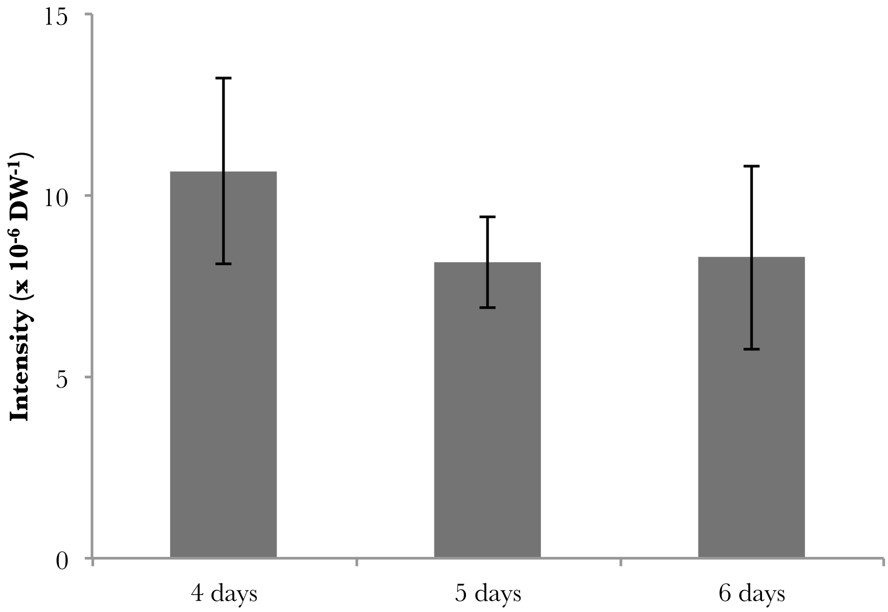
R^2 values for linear regression of all replicate data in the region of linearity, along with the corresponding values from peak areas, were as follows.

	Integrated peak ($Sterol_{Area}$ / NDA_{Area})	**Peak height ($Sterol_{Height}$ / NDA_{Height})**
Brassicasterol (1TMS)	0.990	0.980
Campesterol (1TMS)	0.985	0.976
Stigmasterol (1TMS)	0.989	0.987
Sitosterol (1TMS)	0.985	0.931
All sterols	**0.986**	**0.965**

In each case the spread of data for the peak areas is narrower than for peak heights.

Appendix 3.3. Ribitol (5TMS) mass tag 217 intensity in metabolome dataset

Mass tag (m/z) 217 of the GC-MS spectrum identified as ribitol (5TMS) gave the highest intensity measurements. Comparisons between the age groups for this mass tag after normalisation to dry weight did not indicate significant differences. Graph columns represent mean values of four biological replicates for four and six days, and three biological replicates for five days. Error bars represent SE.

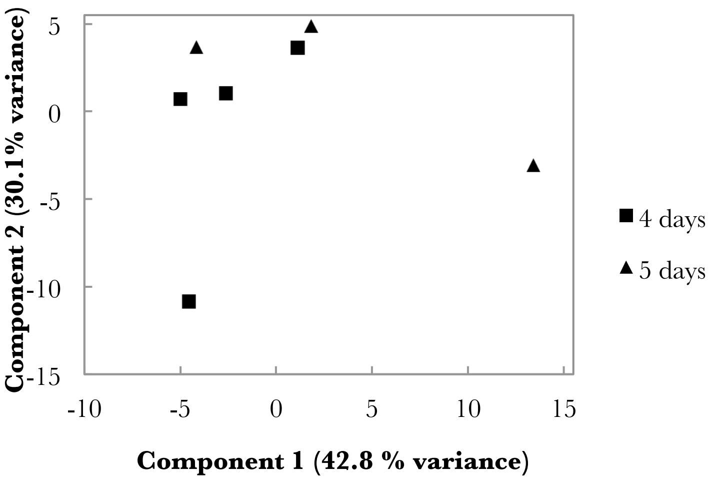


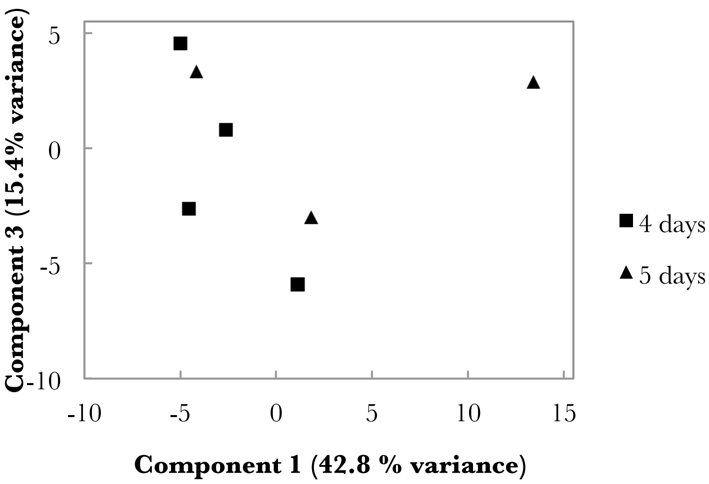
Appendix 3.4. Principal component analysis pairwise comparisons of metabolome data by age

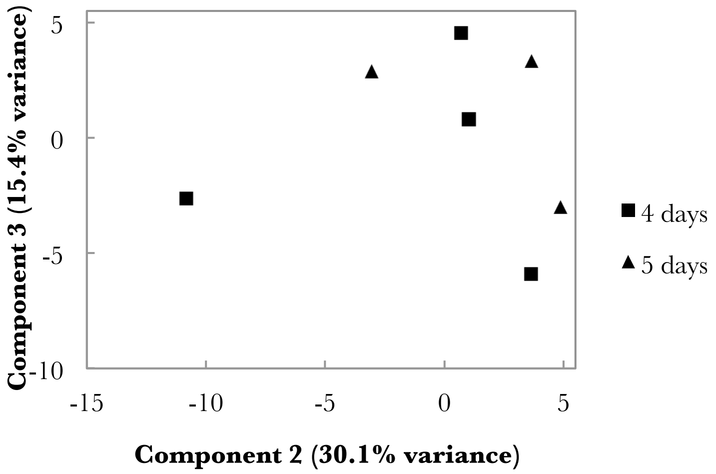
Principal component analysis was performed separately on age pairings of metabolome data.

Days four and five

Three significant components were identified accounting for 88.3% of inter-sample variance. MANOVA and student's *t* tests of component scores did not indicate significant differences between the age groups:

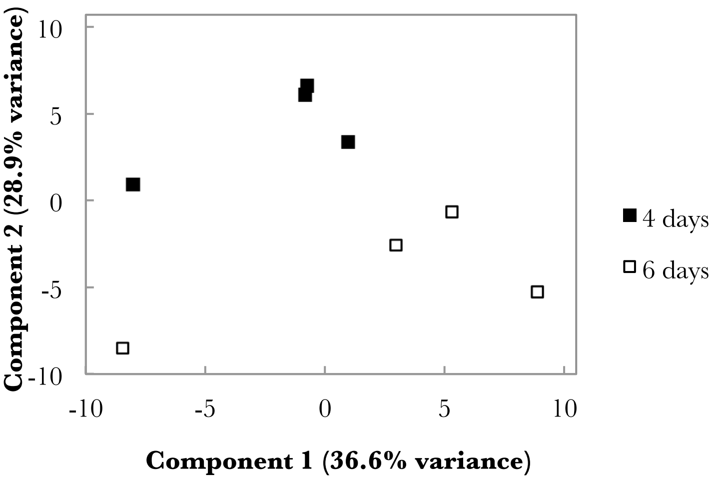


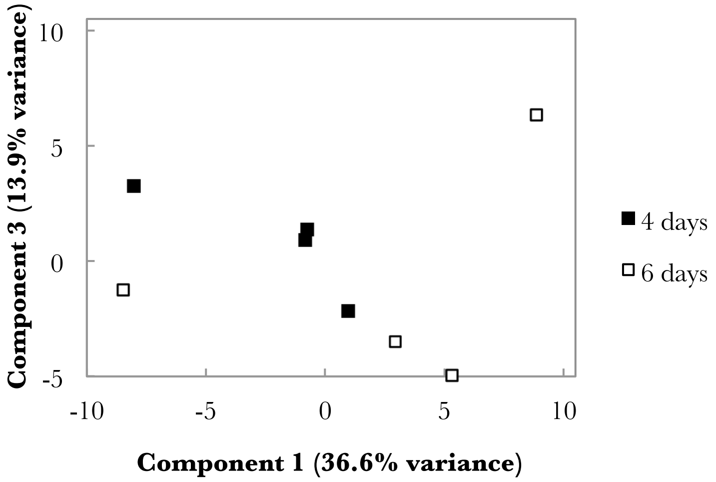


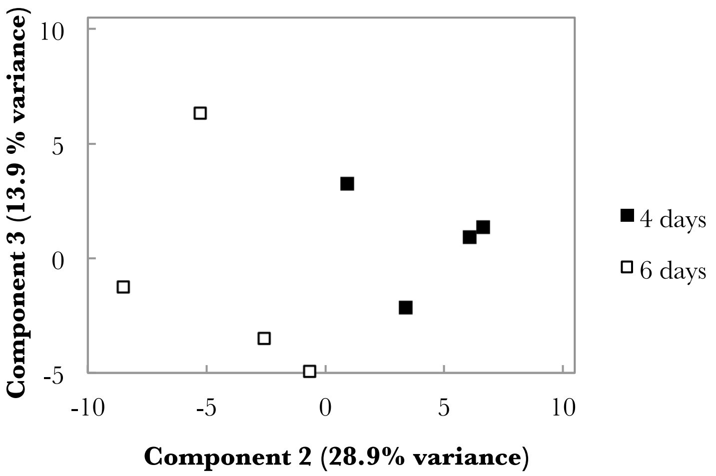


Days four and six

Three significant components were identified accounting for 79.4% of inter-sample variance. MANOVA indicated significant differences between the data of the two ages ($p < 0.01$). Student's *t* tests of component scores suggest that the majority of the differences between the ages are within component two ($p < 0.01$), which accounts for 28.9% of variance. Scores for components one and three were not significantly different:

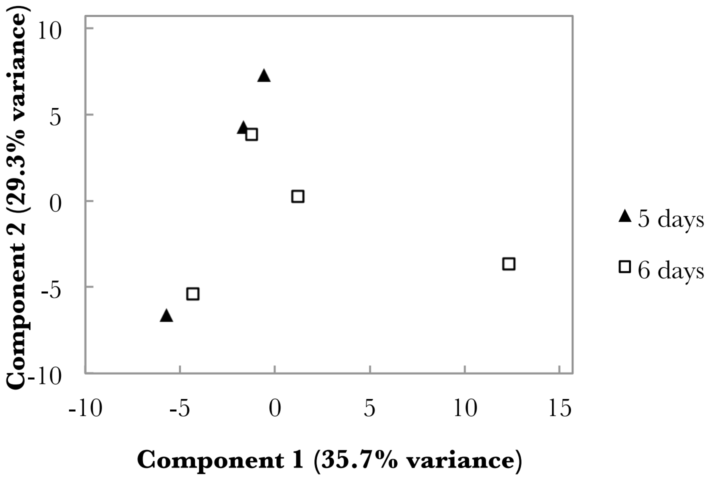


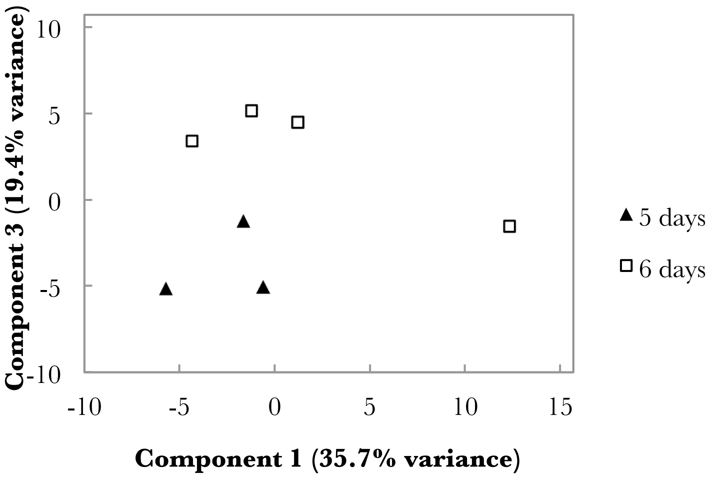


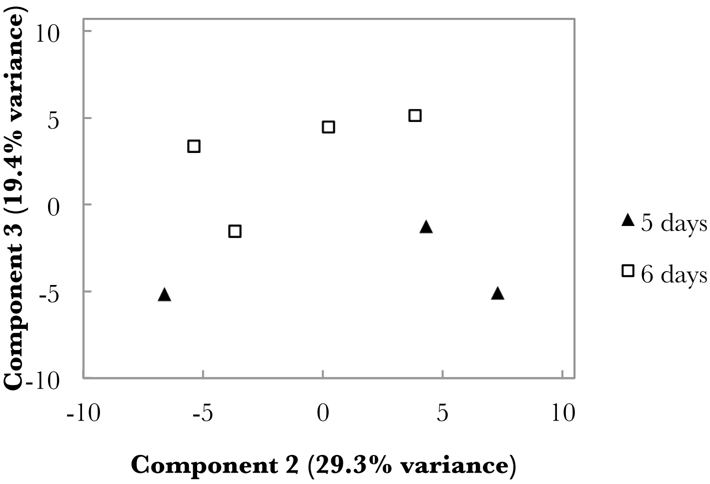


Days five and six

Three significant components were identified accounting for 84.4% of inter-sample variance. MANOVA indicated significant differences between the data of the two ages ($p < 0.05$). Student's *t* tests of component scores suggest that the majority of the differences between the ages are within component three ($p < 0.05$), which accounts for 19.4 % of variance. Scores for components one and two were not significantly different:







Analytes implicated by loading scores to alter in abundance as cultures age

Loading values for component two of four- and six-day comparisons, and component three of five- and six-day comparisons, were compared. Values in **bold** (less than -0.05 for four versus six days, component two; greater than 0.05 for five versus six days, component three) are relatively enriched at six days. Values underlined (greater than 0.05 for four versus six days, component two; less than -0.05 for five versus six days, component three) are relatively depleted at six days.

Analyte	Loading: 4 versus 6 days, component 2	Loading: 5 versus 6 days, component 3	Category
Aconitic acid, cis- (3TMS)	-0.039	-0.058	Organic acid
Alanine (2TMS)	**-0.095**	-0.098	Amino acid
Alanine (3TMS)	**-0.133**	0.042	Amino acid
Alanine [+CO_2] (2TMS)	**-0.110**	**0.157**	Amino acid
Alanine, beta- (3TMS)	**-0.172**	**0.170**	Amino acid
Arabinose (1MEOX) (4TMS) MP	0.008	-0.099	Sugar
Asparagine (2TMS)	-0.041	**0.112**	Amino acid
Asparagine (3TMS)	**-0.085**	**0.057**	Amino acid
Asparagine [-H_2O] (2TMS)	**-0.082**	**0.065**	Amino acid
Aspartic acid (2TMS)	-0.021	**0.118**	Amino acid
Aspartic acid (3TMS)	**-0.062**	-0.141	Amino acid
Butanoic acid, 2-amino- (2TMS)	**-0.107**	-0.084	Organic acid
Butanoic acid, 2,4-dihydroxy- (3TMS)	0.062	-0.142	Organic acid
Butanoic acid, 4-amino- (3TMS)	**-0.111**	-0.036	Organic acid
Butanoic acid, 4-hydroxy- (2TMS)	**-0.071**	-0.055	Organic acid
Butyro-1,4-lactam (1TMS)	-0.002	0.013	Organic acid
Campesterol (1TMS)	-0.006	**0.099**	Sterol
Citric acid (4TMS)	**-0.104**	**0.072**	Sterol
Dehydroascorbic acid dimer (2MEOX) MP	**-0.122**	0.047	Organic acid
Eicosanoic acid (1TMS)	-0.006	-0.045	Organic acid
Erythronic acid (4TMS)	-0.030	-0.068	Organic acid
Ethanolamine (3TMS)	**-0.166**	**0.175**	Primary amine
Fructose (1MEOX) (5TMS) BP	**-0.132**	-0.052	Sugar
Fructose (1MEOX) (5TMS) MP	**-0.133**	-0.053	Sugar
Fucosterol (1TMS)	0.018	0.002	Sterol
Fumaric acid (2TMS)	-0.047	0.005	Organic acid
Galactinol (9TMS)	0.007	**0.161**	Other metabolite
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)	**-0.073**	**0.173**	Other metabolite
Galactose-6-phosphate (1MEOX) (6TMS) early peak	0.134	-0.136	Sugar
Galactose-6-phosphate (1MEOX) (6TMS) late peak	0.149	-0.162	Sugar
Gluconic acid (6TMS)	0.053	-0.085	Organic acid
Glucopyranose, D- (5TMS)	**-0.173**	0.022	Sugar
Glucose (1MEOX) (5TMS) BP	0.011	-0.003	Sugar
Glucose (1MEOX) (5TMS) MP	0.002	-0.026	Sugar
Glucose-6-phosphate (1MEOX) (6TMS) MP	0.164	-0.166	Sugar
Glucose-6-phosphate (6TMS)	**-0.115**	**0.168**	Sugar

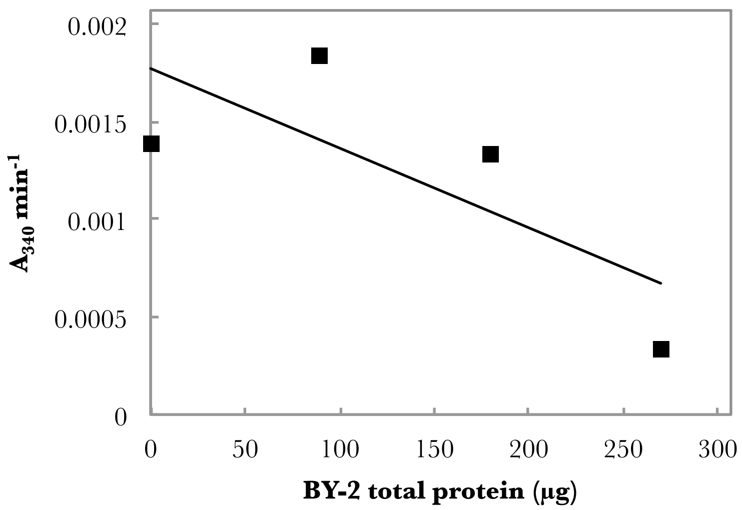
Analyte	Loading: 4 versus 6 days, component 2	Loading: 5 versus 6 days, component 3	Category
Glutamic acid (2TMS)	**-0.092**	0.008	Amino acid
Glutamic acid (3TMS)	**-0.124**	-0.013	Amino acid
Glutamine [-H_2O] (2TMS) BP	**-0.100**	-0.006	Amino acid
Glutamine [-H_2O] (3TMS) MP	**-0.127**	-0.006	Amino acid
Glutamine, DL- (3TMS)	**-0.077**	**0.056**	Amino acid
Glutamine, DL- (4TMS)	-0.003	**0.089**	Amino acid
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	**-0.119**	**0.201**	Organic acid
Glyceric acid (3TMS)	0.073	-0.115	Organic acid
Glycerol-2-phosphate (4TMS)	-0.041	-0.069	Triacylglycerol component
Glycerol-3-phosphate (4TMS)	0.068	-0.095	Triacylglycerol component
Glycerophosphoglycerol (5TMS)	0.125	**0.057**	Triacylglycerol component
Glycine (2TMS)	**-0.120**	-0.119	Amino acid
Glycine (3TMS)	**-0.181**	**0.078**	Amino acid
Hexadecanoic acid (1TMS)	**-0.067**	-0.055	Triacylglycerol component
Homoserine (3TMS)	**-0.181**	0.039	Amino acid
Inositol, myo- (6TMS)	**-0.076**	-0.054	Triacylglycerol component
Isoleucine (1TMS)	-0.005	**0.083**	Amino acid
Lactic acid, DL- (2TMS)	**-0.120**	-0.036	Organic acid
Leucine (1TMS)	-0.024	**0.143**	Amino acid
Lyxonic acid (5TMS)	-0.031	-0.078	Organic acid
Lyxose (1MEOX) (4TMS) MP	0.018	0.045	Sugar
Malic acid (3TMS)	**-0.161**	-0.009	Organic acid
Malic acid, 2-methyl- (3TMS)	0.133	-0.174	Organic acid
Maltose (1MEOX) (8TMS) BP	0.004	**0.130**	Sugar
Maltose (1MEOX) (8TMS) MP	0.144	-0.121	Sugar
Methionine (1TMS)	**-0.083**	**0.174**	Amino acid
Methionine (2TMS)	**-0.178**	**0.116**	Amino acid
myo-Inositol-1-phosphate (7TMS)	0.081	-0.058	Triacylglycerol component
Norleucine (2TMS)	**-0.088**	-0.082	Amino acid
Octadecadienoic acid, n- (1TMS)	-0.014	**0.096**	Triacylglycerol component
Octadecan-1-ol, n- (1TMS)	-0.050	-0.031	Triacylglycerol component
Octadecanoic acid (1TMS)	0.003	0.010	Triacylglycerol component
Ornithine-1,5-lactam (2TMS)	0.097	N/A	Amino acid
Phenylalanine (2TMS)	**-0.118**	**0.131**	Amino acid
Phosphoric acid (3TMS)	0.110	-0.168	Organic acid
Putrescine (4TMS)	-0.047	**0.148**	Amino acid

Analyte	Loading: 4 versus 6 days, component 2	Loading: 5 versus 6 days, component 3	Category
Pyroglutamic acid (2TMS)	**-0.171**	-0.006	Organic acid
Ribonic acid (5TMS) early peak	**-0.101**	-0.062	Organic acid
Ribonic acid (5TMS) late peak	**-0.105**	-0.009	Organic acid
Ribose (1MEOX) (4TMS) BP	-0.028	-0.097	Sugar
Salicin (5TMS)	-0.002	**0.064**	Other metabolite
Serine (2TMS)	**-0.056**	**0.150**	Amino acid
Serine (3TMS)	**-0.146**	-0.018	Amino acid
Serine (4TMS)	**-0.055**	**0.102**	Amino acid
Serine, O-acetyl- (2TMS)	**-0.174**	**0.133**	Amino acid
Sitosterol, beta- (1TMS)	-0.004	**0.101**	Sterol
Stigmasterol (1TMS)	-0.009	**0.115**	Sterol
Succinic acid (2TMS)	**-0.143**	**0.147**	Organic acid
Sucrose (8TMS)	-0.003	-0.012	Sugar
Tagatose (1MEOX) (5TMS) BP	**-0.113**	-0.038	Sugar
Threonic acid (4TMS)	0.171	-0.174	Organic acid
Threonine (3TMS)	**-0.154**	-0.042	Amino acid
Threonine, DL- (2TMS)	-0.032	**0.140**	Amino acid
Turanose (1MEOX) (8TMS) BP	0.092	-0.039	Sugar
Tyrosine (3TMS)	**-0.067**	**0.146**	Amino acid
Uracil (2TMS)	0.028	-0.080	Other metabolite
Uric acid (4TMS)	-0.039	**0.136**	Organic acid
Uridine (4TMS)	0.126	-0.124	Other metabolite
Valine (1TMS)	**-0.118**	-0.120	Amino acid
Valine (2TMS)	**-0.160**	-0.034	Amino acid
Xylitol (5TMS)	0.020	-0.036	Other metabolite
Xylose (1MEOX) (4TMS) MP	**-0.105**	-0.012	Sugar
Xylulose-5-phosphate (1MEOX) (5TMS) BP	0.164	-0.156	Sugar

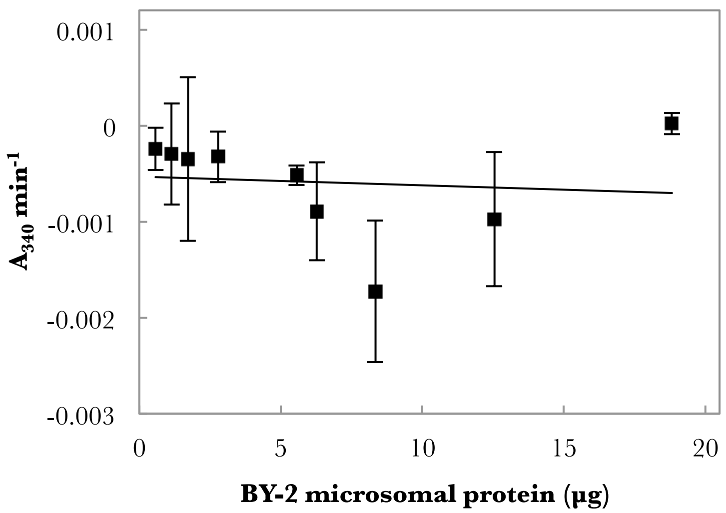
Appendix 3.5. Additional HMGR assay data

Data from ΔA_{340} assays of HMGR activity

ΔA_{340} resulting from measurement of HMGR activity in desalted total protein extracts did not change linearly with protein content when recorded using a spectrophotometer. ($R^2 = 0.558$)

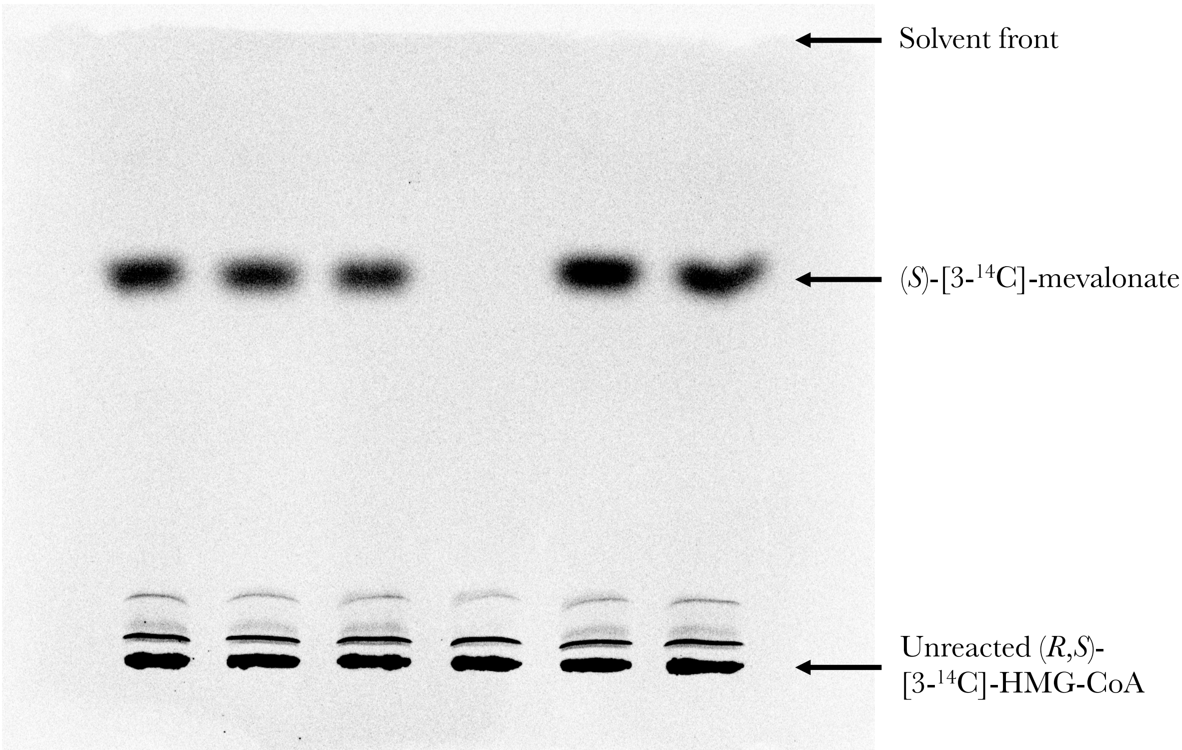


ΔA_{340} resulting from measurement of HMGR activity in microsomal protein extracts did not change linearly with protein content when recorded using a microplate reader. ($R^2 = 0.005$. Data points represent mean ± SE.)



An example phosphorimaged thin layer chromatography plate from the ^{14}C HMGR assay

The following is a typical phosphorimaging result for WT BY-2 microsomal protein extract. The contrast of the image was boosted to enable better visualisation of the mevalonate and HMG-CoA positions. This does not affect reaction calculations. Lane four is a negative control, with heat-denatured microsomal extract. Other lanes contained unheated microsomal extracts.



Appendix 4.1. pH7WG2D-*mCherry* expression vector sequence

Bases	Feature
25-419	*rolD* promoter
573-1370	*Egfp* (enhanced green fluorescent protein)
1407-1624	Cauliflower mosaic virus (CaMV) *35S* promoter
1636-1835	Right transfer DNA border
6739-7988	*Sm/SpR* (Bacterial streptomycin/spectinomycin resistance cassette)
7994-8326	Left transfer DNA border
8330-10116	*hpt* (hygromycin phosphotransferase, including *nos* promoter and terminator)
10171-10396	CaMV *35S* terminator
10393-10411	p7WG2-ins-R primer binding site
10406-10430	attB2 (Gateway recombination site)
10442-11152	*mCherry*
10442-10464	mCherry-R primer binding site
11135-11152	mCherry-F primer binding site (antiparallel sequence)
11167-11191	attB1 (Gateway recombination site)
11219-12245	CaMV *35S* promoter
11290-11311	p7WG2-ins-F primer binding site (antiparallel sequence)

5' Base	Sequence
1	AGCTTGCATGCCTGCAGGTTAGCTT**GCATGCTGCAGGTCGACTCTCTAGGAATTTGTTCG**
61	**TGAACTATTAGTTGCGGGCCTTGGCATCCGACTACCTCTGCGGCAATATTATATTCCCTG**
121	**GGCCCACCGTGAACCCAATTTCGCCTATTTATTCATTACCCCCATTAACATTGAAGTAGT**
181	**CATGATGGGCCTGCAGCACGTTGGTGAGGCTGGCACAACTCATCCATATACTTTCTGACC**
241	**GGATCGGCACATTATTGTAGAAAACGCGGACCCACAGCGCACTTTCCAAAGCGGTGCCGC**
301	**GTCAGAATGCGCTGGCAGAAAAAAATTAATCCAAAAGTACCCTCCAAGCAGCCCATATAA**
361	**ACGCGTTTACAAATCCGCTAACCTCAACAATTTGAGCAGAGAAAATTCGCTAGAGGAT**CC
421	CCGGGTACCGAGCTCGAATTCTCAACACAACATATACAAAACAAACGAATCTCAAGCAAT
481	CAAGCATTCTACTTCTATTGCAGCAATTTAAATCATTTCTTTTAAAGCAAAAGCTATTTT
541	CTGAAAATTTTCACCATTTACGAACGATAGCC**ATGGTGAAGACTAATCTTTTTCTCTTTT**
601	**TCATCTTTTCACTTCTCCTATCATTATCCTCGGCCGACATGGTGAGCAAGGGCGAGGAGC**
661	**TGTTCACCGGGGTGGTGCCCATCCTGGTCGAGCTGGACGGCGACGTAAACGGCCACAAGT**
721	**TCAGCGTGTCCGGCGAGGGCGAGGGCGATGCCACCTACGGCAAGCTGACCCTGAAGTTCA**
781	**TCTGCACCACCGGCAAGCTGCCCGTGCCCTGGCCCACCCTCGTGACCACCCTGACCTACG**
841	**GCGTGCAGTGCTTCAGCCGCTACCCCGACCACATGAAGCAGCACGACTTCTTCAAGTCCG**
901	**CCATGCCCGAAGGCTACGTCCAGGAGCGCACCATCTTCTTCAAGGACGACGGCAACTACA**
961	**AGACCCGCGCCGAGGTGAAGTTCGAGGGCGACACCCTGGTGAACCGCATCGAGCTGAAGG**
1021	**GCATCGACTTCAAGGAGGACGGCAACATCCTGGGGCACAAGCTGGAGTACAACTACAACA**
1081	**GCCACAACGTCTATATCATGGCCGACAAGCAGAAGAACGGCATCAAGGTGAACTTCAAGA**
1141	**TCCGCCACAACATCGAGGACGGCAGCGTGCAGCTCGCCGACCACTACCAGCAGAACACCC**
1201	**CCATCGGCGACGGCCCCGTGCTGCTGCCCGACAACCACTACCTGAGCACCCAGTCCGCCC**
1261	**TGAGCAAAGACCCCAACGAGAAGCGCGATCACATGGTCCTGCTGGAGTTCGTGACCGCCG**
1321	**CCGGGATCACTCTCGGCATGGACGAGCTGTACAAGAAGGACGAGCTGTAA**GCGCCGCCCG
1381	GCTGCAGCCCGGGGGATCCACTAGTT**CTAGAGTCCGCAAAAATCACCAGTCTCTCTCTAC**
1441	**AAATCTATCTCTCTCTATTTTTCTCCAGAATAATGTGTGAGTAGTTCCCACATAAGGGAA**
1501	**TTAGGGTTCTTATAGGGTTTCGCTCATGTGTTGAGCATATAAGAAACCCTTAGTATGTAT**
1561	**TTGTATTTGTAAAATACTTCTATCAATAAAATTTCTAATTCCTAAAACCAAAATCCAGTG**
1621	**ACCT**GCAGGCATGCA**AGCTTAGCTTGAGCTTGGATCAGATTGTCGTTTCCCGCCTTCAGT**
1681	**TTAAACTATCAGTGTTTGACAGGATATATTGGCGGGTAAACCTAAGAGAAAAGAGCGTTT**
1741	**ATTAGAATAACGGATATTTAAAAGGGCGTGAAAAGGTTTATCCGTTCGTCCATTTGTATG**
1801	**TGCATGCCAACCACAGGGTTCCCCTCGGGATCAAA**GTACTTTGATCCAACCCCTCCGCTG

5' Base	Sequence
1861	CTATAGTGCAGTCGGCTTCTGACGTTCAGTGCAGCCGTCTTCTGAAAACGACATGTCGCA
1921	CAAGTCCTAAGTTACGCGACAGGCTGCCGCCCTGCCCTTTTCCTGGCGTTTTCTTGTCGC
1981	GTGTTTTAGTCGCATAAAGTAGAATACTTGCGACTAGAACCGGAGACATTACGCCATGAA
2041	CAAGAGCGCCGCCGCTGGCCTGCTGGGCTATGCCCGCGTCAGCACCGACGACCAGGACTT
2101	GACCAACCAACGGGCCGAACTGCACGCGGCCGGCTGCACCAAGCTGTTTTCCGAGAAGAT
2161	CACCGGCACCAGGCGCGACCGCCCGGAGCTGGCCAGGATGCTTGACCACCTACGCCCTGG
2221	CGACGTTGTGACAGTGACCAGGCTAGACCGCCTGGCCCGCAGCACCCGCGACCTACTGGA
2281	CATTGCCGAGCGCATCCAGGAGGCCGGCGCGGGCCTGCGTAGCCTGGCAGAGCCGTGGGC
2341	CGACACCACCACGCCGGCCGGCCGCATGGTGTTGACCGTGTTCGCCGGCATTGCCGAGTT
2401	CGAGCGTTCCCTAATCATCGACCGCACCCGGAGCGGGCGCGAGGCCGCCAAGGCCCGAGG
2461	CGTGAAGTTTGGCCCCCGCCCTACCCTCACCCCGGCACAGATCGCGCACGCCCGCGAGCT
2521	GATCGACCAGGAAGGCCGCACCGTGAAAGAGGCGGCTGCACTGCTTGGCGTGCATCGCTC
2581	GACCCTGTACCGCGCACTTGAGCGCAGCGAGGAAGTGACGCCCACCGAGGCCAGGCGGCG
2641	CGGTGCCTTCCGTGAGGACGCATTGACCGAGGCCGACGCCCTGGCGGCCGCCGAGAATGA
2701	ACGCCAAGAGGAACAAGCATGAAACCGCACCAGGACGGCCAGGACGAACCGTTTTTCATT
2761	ACCGAAGAGATCGAGGCGGAGATGATCGCGGCCGGGTACGTGTTCGAGCCGCCCGCGCAC
2821	GTCTCAACCGTGCGGCTGCATGAAATCCTGGCCGGTTTGTCTGATGCCAAGCTGGCGGCC
2881	TGGCCGGCCAGCTTGGCCGCTGAAGAAACCGAGCGCCGCCGTCTAAAAAGGTGATGTGTA
2941	TTTGAGTAAAACAGCTTGCGTCATGCGGTCGCTGCGTATATGATGCGATGAGTAAATAAA
3001	CAAATACGCAAGGGGAACGCATGAAGGTTATCGCTGTACTTAACCAGAAAGGCGGGTCAG
3061	GCAAGACGACCATCGCAACCCATCTAGCCCGCGCCCTGCAACTCGCCGGGGCCGATGTTC
3121	TGTTAGTCGATTCCGATCCCCAGGGCAGTGCCCGCGATTGGGCGGCCGTGCGGGAAGATC
3181	AACCGCTAACCGTTGTCGGCATCGACCGCCCGACGATTGACCGCGACGTGAAGGCCATCG
3241	GCCGGCGCGACTTCGTAGTGATCGACGGAGCGCCCCAGGCGGCGGACTTGGCTGTGTCCG
3301	CGATCAAGGCAGCCGACTTCGTGCTGATTCCGGTGCAGCCAAGCCCTTACGACATATGGG
3361	CCACCGCCGACCTGGTGGAGCTGGTTAAGCAGCGCATTGAGGTCACGGATGGAAGGCTAC
3421	AAGCGGCCTTTGTCGTGTCGCGGGCGATCAAAGGCACGCGCATCGGCGGTGAGGTTGCCG
3481	AGGCGCTGGCCGGGTACGAGCTGCCCATTCTTGAGTCCCGTATCACGCAGCGCGTGAGCT
3541	ACCCAGGCACTGCCGCCGCCGGCACAACCGTTCTTGAATCAGAACCCGAGGGCGACGCTG
3601	CCCGCGAGGTCCAGGCGCTGGCCGCTGAAATTAAATCAAAACTCATTTGAGTTAATGAGG
3661	TAAAGAGAAAATGAGCAAAAGCACAAACACGCTAAGTGCCGGCCGTCCGAGCGCACGCAG
3721	CAGCAAGGCTGCAACGTTGGCCAGCCTGGCAGACACGCCAGCCATGAAGCGGGTCAACTT
3781	TCAGTTGCCGGCGGAGGATCACACCAAGCTGAAGATGTACGCGGTACGCCAAGGCAAGAC
3841	CATTACCGAGCTGCTATCTGAATACATCGCGCAGCTACCAGAGTAAATGAGCAAATGAAT
3901	AAATGAGTAGATGAATTTTAGCGGCTAAAGGAGGCGGCATGGAAAATCAAGAACAACCAG
3961	GCACCGACGCCGTGGAATGCCCCATGTGTGGAGGAACGGGCGGTTGGCCAGGCGTAAGCG
4021	GCTGGGTTGTCTGCCGGCCCTGCAATGGCACTGGAACCCCCAAGCCCGAGGAATCGGCGT
4081	GACGGTCGCAAACCATCCGGCCCGGTACAAATCGGCGCGGCGCTGGGTGATGACCTGGTG
4141	GAGAAGTTGAAGGCCGCGCAGGCCGCCCAGCGGCAACGCATCGAGGCAGAAGCACGCCCC
4201	GGTGAATCGTGGCAAGCGGCCGCTGATCGAATCCGCAAAGAATCCCGGCAACCGCCGGCA
4261	GCCGGTGCGCCGTCGATTAGGAAGCCGCCCAAGGGCGACGAGCAACCAGATTTTTTCGTT
4321	CCGATGCTCTATGACGTGGGCACCCGCGATAGTCGCAGCATCATGGACGTGGCCGTTTTC
4381	CGTCTGTCGAAGCGTGACCGACGAGCTGGCGAGGTGATCCGCTACGAGCTTCCAGACGGG
4441	CACGTAGAGGTTTCCGCAGGGCCGGCCGGCATGGCCAGTGTGTGGGATTACGACCTGGTA
4501	CTGATGGCGGTTTCCCATCTAACCGAATCCATGAACCGATACCGGGAAGGGAAGGGAGAC
4561	AAGCCCGGCCGCGTGTTCCGTCCACACGTTGCGGACGTACTCAAGTTCTGCCGGCGAGCC
4621	GATGGCGGAAAGCAGAAAGACGACCTGGTAGAAACCTGCATTCGGTTAAACACCACGCAC
4681	GTTGCCATGCAGCGTACGAAGAAGGCCAAGAACGGCCGCCTGGTGACGGTATCCGAGGGT
4741	GAAGCCTTGATTAGCCGCTACAAGATCGTAAAGAGCGAAACCGGGCGGCCGGAGTACATC
4801	GAGATCGAGCTAGCTGATTGGATGTACCGCGAGATCACAGAAGGCAAGAACCCGGACGTG
4861	CTGACGGTTCACCCCGATTACTTTTTGATCGATCCCGGCATCGGCCGTTTTCTCTACCGC
4921	CTGGCACGCCGCGCCGCAGGCAAGGCAGAAGCCAGATGGTTGTTCAAGACGATCTACGAA
4981	CGCAGTGGCAGCGCCGGAGAGTTCAAGAAGTTCTGTTTCACCGTGCGCAAGCTGATCGGG
5041	TCAAATGACCTGCCGGAGTACGATTTGAAGGAGGAGGCGGGGCAGGCTGGCCCGATCCTA
5101	GTCATGCGCTACCGCAACCTGATCGAGGGCGAAGCATCCGCCGGTTCCTAATGTACGGAG
5161	CAGATGCTAGGGCAAATTGCCCTAGCAGGGGAAAAAGGTCGAAAAGGTCTCTTTCCTGTG
5221	GATAGCACGTACATTGGGAACCCAAAGCCGTACATTGGGAACCGGAACCCGTACATTGGG
5281	AACCCAAAGCCGTACATTGGGAACCGGTCACACATGTAAGTGACTGATATAAAAGAGAAA
5341	AAAGGCGATTTTTCCGCCTAAAACTCTTTAAAACTTATTAAAACTCTTAAAACCCGCCTG

5' Base	Sequence
5401	GCCTGTGCATAACTGTCTGGCCAGCGCACAGCCGAAGAGCTGCAAAAAGCGCCTACCCTT
5461	CGGTCGCTGCGCTCCCTACGCCCCGCCGCTTCGCGTCGGCCTATCGCGGCCGCTGGCCGC
5521	TCAAAAATGGCTGGCCTACGGCCAGGCAATCTACCAGGGCGCGGACAAGCCGCGCCGTCG
5581	CCACTCGACCGCCGGCGCCCACATCAAGGCACCCTGCCTCGCGCGTTTCGGTGATGACGG
5641	TGAAAACCTCTGACACATGCAGCTCCCGGAGACGGTCACAGCTTGTCTGTAAGCGGATGC
5701	CGGGAGCAGACAAGCCCGTCAGGGCGCGTCAGCGGGTGTTGGCGGGTGTCGGGGCGCAGC
5761	CATGACCCAGTCACGTAGCGATAGCGGAGTGTATACTGGCTTAACTATGCGGCATCAGAG
5821	CAGATTGTACTGAGAGTGCACCATATGCGGTGTGAAATACCGCACAGATGCGTAAGGAGA
5881	AAATACCGCATCAGGCGCTCTTCCGCTTCCTCGCTCACTGACTCGCTGCGCTCGGTCGTT
5941	CGGCTGCGGCGAGCGGTATCAGCTCACTCAAAGGCGGTAATACGGTTATCCACAGAATCA
6001	GGGGATAACGCAGGAAAGAACATGTGAGCAAAAGGCCAGCAAAAGGCCAGGAACCGTAAA
6061	AAGGCCGCGTTGCTGGCGTTTTTCCATAGGCTCCGCCCCCCTGACGAGCATCACAAAAAT
6121	CGACGCTCAAGTCAGAGGTGGCGAAACCCGACAGGACTATAAAGATACCAGGCGTTTCCC
6181	CCTGGAAGCTCCCTCGTGCGCTCTCCTGTTCCGACCCTGCCGCTTACCGGATACCTGTCC
6241	GCCTTTCTCCCTTCGGGAAGCGTGGCGCTTTCTCATAGCTCACGCTGTAGGTATCTCAGT
6301	TCGGTGTAGGTCGTTCGCTCCAAGCTGGGCTGTGTGCACGAACCCCCCGTTCAGCCCGAC
6361	CGCTGCGCCTTATCCGGTAACTATCGTCTTGAGTCCAACCCGGTAAGACACGACTTATCG
6421	CCACTGGCAGCAGCCACTGGTAACAGGATTAGCAGAGCGAGGTATGTAGGCGGTGCTACA
6481	GAGTTCTTGAAGTGGTGGCCTAACTACGGCTACACTAGAAGGACAGTATTTGGTATCTGC
6541	GCTCTGCTGAAGCCAGTTACCTTCGGAAAAAGAGTTGGTAGCTCTTGATCCGGCAAACAA
6601	ACCACCGCTGGTAGCGGTGGTTTTTTTGTTTGCAAGCAGCAGATTACGCGCAGAAAAAAA
6661	GGATCTCAAGAAGATCCTTTGATCTTTTCTACGGGGTCTGACGCTCAGTGGAACGAAAAC
6721	TCACGTTAAGGGATTTTG**GTCATGCATGATATATCTCCCAATTTGTGTAGGGCTTATTAT**
6781	**GCACGCTTAAAAATAATAAAAGCAGACTTGACCTGATAGTTTGGCTGTGAGCAATTATGT**
6841	**GCTTAGTGCATCTAATCGCTTGAGTTAACGCCGGCGAAGCGGCGTCGGCTTGAACGAATT**
6901	**TCTAGCTAGACATTATTTGCCGACTACCTTGGTGATCTCGCCTTTCACGTAGTGGACAAA**
6961	**TTCTTCCAACTGATCTGCGCGCGAGGCCAAGCGATCTTCTTCTTGTCCAAGATAAGCCTG**
7021	**TCTAGCTTCAAGTATGACGGGCTGATACTGGGCCGGCAGGCGCTCCATTGCCCAGTCGGC**
7081	**AGCGACATCCTTCGGCGCGATTTTGCCGGTTACTGCGCTGTACCAAATGCGGGACAACGT**
7141	**AAGCACTACATTTCGCTCATCGCCAGCCCAGTCGGGCGGCGAGTTCCATAGCGTTAAGGT**
7201	**TTCATTTAGCGCCTCAAATAGATCCTGTTCAGGAACCGGATCAAAGAGTTCCTCCGCCGC**
7261	**TGGACCTACCAAGGCAACGCTATGTTCTCTTGCTTTTGTCAGCAAGATAGCCAGATCAAT**
7321	**GTCGATCGTGGCTGGCTCGAAGATACCTGCAAGAATGTCATTGCGCTGCCATTCTCCAAA**
7381	**TTGCAGTTCGCGCTTAGCTGGATAACGCCACGGAATGATGTCGTCGTGCACAACAATGGT**
7441	**GACTTCTACAGCGCGGAGAATCTCGCTCTCTCCAGGGGAAGCCGAAGTTTCCAAAAGGTC**
7501	**GTTGATCAAAGCTCGCCGCGTTGTTTCATCAAGCCTTACGGTCACCGTAACCAGCAAATC**
7561	**AATATCACTGTGTGGCTTCAGGCCGCCATCCACTGCGGAGCCGTACAAATGTACGGCCAG**
7621	**CAACGTCGGTTCGAGATGGCGCTCGATGACGCCAACTACCTCTGATAGTTGAGTCGATAC**
7681	**TTCGGCGATCACCGCTTCCCCCATGATGTTTAACTTTGTTTTAGGGCGACTGCCCTGCTG**
7741	**CGTAACATCGTTGCTGCTCCATAACATCAAACATCGACCCACGGCGTAACGCGCTTGCTG**
7801	**CTTGGATGCCCGAGGCATAGACTGTACCCCAAAAAAACATGTCATAACAAGAAGCCATGA**
7861	**AAACCGCCACTGCGCCGTTACCACCGCTGCGTTCGGTCAAGGTTCTGGACCAGTTGCGTG**
7921	**ACGGCAGTTACGCTACTTGCATTACAGCTTACGAACCGAACGAGGCTTATGTCCACTGGG**
7981	**TTCGTGCC**CGAAT**TGATCACAGGCAGCAACGCTCTGTCATCGTTACAATCAACATGCTAC**
8041	**CCTCCGCGAGATCATCCGTGTTTCAAACCCGGCAGCTTAGTTGCCGTTCTTCCGAATAGC**
8101	**ATCGGTAACATGAGCAAAGTCTGCCGCCTTACAACGGCTCTCCCGCTGACGCCGTCCCGG**
8161	**ACTGATGGGCTGCCTGTATCGAGTGGTGATTTTGTGCCGAGCTGCCGGTCGGGGAGCTGT**
8221	**TGGCTGGCTGGTGGCAGGATATATTGTGGTGTAAACAAATTGACGCTTAGACAACTTAAT**
8281	**AACACATTGCGGACGTTTTTAATGTACTGAATTAACGCCGAATTG**AATT**ATCAGCTTGCA**
8341	**TGCCGGTCGATCTAGTAACATAGATGACACCGCGCGATAATTTATCCTAGTTTGCGCG**
8401	**CTATATTTTGTTTTCTATCGCGTATTAAATGTATAATTGCGGGACTCTAATCATAAAAAC**
8461	**CCATCTCATAAATAACGTCATGCATTACATGTTAATTATTACATGCTTAACGTAATTCAA**
8521	**CAGAAATTATATGATAATCATCGCAAGACCGGCAACAGGATTCAATCTTAAGAAACTTTA**
8581	**TTGCCAAATGTTTGAACGATCTGCTTGACTCTAGGGAATTAATTCCTGAATCACTGCGAC**
8641	**CGGCCCTCCCGCGACCCAGCCGAGCGAGCTTAGCGAACTGTGGACGAGAACTGTGCCACC**
8701	**AAGCGTAAGGCCGTTCTCTCGCATTTGCCTTGCTAGGCTCGCGCGAGTTGCTGGCTGAGG**
8761	**CGTTCTCGAAATCAGCTCTTGTTCGGTCGGCATCTACTCTATTCCTTTGCCCTCGGACGA**
8821	**GTGCTGGGGCGTCGGTTTCCACTATCGGCGAGTACTTCTACACAGCCATCGGTCCAGACG**
8881	**GCCGCGCTTCTGCGGGCGATTTGTGTACGCCCGACAGTCCCGGCTCCGGATCGGACGATT**

5' Base	Sequence
8941	**GCGTCGCATCGACCCTGCGCCCAAGCTGCATCATCGAAATTGCCGTCAACCAAGCTCTGA**
9001	**TAGAGTTGGTCAAGACCAATGCGGAGCATATACGCCCGGAGCCTTGGCGATCCTGCAAGC**
9061	**TCCGGATGCCTCCGCTCGAAGTAGCGCGTCTGCTGCTCCATACAAGCCAACCACGGCCTC**
9121	**CAGAAGAAGATGTTGGCGACCTCGTATTGGGAATCCCCGAACATCGCCTCGCTCCAGTCA**
9181	**ATGACCGCTGTTATGCGGCCATTGTCCGTCAGGACATTGTTGGAGCCGAATCCGCGTGCA**
9241	**CGAGTGCCGGACTTCGGGGCAGTCCTCGCCCAAAGCATCAGCTCATCGAGAGCCTGCGCG**
9301	**ACGGACGCACTGACGGTGTCGTCCATCACAGTTTGCCAGTGATACACATGGGGATCAGCA**
9361	**ATCGCGCATATGAAATCACGCCATGTAGTGTATTGACCGATTCCTTGCGGTCCGAATGGG**
9421	**CCGAACCCGCTCGTCTGGCTAAGATCGGCCGCAGCGATAGCATCCATAGCCTCCGCGACC**
9481	**GGCTGAAGAACAGCGGGCAGTTCGGTTTCAGGCAGGTCTTGCAACGTGACACCCTGTGCA**
9541	**CGGCGGGAGATGCAATAGGTCAGGCTCTCGCTGAACTCCCCAATGTCAAGCACTTCCGGA**
9601	**ATCGGGAGCGCGGCCGATGCAAAGTGCCGATAAACATAACGATCTTTGTAGAAACCATCG**
9661	**GCGCAGCTATTTACCCGCAGGACATATCCACGCCCTCCTACATCGAAGCTGAAAGCACGA**
9721	**GATTCTTCGCCCTCCGAGAGCTGCATCAGGTCGGAGACGCTGTCGAACTTTTCGATCAGA**
9781	**AACTTCTCGACAGACGTCGCGGTGAGTTCAGGCTTTTTCATAGGGGGGATTCGAGTTGAG**
9841	**AGTGAATATGAGACTCTAATTGGATACCGAGGGGAATTTATGGAACGTCAGTGGAGCATT**
9901	**TTTGACAAGAAATATTTGCTAGCTGATAGTGACCTTAGGCGACTTTTGAACGCGCAATAA**
9961	**TGGTTTCTGACGTATGTGCTTAGCTCATTAAACTCCAGAAACCCGCGGCTCAGTGGCTCC**
10021	**TTCAACGTTGCGGTTCTGTCAGTTCCAAACGTAAAACGGCTTGTCCCGCGTCATCGGCGG**
10081	**GGTCATAACGTGACTCCCTTAATTCTCATGTATGATAATT**CGAGGGTACCCGGGGATCCT
10141	CTAGAGGGCCCGACGTCGCATGCCTGC**AGGTCACTGGATTTTGGTTTTAGGAATTAGAAA**
10201	**TTTTATTGATAGAAGTATTTTACAAATACAAATACATACTAAGGGTTTCTTATATGCTCA**
10261	**ACACATGAGCGAAACCCTATAAGAACCCTAATTCCCTTATCTGGGAACTACTCACACATT**
10321	**ATTCTGGAGAAAAATAGAGAGAGATAGATTTGTAGAGAGAGACTGGTGATTTTTGCGGAC**
10381	**TCTAGCATGGCCG**CGGGATATCACC**ACTTTGTACAAGAAAGCTGGTCGA**ATTCGCCCTT
10441	T**TTACTTGTACAGCTCGTCCATGCCGCCGGTGGAGTGGCGGCCCTCGGCGCGTTCGTACT**
10501	**GTTCCACGATGGTGTAGTCCTCGTTGTGGGAGGTGATGTCCAACTTGATGTTGACGTTGT**
10561	**AGGCGCCGGGCAGCTGCACGGGCTTCTTGGCCTTGTAGGTGGTCTTGACCTCAGCGTCGT**
10621	**AGTGGCCGCCGTCCTTCAGCTTCAGCCTCTGCTTGATCTCGCCCTTCAGGGCGCCGTCCT**
10681	**CGGGGTACATCCGCTCGGAGGAGGCCTCCCAGCCCATGGTCTTCTTCTGCATTACGGGGC**
10741	**CGTCGGAGGGGAAGTTGGTGCCGCGCAGCTTCACCTTGTAGATGAACTCGCCGTCCTGCA**
10801	**GGGAGGAGTCCTGGGTCACGGTCACCACGCCGCCGTCCTCGAAGTTCATCACGCGCTCCC**
10861	**ACTTGAAGCCCTCGGGGAAGGACAGCTTCAAGTAGTCGGGGATGTCGGCGGGGTGCTTCA**
10921	**CGTAGGCCTTGGAGCCGTACATGAACTGAGGGGACAGGATGTCCCAGGCGAAGGGCAGGG**
10981	**GGCCACCCTTGGTCACCTTCAGCTTGGCGGTCTGGGTGCCCTCGTAGGGGCGGCCCTCGC**
11041	**CCTCGCCCTCGATCTCGAACTCGTGGCCGTTCACGGAGCCCTCCATGTGCACCTTGAAGC**
11101	**GCATGAACTCCTTGATGATGGCCATGTTATCCTCCTCGCCCTTGCTCACCAT**AAGGGCGA
11161	ATTCGG**AGCCTGCTTTTTTGTACAAACTTGT**GATATCACTAGTGCGGCCGCCTGCAGG**TC**
11221	**GACTAGAATAGTAAATTGTAATGTTGTTTGTTGTTTGTTTTGTTGTGGTATTGTTGTAAA**
11281	**AATACCGGAGTCCTCTCCAAATGAAATGAACTTCCTTATATAGAGGAAGGGTCTTGCGAA**
11341	**GGATAGTGGGATTGTGCGTCATCCCTTACGTCAGTGGAGATATCACATCAATCCACTTGC**
11401	**TTTGAAGACGTGGTTGGAACGTCTTCTTTTTCCACGATGCTCCTCGTGGGTGGGGGTCCA**
11461	**TCTTTGGGACCACTGTCGGCAGAGGCATCTTGAACGATAGCCTTTCCTTTATCGCAATGA**
11521	**TGGCATTTGTAGGTGCCACCTTCCTTTTCTACTGTCCTTTTGATGAAGTGACAGATAGCT**
11581	**GGGCAATGGAATCCGAGGAGGTTTCCCGATATTACCCTTTGTTGAAAAGTCTCAATAGCC**
11641	**CTTTGGTCTTCTGAGACTGTATCTTTGATATTCTTGGAGTAGACGAGAGTGTCGTGCTCC**
11701	**ACCATGTTGACGAAGATTTTCTTCTTGTCATTGAGTCGTAAAAGACTCTGTATGAACTGT**
11761	**TCGCCAGTCTTCACGGCGAGTTCTGTTAGATCCTCGATCTGAATTTTTGACTCCATGGCC**
11821	**TTTGATTCAGTAGGAACTACTTTCTTAGAGACTCCAATCTCTATTACTTGCCTTGGTTTA**
11881	**TGAAGCAAGCCTTGAATCGTCCATACTGGAATAGTACTTCTGATCTTGAGAAATATATCT**
11941	**TTCTCTGTGTTCTTGATGCAGTTAGTCCTGAATCTTTTGACTGCATCTTTAACCTTCTTG**
12001	**GGAAGGTATTTGATCTCCTGGAGATTATTACTCGGGTAGATCGTCTTGATGAGACCTGCC**
12061	**GCGTAGGCCTCTCTAACCATCTGTGGGTCAGCATTCTTTCTGAAATTGAAGAGGCTAATC**
12121	**TTCTCATTATCGGTGGTGAACATGGTATCGTCACCTTCTCCGTCGAACTTTCTTCCTAGA**
12181	**TCGTAGAGATAGAGAAAGTCGTCCATGGTGATCTCCGGGGCAAAGGAGATCAGCTTGGCT**
12241	**CTAGT**CGACCATATGGGAGAGCTCA

Appendix 4.2. pH7WG2D-*ATCS* expression vector sequence

Bases	Feature
25-419	*rolD* promoter
573-1370	*Egfp* (enhanced green fluorescent protein)
1407-1624	CaMV *35S* terminator
1636-1835	Right transfer DNA border
6739-7988	*Sm/SpR* (Bacterial streptomycin/spectinomycin resistance cassette)
7994-8326	Left transfer DNA border
8330-10116	*hpt* (hygromycin phosphotransferase, including *nos* promoter and terminator)
10171-10396	CaMV *35S* terminator
10393-10411	p7WG2-ins-R primer binding site
10406-10430	attB2 (Gateway recombination site)
10442-10464	CS-OX-R primer binding site
10451-11872	*ATCS* (At2g44350) coding sequence
11886-11905	CS-OX-F primer binding site (antiparallel sequence)
11923-11967	attB1 (Gateway recombination site)
11975-13001	CaMV *35S* promoter
12043-12064	p7WG2-ins-F primer binding site (antiparallel sequence)

5' Base	Sequence
1	AGCTTGCATGCCTGCAGGTTAGCTT**GCATGCTGCAGGTCGACTCTCTAGGAATTTGTTCG**
61	**TGAACTATTAGTTGCGGGCCTTGGCATCCGACTACCTCTGCGGCAATATTATATTCCCTG**
121	**GGCCCACCGTGAACCCAATTTCGCCTATTTATTCATTACCCCCATTAACATTGAAGTAGT**
181	**CATGATGGGCCTGCAGCACGTTGGTGAGGCTGGCACAACTCATCCATATACTTTCTGACC**
241	**GGATCGGCACATTATTGTAGAAAACGCGGACCCACAGCGCACTTTCCAAAGCGGTGCCGC**
301	**GTCAGAATGCGCTGGCAGAAAAAAATTAATCCAAAAGTACCCTCCAAGCAGCCCATATAA**
361	**ACGCGTTTACAAATCCGCTAACCTCAACAATTTGAGCAGAGAAAATTCGCTAGAGGAT**CC
421	CCGGGTACCGAGCTCGAATTCTCAACACAACATATACAAAACAAACGAATCTCAAGCAAT
481	CAAGCATTCTACTTCTATTGCAGCAATTTAAATCATTTCTTTTAAAGCAAAAGCTATTTT
541	CTGAAAATTTTCACCATTTACGAACGATAGCC**ATGGTGAAGACTAATCTTTTTCTCTTTT**
601	**TCATCTTTTCACTTCTCCTATCATTATCCTCGGCCGACATGGTGAGCAAGGGCGAGGAGC**
661	**TGTTCACCGGGGTGGTGCCCATCCTGGTCGAGCTGGACGGCGACGTAAACGGCCACAAGT**
721	**TCAGCGTGTCCGGCGAGGGCGAGGGCGATGCCACCTACGGCAAGCTGACCCTGAAGTTCA**
781	**TCTGCACCACCGGCAAGCTGCCCGTGCCCTGGCCCACCCTCGTGACCACCCTGACCTACG**
841	**GCGTGCAGTGCTTCAGCCGCTACCCCGACCACATGAAGCAGCACGACTTCTTCAAGTCCG**
901	**CCATGCCCGAAGGCTACGTCCAGGAGCGCACCATCTTCTTCAAGGACGACGGCAACTACA**
961	**AGACCCGCGCCGAGGTGAAGTTCGAGGGCGACACCCTGGTGAACCGCATCGAGCTGAAGG**
1021	**GCATCGACTTCAAGGAGGACGGCAACATCCTGGGGCACAAGCTGGAGTACAACTACAACA**
1081	**GCCACAACGTCTATATCATGGCCGACAAGCAGAAGAACGGCATCAAGGTGAACTTCAAGA**
1141	**TCCGCCACAACATCGAGGACGGCAGCGTGCAGCTCGCCGACCACTACCAGCAGAACACCC**
1201	**CCATCGGCGACGGCCCCGTGCTGCTGCCCGACAACCACTACCTGAGCACCCAGTCCGCCC**
1261	**TGAGCAAAGACCCCAACGAGAAGCGCGATCACATGGTCCTGCTGGAGTTCGTGACCGCCG**
1321	**CCGGGATCACTCTCGGCATGGACGAGCTGTACAAGAAGGACGAGCTGTAA**GCGCCGCCCG
1381	GCTGCAGCCCGGGGGATCCACTAGTT**CTAGAGTCCGCAAAAATCACCAGTCTCTCTCTAC**
1441	**AAATCTATCTCTCTCTATTTTTCTCCAGAATAATGTGTGAGTAGTTCCCACATAAGGGAA**
1501	**TTAGGGTTCTTATAGGGTTTCGCTCATGTGTTGAGCATATAAGAAACCCTTAGTATGTAT**
1561	**TTGTATTTGTAAAATACTTCTATCAATAAAATTTCTAATTCCTAAAACCAAAATCCAGTG**
1621	**ACCT**GCAGGCATGCA**AGCTTAGCTTGAGCTTGGATCAGATTGTCGTTTCCCGCCTTCAGT**
1681	**TTAAACTATCAGTGTTTGACAGGATATATTGGCGGGTAAACCTAAGAGAAAAGAGCGTTT**
1741	**ATTAGAATAACGGATATTTAAAAGGGCGTGAAAAGGTTTATCCGTTCGTCCATTTGTATG**
1801	**TGCATGCCAACCACAGGGTTCCCCTCGGGATCAAA**GTACTTTGATCCAACCCCTCCGCTG

5' Base	Sequence
1861	CTATAGTGCAGTCGGCTTCTGACGTTCAGTGCAGCCGTCTTCTGAAAACGACATGTCGCA
1921	CAAGTCCTAAGTTACGCGACAGGCTGCCGCCCTGCCCTTTTCCTGGCGTTTTCTTGTCGC
1981	GTGTTTTAGTCGCATAAAGTAGAATACTTGCGACTAGAACCGGAGACATTACGCCATGAA
2041	CAAGAGCGCCGCCGCTGGCCTGCTGGGCTATGCCCGCGTCAGCACCGACGACCAGGACTT
2101	GACCAACCAACGGGCCGAACTGCACGCGGCCGGCTGCACCAAGCTGTTTTCCGAGAAGAT
2161	CACCGGCACCAGGCGCGACCGCCCGGAGCTGGCCAGGATGCTTGACCACCTACGCCCTGG
2221	CGACGTTGTGACAGTGACCAGGCTAGACCGCCTGGCCCGCAGCACCCGCGACCTACTGGA
2281	CATTGCCGAGCGCATCCAGGAGGCCGGCGCGGGCCTGCGTAGCCTGGCAGAGCCGTGGGC
2341	CGACACCACCACGCCGGCCGGCCGCATGGTGTTGACCGTGTTCGCCGGCATTGCCGAGTT
2401	CGAGCGTTCCCTAATCATCGACCGCACCCGGAGCGGGCGCGAGGCCGCCAAGGCCCGAGG
2461	CGTGAAGTTTGGCCCCCGCCCTACCCTCACCCCGGCACAGATCGCGCACGCCCGCGAGCT
2521	GATCGACCAGGAAGGCCGCACCGTGAAAGAGGCGGCTGCACTGCTTGGCGTGCATCGCTC
2581	GACCCTGTACCGCGCACTTGAGCGCAGCGAGGAAGTGACGCCCACCGAGGCCAGGCGGCG
2641	CGGTGCCTTCCGTGAGGACGCATTGACCGAGGCCGACGCCCTGGCGGCCGCCGAGAATGA
2701	ACGCCAAGAGGAACAAGCATGAAACCGCACCAGGACGGCCAGGACGAACCGTTTTTCATT
2761	ACCGAAGAGATCGAGGCGGAGATGATCGCGGCCGGGTACGTGTTCGAGCCGCCCGCGCAC
2821	GTCTCAACCGTGCGGCTGCATGAAATCCTGGCCGGTTTGTCTGATGCCAAGCTGGCGGCC
2881	TGGCCGGCCAGCTTGGCCGCTGAAGAAACCGAGCGCCGCCGTCTAAAAAGGTGATGTGTA
2941	TTTGAGTAAAACAGCTTGCGTCATGCGGTCGCTGCGTATATGATGCGATGAGTAAATAAA
3001	CAAATACGCAAGGGGAACGCATGAAGGTTATCGCTGTACTTAACCAGAAAGGCGGGTCAG
3061	GCAAGACGACCATCGCAACCCATCTAGCCCGCGCCCTGCAACTCGCCGGGGCCGATGTTC
3121	TGTTAGTCGATTCCGATCCCCAGGGCAGTGCCCGCGATTGGGCGGCCGTGCGGGAAGATC
3181	AACCGCTAACCGTTGTCGGCATCGACCGCCCGACGATTGACCGCGACGTGAAGGCCATCG
3241	GCCGGCGCGACTTCGTAGTGATCGACGGAGCGCCCCAGGCGGCGGACTTGGCTGTGTCCG
3301	CGATCAAGGCAGCCGACTTCGTGCTGATTCCGGTGCAGCCAAGCCCTTACGACATATGGG
3361	CCACCGCCGACCTGGTGGAGCTGGTTAAGCAGCGCATTGAGGTCACGGATGGAAGGCTAC
3421	AAGCGGCCTTTGTCGTGTCGCGGGCGATCAAAGGCACGCGCATCGGCGGTGAGGTTGCCG
3481	AGGCGCTGGCCGGGTACGAGCTGCCCATTCTTGAGTCCCGTATCACGCAGCGCGTGAGCT
3541	ACCCAGGCACTGCCGCCGCCGGCACAACCGTTCTTGAATCAGAACCCGAGGGCGACGCTG
3601	CCCGCGAGGTCCAGGCGCTGGCCGCTGAAATTAAATCAAAACTCATTTGAGTTAATGAGG
3661	TAAAGAGAAAATGAGCAAAAGCACAAACACGCTAAGTGCCGGCCGTCCGAGCGCACGCAG
3721	CAGCAAGGCTGCAACGTTGGCCAGCCTGGCAGACACGCCAGCCATGAAGCGGGTCAACTT
3781	TCAGTTGCCGGCGGAGGATCACACCAAGCTGAAGATGTACGCGGTACGCCAAGGCAAGAC
3841	CATTACCGAGCTGCTATCTGAATACATCGCGCAGCTACCAGAGTAAATGAGCAAATGAAT
3901	AAATGAGTAGATGAATTTTAGCGGCTAAAGGAGGCGGCATGGAAAATCAAGAACAACCAG
3961	GCACCGACGCCGTGGAATGCCCCATGTGTGGAGGAACGGGCGGTTGGCCAGGCGTAAGCG
4021	GCTGGGTTGTCTGCCGGCCCTGCAATGGCACTGGAACCCCCAAGCCCGAGGAATCGGCGT
4081	GACGGTCGCAAACCATCCGGCCCGGTACAAATCGGCGCGGCGCTGGGTGATGACCTGGTG
4141	GAGAAGTTGAAGGCCGCGCAGGCCGCCCAGCGGCAACGCATCGAGGCAGAAGCACGCCCC
4201	GGTGAATCGTGGCAAGCGGCCGCTGATCGAATCCGCAAAGAATCCCGGCAACCGCCGGCA
4261	GCCGGTGCGCCGTCGATTAGGAAGCCGCCCAAGGGCGACGAGCAACCAGATTTTTTCGTT
4321	CCGATGCTCTATGACGTGGGCACCCGCGATAGTCGCAGCATCATGGACGTGGCCGTTTTC
4381	CGTCTGTCGAAGCGTGACCGACGAGCTGGCGAGGTGATCCGCTACGAGCTTCCAGACGGG
4441	CACGTAGAGGTTTCCGCAGGGCCGGCCGGCATGGCCAGTGTGTGGGATTACGACCTGGTA
4501	CTGATGGCGGTTTCCCATCTAACCGAATCCATGAACCGATACCGGGAAGGGAAGGGAGAC
4561	AAGCCCGGCCGCGTGTTCCGTCCACACGTTGCGGACGTACTCAAGTTCTGCCGGCGAGCC
4621	GATGGCGGAAAGCAGAAAGACGACCTGGTAGAAACCTGCATTCGGTTAAACACCACGCAC
4681	GTTGCCATGCAGCGTACGAAGAAGGCCAAGAACGGCCGCCTGGTGACGGTATCCGAGGGT
4741	GAAGCCTTGATTAGCCGCTACAAGATCGTAAAGAGCGAAACCGGGCGGCCGGAGTACATC
4801	GAGATCGAGCTAGCTGATTGGATGTACCGCGAGATCACAGAAGGCAAGAACCCGGACGTG
4861	CTGACGGTTCACCCCGATTACTTTTTGATCGATCCCGGCATCGGCCGTTTTCTCTACCGC
4921	CTGGCACGCCGCGCCGCAGGCAAGGCAGAAGCCAGATGGTTGTTCAAGACGATCTACGAA
4981	CGCAGTGGCAGCGCCGGAGAGTTCAAGAAGTTCTGTTTCACCGTGCGCAAGCTGATCGGG
5041	TCAAATGACCTGCCGGAGTACGATTTGAAGGAGGAGGCGGGGCAGGCTGGCCCGATCCTA
5101	GTCATGCGCTACCGCAACCTGATCGAGGGCGAAGCATCCGCCGGTTCCTAATGTACGGAG
5161	CAGATGCTAGGGCAAATTGCCCTAGCAGGGGAAAAAGGTCGAAAAGGTCTCTTTCCTGTG
5221	GATAGCACGTACATTGGGAACCCAAAGCCGTACATTGGGAACCGGAACCCGTACATTGGG
5281	AACCCAAAGCCGTACATTGGGAACCGGTCACACATGTAAGTGACTGATATAAAAGAGAAA
5341	AAAGGCGATTTTTCCGCCTAAAACTCTTTAAAACTTATTAAAACTCTTAAAACCCGCCTG

5' Base	Sequence
5401	GCCTGTGCATAACTGTCTGGCCAGCGCACAGCCGAAGAGCTGCAAAAAGCGCCTACCCTT
5461	CGGTCGCTGCGCTCCCTACGCCCCGCCGCTTCGCGTCGGCCTATCGCGGCCGCTGGCCGC
5521	TCAAAAATGGCTGGCCTACGGCCAGGCAATCTACCAGGGCGCGGACAAGCCGCGCCGTCG
5581	CCACTCGACCGCCGGCGCCCACATCAAGGCACCCTGCCTCGCGCGTTTCGGTGATGACGG
5641	TGAAAACCTCTGACACATGCAGCTCCCGGAGACGGTCACAGCTTGTCTGTAAGCGGATGC
5701	CGGGAGCAGACAAGCCCGTCAGGGCGCGTCAGCGGGTGTTGGCGGGTGTCGGGGCGCAGC
5761	CATGACCCAGTCACGTAGCGATAGCGGAGTGTATACTGGCTTAACTATGCGGCATCAGAG
5821	CAGATTGTACTGAGAGTGCACCATATGCGGTGTGAAATACCGCACAGATGCGTAAGGAGA
5881	AAATACCGCATCAGGCGCTCTTCCGCTTCCTCGCTCACTGACTCGCTGCGCTCGGTCGTT
5941	CGGCTGCGGCGAGCGGTATCAGCTCACTCAAAGGCGGTAATACGGTTATCCACAGAATCA
6001	GGGGATAACGCAGGAAAGAACATGTGAGCAAAAGGCCAGCAAAAGGCCAGGAACCGTAAA
6061	AAGGCCGCGTTGCTGGCGTTTTTCCATAGGCTCCGCCCCCCTGACGAGCATCACAAAAAT
6121	CGACGCTCAAGTCAGAGGTGGCGAAACCCGACAGGACTATAAAGATACCAGGCGTTTCCC
6181	CCTGGAAGCTCCCTCGTGCGCTCTCCTGTTCCGACCCTGCCGCTTACCGGATACCTGTCC
6241	GCCTTTCTCCCTTCGGGAAGCGTGGCGCTTTCTCATAGCTCACGCTGTAGGTATCTCAGT
6301	TCGGTGTAGGTCGTTCGCTCCAAGCTGGGCTGTGTGCACGAACCCCCCGTTCAGCCCGAC
6361	CGCTGCGCCTTATCCGGTAACTATCGTCTTGAGTCCAACCCGGTAAGACACGACTTATCG
6421	CCACTGGCAGCAGCCACTGGTAACAGGATTAGCAGAGCGAGGTATGTAGGCGGTGCTACA
6481	GAGTTCTTGAAGTGGTGGCCTAACTACGGCTACACTAGAAGGACAGTATTTGGTATCTGC
6541	GCTCTGCTGAAGCCAGTTACCTTCGGAAAAAGAGTTGGTAGCTCTTGATCCGGCAAACAA
6601	ACCACCGCTGGTAGCGGTGGTTTTTTTGTTTGCAAGCAGCAGATTACGCGCAGAAAAAAA
6661	GGATCTCAAGAAGATCCTTTGATCTTTTCTACGGGGTCTGACGCTCAGTGGAACGAAAAC
6721	TCACGTTAAGGGATTTTG**GTCATGCATGATATATCTCCCAATTTGTGTAGGGCTTATTAT**
6781	**GCACGCTTAAAAATAATAAAAGCAGACTTGACCTGATAGTTTGGCTGTGAGCAATTATGT**
6841	**GCTTAGTGCATCTAATCGCTTGAGTTAACGCCGGCGAAGCGGCGTCGGCTTGAACGAATT**
6901	**TCTAGCTAGACATTATTTGCCGACTACCTTGGTGATCTCGCCTTTCACGTAGTGGACAAA**
6961	**TTCTTCCAACTGATCTGCGCGCGAGGCCAAGCGATCTTCTTCTTGTCCAAGATAAGCCTG**
7021	**TCTAGCTTCAAGTATGACGGGCTGATACTGGGCCGGCAGGCGCTCCATTGCCCAGTCGGC**
7081	**AGCGACATCCTTCGGCGCGATTTTGCCGGTTACTGCGCTGTACCAAATGCGGGACAACGT**
7141	**AAGCACTACATTTCGCTCATCGCCAGCCCAGTCGGGCGGCGAGTTCCATAGCGTTAAGGT**
7201	**TTCATTTAGCGCCTCAAATAGATCCTGTTCAGGAACCGGATCAAAGAGTTCCTCCGCCGC**
7261	**TGGACCTACCAAGGCAACGCTATGTTCTCTTGCTTTTGTCAGCAAGATAGCCAGATCAAT**
7321	**GTCGATCGTGGCTGGCTCGAAGATACCTGCAAGAATGTCATTGCGCTGCCATTCTCCAAA**
7381	**TTGCAGTTCGCGCTTAGCTGGATAACGCCACGGAATGATGTCGTCGTGCACAACAATGGT**
7441	**GACTTCTACAGCGCGGAGAATCTCGCTCTCTCCAGGGGAAGCCGAAGTTTCCAAAAGGTC**
7501	**GTTGATCAAAGCTCGCCGCGTTGTTTCATCAAGCCTTACGGTCACCGTAACCAGCAAATC**
7561	**AATATCACTGTGTGGCTTCAGGCCGCCATCCACTGCGGAGCCGTACAAATGTACGGCCAG**
7621	**CAACGTCGGTTCGAGATGGCGCTCGATGACGCCAACTACCTCTGATAGTTGAGTCGATAC**
7681	**TTCGGCGATCACCGCTTCCCCCATGATGTTTAACTTTGTTTTAGGGCGACTGCCCTGCTG**
7741	**CGTAACATCGTTGCTGCTCCATAACATCAAACATCGACCCACGGCGTAACGCGCTTGCTG**
7801	**CTTGGATGCCCGAGGCATAGACTGTACCCCAAAAAAACATGTCATAACAAGAAGCCATGA**
7861	**AAACCGCCACTGCGCCGTTACCACCGCTGCGTTCGGTCAAGGTTCTGGACCAGTTGCGTG**
7921	**ACGGCAGTTACGCTACTTGCATTACAGCTTACGAACCGAACGAGGCTTATGTCCACTGGG**
7981	**TTCGTGCC**CGAAT**TGATCACAGGCAGCAACGCTCTGTCATCGTTACAATCAACATGCTAC**
8041	**CCTCCGCGAGATCATCCGTGTTTCAAACCCGGCAGCTTAGTTGCCGTTCTTCCGAATAGC**
8101	**ATCGGTAACATGAGCAAAGTCTGCCGCCTTACAACGGCTCTCCCGCTGACGCCGTCCCGG**
8161	**ACTGATGGGCTGCCTGTATCGAGTGGTGATTTTGTGCCGAGCTGCCGGTCGGGGAGCTGT**
8221	**TGGCTGGCTGGTGGCAGGATATATTGTGGTGTAAACAAATTGACGCTTAGACAACTTAAT**
8281	**AACACATTGCGGACGTTTTTAATGTACTGAATTAACGCCGAATTG**AATT**ATCAGCTTGCA**
8341	**TGCCGGTCGATCTAGTAACATAGATGACACCGCGCGCGATAATTTATCCTAGTTTGCGCG**
8401	**CTATATTTTGTTTTCTATCGCGTATTAAATGTATAATTGCGGGACTCTAATCATAAAAAC**
8461	**CCATCTCATAAATAACGTCATGCATTACATGTTAATTATTACATGCTTAACGTAATTCAA**
8521	**CAGAAATTATATGATAATCATCGCAAGACCGGCAACAGGATTCAATCTTAAGAAACTTTA**
8581	**TTGCCAAATGTTTGAACGATCTGCTTGACTCTAGGGAATTAATTCCTGAATCACTGCGAC**
8641	**CGGCCCTCCCGCGACCCAGCCGAGCGAGCTTAGCGAACTGTGGACGAGAACTGTGCCACC**
8701	**AAGCGTAAGGCCGTTCTCTCGCATTTGCCTTGCTAGGCTCGCGCGAGTTGCTGGCTGAGG**
8761	**CGTTCTCGAAATCAGCTCTTGTTCGGTCGGCATCTACTCTATTCCTTTGCCCTCGGACGA**
8821	**GTGCTGGGGCGTCGGTTTCCACTATCGGCGAGTACTTCTACACAGCCATCGGTCCAGACG**
8881	**GCCGCGCTTCTGCGGGCGATTTGTGTACGCCCGACAGTCCCGGCTCCGGATCGGACGATT**

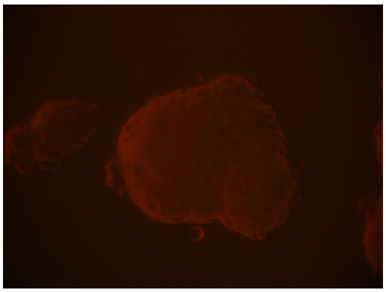
5' Base	Sequence
8941	**GCGTCGCATCGACCCTGCGCCCAAGCTGCATCATCGAAATTGCCGTCAACCAAGCTCTGA**
9001	**TAGAGTTGGTCAAGACCAATGCGGAGCATATACGCCCGGAGCCTTGGCGATCCTGCAAGC**
9061	**TCCGGATGCCTCCGCTCGAAGTAGCGCGTCTGCTGCTCCATACAAGCCAACCACGGCCTC**
9121	**CAGAAGAAGATGTTGGCGACCTCGTATTGGGAATCCCCGAACATCGCCTCGCTCCAGTCA**
9181	**ATGACCGCTGTTATGCGGCCATTGTCCGTCAGGACATTGTTGGAGCCGAATCCGCGTGCA**
9241	**CGAGTGCCGGACTTCGGGGCAGTCCTCGCCCAAAGCATCAGCTCATCGAGAGCCTGCGCG**
9301	**ACGGACGCACTGACGGTGTCGTCCATCACAGTTTGCCAGTGATACACATGGGGATCAGCA**
9361	**ATCGCGCATATGAAATCACGCCATGTAGTGTATTGACCGATTCCTTGCGGTCCGAATGGG**
9421	**CCGAACCCGCTCGTCTGGCTAAGATCGGCCGCAGCGATAGCATCCATAGCCTCCGCGACC**
9481	**GGCTGAAGAACAGCGGGCAGTTCGGTTTCAGGCAGGTCTTGCAACGTGACACCCTGTGCA**
9541	**CGGCGGGAGATGCAATAGGTCAGGCTCTCGCTGAACTCCCCAATGTCAAGCACTTCCGGA**
9601	**ATCGGGAGCGCGGCCGATGCAAAGTGCCGATAAACATAACGATCTTTGTAGAAACCATCG**
9661	**GCGCAGCTATTTACCCGCAGGACATATCCACGCCCTCCTACATCGAAGCTGAAAGCACGA**
9721	**GATTCTTCGCCCTCCGAGAGCTGCATCAGGTCGGAGACGCTGTCGAACTTTTCGATCAGA**
9781	**AACTTCTCGACAGACGTCGCGGTGAGTTCAGGCTTTTTCATAGGGGGGATTCGAGTTGAG**
9841	**AGTGAATATGAGACTCTAATTGGATACCGAGGGGAATTTATGGAACGTCAGTGGAGCATT**
9901	**TTTGACAAGAAATATTTGCTAGCTGATAGTGACCTTAGGCGACTTTTGAACGCGCAATAA**
9961	**TGGTTTCTGACGTATGTGCTTAGCTCATTAAACTCCAGAAACCCGCGGCTCAGTGGCTCC**
10021	**TTCAACGTTGCGGTTCTGTCAGTTCCAAACGTAAAACGGCTTGTCCCGCGTCATCGGCGG**
10081	**GGTCATAACGTGACTCCCTTAATTCTCATGTATGATAATT**CGAGGGTACCCGGGGATCCT
10141	CTAGAGGGCCCGACGTCGCATGCCTGC**AGGTCACTGGATTTTGGTTTTAGGAATTAGAAA**
10201	**TTTTATTGATAGAAGTATTTTACAAATACAAATACATACTAAGGGTTTCTTATATGCTCA**
10261	**ACACATGAGCGAAACCCTATAAGAACCCTAATTCCCTTATCTGGGAACTACTCACACATT**
10321	**ATTCTGGAGAAAAATAGAGAGAGATAGATTTGTAGAGAGAGACTGGTGATTTTTGCGGAC**
10381	**TCTAGCATGGCCG**CGGGATATCACC**ACTTTGTACAAGAAAGCTGGGTCGA**ATTCGCCCTT
10441	TGGTGAC**TTAAGCAGATGAAGCTTTCTTACAATGGGCTTCAAGCCAGTCCATGGTAACAC**
10501	**TCTTTGGCCTCTCAAGTGCAAGTCCAAGAGCTCGGTCCCATATAAGCTGAGAGCAGATGC**
10561	**CAAGACTCCTTGAAACACCAAAGAGCACGGTGTAGTACCTTGCTTCGGTTAGACCATAGT**
10621	**GGTTCAGCAAGACCCCACTGTGAGCATCAACATTTGGCCACGGGTTCTTCACCTTTCCAA**
10681	**GCTCAGTGAGAACAGGAGGCACAACTTCATAAAGCTTTGACACCAGCTGGAAAAGAGGGT**
10741	**CGTCAGGTAGATGCTTCAAGGCAAATTCTCTTTGGCATACATATCTTGGATCAGTATTGC**
10801	**GCAGAACACCGTGACCATATCCCGGAATAACCTTGCCACTGTTTAATGTTTTCCAAACAT**
10861	**ATTCTTTCAACTGTTCTTTTGATATATCTTCTCCACATTCCTCTACGACTGATTTGATCC**
10921	**AAAGCAAAACTTCCTGATTAGCCAAACCATGGAGTGGCCCAGCTAAACCATTTAATGCAG**
10981	**CTGCAAATGACAGATATGGGTCTGAAAGTGCACTACCAACCAGGTGACCAGTGTGAGCAC**
11041	**TAACATTTCCACCTTCATGATCACTGTGGATGGTGATGTAAAGCCTCATGAGCTCTTTCA**
11101	**CCTTTTCATCATCAAATCCCAACATGTGGGAAAAATTTGCACCATAATCCAAAGATTTAT**
11161	**CTGAGGGAATGGAATCACCATTCTTATACATCCTTCGATAAACATATGCAGCTACAACAG**
11221	**GAACACGAGCAATCAGGTTGAGGCAATCCTCATATGTTGGCTCCCAGAACTTTGACTTAT**
11281	**GAATTCCATTCTCATATGCCTTTTGAAACTCACTTTGCACCTGGAGGGCCATAACACCGC**
11341	**TAGCAAATTGAGTCATTGGATGAGCTGTGGAAGGCAGAGCATCGATGGCATTGTACACAT**
11401	**AATCTGGCACAGCAGCACGGTTCGCCAAGTCTTTCGACAGTGCTTCAACTTGCTCTTTGC**
11461	**TAGGTACCTTTCCAGTTAAGAGAAGCCACAAAAGACCCTCCGGTAATGGTTCAGCTCCAG**
11521	**ACTGGGCAGTAGGTAATACTTTCTGGCACTCAGGAATCGACAATCCCCTAAAGCGAATAC**
11581	**CCTCTTCCGGGTCAAGCAATGAGGTTTCCCAAAGCAATCCAGTCATCCCTCTCATTCCAC**
11641	**CAATAACCATATCAACAGTGATGTTTCCCAGTTGGACCTTCCCATGTTCTGACTTCAGTT**
11701	**TCTTCAGACGGTCCTGCTGTTCCGGAATTAACTCTTGCAGCTGCGACTTCAGGTCCAGGT**
11761	**CGGTAGAGCTCTGCATCTGAATCCATCTGACAGAATTGCTGAGTGAAGATTGTTGGCCGA**
11821	**CGCGAGACCTCAGCCTAGTAAAGGCCGATACGCTGCGGAAAAACACCAT**TCTCCAAAACT
11881	CAAAACCAGAGATTCGAGAGCTTCAAAGGGCGAATTCGG*AGCCTGCTTTTTTGTACAAAC*
11941	*TTGT*GATATCACTAGTGCGGCCGCCTGCAGG**TCGACTAGAATAGTAAATTGTAATGTTGT**
12001	**TTGTTGTTTGTTTTGTTGTGGTATTGTTGTAAAAATACCGGAGTCCTCTCCAAATGAAAT**
12061	**GAACTTCCTTATATAGAGGAAGGGTCTTGCGAAGGATAGTGGGATTGTGCGTCATCCCTT**
12121	**ACGTCAGTGGAGATATCACATCAATCCACTTGCTTTGAAGACGTGGTTGGAACGTCTTCT**
12181	**TTTTCCACGATGCTCCTCGTGGGTGGGGGTCCATCTTTGGGACCACTGTCGGCAGAGGCA**
12241	**TCTTGAACGATAGCCTTTCCTTTATCGCAATGATGGCATTTGTAGGTGCCACCTTCCTTT**
12301	**TCTACTGTCCTTTTGATGAAGTGACAGATAGCTGGGCAATGGAATCCGAGGAGGTTTCCC**
12361	**GATATTACCCTTTGTTGAAAAGTCTCAATAGCCCTTTGGTCTTCTGAGACTGTATCTTTG**
12421	**ATATTCTTGGAGTAGACGAGAGTGTCGTGCTCCACCATGTTGACGAAGATTTTCTTCTTG**

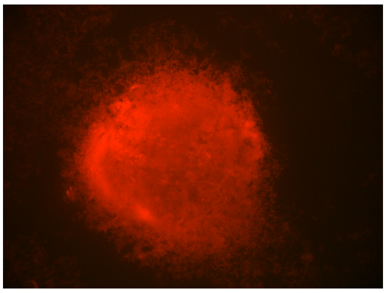
5' Base	Sequence
12481	**TCATTGAGTCGTAAAAGACTCTGTATGAACTGTTCGCCAGTCTTCACGGCGAGTTCTGTT**
12541	**AGATCCTCGATCTGAATTTTTGACTCCATGGCCTTTGATTCAGTAGGAACTACTTTCTTA**
12601	**GAGACTCCAATCTCTATTACTTGCCTTGGTTTATGAAGCAAGCCTTGAATCGTCCATACT**
12661	**GGAATAGTACTTCTGATCTTGAGAAATATATCTTTCTCTGTGTTCTTGATGCAGTTAGTC**
12721	**CTGAATCTTTTGACTGCATCTTTAACCTTCTTGGGAAGGTATTTGATCTCCTGGAGATTA**
12781	**TTACTCGGGTAGATCGTCTTGATGAGACCTGCCGCGTAGGCCTCTCTAACCATCTGTGGG**
12841	**TCAGCATTCTTTCTGAAATTGAAGAGGCTAATCTTCTCATTATCGGTGGTGAACATGGTA**
12901	**TCGTCACCTTCTCCGTCGAACTTTCTTCCTAGATCGTAGAGATAGAGAAAGTCGTCCATG**
12961	**GTGATCTCCGGGGCAAAGGAGATCAGCTTGGCTCTAGT**CGACCATATGGGAGAGCTCA

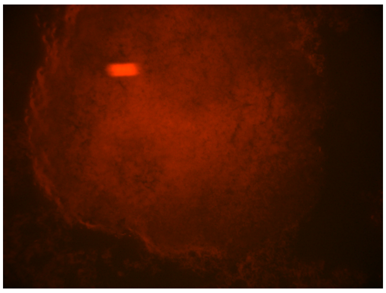
Appendix 4.3. Fluorescence of transformed calli

A subset of transgenic calli were screened by epifluorescence microscopy. *ATCS* and control constructs encode for GFP, which fluoresces green under yellow light. The control construct also encodes mCherry, which fluoresces red under violet light. Note that there is minor excitation of GFP under violet light, which accounts for the red fluorescence of *ATCS*. Images were captured at 1x magnification with an exposure of 8.58 s.

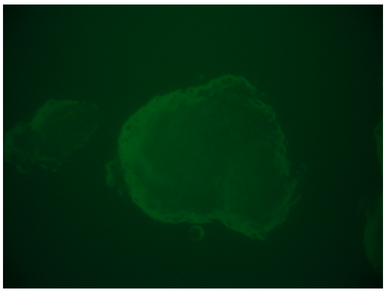
Red fluorescence

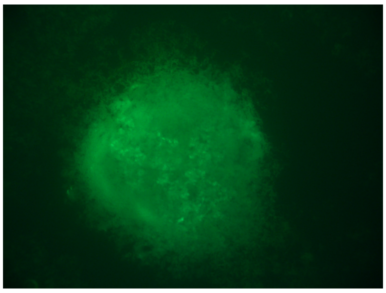

WT

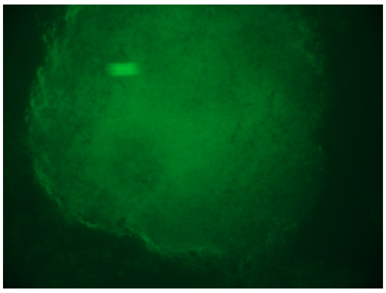

Control (*mCherry-GFP*)


ATCS (*ATCS-GFP*)

Green fluorescence

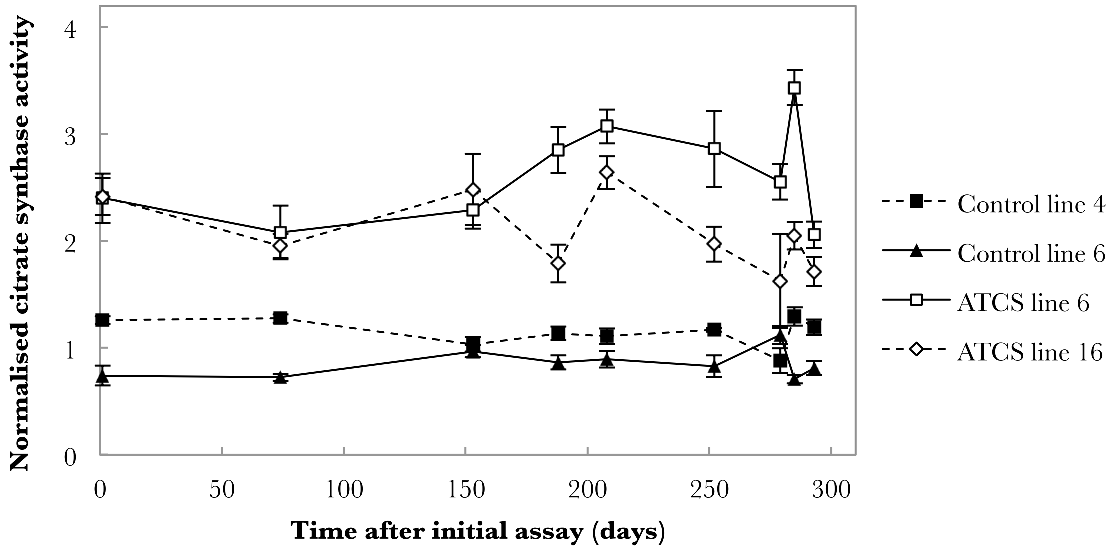

WT


Control (*mCherry-GFP*)


ATCS (*ATCS-GFP*)

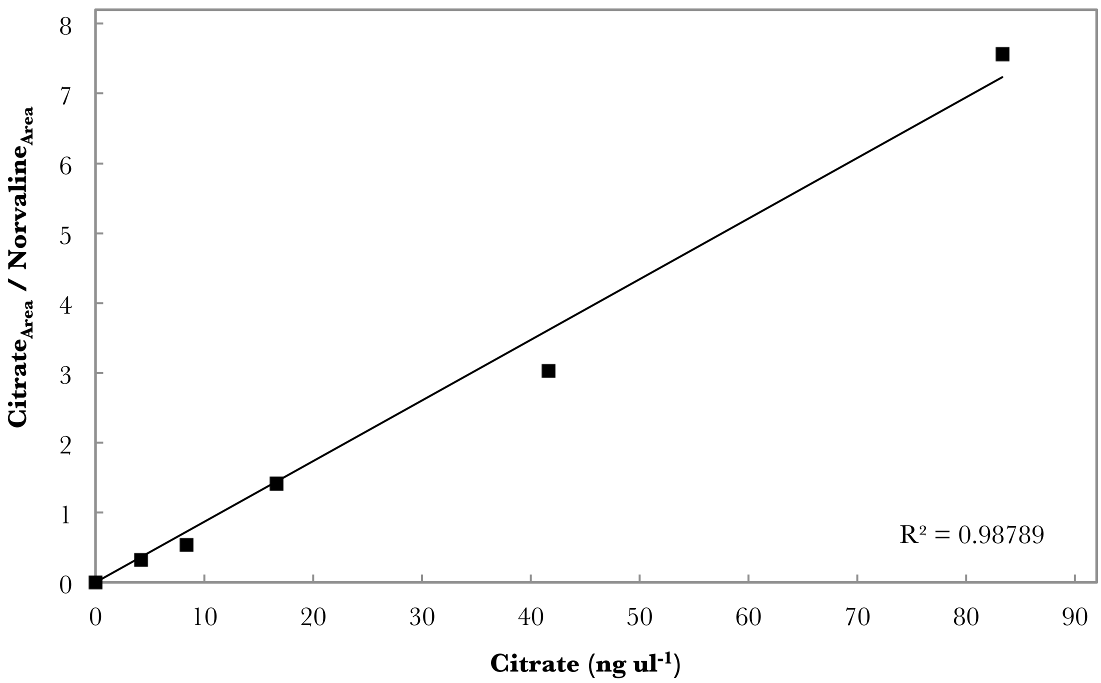
Appendix 4.4. Citrate synthase activity over time

At each time-point citrate synthase activity (measured by acetyl-CoA consumption) in desalted protein extracts was normalised to the mean activity of the two control lines. Each data point represents the mean of three biological replicates. Error bars indicate standard error.



Appendix 4.5. Calibration of GC-MS response to varying concentrations of citrate

Citrate was quantified by GC-MS relative to the internal standard norvaline. Calibration of GC-MS response to citrate content was conducted by Mr Pedro Bota. This gave the following results:

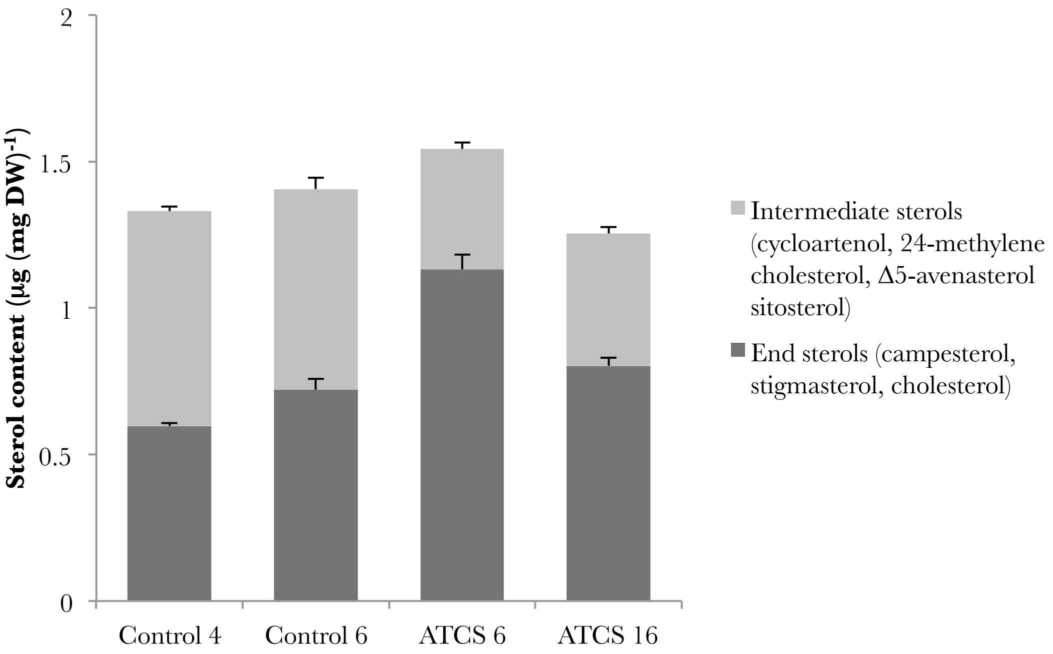


Linear regression gave the following quantification formula:

$$Citrate_{ng.\mu l^{-1}} = 11.52 \times \left(\frac{Citrate_{area}}{Norvaline_{area}}\right)$$

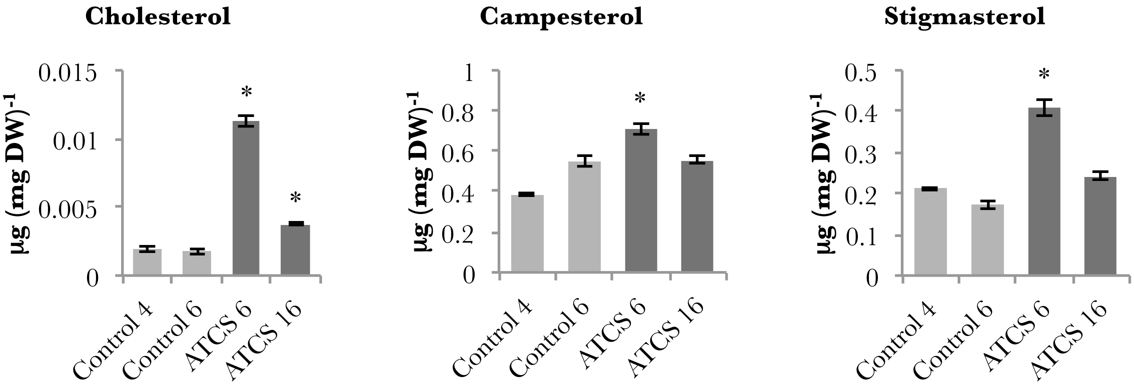
Appendix 4.6. Unconjugated sterol levels in *ATCS* and control lines

There were no statistically significant differences in cumulative unconjugated sterol levels between the four lines. However, *ATCS* lines 6 and 16 each had significantly lower intermediate sterol levels ($p < 0.01$) than controls. *ATCS* line 6 had significantly higher end product sterol levels ($p < 0.005$), but *ATCS* line 16 did not.



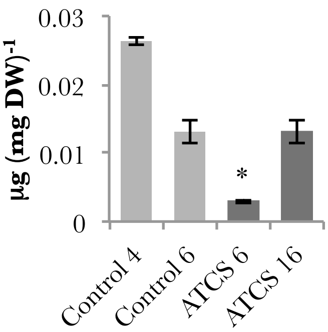
The following is data on individual free sterol levels from log-phase *ATCS* lines 6 and 16, and control lines 4 and 6 (following hexane extraction without prior saponification). Measurements marked with "*" are significantly different to each of the control lines ($p < 0.05$). Error bars represent SE, n = 3.

End product sterols

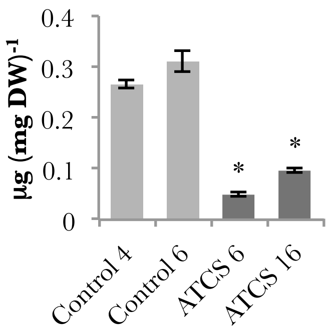


Pathway intermediate sterols

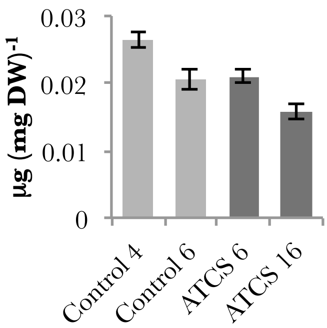
Cycloartenol



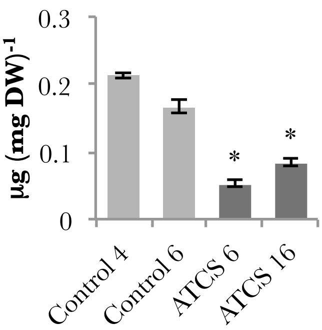
24-methylene cholesterol



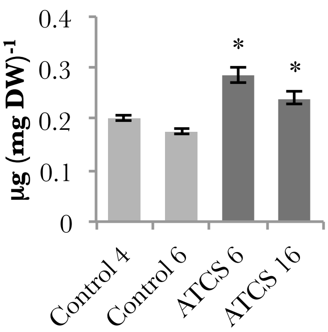
Δ^5-avenasterol



Fucosterol

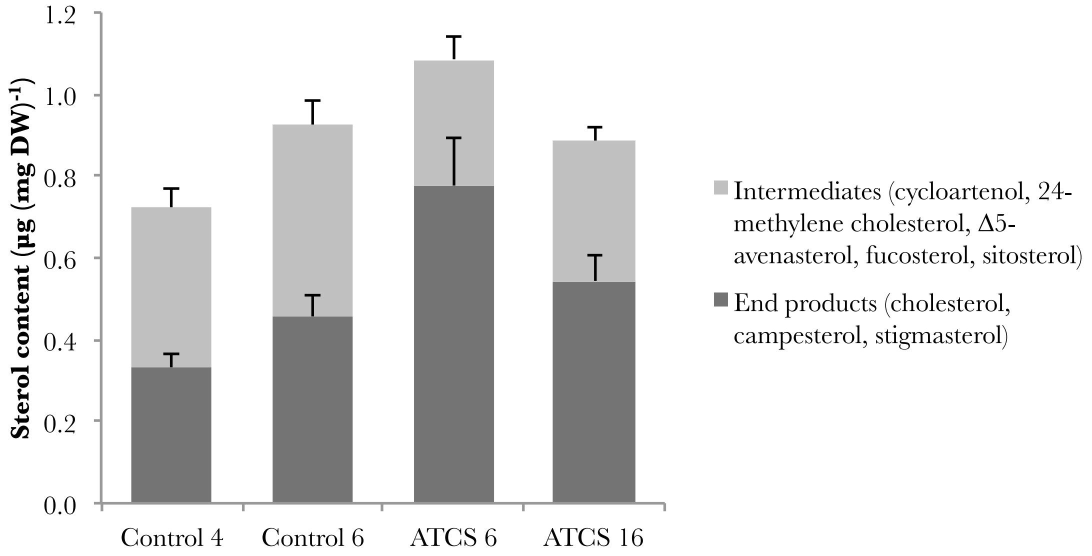


Sitosterol



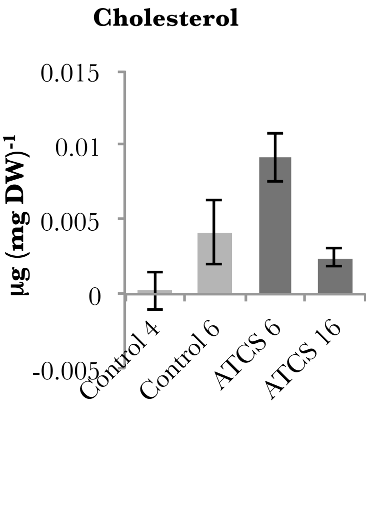
Appendix 4.7. Estimated conjugated sterol levels in *ATCS* and control lines

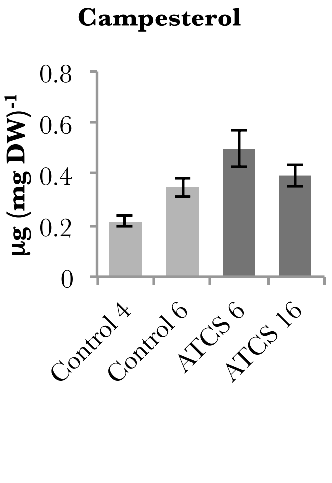
There were no statistically significant differences in predicted total conjugated sterol levels between the four lines. Similarly, there were no significant differences in the predicted cumulative levels of intermediate sterols or end product sterols.

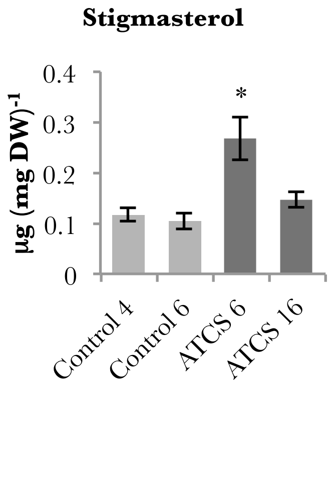


The following is data on individual free sterol levels from log-phase *ATCS* lines 6 and 16, and control lines 4 and 6 (following hexane extraction without prior saponification). Measurements marked with "*" are significantly different to each of the control lines ($p < 0.05$). Error bars represent SE, $n = 3$. *ATCS* lines 6 and 16 Δ^5-avenasterol content is less than 0 µg (mg DW^{-1}). This could be an indication that a significant proportion of this sterol is degraded during the alkaline hydrolysis step of total sterol extraction.

End product sterols

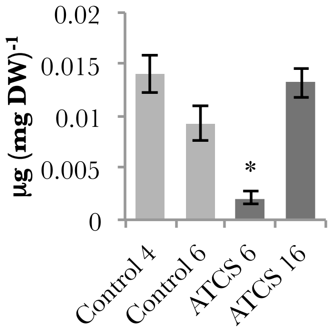




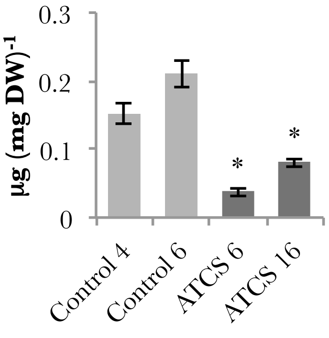


Pathway intermediate sterols

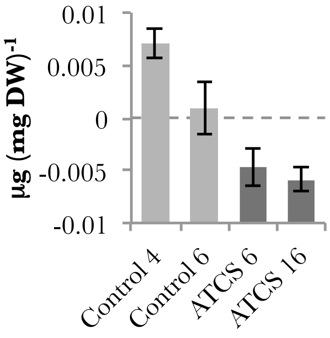
Cycloartenol



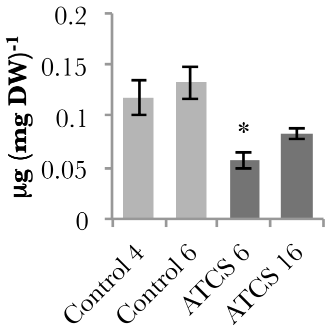
24-methylene cholesterol



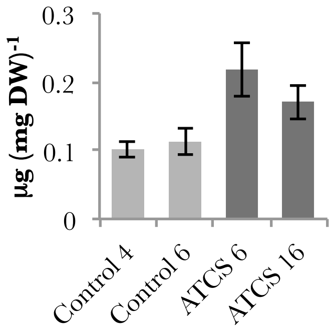
Δ^5-avenasterol



Fucosterol



Sitosterol



Appendix 4.8. Control line 4 metabolome data by day

	Days post-subculture			
Analyte	**4**	**5**	**6**	**7**
Aconitic acid, cis- (3TMS)	1.26 ± 0.78	1.87 ± 0.22	-0.12 ± 0.07	1.00 ± 1.11
Alanine (2TMS)	1.68 ± 1.68	0.00 ± 0.00	1.12 ± 1.12	1.21 ± 1.21
Alanine (3TMS)	0.64 ± 0.14	0.66 ± 0.16	1.34 ± 0.23	1.36 ± 0.14
Alanine [+CO2] (2TMS)	0.46 ± 0.29	0.67 ± 0.12	1.60 ± 0.81	1.28 ± 0.69
Alanine, beta- (3TMS)	0.67 ± 0.05	0.67 ± 0.06	1.29 ± 0.02	1.36 ± 0.15
Arabinose (1MEOX) (4TMS) MP	1.02 ± 0.16	1.12 ± 0.10	1.03 ± 0.07	0.83 ± 0.23
Asparagine (2TMS)	0.29 ± 0.15	0.44 ± 0.06	1.40 ± 0.65	1.87 ± 1.39
Asparagine (3TMS)	0.42 ± 0.29	1.00 ± 0.13	1.05 ± 0.45	1.53 ± 0.52
Asparagine [-H2O] (2TMS)	0.26 ± 0.18	0.38 ± 0.12	1.41 ± 0.20	1.95 ± 0.33
Aspartic acid (2TMS)	0.72 ± 0.41	0.29 ± 0.20	1.78 ± 0.08	1.21 ± 0.66
Aspartic acid (3TMS)	1.87 ± 0.71	1.96 ± 0.20	0.06 ± 0.05	0.11 ± 0.03
Butanoic acid, 2-amino- (2TMS)	2.30 ± 2.30	0.00 ± 0.00	0.99 ± 0.99	0.71 ± 0.71
Butanoic acid, 2,4-dihydroxy- (3TMS)	1.17 ± 0.15	1.07 ± 0.04	1.02 ± 0.07	0.74 ± 0.13
Butanoic acid, 4-amino- (3TMS)	0.76 ± 0.09	1.29 ± 0.35	0.99 ± 0.12	0.97 ± 0.13
Butanoic acid, 4-hydroxy- (2TMS)	0.19 ± 1.25	2.68 ± 1.59	1.48 ± 0.37	-0.35 ± 1.43
Butyro-1,4-lactam (1TMS)	0.23 ± 0.28	0.75 ± 0.17	1.74 ± 1.10	1.28 ± 0.67
Campesterol (1TMS)	0.74 ± 0.38	0.65 ± 0.28	1.20 ± 0.78	1.42 ± 0.03
Citric acid (4TMS)	0.47 ± 0.35	0.91 ± 0.11	1.35 ± 0.15	1.26 ± 0.32
Cycloartenol (1TMS)	1.13 ± 1.13	0.40 ± 0.40	1.39 ± 1.39	1.08 ± 0.54
Dehydroascorbic acid dimer (2MEOX) MP	1.31 ± 0.08	1.22 ± 0.04	0.78 ± 0.16	0.69 ± 0.18
Eicosanoic acid (1TMS)	0.61 ± 0.62	0.88 ± 0.46	1.12 ± 0.76	1.39 ± 0.18
Erythronic acid (4TMS)	1.16 ± 0.16	0.95 ± 0.06	1.03 ± 0.12	0.86 ± 0.16
Ethanolamine (3TMS)	0.14 ± 0.05	0.13 ± 0.06	1.12 ± 0.09	2.61 ± 0.56
Fructose (1MEOX) (5TMS) BP	1.36 ± 0.64	0.66 ± 0.05	0.92 ± 0.32	1.06 ± 0.58
Fructose (1MEOX) (5TMS) MP	1.38 ± 0.64	0.67 ± 0.09	0.90 ± 0.32	1.06 ± 0.63
Fucosterol (1TMS)	1.19 ± 0.67	0.83 ± 0.37	1.02 ± 0.75	0.97 ± 0.08
Fumaric acid (2TMS)	0.98 ± 0.26	1.23 ± 0.13	0.96 ± 0.06	0.83 ± 0.14
Galactinol (9TMS)	0.56 ± 0.28	0.68 ± 0.14	1.19 ± 0.35	1.57 ± 0.02
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)	0.10 ± 0.08	0.18 ± 0.02	1.60 ± 0.80	2.11 ± 0.56
Galactose-6-phosphate (1MEOX) (6TMS) early peak	1.83 ± 0.64	1.03 ± 0.05	0.70 ± 0.16	0.44 ± 0.04
Galactose-6-phosphate (1MEOX) (6TMS) late peak	1.57 ± 0.63	1.13 ± 0.07	0.79 ± 0.14	0.51 ± 0.04
Gluconic acid (6TMS)	0.88 ± 0.15	0.86 ± 0.08	1.20 ± 0.22	1.06 ± 0.21
Glucopyranose, D- (5TMS)	0.07 ± 0.01	0.07 ± 0.01	1.80 ± 0.53	2.06 ± 0.82
Glucose (1MEOX) (5TMS) BP	0.67 ± 0.37	0.92 ± 0.11	1.15 ± 0.28	1.26 ± 0.53
Glucose (1MEOX) (5TMS) MP	1.18 ± 0.29	0.79 ± 0.10	0.92 ± 0.42	1.10 ± 0.79
Glucose-6-phosphate (1MEOX) (6TMS) MP	1.48 ± 0.55	1.17 ± 0.05	0.82 ± 0.14	0.52 ± 0.03
Glucose-6-phosphate (6TMS)	0.01 ± 0.01	0.02 ± 0.01	1.84 ± 0.79	2.13 ± 0.33

	Days post-subculture			
Analyte	**4**	**5**	**6**	**7**
Glutamic acid (2TMS)	1.94 ± 1.04	0.92 ± 0.25	0.58 ± 0.26	0.56 ± 0.40
Glutamic acid (3TMS)	0.92 ± 0.28	1.27 ± 0.14	0.90 ± 0.17	0.91 ± 0.11
Glutamine [-H2O] (2TMS) BP	0.35 ± 0.31	0.69 ± 0.15	1.23 ± 0.41	1.73 ± 0.63
Glutamine [-H2O] (3TMS) MP	0.22 ± 0.20	0.34 ± 0.14	1.39 ± 0.31	2.04 ± 0.21
Glutamine, DL- (3TMS)	0.35 ± 0.35	0.35 ± 0.35	1.47 ± 0.79	1.83 ± 0.98
Glutamine, DL- (4TMS)	0.16 ± 0.16	0.24 ± 0.14	1.67 ± 0.85	1.93 ± 0.96
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	0.66 ± 0.12	0.89 ± 0.11	1.13 ± 0.33	1.32 ± 0.60
Glyceric acid (3TMS)	0.92 ± 0.12	0.87 ± 0.09	1.17 ± 0.02	1.04 ± 0.27
Glycerol-2-phosphate (4TMS)	0.86 ± 0.53	0.85 ± 0.50	1.06 ± 0.45	1.23 ± 0.38
Glycerol-3-phosphate (4TMS)	1.36 ± 0.41	1.17 ± 0.27	0.79 ± 0.12	0.69 ± 0.08
Glycerophosphoglycerol (5TMS)	3.10 ± 2.74	0.63 ± 0.06	0.18 ± 0.03	0.10 ± 0.03
Glycine (2TMS)	0.13 ± 0.13	0.00 ± 0.00	0.00 ± 0.00	3.87 ± 3.87
Glycine (3TMS)	0.44 ± 0.15	0.52 ± 0.12	1.38 ± 0.01	1.65 ± 0.28
Heptadecanoic acid (1TMS)	1.32 ± 0.75	0.87 ± 0.87	1.35 ± 0.72	0.46 ± 0.46
Hexadecanoic acid (1TMS)	0.76 ± 0.50	0.98 ± 0.38	1.26 ± 0.40	1.00 ± 0.09
Homoserine (3TMS)	0.43 ± 0.15	0.61 ± 0.04	1.57 ± 0.18	1.39 ± 0.10
Inositol, *myo*- (6TMS)	1.02 ± 0.16	1.11 ± 0.11	1.07 ± 0.06	0.80 ± 0.06
Isoleucine (1TMS)	0.58 ± 0.29	0.86 ± 0.09	1.31 ± 0.06	1.25 ± 0.05
Isomaltose (1MEOX) (8TMS) BP	1.18 ± 0.66	1.00 ± 0.52	0.92 ± 0.47	0.90 ± 0.45
Lactic acid, DL- (2TMS)	0.95 ± 0.95	0.00 ± 0.00	0.89 ± 0.88	2.16 ± 2.16
Leucine (1TMS)	0.59 ± 0.30	0.96 ± 0.08	1.25 ± 0.05	1.20 ± 0.12
Lyxonic acid (5TMS)	1.26 ± 0.68	0.59 ± 0.11	0.94 ± 0.31	1.20 ± 0.32
Lyxose (1MEOX) (4TMS) MP	0.86 ± 0.45	1.31 ± 0.08	1.00 ± 0.10	0.83 ± 0.24
Malic acid (3TMS)	0.94 ± 0.12	0.93 ± 0.12	1.05 ± 0.23	1.08 ± 0.41
Malic acid, 2-methyl- (3TMS)	1.37 ± 0.19	1.34 ± 0.09	0.86 ± 0.05	0.43 ± 0.10
Maltose (1MEOX) (8TMS) BP	0.74 ± 0.37	0.94 ± 0.13	1.15 ± 0.23	1.16 ± 0.21
Maltose (1MEOX) (8TMS) MP	1.24 ± 0.63	1.83 ± 0.18	0.27 ± 0.27	0.66 ± 0.66
Methionine (1TMS)	0.26 ± 0.15	0.37 ± 0.09	1.28 ± 0.04	2.10 ± 0.12
Methionine (2TMS)	0.27 ± 0.12	0.31 ± 0.05	1.21 ± 0.06	2.21 ± 0.38
myo-Inositol-1-phosphate (7TMS)	1.28 ± 0.43	1.05 ± 0.25	0.86 ± 0.30	0.81 ± 0.04
Norleucine (2TMS)	2.04 ± 0.94	0.88 ± 0.03	0.69 ± 0.03	0.39 ± 0.01
Octadecadienoic acid, n- (1TMS)	0.77 ± 0.44	0.88 ± 0.41	1.28 ± 0.80	1.07 ± 0.34
Octadecan-1-ol, n- (1TMS)	0.91 ± 0.55	1.18 ± 0.27	1.43 ± 0.30	0.48 ± 0.70
Octadecanoic acid (1TMS)	0.77 ± 0.65	1.07 ± 0.45	1.15 ± 0.17	1.02 ± 0.15
Ornithine-1,5-lactam (2TMS)	0.89 ± 0.45	1.19 ± 0.16	0.27 ± 0.27	1.64 ± 0.82
Phenylalanine (2TMS)	0.58 ± 0.25	0.85 ± 0.10	1.29 ± 0.09	1.28 ± 0.08
Phosphoric acid (3TMS)	2.07 ± 0.59	1.08 ± 0.08	0.52 ± 0.03	0.33 ± 0.06
Putrescine (4TMS)	0.39 ± 0.18	0.55 ± 0.11	1.34 ± 0.04	1.72 ± 0.15
Pyroglutamic acid (2TMS)	0.70 ± 0.18	0.83 ± 0.09	1.18 ± 0.17	1.29 ± 0.45
Pyruvic acid (1MEOX) (1TMS)	0.22 ± 0.22	0.00 ± 0.00	1.54 ± 1.54	2.24 ± 2.24
Ribonic acid (5TMS) early peak	0.89 ± 0.07	0.89 ± 0.08	1.11 ± 0.18	1.11 ± 0.27
Ribonic acid (5TMS) late peak	0.87 ± 0.42	1.07 ± 0.06	1.08 ± 0.16	0.98 ± 0.23
Ribose (1MEOX) (4TMS) BP	0.89 ± 0.19	1.08 ± 0.10	1.14 ± 0.10	0.89 ± 0.17

	Days post-subculture			
Analyte	**4**	**5**	**6**	**7**
Salicin (5TMS)	-0.13 ± 0.22	0.00 ± 0.38	3.52 ± 3.89	0.62 ± 0.99
Serine (2TMS)	0.45 ± 0.23	0.71 ± 0.06	1.33 ± 0.13	1.51 ± 0.25
Serine (3TMS)	1.12 ± 0.33	0.64 ± 0.03	0.99 ± 0.16	1.25 ± 0.30
Serine (4TMS)	0.39 ± 0.21	0.49 ± 0.16	1.49 ± 0.18	1.63 ± 0.16
Serine, O-acetyl- (2TMS)	0.56 ± 0.13	0.67 ± 0.11	1.34 ± 0.33	1.43 ± 0.22
Sitosterol, beta- (1TMS)	0.88 ± 0.47	0.68 ± 0.29	1.17 ± 0.83	1.27 ± 0.12
Stigmasterol (1TMS)	0.84 ± 0.43	0.68 ± 0.31	1.19 ± 0.84	1.29 ± 0.03
Succinic acid (2TMS)	0.83 ± 0.31	1.07 ± 0.21	1.10 ± 0.10	1.00 ± 0.30
Sucrose (8TMS)	0.49 ± 0.55	0.90 ± 0.13	1.21 ± 0.37	1.40 ± 0.74
Tagatose (1MEOX) (5TMS) BP	0.88 ± 0.12	0.62 ± 0.11	2.53 ± 1.55	-0.04 ± 0.04
Threonic acid (4TMS)	0.89 ± 0.28	1.17 ± 0.10	1.21 ± 0.14	0.73 ± 0.18
Threonine (3TMS)	0.96 ± 0.16	0.70 ± 0.03	1.09 ± 0.29	1.25 ± 0.39
Threonine, DL- (2TMS)	0.49 ± 0.25	0.81 ± 0.03	1.39 ± 0.11	1.32 ± 0.02
Turanose (1MEOX) (8TMS) BP	1.21 ± 0.61	1.37 ± 0.17	0.81 ± 0.41	0.61 ± 0.06
Tyrosine (3TMS)	0.29 ± 0.26	0.40 ± 0.22	1.43 ± 0.73	1.89 ± 0.95
Uracil (2TMS)	0.71 ± 0.49	1.14 ± 0.32	1.12 ± 0.42	1.03 ± 0.39
Uric acid (4TMS)	0.36 ± 0.36	0.76 ± 0.38	1.34 ± 0.67	1.54 ± 0.80
Uridine (4TMS)	1.43 ± 0.75	2.02 ± 0.70	0.29 ± 0.18	0.26 ± 0.13
Valine (1TMS)	0.00 ± 0.00	0.00 ± 0.00	2.32 ± 2.32	1.68 ± 1.68
Valine (2TMS)	1.07 ± 0.44	0.65 ± 0.05	1.02 ± 0.17	1.26 ± 0.21
Xylitol (5TMS)	0.88 ± 0.37	1.06 ± 0.05	1.08 ± 0.12	0.98 ± 0.18
Xylose (1MEOX) (4TMS) MP	1.76 ± 0.86	0.89 ± 0.04	0.73 ± 0.08	0.62 ± 0.17
Xylulose-5-phosphate (1MEOX) (5TMS) BP	1.78 ± 1.12	1.51 ± 0.21	0.46 ± 0.09	0.25 ± 0.02

Appendix 4.9. Control line 6 metabolome data by day

	Days post-subculture		
Analyte	**4**	**5**	**6**
Aconitic acid, cis- (3TMS)	1.12 ± 0.36	1.40 ± 0.40	0.48 ± 0.55
Alanine (3TMS)	0.53 ± 0.14	0.82 ± 0.29	1.65 ± 0.23
Alanine [+CO_2] (2TMS)	0.63 ± 0.22	0.95 ± 0.27	1.42 ± 0.28
Alanine, beta- (3TMS)	0.62 ± 0.12	0.80 ± 0.20	1.58 ± 0.04
Arabinose (1MEOX) (4TMS) MP	0.83 ± 0.10	1.20 ± 0.31	0.97 ± 0.06
Asparagine (2TMS)	0.61 ± 0.16	0.81 ± 0.21	1.57 ± 0.14
Asparagine (3TMS)	0.25 ± 0.07	0.31 ± 0.18	2.43 ± 0.41
Asparagine [-H2O] (2TMS)	0.32 ± 0.09	0.82 ± 0.28	1.86 ± 0.24
Aspartic acid (2TMS)	0.03 ± 0.06	1.66 ± 0.55	1.31 ± 0.24
Aspartic acid (3TMS)	1.58 ± 0.26	0.70 ± 0.53	0.71 ± 0.24
Butanoic acid, 2,4-dihydroxy- (3TMS)	0.96 ± 0.14	1.22 ± 0.39	0.83 ± 0.03
Butanoic acid, 4-amino- (3TMS)	2.08 ± 0.84	0.35 ± 0.09	0.57 ± 0.08
Butanoic acid, 4-hydroxy- (2TMS)	2.94 ± 1.42	0.02 ± 0.03	0.04 ± 0.02
Butyro-1,4-lactam (1TMS)	2.04 ± 1.09	0.37 ± 0.11	0.59 ± 0.17
Campesterol (1TMS)	0.42 ± 0.19	0.81 ± 0.27	1.76 ± 0.55
Citric acid (4TMS)	0.44 ± 0.14	1.21 ± 0.31	1.34 ± 0.12
Cycloartenol (1TMS)	0.00 ± 0.00	1.53 ± 1.53	1.47 ± 1.47
Dehydroascorbic acid dimer (2MEOX) MP	1.35 ± 0.38	0.91 ± 0.31	0.73 ± 0.04
Eicosanoic acid (1TMS)	0.25 ± 0.72	0.95 ± 0.69	1.80 ± 0.50
Erythronic acid (4TMS)	0.91 ± 0.18	1.15 ± 0.42	0.94 ± 0.02
Ethanolamine (3TMS)	0.16 ± 0.05	0.39 ± 0.08	2.44 ± 0.10
Fructose (1MEOX) (5TMS) BP	1.01 ± 0.40	0.95 ± 0.30	1.04 ± 0.14
Fructose (1MEOX) (5TMS) MP	1.01 ± 0.42	0.97 ± 0.40	1.02 ± 0.14
Fucosterol (1TMS)	0.67 ± 0.34	1.12 ± 0.55	1.21 ± 0.41
Fumaric acid (2TMS)	1.54 ± 0.56	0.88 ± 0.17	0.58 ± 0.04
Galactinol (9TMS)	0.51 ± 0.08	0.77 ± 0.18	1.72 ± 0.06
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)	0.33 ± 0.04	0.40 ± 0.10	2.26 ± 0.87
Galactose-6-phosphate (1MEOX) (6TMS) early peak	0.83 ± 0.07	1.19 ± 0.31	0.98 ± 0.10
Galactose-6-phosphate (1MEOX) (6TMS) late peak	1.25 ± 0.35	1.00 ± 0.24	0.76 ± 0.08
Gluconic acid (6TMS)	0.69 ± 0.17	1.28 ± 0.27	1.03 ± 0.08
Glucopyranose, D- (5TMS)	0.14 ± 0.09	0.16 ± 0.01	2.69 ± 0.91
Glucose (1MEOX) (5TMS) BP	1.01 ± 0.30	0.97 ± 0.24	1.01 ± 0.08
Glucose (1MEOX) (5TMS) MP	1.07 ± 0.45	0.97 ± 0.41	0.96 ± 0.17
Glucose-6-phosphate (1MEOX) (6TMS) MP	1.26 ± 0.36	0.98 ± 0.24	0.76 ± 0.07
Glucose-6-phosphate (6TMS)	0.06 ± 0.01	0.05 ± 0.01	2.89 ± 1.71
Glutamic acid (2TMS)	0.70 ± 0.10	1.71 ± 0.44	0.59 ± 0.13
Glutamic acid (3TMS)	0.53 ± 0.13	0.86 ± 0.21	1.60 ± 0.27
Glutamine [-H_2O] (2TMS) BP	0.54 ± 0.27	0.85 ± 0.42	1.61 ± 0.24
Glutamine [-H_2O] (3TMS) MP	0.14 ± 0.06	0.75 ± 0.35	2.12 ± 0.34
Glutamine, DL- (3TMS)	0.00 ± 0.00	0.56 ± 0.39	2.44 ± 0.33

	Days post-subculture		
Analyte	**4**	**5**	**6**
Glutamine, DL- (4TMS)	0.02 ± 0.02	0.73 ± 0.59	2.25 ± 0.71
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	0.80 ± 0.17	1.12 ± 0.31	1.07 ± 0.38
Glyceric acid (3TMS)	0.85 ± 0.21	1.12 ± 0.25	1.03 ± 0.14
Glycerol-2-phosphate (4TMS)	0.95 ± 0.52	1.39 ± 0.91	0.66 ± 0.13
Glycerol-3-phosphate (4TMS)	1.51 ± 0.34	0.90 ± 0.14	0.59 ± 0.10
Glycerophosphoglycerol (5TMS)	2.67 ± 0.41	0.27 ± 0.06	0.06 ± 0.01
Glycine (3TMS)	0.27 ± 0.07	0.73 ± 0.23	2.00 ± 0.25
Heptadecanoic acid (1TMS)	1.61 ± 0.16	0.51 ± 0.51	0.88 ± 0.88
Hexadecanoic acid (1TMS)	0.84 ± 0.16	0.90 ± 0.20	1.26 ± 0.24
Homoserine (3TMS)	0.25 ± 0.04	0.68 ± 0.25	2.07 ± 0.35
Inositol, *myo*- (6TMS)	0.87 ± 0.22	1.05 ± 0.24	1.07 ± 0.05
Isoleucine (1TMS)	0.47 ± 0.10	0.87 ± 0.20	1.66 ± 0.09
Isomaltose (1MEOX) (8TMS) BP	0.29 ± 0.29	0.93 ± 0.53	1.78 ± 0.37
Lactic acid, DL- (2TMS)	0.40 ± 0.40	2.60 ± 2.36	0.00 ± 0.00
Leucine (1TMS)	0.54 ± 0.14	0.82 ± 0.21	1.64 ± 0.07
Lyxonic acid (5TMS)	1.17 ± 0.37	0.91 ± 0.22	0.92 ± 0.36
Lyxose (1MEOX) (4TMS) MP	1.00 ± 0.22	1.08 ± 0.29	0.93 ± 0.01
Malic acid (3TMS)	0.93 ± 0.27	1.05 ± 0.26	1.02 ± 0.07
Malic acid, 2-methyl- (3TMS)	1.17 ± 0.32	1.22 ± 0.30	0.60 ± 0.05
Maltose (1MEOX) (8TMS) BP	1.22 ± 0.44	0.64 ± 0.16	1.14 ± 0.08
Maltose (1MEOX) (8TMS) MP	2.46 ± 1.13	0.31 ± 0.05	0.23 ± 0.02
Methionine (1TMS)	0.07 ± 0.02	0.40 ± 0.02	2.53 ± 0.57
Methionine (2TMS)	0.20 ± 0.03	0.34 ± 0.10	2.47 ± 0.27
myo-Inositol-1-phosphate (7TMS)	1.02 ± 0.29	0.99 ± 0.14	0.98 ± 0.19
Norleucine (2TMS)	1.44 ± 0.54	0.77 ± 0.17	0.78 ± 0.09
Octadecadienoic acid, n- (1TMS)	0.77 ± 0.51	1.26 ± 0.85	0.97 ± 0.28
Octadecan-1-ol, n- (1TMS)	0.86 ± 0.05	1.17 ± 0.31	0.98 ± 0.12
Octadecanoic acid (1TMS)	0.90 ± 0.31	0.74 ± 0.19	1.36 ± 0.08
Ornithine-1,5-lactam (2TMS)	3.00 ± 1.24	0.00 ± 0.00	0.00 ± 0.00
Phenylalanine (2TMS)	0.45 ± 0.09	0.88 ± 0.20	1.67 ± 0.02
Phosphoric acid (3TMS)	1.73 ± 0.51	0.89 ± 0.19	0.38 ± 0.02
Putrescine (4TMS)	0.29 ± 0.08	0.85 ± 0.24	1.86 ± 0.08
Pyroglutamic acid (2TMS)	0.56 ± 0.10	1.12 ± 0.30	1.32 ± 0.12
Ribonic acid (5TMS) early peak	0.86 ± 0.21	0.98 ± 0.29	1.16 ± 0.04
Ribonic acid (5TMS) late peak	0.90 ± 0.23	1.07 ± 0.40	1.02 ± 0.02
Ribose (1MEOX) (4TMS) BP	0.88 ± 0.25	1.10 ± 0.23	1.02 ± 0.06
Salicin (5TMS)	0.27 ± 0.45	2.95 ± 3.02	-0.23 ± 0.13
Serine (2TMS)	0.18 ± 0.03	0.77 ± 0.20	2.05 ± 0.10
Serine (3TMS)	0.86 ± 0.33	0.57 ± 0.14	1.57 ± 0.10
Serine (4TMS)	0.17 ± 0.02	0.94 ± 0.34	1.89 ± 0.28
Serine, O-acetyl- (2TMS)	0.52 ± 0.13	0.59 ± 0.17	1.89 ± 0.22
Sitosterol, beta- (1TMS)	0.50 ± 0.22	0.85 ± 0.32	1.65 ± 0.53
Stigmasterol (1TMS)	0.44 ± 0.22	0.83 ± 0.32	1.73 ± 0.55

	Days post-subculture		
Analyte	**4**	**5**	**6**
Succinic acid (2TMS)	1.62 ± 0.70	0.82 ± 0.19	0.56 ± 0.05
Sucrose (8TMS)	1.12 ± 0.43	0.89 ± 0.28	0.99 ± 0.11
Tagatose (1MEOX) (5TMS) BP	1.85 ± 0.93	1.29 ± 0.69	-0.14 ± 0.14
Threonic acid (4TMS)	0.75 ± 0.14	1.30 ± 0.34	0.94 ± 0.03
Threonine (3TMS)	0.95 ± 0.28	0.66 ± 0.14	1.39 ± 0.15
Threonine, DL- (2TMS)	0.29 ± 0.08	0.82 ± 0.23	1.89 ± 0.08
Turanose (1MEOX) (8TMS) BP	0.73 ± 0.15	1.11 ± 0.37	1.15 ± 0.15
Tyrosine (3TMS)	0.02 ± 0.02	0.45 ± 0.32	2.54 ± 0.31
Uracil (2TMS)	1.67 ± 0.71	0.76 ± 0.13	0.57 ± 0.08
Uric acid (4TMS)	0.33 ± 0.33	0.27 ± 0.27	2.39 ± 0.46
Uridine (4TMS)	2.68 ± 1.19	0.25 ± 0.07	0.06 ± 0.03
Valine (2TMS)	0.48 ± 0.11	0.67 ± 0.21	1.85 ± 0.26
Xylitol (5TMS)	0.92 ± 0.19	1.07 ± 0.28	1.01 ± 0.03
Xylose (1MEOX) (4TMS) MP	1.00 ± 0.23	1.08 ± 0.29	0.93 ± 0.05
Xylulose-5-phosphate (1MEOX) (5TMS) BP	1.54 ± 0.27	1.07 ± 0.19	0.38 ± 0.05

Appendix 4.10. *ATCS* line 6 metabolome data by day

	Days post-subculture			
Analyte	**4**	**5**	**6**	**7**
Aconitic acid, cis- (3TMS)	1.47 ± 0.21	0.89 ± 0.45	0.58 ± 0.72	1.06 ± 0.65
Alanine (3TMS)	0.87 ± 0.16	0.68 ± 0.13	1.49 ± 0.50	0.95 ± 0.37
Alanine [+CO2] (2TMS)	0.81 ± 0.08	0.58 ± 0.09	1.46 ± 0.66	1.15 ± 0.72
Alanine, beta- (3TMS)	0.97 ± 0.12	0.97 ± 0.06	1.24 ± 0.12	0.82 ± 0.40
Arabinose (1MEOX) (4TMS) MP	1.07 ± 0.14	0.87 ± 0.15	0.95 ± 0.10	1.10 ± 0.37
Asparagine (2TMS)	0.72 ± 0.27	1.04 ± 0.41	1.37 ± 0.20	0.87 ± 0.41
Asparagine (3TMS)	0.36 ± 0.15	0.84 ± 0.17	0.98 ± 0.64	1.81 ± 1.37
Asparagine [-H2O] (2TMS)	0.44 ± 0.13	0.84 ± 0.21	1.28 ± 0.21	1.44 ± 0.83
Aspartic acid (2TMS)	0.32 ± 0.38	1.44 ± 0.21	1.48 ± 0.76	0.76 ± 0.38
Aspartic acid (3TMS)	1.89 ± 0.81	0.03 ± 0.03	0.04 ± 0.04	2.05 ± 1.97
Butanoic acid, 2,4-dihydroxy- (3TMS)	1.97 ± 0.36	0.95 ± 0.05	0.67 ± 0.13	0.41 ± 0.18
Butanoic acid, 4-amino- (3TMS)	2.68 ± 0.80	0.50 ± 0.04	0.42 ± 0.09	0.40 ± 0.26
Butanoic acid, 4-hydroxy- (2TMS)	3.80 ± 1.72	-0.01 ± 0.05	-0.01 ± 0.04	0.22 ± 0.24
Butyro-1,4-lactam (1TMS)	2.88 ± 1.07	0.36 ± 0.06	0.50 ± 0.11	0.26 ± 0.24
Campesterol (1TMS)	0.53 ± 0.46	1.52 ± 1.08	1.41 ± 0.57	0.53 ± 0.09
Citric acid (4TMS)	0.37 ± 0.05	0.85 ± 0.07	1.52 ± 0.27	1.26 ± 0.53
Dehydroascorbic acid dimer (2MEOX) MP	2.14 ± 0.71	0.63 ± 0.04	0.60 ± 0.19	0.63 ± 0.26
Eicosanoic acid (1TMS)	0.74 ± 0.96	0.94 ± 0.52	1.55 ± 0.72	0.77 ± 0.30
Erythronic acid (4TMS)	1.54 ± 0.20	1.01 ± 0.10	0.93 ± 0.11	0.52 ± 0.10
Ethanolamine (3TMS)	0.17 ± 0.04	0.80 ± 0.27	1.25 ± 0.21	1.79 ± 1.17
Fructose (1MEOX) (5TMS) BP	1.44 ± 0.42	0.72 ± 0.11	0.79 ± 0.08	1.05 ± 0.79
Fructose (1MEOX) (5TMS) MP	1.44 ± 0.45	0.67 ± 0.11	0.78 ± 0.10	1.11 ± 0.95
Fucosterol (1TMS)	1.19 ± 1.19	2.05 ± 2.05	0.76 ± 0.76	0.00 ± 0.00
Fumaric acid (2TMS)	1.67 ± 0.35	0.91 ± 0.24	0.90 ± 0.21	0.52 ± 0.08
Galactinol (9TMS)	0.72 ± 0.03	1.14 ± 0.07	1.49 ± 0.11	0.65 ± 0.27
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)	0.54 ± 0.45	1.29 ± 0.57	1.71 ± 0.48	0.46 ± 0.11
Galactose-6-phosphate (1MEOX) (6TMS) early peak	1.42 ± 0.37	1.03 ± 0.23	0.92 ± 0.22	0.63 ± 0.26
Galactose-6-phosphate (1MEOX) (6TMS) late peak	1.79 ± 0.56	0.89 ± 0.18	0.73 ± 0.18	0.58 ± 0.30
Gluconic acid (6TMS)	0.77 ± 0.06	1.63 ± 0.19	1.07 ± 0.14	0.53 ± 0.13
Glucopyranose, D- (5TMS)	0.47 ± 0.42	1.32 ± 0.14	1.47 ± 0.18	0.73 ± 0.05
Glucose (1MEOX) (5TMS) BP	1.38 ± 0.34	0.76 ± 0.09	0.82 ± 0.09	1.04 ± 0.61
Glucose (1MEOX) (5TMS) MP	1.67 ± 0.58	0.55 ± 0.20	0.56 ± 0.09	1.22 ± 1.12
Glucose-6-phosphate (1MEOX) (6TMS) MP	1.81 ± 0.56	0.89 ± 0.18	0.71 ± 0.16	0.59 ± 0.32
Glucose-6-phosphate (6TMS)	0.61 ± 0.59	1.19 ± 0.56	1.89 ± 0.69	0.30 ± 0.17
Glutamic acid (2TMS)	2.09 ± 0.63	1.29 ± 0.36	0.12 ± 0.35	0.51 ± 0.27
Glutamic acid (3TMS)	1.28 ± 0.10	0.90 ± 0.10	0.99 ± 0.20	0.83 ± 0.54
Glutamine [-H2O] (2TMS) BP	1.03 ± 0.57	0.87 ± 0.23	1.43 ± 0.60	0.68 ± 0.38
Glutamine [-H2O] (3TMS) MP	0.35 ± 0.17	0.81 ± 0.41	1.03 ± 0.07	1.80 ± 1.41
Glutamine, DL- (3TMS)	0.00 ± 0.00	1.30 ± 0.92	1.63 ± 1.36	1.08 ± 0.56

	Days post-subculture			
Analyte	**4**	**5**	**6**	**7**
Glutamine, DL- (4TMS)	0.13 ± 0.13	1.41 ± 0.33	2.07 ± 0.02	0.40 ± 0.22
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	1.03 ± 0.16	0.71 ± 0.25	1.21 ± 0.27	1.06 ± 0.46
Glyceric acid (3TMS)	0.82 ± 0.10	0.97 ± 0.09	1.35 ± 0.23	0.85 ± 0.29
Glycerol-2-phosphate (4TMS)*	1.15 ± 0.43	0.24 ± 0.49	1.46 ± 0.61	1.15 ± 0.49
Glycerol-3-phosphate (4TMS)	1.88 ± 0.11	0.70 ± 0.26	0.87 ± 0.24	0.55 ± 0.13
Glycerophosphoglycerol (5TMS)	3.53 ± 2.00	0.18 ± 0.07	0.23 ± 0.11	0.06 ± 0.01
Glycine (3TMS)	0.46 ± 0.04	0.78 ± 0.07	1.59 ± 0.27	1.18 ± 0.69
Heptadecanoic acid (1TMS)	1.01 ± 1.01	0.73 ± 0.73	2.27 ± 1.17	0.00 ± 0.00
Hexadecanoic acid (1TMS)	1.37 ± 0.11	0.76 ± 0.20	1.32 ± 0.35	0.55 ± 0.14
Homoserine (3TMS)	0.79 ± 0.07	0.89 ± 0.07	1.44 ± 0.21	0.87 ± 0.40
Inositol, *myo*- (6TMS)	1.40 ± 0.28	0.89 ± 0.10	0.96 ± 0.11	0.75 ± 0.27
Isoleucine (1TMS)	1.02 ± 0.08	1.01 ± 0.06	1.47 ± 0.12	0.50 ± 0.13
Isomaltose (1MEOX) (8TMS) BP	0.70 ± 0.70	1.78 ± 0.41	1.21 ± 0.72	0.30 ± 0.30
Lactic acid, DL- (2TMS)	0.01 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	3.99 ± 3.69
Leucine (1TMS)	1.07 ± 0.08	1.00 ± 0.04	1.56 ± 0.15	0.37 ± 0.22
Lyxonic acid (5TMS)	2.00 ± 0.62	0.52 ± 0.08	0.78 ± 0.11	0.70 ± 0.38
Lyxose (1MEOX) (4TMS) MP	1.34 ± 0.32	0.81 ± 0.13	0.75 ± 0.14	1.09 ± 0.42
Malic acid (3TMS)	0.98 ± 0.11	0.88 ± 0.08	1.02 ± 0.13	1.12 ± 0.57
Malic acid, 2-methyl- (3TMS)	1.49 ± 0.10	1.22 ± 0.27	0.88 ± 0.22	0.41 ± 0.16
Maltose (1MEOX) (8TMS) BP	0.93 ± 0.11	0.99 ± 0.02	1.37 ± 0.10	0.72 ± 0.33
Maltose (1MEOX) (8TMS) MP	2.12 ± 0.84	0.53 ± 0.03	0.69 ± 0.05	0.66 ± 0.46
Methionine (1TMS)	0.12 ± 0.09	0.48 ± 0.07	2.08 ± 0.34	1.33 ± 0.57
Methionine (2TMS)	0.31 ± 0.06	0.36 ± 0.07	1.19 ± 0.06	2.13 ± 1.18
myo-Inositol-1-phosphate (7TMS)	1.57 ± 0.03	1.06 ± 0.49	0.89 ± 0.26	0.48 ± 0.14
Norleucine (2TMS)	1.43 ± 0.32	1.13 ± 0.10	0.95 ± 0.11	0.49 ± 0.32
Octadecadienoic acid, n- (1TMS)	1.03 ± 0.72	0.74 ± 0.46	1.44 ± 0.51	0.79 ± 0.40
Octadecan-1-ol, n- (1TMS)	1.25 ± 0.17	0.83 ± 0.27	1.17 ± 0.26	0.75 ± 0.28
Octadecanoic acid (1TMS)	1.24 ± 0.13	0.88 ± 0.10	1.36 ± 0.35	0.52 ± 0.14
Ornithine-1,5-lactam (2TMS)	1.98 ± 0.99	0.00 ± 0.00	1.14 ± 1.14	0.88 ± 0.88
Phenylalanine (2TMS)	0.93 ± 0.08	0.87 ± 0.05	1.21 ± 0.24	0.99 ± 0.25
Phosphoric acid (3TMS)	2.68 ± 0.70	0.52 ± 0.13	0.46 ± 0.12	0.34 ± 0.29
Putrescine (4TMS)	0.34 ± 0.08	1.09 ± 0.08	1.72 ± 0.27	0.85 ± 0.44
Pyroglutamic acid (2TMS)	0.80 ± 0.05	0.98 ± 0.11	0.95 ± 0.10	1.26 ± 0.68
Ribonic acid (5TMS) early peak	1.32 ± 0.26	0.85 ± 0.08	1.03 ± 0.12	0.80 ± 0.28
Ribonic acid (5TMS) late peak	1.51 ± 0.21	0.86 ± 0.04	0.92 ± 0.12	0.72 ± 0.24
Ribose (1MEOX) (4TMS) BP	1.13 ± 0.24	1.16 ± 0.14	0.89 ± 0.14	0.82 ± 0.31
Salicin (5TMS)	0.18 ± 0.18	-0.07 ± 0.04	0.01 ± 0.03	3.88 ± 3.61
Serine (2TMS)	0.87 ± 0.05	1.01 ± 0.06	1.54 ± 0.23	0.58 ± 0.17
Serine (3TMS)	1.09 ± 0.33	0.54 ± 0.09	0.96 ± 0.08	1.41 ± 0.99
Serine (4TMS)	0.56 ± 0.11	0.81 ± 0.10	1.48 ± 0.30	1.15 ± 0.16
Serine, O-acetyl- (2TMS)	1.04 ± 0.21	0.69 ± 0.04	1.31 ± 0.23	0.96 ± 0.49
Sitosterol, beta- (1TMS)	0.61 ± 0.52	1.62 ± 1.21	1.33 ± 0.54	0.44 ± 0.15
Stigmasterol (1TMS)	0.45 ± 0.38	1.40 ± 1.01	1.54 ± 0.59	0.61 ± 0.15

	Days post-subculture			
Analyte	**4**	**5**	**6**	**7**
Succinic acid (2TMS)	1.83 ± 0.43	0.78 ± 0.26	0.94 ± 0.27	0.45 ± 0.13
Sucrose (8TMS)	1.55 ± 0.44	0.69 ± 0.07	0.76 ± 0.11	1.01 ± 0.77
Tagatose (1MEOX) (5TMS) BP	1.12 ± 0.56	2.96 ± 1.70	-0.04 ± 0.04	-0.04 ± 0.04
Threonic acid (4TMS)	0.77 ± 0.20	1.34 ± 0.12	1.19 ± 0.20	0.71 ± 0.20
Threonine (3TMS)	1.25 ± 0.30	0.58 ± 0.10	0.82 ± 0.05	1.34 ± 0.86
Threonine, DL- (2TMS)	0.79 ± 0.12	1.10 ± 0.11	1.53 ± 0.14	0.58 ± 0.20
Turanose (1MEOX) (8TMS) BP	0.69 ± 0.12	1.21 ± 0.28	1.30 ± 0.26	0.81 ± 0.56
Tyrosine (3TMS)	0.05 ± 0.05	0.97 ± 0.22	2.33 ± 0.82	0.64 ± 0.41
Uracil (2TMS)	2.07 ± 0.38	0.86 ± 0.38	0.67 ± 0.06	0.39 ± 0.20
Uric acid (4TMS)	1.87 ± 1.10	0.84 ± 0.31	1.03 ± 0.26	0.26 ± 0.26
Uridine (4TMS)	3.39 ± 0.89	0.32 ± 0.15	0.16 ± 0.09	0.13 ± 0.07
Valine (2TMS)	0.85 ± 0.16	0.78 ± 0.12	1.09 ± 0.15	1.29 ± 1.02
Xylitol (5TMS)	1.43 ± 0.21	0.92 ± 0.06	0.96 ± 0.15	0.69 ± 0.20
Xylose (1MEOX) (4TMS) MP	1.28 ± 0.32	0.84 ± 0.13	0.78 ± 0.12	1.11 ± 0.40
Xylulose-5-phosphate (1MEOX) (5TMS) BP	2.21 ± 0.39	0.83 ± 0.18	0.51 ± 0.10	0.44 ± 0.24

* Glycerol-2-phosphate (4TMS) levels are significantly different between days five and seven ($p < 0.0005$).

Appendix 4.11. *ATCS* line 16 metabolome data by day

	Days post-subculture		
Analyte	**4**	**5**	**6**
Aconitic acid, cis- (3TMS)	1.72 ± 0.50	0.95 ± 0.56	0.33 ± 0.41
Alanine (3TMS)	0.81 ± 0.12	0.90 ± 0.03	1.29 ± 0.13
Alanine [+CO2] (2TMS)	0.82 ± 0.15	0.85 ± 0.35	1.33 ± 0.41
Alanine, beta- (3TMS)	1.05 ± 0.16	1.03 ± 0.07	0.93 ± 0.12
Arabinose (1MEOX) (4TMS) MP	1.29 ± 0.15	1.20 ± 0.06	0.51 ± 0.08
Asparagine (2TMS)	1.05 ± 0.47	1.02 ± 0.51	0.93 ± 0.41
Asparagine (3TMS)	0.78 ± 0.32	1.07 ± 0.63	1.15 ± 0.47
Asparagine [-H2O] (2TMS)	1.06 ± 0.46	1.07 ± 0.52	0.86 ± 0.11
Aspartic acid (2TMS)	1.23 ± 1.28	0.27 ± 0.33	1.50 ± 0.49
Aspartic acid (3TMS)	1.91 ± 0.92	1.14 ± 0.68	-0.05 ± 0.01
Butanoic acid, 2,4-dihydroxy- (3TMS)	1.43 ± 0.11	1.10 ± 0.27	0.47 ± 0.04
Butanoic acid, 4-amino- (3TMS)	1.35 ± 0.47	1.28 ± 0.68	0.37 ± 0.02
Butanoic acid, 4-hydroxy- (2TMS)	1.47 ± 1.00	1.47 ± 1.36	0.06 ± 0.02
Butyro-1,4-lactam (1TMS)	1.43 ± 0.44	1.25 ± 0.67	0.32 ± 0.03
Campesterol (1TMS)	1.40 ± 0.72	0.93 ± 0.54	0.67 ± 0.39
Citric acid (4TMS)	1.04 ± 0.36	1.06 ± 0.37	0.91 ± 0.12
Dehydroascorbic acid dimer (2MEOX) MP	1.33 ± 0.20	1.25 ± 0.35	0.43 ± 0.10
Eicosanoic acid (1TMS)	1.18 ± 0.84	1.12 ± 0.32	0.69 ± 0.13
Erythronic acid (4TMS)	1.44 ± 0.21	1.08 ± 0.17	0.48 ± 0.06
Ethanolamine (3TMS)	0.94 ± 0.43	0.50 ± 0.16	1.56 ± 0.28
Fructose (1MEOX) (5TMS) BP	1.36 ± 0.07	1.10 ± 0.11	0.54 ± 0.11
Fructose (1MEOX) (5TMS) MP	1.35 ± 0.05	1.12 ± 0.21	0.53 ± 0.12
Fucosterol (1TMS)	2.38 ± 1.67	0.62 ± 0.62	0.00 ± 0.00
Fumaric acid (2TMS)	1.33 ± 0.11	1.14 ± 0.30	0.54 ± 0.05
Galactinol (9TMS)	1.09 ± 0.22	1.12 ± 0.15	0.79 ± 0.14
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)	0.45 ± 0.05	0.53 ± 0.08	2.02 ± 0.69
Galactose-6-phosphate (1MEOX) (6TMS) early peak	1.20 ± 0.22	1.31 ± 0.12	0.49 ± 0.11
Galactose-6-phosphate (1MEOX) (6TMS) late peak	1.36 ± 0.12	1.31 ± 0.21	0.33 ± 0.05
Gluconic acid (6TMS)	1.26 ± 0.08	0.99 ± 0.13	0.76 ± 0.15
Glucopyranose, D- (5TMS)	0.17 ± 0.09	0.41 ± 0.02	2.42 ± 0.32
Glucose (1MEOX) (5TMS) BP	1.27 ± 0.05	1.12 ± 0.15	0.61 ± 0.09
Glucose (1MEOX) (5TMS) MP	1.38 ± 0.07	1.16 ± 0.21	0.46 ± 0.13
Glucose-6-phosphate (1MEOX) (6TMS) MP	1.35 ± 0.07	1.32 ± 0.18	0.33 ± 0.05
Glucose-6-phosphate (6TMS)	0.10 ± 0.01	0.18 ± 0.03	2.72 ± 0.12
Glutamic acid (2TMS)	1.15 ± 0.31	1.32 ± 0.32	0.53 ± 0.10
Glutamic acid (3TMS)	1.16 ± 0.21	1.12 ± 0.46	0.72 ± 0.21
Glutamine [-H2O] (2TMS) BP	0.73 ± 0.30	1.09 ± 0.53	1.18 ± 0.32
Glutamine [-H2O] (3TMS) MP	0.67 ± 0.48	1.23 ± 0.72	1.10 ± 0.15
Glutamine, DL- (3TMS)	0.00 ± 0.00	1.05 ± 0.94	1.95 ± 0.74
Glutamine, DL- (4TMS)	0.43 ± 0.43	0.89 ± 0.56	1.68 ± 0.58

	Days post-subculture		
Analyte	**4**	**5**	**6**
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	1.15 ± 0.11	0.98 ± 0.08	0.87 ± 0.07
Glyceric acid (3TMS)	1.32 ± 0.06	1.26 ± 0.12	0.41 ± 0.07
Glycerol-2-phosphate (4TMS)	1.50 ± 0.86	0.95 ± 0.31	0.55 ± 0.24
Glycerol-3-phosphate (4TMS)	1.54 ± 0.54	1.09 ± 0.35	0.36 ± 0.09
Glycerophosphoglycerol (5TMS)	1.19 ± 0.95	1.70 ± 1.52	0.10 ± 0.05
Glycine (3TMS)	0.77 ± 0.25	0.96 ± 0.32	1.28 ± 0.15
Heptadecanoic acid (1TMS)	1.37 ± 0.69	1.02 ± 1.02	0.61 ± 0.31
Hexadecanoic acid (1TMS)	1.14 ± 0.31	1.21 ± 0.34	0.66 ± 0.16
Homoserine (3TMS)	0.60 ± 0.36	1.15 ± 0.59	1.25 ± 0.08
Inositol, *myo*- (6TMS)	1.20 ± 0.09	1.16 ± 0.12	0.64 ± 0.07
Isoleucine (1TMS)	1.02 ± 0.30	1.24 ± 0.00	0.75 ± 0.12
Isomaltose (1MEOX) (8TMS) BP	1.49 ± 0.16	1.17 ± 0.62	0.34 ± 0.17
Leucine (1TMS)	0.95 ± 0.28	1.23 ± 0.04	0.82 ± 0.16
Lyxonic acid (5TMS)	1.52 ± 0.24	1.30 ± 0.44	0.18 ± 0.09
Lyxose (1MEOX) (4TMS) MP	1.19 ± 0.08	1.16 ± 0.09	0.65 ± 0.11
Malic acid (3TMS)	1.26 ± 0.09	1.03 ± 0.18	0.71 ± 0.10
Malic acid, 2-methyl- (3TMS)	1.36 ± 0.32	1.15 ± 0.14	0.50 ± 0.12
Maltose (1MEOX) (8TMS) BP	1.14 ± 0.41	1.43 ± 0.86	0.43 ± 0.05
Maltose (1MEOX) (8TMS) MP	1.32 ± 0.62	1.60 ± 1.32	0.08 ± 0.02
Methionine (1TMS)	0.54 ± 0.31	0.37 ± 0.16	2.09 ± 0.63
Methionine (2TMS)	0.72 ± 0.24	0.80 ± 0.33	1.47 ± 0.28
myo-Inositol-1-phosphate (7TMS)	1.46 ± 0.53	1.08 ± 0.23	0.46 ± 0.17
Norleucine (2TMS)	1.62 ± 0.48	1.00 ± 0.15	0.38 ± 0.08
Octadecadienoic acid, n- (1TMS)	1.19 ± 0.74	0.95 ± 0.59	0.86 ± 0.36
Octadecan-1-ol, n- (1TMS)	1.13 ± 0.05	1.19 ± 0.31	0.68 ± 0.11
Octadecanoic acid (1TMS)	1.13 ± 0.17	1.23 ± 0.30	0.64 ± 0.19
Ornithine-1,5-lactam (2TMS)	1.50 ± 1.50	1.11 ± 1.11	0.39 ± 0.39
Phenylalanine (2TMS)	1.06 ± 0.33	1.11 ± 0.28	0.83 ± 0.15
Phosphoric acid (3TMS)	1.64 ± 0.58	1.14 ± 0.52	0.22 ± 0.03
Putrescine (4TMS)	0.68 ± 0.40	1.09 ± 0.48	1.23 ± 0.21
Pyroglutamic acid (2TMS)	1.08 ± 0.16	1.13 ± 0.38	0.79 ± 0.14
Ribonic acid (5TMS) early peak	1.28 ± 0.14	1.18 ± 0.25	0.54 ± 0.08
Ribonic acid (5TMS) late peak	1.32 ± 0.10	1.14 ± 0.16	0.53 ± 0.06
Ribose (1MEOX) (4TMS) BP	1.28 ± 0.30	1.27 ± 0.09	0.44 ± 0.07
Salicin (5TMS)	1.11 ± 0.43	1.41 ± 0.39	0.47 ± 0.19
Serine (2TMS)	0.72 ± 0.43	0.89 ± 0.29	1.39 ± 0.29
Serine (3TMS)	1.23 ± 0.17	1.06 ± 0.31	0.71 ± 0.15
Serine (4TMS)	0.91 ± 0.50	0.87 ± 0.28	1.22 ± 0.11
Serine, O-acetyl- (2TMS)	0.87 ± 0.12	1.16 ± 0.29	0.97 ± 0.11
Sitosterol, beta- (1TMS)	1.34 ± 0.75	0.93 ± 0.50	0.73 ± 0.38
Stigmasterol (1TMS)	1.32 ± 0.69	0.90 ± 0.54	0.78 ± 0.45
Succinic acid (2TMS)	1.29 ± 0.35	1.25 ± 0.55	0.46 ± 0.09
Sucrose (8TMS)	1.34 ± 0.05	1.10 ± 0.16	0.56 ± 0.11

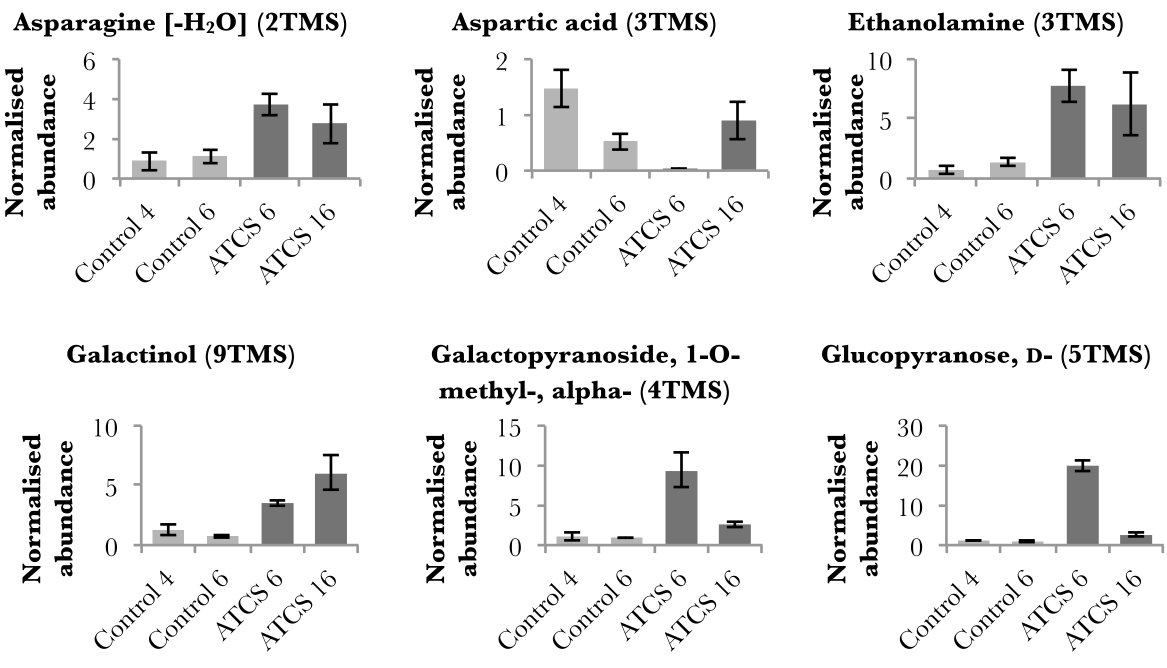
	Days post-subculture		
Analyte	**4**	**5**	**6**
Tagatose (1MEOX) (5TMS) BP	1.79 ± 0.46	1.26 ± 0.98	-0.05 ± 0.05
Threonic acid (4TMS)	1.38 ± 0.32	1.10 ± 0.22	0.52 ± 0.11
Threonine (3TMS)	1.29 ± 0.22	1.26 ± 0.31	0.46 ± 0.07
Threonine, DL- (2TMS)	0.88 ± 0.40	1.03 ± 0.09	1.09 ± 0.25
Turanose (1MEOX) (8TMS) BP	1.15 ± 0.28	1.17 ± 0.33	0.68 ± 0.10
Tyrosine (3TMS)	0.16 ± 0.13	1.31 ± 0.72	1.53 ± 0.47
Uracil (2TMS)	1.54 ± 0.14	1.16 ± 0.43	0.31 ± 0.03
Uric acid (4TMS)	0.00 ± 0.00	0.66 ± 0.66	2.34 ± 0.84
Uridine (4TMS)	1.49 ± 0.76	1.49 ± 1.31	0.02 ± 0.01
Valine (2TMS)	0.82 ± 0.21	1.37 ± 0.67	0.81 ± 0.11
Xylitol (5TMS)	1.29 ± 0.08	1.14 ± 0.09	0.57 ± 0.08
Xylose (1MEOX) (4TMS) MP	1.18 ± 0.11	1.15 ± 0.14	0.67 ± 0.13
Xylulose-5-phosphate (1MEOX) (5TMS) BP	1.43 ± 0.30	1.37 ± 0.75	0.20 ± 0.03

Appendix 4.12. Metabolome comparisons of *ATCS* and control lines, normalised using ribitol

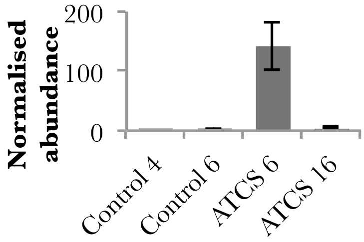
As a means of limiting the likelihood of false negatives arrising from Bonferroni correction for multiple comparisons, analytes were judged to have altered levels in *ATCS* lines if each of the p-values arising from *t* tests between the test line and each of the control lines were less than 0.05 and if the product of these p-values was less than the critical p value after Bonferroni correction (approximately 0.0005). This revealed 12 analytes with significantly increased levels in *ATCS* line 6, and one with decreased levels. 26 analytes were significantly more abundant in *ATCS* line 16 than in the controls, and none were decreased. The sum of peak areas normalised to ribitol and DW was 2.4 ± 0.4 times that of *ATCS* line 16 than controls ($p < 0.05$ follow student's *t* test comparisons with each control line).

Analytes at altered levels in *ATCS* line 6 methanol extracts.

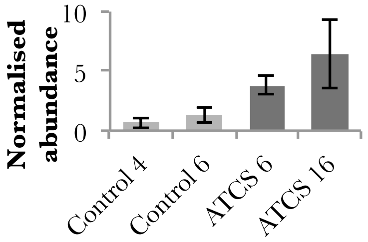
TMS and MEOX derivatives of metabolites determined to be significantly different levels in *ATCS* line 6 extracts than extracts from each of the control lines (Values normalised to mean of controls. Error bars represent SE, n = 6.)



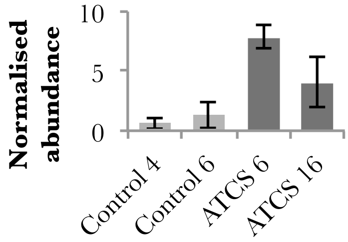
Glucose-6-phosphate (6TMS)



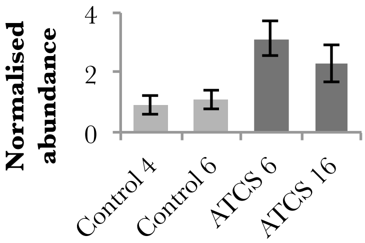
Glutamine [-H2O] (3TMS) MP



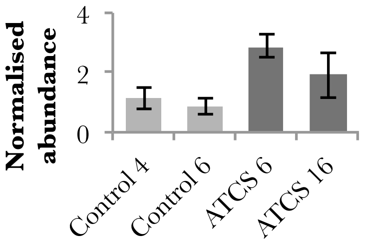
Glutamine, DL- (4TMS)



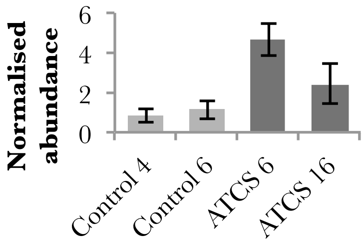
Glycine (3TMS)



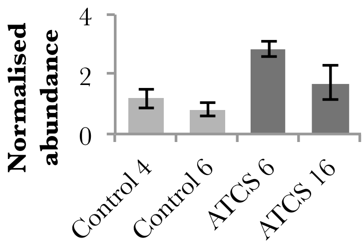
Serine (2TMS)



Serine (4TMS)



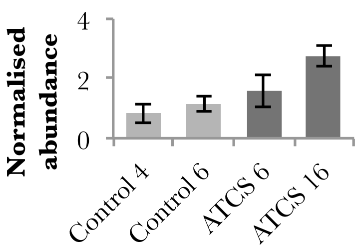
Threonine, DL- (2TMS)



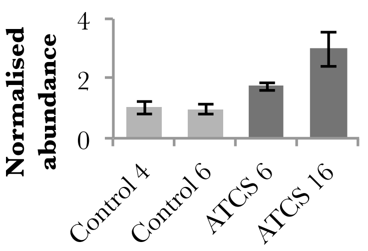
Analytes at altered levels in *ATCS* line 16 methanol extracts

TMS and MEOX derivatives of metabolites determined to be at significantly different levels in *ATCS* line 16 extracts than extracts from each of the control lines (*ATCS* line 6 bars on galactopyranoside, 1-O-methyl-, alpha- (4TMS), glucopyranose, D- (5TMS), and Glucose-6-phosphate (6TMS) graphs are clipped to avoid compression of the y-axis. For visualisation of *ATCS* line 6 data on these analytes, see the graphs presented earlier in Appendix 4.12. Values normalised to mean of controls. Error bars represent SE, n = 6.)

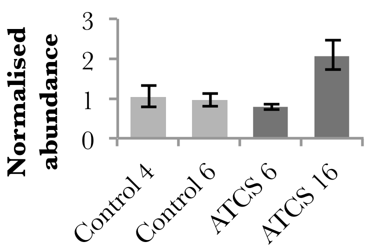
Alanine [+CO_2] (2TMS)



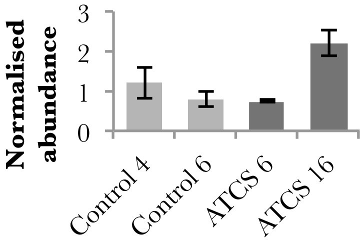
Alanine, beta- (3TMS)



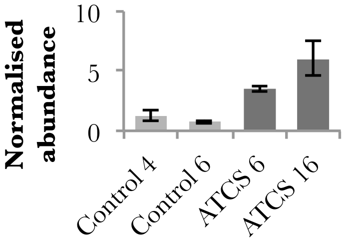
Arabinose (1MEOX) (4TMS) MP



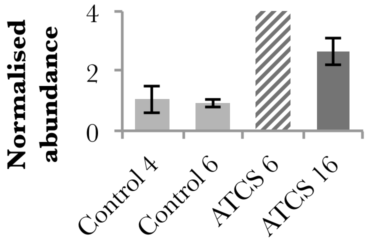
Fructose (1MEOX) (5TMS) BP



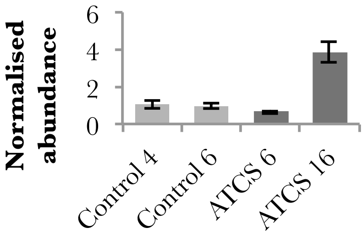
Galactinol (9TMS)



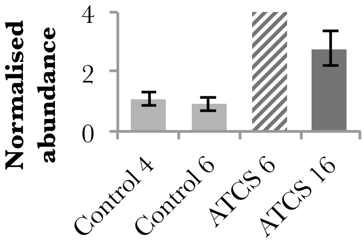
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)



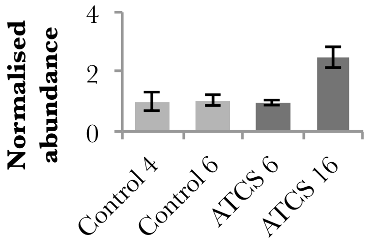
Galactose-6-phosphate (1MEOX) (6TMS) late peak



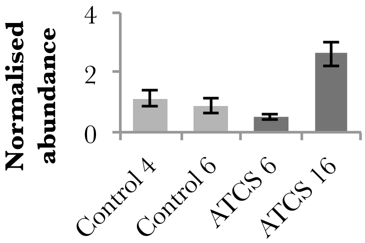
Glucopyranose, D- (5TMS)



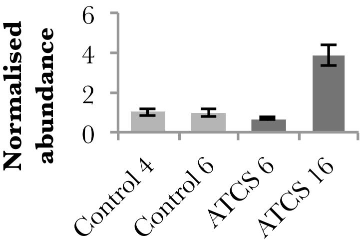
Glucose (1MEOX) (5TMS) BP



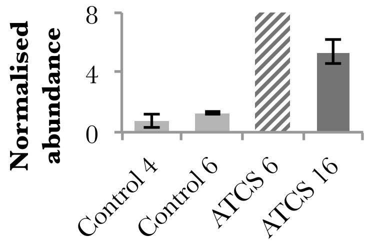
Glucose (1MEOX) (5TMS) MP



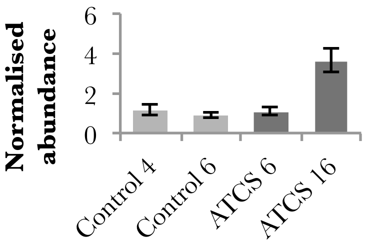
Glucose-6-phosphate (1MEOX) (6TMS) MP



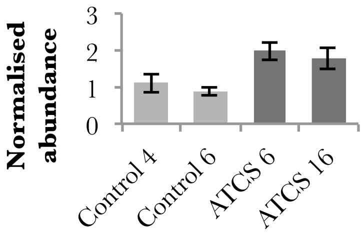
Glucose-6-phosphate (6TMS)



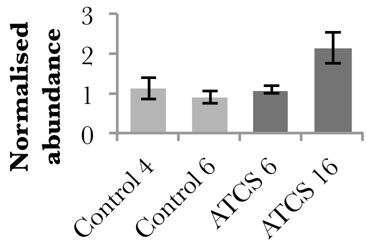
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP



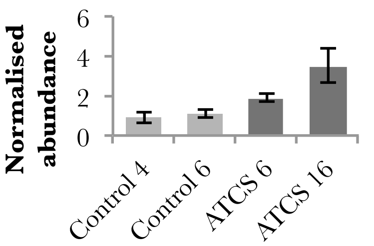
Glyceric acid (3TMS)



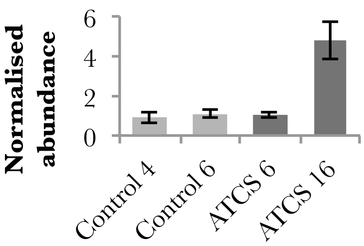
Inositol, *myo*- (6TMS)



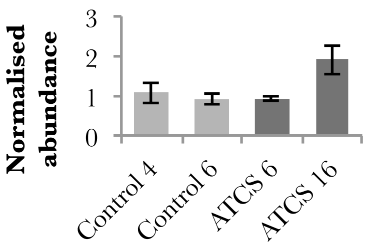
Leucine (1TMS)

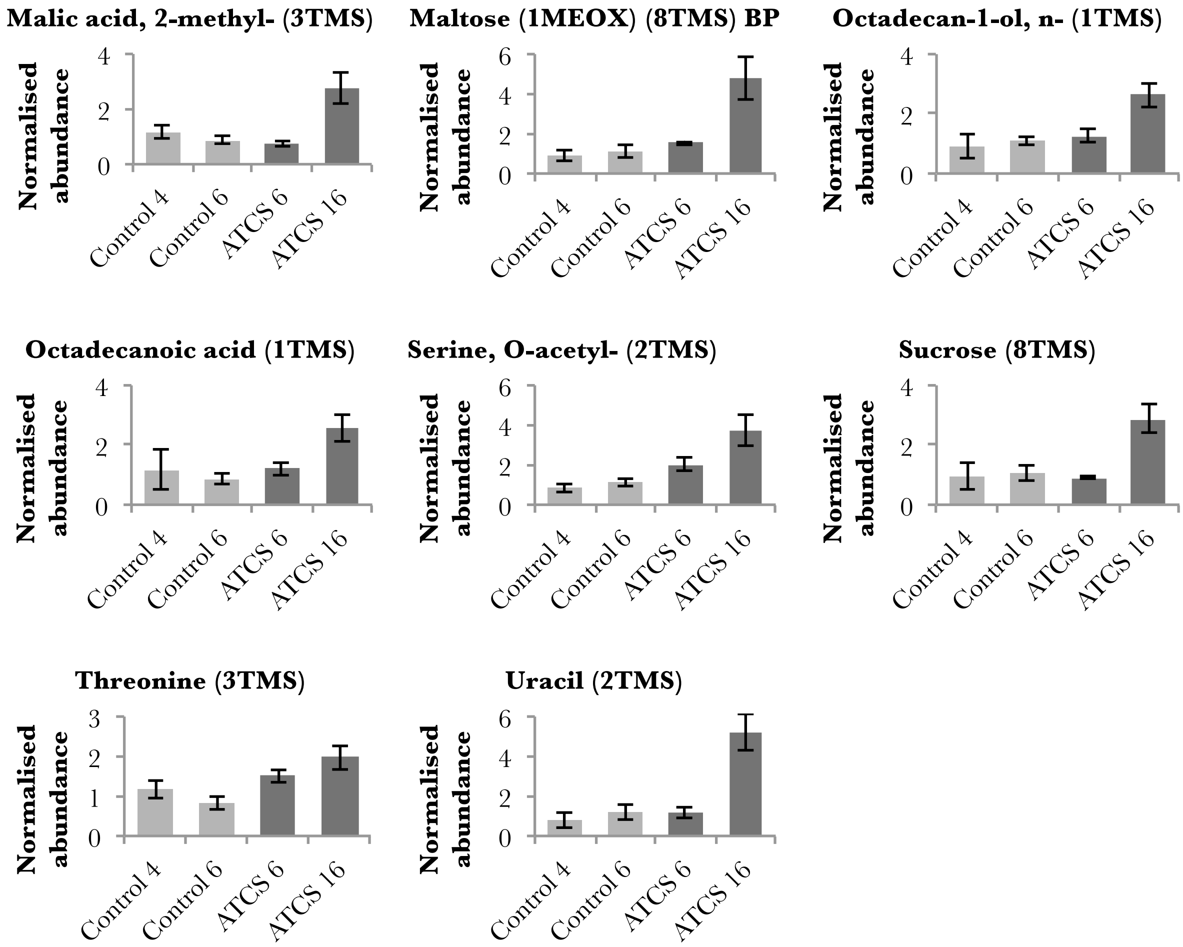


Lyxonic acid (5TMS)



Malic acid (3TMS)





Galactinol (9TMS), α-1-O-methyl-galactopyranoside (4TMS), D-glucopyranose (5TMS), and glucose-6-phosphate (6TMS) were the only analytes found at increased levels in extracts from both of the *ATCS* lines.

The metabolome data was probed further to determine if the altered analyte levels may reflect differences in metabolite levels in the *ATCS* lines. Ethanolamine, galactinol and α-1-O-methyl-galactopyranoside, which were increased in *ATCS* line 6, each had only one derivative, and so the increases in their derivatives were accepted to reflect increased *in vivo* concentrations. β-alanine, arabinose, α-1-O-methyl-galactopyranoside, 2-oxo-glutaric acid, glyceric acid, *myo*-inositol, leucine, lyxonic acid, malic acid, 2-methyl-malic acid, octadecan-1-ol, octadecanoic acid, O-acetyl-serine, sucrose and uracil, which were all increased in *ATCS* line 16 extracts, only had one derivative. Increased *in vivo* levels of these metabolites were also accepted. Other metabolites had more than one derivative. All derivatives were compared to determine if *in vivo* levels were likely to be altered in the *ATCS* lines.

Alanine

Alanine [+CO_2] (2TMS) was 2.8 times that of *ATCS* line 16 extracts ($p < 0.0005$). Average alanine (3TMS) levels were 2.5 times those of control lines. Only one replicate of alanine (2TMS) was identified in each of the control lines and *ATCS* line 16, but the levels in the *ATCS* line 16 extract were the highest. Together, this data is suggestive of increased alanine levels in *ATCS* line 16.

Asparagine

Asparagine [-H_2O] (2TMS) content in *ATCS* line 6 extracts was 3.7 times that of controls ($p < 0.0005$). Average asparagine (2TMS) levels were 2.0 times those of control extracts. However, average asparagine (3TMS) levels were less than in control line 4 extracts. As such, it could not be concluded that *in vivo* asparagine levels in *ATCS* line 6 differed to those of the control lines.

Aspartate

Aspartic acid (3TMS) levels in control extracts varied widely. Control line 4 levels were three times those of control line 6 ($p < 0.05$). *ATCS* line 6 extract contained less than 4% aspartic acid (3TMS) than control line 6 ($p < 0.0005$). However, average levels of aspartic acid (2TMS) were 1.73 times those of controls. This picture is complicated by altered ratios of the two derivatives in each line. While the peak area of the 3TMS derivative was usually higher than the peak area of the 2TMS derivative in the controls and *ATCS* line 16, this tended not to be the case in *ATCS* line 6 extracts. As such, it is not possible to conclude that aspartate levels were lower in *ATCS* line 6.

Fructose

Fructose (1MEOX) (5TMS) BP content in *ATCS* line 16 extracts was 2.2 times the content in control extracts ($p < 0.0005$). Average fructose (1MEOX) (5TMS) MP levels were 2.3 times those in control extracts. This was significant against control line 6 ($p < 0.01$), but was just short of significance against control line 4 ($p = 0.0505$). Due to the significance in the increase of the BP peak, and the similarity in the average increases in each peak, it is reasonable to conclude that fructose levels in *ATCS* line 16 were higher than in control lines.

Galactose-6-phosphate

The second galactose-6-phosphate (1MEOX) (6TMS) elution peak in *ATCS* line 16 extracts was 2.2 times the size of that of the control average ($p < 0.0005$). The mean of the earlier peak was 2.3 times the size of the control average. *t* tests between *ATCS* line 16 and each control line gave p values less than 0.05. These results suggest increases in *in vivo* galactose-6-phosphate content in *ATCS* line 16.

Glucose

Levels of all glucose derivatives were increased in *ATCS* line 16 extracts to 2.5-2.8 times the control levels ($p < 0.0005$). Levels of D-glucopyranose (5TMS) in *ATCS* line 6 extracts were 20 times those of controls ($p < 0.0005$), but the glucose (1MEOX) (5TMS) peaks were smaller on average than peaks from the other derivatives (by 5% and 50% compared to BP and MP peaks, respectively). Except in the case of *ATCS* line 6, D-glucopyranose (5TMS) peaks were about 2% the size of each of the glucose (1MEOX) (5TMS) peaks. D-glucopyranose (5TMS) was still the smaller peak in *ATCS* line 6 extracts. Therefore it was concluded that glucose levels in *ATCS* line 6 were not different to the control lines.

Glucose-6-phosphate

Both glucose-6-phosphate derivatives gave significantly larger peaks in *ATCS* line 16 extracts than control extracts, by 3.9 times for glucose-6-phosphate (1MEOX) (6TMS) MP and 5.4 times for glucose-6-phosphate (6TMS) ($p < 0.0005$). Glucose-6-phosphate (6TMS) yields in *ATCS* line 6 extracts were 142 times those of control extracts ($p < 0.0005$), but the (1MEOX) (6TMS) derivative was identified at an average of 67% of control levels. The (1MEOX) (6TMS) derivative is the primary derivative of glucose-6-phosphate in each of the extracts, and is even present in *ATCS* line 6 extracts at more than 10 times the level of the (6TMS) derivative. Therefore it was concluded that *ATCS* line 6 glucose-6-phosphate levels are not increased.

Glutamine

Glutamine [-H_2O] (2TMS) MP and DL-glutamine (4TMS) in *ATCS* line 6 extracts were detected at 3.8 and 7.9 times the levels in control extracts, respectively ($p < 0.0005$). Average levels of glutamine [-H_2O] (2TMS) BP and DL-glutamine (3TMS) in *ATCS* line 6 extracts were 1.5 and 2.5 times the levels in control extracts. In neither case were these levels significantly different to either of the control lines. However, as average levels are higher than in either of the control lines in all cases, it was accepted that glutamine levels are likely to be increased *in vivo* in *ATCS* line 6.

Glycine

Two glycine derivatives were detected in the dataset. Glycine (2TMS) was only identified in one replicate of control line 4 and one replicate of *ATCS* line 16. It was not detected in extracts from control line 6 or *ATCS* line 6. Glycine (3TMS), by contrast, was detected in every sample. Levels of this derivative in *ATCS* line 6 extracts were 3.1 times those of control extracts ($p < 0.0005$). It was therefore concluded that glycine levels in *ATCS* line 6 were increased.

Maltose

Maltose (1MEOX) (8TMS) BP in *ATCS* line 16 extracts was 4.8 times as abundant as in control extracts ($p < 0.0005$). Maltose (1MEOX) (8TMS) MP was 8.4 times as abundant on average. This was significantly higher than in control line 4 extracts ($p < 0.05$), but not significantly different control line 6 ($p = 0.06$). However, given the significance of the increase in the BP peak, it was concluded that maltose levels were likely to be increased in *ATCS* line 16.

Serine

Serine (2TMS) and (4TMS) derivatives were 2.9 and 4.7 times as abundant in *ATCS* line 6 extracts as in control line extracts, respectively ($p < 0.0005$). Serine (3TMS) was 1.6 times as abundant. This was statistically significant compared to each of the control lines ($p < 0.05$). Thus, it was concluded that serine levels were increased in *ATCS* line 6.

Threonine

Two threonine derivatives were identified. DL-threonine (2TMS) levels in *ATCS* line 6 extracts were 2.9 times those of the controls ($p < 0.0005$). Threonine (3TMS) levels in *ATCS* line 6 extracts were, on average, 1.5 times those of controls. This difference was significant when compared to control line 6 ($p < 0.05$), but it was not significant when compared to control line 4. Given the general trend of increased threonine derivative levels in *ATCS* line 6 extracts, and the significance of the change in DL-threonine (2TMS) levels, it was concluded that threonine levels were increased in *ATCS* line 6.

Threonine (3TMS) in *ATCS* line 16 extracts was present at double the control extract levels ($p < 0.0005$). DL-threonine (2TMS) levels were, on average, 1.7 times the control levels, but this was not significant when compared to either control line. However, given the trend of increased threonine derivatives, and the similarity in the average degree of increase, it was concluded that *ATCS* line 16 did have increased threonine levels.

Summary of individual metabolite changes

To summarise the above discussion, it was concluded *ATCS* line 6 had increased levels of ethanolamine, galactinol, galactose, and the biosynthetically related glutamine, glycine, serine and threonine. With the exception of increases in galactinol and galactose, *ATCS* line 16 exhibited changes in entirely different metabolites. It had increased levels of β-alanine and uracil, soluble sugars (arabinose, fructose, galactose-6-phosphate, glucose and glucose-6-phosphate, maltose, sucrose), the citric acid cycle intermediates 2-oxo-glutarate and malate, O-acetyl-serine, alanine, glycerate, leucine, lyxonate, 2-methyl-malate, *myo*-inositol, octadecan-1-ol, octadecanoic acid and threonine.

Table of analyte abundance normalised average of control values

Levels expressed relative to the mean of the two control lines. *ATCS* values in bold are those that are significantly different to the two control lines. (Significance was defined as the product of the p values resulting from *t* tests between the *ATCS* line and each of the control lines being less than the p-critical value after Bonferroni-correction for multiple comparisons. This p value was approximately 0.0005. Furthermore, p values of each *ATCS* versus control student's *t* test had to be less than 0.05.)

	Line			
Analyte	**Control 4**	**Control 6**	***ATCS* 6**	***ATCS* 16**
Aconitic acid, cis- (3TMS)	0.90 ± 0.33	1.10 ± 0.22	0.55 ± 0.29	2.08 ± 0.86
Alanine (2TMS)	1.56 ± 1.56	0.44 ± 0.44	0.00 ± 0.00	2.11 ± 2.11
Alanine (3TMS)	0.87 ± 0.29	1.13 ± 0.26	2.55 ± 0.68	2.43 ± 0.43
Alanine [+CO_2] (2TMS)	0.85 ± 0.33	1.15 ± 0.25	1.56 ± 0.54	**2.75 ± 0.33**
Alanine, beta- (3TMS)	1.04 ± 0.23	0.96 ± 0.15	1.73 ± 0.13	**2.98 ± 0.57**
Arabinose (1MEOX) (4TMS) MP	1.04 ± 0.27	0.96 ± 0.16	0.76 ± 0.07	**2.09 ± 0.39**
Asparagine (2TMS)	1.14 ± 0.42	0.86 ± 0.15	2.01 ± 0.36	1.54 ± 0.44
Asparagine (3TMS)	1.48 ± 0.64	0.52 ± 0.16	1.19 ± 0.39	1.89 ± 0.64
Asparagine [-H_2O] (2TMS)	0.89 ± 0.47	1.11 ± 0.34	**3.74 ± 0.58**	2.78 ± 1.00
Aspartic acid (2TMS)	0.75 ± 0.43	1.25 ± 0.65	1.73 ± 0.42	1.14 ± 1.01
Aspartic acid (3TMS)	1.47 ± 0.33	0.53 ± 0.15	**0.02 ± 0.01**	0.88 ± 0.33
Butanoic acid, 2-amino- (2TMS)	1.49 ± 1.49	0.51 ± 0.51	0.00 ± 0.00	2.36 ± 2.36
Butanoic acid, 2,4-dihydroxy- (3TMS)	1.11 ± 0.20	0.89 ± 0.16	0.86 ± 0.09	1.50 ± 0.24
Butanoic acid, 4-amino- (3TMS)	0.66 ± 0.15	1.34 ± 0.60	0.55 ± 0.06	2.38 ± 0.51
Butanoic acid, 4-hydroxy- (2TMS)	0.05 ± 0.03	1.95 ± 1.21	-0.01 ± 0.02	5.24 ± 2.55
Butyro-1,4-lactam (1TMS)	0.41 ± 0.17	1.59 ± 0.81	0.55 ± 0.08	3.27 ± 0.68
Campesterol (1TMS)	1.10 ± 0.53	0.90 ± 0.25	1.84 ± 0.69	3.23 ± 1.23
Citric acid (4TMS)	0.93 ± 0.41	1.07 ± 0.30	1.01 ± 0.17	2.71 ± 0.87
Cycloartenol (1TMS)	1.45 ± 1.07	0.55 ± 0.55	0.00 ± 0.00	0.00 ± 0.00
Dehydroascorbic acid dimer (2MEOX) MP	1.25 ± 0.20	0.75 ± 0.16	0.30 ± 0.04	1.28 ± 0.14
Eicosanoic acid (1TMS)	1.39 ± 1.10	0.61 ± 0.48	1.61 ± 0.54	3.41 ± 1.25
Erythronic acid (4TMS)	1.11 ± 0.20	0.89 ± 0.18	0.73 ± 0.05	1.64 ± 0.23
Ethanolamine (3TMS)	0.68 ± 0.33	1.32 ± 0.32	**7.69 ± 1.37**	6.24 ± 2.61
Fructose (1MEOX) (5TMS) BP	1.21 ± 0.39	0.79 ± 0.18	0.75 ± 0.06	**2.22 ± 0.34**
Fructose (1MEOX) (5TMS) MP	1.22 ± 0.42	0.78 ± 0.20	0.68 ± 0.07	2.30 ± 0.38
Fucosterol (1TMS)	1.20 ± 0.56	0.80 ± 0.27	0.24 ± 0.18	0.83 ± 0.45
Fumaric acid (2TMS)	0.84 ± 0.21	1.16 ± 0.29	0.73 ± 0.11	0.95 ± 0.13
Galactinol (9TMS)	1.24 ± 0.48	0.76 ± 0.12	**3.53 ± 0.27**	**6.07 ± 1.44**
Galactopyranoside, 1-O-methyl-, alpha- (4TMS)	1.07 ± 0.47	0.93 ± 0.13	**9.41 ± 2.18**	**2.64 ± 0.43**
Galactose-6-phosphate (1MEOX) (6TMS) early peak	1.29 ± 0.25	0.71 ± 0.12	0.63 ± 0.09	2.90 ± 0.59
Galactose-6-phosphate (1MEOX) (6TMS) late peak	1.05 ± 0.21	0.95 ± 0.17	0.66 ± 0.10	**3.85 ± 0.53**
Gluconic acid (6TMS)	1.09 ± 0.27	0.91 ± 0.18	1.93 ± 0.23	0.89 ± 0.15
Glucopyranose, D- (5TMS)	1.08 ± 0.21	0.92 ± 0.24	**19.92 ± 1.54**	**2.76 ± 0.59**
Glucose (1MEOX) (5TMS) BP	0.97 ± 0.32	1.03 ± 0.18	0.95 ± 0.07	**2.51 ± 0.36**
Glucose (1MEOX) (5TMS) MP	1.12 ± 0.28	0.88 ± 0.24	0.50 ± 0.09	**2.64 ± 0.42**
Glucose-6-phosphate (1MEOX) (6TMS) MP	1.03 ± 0.19	0.97 ± 0.18	0.67 ± 0.09	**3.86 ± 0.51**
Glucose-6-phosphate (6TMS)	0.74 ± 0.41	1.26 ± 0.10	**141.56 ± 39.11**	**5.40 ± 0.88**
Glutamic acid (2TMS)	1.51 ± 0.57	0.49 ± 0.12	0.22 ± 0.11	0.65 ± 0.09
Glutamic acid (3TMS)	1.33 ± 0.25	0.67 ± 0.13	0.81 ± 0.09	2.06 ± 0.45

	Line			
Analyte	**Control 4**	**Control 6**	***ATCS* 6**	***ATCS* 16**
Glutamine [-H_2O] (2TMS) BP	0.78 ± 0.36	1.22 ± 0.41	1.52 ± 0.42	3.25 ± 1.11
Glutamine [-H_2O] (3TMS) MP	0.68 ± 0.44	1.32 ± 0.62	**3.78 ± 0.78**	6.41 ± 2.82
Glutamine, DL- (3TMS)	1.08 ± 1.08	0.92 ± 0.70	2.48 ± 1.25	1.92 ± 1.75
Glutamine, DL- (4TMS)	0.66 ± 0.50	1.34 ± 1.11	**7.87 ± 0.94**	4.05 ± 2.06
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	1.12 ± 0.26	0.88 ± 0.16	1.07 ± 0.22	**3.65 ± 0.58**
Glyceric acid (3TMS)	1.12 ± 0.26	0.88 ± 0.14	1.98 ± 0.24	**1.79 ± 0.30**
Glycerol-2-phosphate (4TMS)	0.72 ± 0.44	1.28 ± 0.53	0.66 ± 0.34	1.00 ± 0.34
Glycerol-3-phosphate (4TMS)	1.05 ± 0.29	0.95 ± 0.17	0.45 ± 0.09	1.26 ± 0.27
Glycerophosphoglycerol (5TMS)	1.24 ± 0.73	0.76 ± 0.29	0.08 ± 0.02	0.78 ± 0.39
Glycine (2TMS)	2.00 ± 2.00	0.00 ± 0.00	0.00 ± 0.00	18.73 ± 18.73
Glycine (3TMS)	0.91 ± 0.35	1.09 ± 0.33	**3.12 ± 0.58**	2.32 ± 0.63
Heptadecanoic acid (1TMS)	1.17 ± 0.76	0.83 ± 0.27	1.04 ± 0.49	1.74 ± 0.79
Hexadecanoic acid (1TMS)	1.03 ± 0.55	0.97 ± 0.13	1.00 ± 0.21	2.14 ± 0.46
Homoserine (3TMS)	0.78 ± 0.25	1.22 ± 0.39	1.96 ± 0.26	4.21 ± 1.66
Inosine (4TMS)	1.09 ± 1.09	0.91 ± 0.91	0.00 ± 0.00	0.00 ± 0.00
Inositol, *myo*- (6TMS)	1.11 ± 0.27	0.89 ± 0.14	1.08 ± 0.08	**2.13 ± 0.38**
Isoleucine (1TMS)	1.01 ± 0.35	0.99 ± 0.20	1.74 ± 0.17	2.43 ± 0.57
Isomaltose (1MEOX) (8TMS) BP	1.62 ± 0.74	0.38 ± 0.19	0.83 ± 0.22	2.10 ± 0.51
Lactic acid, DL- (2TMS)	1.84 ± 1.84	0.16 ± 0.12	0.00 ± 0.00	4.47 ± 4.47
Leucine (1TMS)	0.92 ± 0.30	1.08 ± 0.21	1.88 ± 0.21	**3.50 ± 0.83**
Lyxonic acid (5TMS)	0.92 ± 0.29	1.08 ± 0.21	1.03 ± 0.13	**4.77 ± 0.95**
Lyxose (1MEOX) (4TMS) MP	1.05 ± 0.33	0.95 ± 0.15	0.78 ± 0.09	1.43 ± 0.23
Malic acid (3TMS)	1.09 ± 0.27	0.91 ± 0.16	0.95 ± 0.07	**1.92 ± 0.37**
Malic acid, 2-methyl- (3TMS)	1.15 ± 0.24	0.85 ± 0.14	0.74 ± 0.12	**2.78 ± 0.58**
Maltose (1MEOX) (8TMS) BP	0.90 ± 0.31	1.10 ± 0.29	1.52 ± 0.12	**4.78 ± 1.09**
Maltose (1MEOX) (8TMS) MP	0.26 ± 0.08	1.74 ± 0.88	0.44 ± 0.03	8.36 ± 2.90
Methionine (1TMS)	1.16 ± 0.54	0.84 ± 0.27	4.37 ± 1.33	2.76 ± 1.34
Methionine (2TMS)	0.94 ± 0.32	1.06 ± 0.23	3.22 ± 0.79	6.60 ± 2.07
myo-Inositol-1-phosphate (7TMS)	1.24 ± 0.34	0.76 ± 0.11	0.62 ± 0.16	1.56 ± 0.36
Norleucine (2TMS)	1.20 ± 0.41	0.80 ± 0.21	0.96 ± 0.07	2.11 ± 0.49
Octadecadienoic acid, n- (1TMS)	1.00 ± 0.55	1.00 ± 0.45	0.97 ± 0.31	1.07 ± 0.41
Octadecan-1-ol, n- (1TMS)	0.90 ± 0.40	1.10 ± 0.17	1.24 ± 0.23	**2.62 ± 0.39**
Octadecanoic acid (1TMS)	1.15 ± 0.68	0.85 ± 0.17	1.20 ± 0.21	**2.56 ± 0.45**
Ornithine-1,5-lactam (2TMS)	1.49 ± 0.54	0.51 ± 0.30	0.37 ± 0.37	0.66 ± 0.46
Phenylalanine (2TMS)	0.79 ± 0.26	1.21 ± 0.25	0.80 ± 0.10	1.29 ± 0.38
Phosphoric acid (3TMS)	1.15 ± 0.23	0.85 ± 0.20	0.33 ± 0.05	1.55 ± 0.37
Putrescine (4TMS)	1.08 ± 0.46	0.92 ± 0.27	2.66 ± 0.36	2.86 ± 1.08
Pyroglutamic acid (2TMS)	0.99 ± 0.30	1.01 ± 0.23	1.22 ± 0.09	2.62 ± 0.63
Ribonic acid (5TMS) early peak	0.98 ± 0.21	1.02 ± 0.18	0.77 ± 0.06	1.07 ± 0.15
Ribonic acid (5TMS) late peak	1.05 ± 0.30	0.95 ± 0.20	0.62 ± 0.04	1.61 ± 0.20
Ribose (1MEOX) (4TMS) BP	0.95 ± 0.26	1.05 ± 0.17	1.01 ± 0.11	2.03 ± 0.51
Salicin (5TMS)	-0.18 ± 0.32	2.18 ± 2.01	-0.12 ± 0.12	1.66 ± 0.33
Serine (2TMS)	1.14 ± 0.38	0.86 ± 0.29	**2.88 ± 0.36**	1.91 ± 0.75
Serine (3TMS)	1.21 ± 0.29	0.79 ± 0.19	1.63 ± 0.24	1.97 ± 0.33
Serine (4TMS)	0.84 ± 0.39	1.16 ± 0.48	**4.65 ± 0.84**	2.43 ± 1.01
Serine, O-acetyl- (2TMS)	0.86 ± 0.23	1.14 ± 0.21	1.99 ± 0.34	**3.75 ± 0.78**
Sitosterol, beta- (1TMS)	1.20 ± 0.55	0.80 ± 0.22	2.21 ± 0.89	2.48 ± 0.91

	Line			
Analyte	**Control 4**	**Control 6**	***ATCS* 6**	***ATCS* 16**
Stigmasterol (1TMS)	1.24 ± 0.60	0.76 ± 0.23	2.34 ± 0.84	3.72 ± 1.40
Succinic acid (2TMS)	0.78 ± 0.28	1.22 ± 0.37	1.16 ± 0.23	1.80 ± 0.30
Sucrose (8TMS)	0.94 ± 0.45	1.06 ± 0.25	0.91 ± 0.08	**2.87 ± 0.46**
Tagatose (1MEOX) (5TMS) BP	1.32 ± 0.23	0.68 ± 0.23	2.08 ± 1.44	1.90 ± 0.54
Threonic acid (4TMS)	1.03 ± 0.33	0.97 ± 0.19	1.08 ± 0.09	2.54 ± 0.68
Threonine (3TMS)	1.17 ± 0.22	0.83 ± 0.16	1.51 ± 0.16	**1.98 ± 0.31**
Threonine, DL- (2TMS)	1.20 ± 0.34	0.80 ± 0.23	**2.87 ± 0.27**	1.72 ± 0.56
Turanose (1MEOX) (8TMS) BP	0.87 ± 0.28	1.13 ± 0.24	2.63 ± 0.36	4.25 ± 1.15
Tyrosine (3TMS)	0.93 ± 0.70	1.07 ± 0.79	4.57 ± 1.35	2.71 ± 1.44
Uracil (2TMS)	0.80 ± 0.38	1.20 ± 0.38	1.18 ± 0.27	**5.23 ± 0.92**
Uric acid (4TMS)	1.63 ± 1.08	0.37 ± 0.24	0.77 ± 0.15	0.53 ± 0.53
Uridine (4TMS)	0.51 ± 0.17	1.49 ± 0.77	0.15 ± 0.05	2.89 ± 1.12
Valine (1TMS)	0.00 ± 0.00	2.00 ± 2.00	0.00 ± 0.00	5.32 ± 5.32
Valine (2TMS)	1.11 ± 0.33	0.89 ± 0.18	1.62 ± 0.19	3.26 ± 1.05
Xylitol (5TMS)	1.03 ± 0.27	0.97 ± 0.15	1.11 ± 0.09	1.68 ± 0.26
Xylose (1MEOX) (4TMS) MP	1.32 ± 0.44	0.68 ± 0.11	0.61 ± 0.06	1.03 ± 0.17
Xylulose-5-phosphate (1MEOX) (5TMS) BP	1.10 ± 0.34	0.90 ± 0.13	0.31 ± 0.05	2.12 ± 0.37

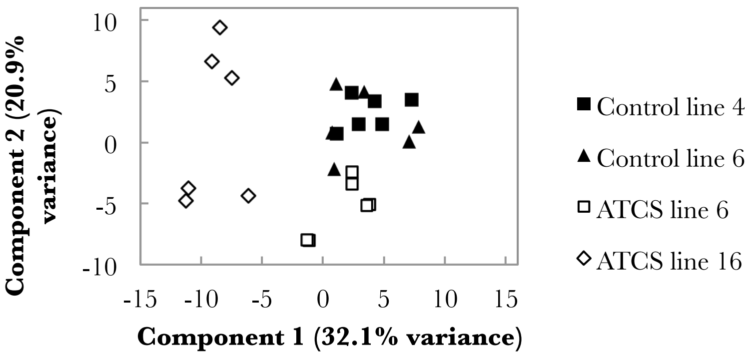
It is important to note that an average 2.4-fold increase in the level of each analyte in *ATCS* line 16, as determined by normalisation of metabolomic GC-MS data to ribitol, is in no way suggestive of a 2.4-fold increase in the total soluble metabolite content of *ATCS* line 16. However, the fact that 92 of the 103 analytes identified were increased by this measure would suggest a significant increase in methanol-soluble metabolites in this line. This observation, coupled with the observation that ribitol abundance in extracts from this line was half the value of other lines, gives credence to the suggestion that ribitol recovery or quantification from this line was compromised. The metabolome will be investigated further in Chapter 5, when the redistribution of ^{14}C from [U-^{14}C]glucose into various metabolite groups will be examined.

Multivariate analyses of metabolome extracts

Principal component analysis also indicated a consistent increase in the abundance of individual analytes in *ATCS* line 16. *ATCS* line 16 had a significantly lower score on component one, which explained 32.1% of inter-sample variance ($p < 0.001$ resulted from student's *t* test with each other line). While most samples had positive scores for this component, all *ATCS* line 16 samples were negative. Over 90% of analyte loadings for component one were negative, suggesting increased abundance in *ATCS* line 16.

Component scores

PCA was performed on the logarithmic growth metabolome data. This identified two statistically significant principal components accounting for 53% of inter-sample variance. MANOVA of principal component scores revealed differences between each pairwise transgenic line comparison ($p < 0.005$), except between the two control lines. ANOVA of each component revealed significant differences between lines ($p < 0.01$). Student's *t* tests subsequently revealed differences in component one between *ATCS* line 6 and control line 4 ($p < 0.05$), but not between *ATCS* line 6 and control line 6. Differences in component one between *ATCS* line 16 and each control line were more significant ($p < 0.0001$), and *ATCS* line 16 was also highly significantly different to *ATCS* line 6 ($p < 0.001$). *ATCS* line 16 was not significantly different to either of the control lines for principal component two. But *ATCS* line 6 was significantly different to each of the control lines ($p < 0.001$), as well as *ATCS* line 16 ($p < 0.05$).

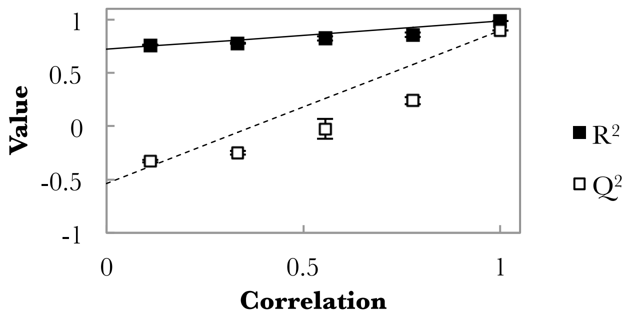


Partial least squares projection to latent structures

To determine if PCA data was over-determined, partial least squares projection to latent structures was performed on the metabolome data. This was done by randomly assigning samples 999 times to one of two groups, one of which initially contained one of the *ATCS* lines, the other of which contained the remaining samples, and by jack-knifing of the data. In each case, the explanatory quality and predictive quality of the latent variables of the simulated groupings reduced as correlation to the true grouping reduced. This suggested that the data was not over-fitted by PCA.

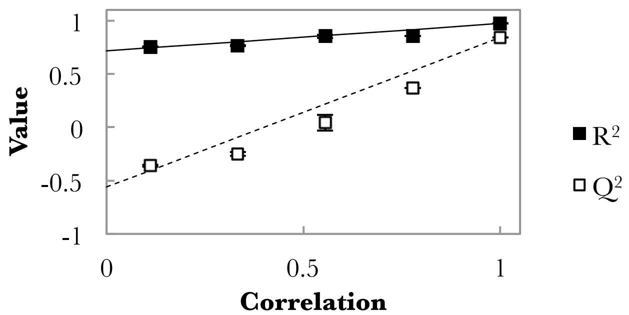
Partial least squares projection to latent structures validation of *ATCS* line 6

Samples were randomly assigned to either "*ATCS* line 6" or "other lines" groups 999 times. R^2 y-intercept = 0.720, Q^2 y-intercept = -0.538.



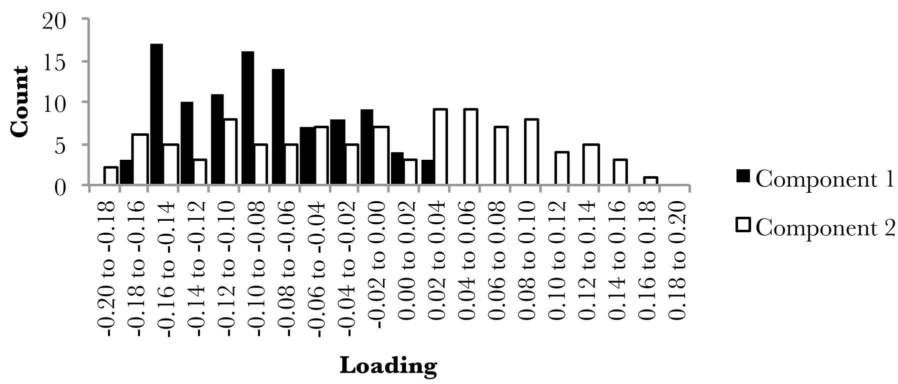
Partial least squares projection to latent structures validation of *ATCS* line 16

R^2 y-intercept = 0.715, Q^2 y-intercept = -0.560



Distribution of loadings for PCA components one and two

Metabolite loadings were investigated for each principal component to gain further understanding into the differences between each *ATCS* line and the control lines.



Categorisation of analytes based on loadings for principal component one, which separates *ATCS* line 16 from control lines.

ATCS line 16 had a lower score on principal component one. 91% of analytes had negative loadings (ranging from -0.17 to 0). Positive loadings reached only as high 0.05. This suggested that *ATCS* line 16 had higher levels of most metabolites than the other lines. Indeed, when peak areas (normalised to cell DW) were summed for each sample, abundance of analytes in *ATCS* line 16 was estimated to be 2.4 times that of each control line ($p < 0.05$). 30 of the 102 analytes had loadings greater than -0.05, suggesting that there was little difference between the lines in these analytes. The remainder appear to be more abundant, to a greater or lesser extent, in *ATCS* line 16. Breakdown of these loadings by metabolite grouping and loading score indicated that sugars, in particular, were more abundant in *ATCS* line 16.

	Loading			
Identity	**-0.17 to -0.10 (Considerably more abundant in *ATCS* 16)**	**-0.10 to -0.05 (Slight increase in abundance in *ATCS* 16)**	**-0.05 to 0.05 (Little difference between lines)**	**All**
Amino acids	10	12	13	35
Organic acids	11	8	5	24
Sterols	0	3	2	5
Sugars	13	3	4	20
Triacylglycerol components	4	3	3	10
Other metabolites	3	2	3	8
Total	**41**	**31**	**30**	**102**

Categorisation of analytes based on loadings for principal component two, which separates *ATCS* line 6 from control lines.

ATCS line 6 had a lower score on principal component two. Loadings were split evenly between positive and negative values for this component. 33 analytes had loadings between -0.05 and 0.05, suggesting that there was little difference between the lines in these analytes. 36 analytes had loadings less than -0.05, and 33 had loadings greater than 0.05. This suggests that there was no difference in the abundance of approximately a third of the analytes, a third were more abundant in *ATCS* line 6, and a third were less abundant. Breakdown of these numbers by metabolite type suggest enrichment of amino acids, at the expense of soluble sugars and organic acids, in *ATCS* line 6.

	Loading			
Identity	**-0.19 to -0.05 (Increased abundance in *ATCS* 6)**	**-0.05 to 0.05 (Little difference between lines)**	**0.05 to 0.18 (Decreased abundance in *ATCS* 6)**	**All**
Amino acids	23	8	4	35
Organic acids	4	9	11	24
Sterols	3	1	1	5
Sugars	3	6	11	20
Triacylglycerol components	0	6	4	10
Other metabolites	3	3	2	8
Total	**36**	**33**	**33**	**102**

Analyte loadings by principal components

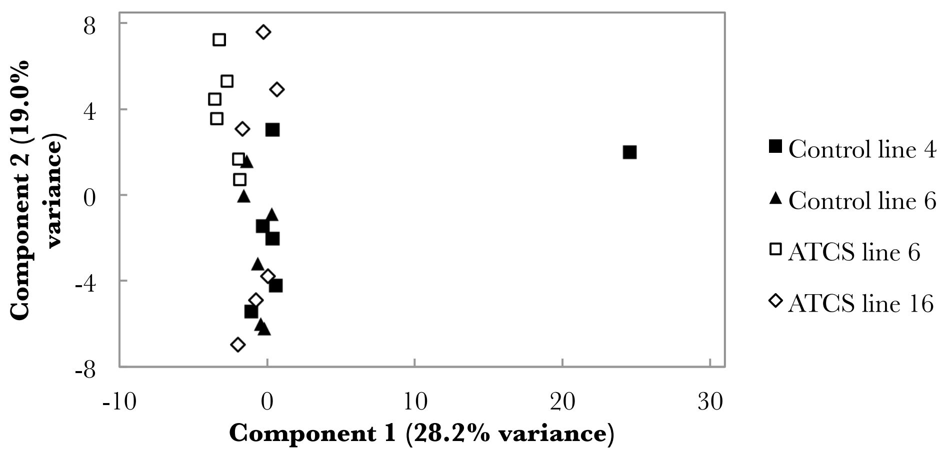
Analyte	**Loading by principal component**		**Category**
	1	**2**	
Aconitic acid, cis- (3TMS)	-0.111	0.026	Organic acid
Alanine (2TMS)	-0.029	-0.016	Amino acid
Alanine (3TMS)	-0.091	-0.112	Amino acid
Alanine [+CO_2] (2TMS)	-0.122	0.040	Amino acid
Alanine, beta- (3TMS)	-0.158	-0.043	Amino acid
Arabinose (1MEOX) (4TMS) MP	-0.157	0.028	Sugar
Asparagine (2TMS)	-0.041	-0.113	Amino acid
Asparagine (3TMS)	-0.068	-0.094	Amino acid
Asparagine [-H_2O] (2TMS)	-0.066	-0.179	Amino acid
Aspartic acid (2TMS)	-0.004	-0.113	Amino acid
Aspartic acid (3TMS)	-0.025	0.134	Amino acid
Butanoic acid, 2-amino- (2TMS)	-0.035	-0.020	Organic acid
Butanoic acid, 2,4-dihydroxy- (3TMS)	-0.114	0.109	Organic acid
Butanoic acid, 4-amino- (3TMS)	-0.089	0.131	Organic acid
Butanoic acid, 4-hydroxy- (2TMS)	-0.078	0.133	Organic acid
Butyro-1,4-lactam (1TMS)	-0.100	0.124	Organic acid
Campesterol (1TMS)	-0.082	-0.054	Sterol
Citric acid (4TMS)	-0.129	-0.089	Organic acid
Cycloartenol (1TMS)	0.039	0.040	Sterol
Dehydroascorbic acid dimer (2MEOX) MP	-0.075	0.168	Organic acid
Eicosanoic acid (1TMS)	-0.092	-0.023	Organic acid
Erythronic acid (4TMS)	-0.121	0.119	Organic acid
Ethanolamine (3TMS)	-0.062	-0.143	Primary amine
Fructose (1MEOX) (5TMS) BP	-0.110	0.064	Sugar

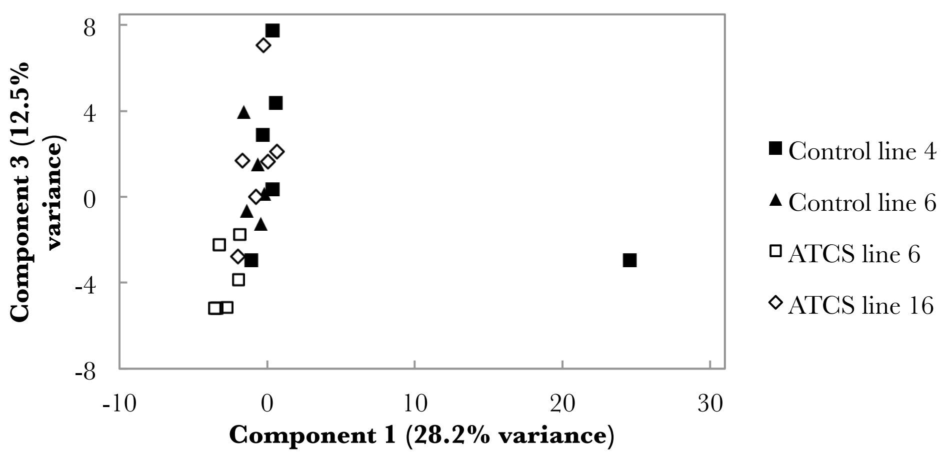
Analyte	Loading by principal component		Category
	1	2	
Fructose (1MEOX) (5TMS) MP	-0.114	0.055	Sugar
Fucosterol (1TMS)	-0.004	0.058	Sterol
Fumaric acid (2TMS)	-0.037	0.095	Organic acid
Galactinol (9TMS)	-0.150	-0.081	Other metabolite
Galactopyranoside, 1-O-methyl-, α- (4TMS)	-0.012	-0.142	Other metabolite
Galactose-6-phosphate (1MEOX) (6TMS) early peak	-0.137	0.035	Sugar
Galactose-6-phosphate (1MEOX) (6TMS) late peak	-0.150	0.084	Sugar
Gluconic acid (6TMS)	0.020	-0.107	Organic acid
Glucopyranose, D- (5TMS)	0.009	-0.150	Sugar
Glucose (1MEOX) (5TMS) BP	-0.160	0.039	Sugar
Glucose (1MEOX) (5TMS) MP	-0.141	0.068	Sugar
Glucose-6-phosphate (1MEOX) (6TMS) MP	-0.152	0.080	Sugar
Glucose-6-phosphate (6TMS)	0.009	-0.138	Sugar
Glutamic acid (2TMS)	0.030	0.078	Amino acid
Glutamic acid (3TMS)	-0.111	-0.019	Amino acid
Glutamine [-H_2O] (2TMS) BP	-0.086	-0.110	Amino acid
Glutamine [-H_2O] (3TMS) MP	-0.098	-0.141	Amino acid
Glutamine, DL- (3TMS)	-0.019	-0.107	Amino acid
Glutamine, DL- (4TMS)	-0.029	-0.189	Amino acid
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	-0.162	0.017	Organic acid
Glyceric acid (3TMS)	-0.094	-0.128	Organic acid
Glycerol-2-phosphate (4TMS)	-0.004	-0.001	Triacylglycerol component
Glycerol-3-phosphate (4TMS)	-0.066	0.152	Triacylglycerol component
Glycerophosphoglycerol (5TMS)	-0.007	0.132	Triacylglycerol component
Glycine (2TMS)	-0.066	-0.042	Amino acid
Glycine (3TMS)	-0.066	-0.177	Amino acid
Heptadecanoic acid (1TMS)	-0.063	0.106	Triacylglycerol component
Hexadecanoic acid (1TMS)	-0.113	0.013	Triacylglycerol component
Homoserine (3TMS)	-0.108	-0.124	Amino acid
Inosine (4TMS)	0.028	0.049	Other metabolite
Inositol, *myo*- (6TMS)	-0.165	-0.012	Triacylglycerol component
Isoleucine (1TMS)	-0.135	-0.095	Amino acid
Isomaltose (1MEOX) (8TMS) BP	-0.079	0.060	Sugar
Lactic acid, DL- (2TMS)	-0.049	-0.030	Organic acid
Leucine (1TMS)	-0.149	-0.074	Amino acid
Lyxonic acid (5TMS)	-0.138	0.083	Organic acid
Lyxose (1MEOX) (4TMS) MP	-0.119	0.046	Sugar
Malic acid (3TMS)	-0.153	-0.004	Organic acid
Malic acid, 2-methyl- (3TMS)	-0.143	0.048	Organic acid
Maltose (1MEOX) (8TMS) BP	-0.107	0.090	Sugar
Maltose (1MEOX) (8TMS) MP	-0.092	0.120	Sugar

Analyte	**Loading by principal component**		**Category**
	1	**2**	
Methionine (1TMS)	-0.043	-0.156	Amino acid
Methionine (2TMS)	-0.132	-0.111	Amino acid
myo-Inositol-1-phosphate (7TMS)	-0.083	0.098	Triacylglycerol component
Norleucine (2TMS)	-0.086	0.078	Amino acid
Octadecadienoic acid, n- (1TMS)	-0.005	-0.040	Triacylglycerol component
Octadecan-1-ol, n- (1TMS)	-0.148	0.028	Triacylglycerol component
Octadecanoic acid (1TMS)	-0.140	0.022	Triacylglycerol component
Ornithine-1,5-lactam (2TMS)	-0.001	0.085	Amino acid
Phenylalanine (2TMS)	-0.077	-0.071	Amino acid
Phosphoric acid (3TMS)	-0.063	0.172	Other metabolite
Putrescine (4TMS)	-0.088	-0.178	Amino acid
Pyroglutamic acid (2TMS)	-0.142	-0.075	Organic acid
Ribonic acid (5TMS)	-0.077	0.077	Organic acid
Ribonic acid (5TMS)2	-0.127	0.098	Organic acid
Ribose (1MEOX) (4TMS) BP	-0.146	-0.019	Sugar
Salicin (5TMS)	-0.041	0.035	Other metabolite
Serine (2TMS)	-0.047	-0.189	Amino acid
Serine (3TMS)	-0.094	-0.047	Amino acid
Serine (4TMS)	-0.040	-0.179	Amino acid
Serine, O-acetyl- (2TMS)	-0.149	-0.075	Amino acid
Sitosterol, β- (1TMS)	-0.057	-0.056	Sterol
Stigmasterol (1TMS)	-0.083	-0.062	Sterol
Succinic acid (2TMS)	-0.089	0.077	Organic acid
Sucrose (8TMS)	-0.157	0.034	Sugar
Tagatose (1MEOX) (5TMS) BP	-0.026	0.059	Sugar
Threonic acid (4TMS)	-0.143	-0.035	Organic acid
Threonine (3TMS)	-0.115	-0.027	Amino acid
Threonine, DL- (2TMS)	-0.040	-0.169	Amino acid
Turanose (1MEOX) (8TMS) BP	-0.129	-0.107	Sugar
Tyrosine (3TMS)	-0.037	-0.163	Amino acid
Uracil (2TMS)	-0.138	0.086	Other metabolite
Uric acid (4TMS)	0.004	-0.049	Organic acid
Uridine (4TMS)	-0.074	0.144	Other metabolite
Valine (1TMS)	-0.066	-0.041	Amino acid
Valine (2TMS)	-0.109	-0.088	Amino acid
Xylitol (5TMS)	-0.147	0.016	Other metabolite
Xylose (1MEOX) (4TMS) MP	-0.002	0.056	Sugar
Xylulose-5-phosphate (1MEOX) (5TMS) BP	-0.098	0.151	Sugar

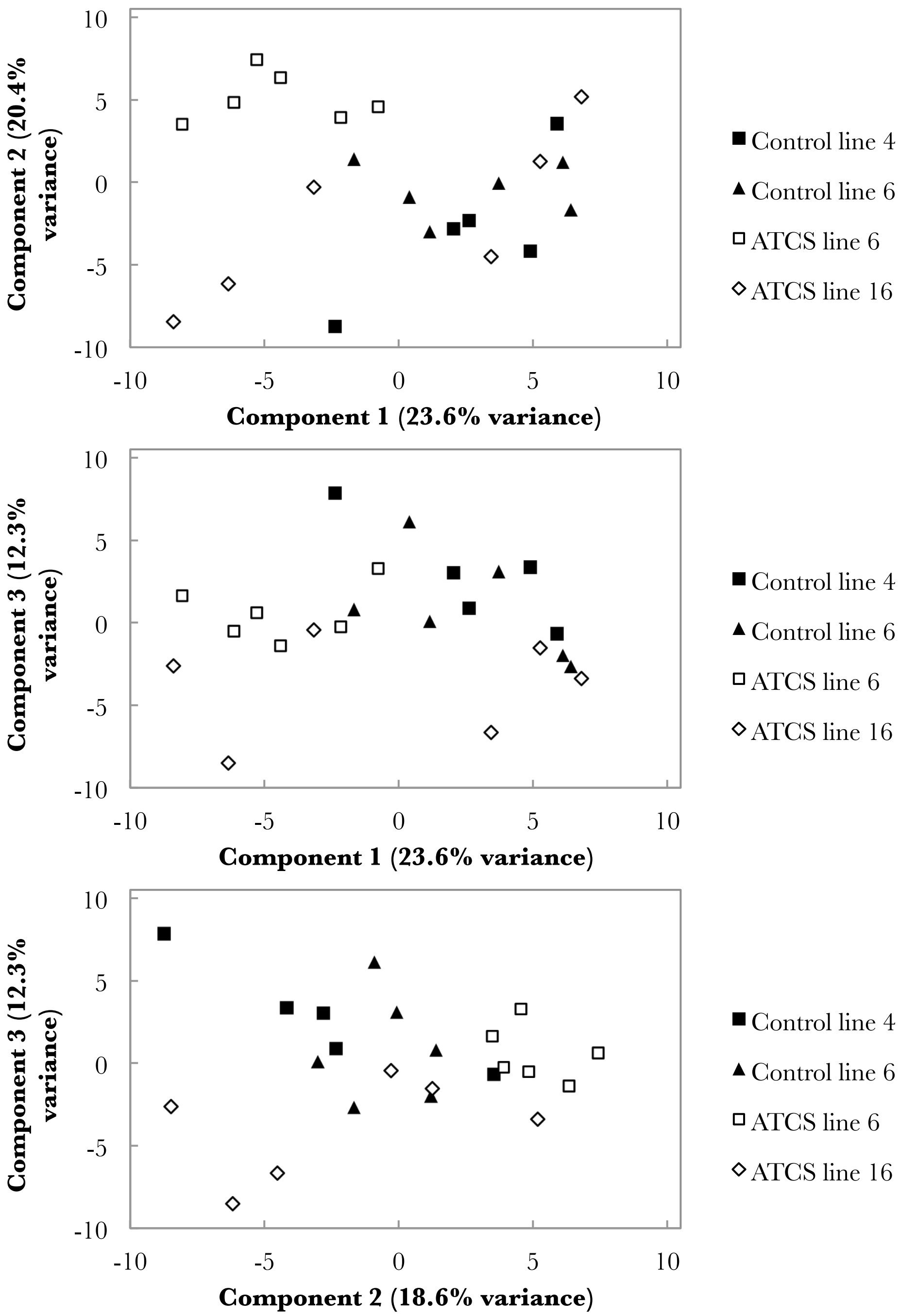
Appendix 4.13. Effects of omitting replicate one of control line 4 from principal component analysis of methanol extract GC-MS data normalised to alkane peak areas

PCA of methanol extract GC-MS data from six replicates for the four transgenic lines resulted in component one separating the first replicate of control line 4 from the other samples:





This potentially anomalous replicate of control line 4 was omitted, and PCA was performed again to see if this resulted in better separation of the samples. PCA of this data revealed three statistically significant principal components accounting for 57% of inter-sample variance:



MANOVA of indicated significant differences between *ATCS* line 6 and control line 4 ($p < 0.0005$), *ATCS* line 6 and control line 6 ($p < 0.005$), *ATCS* lines six and 16 ($p < 0.005$), and *ATCS* line 16 and control line 4 ($p < 0.05$). ANOVA revealed statistically significant differences between lines for each of the three components ($p < 0.05$). *ATCS* line 6 scores on components one and two were significantly different to each control line when assessed using student's *t* tests ($p < 0.005$). *ATCS* line 16 component three scores were significantly different to each of the control lines ($p < 0.05$). *ATCS* line 6 and *ATCS* line 16 had statistically significant scores for components two and three ($p < 0.05$).

Appendix 4.14. Principal component loadings of analytes normalised to alkanes

ATCS line 6 samples had negative scores on component two and positive scores on components one and three, suggesting enrichment of analytes with negative component two loadings and positive component one and three loadings.

Analyte	Loading by principal component			Category
	1	2	3	
Aconitic acid, cis- (3TMS)	-0.035	0.007	0.178	Organic acid
Alanine (2TMS)	0.179	0.032	-0.040	Amino acid
Alanine (3TMS)	0.056	0.156	-0.084	Amino acid
Alanine [+CO_2] (2TMS)	-0.094	0.003	0.041	Amino acid
Alanine, beta- (3TMS)	0.137	0.124	0.015	Amino acid
Arabinose (1MEOX) (4TMS) MP	0.152	0.049	0.129	Sugar
Asparagine (2TMS)	-0.053	0.097	0.006	Amino acid
Asparagine (3TMS)	-0.029	0.100	0.123	Amino acid
Asparagine [-H_2O] (2TMS)	-0.068	0.189	-0.039	Amino acid
Aspartic acid (2TMS)	0.144	0.095	-0.029	Amino acid
Aspartic acid (3TMS)	0.104	-0.080	0.110	Amino acid
Butanoic acid, 2-amino- (2TMS)	0.178	0.034	-0.039	Organic acid
Butanoic acid, 2,4-dihydroxy- (3TMS)	0.171	0.006	0.042	Organic acid
Butanoic acid, 4-amino- (3TMS)	0.043	-0.117	0.021	Organic acid
Butanoic acid, 4-hydroxy- (2TMS)	-0.009	-0.127	-0.001	Organic acid
Butyro-1,4-lactam (1TMS)	-0.029	-0.120	0.021	Organic acid
Campesterol (1TMS)	-0.044	0.084	0.147	Sterol
Citric acid (4TMS)	-0.051	0.129	0.173	Organic acid
Cycloartenol (1TMS)	-0.005	-0.039	0.111	Sterol
Dehydroascorbic acid dimer (2MEOX) MP	0.180	-0.020	0.026	Organic acid
Eicosanoic acid (1TMS)	-0.061	0.049	0.115	Organic acid
Erythronic acid (4TMS)	0.176	-0.007	0.044	Organic acid
Ethanolamine (3TMS)	-0.027	0.165	-0.074	Primary amine
Fructose (1MEOX) (5TMS) BP	0.182	0.020	-0.037	Sugar
Fructose (1MEOX) (5TMS) MP	0.183	0.019	-0.038	Sugar
Fucosterol (1TMS)	-0.015	-0.029	0.180	Sterol
Fumaric acid (2TMS)	0.068	-0.080	0.065	Organic acid
Galactinol (9TMS)	-0.064	0.159	0.052	Other metabolite
Galactopyranoside, 1-O-methyl-, α- (4TMS)	-0.059	0.122	-0.139	Other metabolite
Galactose-6-phosphate (1MEOX) (6TMS) early peak	0.149	0.031	0.089	Sugar
Galactose-6-phosphate (1MEOX) (6TMS) late peak	0.079	-0.017	0.146	Sugar
Gluconic acid (6TMS)	0.078	0.091	-0.057	Organic acid
Glucopyranose, D- (5TMS)	-0.052	0.128	-0.174	Sugar
Glucose (1MEOX) (5TMS) BP	-0.081	0.004	0.179	Sugar
Glucose (1MEOX) (5TMS) MP	0.183	0.007	-0.019	Sugar
Glucose-6-phosphate (1MEOX) (6TMS) MP	0.069	-0.015	0.151	Sugar

Analyte	**Loading by principal component**			**Category**
	1	**2**	**3**	
Glucose-6-phosphate (6TMS)	-0.051	0.117	-0.158	Sugar
Glutamic acid (2TMS)	0.182	0.018	-0.028	Amino acid
Glutamic acid (3TMS)	0.077	0.052	0.162	Amino acid
Glutamine [-H_2O] (2TMS) BP	-0.060	0.089	0.126	Amino acid
Glutamine [-H_2O] (3TMS) MP	-0.040	0.177	0.021	Amino acid
Glutamine, DL- (3TMS)	-0.038	0.120	0.014	Amino acid
Glutamine, DL- (4TMS)	-0.065	0.180	-0.096	Amino acid
Glutaric acid, 2-oxo- (1MEOX) (2TMS) MP	0.102	0.074	0.126	Organic acid
Glyceric acid (3TMS)	0.118	0.135	-0.040	Organic acid
Glycerol-2-phosphate (4TMS)	-0.023	-0.014	0.101	Triacylglycerol component
Glycerol-3-phosphate (4TMS)	0.093	-0.085	0.145	Triacylglycerol component
Glycerophosphoglycerol (5TMS)	-0.006	-0.126	0.074	Triacylglycerol component
Glycine (2TMS)	0.107	0.058	0.002	Amino acid
Glycine (3TMS)	0.006	0.202	-0.068	Amino acid
Heptadecanoic acid (1TMS)	-0.033	-0.066	0.084	Triacylglycerol component
Hexadecanoic acid (1TMS)	0.037	0.026	0.114	Triacylglycerol component
Homoserine (3TMS)	-0.009	0.168	0.075	Amino acid
Inosine (4TMS)	-0.009	-0.082	-0.054	Other metabolite
Inositol, *myo*- (6TMS)	0.154	0.088	0.079	Triacylglycerol component
Isoleucine (1TMS)	-0.088	0.154	0.108	Amino acid
Isomaltose (1MEOX) (8TMS) BP	-0.027	0.006	0.173	Sugar
Lactic acid, DL- (2TMS)	0.173	0.040	-0.033	Organic acid
Leucine (1TMS)	-0.078	0.144	0.099	Amino acid
Lyxonic acid (5TMS)	0.024	-0.023	0.076	Organic acid
Lyxose (1MEOX) (4TMS) MP	-0.066	-0.016	0.197	Sugar
Malic acid (3TMS)	0.171	0.058	0.044	Organic acid
Malic acid, 2-methyl- (3TMS)	0.144	0.035	0.127	Organic acid
Maltose (1MEOX) (8TMS) BP	-0.046	-0.049	0.036	Sugar
Maltose (1MEOX) (8TMS) MP	-0.016	-0.101	0.014	Sugar
Methionine (1TMS)	-0.064	0.161	-0.011	Amino acid
Methionine (2TMS)	-0.030	0.164	0.057	Amino acid
myo-Inositol-1-phosphate (7TMS)	0.089	-0.030	0.169	Triacylglycerol component
Norleucine (2TMS)	0.181	0.020	-0.038	Amino acid
Octadecadienoic acid, n- (1TMS)	-0.032	0.022	0.128	Triacylglycerol component
Octadecan-1-ol, n- (1TMS)	0.076	-0.021	-0.006	Triacylglycerol component
Octadecanoic acid (1TMS)	-0.032	0.037	0.136	Triacylglycerol component
Ornithine-1,5-lactam (2TMS)	0.165	-0.006	-0.012	Amino acid
Phenylalanine (2TMS)	-0.022	0.070	0.160	Amino acid
Phosphoric acid (3TMS)	0.181	-0.026	-0.019	Organic acid
Putrescine (4TMS)	0.003	0.220	0.025	Amino acid
Pyroglutamic acid (2TMS)	0.093	0.148	0.109	Organic acid
Ribonic acid (5TMS) early peak	0.170	0.010	0.016	Organic acid
Ribonic acid (5TMS) late peak	-0.027	-0.056	0.209	Organic acid
Ribose (1MEOX) (4TMS) BP	0.126	0.091	0.115	Sugar
Salicin (5TMS)	0.047	-0.032	-0.015	Other metabolite
Serine (2TMS)	-0.080	0.185	-0.012	Amino acid

Analyte	**Loading by principal component**			**Category**
	1	**2**	**3**	
Serine (3TMS)	0.174	0.048	-0.053	Amino acid
Serine (4TMS)	-0.061	0.183	-0.089	Amino acid
Serine, O-acetyl- (2TMS)	0.027	0.161	0.038	Amino acid
Sitosterol, β- (1TMS)	-0.044	0.064	0.106	Sterol
Stigmasterol (1TMS)	-0.045	0.095	0.127	Sterol
Succinic acid (2TMS)	0.031	-0.048	0.022	Organic acid
Sucrose (8TMS)	-0.123	-0.037	0.140	Sugar
Tagatose (1MEOX) (5TMS) BP	0.089	-0.018	-0.023	Sugar
Threonic acid (4TMS)	0.052	0.122	0.182	Organic acid
Threonine (3TMS)	0.173	0.051	-0.043	Amino acid
Threonine, DL- (2TMS)	-0.083	0.159	-0.038	Amino acid
Turanose (1MEOX) (8TMS) BP	-0.068	0.153	0.061	Sugar
Tyrosine (3TMS)	-0.057	0.163	-0.034	Amino acid
Uracil (2TMS)	-0.031	-0.038	0.096	Other metabolite
Uric acid (4TMS)	-0.017	0.045	0.101	Organic acid
Uridine (4TMS)	-0.014	-0.142	0.032	Other metabolite
Valine (1TMS)	0.006	0.043	0.034	Amino acid
Valine (2TMS)	0.165	0.085	-0.026	Amino acid
Xylitol (5TMS)	-0.025	0.036	0.188	Other metabolite
Xylose (1MEOX) (4TMS) MP	0.182	0.022	-0.031	Sugar
Xylulose-5-phosphate (1MEOX) (5TMS) BP	-0.031	-0.140	0.174	Sugar

Appendix 5.1. Simple hypothetical metabolic model for 13C-FLUX

This is an example of a simple steady state metabolic flux model in 13C-FLUX format featuring a substrate (MAext) labelled at carbon one. It describes the hypothetical metabolic pathway presented in Figure 5.1.

```
PROJECT
    NAME            VERSION         FORMAT          DATE            COMMENT
    MFA_tutorial    1                               05.06.13

NETWORK
    FLUX_NAME       EDUCT_1         EDUCT_2         PRODUCT_1       PRODUCT_2
    Va              MAext                           MA
                    #ABCDEF                         #ABCDEF
    Vb              MA                              MB              MC
                    #ABCDEF                         #ABCD           #EF
    Vc              MB              MC              MD
                    #ABCD           #EF             #ABCDEF
    Vd              MB              MC              MD
                    #ABCD           #EF             #EFABCD
    Vf              MD                              MDout
                    #ABCDEF                         #ABCDEF

FLUXES
    NET
        NAME    FCD    VALUE(F/C)    ED_WEIGHT    LOW(F)    INC(F)    UP(F)
        Va      C      1
        Vb      D
        Vc      D
        Vd      F      0.2
        Vf      D

    XCH
        NAME    FCD    VALUE(F/C)    ED_WEIGHT    LOW(F)    INC(F)    UP(F)
        Va      D
        Vb      F      0
        Vc      C      0
        Vd      C      0
        Vf      D

EQUALITIES
    NET
            VALUE    FORMULA
```

```
    XCH
            VALUE     FORMULA

INEQUALITIES
    NET
            VALUE     COMP          FORMULA

    XCH
            VALUE     COMP          FORMULA

FLUX_MEASUREMENTS
    FLUX_NAME     VALUE               DEVIATION
    Va            1                   0.1

LABEL_INPUT
    META_NAME     ISOTOPOMER          VALUE
    MAext         #100000             1

LABEL_MEASUREMENTS
    META_NAME     CUM_GROUP     VALUE      DEVIATION     CUM_CONSTRAINTS

PEAK_MEASUREMENTS
    META_NAME     PEAK_NO     VALUE_S     VALUE_D-     VALUE_D+     VALUE_DD
      VALUE_T     DEVIATION_S     DEVIATION_D-     DEVIATION_D+     DEVIATION_DD/T

MASS_SPECTROMETRY
    META_NAME     FRAGMENT     WEIGHT     VALUE     DEVIATION
    MD            1,2          0          0.2       0.01
                               1          0.8       0.01
                               2          0         0.01
    MD            3,4,5,6      0          0.8       0.01
                               1          0.2       0.01
                               2          0         0.01
                               3          0         0.01
                               4          0         0.01

OPTIONS
    OPT_NAME      OPT_VALUE
```

Appendix 5.2. Wild-type BY-2 cell suspension culture isotopic steady state ^{13}C fractional enrichment data

The following tables give values of ^{13}C fractional enrichment in soluble amino acids and amino acids from protein hydrolysate in wild-type BY-2 cell cultures at isotopic steady state (mean ± SE). Blank values indicate where fragments were detected in fewer than three replicates for that time-point or in unlabelled control samples, or where the ^{13}C isotopic abundance in the unlabelled samples was calculated not to be at natural abundance (0.0113 ± 0.03).

Values in **bold** indicate significant differences between the two time-points within the amino acid grouping (either soluble and hydrolysate). Underlined values indicate significant within-day differences between soluble amino acids and protein hydrolysate ($p < 0.05$, student's *t* test). It should be noted that glutamine and asparagine are degraded during acid hydrolysis of proteins (Ratcliffe and Shachar-Hill, 2006). Several amino acids or fragments thereof were undetected in soluble amino acid samples as the samples were methanol extracts and so tended to have other metabolites coeluting during GC-MS and have higher levels of noise than protein hydrolysate samples.

Fragments marked with "[1]" (all fragments of glycine and serine, and all fragments, except f302, of methionine, arginine and histidine) are not expected to reach absolute isotopic steady state due to contributions in their biosynthesis of carbon from atmospheric CO_2 and methylene-tetrahydrofolate (Amir, 2010; Masakapalli, 2011).

Values marked with "[2]" indicate those that are not significantly different to ^{13}C fractional enrichment of glucose in cell culture filtrate of 0.213 ± 0.003 ($p > 0.05$, student's *t* test).

	Soluble amino acids		**Protein hydrolysate**	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Alanine-2TBDMS (M-15)	0.195 ± 0.000	0.194 ± 0.001	0.185 ± 0.001	-
Alanine-2TBDMS (M-57)	-	-	0.196 ± 0.000	0.198 ± 0.000
Alanine-2TBDMS (f302)	0.066 ± 0.011	0.073 ± 0.003	0.056 ± 0.001	-
Glycine-2TBDMS (M-57)[1]	-	-	**0.188 ± 0.000**	**0.193 ± 0.000**
Glycine-2TBDMS (M-85)[1]	0.199 ± 0.000	0.199 ± 0.001	**0.188 ± 0.000**	**0.194 ± 0.000**
Valine-2TBDMS (M-85)	-	-	**0.187 ± 0.000**	**0.190 ± 0.000**
Valine-2TBDMS (M-159)	0.205 ± 0.001[2]	0.204 ± 0.000	**0.195 ± 0.000**	**0.203 ± 0.002**
Leucine-2TBDMS (M-159)	-	-	**0.189 ± 0.000**	**0.193 ± 0.000**
Leucine-2TBDMS (f302)	-	-	**0.360 ± 0.001**	**0.368 ± 0.000**
Isoleucine-2TBDMS (M-159)	-	-	**0.185 ± 0.001**	**0.192 ± 0.001**
Proline-2TBDMS (M-159)	-	-	0.146 ± 0.025[2]	0.159 ± 0.006
Methionine-2TBDMS (M-57)[1]	-	-	**0.178 ± 0.001**	**0.183 ± 0.001**
Methionine-2TBDMS (M-85)[1]	-	-	**0.179 ± 0.001**	**0.185 ± 0.001**

	Soluble amino acids		**Protein hydrolysate**	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Methionine-2TBDMS (M-159)[1]	-	-	**0.176 ± 0.001**	**0.183 ± 0.000**
Serine-3TBDMS (M-57)[1]	-	-	0.190 ± 0.002	0.194 ± 0.001
Serine-3TBDMS (M-85)[1]	<u>0.201 ± 0.001</u>	<u>0.203 ± 0.000</u>	<u>**0.194 ± 0.000**</u>	<u>**0.199 ± 0.000**</u>
Serine-3TBDMS (M-159)[1]	-	-	**0.192 ± 0.000**	**0.196 ± 0.000**
Serine-3TBDMS (f302)[1]	<u>0.201 ± 0.001</u>	-	<u>**0.196 ± 0.001**</u>	**0.200 ± 0.000**
Threonine-3TBDMS (M-57)	-	-	**0.183 ± 0.001**	**0.188 ± 0.001**
Phenylalanine-2TBDMS (M-57)	-	-	**0.188 ± 0.000**	**0.193 ± 0.000**
Phenylalanine-2TBDMS (M-85)	-	-	**0.190 ± 0.000**	**0.194 ± 0.001**
Phenylalanine-2TBDMS (f302)	<u>0.176 ± 0.004</u>	-	<u>**0.186 ± 0.000**</u>	**0.190 ± 0.000**
Aspartate-3TBDMS (M-57)	-	-	**0.186 ± 0.000**	**0.191 ± 0.000**
Aspartate-3TBDMS (M-159)	-	-	**0.190 ± 0.000**	**0.195 ± 0.000**
Aspartate-3TBDMS (f302)	<u>0.198 ± 0.000</u>	<u>0.199 ± 0.001</u>	<u>**0.189 ± 0.000**</u>	<u>**0.194 ± 0.000**</u>
Cysteine-3TBDMS (M-159)	-	-	0.134 ± 0.006	0.122 ± 0.008
Glutamate-3TBDMS (M-85)	-	-	**0.191 ± 0.000**	**0.195 ± 0.000**
Glutamate-3TBDMS (M-159)	-	-	**0.190 ± 0.001**	**0.194 ± 0.000**
Glutamate-3TBDMS (f302)	<u>0.197 ± 0.002</u>	<u>0.202 ± 0.002</u>	<u>**0.185 ± 0.001**</u>	<u>**0.189 ± 0.001**</u>
Lysine-3TBDMS (M-159)	-	-	0.182 ± 0.001	0.183 ± 0.002
Lysine-3TBDMS (f302)	-	-	**0.214 ± 0.001**[2]	**0.219 ± 0.001**[2]
Histidine-3TBDMS (M-57)[1]	-	-	**0.188 ± 0.001**	**0.193 ± 0.000**
Histidine-3TBDMS (f302)	-	<u>0.325 ± 0.003</u>	**0.180 ± 0.001**	<u>**0.185 ± 0.002**</u>
Tyrosine-3TBDMS (f302)	<u>**0.288 ± 0.024**</u>	<u>**0.202 ± 0.000**</u>	<u>**0.189 ± 0.000**</u>	<u>**0.192 ± 0.001**</u>

Appendix 5.3. Isotopic steady state ^{13}C fractional enrichment data for transgenic BY-2 cell suspension cultures

The following tables give ^{13}C fractional enrichment in soluble amino acids and amino acids from protein hydrolysate in transgenic BY-2 cell lines (control lines 4 and 6, and *ATCS* lines 6 and 16) at isotopic steady state (mean ± SE). Blank values indicate where fragments were detected in fewer than three replicates for that time-point or in unlabelled control samples, or where the ^{13}C isotopic abundance in the unlabelled samples was calculated not to be at natural abundance (0.0113 ± 0.03).

Values in **bold** indicate significant differences between the two time-points within the amino acid grouping (either soluble and hydrolysate). Underlined values indicate significant within-day differences between soluble amino acids and protein hydrolysate ($p < 0.05$, student's *t* test). It should be noted that glutamine and asparagine are degraded during acid hydrolysis of proteins (Ratcliffe and Shachar-Hill, 2006). Several amino acids or fragments thereof were undetected in soluble amino acid samples as the samples were methanol extracts and so tended to have other metabolites coeluting during GC-MS and have higher levels of noise than protein hydrolysate samples.

Fragments marked with "[1]" (all fragments of glycine and serine, and all fragments, except f302, of methionine, arginine and histidine) are not expected to reach absolute isotopic steady state due to contributions in their biosynthesis of carbon from atmospheric CO_2 and methylene-tetrahydrofolate (Amir, 2010; Masakapalli, 2011).

"[2]" denotes values that are not significantly different to ^{13}C fractional enrichment of glucose in cell culture filtrate ($p > 0.05$, student's *t* test).

Control line 4

^{13}C fractional enrichment of glucose in cell culture filtrate = 0.212 ± 0.002

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Alanine-2TBDMS (M-15)	0.192 ± 0.000	0.193 ± 0.002	-	-
Alanine-2TBDMS (M-57)	0.198 ± 0.000	0.198 ± 0.001	**0.194 ± 0.000**	**0.197 ± 0.000**
Alanine-2TBDMS (M-85)	0.201 ± 0.000	0.201 ± 0.000	-	-
Alanine-2TBDMS (f302)	**0.095 ± 0.005**	**0.063 ± 0.002**	0.055 ± 0.000	0.056 ± 0.001
Glycine-2TBDMS (M-15)[1]	-	-	0.189 ± 0.002	0.191 ± 0.002
Glycine-2TBDMS (M-57)[1]	0.194 ± 0.001	0.195 ± 0.000	**0.188 ± 0.001**	**0.192 ± 0.000**
Glycine-2TBDMS (M-85)[1]	**0.193 ± 0.001**	**0.196 ± 0.000**	**0.187 ± 0.000**	**0.191 ± 0.000**
Valine-2TBDMS (M-15)	0.194 ± 0.008[2]	0.191 ± 0.004	-	-
Valine-2TBDMS (M-57)	0.193 ± 0.001	0.195 ± 0.000	-	-

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Valine-2TBDMS (M-85)	0.193 ± 0.001	0.198 ± 0.000	**0.179 ± 0.002**	**0.187 ± 0.001**
Valine-2TBDMS (M-159)	**0.208 ± 0.002**[2]	**0.205 ± 0.001**	0.197 ± 0.001	0.198 ± 0.000
Valine-2TBDMS (f302)	0.208 ± 0.001[2]	0.209 ± 0.003[2]	0.199 ± 0.001	0.205 ± 0.000[2]
Leucine-2TBDMS (M-15)	0.161 ± 0.002	0.168 ± 0.002	-	-
Leucine-2TBDMS (M-57)	0.182 ± 0.001	0.184 ± 0.001	-	-
Leucine-2TBDMS (M-85)	**0.161 ± 0.005**	**0.098 ± 0.010**	-	-
Leucine-2TBDMS (M-159)	0.192 ± 0.001	0.195 ± 0.001	**0.188 ± 0.000**	**0.192 ± 0.000**
Leucine-2TBDMS (f302)	0.372 ± 0.002	0.375 ± 0.003	-	-
Isoleucine-2TBDMS (M-159)	-	-	0.191 ± 0.001	0.193 ± 0.000
Proline-2TBDMS (M-85)	**0.204 ± 0.002**	**0.243 ± 0.004**	**0.186 ± 0.000**	**0.190 ± 0.001**
Methionine-2TBDMS (M-57)[1]	0.179 ± 0.006	0.172 ± 0.005	**0.176 ± 0.000**	**0.178 ± 0.000**
Methionine-2TBDMS (M-85)[1]	**0.104 ± 0.005**	**0.148 ± 0.007**	-	-
Methionine-2TBDMS (M-159)[1]	0.168 ± 0.004	0.184 ± 0.005	**0.173 ± 0.000**	**0.176 ± 0.000**
Serine-3TBDMS (M-15)[1]	0.196 ± 0.002	0.197 ± 0.001	0.192 ± 0.002	0.194 ± 0.002
Serine-3TBDMS (M-57)[1]	0.200 ± 0.000	0.200 ± 0.000	**0.193 ± 0.001**	**0.196 ± 0.000**
Serine-3TBDMS (M-85)[1]	0.199 ± 0.000	0.200 ± 0.001	**0.194 ± 0.001**	**0.197 ± 0.000**
Serine-3TBDMS (M-159)[1]	**0.196 ± 0.000**	**0.197 ± 0.000**	**0.191 ± 0.000**	**0.195 ± 0.000**
Serine-3TBDMS (f302)[1]	0.198 ± 0.001	0.198 ± 0.000	0.193 ± 0.000	0.198 ± 0.001
Threonine-3TBDMS (M-57)	0.178 ± 0.004	0.173 ± 0.002	-	-
Threonine-3TBDMS (M-85)	**0.155 ± 0.007**	**0.189 ± 0.005**	**0.184 ± 0.001**	**0.190 ± 0.001**
Phenylalanine-2TBDMS (M-85)	0.187 ± 0.004	0.188 ± 0.002	-	-
Phenylalanine-2TBDMS (M-159)	0.189 ± 0.005	0.187 ± 0.007	**0.188 ± 0.000**	**0.192 ± 0.000**
Phenylalanine-2TBDMS (f302)	0.191 ± 0.002	0.197 ± 0.002	**0.184 ± 0.001**	**0.188 ± 0.001**
Aspartate-3TBDMS (M-15)	0.192 ± 0.003	0.195 ± 0.001	0.185 ± 0.001	0.190 ± 0.001
Aspartate-3TBDMS (M-57)	0.195 ± 0.000	0.196 ± 0.001	**0.187 ± 0.000**	**0.191 ± 0.000**
Aspartate-3TBDMS (M-85)	**0.189 ± 0.002**	**0.193 ± 0.000**	**0.188 ± 0.000**	**0.192 ± 0.000**
Aspartate-3TBDMS (M-159)	0.204 ± 0.002	0.200 ± 0.001	**0.190 ± 0.000**	**0.194 ± 0.000**
Aspartate-3TBDMS (f302)	0.196 ± 0.001	0.198 ± 0.001	**0.188 ± 0.000**	**0.192 ± 0.000**
Cysteine-3TBDMS (M-159)	-	-	0.115 ± 0.010	0.142 ± 0.008
Glutamate-3TBDMS (M-0)	0.190 ± 0.002	0.187 ± 0.001	-	-
Glutamate-3TBDMS (M-15)	0.194 ± 0.001	0.190 ± 0.002	-	-
Glutamate-3TBDMS (M-57)	0.196 ± 0.000	0.196 ± 0.000	-	-
Glutamate-3TBDMS (M-85)	0.197 ± 0.001	0.197 ± 0.001	**0.190 ± 0.000**	**0.194 ± 0.000**
Glutamate-3TBDMS (M-159)	0.196 ± 0.000	0.196 ± 0.000	**0.190 ± 0.000**	**0.193 ± 0.000**
Glutamate-3TBDMS (f302)	-	-	0.188 ± 0.001	0.194 ± 0.003
Lysine-3TBDMS (M-159)	-	-	0.178 ± 0.002	0.184 ± 0.001
Lysine-3TBDMS (f302)	-	-	0.214 ± 0.001	0.216 ± 0.000
Arginine (-NH2)-3TBDMS (M-159)[1]	-	-	**0.159 ± 0.005**	**0.180 ± 0.002**
Arginine (-NH2)-3TBDMS (f302)	-	-	**0.196 ± 0.029**[2]	**0.293 ± 0.024**
Histidine-3TBDMS (M-159)[1]	-	-	**0.194 ± 0.001**	**0.200 ± 0.000**
Histidine-3TBDMS (f302)	-	-	0.185 ± 0.003	0.191 ± 0.002
Tyrosine-3TBDMS (M-57)	-	-	0.194 ± 0.001	0.198 ± 0.002
Tyrosine-3TBDMS (f302)	-	-	**0.185 ± 0.000**	**0.190 ± 0.000**

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
ProlineUK01-2TBDMS (M-85)	-	-	**0.188 ± 0.000**	**0.192 ± 0.000**
ProlineUK01-2TBDMS (M-159)	-	-	**0.182 ± 0.000**	**0.186 ± 0.001**
Glutamine-3TBDMS (M-0)	**0.216 ± 0.003**	**0.203 ± 0.000**	-	-
Glutamine-3TBDMS (M-15)	**0.186 ± 0.001**	**0.191 ± 0.000**	-	-
Glutamine-3TBDMS (M-57)	**0.197 ± 0.000**	**0.198 ± 0.000**	-	-
Glutamine-4TBDMS (M-57)	**0.196 ± 0.000**	**0.199 ± 0.000**	-	-
GABA-2TBDMS (M-57)	0.174 ± 0.004	0.176 ± 0.010	-	-
GABA-2TBDMS (M-85)	0.203 ± 0.004[2]	0.198 ± 0.005	-	-

Control line 6

^{13}C fractional enrichment of glucose in cell culture filtrate = 0.210 ± 0.004

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Alanine-2TBDMS (M-57)	0.203 ± 0.001[2]	0.204 ± 0.000[2]	**0.195 ± 0.000**	**0.198 ± 0.000**
Alanine-2TBDMS (M-85)	-	-	-	-
Alanine-2TBDMS (f302)	0.058 ± 0.004	-	**0.050 ± 0.002**	**0.065 ± 0.001**
Glycine-2TBDMS (M-57)[1]	-	0.198 ± 0.000[2]	**0.188 ± 0.000**	**0.192 ± 0.001**
Glycine-2TBDMS (M-85)[1]	0.196 ± 0.001	0.198 ± 0.001[2]	**0.186 ± 0.001**	**0.190 ± 0.000**
Valine-2TBDMS (M-85)	-	-	0.181 ± 0.001	0.183 ± 0.001
Valine-2TBDMS (M-159)	-	0.203 ± 0.001[2]	**0.196 ± 0.001**	**0.199 ± 0.001**
Valine-2TBDMS (f302)	0.209 ± 0.002[2]	0.210 ± 0.000[2]	-	-
Leucine-2TBDMS (M-159)	-	-	**0.190 ± 0.000**	**0.193 ± 0.001**
Isoleucine-2TBDMS (M-159)	-	-	0.190 ± 0.001	0.194 ± 0.001
Proline-2TBDMS (M-85)	**0.201 ± 0.001**[2]	**0.218 ± 0.002**[2]	-	-
Methionine-2TBDMS (M-57)[1]	-	-	**0.174 ± 0.001**	**0.178 ± 0.001**
Methionine-2TBDMS (M-85)[1]	-0.451 ± 0.369[2]	0.193 ± 0.000	-	-
Methionine-2TBDMS (M-159)[1]	-	-	**0.171 ± 0.001**	**0.177 ± 0.001**
Serine-3TBDMS (M-15)[1]	0.197 ± 0.003[2]	0.201 ± 0.001[2]	-	0.194 ± 0.002[2]
Serine-3TBDMS (M-57)[1]	-	-	**0.193 ± 0.001**	**0.197 ± 0.000**
Serine-3TBDMS (M-85)[1]	0.201 ± 0.002[2]	0.203 ± 0.000[2]	**0.194 ± 0.000**	**0.197 ± 0.000**
Serine-3TBDMS (M-159)[1]	**0.199 ± 0.000**[2]	**0.201 ± 0.000**[2]	**0.192 ± 0.000**	**0.195 ± 0.000**
Serine-3TBDMS (f302)[1]	**0.197 ± 0.000**[2]	**0.202 ± 0.001**[2]	**0.194 ± 0.000**	**0.197 ± 0.000**
Threonine-3TBDMS (M-85)	**0.141 ± 0.006**	**0.194 ± 0.001**	-	-
Phenylalanine-2TBDMS (M-159)	0.172 ± 0.007	0.185 ± 0.001	**0.190 ± 0.000**	**0.193 ± 0.001**
Phenylalanine-2TBDMS (f302)	-	-	**0.187 ± 0.001**	**0.191 ± 0.001**
Aspartate-3TBDMS (M-57)	0.195 ± 0.001	0.196 ± 0.000	**0.186 ± 0.001**	**0.190 ± 0.001**
Aspartate-3TBDMS (M-85)	**0.191 ± 0.002**	**0.198 ± 0.001**[2]	-	-
Aspartate-3TBDMS (M-159)	-	-	**0.188 ± 0.000**	**0.193 ± 0.000**
Aspartate-3TBDMS (f302)	0.199 ± 0.001[2]	0.200 ± 0.001[2]	**0.187 ± 0.000**	**0.192 ± 0.000**

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Cysteine-3TBDMS (M-159)	-	-	0.131 ± 0.011	0.130 ± 0.010
Glutamate-3TBDMS (M-57)	**0.197 ± 0.001**	**0.199 ± 0.000**	-	-
Glutamate-3TBDMS (M-85)	0.198 ± 0.001[2]	0.200 ± 0.001[2]	**0.188 ± 0.000**	**0.192 ± 0.001**
Glutamate-3TBDMS (M-159)	**0.196 ± 0.001**	**0.199 ± 0.000**	**0.189 ± 0.000**	**0.193 ± 0.000**
Glutamate-3TBDMS (f302)	0.226 ± 0.012[2]	0.203 ± 0.003[2]	0.190 ± 0.001	0.192 ± 0.000
Asparagine-3TBDMS (M-57)	0.072 ± 0.016	0.303 ± 0.182[2]	-	-
Asparagine-3TBDMS (f302)	0.223 ± 0.001[2]	0.243 ± 0.024[2]	-	-
Lysine-3TBDMS (M-159)	-	-	**0.180 ± 0.000**	**0.184 ± 0.001**
Lysine-3TBDMS (f302)	-	-	0.214 ± 0.001[2]	0.216 ± 0.001[2]
Arginine (-NH2)-3TBDMS (f302)	-	-	0.238 ± 0.030[2]	0.245 ± 0.032[2]
Histidine-3TBDMS (M-159)[1]	-	-	**0.197 ± 0.001**	**0.200 ± 0.001**[2]
Histidine-3TBDMS (f302)	**0.338 ± 0.003**	**0.284 ± 0.008**	0.186 ± 0.001	0.190 ± 0.001
Tyrosine-3TBDMS (M-57)	-	-	0.196 ± 0.002	0.199 ± 0.001[2]
Tyrosine-3TBDMS (M-85)	-	-	0.203 ± 0.002[2]	0.207 ± 0.002[2]
Tyrosine-3TBDMS (f302)	**0.262 ± 0.008**	**0.205 ± 0.004**[2]	**0.187 ± 0.000**	**0.190 ± 0.000**
ProlineUK01-2TBDMS (M-85)	-	-	**0.186 ± 0.000**	**0.191 ± 0.001**
ProlineUK01-2TBDMS (M-159)	-	-	**0.181 ± 0.001**	**0.184 ± 0.000**
Glutamine-3TBDMS (M-0)	0.199 ± 0.001[2]	0.199 ± 0.000	-	-
Glutamine-3TBDMS (M-15)	**0.188 ± 0.001**	**0.194 ± 0.000**	-	-
Glutamine-3TBDMS (M-57)	**0.197 ± 0.001**[2]	**0.200 ± 0.000**[2]	-	-
Glutamine-3TBDMS (M-159)	**0.228 ± 0.003**	**0.214 ± 0.001**	-	-
Glutamine-4TBDMS (M-57)	0.198 ± 0.001[2]	0.200 ± 0.000[2]	-	-

ATCS line 6

^{13}C fractional enrichment of glucose in cell culture filtrate = 0.214 ± 0.002

	Soluble amino acids		Protein hydrolysate	
Identity	**5 days**	**6 days**	**5 days**	**6 days**
Alanine-2TBDMS (M-15)	0.192 ± 0.002	0.199 ± 0.002	0.186 ± 0.002	-
Alanine-2TBDMS (M-57)	**0.200 ± 0.000**	**0.205 ± 0.000**	**0.195 ± 0.000**	**0.199 ± 0.001**
Alanine-2TBDMS (f302)	0.081 ± 0.009	0.089 ± 0.001	0.070 ± 0.001	-
Glycine-2TBDMS (M-57)[1]	**0.195 ± 0.000**	**0.200 ± 0.000**	**0.188 ± 0.000**	**0.194 ± 0.000**
Glycine-2TBDMS (M-85)[1]	0.195 ± 0.000	-	**0.187 ± 0.001**	**0.195 ± 0.001**
Valine-2TBDMS (M-85)	-	-	**0.185 ± 0.000**	**0.180 ± 0.002**
Valine-2TBDMS (M-159)	0.204 ± 0.001	0.206 ± 0.000	**0.193 ± 0.000**	**0.211 ± 0.002**[2]
Valine-2TBDMS (f302)	0.209 ± 0.002[2]	0.212 ± 0.001[2]	0.199 ± 0.000	-
Leucine-2TBDMS (M-159)	-	-	**0.188 ± 0.001**	**0.201 ± 0.005**[2]
Leucine-2TBDMS (f302)	0.375 ± 0.001	0.376 ± 0.002	**0.361 ± 0.001**	**0.370 ± 0.001**
Isoleucine-2TBDMS (M-159)	-	-	**0.184 ± 0.001**	**0.210 ± 0.003**[2]
Proline-2TBDMS (M-85)	0.217 ± 0.003[2]	0.216 ± 0.002[2]	**0.184 ± 0.001**	**0.200 ± 0.004**

	Soluble amino acids		Protein hydrolysate	
Identity	**5 days**	**6 days**	**5 days**	**6 days**
Proline-2TBDMS (M-159)	-	-	**0.166 ± 0.002**	**0.123 ± 0.007**
Methionine-2TBDMS (M-57)[1]	-	-	**0.175 ± 0.001**	**0.188 ± 0.001**
Methionine-2TBDMS (M-85)[1]	-	-	**0.174 ± 0.003**	**0.190 ± 0.003**
Methionine-2TBDMS (M-159)[1]	-	-	**0.174 ± 0.002**	**0.180 ± 0.001**
Serine-3TBDMS (M-15)[1]	0.200 ± 0.001	-	0.191 ± 0.000	-
Serine-3TBDMS (M-57)[1]	-	-	**0.192 ± 0.001**	**0.198 ± 0.001**
Serine-3TBDMS (M-85)[1]	**0.200 ± 0.000**	**0.206 ± 0.000**	0.194 ± 0.000	0.195 ± 0.001
Serine-3TBDMS (M-159)[1]	**0.198 ± 0.000**	**0.203 ± 0.000**	**0.192 ± 0.000**	**0.197 ± 0.001**
Serine-3TBDMS (f302)[1]	0.199 ± 0.001	0.201 ± 0.001	**0.195 ± 0.001**	**0.199 ± 0.000**
Threonine-3TBDMS (M-57)	0.192 ± 0.001	0.188 ± 0.001	0.178 ± 0.001	0.176 ± 0.003
Phenylalanine-2TBDMS (M-85)	-	-	**0.190 ± 0.000**	**0.198 ± 0.001**
Phenylalanine-2TBDMS (M-159)	-	-	**0.189 ± 0.000**	**0.193 ± 0.001**
Phenylalanine-2TBDMS (f302)	-	-	**0.185 ± 0.000**	**0.190 ± 0.001**
Aspartate-3TBDMS (M-57)	0.196 ± 0.000	0.196 ± 0.000	**0.186 ± 0.001**	**0.193 ± 0.000**
Aspartate-3TBDMS (M-159)	**0.194 ± 0.001**	**0.201 ± 0.000**	**0.189 ± 0.001**	**0.194 ± 0.000**
Aspartate-3TBDMS (f302)	0.198 ± 0.000	0.200 ± 0.001	**0.187 ± 0.001**	**0.194 ± 0.000**
Cysteine-3TBDMS (M-159)	-	-	0.128 ± 0.003	0.113 ± 0.019
Glutamate-3TBDMS (M-57)	**0.197 ± 0.000**	**0.193 ± 0.000**	**0.191 ± 0.000**	**0.202 ± 0.004**
Glutamate-3TBDMS (M-85)	**0.198 ± 0.000**	**0.202 ± 0.001**	**0.191 ± 0.001**	**0.196 ± 0.001**
Glutamate-3TBDMS (M-159)	**0.197 ± 0.000**	**0.202 ± 0.000**	0.190 ± 0.001	0.193 ± 0.001
Glutamate-3TBDMS (f302)	-	-	**0.188 ± 0.002**	**0.193 ± 0.000**
Asparagine-3TBDMS (M-57)	0.157 ± 0.011	0.178 ± 0.000	-	-
Asparagine-3TBDMS (f302)	0.210 ± 0.002[2]	0.210 ± 0.000[2]	-	-
Lysine-3TBDMS (M-159)	-	-	**0.179 ± 0.001**	**0.164 ± 0.005**
Lysine-3TBDMS (f302)	-	-	**0.211 ± 0.001**[2]	**0.231 ± 0.006**[2]
Histidine-3TBDMS (f302)	0.339 ± 0.004	0.266 ± 0.002	0.186 ± 0.001	0.170 ± 0.011
Tyrosine-3TBDMS (f302)	0.238 ± 0.013[2]	0.198 ± 0.002	**0.187 ± 0.000**	**0.192 ± 0.002**
ProlineUK01-2TBDMS (M-85)	-	-	**0.186 ± 0.001**	**0.193 ± 0.001**
ProlineUK01-2TBDMS (M-159)	-	-	0.181 ± 0.001	0.186 ± 0.001
Glutamine-3TBDMS (M-15)	**0.192 ± 0.001**	**0.199 ± 0.001**	-	-
Glutamine-3TBDMS (M-57)	**0.198 ± 0.000**	**0.204 ± 0.000**	-	-

ATCS line 16

^{13}C fractional enrichment of glucose in cell culture filtrate = 0.215 ± 0.002

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Alanine-2TBDMS (M-57)	0.201 ± 0.000	0.201 ± 0.000	**0.192 ± 0.000**	**0.197 ± 0.001**
Glycine-2TBDMS (M-15)[1]	-	-	**0.185 ± 0.001**	**0.199 ± 0.000**
Glycine-2TBDMS (M-57)[1]	-	-	**0.184 ± 0.001**	**0.192 ± 0.000**

	Soluble amino acids		Protein hydrolysate	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
Glycine-2TBDMS (M-85)[1]	<u>0.194 ± 0.001</u>	-	<u>**0.184 ± 0.000**</u>	**0.192 ± 0.001**
Valine-2TBDMS (M-85)	-	-	0.180 ± 0.001	0.178 ± 0.004
Valine-2TBDMS (M-159)	-	-	**0.189 ± 0.000**	**0.202 ± 0.002**
Valine-2TBDMS (f302)	-	<u>0.210 ± 0.002</u>[2]	-	<u>0.202 ± 0.000</u>
Leucine-2TBDMS (M-159)	-	-	**0.184 ± 0.000**	**0.192 ± 0.000**
Leucine-2TBDMS (f302)	-	<u>0.382 ± 0.001</u>	**0.352 ± 0.000**	<u>**0.368 ± 0.002**</u>
Isoleucine-2TBDMS (M-159)	-	-	**0.181 ± 0.000**	**0.197 ± 0.002**
Isoleucine-2TBDMS (f302)	-	-	**0.256 ± 0.000**	**0.272 ± 0.001**
Proline-2TBDMS (M-85)	<u>**0.199 ± 0.000**</u>	<u>**0.223 ± 0.004**</u>[2]	<u>**0.178 ± 0.000**</u>	<u>**0.192 ± 0.002**</u>
Methionine-2TBDMS (M-57)[1]	-	-	**0.172 ± 0.001**	**0.180 ± 0.001**
Methionine-2TBDMS (M-85)[1]	-	-	**0.172 ± 0.000**	**0.180 ± 0.001**
Methionine-2TBDMS (M-159)[1]	-	-	**0.171 ± 0.000**	**0.180 ± 0.001**
Serine-3TBDMS (M-15)[1]	0.192 ± 0.002	0.198 ± 0.002	0.189 ± 0.001	-
Serine-3TBDMS (M-57)[1]	-	-	**0.188 ± 0.001**	**0.194 ± 0.001**
Serine-3TBDMS (M-85)[1]	<u>**0.199 ± 0.000**</u>	<u>**0.202 ± 0.000**</u>	<u>**0.191 ± 0.000**</u>	<u>**0.195 ± 0.001**</u>
Serine-3TBDMS (M-159)[1]	-	-	**0.189 ± 0.000**	**0.194 ± 0.001**
Serine-3TBDMS (f302)[1]	-	-	**0.191 ± 0.000**	**0.195 ± 0.001**
Phenylalanine-2TBDMS (M-15)	-	-	0.205 ± 0.004	0.197 ± 0.004
Phenylalanine-2TBDMS (M-85)	-	-	**0.187 ± 0.000**	**0.193 ± 0.001**
Phenylalanine-2TBDMS (M-159)	-	-	**0.186 ± 0.000**	**0.193 ± 0.000**
Phenylalanine-2TBDMS (f302)	-	-	**0.183 ± 0.000**	**0.190 ± 0.001**
Aspartate-3TBDMS (M-15)	-	-	**0.181 ± 0.001**	**0.191 ± 0.001**
Aspartate-3TBDMS (M-57)	<u>0.196 ± 0.001</u>	<u>0.198 ± 0.001</u>	<u>**0.181 ± 0.000**</u>	<u>**0.190 ± 0.000**</u>
Aspartate-3TBDMS (M-85)	0.188 ± 0.002	0.191 ± 0.002	-	0.191 ± 0.002
Aspartate-3TBDMS (M-159)	-	-	**0.184 ± 0.000**	**0.192 ± 0.001**
Aspartate-3TBDMS (f302)	<u>0.199 ± 0.001</u>	<u>0.198 ± 0.001</u>	<u>**0.183 ± 0.000**</u>	<u>**0.192 ± 0.000**</u>
Cysteine-3TBDMS (M-159)	-	-	0.128 ± 0.002	0.124 ± 0.004
Glutamate-3TBDMS (M-57)	**0.189 ± 0.003**	**0.197 ± 0.000**	-	-
Glutamate-3TBDMS (M-85)	<u>0.196 ± 0.001</u>	<u>0.199 ± 0.001</u>	<u>**0.184 ± 0.000**</u>	<u>**0.193 ± 0.001**</u>
Glutamate-3TBDMS (M-159)	<u>**0.194 ± 0.001**</u>	<u>**0.198 ± 0.000**</u>	<u>**0.185 ± 0.000**</u>	<u>**0.192 ± 0.001**</u>
Glutamate-3TBDMS (f302)	-	-	0.188 ± 0.003	0.193 ± 0.002
Asparagine-3TBDMS (M-57)	0.171 ± 0.015	-0.165 ± 0.228[2]	-	-
Asparagine-3TBDMS (f302)	**0.203 ± 0.007**[2]	**0.233 ± 0.009**[2]	-	-
Lysine-3TBDMS (M-159)	-	-	0.174 ± 0.001	0.177 ± 0.002
Lysine-3TBDMS (f302)	-	-	**0.208 ± 0.001**	**0.215 ± 0.001**[2]
Arginine (-NH2)-3TBDMS (M-159)[1]	-	-	0.166 ± 0.003	0.137 ± 0.019
Arginine (-NH2)-3TBDMS (f302)	-	-	**0.275 ± 0.036**[2]	**0.155 ± 0.019**
Histidine-3TBDMS (M-85)[1]	-	-	0.196 ± 0.005	0.194 ± 0.002
Histidine-3TBDMS (M-159)[1]	-	-	**0.190 ± 0.001**	**0.197 ± 0.000**
Histidine-3TBDMS (f302)	<u>**0.343 ± 0.002**</u>	<u>**0.316 ± 0.007**</u>	<u>0.183 ± 0.002</u>	<u>0.182 ± 0.001</u>
Tyrosine-3TBDMS (M-57)	-	-	**0.189 ± 0.001**	**0.196 ± 0.002**
Tyrosine-3TBDMS (M-85)	-	-	**0.186 ± 0.001**	**0.196 ± 0.001**
Tyrosine-3TBDMS (f302)	-	-	**0.183 ± 0.000**	**0.190 ± 0.000**

	Soluble amino acids		**Protein hydrolysate**	
Identity	**4 days**	**5 days**	**4 days**	**5 days**
ProlineUK01-2TBDMS (M-85)	-	-	**0.179 ± 0.001**	**0.188 ± 0.001**
ProlineUK01-2TBDMS (M-159)	-	-	**0.173 ± 0.001**	**0.183 ± 0.001**
Glutamine-3TBDMS (M-57)	**0.188 ± 0.002**	**0.199 ± 0.000**	-	-
Glutamine-4TBDMS (M-57)	0.199 ± 0.000	0.200 ± 0.000	-	-

Appendix 5.4. BY-2 metabolic model ftbl file structure

The network, fluxes, equalities, inequalities, flux measurements, label input, label measurements and peak measurements sections were structurally identical for all models. F, C and D in the "FLUXES" section respectively relate to free, constrained and determined flux designations, where free fluxes are varied by 13C-FLUX from values initially provided by the user, constrained fluxes are supplied by the user and are not alterable by the software, and determined fluxes are dependent on the values of the free and constrained fluxes and are calculated by the software.

```
NETWORK
           FLUX_NAME       EDUCT_1     EDUCT_2     PRODUCT_1   PRODUCT_2
// *** [1-13C]glucose ***
// Inputs
           Vupt1           GLC_1                   GLCext                  // [1-13C]glucose uptake
                           #ABCDEF                 #ABCDEF
           Vupt0           GLC_0                   GLCext                  // Unlabelled glucose uptake
                           #ABCDEF                 #ABCDEF
           Vco2in          CO2ex                   CO2
                           #A                      #A
           Vmthfin         MTHFex                  MTHF
                           #A                      #A

// Cytosolic hexose/triose phosphate metabolism
           Vg              GLCext                  G6P
                           #ABCDEF                 #ABCDEF
           Vgf             G6P                     F6P
                           #ABCDEF                 #ABCDEF
           Vald            F6P                     DHAP        TP
                           #ABCDEF                 #CBA        #DEF
           Vtpi            DHAP                    TP
                           #ABC                    #ABC
           Vfas2           DHAP                    G3P
                           #ABC                    #ABC
```

```
          Vpk           TP                      PYRc
                        #ABC                    #ABC
          Vpyr          PYRc                    PYRm
                        #ABC                    #ABC
          Vadh          PYRc                    EtOH        CO2
                        #ABC                    #BC         #A

// Cytosolic pentose phosphate pathway
          Vppp1         G6P                     CO2         P5Pp
                        #ABCDEF                 #A          #BCDEF

// Sugars storage
          Vgsuc         G6P                     GSUC
                        #ABCDEF                 #ABCDEF
          Vgsuceff      GSUC                    G6Peff
                        #ABCDEF                 #ABCDEF
          Vfsuc         F6P                     FSUC
                        #ABCDEF                 #ABCDEF
          Vfsuceff      FSUC                    F6Peff
                        #ABCDEF                 #ABCDEF

// Plastidial hexose/triose phosphate metabolism
          Vstsp         G6Pp                    STA
                        #ABCDEF                 #ABCDEF
          Vgfp          G6Pp                    F6Pp
                        #ABCDEF                 #ABCDEF
          Valdp         F6Pp                    TPp         TPp
                        #ABCDEF                 #CBA        #DEF
          Vpkp          TPp                     PYRp
                        #ABC                    #ABC
          Vpdhp         PYRp                    CO2         AcCoAp
                        #ABC                    #A          #BC
          Vfas1         AcCoAp                  AcCoAeff
                        #AB                     #AB
          Vmep          OAA                     PYRp        CO2
                        #ABCD                   #ABC        #D
```

```
// Plastidial pentose phosphate pathway
          Vppp1_p        G6Pp                    CO2         P5Pp
                         #ABCDEF                 #A          #BCDEF
          Vppp2a_p       P5Pp                    TPp         TKC2p       //Half Reaction
                         #ABCDE                  #CDE        #AB
          Vppp2b_p       E4Pp         TKC2p      F6Pp                    //Half Reaction
                         #abcd        #AB        #ABabcd
          Vppp2c_p       P5Pp         TKC2p      S7Pp                    //Half Reaction
                         #abcde       #AB        #ABabcde
          Vppp3a_p       S7Pp                    E4Pp        TAC3p       //Half Reaction
                         #ABCDEFG                #DEFG       #ABC
          Vppp3b_p       TPp          TAC3p      F6Pp                    //Half Reaction
                         #abc         #ABC       #ABCabc

// Cytosol-plastid exchange
          Vhcp           G6P                     G6Pp
                         #ABCDEF                 #ABCDEF
          Vtpt           TP                      TPp
                         #ABC                    #ABC
          Vpyrt          PYRc                    PYRp
                         #ABC                    #ABC

// Citric acid cycle (Malate and oxaloacetate combined)
          Vpdh           PYRm                    CO2         AcCoA
                         #ABC                    #A          #BC
          Vcs            AcCoA        OAA        CIT
                         #AB          #abcd      #ABbcda
          Vca            CIT                     ICIT
                         #ABCDEF                 #EDCBAF
          Vicdh          ICIT                    CO2         AKG
                         #ABCDEF                 #F          #ABCDE
          Vakgdh         AKG                     CO2         SUCC
                         #ABCDE                  #A          #BCDE
          Vsuccdh        SUCC                    FUM
                         #ABCD                   #ABCD
```

```
          Vfum1          FUM                        OAA
                         #ABCD                      #ABCD
          Vfum2          FUM                        OAA
                         #ABCD                      #DCBA
          Vme            OAA                        CO2          PYRm
                         #ABCD                      #D           #ABC
          Vpepc          TP             CO2         OAA
                         #ABC           #a          #ABCa

// Cytosolic mevalonate pathway
          Vacl           CIT                        OAA          AcCoACyt
                         #ABCDEF                    #FCDE        #AB
          Vmva1          AcCoACyt       AcCoACyt    AcAcCoA
                         #AB            #CD         #ABCD
          Vmva2          AcAcCoA        AcCoACyt    IPPc         CO2
                         #ABCD          #EF         #ABCDF       #E
          Vsterol        IPPc                       Sterol
                         #ABCDE                     #ABCDE

//Amino acid Oxidation
          Vthrox         THR                        GLY          AcCoA
                         #ABCD                      #AB          #CD

// Citric acid cycle efflux
          VcitOUT        CIT                        CITeff
                         #ABCDEF                    #ABCDEF
          VsuccOUT       SUCC                       SUCCeff
                         #ABCD                      #ABCD
          VmalOUT        OAA                        MALeff
                         #ABCD                      #ABCD
          Vgabaeff       AKG                        GABA         CO2
                         #ABCDE                     #EDCB        #A
          VgabaOUT       GABA                       GABAeff
                         #ABCD                      #ABCD

// Efflux
```

```
        Vco2out         CO2                         CO2eff
                        #A                          #A
        Vwall           G6P                         WALL
                        #ABCDEF                     #ABCDEF
        Vsta            STA                         STAeff
                        #ABCDEF                     #ABCDEF
        Vadheff         EtOH                        EtOH_out
                        #AB                         #AB
        Vpentan         G6P                         PENTAN      CO2
                        #ABCDEF                     #ABCDE      #F
        Vpentaneff      PENTAN                      PENTANeff
                        #ABCDE                      #ABCDE

// Amino acid metabolism
        Vglu            AKG                         GLU
                        #ABCDE                      #ABCDE
        Vglueff         GLU                         GLUeff
                        #ABCDE                      #ABCDE
        Vasp            OAA                         ASP
                        #ABCD                       #ABCD
        Vaspeff         ASP                         ASPeff
                        #ABCD                       #ABCD
        Varg            AKG         CO2             ARG
                        #ABCDE      #a              #ABCDEa
        Vargeff         ARG                         ARGeff
                        #ABCDEF                     #ABCDEF
        Vasp_arg        ASP                         FUM
                        #ABCD                       #ABCD
        Vser            TPp                         SER
                        #ABC                        #ABC
        Vcys            SER                         CYS
                        #ABC                        #ABC
        Vcyseff         CYS                         CYSeff
                        #ABC                        #ABC
        Vgly            SER                         GLY         MTHF
                        #ABC                        #AB         #C
```

Vglydc	GLY		CO2	MTHF
	#AB		#A	#B
Vglyeff	GLY		GLYeff	
	#AB		#AB	
Vmthfout	MTHF		MTHFeff	
	#A		#A	
Vala	PYRc		ALA	
	#ABC		#ABC	
Valaeff	ALA		ALAeff	
	#ABC		#ABC	
Varo1	E4Pp	TPp	ARO	
	#ABCD	#abc	#abcABCD	
Varo2	E4Pp	TPp	ARO	
	#ABCD	#abc	#abDCBAc	
Vleu1	PYRp	PYRp	ISOVAL	CO2
	#ABC	#abc	#abBCc	#A
Vleu	ISOVAL	AcCoAp	LEU	CO2
	#ABCDE	#ab	#abBCDE	#A
Vleueff	LEU		LEUeff	
	#ABCDEF		#ABCDEF	
Vval	ISOVAL		VAL	
	#ABCDE		#ABCDE	
Vvaleff	VAL		VALeff	
	#ABCDE		#ABCDE	
Vmet	ASP	MTHF	MET	
	#ABCD	#a	#ABCDa	
Vmeteff	MET		METeff	
	#ABCDE		#ABCDE	
Vthr	ASP		THR	
	#ABCD		#ABCD	
Vthreff	THR		THReff	
	#ABCD		#ABCD	
Vile	PYRp	THR	ILE	CO2
	#ABC	#abcd	#abBcdC	#A
Vileeff	ILE		ILEeff	
	#ABCDEF		#ABCDEF	

```
           Vphe_tyr        ARO          TPp          PHE_TYR      CO2         // Flux to phenylalanine and tyrosine
                           #ABCDEFG     #abc         #abcBCDEFG   #A
           Vphe_tyreff     PHE_TYR                   PHE_TYReff
                           #ABCDEFGHI                #ABCDEFGHI
           Vlys            OAA          PYRp         LYS          CO2
                           #ABCD        #abc         #ABCDcb      #a
           Vlys1           OAA          PYRp         LYS          CO2
                           #ABCD        #abc         #abcDCB      #A
           Vlyseff         LYS                       LYSeff
                           #ABCDEF                   #ABCDEF
           Vhis            P5Pp         MTHF         HIS
                           #ABCDE       #a           #EDCBAa
           Vhiseff         HIS                       HISeff
                           #ABCDEF                   #ABCDEF
//For Tryptophan
           Vtrp2ca         P5Pp                      TPp          CCa
                           #ABCDE                    #CDE         #AB
           Vtrp2caeff      CCa                       CCaeff                   // 2C tryptophan fragment
                           #AB                       #AB
           Vtrp2cb         TPp                       CO2          CCb
                           #ABC                      #A           #BC
           Vtrp2cbeff      CCb                       CCbeff                   // 2C tryptophan fragment
                           #AB                       #AB
           Vtrp3c_sereff   SER                       SEReff                   // 3C tryptophan fragment and serine
                           #ABC                      #ABC
           Vtrp4c          E4Pp                      E4Ppeff                  // 4C tryptophan fragment
                           #ABCD                     #ABCD

// Proxy reactions
           Vserin          AA3Cex                    SEReff
                           #ABC                      #ABC
           Vglyin          AA2Cex                    GLYeff
                           #AB                       #AB
           Vargin          AA6Cex                    ARGeff
                           #ABCDEF                   #ABCDEF
           Vhisin          AA6Cex                    HISeff
```

```
                    #ABCDEF           #ABCDEF
        Vmetin      AA5Cex            METeff
                    #ABCDE            #ABCDE
        Vserprotout SEReff            SERProt
                    #ABC              #ABC
        Vglyprotout GLYeff            GLYProt
                    #AB               #AB
        Vargprotout ARGeff            ARGProt
                    #ABCDEF           #ABCDEF
        Vhisprotout HISeff            HISProt
                    #ABCDEF           #ABCDEF
        Vmetprotout METeff            METProt
                    #ABCDE            #ABCDE

// *** 20% [U-13C]glucose ***
// Inputs
        VUuptU      GLC_U             GLCext_U            // [13C6]glucose uptake
                    #ABCDEF           #ABCDEF
        VUupt0      GLC_0             GLCext_U            // Unlabelled glucose uptake
                    #ABCDEF           #ABCDEF
//      VUco2in     CO2ex             CO2_U               // Omitted - did not affect residuum
//                  #A                #A
        VUmthfin    MTHFex            MTHF_U
                    #A                #A

// Cytosolic hexose/triose phosphate metabolism
        VUg         GLCext_U          G6P_U
                    #ABCDEF           #ABCDEF
        VUgf        G6P_U             F6P_U
                    #ABCDEF           #ABCDEF
        VUald       F6P_U             DHAP_U      TP_U
                    #ABCDEF           #CBA        #DEF
        VUtpi       DHAP_U            TP_U
                    #ABC              #ABC
        VUfas2      DHAP_U            G3P_U
                    #ABC              #ABC
```

```
          VUpk            TP_U                    PYRc_U
                          #ABC                    #ABC
          VUpyr           PYRc_U                  PYRm_U
                          #ABC                    #ABC
          VUadh           PYRc_U                  EtOH_U       CO2_U
                          #ABC                    #BC          #A

// Cytosolic pentose phosphate pathway
          VUppp1          G6P_U                   CO2_U        P5Pp_U
                          #ABCDEF                 #A           #BCDEF

// Sugars storage
          VUgsuc          G6P_U                   GSUC_U
                          #ABCDEF                 #ABCDEF
          VUgsuceff       GSUC_U                  G6Peff_U
                          #ABCDEF                 #ABCDEF
          VUfsuc          F6P_U                   FSUC_U
                          #ABCDEF                 #ABCDEF
          VUfsuceff       FSUC_U                  F6Peff_U
                          #ABCDEF                 #ABCDEF

// Plastidial hexose/triose phosphate metabolism
          VUstsp          G6Pp_U                  STA_U
                          #ABCDEF                 #ABCDEF
          VUgfp           G6Pp_U                  F6Pp_U
                          #ABCDEF                 #ABCDEF
          VUaldp          F6Pp_U                  TPp_U        TPp_U
                          #ABCDEF                 #CBA         #DEF
          VUpkp           TPp_U                   PYRp_U
                          #ABC                    #ABC
          VUpdhp          PYRp_U                  CO2_U        AcCoAp_U
                          #ABC                    #A           #BC
          VUfas1          AcCoAp_U                AcCoAeff_U
                          #AB                     #AB
          VUmep           OAA_U                   PYRp_U       CO2_U
                          #ABCD                   #ABC         #D
```

```
// Plastidial pentose phosphate pathway
          VUppp1_p        G6Pp_U                      CO2_U       P5Pp_U
                          #ABCDEF                     #A          #BCDEF
          VUppp2a_p       P5Pp_U                      TPp_U       TKC2p_U     //Half Reaction
                          #ABCDE                      #CDE        #AB
          VUppp2b_p       E4Pp_U        TKC2p_U       F6Pp_U                  //Half Reaction
                          #abcd         #AB           #ABabcd
          VUppp2c_p       P5Pp_U        TKC2p_U       S7Pp_U                  //Half Reaction
                          #abcde        #AB           #ABabcde
          VUppp3a_p       S7Pp_U                      E4Pp_U      TAC3p_U     //Half Reaction
                          #ABCDEFG                    #DEFG       #ABC
          VUppp3b_p       TPp_U         TAC3p_U       F6Pp_U                  //Half Reaction
                          #abc          #ABC          #ABCabc

// Cytosol-plastid exchange
          VUhcp           G6P_U                       G6Pp_U
                          #ABCDEF                     #ABCDEF
          VUtpt           TP_U                        TPp_U
                          #ABC                        #ABC
          VUpyrt          PYRc_U                      PYRp_U
                          #ABC                        #ABC

// Citric acid cycle (Malate and oxaloacetate combined)
          VUpdh           PYRm_U                      CO2_U       AcCoA_U
                          #ABC                        #A          #BC
          VUcs            AcCoA_U       OAA_U         CIT_U
                          #AB           #abcd         #ABbcda
          VUca            CIT_U                       ICIT_U
                          #ABCDEF                     #EDCBAF
          VUicdh          ICIT_U                      CO2_U       AKG_U
                          #ABCDEF                     #F          #ABCDE
          VUakgdh         AKG_U                       CO2_U       SUCC_U
                          #ABCDE                      #A          #BCDE
          VUsuccdh        SUCC_U                      FUM_U
                          #ABCD                       #ABCD
```

```
          VUfum1          FUM_U                       OAA_U
                          #ABCD                       #ABCD
          VUfum2          FUM_U                       OAA_U
                          #ABCD                       #DCBA
          VUme            OAA_U                       CO2_U        PYRm_U
                          #ABCD                       #D           #ABC
          VUpepc          TP_U          CO2_U         OAA_U
                          #ABC          #a            #ABCa

// Cytosolic mevalonate pathway
          VUacl           CIT_U                       OAA_U        AcCoACyt_U
                          #ABCDEF                     #FCDE        #AB
          VUmva1          AcCoACyt_U    AcCoACyt_U    AcAcCoA_U
                          #AB           #CD           #ABCD
          VUmva2          AcAcCoA_U     AcCoACyt_U    IPPc_U       CO2_U
                          #ABCD         #EF           #ABCDF       #E
          VUsterol        IPPc_U                      Sterol_U
                          #ABCDE                      #ABCDE

//Amino acid Oxidation
//        VUthrox         THR_U                       GLY_U        AcCoA_U      // Omitted - did not affect residuum
//                        #ABCD                       #AB          #CD

// Citric acid cycle efflux
          VUcitOUT        CIT_U                       CITeff_U
                          #ABCDEF                     #ABCDEF
          VUsuccOUT       SUCC_U                      SUCCeff_U
                          #ABCD                       #ABCD
          VUmalOUT        OAA_U                       MALeff_U
                          #ABCD                       #ABCD
          VUgabaeff       AKG_U                       GABA_U       CO2_U
                          #ABCDE                      #EDCB        #A
          VUgabaOUT       GABA_U                      GABAeff_U
                          #ABCD                       #ABCD

// Efflux
```

```
        VUco2out       CO2_U                  CO2eff_U
                       #A                     #A
        VUwall         G6P_U                  WALL_U
                       #ABCDEF                #ABCDEF
        VUsta          STA_U                  STAeff_U
                       #ABCDEF                #ABCDEF
        VUadheff       EtOH_U                 EtOH_out_U
                       #AB                    #AB
        VUpentan       G6P_U                  PENTAN_U    CO2_U
                       #ABCDEF                #ABCDE      #F
        VUpentaneff    PENTAN_U               PENTANeff_U
                       #ABCDE                 #ABCDE

// Amino acid metabolism
        VUglu          AKG_U                  GLU_U
                       #ABCDE                 #ABCDE
        VUglueff       GLU_U                  GLUeff_U
                       #ABCDE                 #ABCDE
        VUasp          OAA_U                  ASP_U
                       #ABCD                  #ABCD
        VUaspeff       ASP_U                  ASPeff_U
                       #ABCD                  #ABCD
        VUarg          AKG_U      CO2_U       ARG_U
                       #ABCDE     #a          #ABCDEa
        VUargeff       ARG_U                  ARGeff_U
                       #ABCDEF                #ABCDEF
        VUasp_arg      ASP_U                  FUM_U
                       #ABCD                  #ABCD
        VUser          TPp_U                  SER_U
                       #ABC                   #ABC
        VUcys          SER_U                  CYS_U
                       #ABC                   #ABC
        VUcyseff       CYS_U                  CYSeff_U
                       #ABC                   #ABC
        VUgly          SER_U                  GLY_U       MTHF_U
                       #ABC                   #AB         #C
```

VUglydc	GLY_U		CO2_U	MTHF_U
	#AB		#A	#B
VUglyeff	GLY_U		GLYeff_U	
	#AB		#AB	
VUmthfout	MTHF_U		MTHFeff_U	
	#A		#A	
VUala	PYRc_U		ALA_U	
	#ABC		#ABC	
VUalaeff	ALA_U		ALAeff_U	
	#ABC		#ABC	
VUaro1	E4Pp_U	TPp_U	ARO_U	
	#ABCD	#abc	#abcABCD	
VUaro2	E4Pp_U	TPp_U	ARO_U	
	#ABCD	#abc	#abDCBAc	
VUleu1	PYRp_U	PYRp_U	ISOVAL_U	CO2_U
	#ABC	#abc	#abBCc	#A
VUleu	ISOVAL_U	AcCoAp_U	LEU_U	CO2_U
	#ABCDE	#ab	#abBCDE	#A
VUleueff	LEU_U		LEUeff_U	
	#ABCDEF		#ABCDEF	
VUval	ISOVAL_U		VAL_U	
	#ABCDE		#ABCDE	
VUvaleff	VAL_U		VALeff_U	
	#ABCDE		#ABCDE	
VUmet	ASP_U	MTHF_U	MET_U	
	#ABCD	#a	#ABCDa	
VUmeteff	MET_U		METeff_U	
	#ABCDE		#ABCDE	
VUthr	ASP_U		THR_U	
	#ABCD		#ABCD	
VUthreff	THR_U		THReff_U	
	#ABCD		#ABCD	
VUile	PYRp_U	THR_U	ILE_U	CO2_U
	#ABC	#abcd	#abBcdC	#A
VUileeff	ILE_U		ILEeff_U	
	#ABCDEF		#ABCDEF	

```
           VUphe_tyr        ARO_U        TPp_U        PHE_TYR_U   CO2_U        // Flux to phenylalanine and tyrosine
                            #ABCDEFG     #abc         #abcBCDEFG  #A
           VUphe_tyreff     PHE_TYR_U                 PHE_TYReff_U
                            #ABCDEFGHI                #ABCDEFGHI
           VUlys            OAA_U        PYRp_U       LYS_U       CO2_U
                            #ABCD        #abc         #ABCDcb     #a
           VUlys1           OAA_U        PYRp_U       LYS_U       CO2_U
                            #ABCD        #abc         #abcDCB     #A
           VUlyseff         LYS_U                     LYSeff_U
                            #ABCDEF                   #ABCDEF
           VUhis            P5Pp_U       MTHF_U       HIS_U
                            #ABCDE       #a           #EDCBAa
           VUhiseff         HIS_U                     HISeff_U
                            #ABCDEF                   #ABCDEF
//For Tryptophan
           VUtrp2ca         P5Pp_U                    TPp_U       CCa_U
                            #ABCDE                    #CDE        #AB
           VUtrp2caeff      CCa_U                     CCaeff_U                 // 2C tryptophan fragment
                            #AB                       #AB
           VUtrp2cb         TPp_U                     CO2_U       CCb_U
                            #ABC                      #A          #BC
           VUtrp2cbeff      CCb_U                     CCbeff_U                 // 2C tryptophan fragment
                            #AB                       #AB
           VUtrp3c_sereff   SER_U                     SEReff_U                 // 3C tryptophan fragment and serine
                            #ABC                      #ABC
           VUtrp4c          E4Pp_U                    E4Ppeff_U                // 4C tryptophan fragment
                            #ABCD                     #ABCD

// Proxy reactions
           VUserin          AA3Cex                    SEReff_U
                            #ABC                      #ABC
           VUglyin          AA2Cex                    GLYeff_U
                            #AB                       #AB
           VUargin          AA6Cex                    ARGeff_U
                            #ABCDEF                   #ABCDEF
           VUhisin          AA6Cex                    HISeff_U
```

```
                #ABCDEF                #ABCDEF
VUmetin         AA5Cex                 METeff_U
                #ABCDE                 #ABCDE
VUserprotout    SEReff_U               SERProt_U
                #ABC                   #ABC
VUglyprotout    GLYeff_U               GLYProt_U
                #AB                    #AB
VUargprotout    ARGeff_U               ARGProt_U
                #ABCDEF                #ABCDEF
VUhisprotout    HISeff_U               HISProt_U
                #ABCDEF                #ABCDEF
VUmetprotout    METeff_U               METProt_U
                #ABCDE                 #ABCDE


FLUXES
          NET
                     NAME            FCD        VALUE(F/C)  ED_WEIGHT  LOW(F)     INC(F)     UP(F)
// *** [1-13C]glucose ***
                     Vupt1           D
                     Vupt0           F
                     Vg              C
                     Vco2in          F
                     Vmthfin         F
                     Vgf             F
                     Vald            D
                     Vtpi            D
                     Vfas2           C
                     Vpk             D
                     Vpyr            D
                     Vadh            D
                     Vppp1           F
                     Vgsuc           C
                     Vgsuceff        D
                     Vfsuc           C
```

Vfsuceff	D
Vhcp	D
Vstsp	D
Vgfp	D
Valdp	D
Vpkp	F
Vpdhp	D
Vfas1	C
Vmep	D
Vppp1_p	F
Vppp2a_p	D
Vppp2b_p	D
Vppp2c_p	D
Vppp3a_p	D
Vppp3b_p	D
Vtpt	D
Vpyrt	F
Vpdh	D
Vcs	D
Vca	D
Vicdh	D
Vakgdh	D
Vsuccdh	D
Vfum1	D
Vfum2	D
Vme	F
Vpepc	D
Vacl	D
Vmva1	D
Vmva2	D
Vsterol	C
Vthrox	F
VcitOUT	C
VsuccOUT	C
VmalOUT	C
Vgabaeff	D

```
VgabaOUT        C
Vco2out         D
Vwall           C
Vsta            C
Vadheff         C
Vpentan         D
Vpentaneff      C
Vglu            D
Vglueff         C
Vasp            D
Vaspeff         C
Varg            D
Vargeff         C
Vasp_arg        D
Vser            D
Vcys            D
Vcyseff         C
Vgly            D
Vglydc          F
Vglyeff         C
Vmthfout        D
Vala            D
Valaeff         C
Varo1           D
Varo2           D
Vleu1           D
Vleu            D
Vleueff         C
Vval            D
Vvaleff         C
Vmet            D
Vmeteff         C
Vthr            D
Vthreff         C
Vile            D
Vileeff         C
```

```
                      Vphe_tyr         D
                      Vphe_tyreff      C
                      Vlys             D
                      Vlys1            F
                      Vlyseff          C
                      Vhis             D
                      Vhiseff          C
                      Vtrp2ca          D
                      Vtrp2caeff       C
                      Vtrp2cb          D
                      Vtrp2cbeff       C
                      Vtrp3c_sereff    C
                      Vtrp4c           C
                      Vserin           F
                      Vglyin           F
                      Vserprotout      D
                      Vglyprotout      D
                      Vargin           F
                      Vhisin           F
                      Vmetin           F
                      Vargprotout      D
                      Vhisprotout      D
                      Vmetprotout      D

// *** 20% [U-13C]glucose ***
                      VUuptU           F
                      VUupt0           D
                      VUg              D
                      VUco2in          D
                      VUmthfin         D
                      VUgf             D
                      VUald            D
                      VUtpi            D
                      VUfas2           D
                      VUpk             D
                      VUpyr            D
```

```
VUadh          D
VUppp1         D
VUgsuc         D
VUgsuceff      D
VUfsuc         D
VUfsuceff      D
VUhcp          D
VUstsp         D
VUgfp          D
VUaldp         D
VUpkp          D
VUpdhp         D
VUfas1         D
VUmep          D
VUppp1_p       D
VUppp2a_p      D
VUppp2b_p      D
VUppp2c_p      D
VUppp3a_p      D
VUppp3b_p      D
VUtpt          D
VUpyrt         D
VUpdh          D
VUcs           D
VUca           D
VUicdh         D
VUakgdh        D
VUsuccdh       D
VUfum1         D
VUfum2         D
VUme           D
VUpepc         D
VUacl          D
VUmva1         D
VUmva2         D
VUsterol       D
```

```
VUthrox         D
VUcitOUT        D
VUsuccOUT       D
VUmalOUT        D
VUgabaeff       D
VUgabaOUT       D
VUco2out        D
VUwall          D
VUsta           D
VUadheff        D
VUpentan        D
VUpentaneff     D
VUglu           D
VUglueff        D
VUasp           D
VUaspeff        D
VUarg           D
VUargeff        D
VUasp_arg       D
VUser           D
VUcys           D
VUcyseff        D
VUgly           D
VUglydc         D
VUglyeff        D
VUmthfout       D
VUala           D
VUalaeff        D
VUaro1          D
VUaro2          D
VUleu1          D
VUleu           D
VUleueff        D
VUval           D
VUvaleff        D
VUmet           D
```

```
                    VUmeteff        D
                    VUthr           D
                    VUthreff        D
                    VUile           D
                    VUileeff        D
                    VUphe_tyr       D
                    VUphe_tyreff    D
                    VUlys           D
                    VUlys1          D
                    VUlyseff        D
                    VUhis           D
                    VUhiseff        D
                    VUtrp2ca        D
                    VUtrp2caeff     D
                    VUtrp2cb        D
                    VUtrp2cbeff     D
                    VUtrp3c_sereff  D
                    VUtrp4c         D
                    VUserin         D
                    VUglyin         D
                    VUserprotout    D
                    VUglyprotout    D
                    VUargin         D
                    VUhisin         D
                    VUmetin         D
                    VUargprotout    D
                    VUhisprotout    D
                    VUmetprotout    D

          XCH
                    NAME            FCD        VALUE(F/C)  ED_WEIGHT  LOW(F)     INC(F)     UP(F)
// *** [1-13C]glucose ***
                    Vupt1           D
                    Vupt0           D
                    Vg              C          0
                    Vco2in          D
```

Vmthfin	D	
Vgf	F	
Vald	F	
Vtpi	F	
Vfas2	D	
Vpk	C	0
Vpyr	C	0
Vadh	C	0
Vppp1	C	0
Vgsuc	C	0
Vgsuceff	D	
Vfsuc	C	0
Vfsuceff	D	
Vhcp	F	
Vstsp	C	0
Vgfp	F	
Valdp	C	0
Vpkp	C	0
Vpdhp	C	0
Vfas1	D	
Vmep	C	0
Vppp1_p	C	0
Vppp2a_p	F	
Vppp2b_p	F	
Vppp2c_p	F	
Vppp3a_p	F	
Vppp3b_p	F	
Vtpt	F	
Vpyrt	C	0
Vpdh	C	0
Vcs	C	0
Vca	C	0
Vicdh	C	0
Vakgdh	C	0
Vsuccdh	C	0
Vfum1	F	

Vfum2	D	
Vme	C	0
Vpepc	F	
Vacl	C	0
Vmva1	C	0
Vmva2	C	0
Vsterol	D	
Vthrox	F	
VcitOUT	D	
VsuccOUT	D	
VmalOUT	D	
Vgabaeff	C	0
VgabaOUT	D	
Vco2out	D	
Vwall	C	0
Vsta	C	0
Vadheff	D	
Vpentan	C	0
Vpentaneff	D	
Vglu	F	
Vglueff	D	
Vasp	C	0
Vaspeff	D	
Varg	C	0
Vargeff	C	0
Vasp_arg	C	0
Vser	C	0
Vcys	C	0
Vcyseff	D	
Vgly	F	
Vglydc	F	
Vglyeff	C	0
Vmthfout	D	
Vala	C	0
Valaeff	D	
Varo1	C	0

Varo2	C	0
Vleu1	C	0
Vleu	C	0
Vleueff	D	
Vval	C	0
Vvaleff	D	
Vmet	C	0
Vmeteff	C	0
Vthr	C	0
Vthreff	D	
Vile	C	0
Vileeff	D	
Vphe_tyr	C	0
Vphe_tyreff	D	
Vlys	C	0
Vlys1	C	0
Vlyseff	D	
Vhis	C	0
Vhiseff	C	0
Vtrp2ca	C	0
Vtrp2caeff	D	
Vtrp2cb	C	0
Vtrp2cbeff	D	
Vtrp3c_sereff	C	0
Vtrp4c	D	
Vserin	D	
Vglyin	D	
Vserprotout	D	
Vglyprotout	D	
Vargin	D	
Vhisin	D	
Vmetin	D	
Vargprotout	D	
Vhisprotout	D	
Vmetprotout	D	

```
// *** 20% [U-13C]glucose ***
                      VUuptU          D
                      VUupt0          D
                      VUg             D
                      VUco2in         D
                      VUmthfin        D
                      VUgf            D
                      VUald           D
                      VUtpi           D
                      VUfas2          D
                      VUpk            D
                      VUpyr           D
                      VUadh           D
                      VUppp1          D
                      VUgsuc          D
                      VUgsuceff       D
                      VUfsuc          D
                      VUfsuceff       D
                      VUhcp           D
                      VUstsp          D
                      VUgfp           D
                      VUaldp          D
                      VUpkp           D
                      VUpdhp          D
                      VUfas1          D
                      VUmep           D
                      VUppp1_p        D
                      VUppp2a_p       D
                      VUppp2b_p       D
                      VUppp2c_p       D
                      VUppp3a_p       D
                      VUppp3b_p       D
                      VUtpt           D
                      VUpyrt          D
                      VUpdh           D
                      VUcs            D
```

```
VUca            D
VUicdh          D
VUakgdh         D
VUsuccdh        D
VUfum1          D
VUfum2          D
VUme            D
VUpepc          D
VUacl           D
VUmva1          D
VUmva2          D
VUsterol        D
VUthrox         D
VUcitOUT        D
VUsuccOUT       D
VUmalOUT        D
VUgabaeff       D
VUgabaOUT       D
VUco2out        D
VUwall          D
VUsta           D
VUadheff        D
VUpentan        D
VUpentaneff     D
VUglu           D
VUglueff        D
VUasp           D
VUaspeff        D
VUarg           D
VUargeff        D
VUasp_arg       D
VUser           D
VUcys           D
VUcyseff        D
VUgly           D
VUglydc         D
```

```
VUglyeff        D
VUmthfout       D
VUala           D
VUalaeff        D
VUaro1          D
VUaro2          D
VUleu1          D
VUleu           D
VUleueff        D
VUval           D
VUvaleff        D
VUmet           D
VUmeteff        D
VUthr           D
VUthreff        D
VUile           D
VUileeff        D
VUphe_tyr       D
VUphe_tyreff    D
VUlys           D
VUlys1          D
VUlyseff        D
VUhis           D
VUhiseff        D
VUtrp2ca        D
VUtrp2caeff     D
VUtrp2cb        D
VUtrp2cbeff     D
VUtrp3c_sereff  D
VUtrp4c         D
VUserin         D
VUglyin         D
VUserprotout    D
VUglyprotout    D
VUargin         D
VUhisin         D
```

```
            VUmetin         D
            VUargprotout    D
            VUhisprotout    D
            VUmetprotout    D


EQUALITIES
     NET
             VALUE      FORMULA
             0          Vfum1-Vfum2
             0          Varo1-Varo2
             0          Vasp_arg-Varg
             0          VUfum1-VUfum2
             0          VUaro1-VUaro2
             0          VUasp_arg-VUarg

             0          Vg-VUg
             0          Vco2in-VUco2in
             0          Vmthfin-VUmthfin
             0          Vgf-VUgf
             0          Vfas2-VUfas2
             0          Vppp1-VUppp1
             0          Vgsuc-VUgsuc
             0          Vfsuc-VUfsuc
             0          Vpkp-VUpkp
             0          Vfas1-VUfas1
             0          Vppp1_p-VUppp1_p
             0          Vpyrt-VUpyrt
             0          Vme-VUme
             0          Vsterol-VUsterol
             0          Vthrox-VUthrox
             0          VcitOUT-VUcitOUT
             0          VsuccOUT-VUsuccOUT
             0          VmalOUT-VUmalOUT
             0          VgabaOUT-VUgabaOUT
```

```
                0           Vco2out-VUco2out
                0           Vwall-VUwall
                0           Vsta-VUsta
                0           Vadheff-VUadheff
                0           Vpentaneff-VUpentaneff
                0           Vglueff-VUglueff
                0           Vaspeff-VUaspeff
                0           Vargeff-VUargeff
                0           Vcyseff-VUcyseff
                0           Vglydc-VUglydc
                0           Valaeff-VUalaeff
                0           Vleueff-VUleueff
                0           Vvaleff-VUvaleff
                0           Vmeteff-VUmeteff
                0           Vthreff-VUthreff
                0           Vileeff-VUileeff
                0           Vphe_tyreff-VUphe_tyreff
                0           Vlys1-VUlys1
                0           Vhiseff-VUhiseff
                0           Vtrp2caeff-VUtrp2caeff
                0           Vtrp2cbeff-VUtrp2cbeff
                0           Vtrp4c-VUtrp4c
                0           Vserin-VUserin
                0           Vglyin-VUglyin
                0           Vargin-VUargin
                0           Vhisin-VUhisin
                0           Vmetin-VUmetin
                0           Vserprotout-VUserprotout
                0           Vglyprotout-VUglyprotout
//              *           Vco2out-Vco2in          // *Value derived from measurement of 14CO2. Optional;
                                                    included to constrain 13CO2 output by the model.

        XCH
                VALUE       FORMULA
                0           Vfum1-Vfum2
                0           VUfum1-VUfum2
```

```
0           Vg-VUg
0           Vgf-VUgf
0           Vald-VUald
0           Vtpi-VUtpi
0           Vpk-VUpk
0           Vpyr-VUpyr
0           Vadh-VUadh
0           Vppp1-VUppp1
0           Vgsuc-VUgsuc
0           Vfsuc-VUfsuc
0           Vhcp-VUhcp
0           Vstsp-VUstsp
0           Vgfp-VUgfp
0           Valdp-VUaldp
0           Vpkp-VUpkp
0           Vpdhp-VUpdhp
0           Vmep-VUmep
0           Vppp1_p-VUppp1_p
0           Vppp2a_p-VUppp2a_p
0           Vppp2b_p-VUppp2b_p
0           Vppp2c_p-VUppp2c_p
0           Vppp3a_p-VUppp3a_p
0           Vppp3b_p-VUppp3b_p
0           Vtpt-VUtpt
0           Vpyrt-VUpyrt
0           Vpdh-VUpdh
0           Vcs-VUcs
0           Vca-VUca
0           Vicdh-VUicdh
0           Vakgdh-VUakgdh
0           Vsuccdh-VUsuccdh
0           Vfum1-VUfum1
0           Vme-VUme
0           Vpepc-VUpepc
0           Vacl-VUacl
0           Vmva1-VUmva1
```

0	Vmva2-VUmva2
0	Vthrox-VUthrox
0	Vgabaeff-VUgabaeff
0	Vpentan-VUpentan
0	Vglu-VUglu
0	Vasp-VUasp
0	Varg-VUarg
0	Vasp_arg-VUasp_arg
0	Vser-VUser
0	Vcys-VUcys
0	Vgly-VUgly
0	Vglydc-VUglydc
0	Vala-VUala
0	Varo1-VUaro1
0	Varo2-VUaro2
0	Vleu1-VUleu1
0	Vleu-VUleu
0	Vval-VUval
0	Vmet-VUmet
0	Vthr-VUthr
0	Vile-VUile
0	Vphe_tyr-VUphe_tyr
0	Vlys-VUlys
0	Vlys1-VUlys1
0	Vhis-VUhis
0	Vtrp2ca-VUtrp2ca
0	Vtrp2cb-VUtrp2cb
0	Vglyeff-VUglyeff
0	Vtrp3c_sereff-VUtrp3c_sereff
0	Vmeteff-VUmeteff
0	Vhiseff-VUhiseff
0	Vargeff-VUargeff
0	Vwall-VUwall
0	Vsta-VUsta

```
INEQUALITIES
  NET
                    VALUE     COMP      FORMULA
                    0         <=        Vpepc
                    0         <=        Vme
                    0         <=        Vpk
                    0         <=        Vpyr
                    0         <=        Vpyrt
                    0         <=        Vadh
                    0         <=        Vppp1
                    0         <=        Vstsp
                    0         <=        Valdp
                    0         <=        Vpkp
                    0         <=        Vpdhp
                    0         <=        Vmep
                    0         <=        Vppp1_p
                    0         <=        Vpdh
                    0         <=        Vasp
                    0         <=        Varg
                    0         <=        Vser
                    0         <=        Vcys
                    0         <=        Vala
                    0         <=        Varo1
                    0         <=        Varo2
                    0         <=        Vleu1
                    0         <=        Vleu
                    0         <=        Vile
                    0         <=        Vval
                    0         <=        Vmet
                    0         <=        Vphe_tyr
                    0         <=        Vlys
                    0         <=        Vlys1
                    0         <=        Vhis
                    0         <=        Vtrp2ca
                    0         <=        Vtrp2cb
                    0         <=        Vtrp3c_sereff
```

```
                    0           <=          Vglyeff
                    0           <=          Vargeff
                    0           <=          Vhiseff
                    0           <=          Vmeteff
                    0           <=          Vacl
                    0           <=          Vmva1

  XCH
                    VALUE       COMP        FORMULA



FLUX_MEASUREMENTS
    FLUX_NAME       VALUE       DEVIATION

    Vg              10          0.1
//  Vupt1
//  VUuptU
//  Vfas2
//  Vgsuc
//  Vfsuc
//  Vfas1
//  Vsterol
//  VcitOUT
//  VsuccOUT
//  VmalOUT
//  VgabaOUT
//  Vwall
//  Vsta
//  Vadheff
//  Vpentaneff
//  Vglueff
//  Vaspeff
//  Vargeff
//  Vcyseff
//  Vglyeff
```

```
//  Valaeff
//  Vleueff
//  Vvaleff
//  Vmeteff
//  Vthreff
//  Vileeff
//  Vphe_tyreff
//  Vlyseff
//  Vhiseff
//  Vtrp2caeff
//  Vtrp2cbeff
//  Vtrp3c_sereff
//  Vtrp4c


LABEL_INPUT
    META_NAME         ISOTOPOMER  VALUE

    GLC_0             #000000     0.934086736  // 13C natural abundance = 0.0113
                      #100000     0.010675817
                      #010000     0.010675817
                      #001000     0.010675817
                      #000100     0.010675817
                      #000010     0.010675817
                      #000001     0.010675817
                      #110000     0.000122016
                      #101000     0.000122016
                      #100100     0.000122016
                      #100010     0.000122016
                      #100001     0.000122016
                      #011000     0.000122016
                      #010100     0.000122016
                      #010010     0.000122016
                      #010001     0.000122016
                      #001100     0.000122016
```

#001010	0.000122016
#001001	0.000122016
#000110	0.000122016
#000101	0.000122016
#000011	0.000122016
#000111	1.39E-06
#001011	1.39E-06
#001101	1.39E-06
#001110	1.39E-06
#010011	1.39E-06
#010101	1.39E-06
#010110	1.39E-06
#011001	1.39E-06
#011010	1.39E-06
#011100	1.39E-06
#100011	1.39E-06
#100101	1.39E-06
#100110	1.39E-06
#101001	1.39E-06
#101010	1.39E-06
#101100	1.39E-06
#110001	1.39E-06
#110010	1.39E-06
#110100	1.39E-06
#111000	1.39E-06
#001111	1.59E-08
#010111	1.59E-08
#011011	1.59E-08
#011101	1.59E-08
#011110	1.59E-08
#100111	1.59E-08
#101011	1.59E-08
#101101	1.59E-08
#101110	1.59E-08
#110011	1.59E-08
#110101	1.59E-08

	#110110	1.59E-08	
	#111001	1.59E-08	
	#111010	1.59E-08	
	#111100	1.59E-08	
	#011111	1.82E-10	
	#101111	1.82E-10	
	#110111	1.82E-10	
	#111011	1.82E-10	
	#111101	1.82E-10	
	#111110	1.82E-10	
	#111111	2.08E-12	
GLC_1	#000000	0.009447626	// 99% C1 = ^{13}C
	#100000	0.935314927	
	#110000	0.010689854	
	#101000	0.010689854	
	#100100	0.010689854	
	#100010	0.010689854	
	#100001	0.010689854	
	#111000	0.000122176	
	#110100	0.000122176	
	#110010	0.000122176	
	#110001	0.000122176	
	#101100	0.000122176	
	#101010	0.000122176	
	#101001	0.000122176	
	#100110	0.000122176	
	#100101	0.000122176	
	#100011	0.000122176	
	#111100	1.40E-06	
	#111010	1.40E-06	
	#111001	1.40E-06	
	#110110	1.40E-06	
	#110101	1.40E-06	
	#110011	1.40E-06	
	#101110	1.40E-06	

#101101	1.40E-06
#101011	1.40E-06
#100111	1.40E-06
#101111	1.60E-08
#110111	1.60E-08
#111011	1.60E-08
#111101	1.60E-08
#111110	1.60E-08
#111111	1.82E-10
#010000	0.000107978
#001000	0.000107978
#000100	0.000107978
#000010	0.000107978
#000001	0.000107978
#011000	1.23E-06
#010100	1.23E-06
#010010	1.23E-06
#010001	1.23E-06
#001100	1.23E-06
#001010	1.23E-06
#001001	1.23E-06
#000110	1.23E-06
#000101	1.23E-06
#000011	1.23E-06
#000111	1.41E-08
#001011	1.41E-08
#001101	1.41E-08
#001110	1.41E-08
#010011	1.41E-08
#010101	1.41E-08
#010110	1.41E-08
#011001	1.41E-08
#011010	1.41E-08
#011100	1.41E-08
#001111	1.61E-10
#010111	1.61E-10

```
                  #011011     1.61E-10
                  #011101     1.61E-10
                  #011110     1.61E-10
                  #011111     1.84E-12

GLC_U             #000000     1.00E-12     // 99% 13C
                  #111111     0.941480149
                  #011111     0.0095099
                  #101111     0.0095099
                  #110111     0.0095099
                  #111011     0.0095099
                  #111101     0.0095099
                  #111110     0.0095099
                  #001111     9.61E-05
                  #010111     9.61E-05
                  #011011     9.61E-05
                  #011101     9.61E-05
                  #011110     9.61E-05
                  #100111     9.61E-05
                  #101011     9.61E-05
                  #101101     9.61E-05
                  #101110     9.61E-05
                  #110011     9.61E-05
                  #110101     9.61E-05
                  #110110     9.61E-05
                  #111001     9.61E-05
                  #111010     9.61E-05
                  #111100     9.61E-05
                  #000111     9.70E-07
                  #001011     9.70E-07
                  #001101     9.70E-07
                  #001110     9.70E-07
                  #010011     9.70E-07
                  #010101     9.70E-07
                  #010110     9.70E-07
                  #011001     9.70E-07
```

	#011010	9.70E-07
	#011100	9.70E-07
	#100011	9.70E-07
	#100101	9.70E-07
	#100110	9.70E-07
	#101001	9.70E-07
	#101010	9.70E-07
	#101100	9.70E-07
	#110001	9.70E-07
	#110010	9.70E-07
	#110100	9.70E-07
	#111000	9.70E-07
	#000011	9.80E-09
	#000101	9.80E-09
	#000110	9.80E-09
	#001001	9.80E-09
	#001010	9.80E-09
	#001100	9.80E-09
	#010001	9.80E-09
	#010010	9.80E-09
	#010100	9.80E-09
	#011000	9.80E-09
	#100001	9.80E-09
	#100010	9.80E-09
	#100100	9.80E-09
	#101000	9.80E-09
	#110000	9.80E-09
	#100000	9.90E-11
	#010000	9.90E-11
	#001000	9.90E-11
	#000100	9.90E-11
	#000010	9.90E-11
	#000001	9.90E-11
MTHFex	#0	0.9887
	#1	0.0113

CO2ex	#0	0.9887
	#1	0.0113
AA3Cex	#000	0.966481627
	#100	0.011046063
	#010	0.011046063
	#001	0.011046063
	#110	0.000126247
	#011	0.000126247
	#101	0.000126247
	#111	1.44E-06
AA2Cex	#00	0.97752769
	#10	0.01117231
	#01	0.01117231
	#11	0.00012769
AA6Cex	#000000	0.934086736
	#100000	0.010675817
	#010000	0.010675817
	#001000	0.010675817
	#000100	0.010675817
	#000010	0.010675817
	#000001	0.010675817
	#110000	0.000122016
	#101000	0.000122016
	#100100	0.000122016
	#100010	0.000122016
	#100001	0.000122016
	#011000	0.000122016
	#010100	0.000122016
	#010010	0.000122016
	#010001	0.000122016
	#001100	0.000122016
	#001010	0.000122016
	#001001	0.000122016

#000110	0.000122016
#000101	0.000122016
#000011	0.000122016
#000111	1.39E-06
#001011	1.39E-06
#001101	1.39E-06
#001110	1.39E-06
#010011	1.39E-06
#010101	1.39E-06
#010110	1.39E-06
#011001	1.39E-06
#011010	1.39E-06
#011100	1.39E-06
#100011	1.39E-06
#100101	1.39E-06
#100110	1.39E-06
#101001	1.39E-06
#101010	1.39E-06
#101100	1.39E-06
#110001	1.39E-06
#110010	1.39E-06
#110100	1.39E-06
#111000	1.39E-06
#001111	1.59E-08
#010111	1.59E-08
#011011	1.59E-08
#011101	1.59E-08
#011110	1.59E-08
#100111	1.59E-08
#101011	1.59E-08
#101101	1.59E-08
#101110	1.59E-08
#110011	1.59E-08
#110101	1.59E-08
#110110	1.59E-08
#111001	1.59E-08

	#111010	1.59E-08
	#111100	1.59E-08
	#011111	1.82E-10
	#101111	1.82E-10
	#110111	1.82E-10
	#111011	1.82E-10
	#111101	1.82E-10
	#111110	1.82E-10
	#111111	2.08E-12
AA5Cex	#00000	0.944762552
	#00001	0.010797832
	#00010	0.010797832
	#00100	0.010797832
	#01000	0.010797832
	#10000	0.010797832
	#00011	0.00012341
	#00101	0.00012341
	#00110	0.00012341
	#01001	0.00012341
	#01010	0.00012341
	#01100	0.00012341
	#10001	0.00012341
	#10010	0.00012341
	#10100	0.00012341
	#11000	0.00012341
	#00111	1.41E-06
	#01011	1.41E-06
	#01101	1.41E-06
	#01110	1.41E-06
	#10011	1.41E-06
	#10101	1.41E-06
	#10110	1.41E-06
	#11001	1.41E-06
	#11010	1.41E-06
	#11100	1.41E-06

```
                        #01111      1.61E-08
                        #10111      1.61E-08
                        #11011      1.61E-08
                        #11101      1.61E-08
                        #11110      1.61E-08
                        #11111      1.84E-10


LABEL_MEASUREMENTS
  META_NAME             CUM_GROUP  VALUE      DEVIATION  CUM_CONSTRAINTS


PEAK_MEASUREMENTS
  META_NAME             PEAK_NO    VALUE_S    VALUE_D-   VALUE_D+   VALUE_DD   VALUE_T    DEVIATION_S
                                                                        DEVIATION_D-    DEVIATION_D+   DEVIATION_DD/T


MASS_SPECTROMETRY
  META_NAME             FRAGMENT   WEIGHT     VALUE      DEVIATION


OPTIONS
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Appendix 5.5. ^{14}C uptake by *ATCS* and control line BY-2 cell suspension culture supplemented with [U-^{14}C]glucose

5 ml culture samples at metabolic steady state were supplemented with 7.4 kBq [U-^{14}C]glucose for 24 h. Total metabolised ^{14}C was calculated by summing the ^{14}C measured in CO_2, methanol and chloroform extracts, insoluble residue, and organic acid, protein and ethanol extracts from cell culture filtrate. Student's *t* tests did not reveal significant differences in the amount of ^{14}C metabolised between control and *ATCS* lines. Values are the means of four replicates ± SE.

	Total ^{14}C metabolised
Control line 4	132,676 ± 2,267
Control line 6	150,496 ± 3,347
***ATCS* line 6**	129,884 ± 2,037
***ATCS* line 16**	141,981 ± 7,515

Appendix 5.6. ^{14}C biomass redistribution comparisons of *ATCS* and control lines with wild-type BY-2 cell cultures

Data on ^{14}C redistribution after feeding of cell cultures with [U-^{14}C]glucose for 24 h is presented below. *ATCS* and control line data is presented in Figure 5.5. Wild-type data is from Table 5.1. Values are means of four biological replicates ± SE. Wild-type data is from a separate experiment to that of the transgenic lines.

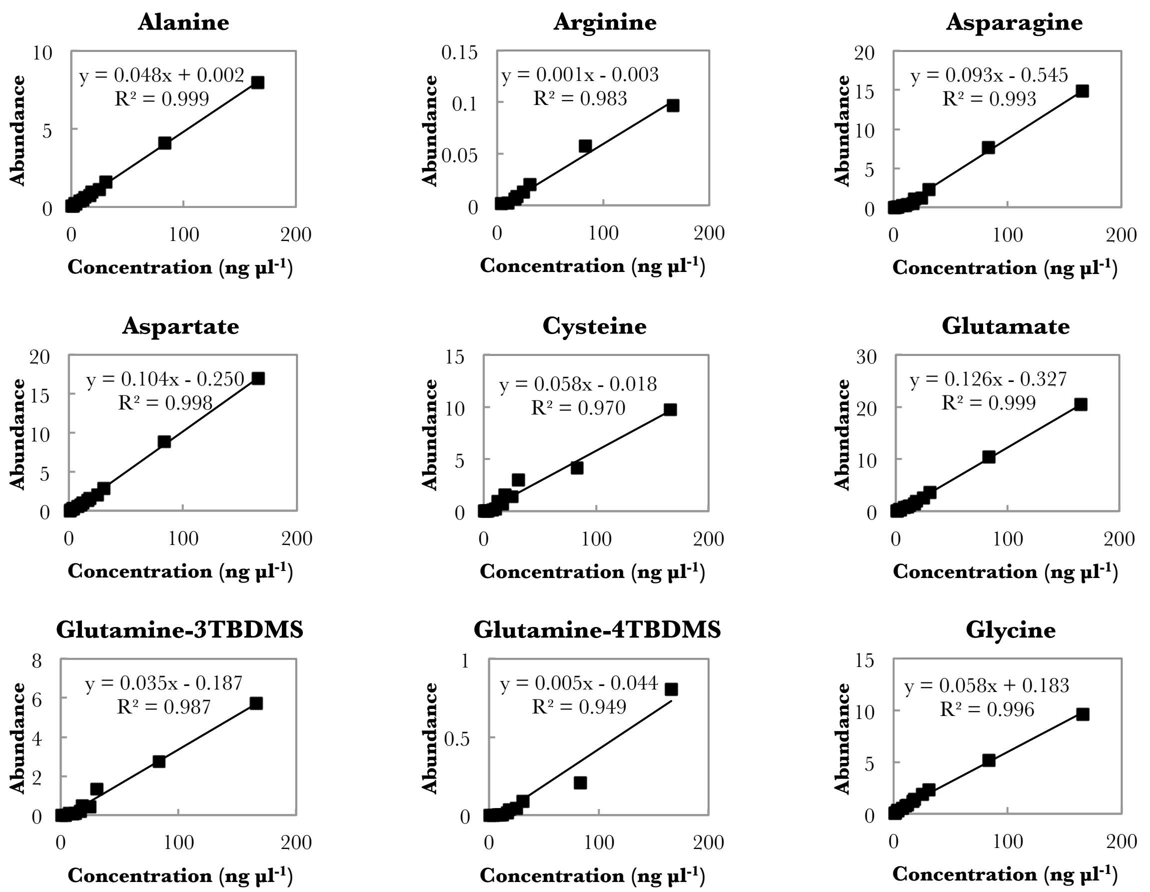
		Radioactivity (% of ^{14}C uptake)			
Metabolic fraction	Wild-type	Control line 4	Control line 6	*ATCS* line 6	*ATCS* line 16
CO_2	38.3 ± 2.4	39.7 ± 0.7	36.1 ± 1.6	40.1 ± 0.5	35.9 ± 1.1
Cell culture filtrate organic acids	0.7 ± 0.1	0.7 ± 0.0	0.8 ± 0.1	0.8 ± 0.1	0.9 ± 0.1
Cell culture filtrate protein	1.1 ± 0.2	1.9 ± 0.1	2.8 ± 0.3	2.3 ± 0.5	3.4 ± 0.1
Ethanol	0.5 ± 0.1	0.2 ± 0.0	0.2 ± 0.0	0.2 ± 0.0	0.2 ± 0.1
Chloroform-soluble (lipids)	2.0 ± 0.1	3.3 ± 0.2	2.5 ± 0.0	2.5 ± 0.2	2.7 ± 0.3
Methanol-soluble	36.7 ± 1.6	31.5 ± 0.4	35.5 ± 1.0	32.9 ± 1.1	27.6 ± 1.6
Sugars	14.1 ± 0.7	17.3 ± 0.5	17.4 ± 0.9	16.9 ± 0.7	14.6 ± 0.9
Amino acids	17.1 ± 1.3	10.9 ± 0.4	14.7 ± 1.1	12.9 ± 0.8	10.4 ± 0.8
Organic acids	5.4 ± 0.4	3.3 ± 0.1	3.4 ± 0.1	3.1 ± 0.2	2.6 ± 0.2
Methanol-insoluble	20.8 ± 0.9	22.8 ± 0.4	22.1 ± 0.7	21.1 ± 1.1	29.2 ± 1.0
Starch	2.5 ± 0.1	2.7 ± 0.3	2.5 ± 0.2	2.1 ± 0.2	5.1 ± 0.2
Protein	5.7 ± 0.2	4.5 ± 0.2	3.5 ± 0.2	3.7 ± 0.4	5.3 ± 0.6
Digestible cell wall	1.5 ± 0.1	1.2 ± 0.0	1.1 ± 0.1	1.1 ± 0.1	1.3 ± 0.1
Indigestible cell wall	11.1 ± 1.1	14.4 ± 0.1	15.1 ± 0.3	14.3 ± 0.7	17.7 ± 0.5

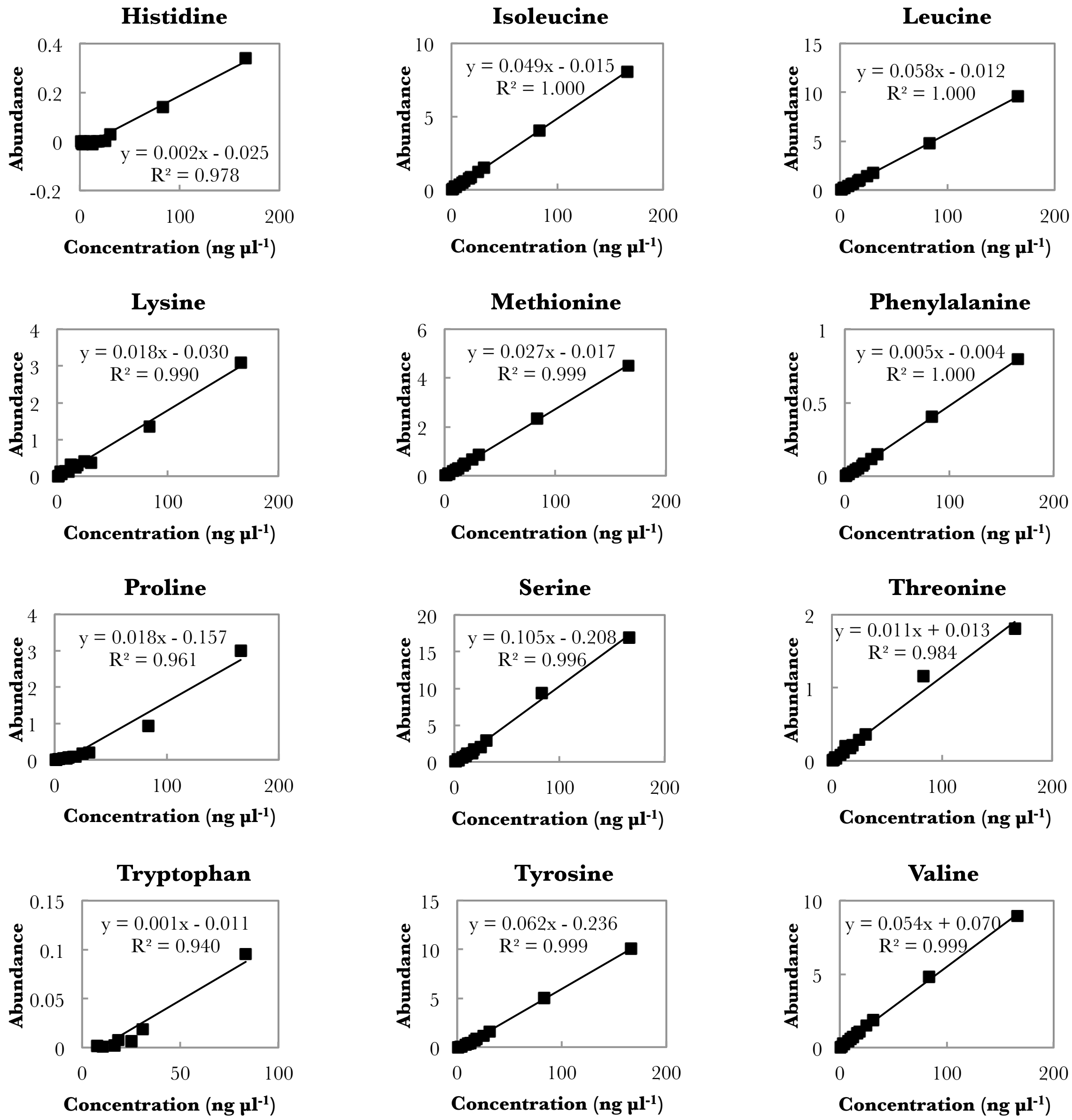
Appendix 5.7. GC-MS standard curves for amino acid and organic acid TBDMS derivatives

GC-MS standard curves of amino acid and organic acid TBDMS ethers were created by Mr Pedro Bota.

Amino acids

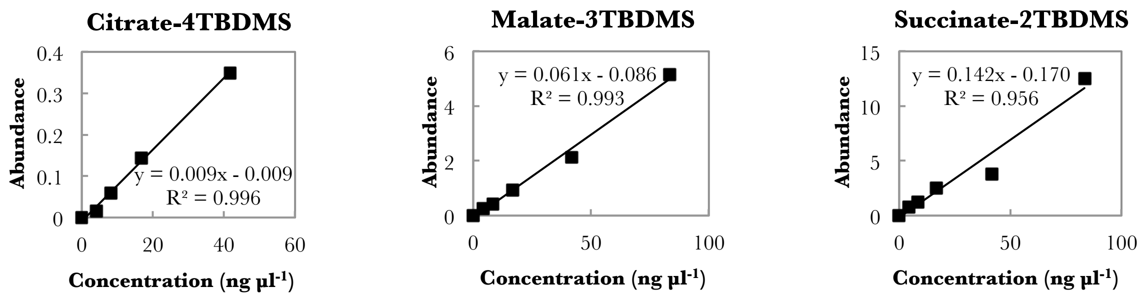
Alanine, glycine, isoleucine, leucine, methionine, phenylalanine, proline, tryptophan and valine were identified as 2TBDMS derivatives. Arginine, asparagine, aspartate, cysteine, glutamate, histidine, lysine, serine, threonine and tyrosine formed 3TBDMS derivatives. Glutamine was identified as both 3- and 4TBDMS derivatives. M-57 counts were normalised to M-57 of a norvaline internal standard to created standard curves of all amino acids except cysteine, which did not have reliable M-57 measurements. Instead, the total ion count for the cysteine peak was normalised to M-57 of norvaline.





Organic acids

Organic acids were also quantified relative to norvaline using M-57 fragments.



Appendix 5.8. Mathematical correction of ^{13}C fractional enrichment

Mathematical correction of ^{13}C fractional enrichment of cell wall, starch and protein components was achieved by methods described by Masakapalli et al. (2013). This was done by deriving a correction factor (Δ) for each mass isotopomer. This was defined as:

$$\Delta = \frac{F_S - F_P}{F_S - 0.0113}$$

where F_S is the expected ^{13}C fractional enrichment based on the fractional enrichment in precursor metabolites, F_P is the measured fractional enrichment in that fragment, and 0.0113 is the ^{13}C natural abundance. The product of Δ and the expected natural abundance of the mass isotopomer was subtracted from the normalised abundance of the mass isotopomer. This value was then normalised to the sum of the corrected mass isotopomers for that metabolite fragment.

Component	**Metabolite**	**Defined in model as:**	**Carbons**	**Precursor**	**Defined in model as:**	**Carbons**
Cell wall	Arabinose MeOX 4TMS (M-364)	PENTAN	5	Average of methanol-soluble glucose1 5TMS (M-250) and methanol-soluble glucose2 5TMS (M-250)	Not included	3,4,5,6
	Arabinose MeOX 4TMS (M-250)	PENTAN	3,4,5			
	Arabinose MeOX 4TMS (M-160)	PENTAN	3,4,5			
	Arabinose MeOX 4TMS (M-307)	PENTAN	1,2			
	Xylose MeOX 4TMS major (M-364)	PENTAN	5			
	Xylose MeOX 4TMS major (M-250)	PENTAN	3,4,5			
	Xylose MeOX 4TMS major (M-160)	PENTAN	3,4,5			
	Xylose MeOX 4TMS major (M-307)	PENTAN	1,2			
	Xylose MeOX 4TMS minor (M-364)	PENTAN	5			
	Xylose MeOX 4TMS minor (M-250)	PENTAN	3,4,5			
	Xylose MeOX 4TMS minor (M-160)	PENTAN	3,4,5			
	Xylose MeOX 4TMS minor (M-307)	PENTAN	1,2			
	Galactose 5TMS (M-409)	WALL	1,2			
	Galactose 5TMS (M-250)	WALL	3,4,5,6			
	Mannose 5TMS (M-409)	WALL	1,2			

Component	**Metabolite**	**Defined in model as:**	**Carbons**	**Precursor**	**Defined in model as:**	**Carbons**
	Mannose 5TMS (M-250)	WALL	3,4,5,6			
	Glucose1 5TMS (M-409)	WALL	1,2	Methanol-soluble glucose1 5TMS (M-409)	Not included	1,2
	Glucose1 5TMS (M-250)	WALL	3,4,5,6	Methanol-soluble glucose1 5TMS (M-250)	Not included	3,4,5,6
	Glucose2 5TMS (M-409)	WALL	1,2	Methanol-soluble glucose2 5TMS (M-409)	Not included	1,2
	Glucose2 5TMS (M-250)	WALL	3,4,5,6	Methanol-soluble glucose2 5TMS (M-250)	Not included	3,4,5,6
Starch	Glucose1 5TMS (M-409)	STA	1,2	Methanol-soluble glucose1 5TMS (M-409)	Not included	1,2
	Glucose1 5TMS (M-250)	STA	3,4,5,6	Methanol-soluble glucose1 5TMS (M-250)	Not included	3,4,5,6
	Glucose2 5TMS (M-409)	STA	1,2	Methanol-soluble glucose2 5TMS (M-409)	Not included	1,2
	Glucose2 5TMS (M-250)	STA	3,4,5,6	Methanol-soluble glucose2 5TMS (M-250)	Not included	3,4,5,6
Protein	Alanine-2TBDMS (M-0)	ALA	1,2,3	Average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85)	ALA	1,2,3; 1,2,3; 2,3
	Alanine-2TBDMS (M-15)	ALA	1,2,3	methanol-soluble alanine-2TBDMS (M-15)	ALA	1,2,3
	Alanine-2TBDMS (M-57)	ALA	1,2,3	methanol-soluble alanine-2TBDMS (M-57)	ALA	1,2,3
	Alanine-2TBDMS (M-85)	ALA	2,3	methanol-soluble alanine-2TBDMS (M-85)	ALA	1,2,3
	Alanine-2TBDMS (M-159)	ALA	2,3	Average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85)	ALA	1,2,3; 1,2,3; 2,3
	Alanine-2TBDMS (f302)	ALA	1,2			
	Aspartate-3TBDMS (M-0)	ASP	1,2,3,4	Average of malic acid-3TBDMS (M-15), (M-57) and TCA-4TBDMS (M-57)	MAL, CIT	1,2,3,4 (MAL); 1,2,3,4 (CIT)
	Aspartate-3TBDMS (M-15)	ASP	1,2,3,4			
	Aspartate-3TBDMS (M-57)	ASP	1,2,3,4			
	Aspartate-3TBDMS (M-85)	ASP	2,3,4			
	Aspartate-3TBDMS (M-159)	ASP	2,3,4			
	Aspartate-3TBDMS (f302)	ASP	1,2			
	Glutamate-3TBDMS (M-0)	GLU	1,2,3,4,5			
	Glutamate-3TBDMS (M-15)	GLU	1,2,3,4,5			
	Glutamate-3TBDMS (M-57)	GLU	1,2,3,4,5			
	Glutamate-3TBDMS (M-85)	GLU	2,3,4,5			
	Glutamate-3TBDMS (M-159)	GLU	2,3,4,5			
	Glutamate-3TBDMS (f302)	GLU	1,2			
	Proline-2TBDMS (M-0)	GLU	1,2,3,4,5			
	Proline-2TBDMS (M-15)	GLU	1,2,3,4,5			
	Proline-2TBDMS (M-57)	GLU	1,2,3,4,5			
	Proline-2TBDMS (M-85)	GLU	2,3,4,5			
	Proline-2TBDMS (M-159)	GLU	2,3,4,5			
	ProlineUK01-2TBDMS (M-0)	GLU	1,2,3,4,5			
	ProlineUK01-2TBDMS (M-15)	GLU	1,2,3,4,5			
	ProlineUK01-2TBDMS (M-57)	GLU	1,2,3,4,5			

Component	**Metabolite**	**Defined in model as:**	**Carbons**	**Precursor**	**Defined in model as:**	**Carbons**
	ProlineUK01-2TBDMS (M-85)	GLU	2,3,4,5			
	ProlineUK01-2TBDMS (M-159)	GLU	2,3,4,5			
	ProlineUK02-2TBDMS (M-0)	GLU	1,2,3,4,5			
	ProlineUK02-2TBDMS (M-15)	GLU	1,2,3,4,5			
	ProlineUK02-2TBDMS (M-57)	GLU	1,2,3,4,5			
	ProlineUK02-2TBDMS (M-85)	GLU	2,3,4,5			
	ProlineUK02-2TBDMS (M-159)	GLU	2,3,4,5			
	Isoleucine-2TBDMS (M-0) Isoleucine-2TBDMS (M-15) Isoleucine-2TBDMS (M-57)	ILE ILE ILE	1,2,3,4,5,6 1,2,3,4,5,6 1,2,3,4,5,6	4 x the average of malic acid-3TBDMS (M-15) and (M-57) plus 2x the average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85), all divided by 6	MAL, ALA	1,2,3,4 (MAL); 1,2,3 (ALA); 2,3 (ALA)
	Isoleucine-2TBDMS (M-85) Isoleucine-2TBDMS (M-159)	ILE ILE	2,3,4,5,6 2,3,4,5,6	3 x the average of malic acid-3TBDMS (M-15) and (M-57) plus 2x the average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85), all divided by 6	MAL, ALA	1,2,3,4 (MAL); 1,2,3 (ALA); 2,3 (ALA)
	Isoleucine-2TBDMS (f302) Leucine-2TBDMS (M-0) Leucine-2TBDMS (M-15) Leucine-2TBDMS (M-57) Leucine-2TBDMS (M-85) Leucine-2TBDMS (M-159) Leucine-2TBDMS (f302)	ILE LEU LEU LEU LEU LEU LEU	1,2 1,2,3,4,5,6 1,2,3,4,5,6 1,2,3,4,5,6 2,3,4,5,6 2,3,4,5,6 1,2	Average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85)	ALA	1,2,3; 1,2,3; 2,3
	Lysine-3TBDMS (M-0) Lysine-3TBDMS (M-15) Lysine-3TBDMS (M-57) Lysine-3TBDMS (M-85) Lysine-3TBDMS (M-159) Lysine-3TBDMS (f302) Lysine-3TBDMS (sc)	LYS LYS LYS LYS LYS LYS LYS	1,2,3,4,5,6 1,2,3,4,5,6 1,2,3,4,5,6 2,3,4,5,6 2,3,4,5,6 1,2 3,4,5	7 x the average of malic acid-3TBDMS (M-15) and (M-57) plus 5x the average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85), all divided by 12	MAL, ALA	1,2,3,4 (MAL); 1,2,3 (ALA); 2,3 (ALA)
	Phenylalanine-2TBDMS (M-0) Phenylalanine-2TBDMS (M-15) Phenylalanine-2TBDMS (M-57) Phenylalanine-2TBDMS (M-85) Phenylalanine-2TBDMS (M-159) Phenylalanine-2TBDMS (f302) Phenylalanine-2TBDMS (Sc)	PHE_TYR PHE_TYR PHE_TYR PHE_TYR PHE_TYR PHE_TYR PHE_TYR	1,2,3,4,5,6,7,8,9 1,2,3,4,5,6,7,8,9 1,2,3,4,5,6,7,8,9 2,3,4,5,6,7,8,9 2,3,4,5,6,7,8,9 1,2 3,4,5,6,7,8,9	Average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85)	ALA	1,2,3; 1,2,3; 2,3

Component	**Metabolite**	**Defined in model as:**	**Carbons**	**Precursor**	**Defined in model as:**	**Carbons**
	Tyrosine-3TBDMS (M-0)	PHE_TYR	1,2,3,4,5,6,7,8,9			
	Tyrosine-3TBDMS (M-15)	PHE_TYR	1,2,3,4,5,6,7,8,9			
	Tyrosine-3TBDMS (M-57)	PHE_TYR	1,2,3,4,5,6,7,8,9			
	Tyrosine-3TBDMS (M-85)	PHE_TYR	2,3,4,5,6,7,8,9			
	Tyrosine-3TBDMS (M-159)	PHE_TYR	2,3,4,5,6,7,8,9			
	Tyrosine-3TBDMS (f302)	PHE_TYR	1,2			
	Tyrosine-3TBDMS (sc)	PHE_TYR	3,4,5,6,7,8,9			
	Threonine-3TBDMS (M-0)	THR	1,2,3,4	Average of malic acid-3TBDMS (M-15), (M-57) and TCA-4TBDMS (M-57)	MAL, CIT	1,2,3,4 (MAL); 1,2,3,4 (CIT)
	Threonine-3TBDMS (M-15)	THR	1,2,3,4			
	Threonine-3TBDMS (M-57)	THR	1,2,3,4			
	Threonine-3TBDMS (M-85)	THR	2,3,4			
	Threonine-3TBDMS (M-159)	THR	2,3,4			
	Valine-2TBDMS (M-0)	VAL	1,2,3,4,5	Average of methanol-soluble alanine-2TBDMS (M-15), (M-57) and (M-85)	ALA	1,2,3; 1,2,3; 2,3
	Valine-2TBDMS (M-15)	VAL	1,2,3,4,5			
	Valine-2TBDMS (M-57)	VAL	1,2,3,4,5			
	Valine-2TBDMS (M-85)	VAL	2,3,4,5			
	Valine-2TBDMS (M-159)	VAL	2,3,4,5			
	Valine-2TBDMS (f302)	VAL	1,2			

Appendix 5.9. Fluxes and deviations derived by linear and non-linear statistical analyses for each BY-2 cell line

Best-fit fluxes are the flux values from the best-fit flux solution with lowest residuum. Deviations are derived by linear statistical analysis of the solution using the EstimateStat component of 13C-FLUX. 68% confidence limits were the range of the middle 68% of values for each flux of the feasible solutions below the cut-off residuum after one thousand Monte Carlo simulations with bootstrap sampling. 95% confidence intervals were derived using the non-linear sampling of each flux in turn using a confidence interval tool designed for use with 13C-FLUX (Antoniewicz et al., 2006). Deviations marked "ND" were not determinable by EstimateStat. Net flux lower confidence intervals marked as "<0" were within the 95% confidence residuum range down to a flux of 0, but lower values were not testable due to constraints imposed by other fluxes or in the inequalities section of the model. Exchange fluxes that were within the 95% confidence range with a flux of 0.99 were designated as having an upper confidence interval of infinity (∞).

Wild-type

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Inputs						
Vupt1	10.000 ± 0.179			0.000		
Vupt0	0.000 ± 0.179	0.000, 0.763	<0, 0.103	0.000		
VUuptU	1.989 ± 0.006	0.385, 1.989	1.977, 2.002	0.000		
VUupt0	8.011 ± 0.006			0.000		
Vco2in	0.000 ± 0.882	0.151, 1.562	0.000, 1.639	0.000		
Vmthfin	3.316 ± 0.528	0.409, 3.569	2.735, 4.787	0.000		
Cytosolic hexose/triose phosphate metabolism						
Vg	10.000			0.000		
Vgf	4.786 ± 1.120	0.037, 4.196	2.839, 6.731	0.99 ± 0.003	0.739, 0.99	0.987, ∞
Vald	4.266 ± 1.120			0.862 ± 0.007	0.679, 0.870	0.841, 0.873
Vtpi	4.086 ± 1.120			0.918 ± 0.018	0.677, 0.950	0.896, 0.936

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vfas2	0.180			0.000		
Vpk	4.510 ± 0.356			0.000		
Vpyr	3.912 ± 0.355			0.000		
Vadh	0.140			0.000		
Cytosolic pentose phosphate pathway						
Vppp1	3.363 ± 2.915	0.481, 2.128	1.681, 4.036	0.000		
Sugars storage						
Vgsuc	0.510			0.000		
Vgsuceff	0.510			0.000		
Vfsuc	0.520			0.000		
Vfsuceff	0.520			0.000		
Plastidial hexose/triose phosphate metabolism						
Vstsp	0.250			0.000		
Vgfp	0.542 ± 1.229			0.951 ± 0.040	0.351, 0.99	0.903, 0.968
Valdp	3.022 ± 1.081			0.000		
Vpkp	0.457 ± 0.060	0.340, 0.540	0.343, 0.686	0.000		
Vpdhp	0.658			0.000		
Vfas1	0.590			0.000		
Vmep	0.122 ± 0.010			0.000		
Plastidial pentose phosphate pathway						
Vppp1_p	0.394 ± 3.741	0.138, 2.423	<0, 3.277	0.000		
Vppp2a_p	2.480 ± 0.587			0.941 ± 0.016	0.471, 0.957	0.894, 0.954
Vppp2b_p	1.210 ± 0.293			0.872 ± 0.055	0.554, 0.880	0.788, 0.898
Vppp2c_p	1.270 ± 0.293			0.852 ± 164714.000	0.192, 0.870	0.763, 0.874
Vppp3a_p	1.270 ± 0.293			0.935 ± 176735.000	0.216, 0.931	0.840, 0.979
Vppp3b_p	1.270 ± 0.293			0.253 ± 0.200	0.145, 0.837	0.023, 0.684
Cytosol-plastid exchange						

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Vhcp	1.186 ± 3.374			0.931 ± 0.006	0.429, 0.935	0.919, 0.938
Vtpt	1.952 ± 2.195			0.928 ± 0.019	0.017, 0.926	0.836, 0.959
Vpyrt	0.401 ± 0.062	0.329, 0.524	0.201, 0.502	0.000		
TCA cycle						
Vpdh	4.307 ± 0.374			0.000		
Vcs	4.307 ± 0.375			0.000		
Vca	4.235 ± 0.375			0.000		
Vicdh	4.235 ± 0.375			0.000		
Vakgdh	3.521 ± 0.375			0.000		
Vsuccdh	3.507 ± 0.375			0.000		
Vfum1	1.755 ± 0.188			0.972 ± 0.013	0.464, 0.99	0.947, ∞
Vfum2	1.755 ± 0.188			0.972 ± 0.013		
Vme	0.395 ± 0.114	0.270, 1.559	0.293, 0.587	0.000		
Vpepc	1.891 ± 0.101			0.000 ± 0.201	0.000, 0.661	0.000, 0.205
Cytosolic mevalonate pathway						
Vacl	0.054			0.000		
Vmva1	0.018			0.000		
Vmva2	0.018			0.000		
Vsterol	0.018			0.000		
TCA cycle efflux						
VcitOUT	0.018			0.000		
VsuccOUT	0.014			0.000		
VmalOUT	0.250			0.000		
Vgabaeff	0.000			0.000		
VgabaOUT	0.000			0.000		
Efflux						
Vco2out	24.128 ± 1.235			0.000		
Vwall	0.069			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vsta	0.250			0.000		
Vadheff	0.140			0.000		
Vpentan	0.086			0.000		
Vpentaneff	0.086			0.000		
Amino acid oxidation						
Vthrox	0.000 ± 0.119	0.000, 0.285	-0.003, 0.205	0.000 ± 0.002	0.000, 0.394	<0, 0.003
Amino acid metabolism						
Vglu	0.710			0.482 ± 14374700.000	0.102, 0.807	0.000, ∞
Vglueff	0.710			0.000		
Vasp	0.349 ± 0.119			0.000		
Vaspeff	0.260			0.000		
Varg	0.004			0.000		
Vargeff	0.004			0.000		
Vasp_arg	0.004			0.000		
Vser	8.628 ± 0.332			0.000		
Vcys	0.007			0.000		
Vcyseff	0.007			0.000		
Vgly	8.521 ± 0.332			0.874 ± 0.005	0.536, 0.873	0.852, 0.895
Vglydc	8.464 ± 0.356	0.550, 8.437	7.600, 9.289	0.716 ± 0.018	0.327, 0.727	0.644, 0.788
Vglyeff	0.058			0.000		
Vmthfout	20.281 ± 0.917			0.000		
Vala	0.056			0.000		
Valaeff	0.056			0.000		
Varo1	0.030			0.000		
Varo2	0.030			0.000		
Vleu1	0.128			0.000		
Vleu	0.068			0.000		
Vleueff	0.068			0.000		
Vval	0.060			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vvaleff	0.060			0.000		
Vmet	0.013			0.000		
Vmeteff	0.013			0.000		
Vthr	0.072 ± 0.119			0.000		
Vthreff	0.039			0.000		
Vile	0.033			0.000		
Vileeff	0.033			0.000		
Vphe_tyr	0.060			0.000		
Vphe_tyreff	0.060			0.000		
Vlys	0.019 ± 0.001			0.000		
Vlys1	0.014 ± 0.001	0.013, 0.033	0.010, 0.017	0.000		
Vlyseff	0.033			0.000		
Vhis	0.007			0.000		
Vhiseff	0.007			0.000		
Vtrp2ca	0.000			0.000		
Vtrp2caeff	0.000			0.000		
Vtrp2cb	0.000			0.000		
Vtrp2cbeff	0.000			0.000		
Vtrp3c_sereff	0.100			0.000		
Vtrp4c	0.000			0.000		
Proxy reactions						
Vserin	0.005 ± 0.001	0.005, 0.326	0.003, 0.008	0.000		
Vglyin	0.002 ± 0.001	0.000, 0.438	<0, 0.008	0.000		
Vargin	0.000 ± 0.000	0.000, 0.592	0.000, 0.000	0.000		
Vhisin	0.000 ± 0.000	0.000, 0.273	0.000, 0.001	0.000		
Vmetin	0.001 ± 0.000	0.001, 0.383	0.001, 0.001	0.000		
Vserprotout	0.105 ± 0.001			0.000		
Vglyprotout	0.060 ± 0.001			0.000		
Vargprotout	0.005 ± 0.000			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Vhisprotout	0.008 ± 0.000			0.000		
Vmetprotout	0.014 ± 0.000			0.000		

Control line 4

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Inputs						
Vupt1	9.669 ± 0.179			0.000		
Vupt0	0.331 ± 0.179	0.000, 0.450	0.000, 0.630	0.000		
VUuptU	1.883 ± 0.006	1.874, 1.886	1.871, 1.895	0.000		
VUupt0	8.117 ± 0.006			0.000		
Vco2in	0.100 ± 0.969	0.000, 0.871	<0, 3.298	0.000		
Vmthfin	3.229 ± 0.574	1.333, 3.455	2.617, 4.451	0.000		
Cytosolic hexose/triose phosphate metabolism						
Vg	10.000			0.000		
Vgf	3.440 ± 2.204	-0.756, 3.603	0.926, 5.953	0.99 ± 0.002	0.99, 0.99	0.989, ∞
Vald	2.670 ± 2.204			0.929 ± 0.004	0.908, 0.932	0.923, 0.933
Vtpi	2.627 ± 2.204			0.963 ± 0.007	0.959, 0.981	0.951, 0.976
Vfas2	0.043			0.000		
Vpk	3.778 ± 0.496			0.000		
Vpyr	3.466 ± 0.458			0.000		
Vadh	0.049			0.000		
Cytosolic pentose phosphate pathway						
Vppp1	3.411 ± 4.740	2.210, 3.859	3.241, 6.141	0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Sugars storage						
Vgsuc	0.770			0.000		
Vgsuceff	0.770			0.000		
Vfsuc	0.770			0.000		
Vfsuceff	0.770			0.000		
Plastidial hexose/triose phosphate metabolism						
Vstsp	0.270			0.000		
Vgfp	1.990 ± 2.380			0.99 ± 0.024	0.988, 0.99	0.965, ∞
Valdp	4.239 ± 2.225			0.000		
Vpkp	1.021 ± 0.290	0.657, 1.200	0.511, 1.338	0.000		
Vpdhp	1.056			0.000		
Vfas1	1.000			0.000		
Vmep	0.130 ± 0.015			0.000		
Plastidial pentose phosphate pathway						
Vppp1_p	0.000 ± 5.549	0.000, 1.116	<0, 2.670	0.000		
Vppp2a_p	2.249 ± 0.595			0.941 ± 0.016	0.921, 0.963	0.894, 0.953
Vppp2b_p	1.095 ± 0.297			0.919 ± 0.036	0.886, 0.928	0.907, 0.928
Vppp2c_p	1.154 ± 0.297			0.969 ± ND	0.865, 0.982	0.775, 0.99
Vppp3a_p	1.154 ± 0.297			0.859 ± ND	0.830, 0.935	0.769, 0.881
Vppp3b_p	1.154 ± 0.297			0.546 ± 0.098	0.436, 0.869	0.434, 0.769
Cytosol-plastid exchange						
Vhcp	2.260 ± 5.202			0.959 ± 0.005	0.952, 0.965	0.947, 0.967
Vtpt	0.189 ± 4.318			0.969 ± 0.011	0.369, 0.973	0.944, 0.99
Vpyrt	0.199 ± 0.290	0.000, 0.254	<0, 0.545	0.000		
TCA cycle						
Vpdh	3.584 ± 0.455			0.000		
Vcs	3.584 ± 0.464			0.000		

	Net fluxes			**Exchange fluxes**		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vca	3.431 ± 0.464			0.000		
Vicdh	3.431 ± 0.464			0.000		
Vakgdh	2.946 ± 0.464			0.000		
Vsuccdh	2.941 ± 0.464			0.000		
Vfum1	1.473 ± 0.232			0.963 ± 0.019	0.960, 0.988	0.915, ∞
Vfum2	1.473 ± 0.232			0.963 ± 0.019		
Vme	0.118 ± 0.090	0.085, 0.415	0.044, 0.416	0.000		
Vpepc	1.329 ± 0.083			0.000 ± 0.219	0.000, 0.328	0.000, 0.205
Cytosolic mevalonate pathway						
Vacl	0.072			0.000		
Vmva1	0.024			0.000		
Vmva2	0.024			0.000		
Vsterol	0.024			0.000		
TCA cycle efflux						
VcitOUT	0.081			0.000		
VsuccOUT	0.005			0.000		
VmalOUT	0.250			0.000		
Vgabaeff	0.000			0.000		
VgabaOUT	0.000			0.000		
Efflux						
Vco2out	22.342 ± 1.346			0.000		
Vwall	0.059			0.000		
Vsta	0.270			0.000		
Vadheff	0.049			0.000		
Vpentan	0.060			0.000		
Vpentaneff	0.060			0.000		
Amino acid oxidation						
Vthrox	0.000 ± 0.099	0.000, 0.085	-0.003, 0.103	0.000 ± 0.004	0.000, 0.101	<0, 0.003

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Amino acid metabolism						
Vglu	0.480			0.533 ± 7315230.000	0.165, 0.877	0.000, ∞
Vglueff	0.480			0.000		
Vasp	0.225 ± 0.099			0.000		
Vaspeff	0.130			0.000		
Varg	0.005			0.000		
Vargeff	0.005			0.000		
Vasp_arg	0.005			0.000		
Vser	8.626 ± 0.402			0.000		
Vcys	0.005			0.000		
Vcyseff	0.005			0.000		
Vgly	8.501 ± 0.402			0.898 ± 0.005	0.868, 0.898	0.887, 0.904
Vglydc	8.471 ± 0.416	6.398, 8.507	7.625, 8.896	0.722 ± 0.019	0.618, 0.727	0.686, 0.758
Vglyeff	0.030			0.000		
Vmthfout	20.184 ± 1.027			0.000		
Vala	0.064			0.000		
Valaeff	0.064			0.000		
Varo1	0.029			0.000		
Varo2	0.029			0.000		
Vleu1	0.114			0.000		
Vleu	0.056			0.000		
Vleueff	0.056			0.000		
Vval	0.058			0.000		
Vvaleff	0.058			0.000		
Vmet	0.010			0.000		
Vmeteff	0.010			0.000		
Vthr	0.080 ± 0.099			0.000		
Vthreff	0.054			0.000		
Vile	0.026			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vileeff	0.026			0.000		
Vphe_tyr	0.057			0.000		
Vphe_tyreff	0.057			0.000		
Vlys	0.021 ± 0.002			0.000		
Vlys1	0.019 ± 0.002	0.019, 0.023	0.014, 0.024	0.000		
Vlyseff	0.040			0.000		
Vhis	0.007			0.000		
Vhiseff	0.007			0.000		
Vtrp2ca	0.002			0.000		
Vtrp2caeff	0.002			0.000		
Vtrp2cb	0.002			0.000		
Vtrp2cbeff	0.002			0.000		
Vtrp3c_sereff	0.120			0.000		
Vtrp4c	0.002			0.000		
Proxy reactions						
Vserin	0.003 ± 0.001	0.001, 0.003	0.000, 0.004	0.000		
Vglyin	0.001 ± 0.000	0.001, 0.002	<0, 0.004	0.000		
Vargin	0.000 ± 0.000	0.000, 0.001	0.000, 0.001	0.000		
Vhisin	0.001 ± 0.000	0.001, 0.001	0.000, 0.001	0.000		
Vmetin	0.001 ± 0.000	0.001, 0.001	0.001, 0.001	0.000		
Vserprotout	0.123 ± 0.001			0.000		
Vglyprotout	0.031 ± 0.000			0.000		
Vargprotout	0.005 ± 0.000			0.000		
Vhisprotout	0.008 ± 0.000			0.000		
Vmetprotout	0.011 ± 0.000			0.000		

Control line 6

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Inputs						
Vupt1	10.000 ± 0.157			0.000		
Vupt0	0.000 ± 0.157	0.000, 0.274	<0, 0.205	0.000		
VUuptU	1.969 ± 0.006	1.966, 1.962	1.953, 1.978	0.000		
VUupt0	8.031 ± 0.006			0.000		
Vco2in	1.656 ± 0.972	0.825, 2.371	0.331, 2.981	0.000		
Vmthfin	2.098 ± 0.474	0.466, 2.222	1.694, 2.895	0.000		
Cytosolic hexose/triose phosphate metabolism						
Vg	10.000			0.000		
Vgf	2.523 ± 1.872	0.433, 2.412	0.519, 3.023	0.99 ± 0.003	0.99, 0.99	0.989, ∞
Vald	1.793 ± 1.872			0.892 ± 0.005	0.887, 0.898	0.882, 0.898
Vtpi	1.760 ± 1.872			0.929 ± 0.016	0.906, 0.929	0.905, 0.936
Vfas2	0.033			0.000		
Vpk	4.868 ± 0.419			0.000		
Vpyr	4.207 ± 0.394			0.000		
Vadh	0.058			0.000		
Cytosolic pentose phosphate pathway						
Vppp1	2.318 ± 3.113	1.612, 2.286	2.264, 4.180	0.000		
Sugars storage						
Vgsuc	0.730			0.000		
Vgsuceff	0.730			0.000		
Vfsuc	0.730			0.000		
Vfsuceff	0.730			0.000		
Plastidial hexose/triose phosphate metabolism						
Vstsp	0.260			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vgfp	2.511 ± 1.972			0.961 ± 0.037	0.960, 0.99	0.913, 0.968
Valdp	5.069 ± 1.877			0.000		
Vpkp	0.452 ± 0.174	0.284, 0.717	0.000, 0.901	0.000		
Vpdhp	0.805			0.000		
Vfas1	0.750			0.000		
Vmep	0.080 ± 0.011			0.000		
Plastidial pentose phosphate pathway						
Vppp1_p	1.552 ± 3.752	1.403, 2.230	1.479, 1.714	0.000		
Vppp2a_p	2.557 ± 0.465			0.933 ± 0.013	0.908, 0.942	0.910, 0.948
Vppp2b_p	1.252 ± 0.233			0.892 ± 0.043	0.804, 0.889	0.845, 0.901
Vppp2c_p	1.305 ± 0.233			0.897 ± 218643.000	0.779, 0.931	0.715, 0.917
Vppp3a_p	1.305 ± 0.233			0.897 ± 218643.000	0.764, 0.912	0.715, 0.917
Vppp3b_p	1.305 ± 0.233			0.145 ± 0.227	0.000, 0.393	0.000, 0.378
Cytosol-plastid exchange						
Vhcp	4.323 ± 3.674			0.933 ± 0.008	0.917, 0.940	0.910, 0.947
Vtpt	-2.920 ± 3.743			0.969 ± 0.021	0.009, 0.967	0.956, 0.991
Vpyrt	0.528 ± 0.175	0.230, 0.715	0.000, 1.051	0.000		
TCA cycle						
Vpdh	4.412 ± 0.400			0.000		
Vcs	4.412 ± 0.403			0.000		
Vca	4.208 ± 0.403			0.000		
Vicdh	4.208 ± 0.403			0.000		
Vakgdh	3.495 ± 0.403			0.000		
Vsuccdh	3.491 ± 0.403			0.000		
Vfum1	1.747 ± 0.201			0.988 ± 0.015	0.984, 0.99	0.964, ∞
Vfum2	1.747 ± 0.201			0.988 ± 0.015		
Vme	0.206 ± 0.101	0.208, 0.998	0.153, 0.498	0.000		
Vpepc	1.605 ± 0.098			0.000 ± 0.197	0.000, 0.576	0.000, 0.103

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Cytosolic mevalonate pathway						
Vacl	0.084			0.000		
Vmva1	0.028			0.000		
Vmva2	0.028			0.000		
Vsterol	0.028			0.000		
TCA cycle efflux						
VcitOUT	0.120			0.000		
VsuccOUT	0.004			0.000		
VmalOUT	0.210			0.000		
Vgabaeff	0.000			0.000		
VgabaOUT	0.000			0.000		
Efflux						
Vco2out	25.253 ± 1.313			0.000		
Vwall	0.041			0.000		
Vsta	0.260			0.000		
Vadheff	0.058			0.000		
Vpentan	0.065			0.000		
Vpentaneff	0.065			0.000		
Amino acid oxidation						
Vthrox	0.000 ± 0.112	-0.002, 0.206	-0.001, 0.213	0.000 ± 0.002	0.000, 0.002	<0, 0.002
Amino acid metabolism						
Vglu	0.710			0.513 ± 13705400.000	0.100, 0.856	0.000, ∞
Vglueff	0.710			0.000		
Vasp	0.239 ± 0.112			0.000		
Vaspeff	0.130			0.000		
Varg	0.003			0.000		
Vargeff	0.003			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vasp_arg	0.003			0.000		
Vser	7.918 ± 0.351			0.000		
Vcys	0.004			0.000		
Vcyseff	0.004			0.000		
Vgly	7.764 ± 0.351			0.858 ± 0.006	0.685, 0.859	0.837, 0.869
Vglydc	7.715 ± 0.365	2.658, 7.780	7.543, 8.124	0.655 ± 0.025	0.340, 0.656	0.588, 0.685
Vglyeff	0.049			0.000		
Vmthfout	17.566 ± 0.861			0.000		
Vala	0.076			0.000		
Valaeff	0.076			0.000		
Varo1	0.025			0.000		
Varo2	0.025			0.000		
Vleu1	0.099			0.000		
Vleu	0.055			0.000		
Vleueff	0.055			0.000		
Vval	0.044			0.000		
Vvaleff	0.044			0.000		
Vmet	0.007			0.000		
Vmeteff	0.007			0.000		
Vthr	0.099 ± 0.112			0.000		
Vthreff	0.079			0.000		
Vile	0.020			0.000		
Vileeff	0.020			0.000		
Vphe_tyr	0.050			0.000		
Vphe_tyreff	0.050			0.000		
Vlys	0.021 ± 0.001			0.000		
Vlys1	0.015 ± 0.001	0.014, 0.016	0.011, 0.019	0.000		
Vlyseff	0.036			0.000		
Vhis	0.005			0.000		
Vhiseff	0.005			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vtrp2ca	0.003			0.000		
Vtrp2caeff	0.003			0.000		
Vtrp2cb	0.003			0.000		
Vtrp2cbeff	0.003			0.000		
Vtrp3c_sereff	0.150			0.000		
Vtrp4c	0.003			0.000		
Proxy reactions						
Vserin	0.004 ± 0.001	0.003, 0.007	0.000, 0.009	0.000		
Vglyin	0.001 ± 0.001	0.000, 0.003	<0, 0.004	0.000		
Vargin	0.000 ± 0.000	0.000, 0.000	0.000, 0.000	0.000		
Vhisin	0.000 ± 0.000	0.000, 0.000	0.000, 0.001	0.000		
Vmetin	0.001 ± 0.000	0.001, 0.001	0.001, 0.001	0.000		
Vserprotout	0.154 ± 0.001			0.000		
Vglyprotout	0.050 ± 0.001			0.000		
Vargprotout	0.004 ± 0.000			0.000		
Vhisprotout	0.005 ± 0.000			0.000		
Vmetprotout	0.007 ± 0.000			0.000		

ATCS line 6

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Inputs						
Vupt1	9.039 ± 0.205			0.000		
Vupt0	0.961 ± 0.205	0.827, 1.578	0.585, 1.208	0.000		
VUuptU	1.877 ± 0.006	1.865, 1.876	1.864, 1.887	0.000		
VUupt0	8.123 ± 0.006			0.000		
Vco2in	0.000 ± 1.121	0.000, 0.712	<0, 0.819	0.000		
Vmthfin	2.434 ± 0.486	0.492, 2.165	0.730, 3.407	0.000		
Cytosolic hexose/triose phosphate metabolism						
Vg	10.000			0.000		
Vgf	0.133 ± 2.962	-0.347, 1.907	-0.634, 0.431	0.99 ± 0.006	0.981, 0.99	0.975, ∞
Vald	-0.687 ± 2.962			0.831 ± 0.127	0.761, 0.851	0.754, 0.835
Vtpi	-0.732 ± 2.962			0.99 ± 0.053	0.989, 0.99	0.941, ∞
Vfas2	0.045			0.000		
Vpk	5.916 ± 0.668			0.000		
Vpyr	5.549 ± 0.652			0.000		
Vadh	0.055			0.000		
Cytosolic pentose phosphate pathway						
Vppp1	0.029 ± 1.686	0.111, 1.377	<0, 0.410	0.000	0.029 ± 1.686	
Sugars storage						
Vgsuc	0.810			0.000		
Vgsuceff	0.810			0.000		
Vfsuc	0.820			0.000		
Vfsuceff	0.820			0.000		
Plastidial hexose/triose phosphate metabolism						
Vstsp	0.210			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vgfp	6.180 ± 2.987			0.99 ± 0.006	0.988, 0.99	0.987, ∞
Valdp	7.873 ± 2.963			0.000		
Vpkp	0.645 ± 0.074	0.502, 0.739	0.486, 0.668	0.000		
Vpdhp	0.798			0.000		
Vfas1	0.750			0.000		
Vmep	0.172 ± 0.011			0.000		
Plastidial pentose phosphate pathway						
Vppp1_p	2.542 ± 1.764	0.428, 2.019	1.879, 2.607	0.000		
Vppp2a_p	1.694 ± 0.296			0.857 ± 0.021	0.760, 0.863	0.785, 0.910
Vppp2b_p	0.822 ± 0.148			0.922 ± 0.014	0.909, 0.931	0.905, 0.934
Vppp2c_p	0.872 ± 0.148			0.833 ± ND	0.618, 0.818	0.764, ∞
Vppp3a_p	0.872 ± 0.148			0.827 ± ND	0.682, 0.821	0.758, ∞
Vppp3b_p	0.872 ± 0.148			0.948 ± 0.013	0.950, 0.965	0.933, 0.966
Cytosol-plastid exchange						
Vhcp	8.932 ± 3.933			0.966 ± 0.007	0.959, 0.967	0.960, 0.972
Vtpt	-9.599 ± 5.602			0.794 ± 0.420	0.000, 0.920	0.000, 0.99
Vpyrt	0.232 ± 0.079	0.132, 0.389	0.000, 0.349	0.000		
TCA cycle						
Vpdh	6.396 ± 0.706			0.000		
Vcs	6.396 ± 0.723			0.000		
Vca	6.244 ± 0.723			0.000		
Vicdh	6.244 ± 0.723			0.000		
Vakgdh	5.620 ± 0.723			0.000		
Vsuccdh	5.615 ± 0.723			0.000		
Vfum1	2.809 ± 0.361			0.980 ± 0.012	0.977, 0.99	0.960, ∞
Vfum2	2.809 ± 0.361			0.980 ± 0.012		
Vme	0.847 ± 0.166	0.501, 1.306	0.292, 1.236	0.000		
Vpepc	2.264 ± 0.174			0.074 ± 0.223	0.000, 0.665	<0, 0.221

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Cytosolic mevalonate pathway						
Vacl	0.093			0.000		
Vmva1	0.031			0.000		
Vmva2	0.031			0.000		
Vsterol	0.031			0.000		
TCA cycle efflux						
VcitOUT	0.059			0.000		
VsuccOUT	0.006			0.000		
VmalOUT	0.210			0.000		
Vgabaeff	0.000			0.000		
VgabaOUT	0.000			0.000		
Efflux						
Vco2out	26.835 ± 1.843			0.000		
Vwall	0.044			0.000		
Vsta	0.210			0.000		
Vadheff	0.055			0.000		
Vpentan	0.051			0.000		
Vpentaneff	0.051			0.000		
Amino acid oxidation						
Vthrox	0.000 ± 0.132	-0.003, 0.000	-0.007, 0.058	0.000 ± 0.003	0.000, 0.000	<0, 0.007
Amino acid metabolism						
Vglu	0.620			0.512 ± 10753600.000	0.156, 0.844	0.000, ∞
Vglueff	0.620			0.000		
Vasp	0.313 ± 0.132			0.000		
Vaspeff	0.130			0.000		
Varg	0.003			0.000		
Vargeff	0.003			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vasp_arg	0.003			0.000		
Vser	6.226 ± 0.668			0.000		
Vcys	0.005			0.000		
Vcyseff	0.005			0.000		
Vgly	6.112 ± 0.668			0.826 ± 0.016	0.593, 0.833	0.816, 0.837
Vglydc	6.064 ± 0.660	1.697, 6.297	4.318, 6.386	0.769 ± 0.023	0.500, 0.771	0.750, 0.789
Vglyeff	0.048			0.000		
Vmthfout	14.597 ± 1.634			0.000		
Vala	0.081			0.000		
Valaeff	0.081			0.000		
Varo1	0.025			0.000		
Varo2	0.025			0.000		
Vleu1	0.096			0.000		
Vleu	0.048			0.000		
Vleueff	0.048			0.000		
Vval	0.048			0.000		
Vvaleff	0.048			0.000		
Vmet	0.008			0.000		
Vmeteff	0.008			0.000		
Vthr	0.172 ± 0.132			0.000		
Vthreff	0.150			0.000		
Vile	0.022			0.000		
Vileeff	0.022			0.000		
Vphe_tyr	0.049			0.000		
Vphe_tyreff	0.049			0.000		
Vlys	0.021 ± 0.001			0.000		
Vlys1	0.016 ± 0.001	0.014, 0.019	0.012, 0.020	0.000		
Vlyseff	0.037			0.000		
Vhis	0.005			0.000		
Vhiseff	0.005			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals	Best-fit flux ± deviation	68% confidence limits	95% confidence intervals
Vtrp2ca	0.001			0.000		
Vtrp2caeff	0.001			0.000		
Vtrp2cb	0.001			0.000		
Vtrp2cbeff	0.001			0.000		
Vtrp3c_sereff	0.110			0.000		
Vtrp4c	0.001			0.000		
Proxy reactions						
Vserin	0.004 ± 0.001	0.004, 0.007	0.002, 0.007	0.000		
Vglyin	0.001 ± 0.001	0.001, 0.002	<0, 0.005	0.000		
Vargin	0.000 ± 0.000	0.000, 0.000	0.000, 0.000	0.000		
Vhisin	0.000 ± 0.000	0.000, 0.000	0.000, 0.001	0.000		
Vmetin	0.001 ± 0.000	0.001, 0.001	0.001, 0.001	0.000		
Vserprotout	0.114 ± 0.001			0.000		
Vglyprotout	0.049 ± 0.001			0.000		
Vargprotout	0.004 ± 0.000			0.000		
Vhisprotout	0.006 ± 0.000			0.000		
Vmetprotout	0.009 ± 0.000			0.000		

ATCS line 16

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Inputs						
Vupt1	9.477 ± 0.177			0.000		
Vupt0	0.523 ± 0.177	0.176, 0.638	0.499, 1.054	0.000		
VUuptU	1.927 ± 0.006	1.911, 1.930	1.910, 1.934	0.000		
VUupt0	8.073 ± 0.006			0.000		
Vco2in	1.650 ± 0.941	0.694, 2.811	<0, 2.970	0.000		
Vmthfin	1.310 ± 0.438	0.403, 2.010	0.783, 2.357	0.000		
Cytosolic hexose/triose phosphate metabolism						
Vg	10.000			0.000		
Vgf	4.944 ± 0.601	0.929, 5.054	2.967, 5.193	0.99 ± 0.003	0.99, 0.99	0.988, ∞
Vald	4.344 ± 0.601			0.911 ± 0.005	0.894, 0.918	0.898, 0.920
Vtpi	4.321 ± 0.601			0.904 ± 0.011	0.896, 0.930	0.880, 0.914
Vfas2	0.023			0.000		
Vpk	4.160 ± 0.412			0.000		
Vpyr	3.638 ± 0.402			0.000		
Vadh	0.062			0.000		
Cytosolic pentose phosphate pathway						
Vppp1	0.654 ± 1.602	0.906, 2.025	0.577, 1.310	0.000		
Sugars storage						
Vgsuc	0.600			0.000		
Vgsuceff	0.600			0.000		
Vfsuc	0.600			0.000		
Vfsuceff	0.600			0.000		
Plastidial hexose/triose phosphate metabolism						
Vstsp	0.510			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vgfp	0.160 ± 0.599			0.948 ± 0.013	0.940, 0.988	0.925, 0.959
Valdp	2.579 ± 0.560			0.000		
Vpkp	0.539 ± 0.065	0.494, 0.674	0.404, 0.673	0.000		
Vpdhp	0.786			0.000		
Vfas1	0.720			0.000		
Vmep	0.162 ± 0.012			0.000		
Plastidial pentose phosphate pathway						
Vppp1_p	3.014 ± 1.921	1.522, 2.759	2.942, 5.422	0.000		
Vppp2a_p	2.419 ± 0.306			0.909 ± 0.016	0.897, 0.936	0.882, 0.916
Vppp2b_p	1.179 ± 0.153			0.971 ± 0.016	0.883, 0.972	0.922, 0.980
Vppp2c_p	1.239 ± 0.153			0.826 ± 356690.000	0.567, 0.898	0.484, 0.889
Vppp3a_p	1.239 ± 0.153			0.793 ± 345242.000	0.645, 0.887	0.464, 0.853
Vppp3b_p	1.239 ± 0.153			0.867 ± 0.029	0.732, 0.911	0.792, 0.924
Cytosol-plastid exchange						
Vhcp	3.684 ± 1.813			0.951 ± 0.005	0.945, 0.957	0.945, 0.961
Vtpt	2.426 ± 1.060			0.911 ± 0.020	0.058, 0.921	0.903, 0.951
Vpyrt	0.407 ± 0.068	0.266, 0.463	0.200, 0.601	0.000		
TCA cycle						
Vpdh	4.398 ± 0.480			0.000		
Vcs	4.391 ± 0.468			0.000		
Vca	4.245 ± 0.468			0.000		
Vicdh	4.245 ± 0.468			0.000		
Vakgdh	3.579 ± 0.468			0.000		
Vsuccdh	3.573 ± 0.468			0.000		
Vfum1	1.790 ± 0.234			0.99 ± 0.013	0.985, 0.99	0.965, ∞
Vfum2	1.790 ± 0.234			0.99 ± 0.013		
Vme	0.760 ± 0.161	0.748, 1.453	0.683, 1.222	0.000		
Vpepc	2.079 ± 0.137			0.000 ± 0.235	0.000, 0.48	0.000, 0.103

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Cytosolic mevalonate pathway						
Vacl	0.078			0.000		
Vmva1	0.026			0.000		
Vmva2	0.026			0.000		
Vsterol	0.026			0.000		
TCA cycle efflux						
VcitOUT	0.068			0.000		
VsuccOUT	0.006			0.000		
VmalOUT	0.170			0.000		
Vgabaeff	0.000			0.000		
VgabaOUT	0.000			0.000		
Efflux						
Vco2out	25.580 ± 1.459			0.000		
Vwall	0.063			0.000		
Vsta	0.510			0.000		
Vadheff	0.062			0.000		
Vpentan	0.055			0.000		
Vpentaneff	0.055			0.000		
Amino acid oxidation						
Vthrox	-0.006 ± 0.139	-0.010, 0.021	-0.019, 0.058	0.000 ± 0.150	0, 0.032	<0, 0.026
Amino acid metabolism						
Vglu	0.660			0.512 ± 15946100.000	0.156, 0.802	0.000, ∞
Vglueff	0.660			0.000		
Vasp	0.214 ± 0.139			0.000		
Vaspeff	0.120			0.000		
Varg	0.006			0.000		
Vargeff	0.006			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vasp_arg	0.006			0.000		
Vser	8.106 ± 0.456			0.000		
Vcys	0.005			0.000		
Vcyseff	0.005			0.000		
Vgly	7.980 ± 0.456			0.880 ± 0.007	0.784, 0.885	0.871, 0.893
Vglydc	7.953 ± 0.478	3.693, 8.179	7.789, 8.386	0.779 ± 0.017	0.584, 0.78	0.738, 0.796
Vglyeff	0.021			0.000		
Vmthfout	17.222 ± 1.068			0.000		
Vala	0.054			0.000		
Valaeff	0.054			0.000		
Varo1	0.030			0.000		
Varo2	0.030			0.000		
Vleu1	0.126			0.000		
Vleu	0.066			0.000		
Vleueff	0.066			0.000		
Vval	0.060			0.000		
Vvaleff	0.060			0.000		
Vmet	0.011			0.000		
Vmeteff	0.011			0.000		
Vthr	0.078 ± 0.139			0.000		
Vthreff	0.054			0.000		
Vile	0.030			0.000		
Vileeff	0.030			0.000		
Vphe_tyr	0.059			0.000		
Vphe_tyreff	0.059			0.000		
Vlys	0.018 ± 0.001			0.000		
Vlys1	0.021 ± 0.001	0.019, 0.022	0.016, 0.025	0.000		
Vlyseff	0.039			0.000		
Vhis	0.010			0.000		
Vhiseff	0.010			0.000		

	Net fluxes			Exchange fluxes		
	Best-fit flux ± deviation	**68% confidence limits**	**95% confidence intervals**	**Best-fit flux ± deviation**	**68% confidence limits**	**95% confidence intervals**
Vtrp2ca	0.001			0.000		
Vtrp2caeff	0.001			0.000		
Vtrp2cb	0.001			0.000		
Vtrp2cbeff	0.001			0.000		
Vtrp3c_sereff	0.120			0.000		
Vtrp4c	0.001			0.000		
Proxy reactions						
Vserin	0.001 ± 0.001	0.000, 0.002	<0, 0.003	0.000		
Vglyin	0.000 ± 0.000	0.000, 0.000	<0, 0.001	0.000		
Vargin	0.000 ± 0.000	0.000, 0.000	0.000, 0.000	0.000		
Vhisin	0.001 ± 0.000	0.000, 0.001	0.000, 0.001	0.000		
Vmetin	0.001 ± 0.000	0.001, 0.001	0.001, 0.001	0.000		
Vserprotout	0.121 ± 0.001			0.000		
Vglyprotout	0.021 ± 0.000			0.000		
Vargprotout	0.006 ± 0.000			0.000		
Vhisprotout	0.010 ± 0.000			0.000		
Vmetprotout	0.012 ± 0.000			0.000		

Appendix 5.10. GC-MS-derived mass isotopomer data used in BY-2 metabolic models

The following data is presented in 13C-FLUX ftbl format and represents all mass isotopomer data used in final 13C-FLUX models.

Wild-type

```
MASS_SPECTROMETRY
      META_NAME   FRAGMENT    WEIGHT      VALUE DEVIATION
      ALA   1,2,3 0      0.576 0.01
                  1      0.394 0.01
                  2      0.028 0.01
                  3      0.002 0.01
      ALA   2,3   0      0.597 0.011
                  1      0.39  0.011
                  2      0.012 0.011
      GLY   1,2   0      0.909 0.011
                  1      0.088 0.011
                  2      0.002 0.011
      GLY   2     0      0.977 0.011
                  1      0.023 0.011
      VAL   1,2,3,4,5    0      0.363 0.01
                  1      0.445 0.01
                  2      0.176 0.01
                  3      0.017 0.01
                  4      0.001 0.01
                  5      -0.001      0.01
      VAL   2,3,4,5      0      0.372 0.029
                  1      0.444 0.029
                  2      0.157 0.029
                  3      0.026 0.029
                  4      0.001 0.029
      LEU   2,3,4,5,6    0      0.259 0.011
                  1      0.42  0.011
                  2      0.254 0.011
                  3      0.062 0.011
                  4      0.006 0.011
                  5      0     0.011
      MET   2,3,4,5      0      0.372 0.01
                  1      0.443 0.01
                  2      0.172 0.01
                  3      0.019 0.01
                  4      -0.006      0.01
      SER   1,2,3 0      0.701 0.01
```

		1	0.298	0.01	
		2	0.005	0.01	
		3	-0.005		0.01
SER	1,2,3	0	0.694	0.011	
		1	0.292	0.011	
		2	0.014	0.011	
		3	0.001	0.011	
SER	2,3	0	0.716	0.01	
		1	0.272	0.01	
		2	0.012	0.01	
SER	2,3	0	0.72	0.011	
		1	0.274	0.011	
		2	0.006	0.011	
SER	1,2	0	0.943	0.013	
		1	0.058	0.013	
		2	-0.001		0.013
THR	2,3,4	0	0.467	0.026	
		1	0.42	0.031	
		2	0.118	0.027	
		3	-0.005		0.033
ASP	1,2,3,4		0	0.371	0.01
		1	0.444	0.01	
		2	0.164	0.01	
		3	0.024	0.01	
		4	-0.003		0.01
ASP	2,3,4	0	0.444	0.01	
		1	0.437	0.01	
		2	0.115	0.01	
		3	0.004	0.01	
ASP	1,2	0	0.633	0.013	
		1	0.337	0.013	
		2	0.03	0.013	
GLU	1,2,3,4,5		0	0.253	0.01
		1	0.435	0.01	
		2	0.242	0.01	
		3	0.058	0.01	
		4	0.014	0.01	
		5	-0.002		0.01
GLU	1,2,3,4,5		0	0.262	0.01
		1	0.425	0.01	
		2	0.25	0.01	
		3	0.06	0.01	
		4	0.005	0.01	
		5	-0.001		0.01
GLU	2,3,4,5		0	0.3	0.01
		1	0.446	0.01	
		2	0.214	0.01	
		3	0.036	0.01	
		4	0.004	0.01	
GLU	1,2,3,4,5		0	0.275	0.013
		1	0.434	0.013	
		2	0.245	0.013	
		3	0.05	0.013	

		4	0.002	0.013
		5	-0.005	0.013
GLU	1,2,3,4,5	0	0.266	0.01
		1	0.432	0.01
		2	0.244	0.01
		3	0.056	0.01
		4	0.004	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.267	0.011
		1	0.431	0.011
		2	0.241	0.011
		3	0.057	0.011
		4	0.005	0.011
		5	-0.001	0.011
GABA	1,2,3,4	0	0.313	0.019
		1	0.44	0.019
		2	0.214	0.019
		3	0.032	0.019
		4	0.002	0.019
ALA	1,2,3	0	0.576	0.01
		1	0.396	0.01
		2	0.027	0.01
		3	0.002	0.01
ALA	2,3	0	0.596	0.011
		1	0.391	0.011
		2	0.013	0.011
GLY	1,2	0	0.903	0.011
		1	0.094	0.011
		2	0.002	0.011
GLY	2	0	0.978	0.011
		1	0.022	0.011
VAL	1,2,3,4,5	0	0.381	0.01
		1	0.445	0.01
		2	0.16	0.01
		3	0.016	0.01
		4	0.001	0.01
		5	-0.002	0.01
VAL	1,2,3,4,5	0	0.361	0.01
		1	0.447	0.01
		2	0.171	0.01
		3	0.02	0.01
		4	0.001	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.373	0.029
		1	0.443	0.029
		2	0.161	0.029
		3	0.022	0.029
		4	0.002	0.029
LEU	2,3,4,5,6	0	0.263	0.011
		1	0.413	0.011
		2	0.257	0.011
		3	0.063	0.011
		4	0.005	0.011

		5	-0.001	0.011
MET	2,3,4,5	0	0.372	0.01
		1	0.432	0.01
		2	0.172	0.01
		3	0.028	0.01
		4	-0.004	0.01
SER	1,2,3	0	0.691	0.013
		1	0.292	0.01
		2	0.013	0.01
		3	0.004	0.011
SER	1,2,3	0	0.685	0.011
		1	0.3	0.011
		2	0.015	0.011
		3	0	0.011
SER	2,3	0	0.714	0.019
		1	0.274	0.016
		2	0.012	0.019
SER	2,3	0	0.719	0.011
		1	0.275	0.011
		2	0.006	0.011
SER	1,2	0	0.934	0.013
		1	0.064	0.013
		2	0.002	0.013
THR	2,3,4	0	0.475	0.02
		1	0.431	0.023
		2	0.107	0.02
		3	-0.013	0.024
ASP	1,2,3,4	0	0.374	0.01
		1	0.455	0.011
		2	0.162	0.01
		3	0.017	0.01
		4	-0.008	0.01
ASP	1,2,3,4	0	0.379	0.01
		1	0.436	0.01
		2	0.164	0.01
		3	0.022	0.01
		4	-0.001	0.01
ASP	2,3,4	0	0.44	0.01
		1	0.439	0.01
		2	0.114	0.01
		3	0.006	0.01
ASP	1,2	0	0.634	0.013
		1	0.337	0.013
		2	0.028	0.013
GLU	1,2,3,4,5	0	0.271	0.012
		1	0.422	0.012
		2	0.244	0.012
		3	0.058	0.012
		4	0.004	0.012
		5	0	0.012
GLU	1,2,3,4,5	0	0.259	0.01
		1	0.42	0.01
		2	0.24	0.01

		3	0.061	0.01
		4	0.012	0.01
		5	0.008	0.01
GLU	1,2,3,4,5	0	0.263	0.01
		1	0.425	0.01
		2	0.249	0.01
		3	0.06	0.01
		4	0.005	0.01
		5	-0.001	0.01
GLU	2,3,4,5	0	0.302	0.01
		1	0.442	0.01
		2	0.211	0.01
		3	0.035	0.01
		4	0.01	0.01
GLU	1,2,3,4,5	0	0.281	0.013
		1	0.44	0.018
		2	0.245	0.013
		3	0.046	0.013
		4	-0.006	0.013
		5	-0.007	0.014
GLU	1,2,3,4,5	0	0.267	0.01
		1	0.429	0.01
		2	0.246	0.01
		3	0.056	0.01
		4	0.004	0.01
		5	-0.002	0.01
GLU	1,2,3,4,5	0	0.269	0.011
		1	0.428	0.011
		2	0.242	0.011
		3	0.056	0.011
		4	0.005	0.011
		5	0	0.011
GABA	1,2,3,4	0	0.31	0.019
		1	0.445	0.019
		2	0.216	0.019
		3	0.031	0.019
		4	-0.001	0.019
ALA	1,2,3	0	0.583	0.01
		1	0.391	0.01
		2	0.024	0.01
		3	0.001	0.01
ALA	2,3	0	0.602	0.011
		1	0.389	0.011
		2	0.009	0.011
GLY	1,2	0	0.899	0.011
		1	0.097	0.011
		2	0.004	0.011
GLY	2	0	0.978	0.011
		1	0.022	0.011
VAL	1,2,3,4,5	0	0.368	0.01
		1	0.448	0.01
		2	0.164	0.01
		3	0.02	0.01

		4	0.003	0.01
		5	-0.003	0.01
VAL	2,3,4,5	0	0.371	0.029
		1	0.441	0.029
		2	0.158	0.029
		3	0.029	0.029
		4	0.001	0.029
LEU	2,3,4,5,6	0	0.265	0.011
		1	0.412	0.011
		2	0.257	0.011
		3	0.066	0.011
		4	0.005	0.011
		5	-0.004	0.011
MET	2,3,4,5	0	0.384	0.019
		1	0.425	0.024
		2	0.174	0.018
		3	0.025	0.021
		4	-0.01	0.023
SER	1,2,3	0	0.684	0.012
		1	0.305	0.01
		2	0.014	0.01
		3	-0.003	0.011
SER	1,2,3	0	0.68	0.011
		1	0.303	0.011
		2	0.017	0.011
		3	0	0.011
SER	2,3	0	0.712	0.01
		1	0.281	0.01
		2	0.007	0.01
SER	2,3	0	0.714	0.011
		1	0.281	0.011
		2	0.005	0.011
SER	1,2	0	0.943	0.013
		1	0.061	0.013
		2	-0.003	0.013
THR	2,3,4	0	0.478	0.024
		1	0.389	0.026
		2	0.144	0.023
		3	-0.011	0.029
ASP	1,2,3,4	0	0.39	0.01
		1	0.425	0.01
		2	0.166	0.01
		3	0.021	0.01
		4	-0.001	0.01
ASP	2,3,4	0	0.457	0.01
		1	0.426	0.01
		2	0.113	0.01
		3	0.004	0.01
ASP	1,2	0	0.649	0.013
		1	0.329	0.013
		2	0.022	0.013
GLU	1,2,3,4,5	0	0.261	0.01
		1	0.442	0.01

		2	0.247	0.01
		3	0.051	0.01
		4	0.003	0.01
		5	-0.004	0.01
GLU	1,2,3,4,5	0	0.265	0.01
		1	0.429	0.01
		2	0.243	0.01
		3	0.06	0.01
		4	0.003	0.01
		5	0	0.01
GLU	2,3,4,5	0	0.305	0.01
		1	0.45	0.01
		2	0.208	0.01
		3	0.031	0.01
		4	0.006	0.01
GLU	1,2,3,4,5	0	0.29	0.013
		1	0.443	0.019
		2	0.242	0.013
		3	0.045	0.013
		4	-0.009	0.014
		5	-0.01	0.015
GLU	1,2,3,4,5	0	0.275	0.01
		1	0.435	0.01
		2	0.237	0.01
		3	0.051	0.01
		4	0.003	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.278	0.011
		1	0.432	0.011
		2	0.233	0.011
		3	0.054	0.011
		4	0.003	0.011
		5	0.001	0.011
GABA	1,2,3,4	0	0.317	0.019
		1	0.431	0.019
		2	0.202	0.019
		3	0.04	0.019
		4	0.01	0.019
ALA_U	1,2,3	0	0.716	0.01
		1	0.091	0.01
		2	0.046	0.01
		3	0.147	0.01
ALA_U	2,3	0	0.759	0.011
		1	0.066	0.011
		2	0.176	0.011
GLY_U	1,2	0	0.721	0.011
		1	0.15	0.011
		2	0.128	0.011
GLY_U	2	0	0.796	0.011
		1	0.204	0.011
VAL_U	1,2,3,4,5	0	0.555	0.01
		1	0.142	0.01
		2	0.154	0.01

		3	0.122	0.01
		4	0.014	0.01
		5	0.012	0.01
VAL_U	1,2,3,4,5	0	0.547	0.01
		1	0.127	0.01
		2	0.16	0.01
		3	0.126	0.01
		4	0.019	0.01
		5	0.023	0.01
VAL_U	2,3,4,5	0	0.575	0.029
		1	0.109	0.029
		2	0.253	0.029
		3	0.035	0.029
		4	0.027	0.029
LEU_U	2,3,4,5,6	0	0.465	0.011
		1	0.2	0.011
		2	0.226	0.011
		3	0.072	0.011
		4	0.03	0.011
		5	0.007	0.011
MET_U	2,3,4,5	0	0.514	0.01
		1	0.281	0.01
		2	0.12	0.01
		3	0.074	0.01
		4	0.012	0.01
SER_U	1,2,3	0	0.66	0.01
		1	0.155	0.01
		2	0.083	0.01
		3	0.102	0.01
SER_U	1,2,3	0	0.663	0.011
		1	0.157	0.011
		2	0.077	0.011
		3	0.103	0.011
SER_U	2,3	0	0.708	0.01
		1	0.166	0.01
		2	0.125	0.01
SER_U	2,3	0	0.711	0.011
		1	0.166	0.011
		2	0.123	0.011
SER_U	1,2	0	0.738	0.013
		1	0.115	0.013
		2	0.147	0.013
THR_U	2,3,4	0	0.606	0.018
		1	0.229	0.014
		2	0.118	0.015
		3	0.047	0.016
ASP_U	1,2,3,4	0	0.544	0.011
		1	0.211	0.01
		2	0.134	0.01
		3	0.087	0.01
		4	0.024	0.01
ASP_U	1,2,3,4	0	0.553	0.01
		1	0.214	0.01

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            2     0.141 0.01
            3     0.074 0.01
            4     0.019 0.01
ASP_U 2,3,4 0     0.617 0.01
            1     0.213 0.01
            2     0.124 0.01
            3     0.046 0.01
ASP_U 1,2   0     0.715 0.013
            1     0.169 0.013
            2     0.116 0.013
GLU_U 1,2,3,4,5   0     0.476 0.012
            1     0.213 0.012
            2     0.199 0.012
            3     0.09  0.012
            4     0.012 0.012
            5     0.01  0.012
GLU_U 1,2,3,4,5   0     0.463 0.01
            1     0.208 0.01
            2     0.22  0.01
            3     0.079 0.01
            4     0.026 0.01
            5     0.004 0.01
GLU_U 1,2,3,4,5   0     0.459 0.01
            1     0.214 0.01
            2     0.212 0.01
            3     0.082 0.01
            4     0.024 0.01
            5     0.008 0.01
GLU_U 2,3,4,5     0     0.516 0.01
            1     0.223 0.01
            2     0.197 0.01
            3     0.049 0.01
            4     0.015 0.01
GLU_U 1,2,3,4,5   0     0.474 0.013
            1     0.203 0.013
            2     0.214 0.013
            3     0.081 0.013
            4     0.024 0.013
            5     0.005 0.013
GLU_U 1,2,3,4,5   0     0.462 0.01
            1     0.206 0.01
            2     0.214 0.01
            3     0.084 0.01
            4     0.025 0.01
            5     0.008 0.01
GLU_U 1,2,3,4,5   0     0.469 0.011
            1     0.206 0.011
            2     0.21  0.011
            3     0.083 0.011
            4     0.026 0.011
            5     0.007 0.011
GABA_U      1,2,3,4     0     0.527 0.019
            1     0.219 0.019
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            2     0.206 0.019
            3     0.04  0.019
            4     0.008 0.019
ALA_U 1,2,3 0     0.717 0.01
            1     0.089 0.01
            2     0.044 0.01
            3     0.151 0.01
ALA_U 2,3   0     0.758 0.011
            1     0.063 0.011
            2     0.179 0.011
GLY_U 1,2   0     0.72  0.011
            1     0.156 0.011
            2     0.125 0.011
GLY_U 2     0     0.798 0.011
            1     0.202 0.011
VAL_U 1,2,3,4,5   0     0.562 0.01
            1     0.126 0.01
            2     0.159 0.01
            3     0.115 0.01
            4     0.02  0.01
            5     0.018 0.01
VAL_U 1,2,3,4,5   0     0.55  0.01
            1     0.122 0.01
            2     0.16  0.01
            3     0.128 0.01
            4     0.017 0.01
            5     0.023 0.01
VAL_U 2,3,4,5     0     0.572 0.029
            1     0.11  0.029
            2     0.255 0.029
            3     0.035 0.029
            4     0.028 0.029
LEU_U 2,3,4,5,6   0     0.466 0.011
            1     0.197 0.011
            2     0.23  0.011
            3     0.071 0.011
            4     0.029 0.011
            5     0.007 0.011
MET_U 2,3,4,5     0     0.51  0.01
            1     0.281 0.01
            2     0.122 0.01
            3     0.073 0.01
            4     0.014 0.01
SER_U 1,2,3 0     0.665 0.01
            1     0.155 0.01
            2     0.076 0.01
            3     0.103 0.01
SER_U 1,2,3 0     0.66  0.011
            1     0.158 0.011
            2     0.077 0.011
            3     0.105 0.011
SER_U 2,3   0     0.709 0.01
            1     0.165 0.01
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	2	0.126	0.01
SER_U 2,3	0	0.712	0.011
	1	0.164	0.011
	2	0.124	0.011
SER_U 1,2	0	0.734	0.013
	1	0.114	0.013
	2	0.151	0.013
THR_U 2,3,4	0	0.622	0.01
	1	0.214	0.01
	2	0.119	0.01
	3	0.045	0.01
ASP_U 1,2,3,4	0	0.552	0.01
	1	0.215	0.01
	2	0.137	0.01
	3	0.078	0.01
	4	0.018	0.01
ASP_U 1,2,3,4	0	0.548	0.01
	1	0.214	0.01
	2	0.147	0.01
	3	0.074	0.01
	4	0.017	0.01
ASP_U 2,3,4	0	0.608	0.01
	1	0.225	0.01
	2	0.121	0.01
	3	0.045	0.01
ASP_U 1,2	0	0.718	0.013
	1	0.162	0.013
	2	0.12	0.013
GLU_U 1,2,3,4,5	0	0.476	0.012
	1	0.215	0.012
	2	0.212	0.012
	3	0.08	0.012
	4	0.019	0.012
	5	-0.001	0.012
GLU_U 1,2,3,4,5	0	0.46	0.01
	1	0.209	0.01
	2	0.217	0.01
	3	0.083	0.01
	4	0.023	0.01
	5	0.008	0.01
GLU_U 1,2,3,4,5	0	0.461	0.01
	1	0.212	0.01
	2	0.21	0.01
	3	0.084	0.01
	4	0.025	0.01
	5	0.007	0.01
GLU_U 2,3,4,5	0	0.511	0.01
	1	0.223	0.01
	2	0.197	0.01
	3	0.055	0.01
	4	0.015	0.01
GLU_U 1,2,3,4,5	0	0.479	0.013
	1	0.201	0.013

		2	0.214	0.013
		3	0.079	0.013
		4	0.025	0.013
		5	0.002	0.013
GLU_U	1,2,3,4,5	0	0.46	0.01
		1	0.205	0.01
		2	0.216	0.01
		3	0.085	0.01
		4	0.026	0.01
		5	0.008	0.01
GLU_U	1,2,3,4,5	0	0.467	0.011
		1	0.202	0.011
		2	0.214	0.011
		3	0.084	0.011
		4	0.025	0.011
		5	0.009	0.011
GABA_U	1,2,3,4	0	0.52	0.019
		1	0.224	0.019
		2	0.197	0.019
		3	0.043	0.019
		4	0.015	0.019
ALA_U	1,2,3	0	0.713	0.01
		1	0.09	0.01
		2	0.045	0.01
		3	0.152	0.01
ALA_U	2,3	0	0.754	0.011
		1	0.065	0.011
		2	0.181	0.011
GLY_U	1,2	0	0.716	0.011
		1	0.16	0.011
		2	0.124	0.011
GLY_U	2	0	0.796	0.011
		1	0.204	0.011
VAL_U	1,2,3,4,5	0	0.553	0.01
		1	0.129	0.01
		2	0.16	0.01
		3	0.119	0.01
		4	0.017	0.01
		5	0.022	0.01
VAL_U	1,2,3,4,5	0	0.549	0.01
		1	0.125	0.01
		2	0.16	0.01
		3	0.127	0.01
		4	0.017	0.01
		5	0.023	0.01
VAL_U	2,3,4,5	0	0.571	0.029
		1	0.111	0.029
		2	0.256	0.029
		3	0.034	0.029
		4	0.028	0.029
LEU_U	2,3,4,5,6	0	0.468	0.011
		1	0.199	0.011
		2	0.229	0.011

	3	0.07	0.011	
	4	0.028	0.011	
	5	0.006	0.011	
MET_U 2,3,4,5		0	0.505	0.01
	1	0.287	0.01	
	2	0.122	0.01	
	3	0.074	0.01	
	4	0.012	0.01	
SER_U 1,2,3	0	0.66	0.01	
	1	0.158	0.01	
	2	0.076	0.01	
	3	0.106	0.01	
SER_U 1,2,3	0	0.659	0.011	
	1	0.158	0.011	
	2	0.077	0.011	
	3	0.105	0.011	
SER_U 2,3	0	0.706	0.01	
	1	0.168	0.01	
	2	0.126	0.01	
SER_U 2,3	0	0.708	0.011	
	1	0.167	0.011	
	2	0.125	0.011	
SER_U 1,2	0	0.731	0.013	
	1	0.117	0.013	
	2	0.152	0.013	
THR_U 2,3,4	0	0.621	0.01	
	1	0.218	0.01	
	2	0.116	0.01	
	3	0.045	0.01	
ASP_U 1,2,3,4		0	0.557	0.01
	1	0.21	0.01	
	2	0.161	0.01	
	3	0.063	0.01	
	4	0.009	0.01	
ASP_U 1,2,3,4		0	0.549	0.01
	1	0.213	0.01	
	2	0.145	0.01	
	3	0.074	0.01	
	4	0.019	0.01	
ASP_U 2,3,4	0	0.616	0.01	
	1	0.215	0.01	
	2	0.121	0.01	
	3	0.047	0.01	
ASP_U 1,2	0	0.711	0.013	
	1	0.167	0.013	
	2	0.122	0.013	
GLU_U 1,2,3,4,5		0	0.46	0.012
	1	0.229	0.012	
	2	0.207	0.012	
	3	0.073	0.012	
	4	0.027	0.012	
	5	0.004	0.012	
GLU_U 1,2,3,4,5		0	0.457	0.01

		1	0.213	0.01
		2	0.209	0.01
		3	0.087	0.01
		4	0.026	0.01
		5	0.009	0.01
GLU_U	1,2,3,4,5	0	0.458	0.01
		1	0.213	0.01
		2	0.212	0.01
		3	0.085	0.01
		4	0.024	0.01
		5	0.008	0.01
GLU_U	2,3,4,5	0	0.511	0.01
		1	0.222	0.01
		2	0.197	0.01
		3	0.055	0.01
		4	0.015	0.01
GLU_U	1,2,3,4,5	0	0.481	0.013
		1	0.204	0.013
		2	0.214	0.013
		3	0.079	0.013
		4	0.022	0.013
		5	0.001	0.013
GLU_U	1,2,3,4,5	0	0.459	0.01
		1	0.205	0.01
		2	0.216	0.01
		3	0.086	0.01
		4	0.026	0.01
		5	0.008	0.01
GLU_U	1,2,3,4,5	0	0.464	0.011
		1	0.204	0.011
		2	0.214	0.011
		3	0.085	0.011
		4	0.025	0.011
		5	0.009	0.011
GABA_U	1,2,3,4	0	0.522	0.019
		1	0.223	0.019
		2	0.197	0.019
		3	0.046	0.019
		4	0.012	0.019
FUM	1,2,3,4	0	0.365	0.017
		1	0.391	0.017
		2	0.187	0.017
		3	0.039	0.017
		4	0.018	0.017
OAA	1,2,3,4	0	0.363	0.01
		1	0.439	0.01
		2	0.172	0.01
		3	0.025	0.01
		4	0.001	0.01
CIT	1,2,3,4,5,6	0	0.222	0.01
		1	0.403	0.01
		2	0.278	0.01
		3	0.085	0.01

		4	0.013	0.01
		5	-0.001	0.01
		6	-0.001	0.01
FUM	1,2,3,4	0	0.403	0.017
		1	0.4	0.017
		2	0.155	0.017
		3	0.035	0.017
		4	0.008	0.017
OAA	1,2,3,4	0	0.363	0.011
		1	0.438	0.011
		2	0.172	0.011
		3	0.027	0.011
		4	0	0.011
OAA	1,2,3,4	0	0.362	0.01
		1	0.442	0.01
		2	0.172	0.01
		3	0.024	0.01
		4	0.001	0.01
CIT	1,2,3,4,5,6	0	0.221	0.01
		1	0.404	0.01
		2	0.275	0.01
		3	0.09	0.01
		4	0.01	0.01
		5	0	0.01
		6	0	0.01
OAA	1,2,3,4	0	0.388	0.011
		1	0.406	0.013
		2	0.177	0.011
		3	0.037	0.011
		4	-0.008	0.012
OAA	1,2,3,4	0	0.372	0.01
		1	0.438	0.01
		2	0.167	0.01
		3	0.022	0.01
		4	0.001	0.01
CIT	1,2,3,4,5,6	0	0.228	0.01
		1	0.4	0.01
		2	0.28	0.01
		3	0.077	0.01
		4	0.016	0.01
		5	-0.001	0.01
		6	0	0.01
FUM_U	1,2,3,4	0	0.534	0.021
		1	0.207	0.017
		2	0.135	0.017
		3	0.097	0.017
		4	0.028	0.017
OAA_U	1,2,3,4	0	0.541	0.011
		1	0.224	0.011
		2	0.14	0.011
		3	0.074	0.011
		4	0.021	0.011
OAA_U	1,2,3,4	0	0.54	0.01

		1	0.221	0.01
		2	0.145	0.01
		3	0.075	0.01
		4	0.019	0.01
CIT_U	1,2,3,4,5,6	0	0.408	0.01
		1	0.215	0.01
		2	0.213	0.01
		3	0.106	0.01
		4	0.044	0.01
		5	0.012	0.01
		6	0.003	0.01
FUM_U	1,2,3,4	0	0.524	0.017
		1	0.213	0.017
		2	0.145	0.017
		3	0.09	0.017
		4	0.028	0.017
OAA_U	1,2,3,4	0	0.536	0.011
		1	0.218	0.011
		2	0.15	0.011
		3	0.076	0.011
		4	0.019	0.011
OAA_U	1,2,3,4	0	0.538	0.01
		1	0.22	0.01
		2	0.149	0.01
		3	0.074	0.01
		4	0.019	0.01
CIT_U	1,2,3,4,5,6	0	0.405	0.01
		1	0.213	0.01
		2	0.217	0.01
		3	0.106	0.01
		4	0.044	0.01
		5	0.012	0.01
		6	0.003	0.01
FUM_U	1,2,3,4	0	0.537	0.017
		1	0.203	0.017
		2	0.146	0.017
		3	0.086	0.017
		4	0.027	0.017
OAA_U	1,2,3,4	0	0.535	0.011
		1	0.225	0.011
		2	0.146	0.011
		3	0.075	0.011
		4	0.019	0.011
OAA_U	1,2,3,4	0	0.536	0.01
		1	0.222	0.01
		2	0.15	0.01
		3	0.074	0.01
		4	0.019	0.01
CIT_U	1,2,3,4,5,6	0	0.405	0.01
		1	0.215	0.01
		2	0.216	0.01
		3	0.104	0.01
		4	0.044	0.01

		5	0.012	0.01
		6	0.003	0.01
ALA	1,2,3	0	0.588	0.011
		1	0.387	0.011
		2	0.024	0.011
		3	0.001	0.011
ALA	2,3	0	0.605	0.011
		1	0.389	0.011
		2	0.006	0.011
GLYeff	1,2	0	0.903	0.013
		1	0.094	0.01
		2	0.003	0.01
GLYeff	1,2	0	0.906	0.01
		1	0.091	0.01
		2	0.002	0.01
GLYeff	2	0	0.966	0.01
		1	0.034	0.01
VAL	1,2,3,4,5	0	0.381	0.01
		1	0.466	0.01
		2	0.155	0.01
		3	0.01	0.01
		4	-0.009	0.01
		5	-0.003	0.01
VAL	1,2,3,4,5	0	0.355	0.01
		1	0.469	0.01
		2	0.167	0.01
		3	0.014	0.01
		4	-0.002	0.01
		5	-0.003	0.01
VAL	2,3,4,5	0	0.37	0.01
		1	0.467	0.011
		2	0.157	0.01
		3	0.008	0.01
		4	-0.003	0.01
VAL	2,3,4,5	0	0.383	0.024
		1	0.427	0.024
		2	0.16	0.024
		3	0.028	0.024
		4	0.002	0.024
LEU	1,2,3,4,5,6	0	0.222	0.02
		1	0.431	0.02
		2	0.267	0.02
		3	0.084	0.02
		4	0.003	0.02
		5	-0.006	0.02
		6	-0.001	0.02
LEU	2,3,4,5,6	0	0.253	0.017
		1	0.432	0.017
		2	0.252	0.017
		3	0.058	0.017
		4	0.004	0.017
		5	0.001	0.017
ILE	1,2,3,4,5,6	0	0.208	0.018

		1	0.45	0.018
		2	0.278	0.018
		3	0.079	0.018
		4	-0.005	0.018
		5	-0.011	0.018
		6	0.001	0.018
ILE	2,3,4,5,6	0	0.259	0.01
		1	0.447	0.01
		2	0.236	0.01
		3	0.055	0.01
		4	0.004	0.01
		5	-0.001	0.01
ILE	2,3,4,5,6	0	0.266	0.02
		1	0.44	0.02
		2	0.235	0.02
		3	0.053	0.02
		4	0.005	0.02
		5	0.001	0.02
GLU	2,3,4,5	0	0.342	0.019
		1	0.411	0.019
		2	0.203	0.019
		3	0.049	0.019
		4	-0.005	0.019
METeff	1,2,3,4,5	0	0.371	0.01
		1	0.401	0.01
		2	0.185	0.01
		3	0.039	0.01
		4	0	0.01
		5	0.004	0.01
METeff	2,3,4,5	0	0.416	0.013
		1	0.407	0.013
		2	0.151	0.013
		3	0.023	0.013
		4	0.003	0.013
METeff	2,3,4,5	0	0.413	0.011
		1	0.412	0.011
		2	0.153	0.011
		3	0.023	0.011
		4	0	0.011
SEReff	1,2,3	0	0.712	0.01
		1	0.28	0.01
		2	0.007	0.01
		3	0	0.01
SEReff	1,2,3	0	0.717	0.01
		1	0.279	0.01
		2	0.008	0.01
		3	-0.003	0.01
SEReff	2,3	0	0.743	0.01
		1	0.256	0.01
		2	0.001	0.01
SEReff	2,3	0	0.739	0.011
		1	0.257	0.011
		2	0.004	0.011

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SEReff      1,2   0     0.93  0.018
            1     0.066 0.018
            2     0.004 0.018
THR   1,2,3,4     0     0.357 0.01
            1     0.456 0.01
            2     0.168 0.01
            3     0.02  0.01
            4     0     0.01
THR   2,3,4 0     0.425 0.01
            1     0.455 0.01
            2     0.114 0.01
            3     0.006 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.277 0.015
            1     0.431 0.015
            2     0.226 0.015
            3     0.058 0.015
            4     0.006 0.015
            5     0.002 0.015
            6     0     0.015
            7     -0.001      0.015
            8     0     0.015
            9     0     0.015
PHE_TYR     2,3,4,5,6,7,8,9   0     0.281 0.018
            1     0.439 0.018
            2     0.223 0.018
            3     0.053 0.018
            4     0.004 0.018
            5     0.001 0.018
            6     0     0.018
            7     -0.001      0.018
            8     0     0.018
PHE_TYR     2,3,4,5,6,7,8,9   0     0.274 0.019
            1     0.442 0.019
            2     0.231 0.019
            3     0.052 0.019
            4     0.005 0.019
            5     0     0.019
            6     -0.001      0.019
            7     -0.001      0.019
            8     -0.001      0.019
PHE_TYR     1,2   0     0.955 0.01
            1     0.046 0.01
            2     0     0.01
ASP   1,2,3,4     0     0.378 0.011
            1     0.433 0.011
            2     0.167 0.011
            3     0.018 0.011
            4     0.005 0.011
ASP   1,2,3,4     0     0.367 0.011
            1     0.45  0.011
            2     0.159 0.011
            3     0.024 0.011
            4     0.001 0.011
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ASP	2,3,4	0	0.434	0.01
		1	0.442	0.01
		2	0.115	0.01
		3	0.01	0.01
ASP	2,3,4	0	0.434	0.018
		1	0.436	0.018
		2	0.117	0.018
		3	0.013	0.018
ASP	1,2	0	0.628	0.011
		1	0.338	0.011
		2	0.034	0.011
CYS	1,2,3	0	0.716	0.018
		1	0.308	0.018
		2	-0.012	0.018
		3	-0.012	0.018
CYS	2,3	0	0.735	0.013
		1	0.265	0.01
		2	0	0.013
GLU	1,2,3,4,5	0	0.267	0.01
		1	0.434	0.01
		2	0.239	0.01
		3	0.057	0.01
		4	0.003	0.01
		5	0	0.01
GLU	1,2,3,4,5	0	0.267	0.011
		1	0.435	0.011
		2	0.24	0.011
		3	0.054	0.011
		4	0.004	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.309	0.011
		1	0.459	0.011
		2	0.206	0.011
		3	0.028	0.011
		4	-0.002	0.011
LYS	1,2,3,4,5,6	0	0.237	0.01
		1	0.44	0.01
		2	0.253	0.01
		3	0.073	0.01
		4	0.006	0.01
		5	-0.005	0.01
		6	-0.004	0.01
LYS	1,2,3,4,5,6	0	0.237	0.01
		1	0.439	0.01
		2	0.261	0.01
		3	0.07	0.01
		4	0.002	0.01
		5	-0.002	0.01
		6	-0.007	0.01
LYS	2,3,4,5,6	0	0.27	0.011
		1	0.456	0.016
		2	0.242	0.011
		3	0.045	0.011

	4	-0.001	0.012	
	5	-0.012	0.013	
HISeff	1,2,3,4,5,6	0	0.431	0.013
	1	0.402	0.013	
	2	0.135	0.013	
	3	0.037	0.013	
	4	0	0.013	
	5	-0.003	0.013	
	6	-0.001	0.013	
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.281	0.01
	1	0.419	0.01	
	2	0.247	0.01	
	3	0.055	0.01	
	4	0.006	0.01	
	5	-0.006	0.01	
	6	-0.004	0.01	
	7	0.001	0.01	
	8	0	0.01	
	9	0	0.01	
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.28	0.023
	1	0.427	0.023	
	2	0.228	0.023	
	3	0.05	0.023	
	4	0.006	0.023	
	5	0.001	0.023	
	6	0.002	0.023	
	7	-0.001	0.023	
	8	0.003	0.023	
	9	0.003	0.023	
PHE_TYR	2,3,4,5,6,7,8,9	0	0.294	0.01
	1	0.439	0.01	
	2	0.22	0.01	
	3	0.052	0.01	
	4	0.002	0.01	
	5	-0.001	0.01	
	6	-0.002	0.01	
	7	-0.003	0.01	
	8	-0.001	0.01	
PHE_TYR	2,3,4,5,6,7,8,9	0	0.294	0.013
	1	0.458	0.02	
	2	0.228	0.011	
	3	0.054	0.01	
	4	-0.001	0.01	
	5	-0.007	0.01	
	6	-0.007	0.01	
	7	-0.009	0.011	
	8	-0.01	0.011	
PHE_TYR	1,2	0	0.952	0.01
	1	0.047	0.01	
	2	0.001	0.01	
GLU	1,2,3,4,5	0	0.281	0.01
	1	0.429	0.01	
	2	0.238	0.01	

		3	0.054	0.01
		4	0.002	0.01
		5	-0.004	0.01
GLU	2,3,4,5	0	0.31	0.011
		1	0.458	0.011
		2	0.206	0.011
		3	0.027	0.011
		4	0	0.011
GLU	2,3,4,5	0	0.293	0.012
		1	0.474	0.016
		2	0.208	0.011
		3	0.03	0.014
		4	-0.005	0.015
ALA	1,2,3	0	0.587	0.011
		1	0.388	0.011
		2	0.023	0.011
		3	0.001	0.011
ALA	2,3	0	0.603	0.011
		1	0.389	0.011
		2	0.007	0.011
GLYeff	1,2	0	0.906	0.01
		1	0.093	0.01
		2	0.001	0.01
GLYeff	1,2	0	0.91	0.01
		1	0.088	0.01
		2	0.002	0.01
GLYeff	2	0	0.971	0.01
		1	0.029	0.01
VAL	1,2,3,4,5	0	0.374	0.01
		1	0.46	0.01
		2	0.164	0.01
		3	0.012	0.01
		4	-0.006	0.01
		5	-0.004	0.01
VAL	1,2,3,4,5	0	0.356	0.01
		1	0.469	0.01
		2	0.167	0.01
		3	0.014	0.01
		4	-0.003	0.01
		5	-0.003	0.01
VAL	2,3,4,5	0	0.37	0.013
		1	0.472	0.015
		2	0.154	0.011
		3	0.007	0.013
		4	-0.003	0.014
VAL	2,3,4,5	0	0.381	0.024
		1	0.43	0.024
		2	0.159	0.024
		3	0.028	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.231	0.02
		1	0.429	0.02
		2	0.263	0.02

		3	0.077	0.02
		4	0.007	0.02
		5	-0.006	0.02
		6	-0.001	0.02
LEU	2,3,4,5,6	0	0.253	0.017
		1	0.429	0.017
		2	0.254	0.017
		3	0.06	0.017
		4	0.004	0.017
		5	0	0.017
ILE	1,2,3,4,5,6	0	0.213	0.018
		1	0.435	0.018
		2	0.283	0.018
		3	0.077	0.018
		4	0.005	0.018
		5	-0.014	0.018
		6	0.001	0.018
ILE	2,3,4,5,6	0	0.274	0.017
		1	0.465	0.024
		2	0.243	0.016
		3	0.044	0.017
		4	-0.01	0.019
		5	-0.016	0.02
ILE	2,3,4,5,6	0	0.266	0.02
		1	0.438	0.02
		2	0.235	0.02
		3	0.054	0.02
		4	0.006	0.02
		5	0.001	0.02
GLU	2,3,4,5	0	0.338	0.019
		1	0.431	0.019
		2	0.192	0.019
		3	0.038	0.019
		4	0.001	0.019
METeff	1,2,3,4,5	0	0.373	0.01
		1	0.401	0.01
		2	0.186	0.01
		3	0.036	0.01
		4	0.002	0.01
		5	0.003	0.01
METeff	2,3,4,5	0	0.412	0.013
		1	0.411	0.013
		2	0.154	0.013
		3	0.022	0.013
		4	0.001	0.013
METeff	2,3,4,5	0	0.412	0.011
		1	0.414	0.011
		2	0.155	0.011
		3	0.022	0.011
		4	-0.002	0.011
SEReff	1,2,3	0	0.709	0.01
		1	0.276	0.01
		2	0.017	0.01

		3	-0.002	0.01
SEReff	1,2,3	0	0.718	0.01
		1	0.277	0.01
		2	0.01	0.01
		3	-0.005	0.01
SEReff	2,3	0	0.74	0.01
		1	0.258	0.01
		2	0.002	0.01
SEReff	2,3	0	0.739	0.011
		1	0.257	0.011
		2	0.004	0.011
SEReff	1,2	0	0.928	0.018
		1	0.066	0.018
		2	0.006	0.018
THR	1,2,3,4	0	0.362	0.01
		1	0.451	0.01
		2	0.166	0.01
		3	0.02	0.01
		4	0.001	0.01
THR	2,3,4	0	0.427	0.01
		1	0.44	0.01
		2	0.126	0.01
		3	0.007	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.272	0.015
		1	0.431	0.015
		2	0.233	0.015
		3	0.055	0.015
		4	0.007	0.015
		5	0.002	0.015
		6	0	0.015
		7	-0.001	0.015
		8	0	0.015
		9	0	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.279	0.018
		1	0.438	0.018
		2	0.228	0.018
		3	0.05	0.018
		4	0.005	0.018
		5	0	0.018
		6	0	0.018
		7	0	0.018
		8	0	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.275	0.019
		1	0.441	0.019
		2	0.231	0.019
		3	0.052	0.019
		4	0.005	0.019
		5	0	0.019
		6	-0.001	0.019
		7	-0.001	0.019
		8	-0.001	0.019
PHE_TYR	1,2	0	0.952	0.01
		1	0.045	0.01

		2	0.002	0.01
ASP	1,2,3,4	0	0.377	0.011
		1	0.442	0.011
		2	0.165	0.011
		3	0.016	0.011
		4	0.001	0.011
ASP	1,2,3,4	0	0.37	0.011
		1	0.446	0.011
		2	0.163	0.011
		3	0.02	0.011
		4	0.001	0.011
ASP	2,3,4	0	0.434	0.01
		1	0.44	0.01
		2	0.118	0.01
		3	0.007	0.01
ASP	2,3,4	0	0.437	0.018
		1	0.436	0.018
		2	0.114	0.018
		3	0.013	0.018
ASP	1,2	0	0.627	0.011
		1	0.34	0.011
		2	0.033	0.011
CYS	1,2,3	0	0.718	0.023
		1	0.291	0.018
		2	-0.016	0.018
		3	0.007	0.018
CYS	2,3	0	0.722	0.015
		1	0.266	0.012
		2	0.012	0.015
GLU	1,2,3,4,5	0	0.277	0.01
		1	0.429	0.01
		2	0.232	0.01
		3	0.056	0.01
		4	0.005	0.01
		5	0.001	0.01
GLU	1,2,3,4,5	0	0.267	0.011
		1	0.435	0.011
		2	0.239	0.011
		3	0.056	0.011
		4	0.003	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.308	0.011
		1	0.461	0.011
		2	0.204	0.011
		3	0.029	0.011
		4	-0.002	0.011
LYS	1,2,3,4,5,6	0	0.238	0.01
		1	0.432	0.01
		2	0.256	0.01
		3	0.066	0.01
		4	0.009	0.01
		5	-0.001	0.01
		6	0	0.01

```
LYS	2,3,4,5,6	0	0.267	0.01
	1	0.451	0.013
	2	0.245	0.01
	3	0.048	0.01
	4	-0.002	0.01
	5	-0.01	0.011
HISeff	1,2,3,4,5,6	0	0.422	0.013
	1	0.398	0.013
	2	0.149	0.013
	3	0.024	0.013
	4	0.003	0.013
	5	0.002	0.013
	6	0.001	0.013
HISeff	2,3,4,5,6	0	0.539	0.023
	1	0.362	0.023
	2	0.076	0.023
	3	0.028	0.023
	4	0.003	0.023
	5	-0.007	0.023
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.277	0.01
	1	0.426	0.01
	2	0.241	0.01
	3	0.053	0.01
	4	0.007	0.01
	5	-0.003	0.01
	6	-0.002	0.01
	7	0	0.01
	8	0	0.01
	9	0	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.286	0.023
	1	0.423	0.023
	2	0.226	0.023
	3	0.053	0.023
	4	0.009	0.023
	5	-0.001	0.023
	6	0.001	0.023
	7	-0.001	0.023
	8	0.003	0.023
	9	0.003	0.023
PHE_TYR	2,3,4,5,6,7,8,9	0	0.292	0.01
	1	0.43	0.01
	2	0.223	0.01
	3	0.048	0.01
	4	0.005	0.01
	5	0	0.01
	6	0.001	0.01
	7	-0.001	0.01
	8	0.004	0.01
PHE_TYR	2,3,4,5,6,7,8,9	0	0.29	0.01
	1	0.445	0.01
	2	0.222	0.01
	3	0.053	0.01
	4	0.004	0.01
```

```
            5     -0.001      0.01
            6     -0.004      0.01
            7     -0.004      0.01
            8     -0.004      0.01
PHE_TYR     1,2   0     0.953 0.01
            1     0.046 0.01
            2     0.002 0.01
GLU   1,2,3,4,5   0     0.287 0.01
            1     0.425 0.01
            2     0.231 0.01
            3     0.056 0.01
            4     0.002 0.01
            5     -0.001      0.01
GLU   2,3,4,5     0     0.308 0.011
            1     0.46  0.011
            2     0.203 0.011
            3     0.029 0.011
            4     0     0.011
GLU   2,3,4,5     0     0.295 0.012
            1     0.474 0.016
            2     0.211 0.011
            3     0.026 0.014
            4     -0.004      0.015
ALA   1,2,3 0     0.588 0.011
            1     0.389 0.011
            2     0.021 0.011
            3     0.001 0.011
ALA   2,3   0     0.606 0.011
            1     0.386 0.011
            2     0.008 0.011
GLYeff      1,2   0     0.889 0.014
            1     0.104 0.01
            2     0.007 0.011
GLYeff      1,2   0     0.903 0.01
            1     0.095 0.01
            2     0.002 0.01
GLYeff      2     0     0.969 0.01
            1     0.031 0.01
VAL   1,2,3,4,5   0     0.382 0.01
            1     0.453 0.01
            2     0.159 0.01
            3     0.015 0.01
            4     -0.004      0.01
            5     -0.004      0.01
VAL   1,2,3,4,5   0     0.358 0.01
            1     0.468 0.01
            2     0.166 0.01
            3     0.014 0.01
            4     -0.003      0.01
            5     -0.003      0.01
VAL   2,3,4,5     0     0.372 0.012
            1     0.47  0.014
            2     0.156 0.01
```

		3	0.006	0.012
		4	-0.004	0.013
VAL	2,3,4,5	0	0.384	0.024
		1	0.428	0.024
		2	0.158	0.024
		3	0.028	0.024
		4	0.002	0.024
LEU	1,2,3,4,5,6	0	0.226	0.02
		1	0.433	0.02
		2	0.264	0.02
		3	0.076	0.02
		4	0.005	0.02
		5	-0.002	0.02
		6	-0.002	0.02
LEU	2,3,4,5,6	0	0.258	0.017
		1	0.429	0.017
		2	0.251	0.017
		3	0.058	0.017
		4	0.004	0.017
		5	0	0.017
ILE	1,2,3,4,5,6	0	0.22	0.018
		1	0.45	0.018
		2	0.264	0.018
		3	0.069	0.018
		4	0.007	0.018
		5	-0.01	0.018
		6	0	0.018
ILE	2,3,4,5,6	0	0.272	0.01
		1	0.449	0.01
		2	0.235	0.01
		3	0.05	0.01
		4	0	0.01
		5	-0.006	0.01
ILE	2,3,4,5,6	0	0.273	0.02
		1	0.438	0.02
		2	0.231	0.02
		3	0.052	0.02
		4	0.005	0.02
		5	0.001	0.02
GLU	2,3,4,5	0	0.34	0.019
		1	0.433	0.019
		2	0.193	0.019
		3	0.032	0.019
		4	0.002	0.019
METeff	1,2,3,4,5	0	0.377	0.01
		1	0.405	0.01
		2	0.174	0.01
		3	0.039	0.01
		4	0.002	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.412	0.013
		1	0.408	0.013
		2	0.155	0.013

```
            3     0.024 0.013
            4     0.002 0.013
METeff      2,3,4,5     0     0.412 0.011
            1     0.411 0.011
            2     0.154 0.011
            3     0.023 0.011
            4     0     0.011
SEReff      1,2,3 0     0.705 0.01
            1     0.275 0.01
            2     0.014 0.01
            3     0.005 0.01
SEReff      1,2,3 0     0.71  0.01
            1     0.283 0.01
            2     0.01  0.01
            3     -0.003      0.01
SEReff      2,3   0     0.74  0.01
            1     0.26  0.01
            2     0     0.01
SEReff      2,3   0     0.738 0.011
            1     0.258 0.011
            2     0.004 0.011
SEReff      1,2   0     0.93  0.018
            1     0.065 0.018
            2     0.004 0.018
THR   1,2,3,4     0     0.37  0.01
            1     0.449 0.01
            2     0.155 0.01
            3     0.029 0.01
            4     -0.002      0.01
THR   2,3,4 0     0.444 0.01
            1     0.436 0.01
            2     0.111 0.01
            3     0.009 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.275 0.015
            1     0.428 0.015
            2     0.234 0.015
            3     0.055 0.015
            4     0.006 0.015
            5     0.001 0.015
            6     0.001 0.015
            7     -0.001      0.015
            8     0     0.015
            9     0     0.015
PHE_TYR     2,3,4,5,6,7,8,9   0     0.284 0.018
            1     0.432 0.018
            2     0.228 0.018
            3     0.052 0.018
            4     0.004 0.018
            5     0     0.018
            6     0     0.018
            7     0     0.018
            8     0     0.018
PHE_TYR     2,3,4,5,6,7,8,9   0     0.276 0.019
```

		1	0.438	0.019
		2	0.231	0.019
		3	0.052	0.019
		4	0.005	0.019
		5	-0.001	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.956	0.01
		1	0.044	0.01
		2	0.001	0.01
ASP	1,2,3,4	0	0.38	0.011
		1	0.446	0.011
		2	0.164	0.011
		3	0.016	0.011
		4	-0.006	0.011
ASP	1,2,3,4	0	0.38	0.011
		1	0.443	0.011
		2	0.158	0.011
		3	0.02	0.011
		4	0	0.011
ASP	2,3,4	0	0.441	0.01
		1	0.436	0.01
		2	0.115	0.01
		3	0.008	0.01
ASP	2,3,4	0	0.444	0.018
		1	0.432	0.018
		2	0.112	0.018
		3	0.012	0.018
ASP	1,2	0	0.634	0.011
		1	0.332	0.011
		2	0.033	0.011
CYS	1,2,3	0	0.69	0.023
		1	0.307	0.018
		2	0.022	0.018
		3	-0.019	0.02
GLU	1,2,3,4,5	0	0.279	0.01
		1	0.43	0.01
		2	0.233	0.01
		3	0.054	0.01
		4	0.005	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.275	0.011
		1	0.436	0.011
		2	0.234	0.011
		3	0.052	0.011
		4	0.004	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.316	0.011
		1	0.458	0.011
		2	0.201	0.011
		3	0.026	0.011
		4	-0.001	0.011

```
LYS	1,2,3,4,5,6	0	0.236	0.01
		1	0.424	0.01
		2	0.267	0.01
		3	0.067	0.01
		4	0.01	0.01
		5	-0.002	0.01
		6	-0.001	0.01
LYS	1,2,3,4,5,6	0	0.242	0.01
		1	0.447	0.011
		2	0.258	0.01
		3	0.063	0.01
		4	0.005	0.01
		5	-0.007	0.01
		6	-0.008	0.01
LYS	2,3,4,5,6	0	0.265	0.01
		1	0.45	0.01
		2	0.24	0.01
		3	0.048	0.01
		4	0.001	0.01
		5	-0.005	0.01
ARGeff	1,2,3,4,5,6	0	0.288	0.01
		1	0.404	0.011
		2	0.238	0.01
		3	0.072	0.01
		4	0.013	0.01
		5	-0.006	0.01
		6	-0.01	0.01
HISeff	1,2,3,4,5,6	0	0.43	0.013
		1	0.383	0.013
		2	0.159	0.013
		3	0.023	0.013
		4	0.005	0.013
		5	-0.002	0.013
		6	0.002	0.013
HISeff	2,3,4,5,6	0	0.551	0.023
		1	0.352	0.023
		2	0.088	0.023
		3	0.022	0.023
		4	-0.002	0.023
		5	-0.011	0.023
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.262	0.01
		1	0.454	0.01
		2	0.237	0.01
		3	0.055	0.01
		4	0.005	0.01
		5	-0.003	0.01
		6	-0.006	0.01
		7	0	0.01
		8	-0.001	0.01
		9	-0.002	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.281	0.023
		1	0.427	0.023
		2	0.23	0.023
```

```
            3     0.048 0.023
            4     0.008 0.023
            5     0     0.023
            6     0.001 0.023
            7     -0.001      0.023
            8     0.003 0.023
            9     0.002 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.297 0.01
            1     0.431 0.01
            2     0.231 0.01
            3     0.043 0.01
            4     0.003 0.01
            5     -0.001      0.01
            6     0     0.01
            7     -0.003      0.01
            8     -0.001      0.01
PHE_TYR     2,3,4,5,6,7,8,9   0     0.29  0.01
            1     0.449 0.015
            2     0.231 0.01
            3     0.054 0.01
            4     0.002 0.01
            5     -0.006      0.01
            6     -0.006      0.01
            7     -0.007      0.01
            8     -0.008      0.01
PHE_TYR     1,2   0     0.955 0.01
            1     0.045 0.01
            2     0     0.01
GLU   1,2,3,4,5   0     0.291 0.01
            1     0.429 0.01
            2     0.235 0.01
            3     0.048 0.01
            4     0     0.01
            5     -0.003      0.01
GLU   2,3,4,5     0     0.32  0.011
            1     0.452 0.011
            2     0.198 0.011
            3     0.028 0.011
            4     0.001 0.011
GLU   2,3,4,5     0     0.302 0.01
            1     0.471 0.013
            2     0.205 0.01
            3     0.025 0.011
            4     -0.004      0.012
ALA_U 1,2,3 0     0.726 0.011
            1     0.077 0.011
            2     0.038 0.011
            3     0.158 0.011
ALA_U 2,3   0     0.762 0.011
            1     0.055 0.011
            2     0.183 0.011
GLYeff_U    1,2   0     0.734 0.01
            1     0.136 0.01
```

```
            2     0.129 0.01
GLYeff_U    1,2   0     0.737 0.01
            1     0.134 0.01
            2     0.129 0.01
GLYeff_U    2     0     0.803 0.01
            1     0.197 0.01
VAL_U 1,2,3,4,5   0     0.536 0.01
            1     0.126 0.01
            2     0.173 0.01
            3     0.127 0.01
            4     0.013 0.01
            5     0.025 0.01
VAL_U 1,2,3,4,5   0     0.542 0.01
            1     0.119 0.01
            2     0.166 0.01
            3     0.133 0.01
            4     0.016 0.01
            5     0.024 0.01
VAL_U 2,3,4,5     0     0.571 0.01
            1     0.108 0.01
            2     0.269 0.01
            3     0.023 0.01
            4     0.028 0.01
VAL_U 2,3,4,5     0     0.584 0.024
            1     0.105 0.024
            2     0.269 0.024
            3     0.011 0.024
            4     0.032 0.024
LEU_U 1,2,3,4,5,6 0     0.428 0.02
            1     0.128 0.02
            2     0.308 0.02
            3     0.062 0.02
            4     0.065 0.02
            5     0.004 0.02
            6     0.004 0.02
LEU_U 2,3,4,5,6   0     0.462 0.017
            1     0.194 0.017
            2     0.235 0.017
            3     0.073 0.017
            4     0.029 0.017
            5     0.006 0.017
ILE_U 1,2,3,4,5,6 0     0.394 0.018
            1     0.213 0.018
            2     0.232 0.018
            3     0.1   0.018
            4     0.045 0.018
            5     0.015 0.018
            6     0.001 0.018
ILE_U 2,3,4,5,6   0     0.453 0.01
            1     0.212 0.01
            2     0.222 0.01
            3     0.082 0.01
            4     0.023 0.01
```

```
            5      0.007 0.01
ILE_U 2,3,4,5,6    0      0.461 0.02
            1      0.21   0.02
            2      0.218 0.02
            3      0.08   0.02
            4      0.024 0.02
            5      0.008 0.02
GLU_U 2,3,4,5      0      0.512 0.019
            1      0.231 0.019
            2      0.19   0.019
            3      0.047 0.019
            4      0.02   0.019
METeff_U    1,2,3,4,5    0      0.481 0.01
            1      0.263 0.01
            2      0.128 0.01
            3      0.086 0.01
            4      0.033 0.01
            5      0.01   0.01
METeff_U    2,3,4,5      0      0.546 0.013
            1      0.26   0.013
            2      0.108 0.013
            3      0.074 0.013
            4      0.013 0.013
METeff_U    2,3,4,5      0      0.553 0.011
            1      0.259 0.011
            2      0.108 0.011
            3      0.07   0.011
            4      0.009 0.011
SEReff_U    1,2,3 0      0.686 0.01
            1      0.149 0.01
            2      0.068 0.01
            3      0.098 0.01
SEReff_U    1,2,3 0      0.681 0.01
            1      0.146 0.01
            2      0.074 0.01
            3      0.099 0.01
SEReff_U    2,3    0      0.719 0.01
            1      0.161 0.01
            2      0.12   0.01
SEReff_U    2,3    0      0.718 0.011
            1      0.162 0.011
            2      0.12   0.011
SEReff_U    1,2    0      0.745 0.018
            1      0.102 0.018
            2      0.153 0.018
THR_U 1,2,3,4      0      0.541 0.01
            1      0.215 0.01
            2      0.148 0.01
            3      0.077 0.01
            4      0.018 0.01
THR_U 2,3,4 0      0.605 0.01
            1      0.224 0.01
            2      0.124 0.01
```

```
            3     0.047 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.356 0.015
            1     0.147 0.015
            2     0.135 0.015
            3     0.177 0.015
            4     0.086 0.015
            5     0.048 0.015
            6     0.031 0.015
            7     0.013 0.015
            8     0.004 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.374 0.018
            1     0.139 0.018
            2     0.212 0.018
            3     0.121 0.018
            4     0.084 0.018
            5     0.04  0.018
            6     0.023 0.018
            7     0.005 0.018
            8     0.003 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.369 0.019
            1     0.142 0.019
            2     0.215 0.019
            3     0.121 0.019
            4     0.082 0.019
            5     0.04  0.019
            6     0.022 0.019
            7     0.005 0.019
            8     0.003 0.019
PHE_TYR_U   1,2   0     0.753 0.01
            1     0.081 0.01
            2     0.166 0.01
ASP_U 1,2,3,4     0     0.554 0.011
            1     0.206 0.011
            2     0.147 0.011
            3     0.073 0.011
            4     0.021 0.011
ASP_U 1,2,3,4     0     0.542 0.011
            1     0.216 0.011
            2     0.148 0.011
            3     0.074 0.011
            4     0.019 0.011
ASP_U 2,3,4 0     0.605 0.01
            1     0.227 0.01
            2     0.121 0.01
            3     0.047 0.01
ASP_U 2,3,4 0     0.607 0.018
            1     0.222 0.018
            2     0.122 0.018
            3     0.05  0.018
ASP_U 1,2   0     0.718 0.011
            1     0.159 0.011
            2     0.123 0.011
```

```
CYS_U 1,2,3 0      0.684 0.018
            1      0.134 0.018
            2      0.072 0.018
            3      0.11  0.018
CYS_U 2,3   0      0.718 0.01
            1      0.156 0.01
            2      0.126 0.01
GLU_U 1,2,3,4,5    0      0.465 0.01
            1      0.205 0.01
            2      0.214 0.01
            3      0.083 0.01
            4      0.024 0.01
            5      0.009 0.01
GLU_U 1,2,3,4,5    0      0.469 0.011
            1      0.203 0.011
            2      0.215 0.011
            3      0.081 0.011
            4      0.024 0.011
            5      0.008 0.011
GLU_U 2,3,4,5      0      0.519 0.011
            1      0.221 0.011
            2      0.2   0.011
            3      0.047 0.011
            4      0.014 0.011
LYS_U 1,2,3,4,5,6 0      0.425 0.01
            1      0.209 0.01
            2      0.177 0.01
            3      0.121 0.01
            4      0.045 0.01
            5      0.015 0.01
            6      0.007 0.01
LYS_U 1,2,3,4,5,6 0      0.408 0.01
            1      0.216 0.01
            2      0.184 0.01
            3      0.128 0.01
            4      0.044 0.01
            5      0.016 0.01
            6      0.004 0.01
LYS_U 2,3,4,5,6    0      0.447 0.01
            1      0.218 0.01
            2      0.226 0.01
            3      0.08  0.01
            4      0.022 0.01
            5      0.007 0.01
ARGeff_U    1,2,3,4,5,6 0      0.414 0.01
            1      0.257 0.01
            2      0.195 0.01
            3      0.104 0.01
            4      0.03  0.01
            5      0.007 0.01
            6      -0.006      0.01
HISeff_U    1,2,3,4,5,6 0      0.463 0.013
            1      0.232 0.013
```

```
            2     0.113 0.013
            3     0.105 0.013
            4     0.045 0.013
            5     0.033 0.013
            6     0.009 0.013
HISeff_U    2,3,4,5,6   0     0.508 0.026
            1     0.231 0.019
            2     0.186 0.018
            3     0.075 0.018
            4     0.013 0.02
            5     -0.013      0.022
HISeff_U    2,3,4,5,6   0     0.469 0.023
            1     0.237 0.023
            2     0.173 0.023
            3     0.074 0.023
            4     0.038 0.023
            5     0.01  0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.348 0.01
            1     0.14  0.01
            2     0.14  0.01
            3     0.177 0.01
            4     0.093 0.01
            5     0.047 0.01
            6     0.033 0.01
            7     0.017 0.01
            8     0.004 0.01
            9     0.001 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.359 0.023
            1     0.144 0.023
            2     0.135 0.023
            3     0.172 0.023
            4     0.085 0.023
            5     0.046 0.023
            6     0.032 0.023
            7     0.018 0.023
            8     0.005 0.023
            9     0.004 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.375 0.01
            1     0.14  0.01
            2     0.207 0.01
            3     0.118 0.01
            4     0.082 0.01
            5     0.042 0.01
            6     0.024 0.01
            7     0.008 0.01
            8     0.006 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.371 0.01
            1     0.142 0.01
            2     0.217 0.01
            3     0.122 0.01
            4     0.083 0.01
            5     0.04  0.01
            6     0.022 0.01
```

		7	0.003	0.01
		8	0.001	0.01
PHE_TYR_U	1,2	0	0.753	0.01
		1	0.08	0.01
		2	0.167	0.01
GLU_U	1,2,3,4,5	0	0.465	0.01
		1	0.205	0.01
		2	0.211	0.01
		3	0.084	0.01
		4	0.028	0.01
		5	0.008	0.01
GLU_U	2,3,4,5	0	0.522	0.011
		1	0.22	0.011
		2	0.196	0.011
		3	0.046	0.011
		4	0.015	0.011
GLU_U	2,3,4,5	0	0.517	0.01
		1	0.227	0.01
		2	0.188	0.01
		3	0.052	0.01
		4	0.017	0.01
ALA_U	1,2,3	0	0.728	0.011
		1	0.077	0.011
		2	0.038	0.011
		3	0.158	0.011
ALA_U	2,3	0	0.763	0.011
		1	0.054	0.011
		2	0.183	0.011
VAL_U	1,2,3,4,5	0	0.529	0.01
		1	0.125	0.01
		2	0.175	0.01
		3	0.126	0.01
		4	0.025	0.01
		5	0.022	0.01
VAL_U	1,2,3,4,5	0	0.543	0.01
		1	0.117	0.01
		2	0.165	0.01
		3	0.134	0.01
		4	0.016	0.01
		5	0.024	0.01
VAL_U	2,3,4,5	0	0.573	0.01
		1	0.106	0.01
		2	0.269	0.01
		3	0.023	0.01
		4	0.028	0.01
VAL_U	2,3,4,5	0	0.578	0.024
		1	0.099	0.024
		2	0.259	0.024
		3	0.035	0.024
		4	0.028	0.024
LEU_U	1,2,3,4,5,6	0	0.424	0.02
		1	0.138	0.02
		2	0.306	0.02

		3	0.057	0.02
		4	0.065	0.02
		5	0.007	0.02
		6	0.005	0.02
LEU_U	2,3,4,5,6	0	0.461	0.017
		1	0.195	0.017
		2	0.235	0.017
		3	0.073	0.017
		4	0.029	0.017
		5	0.006	0.017
ILE_U	1,2,3,4,5,6	0	0.391	0.018
		1	0.218	0.018
		2	0.24	0.018
		3	0.096	0.018
		4	0.043	0.018
		5	0.013	0.018
		6	-0.001	0.018
ILE_U	2,3,4,5,6	0	0.458	0.01
		1	0.211	0.01
		2	0.221	0.01
		3	0.081	0.01
		4	0.023	0.01
		5	0.006	0.01
ILE_U	2,3,4,5,6	0	0.46	0.02
		1	0.207	0.02
		2	0.219	0.02
		3	0.082	0.02
		4	0.024	0.02
		5	0.008	0.02
GLU_U	2,3,4,5	0	0.53	0.019
		1	0.218	0.019
		2	0.191	0.019
		3	0.045	0.019
		4	0.016	0.019
METeff_U	1,2,3,4,5	0	0.479	0.01
		1	0.263	0.01
		2	0.132	0.01
		3	0.085	0.01
		4	0.034	0.01
		5	0.007	0.01
METeff_U	2,3,4,5	0	0.541	0.013
		1	0.261	0.013
		2	0.109	0.013
		3	0.075	0.013
		4	0.014	0.013
METeff_U	2,3,4,5	0	0.547	0.011
		1	0.264	0.011
		2	0.107	0.011
		3	0.071	0.011
		4	0.01	0.011
SEReff_U	1,2,3	0	0.693	0.01
		1	0.143	0.01
		2	0.066	0.01

```
            3     0.098 0.01
SEReff_U    1,2,3 0     0.688 0.01
            1     0.144 0.01
            2     0.073 0.01
            3     0.095 0.01
SEReff_U    2,3   0     0.726 0.01
            1     0.159 0.01
            2     0.115 0.01
SEReff_U    2,3   0     0.729 0.011
            1     0.156 0.011
            2     0.115 0.011
SEReff_U    1,2   0     0.755 0.018
            1     0.101 0.018
            2     0.144 0.018
THR_U 1,2,3,4     0     0.553 0.01
            1     0.203 0.01
            2     0.154 0.01
            3     0.073 0.01
            4     0.017 0.01
THR_U 2,3,4 0     0.604 0.01
            1     0.229 0.01
            2     0.128 0.01
            3     0.039 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.358 0.015
            1     0.146 0.015
            2     0.134 0.015
            3     0.177 0.015
            4     0.087 0.015
            5     0.047 0.015
            6     0.031 0.015
            7     0.012 0.015
            8     0.004 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.374 0.018
            1     0.141 0.018
            2     0.212 0.018
            3     0.12  0.018
            4     0.081 0.018
            5     0.041 0.018
            6     0.023 0.018
            7     0.005 0.018
            8     0.003 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.371 0.019
            1     0.142 0.019
            2     0.215 0.019
            3     0.122 0.019
            4     0.083 0.019
            5     0.04  0.019
            6     0.022 0.019
            7     0.004 0.019
            8     0.002 0.019
PHE_TYR_U   1,2   0     0.752 0.01
            1     0.081 0.01
```

```
            2     0.166 0.01
ASP_U 1,2,3,4     0     0.542 0.011
            1     0.213 0.011
            2     0.153 0.011
            3     0.073 0.011
            4     0.019 0.011
ASP_U 1,2,3,4     0     0.544 0.011
            1     0.214 0.011
            2     0.147 0.011
            3     0.076 0.011
            4     0.019 0.011
ASP_U 2,3,4 0     0.609 0.01
            1     0.222 0.01
            2     0.123 0.01
            3     0.046 0.01
ASP_U 2,3,4 0     0.607 0.018
            1     0.221 0.018
            2     0.122 0.018
            3     0.05  0.018
ASP_U 1,2   0     0.719 0.011
            1     0.16  0.011
            2     0.122 0.011
CYS_U 1,2,3 0     0.69  0.018
            1     0.14  0.018
            2     0.059 0.018
            3     0.11  0.018
CYS_U 2,3   0     0.723 0.011
            1     0.166 0.01
            2     0.111 0.01
GLU_U 1,2,3,4,5   0     0.467 0.01
            1     0.206 0.01
            2     0.211 0.01
            3     0.08  0.01
            4     0.026 0.01
            5     0.01  0.01
GLU_U 1,2,3,4,5   0     0.469 0.011
            1     0.201 0.011
            2     0.214 0.011
            3     0.083 0.011
            4     0.024 0.011
            5     0.008 0.011
GLU_U 2,3,4,5     0     0.522 0.011
            1     0.22  0.011
            2     0.2   0.011
            3     0.045 0.011
            4     0.013 0.011
LYS_U 1,2,3,4,5,6 0     0.425 0.01
            1     0.201 0.01
            2     0.182 0.01
            3     0.129 0.01
            4     0.043 0.01
            5     0.017 0.01
            6     0.002 0.01
```

```
LYS_U 1,2,3,4,5,6 0      0.416 0.01
            1     0.218 0.01
            2     0.187 0.01
            3     0.126 0.01
            4     0.04  0.01
            5     0.012 0.01
            6     0     0.01
LYS_U 2,3,4,5,6   0     0.45  0.01
            1     0.218 0.01
            2     0.223 0.01
            3     0.081 0.01
            4     0.022 0.01
            5     0.006 0.01
ARGeff_U    1,2,3,4,5,6 0     0.429 0.013
            1     0.264 0.013
            2     0.195 0.013
            3     0.111 0.013
            4     0.019 0.013
            5     -0.01 0.013
            6     -0.007      0.013
ARGeff_U    1,2,3,4,5,6 0     0.401 0.01
            1     0.259 0.01
            2     0.195 0.01
            3     0.102 0.01
            4     0.035 0.01
            5     0.01  0.01
            6     -0.001      0.01
HISeff_U    1,2,3,4,5,6 0     0.464 0.013
            1     0.229 0.013
            2     0.115 0.013
            3     0.105 0.013
            4     0.046 0.013
            5     0.032 0.013
            6     0.009 0.013
HISeff_U    2,3,4,5,6   0     0.466 0.023
            1     0.237 0.023
            2     0.179 0.023
            3     0.075 0.023
            4     0.034 0.023
            5     0.009 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.354 0.01
            1     0.139 0.01
            2     0.142 0.01
            3     0.186 0.01
            4     0.077 0.01
            5     0.053 0.01
            6     0.036 0.01
            7     0.01  0.01
            8     0.002 0.01
            9     0.001 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.363 0.023
            1     0.145 0.023
            2     0.134 0.023
```

```
            3     0.176 0.023
            4     0.085 0.023
            5     0.045 0.023
            6     0.031 0.023
            7     0.013 0.023
            8     0.005 0.023
            9     0.002 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.382 0.01
            1     0.139 0.01
            2     0.21  0.01
            3     0.115 0.01
            4     0.079 0.01
            5     0.042 0.01
            6     0.022 0.01
            7     0.005 0.01
            8     0.005 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.367 0.01
            1     0.142 0.01
            2     0.215 0.01
            3     0.119 0.01
            4     0.083 0.01
            5     0.045 0.01
            6     0.023 0.01
            7     0.006 0.01
            8     0.002 0.01
PHE_TYR_U   1,2   0     0.753 0.01
            1     0.08  0.01
            2     0.167 0.01
GLU_U 1,2,3,4,5   0     0.47  0.01
            1     0.196 0.01
            2     0.222 0.01
            3     0.08  0.01
            4     0.025 0.01
            5     0.007 0.01
GLU_U 2,3,4,5     0     0.522 0.011
            1     0.221 0.011
            2     0.197 0.011
            3     0.046 0.011
            4     0.014 0.011
GLU_U 2,3,4,5     0     0.518 0.021
            1     0.225 0.012
            2     0.205 0.012
            3     0.042 0.015
            4     0.01  0.016
ALA_U 1,2,3 0     0.723 0.011
            1     0.078 0.011
            2     0.039 0.011
            3     0.16  0.011
ALA_U 2,3   0     0.76  0.011
            1     0.056 0.011
            2     0.185 0.011
GLYeff_U    1,2   0     0.736 0.01
            1     0.142 0.01
```

```
            2     0.122 0.01
GLYeff_U    1,2   0     0.737 0.01
            1     0.139 0.01
            2     0.123 0.01
GLYeff_U    2     0     0.808 0.01
            1     0.192 0.01
VAL_U 1,2,3,4,5   0     0.539 0.012
            1     0.125 0.01
            2     0.176 0.01
            3     0.124 0.01
            4     0.015 0.01
            5     0.021 0.01
VAL_U 1,2,3,4,5   0     0.541 0.01
            1     0.119 0.01
            2     0.168 0.01
            3     0.132 0.01
            4     0.016 0.01
            5     0.024 0.01
VAL_U 2,3,4,5     0     0.573 0.011
            1     0.108 0.01
            2     0.267 0.01
            3     0.025 0.01
            4     0.027 0.01
VAL_U 2,3,4,5     0     0.575 0.024
            1     0.1   0.024
            2     0.26  0.024
            3     0.037 0.024
            4     0.028 0.024
LEU_U 1,2,3,4,5,6 0     0.427 0.02
            1     0.129 0.02
            2     0.309 0.02
            3     0.06  0.02
            4     0.066 0.02
            5     0.005 0.02
            6     0.004 0.02
LEU_U 2,3,4,5,6   0     0.459 0.017
            1     0.195 0.017
            2     0.236 0.017
            3     0.075 0.017
            4     0.029 0.017
            5     0.006 0.017
ILE_U 1,2,3,4,5,6 0     0.396 0.018
            1     0.203 0.018
            2     0.241 0.018
            3     0.101 0.018
            4     0.048 0.018
            5     0.011 0.018
            6     0     0.018
ILE_U 2,3,4,5,6   0     0.454 0.01
            1     0.215 0.01
            2     0.219 0.01
            3     0.08  0.01
            4     0.023 0.01
```

		5	0.008	0.01
ILE_U	2,3,4,5,6	0	0.457	0.02
		1	0.21	0.02
		2	0.218	0.02
		3	0.082	0.02
		4	0.024	0.02
		5	0.008	0.02
GLU_U	2,3,4,5	0	0.525	0.019
		1	0.227	0.019
		2	0.18	0.019
		3	0.049	0.019
		4	0.018	0.019
METeff_U	1,2,3,4,5	0	0.475	0.01
		1	0.266	0.01
		2	0.131	0.01
		3	0.083	0.01
		4	0.034	0.01
		5	0.009	0.01
METeff_U	2,3,4,5	0	0.545	0.013
		1	0.262	0.013
		2	0.109	0.013
		3	0.072	0.013
		4	0.012	0.013
METeff_U	2,3,4,5	0	0.544	0.011
		1	0.262	0.011
		2	0.111	0.011
		3	0.071	0.011
		4	0.012	0.011
SEReff_U	1,2,3	0	0.677	0.01
		1	0.147	0.01
		2	0.077	0.01
		3	0.099	0.01
SEReff_U	1,2,3	0	0.675	0.01
		1	0.148	0.01
		2	0.076	0.01
		3	0.101	0.01
SEReff_U	2,3	0	0.712	0.01
		1	0.165	0.01
		2	0.122	0.01
SEReff_U	2,3	0	0.719	0.011
		1	0.162	0.011
		2	0.12	0.011
SEReff_U	1,2	0	0.741	0.018
		1	0.108	0.018
		2	0.151	0.018
THR_U	1,2,3,4	0	0.539	0.01
		1	0.213	0.01
		2	0.152	0.01
		3	0.078	0.01
		4	0.019	0.01
THR_U	2,3,4	0	0.596	0.01
		1	0.235	0.01
		2	0.123	0.01

```
            3     0.045 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.354 0.015
            1     0.147 0.015
            2     0.135 0.015
            3     0.18  0.015
            4     0.086 0.015
            5     0.047 0.015
            6     0.031 0.015
            7     0.012 0.015
            8     0.004 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.372 0.018
            1     0.14  0.018
            2     0.213 0.018
            3     0.124 0.018
            4     0.081 0.018
            5     0.04  0.018
            6     0.023 0.018
            7     0.005 0.018
            8     0.003 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.365 0.019
            1     0.142 0.019
            2     0.216 0.019
            3     0.123 0.019
            4     0.082 0.019
            5     0.04  0.019
            6     0.023 0.019
            7     0.004 0.019
            8     0.003 0.019
PHE_TYR_U   1,2   0     0.752 0.01
            1     0.082 0.01
            2     0.166 0.01
ASP_U 1,2,3,4     0     0.545 0.011
            1     0.203 0.011
            2     0.155 0.011
            3     0.077 0.011
            4     0.02  0.011
ASP_U 1,2,3,4     0     0.541 0.011
            1     0.216 0.011
            2     0.149 0.011
            3     0.074 0.011
            4     0.02  0.011
ASP_U 2,3,4 0     0.603 0.01
            1     0.226 0.01
            2     0.125 0.01
            3     0.046 0.01
ASP_U 2,3,4 0     0.605 0.018
            1     0.223 0.018
            2     0.122 0.018
            3     0.05  0.018
ASP_U 1,2   0     0.716 0.011
            1     0.16  0.011
            2     0.124 0.011
```

CYS_U 1,2,3	0	0.649	0.018
	1	0.166	0.018
	2	0.093	0.018
	3	0.092	0.018
GLU_U 1,2,3,4,5	0	0.468	0.01
	1	0.203	0.01
	2	0.217	0.01
	3	0.084	0.01
	4	0.02	0.01
	5	0.008	0.01
GLU_U 1,2,3,4,5	0	0.467	0.011
	1	0.202	0.011
	2	0.215	0.011
	3	0.083	0.011
	4	0.024	0.011
	5	0.009	0.011
GLU_U 2,3,4,5	0	0.518	0.011
	1	0.221	0.011
	2	0.201	0.011
	3	0.046	0.011
	4	0.014	0.011
LYS_U 1,2,3,4,5,6	0	0.415	0.01
	1	0.21	0.01
	2	0.186	0.01
	3	0.12	0.01
	4	0.046	0.01
	5	0.02	0.01
	6	0.003	0.01
LYS_U 1,2,3,4,5,6	0	0.409	0.01
	1	0.212	0.01
	2	0.185	0.01
	3	0.128	0.01
	4	0.044	0.01
	5	0.016	0.01
	6	0.005	0.01
LYS_U 2,3,4,5,6	0	0.449	0.01
	1	0.219	0.01
	2	0.223	0.01
	3	0.081	0.01
	4	0.022	0.01
	5	0.005	0.01
ARGeff_U 1,2,3,4,5,6	0	0.441	0.013
	1	0.261	0.013
	2	0.192	0.013
	3	0.097	0.013
	4	0.026	0.013
	5	-0.01	0.013
	6	-0.007	0.013
ARGeff_U 1,2,3,4,5,6	0	0.415	0.011
	1	0.254	0.01
	2	0.198	0.01
	3	0.096	0.01
	4	0.037	0.01

	5	0.007	0.01	
	6	-0.007	0.01	
HISeff_U	1,2,3,4,5,6	0	0.459	0.013
	1	0.232	0.013	
	2	0.115	0.013	
	3	0.106	0.013	
	4	0.046	0.013	
	5	0.034	0.013	
	6	0.008	0.013	
HISeff_U	2,3,4,5,6	0	0.513	0.033
	1	0.233	0.023	
	2	0.187	0.022	
	3	0.059	0.023	
	4	0.019	0.025	
	5	-0.011	0.027	
HISeff_U	2,3,4,5,6	0	0.456	0.023
	1	0.242	0.023	
	2	0.173	0.023	
	3	0.078	0.023	
	4	0.037	0.023	
	5	0.014	0.023	
PHE_TYR_U	1,2,3,4,5,6,7,8,9	0	0.362	0.01
	1	0.142	0.01	
	2	0.14	0.01	
	3	0.177	0.01	
	4	0.084	0.01	
	5	0.053	0.01	
	6	0.033	0.01	
	7	0.011	0.01	
	8	0.002	0.01	
	9	-0.005	0.01	
PHE_TYR_U	1,2,3,4,5,6,7,8,9	0	0.361	0.023
	1	0.148	0.023	
	2	0.135	0.023	
	3	0.174	0.023	
	4	0.084	0.023	
	5	0.046	0.023	
	6	0.03	0.023	
	7	0.012	0.023	
	8	0.006	0.023	
	9	0.003	0.023	
PHE_TYR_U	2,3,4,5,6,7,8,9	0	0.381	0.01
	1	0.137	0.01	
	2	0.208	0.01	
	3	0.121	0.01	
	4	0.082	0.01	
	5	0.039	0.01	
	6	0.024	0.01	
	7	0.004	0.01	
	8	0.004	0.01	
PHE_TYR_U	2,3,4,5,6,7,8,9	0	0.366	0.01
	1	0.144	0.01	
	2	0.215	0.01	

		3	0.122	0.01
		4	0.083	0.01
		5	0.041	0.01
		6	0.023	0.01
		7	0.003	0.01
		8	0.002	0.01
PHE_TYR_U	1,2	0	0.754	0.01
		1	0.079	0.01
		2	0.167	0.01
GLU_U	1,2,3,4,5	0	0.474	0.01
		1	0.196	0.01
		2	0.216	0.01
		3	0.081	0.01
		4	0.024	0.01
		5	0.009	0.01
GLU_U	2,3,4,5	0	0.518	0.011
		1	0.221	0.011
		2	0.199	0.011
		3	0.047	0.011
		4	0.015	0.011
GLU_U	2,3,4,5	0	0.514	0.019
		1	0.223	0.011
		2	0.207	0.011
		3	0.044	0.013
		4	0.011	0.014
STA	1,2	0	0.362	0.01
		1	0.64	0.01
		2	-0.002	0.01
STA	3,4,5,6	0	0.745	0.015
		1	0.232	0.015
		2	0.022	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.361	0.01
		1	0.637	0.013
		2	0.002	0.013
STA	3,4,5,6	0	0.745	0.012
		1	0.236	0.012
		2	0.019	0.012
		3	-0.001	0.012
		4	0.001	0.012
STA	1,2	0	0.367	0.01
		1	0.635	0.01
		2	-0.001	0.01
STA	3,4,5,6	0	0.744	0.015
		1	0.235	0.015
		2	0.021	0.015
		3	0.001	0.015
		4	-0.001	0.015
STA	1,2	0	0.364	0.01
		1	0.636	0.012
		2	0	0.012
STA	3,4,5,6	0	0.747	0.012

		1	0.231	0.012
		2	0.021	0.012
		3	0.001	0.012
		4	0.001	0.012
STA	1,2	0	0.378	0.01
		1	0.625	0.01
		2	-0.003	0.01
STA	3,4,5,6	0	0.746	0.015
		1	0.234	0.015
		2	0.018	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.373	0.012
		1	0.624	0.017
		2	0.003	0.018
STA	3,4,5,6	0	0.751	0.012
		1	0.231	0.012
		2	0.015	0.012
		3	0.005	0.012
		4	-0.003	0.012
STA_U	1,2	0	0.748	0.019
		1	0.097	0.014
		2	0.155	0.013
STA_U	3,4,5,6	0	0.655	0.015
		1	0.139	0.015
		2	0.024	0.015
		3	0.085	0.015
		4	0.096	0.015
STA_U	1,2	0	0.748	0.028
		1	0.105	0.021
		2	0.147	0.02
STA_U	3,4,5,6	0	0.659	0.012
		1	0.137	0.012
		2	0.024	0.012
		3	0.084	0.012
		4	0.096	0.012
STA_U	1,2	0	0.746	0.02
		1	0.099	0.015
		2	0.155	0.014
STA_U	3,4,5,6	0	0.653	0.015
		1	0.139	0.015
		2	0.024	0.015
		3	0.087	0.015
		4	0.097	0.015
STA_U	1,2	0	0.744	0.029
		1	0.106	0.022
		2	0.151	0.021
STA_U	3,4,5,6	0	0.66	0.012
		1	0.137	0.012
		2	0.024	0.012
		3	0.084	0.012
		4	0.095	0.012
STA_U	1,2	0	0.749	0.018

		1	0.097	0.014
		2	0.154	0.013
STA_U	3,4,5,6	0	0.653	0.015
		1	0.139	0.015
		2	0.025	0.015
		3	0.086	0.015
		4	0.097	0.015
STA_U	1,2	0	0.753	0.029
		1	0.101	0.022
		2	0.146	0.021
STA_U	3,4,5,6	0	0.659	0.012
		1	0.136	0.012
		2	0.022	0.012
		3	0.087	0.012
		4	0.095	0.012
WALL	1,2	0	0.249	0.013
		1	0.746	0.02
		2	0.005	0.018
WALL	3,4,5,6	0	0.782	0.012
		1	0.202	0.012
		2	0.015	0.012
		3	0.001	0.012
		4	0.001	0.012
WALL	1,2	0	0.255	0.013
		1	0.741	0.021
		2	0.003	0.019
WALL	3,4,5,6	0	0.782	0.012
		1	0.202	0.012
		2	0.014	0.012
		3	0.001	0.012
		4	0	0.012
WALL	1,2	0	0.264	0.01
		1	0.731	0.016
		2	0.005	0.015
WALL	3,4,5,6	0	0.78	0.012
		1	0.205	0.012
		2	0.014	0.012
		3	0	0.012
		4	0	0.012
WALL_U	3,4,5,6	0	0.675	0.012
		1	0.121	0.012
		2	0.022	0.012
		3	0.071	0.012
		4	0.112	0.012
WALL_U	1,2	0	0.74	0.036
		1	0.108	0.027
		2	0.152	0.025
WALL_U	3,4,5,6	0	0.68	0.012
		1	0.119	0.012
		2	0.019	0.012
		3	0.072	0.012
		4	0.11	0.012
WALL_U	1,2	0	0.755	0.036

```
            1      0.098 0.027
            2      0.146 0.025
WALL_U      3,4,5,6     0      0.677 0.012
            1      0.119 0.012
            2      0.02  0.012
            3      0.07  0.012
            4      0.114 0.012
FSUC  4,5,6 0      0.803 0.014
            1      0.189 0.014
            2      0.008 0.014
            3      0     0.014
FSUC  4,5,6 0      0.818 0.029
            1      0.187 0.014
            2      0.002 0.018
            3      -0.007      0.019
FSUC  1,2,3,4      0     0.245 0.013
            1      0.724 0.013
            2      0.033 0.013
            3      0     0.013
            4      -0.002      0.013
FSUC  4,5,6 0      0.805 0.013
            1      0.188 0.013
            2      0.007 0.013
            3      0     0.013
FSUC  4,5,6 0      0.798 0.031
            1      0.207 0.015
            2      0.002 0.02
            3      -0.007      0.021
FSUC  1,2,3,4      0     0.247 0.011
            1      0.727 0.011
            2      0.031 0.011
            3      -0.001      0.011
            4      -0.004      0.011
FSUC  4,5,6 0      0.804 0.014
            1      0.189 0.014
            2      0.008 0.014
            3      0     0.014
FSUC  4,5,6 0      0.818 0.031
            1      0.188 0.015
            2      0.002 0.019
            3      -0.008      0.02
FSUC  1,2,3,4      0     0.247 0.013
            1      0.724 0.013
            2      0.034 0.013
            3      -0.002      0.013
            4      -0.002      0.013
FSUC  4,5,6 0      0.805 0.013
            1      0.188 0.013
            2      0.008 0.013
            3      -0.001      0.013
FSUC  4,5,6 0      0.797 0.034
            1      0.207 0.017
            2      0.002 0.021
```

		3	-0.006	0.022
FSUC	1,2,3,4	0	0.253	0.011
		1	0.719	0.011
		2	0.036	0.011
		3	-0.005	0.011
		4	-0.003	0.011
FSUC	4,5,6	0	0.801	0.014
		1	0.192	0.014
		2	0.008	0.014
		3	-0.001	0.014
FSUC	4,5,6	0	0.817	0.028
		1	0.191	0.013
		2	0.001	0.017
		3	-0.009	0.018
FSUC	1,2,3,4	0	0.255	0.013
		1	0.711	0.013
		2	0.036	0.013
		3	-0.001	0.013
		4	-0.001	0.013
FSUC	4,5,6	0	0.803	0.013
		1	0.191	0.013
		2	0.007	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.793	0.033
		1	0.211	0.016
		2	0.002	0.021
		3	-0.007	0.022
FSUC	1,2,3,4	0	0.255	0.011
		1	0.718	0.011
		2	0.033	0.011
		3	-0.002	0.011
		4	-0.003	0.011
FSUC_U	4,5,6	0	0.756	0.014
		1	0.046	0.014
		2	0.019	0.014
		3	0.179	0.014
FSUC_U	4,5,6	0	0.778	0.016
		1	0.037	0.01
		2	0.011	0.01
		3	0.174	0.01
FSUC_U	1,2,3,4	0	0.657	0.013
		1	0.138	0.013
		2	0.044	0.013
		3	0.057	0.013
		4	0.105	0.013
FSUC_U	4,5,6	0	0.757	0.013
		1	0.046	0.013
		2	0.019	0.013
		3	0.178	0.013
FSUC_U	4,5,6	0	0.774	0.02
		1	0.041	0.012
		2	0.013	0.012
		3	0.171	0.01

FSUC_U	1,2,3,4	0	0.663	0.011
	1	0.134	0.011	
	2	0.044	0.011	
	3	0.054	0.011	
	4	0.106	0.011	
FSUC_U	4,5,6	0	0.757	0.014
	1	0.044	0.014	
	2	0.019	0.014	
	3	0.18	0.014	
FSUC_U	4,5,6	0	0.778	0.016
	1	0.037	0.01	
	2	0.011	0.01	
	3	0.174	0.01	
FSUC_U	1,2,3,4	0	0.654	0.013
	1	0.137	0.013	
	2	0.047	0.013	
	3	0.056	0.013	
	4	0.106	0.013	
FSUC_U	4,5,6	0	0.758	0.013
	1	0.045	0.013	
	2	0.018	0.013	
	3	0.179	0.013	
FSUC_U	4,5,6	0	0.775	0.019
	1	0.041	0.012	
	2	0.013	0.012	
	3	0.172	0.01	
FSUC_U	1,2,3,4	0	0.658	0.011
	1	0.136	0.011	
	2	0.044	0.011	
	3	0.056	0.011	
	4	0.106	0.011	
FSUC_U	4,5,6	0	0.757	0.014
	1	0.045	0.014	
	2	0.018	0.014	
	3	0.18	0.014	
FSUC_U	4,5,6	0	0.78	0.016
	1	0.036	0.01	
	2	0.01	0.01	
	3	0.174	0.01	
FSUC_U	1,2,3,4	0	0.659	0.013
	1	0.137	0.013	
	2	0.045	0.013	
	3	0.053	0.013	
	4	0.106	0.013	
FSUC_U	4,5,6	0	0.759	0.013
	1	0.044	0.013	
	2	0.018	0.013	
	3	0.179	0.013	
FSUC_U	4,5,6	0	0.776	0.02
	1	0.04	0.012	
	2	0.012	0.013	
	3	0.172	0.01	
FSUC_U	1,2,3,4	0	0.659	0.011

		1	0.135	0.011
		2	0.046	0.011
		3	0.053	0.011
		4	0.106	0.011
PENTAN	5	0	0.998	0.01
		1	0.002	0.01
PENTAN	3,4,5	0	0.936	0.043
		1	0.077	0.02
		2	-0.005	0.022
		3	-0.008	0.023
PENTAN	3,4,5	0	0.941	0.01
		1	0.057	0.01
		2	0.002	0.01
		3	0	0.01
PENTAN	5	0	0.993	0.015
		1	0.007	0.015
PENTAN	3,4,5	0	0.935	0.036
		1	0.074	0.016
		2	-0.001	0.018
		3	-0.009	0.019
PENTAN	3,4,5	0	0.951	0.01
		1	0.053	0.01
		2	-0.004	0.01
		3	0	0.01
PENTAN	5	0	1.001	0.01
		1	-0.001	0.01
PENTAN	3,4,5	0	0.948	0.01
		1	0.052	0.01
		2	0	0.01
		3	0	0.01
WALL	3,4,5,6	0	0.794	0.012
		1	0.192	0.012
		2	0.014	0.012
		3	0	0.012
		4	0	0.012
PENTAN	5	0	0.997	0.01
		1	0.003	0.01
PENTAN	3,4,5	0	0.934	0.042
		1	0.078	0.02
		2	-0.004	0.022
		3	-0.008	0.023
PENTAN	3,4,5	0	0.94	0.01
		1	0.058	0.01
		2	0.002	0.01
		3	0	0.01
PENTAN	5	0	0.991	0.015
		1	0.009	0.015
PENTAN	3,4,5	0	0.935	0.03
		1	0.071	0.016
		2	0.004	0.016
		3	-0.01	0.016
PENTAN	3,4,5	0	0.948	0.01
		1	0.047	0.01

		2	0.005	0.01
		3	0	0.01
PENTAN	5	0	0.999	0.01
		1	0.001	0.01
PENTAN	3,4,5	0	0.949	0.032
		1	0.075	0.029
		2	-0.011	0.029
		3	-0.013	0.029
PENTAN	3,4,5	0	0.942	0.01
		1	0.057	0.01
		2	0	0.01
		3	0	0.01
WALL	3,4,5,6	0	0.789	0.012
		1	0.197	0.012
		2	0.013	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN	5	0	0.996	0.01
		1	0.004	0.01
PENTAN	3,4,5	0	0.935	0.041
		1	0.079	0.02
		2	-0.006	0.021
		3	-0.008	0.022
PENTAN	3,4,5	0	0.938	0.01
		1	0.059	0.01
		2	0.002	0.01
		3	0	0.01
PENTAN	5	0	0.992	0.015
		1	0.008	0.015
PENTAN	3,4,5	0	0.93	0.028
		1	0.081	0.016
		2	-0.003	0.016
		3	-0.008	0.016
PENTAN	3,4,5	0	0.956	0.01
		1	0.054	0.01
		2	-0.008	0.01
		3	-0.002	0.01
PENTAN	5	0	0.998	0.01
		1	0.002	0.01
PENTAN	3,4,5	0	0.95	0.029
		1	0.077	0.029
		2	-0.012	0.029
		3	-0.016	0.029
PENTAN	3,4,5	0	0.943	0.01
		1	0.055	0.01
		2	0.001	0.01
		3	0.001	0.01
WALL	3,4,5,6	0	0.785	0.012
		1	0.202	0.012
		2	0.012	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN_U	5	0	0.794	0.01

```
            1     0.206 0.01
PENTAN_U    3,4,5 0     0.688 0.02
            1     0.127 0.02
            2     0.065 0.02
            3     0.12  0.02
PENTAN_U    3,4,5 0     0.688 0.01
            1     0.119 0.01
            2     0.072 0.01
            3     0.121 0.01
PENTAN_U    5     0     0.794 0.015
            1     0.206 0.015
PENTAN_U    3,4,5 0     0.684 0.016
            1     0.124 0.016
            2     0.077 0.016
            3     0.114 0.016
PENTAN_U    3,4,5 0     0.698 0.01
            1     0.12  0.01
            2     0.066 0.01
            3     0.117 0.01
PENTAN_U    5     0     0.792 0.01
            1     0.208 0.01
PENTAN_U    3,4,5 0     0.688 0.029
            1     0.126 0.029
            2     0.068 0.029
            3     0.118 0.029
PENTAN_U    3,4,5 0     0.694 0.01
            1     0.118 0.01
            2     0.069 0.01
            3     0.119 0.01
WALL_U      3,4,5,6     0     0.679 0.012
            1     0.114 0.012
            2     0.02  0.012
            3     0.067 0.012
            4     0.119 0.012
PENTAN_U    5     0     0.792 0.01
            1     0.208 0.01
PENTAN_U    3,4,5 0     0.683 0.02
            1     0.128 0.02
            2     0.068 0.02
            3     0.12  0.02
PENTAN_U    3,4,5 0     0.692 0.01
            1     0.117 0.01
            2     0.071 0.01
            3     0.12  0.01
PENTAN_U    5     0     0.789 0.015
            1     0.211 0.015
PENTAN_U    3,4,5 0     0.673 0.016
            1     0.136 0.016
            2     0.071 0.016
            3     0.12  0.016
PENTAN_U    3,4,5 0     0.687 0.01
            1     0.119 0.01
            2     0.074 0.01
```

```
            3     0.12  0.01
PENTAN_U    5     0     0.796 0.01
            1     0.204 0.01
PENTAN_U    3,4,5 0     0.681 0.029
            1     0.129 0.029
            2     0.07  0.029
            3     0.119 0.029
PENTAN_U    3,4,5 0     0.689 0.01
            1     0.12  0.01
            2     0.071 0.01
            3     0.119 0.01
WALL_U      3,4,5,6     0     0.681 0.012
            1     0.115 0.012
            2     0.018 0.012
            3     0.068 0.012
            4     0.118 0.012
PENTAN_U    5     0     0.794 0.01
            1     0.206 0.01
PENTAN_U    3,4,5 0     0.688 0.02
            1     0.127 0.02
            2     0.067 0.02
            3     0.119 0.02
PENTAN_U    3,4,5 0     0.693 0.01
            1     0.117 0.01
            2     0.072 0.01
            3     0.118 0.01
PENTAN_U    5     0     0.797 0.015
            1     0.203 0.015
PENTAN_U    3,4,5 0     0.706 0.016
            1     0.105 0.016
            2     0.07  0.016
            3     0.119 0.016
PENTAN_U    3,4,5 0     0.694 0.017
            1     0.105 0.011
            2     0.075 0.011
            3     0.125 0.011
PENTAN_U    5     0     0.793 0.01
            1     0.207 0.01
PENTAN_U    3,4,5 0     0.683 0.029
            1     0.135 0.029
            2     0.065 0.029
            3     0.117 0.029
PENTAN_U    3,4,5 0     0.69  0.01
            1     0.116 0.01
            2     0.073 0.01
            3     0.121 0.01
WALL_U      3,4,5,6     0     0.684 0.012
            1     0.112 0.012
            2     0.018 0.012
            3     0.067 0.012
            4     0.118 0.012
```

Control line 4

```
MASS_SPECTROMETRY
      META_NAME    FRAGMENT    WEIGHT      VALUE DEVIATION
      ALA   1,2,3 0     0.585 0.01
                  1     0.384 0.01
                  2     0.029 0.01
                  3     0.001 0.01
      ALA   2,3   0     0.606 0.011
                  1     0.377 0.011
                  2     0.017 0.011
      GLY   1,2   0     0.896 0.011
                  1     0.098 0.011
                  2     0.006 0.011
      GLY   2     0     0.964 0.011
                  1     0.036 0.011
      VAL   1,2,3,4,5   0     0.394 0.01
                  1     0.435 0.01
                  2     0.154 0.01
                  3     0.016 0.01
                  4     0.001 0.01
                  5     0     0.01
      VAL   2,3,4,5     0     0.401 0.02
                  1     0.452 0.025
                  2     0.151 0.017
                  3     0.002 0.021
                  4     -0.007      0.022
      VAL   2,3,4,5     0     0.398 0.029
                  1     0.426 0.029
                  2     0.142 0.029
                  3     0.032 0.029
                  4     0.003 0.029
      SER   1,2,3 0     0.687 0.011
                  1     0.299 0.011
                  2     0.014 0.011
                  3     0.001 0.011
      SER   2,3   0     0.71  0.011
                  1     0.277 0.011
                  2     0.013 0.011
      SER   1,2   0     0.934 0.013
                  1     0.064 0.013
                  2     0.002 0.013
      PHE_TYR     1,2   0     0.931 0.01
                  1     0.073 0.01
                  2     -0.004      0.01
      ASP   1,2,3,4     0     0.381 0.01
                  1     0.438 0.01
                  2     0.163 0.01
                  3     0.021 0.01
                  4     -0.002      0.01
      ASP   2,3,4 0     0.442 0.01
```

		1	0.435	0.01	
		2	0.117	0.01	
		3	0.006	0.01	
ASP	1,2	0	0.628	0.013	
		1	0.337	0.013	
		2	0.036	0.013	
GLU	1,2,3,4,5	0	0.284	0.012	
		1	0.436	0.012	
		2	0.234	0.012	
		3	0.049	0.012	
		4	-0.002		0.012
		5	-0.001		0.012
GLU	1,2,3,4,5	0	0.269	0.01	
		1	0.417	0.01	
		2	0.241	0.01	
		3	0.057	0.01	
		4	0.009	0.01	
		5	0.006	0.01	
GLU	1,2,3,4,5	0	0.269	0.01	
		1	0.429	0.01	
		2	0.241	0.01	
		3	0.057	0.01	
		4	0.005	0.01	
		5	0	0.01	
GLU	2,3,4,5	0	0.313	0.01	
		1	0.446	0.01	
		2	0.204	0.01	
		3	0.033	0.01	
		4	0.004	0.01	
ASP	1,2	0	0.631	0.01	
		1	0.335	0.01	
		2	0.034	0.01	
GLU	1,2,3,4,5	0	0.283	0.013	
		1	0.433	0.013	
		2	0.234	0.013	
		3	0.044	0.013	
		4	0.004	0.013	
		5	0.002	0.013	
GLU	1,2,3,4,5	0	0.276	0.01	
		1	0.431	0.01	
		2	0.237	0.01	
		3	0.054	0.01	
		4	0.003	0.01	
		5	-0.002		0.01
GLU	1,2,3,4,5	0	0.279	0.011	
		1	0.426	0.011	
		2	0.234	0.011	
		3	0.054	0.011	
		4	0.007	0.011	
		5	0	0.011	
GABA	1,2,3,4	0	0.328	0.019	
		1	0.442	0.019	
		2	0.201	0.019	

		3	0.03	0.019
		4	-0.002	0.019
ALA	1,2,3	0	0.569	0.01
		1	0.392	0.01
		2	0.037	0.01
		3	0.002	0.01
ALA	2,3	0	0.595	0.011
		1	0.387	0.011
		2	0.018	0.011
GLY	1,2	0	0.897	0.011
		1	0.099	0.011
		2	0.004	0.011
GLY	2	0	0.972	0.011
		1	0.028	0.011
VAL	1,2,3,4,5	0	0.376	0.01
		1	0.437	0.01
		2	0.164	0.01
		3	0.022	0.01
		4	0.002	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.387	0.01
		1	0.443	0.01
		2	0.162	0.01
		3	0.009	0.01
		4	-0.002	0.01
VAL	2,3,4,5	0	0.389	0.029
		1	0.431	0.029
		2	0.155	0.029
		3	0.024	0.029
		4	0.001	0.029
SER	1,2,3	0	0.671	0.029
		1	0.297	0.022
		2	0.015	0.024
		3	0.017	0.025
SER	1,2,3	0	0.677	0.011
		1	0.305	0.011
		2	0.018	0.011
		3	0	0.011
SER	2,3	0	0.715	0.011
		1	0.278	0.011
		2	0.007	0.011
SER	1,2	0	0.927	0.013
		1	0.074	0.013
		2	0	0.013
PHE_TYR	1,2	0	0.923	0.01
		1	0.073	0.01
		2	0.004	0.01
ASP	1,2,3,4	0	0.373	0.01
		1	0.44	0.01
		2	0.169	0.01
		3	0.021	0.01
		4	-0.004	0.01
ASP	2,3,4	0	0.444	0.01

		1	0.444	0.01	
		2	0.112	0.01	
		3	0.001	0.01	
ASP	1,2	0	0.625	0.013	
		1	0.345	0.013	
		2	0.03	0.013	
GLU	1,2,3,4,5	0	0.289	0.012	
		1	0.414	0.012	
		2	0.243	0.012	
		3	0.054	0.012	
		4	0.004	0.012	
		5	-0.004		0.012
GLU	1,2,3,4,5	0	0.262	0.01	
		1	0.42	0.01	
		2	0.235	0.01	
		3	0.057	0.01	
		4	0.013	0.01	
		5	0.012	0.01	
GLU	1,2,3,4,5	0	0.268	0.01	
		1	0.426	0.01	
		2	0.245	0.01	
		3	0.057	0.01	
		4	0.005	0.01	
		5	0	0.01	
GLU	2,3,4,5	0	0.31	0.01	
		1	0.441	0.01	
		2	0.206	0.01	
		3	0.036	0.01	
		4	0.007	0.01	
ASP	1,2	0	0.6	0.01	
		1	0.345	0.01	
		2	0.055	0.01	
GLU	1,2,3,4,5	0	0.277	0.013	
		1	0.43	0.013	
		2	0.238	0.013	
		3	0.048	0.013	
		4	0.003	0.013	
		5	0.004	0.013	
GLU	1,2,3,4,5	0	0.269	0.01	
		1	0.428	0.01	
		2	0.244	0.01	
		3	0.057	0.01	
		4	0.004	0.01	
		5	-0.002		0.01
GLU	1,2,3,4,5	0	0.273	0.011	
		1	0.426	0.011	
		2	0.241	0.011	
		3	0.055	0.011	
		4	0.005	0.011	
		5	0	0.011	
GABA	1,2,3,4	0	0.316	0.019	
		1	0.446	0.019	
		2	0.207	0.019	

		3	0.032	0.019
		4	0	0.019
ALA	1,2,3	0	0.57	0.01
		1	0.393	0.01
		2	0.036	0.01
		3	0.002	0.01
ALA	2,3	0	0.596	0.011
		1	0.386	0.011
		2	0.018	0.011
GLY	1,2	0	0.9	0.011
		1	0.099	0.011
		2	0.001	0.011
GLY	2	0	0.968	0.011
		1	0.032	0.011
VAL	1,2,3,4,5	0	0.388	0.01
		1	0.429	0.01
		2	0.163	0.01
		3	0.017	0.01
		4	0.002	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.397	0.011
		1	0.437	0.013
		2	0.161	0.01
		3	0.008	0.012
		4	-0.004	0.012
VAL	2,3,4,5	0	0.398	0.029
		1	0.425	0.029
		2	0.149	0.029
		3	0.026	0.029
		4	0.002	0.029
SER	1,2,3	0	0.678	0.023
		1	0.297	0.017
		2	0.011	0.019
		3	0.014	0.02
SER	1,2,3	0	0.68	0.011
		1	0.303	0.011
		2	0.016	0.011
		3	0	0.011
SER	2,3	0	0.718	0.011
		1	0.274	0.011
		2	0.008	0.011
SER	1,2	0	0.927	0.013
		1	0.074	0.013
		2	-0.001	0.013
PHE_TYR	1,2	0	0.928	0.01
		1	0.065	0.01
		2	0.008	0.01
ASP	1,2,3,4	0	0.374	0.01
		1	0.442	0.01
		2	0.165	0.01
		3	0.022	0.01
		4	-0.003	0.01
ASP	2,3,4	0	0.437	0.01

		1	0.44	0.01	
		2	0.122	0.01	
		3	0.001	0.01	
ASP	1,2	0	0.623	0.013	
		1	0.34	0.013	
		2	0.036	0.013	
GLU	1,2,3,4,5		0	0.285	0.012
		1	0.418	0.012	
		2	0.253	0.012	
		3	0.06	0.012	
		4	-0.007		0.012
		5	-0.009		0.012
GLU	1,2,3,4,5		0	0.262	0.01
		1	0.406	0.01	
		2	0.236	0.01	
		3	0.06	0.01	
		4	0.021	0.01	
		5	0.016	0.01	
GLU	1,2,3,4,5		0	0.267	0.01
		1	0.428	0.01	
		2	0.243	0.01	
		3	0.057	0.01	
		4	0.005	0.01	
		5	0	0.01	
GLU	2,3,4,5		0	0.31	0.01
		1	0.44	0.01	
		2	0.208	0.01	
		3	0.034	0.01	
		4	0.007	0.01	
ASP	1,2	0	0.614	0.01	
		1	0.337	0.01	
		2	0.049	0.01	
GLU	1,2,3,4,5		0	0.274	0.013
		1	0.42	0.013	
		2	0.232	0.013	
		3	0.044	0.013	
		4	0.01	0.013	
		5	0.02	0.013	
GLU	1,2,3,4,5		0	0.272	0.01
		1	0.43	0.01	
		2	0.242	0.01	
		3	0.055	0.01	
		4	0.003	0.01	
		5	-0.002		0.01
GLU	1,2,3,4,5		0	0.274	0.011
		1	0.427	0.011	
		2	0.239	0.011	
		3	0.056	0.011	
		4	0.005	0.011	
		5	0	0.011	
GABA	1,2,3,4		0	0.315	0.019
		1	0.446	0.019	
		2	0.206	0.019	

```
            3      0.033 0.019
            4      0      0.019
ALA_U 1,2,3 0      0.712 0.01
            1      0.106 0.01
            2      0.052 0.01
            3      0.131 0.01
ALA_U 2,3   0      0.761 0.011
            1      0.075 0.011
            2      0.164 0.011
GLY_U 1,2   0      0.726 0.011
            1      0.167 0.011
            2      0.107 0.011
GLY_U 2     0      0.809 0.011
            1      0.191 0.011
VAL_U 1,2,3,4,5    0      0.569 0.01
            1      0.139 0.01
            2      0.15  0.01
            3      0.108 0.01
            4      0.017 0.01
            5      0.018 0.01
VAL_U 2,3,4,5      0      0.596 0.01
            1      0.13  0.01
            2      0.227 0.01
            3      0.025 0.01
            4      0.022 0.01
VAL_U 2,3,4,5      0      0.596 0.029
            1      0.12  0.029
            2      0.226 0.029
            3      0.035 0.029
            4      0.023 0.029
SER_U 1,2,3 0      0.658 0.01
            1      0.183 0.01
            2      0.078 0.01
            3      0.081 0.01
SER_U 1,2,3 0      0.656 0.011
            1      0.182 0.011
            2      0.08  0.011
            3      0.081 0.011
SER_U 2,3   0      0.706 0.01
            1      0.19  0.01
            2      0.104 0.01
SER_U 2,3   0      0.71  0.011
            1      0.186 0.011
            2      0.104 0.011
SER_U 1,2   0      0.736 0.013
            1      0.135 0.013
            2      0.129 0.013
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.416 0.021
            1      0.154 0.021
            2      0.197 0.021
            3      0.115 0.021
            4      0.066 0.021
            5      0.033 0.021
```

```
            6     0.012 0.021
            7     0     0.021
            8     0.008 0.021
PHE_TYR_U   1,2   0     0.757 0.01
            1     0.109 0.01
            2     0.134 0.01
ASP_U 1,2,3,4     0     0.552 0.01
            1     0.222 0.01
            2     0.144 0.01
            3     0.066 0.01
            4     0.016 0.01
ASP_U 2,3,4 0     0.619 0.01
            1     0.226 0.01
            2     0.116 0.01
            3     0.039 0.01
ASP_U 1,2   0     0.717 0.013
            1     0.172 0.013
            2     0.111 0.013
GLU_U 1,2,3,4,5   0     0.476 0.012
            1     0.22  0.012
            2     0.204 0.012
            3     0.077 0.012
            4     0.015 0.012
            5     0.006 0.012
GLU_U 1,2,3,4,5   0     0.469 0.01
            1     0.222 0.01
            2     0.197 0.01
            3     0.084 0.01
            4     0.022 0.01
            5     0.006 0.01
GLU_U 1,2,3,4,5   0     0.473 0.01
            1     0.217 0.01
            2     0.204 0.01
            3     0.079 0.01
            4     0.021 0.01
            5     0.006 0.01
GLU_U 2,3,4,5     0     0.525 0.01
            1     0.228 0.01
            2     0.185 0.01
            3     0.05  0.01
            4     0.012 0.01
ASP_U 1,2   0     0.704 0.01
            1     0.172 0.01
            2     0.124 0.01
GLU_U 1,2,3,4,5   0     0.48  0.013
            1     0.213 0.013
            2     0.203 0.013
            3     0.076 0.013
            4     0.023 0.013
            5     0.005 0.013
GLU_U 1,2,3,4,5   0     0.47  0.01
            1     0.214 0.01
            2     0.208 0.01
```

```
            3     0.079 0.01
            4     0.023 0.01
            5     0.007 0.01
GLU_U 1,2,3,4,5   0     0.476 0.011
            1     0.213 0.011
            2     0.205 0.011
            3     0.077 0.011
            4     0.023 0.011
            5     0.007 0.011
GABA_U      1,2,3,4     0     0.53  0.019
            1     0.234 0.019
            2     0.182 0.019
            3     0.043 0.019
            4     0.011 0.019
ALA_U 1,2,3 0     0.711 0.01
            1     0.109 0.01
            2     0.054 0.01
            3     0.127 0.01
ALA_U 2,3   0     0.762 0.011
            1     0.079 0.011
            2     0.159 0.011
GLY_U 1,2   0     0.729 0.011
            1     0.161 0.011
            2     0.109 0.011
GLY_U 2     0     0.81  0.011
            1     0.19  0.011
VAL_U 1,2,3,4,5   0     0.568 0.01
            1     0.135 0.01
            2     0.151 0.01
            3     0.111 0.01
            4     0.016 0.01
            5     0.02  0.01
VAL_U 2,3,4,5     0     0.589 0.01
            1     0.136 0.01
            2     0.228 0.01
            3     0.022 0.01
            4     0.025 0.01
VAL_U 2,3,4,5     0     0.594 0.029
            1     0.114 0.029
            2     0.232 0.029
            3     0.035 0.029
            4     0.024 0.029
SER_U 1,2,3 0     0.668 0.01
            1     0.172 0.01
            2     0.08  0.01
            3     0.079 0.01
SER_U 1,2,3 0     0.659 0.011
            1     0.177 0.011
            2     0.079 0.011
            3     0.085 0.011
SER_U 2,3   0     0.712 0.01
            1     0.183 0.01
            2     0.105 0.01
```

```
SER_U 2,3   0      0.717 0.011
            1      0.179 0.011
            2      0.104 0.011
SER_U 1,2   0      0.735 0.013
            1      0.134 0.013
            2      0.131 0.013
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.411 0.021
            1      0.15  0.021
            2      0.2   0.021
            3      0.115 0.021
            4      0.068 0.021
            5      0.033 0.021
            6      0.014 0.021
            7      -0.002      0.021
            8      0.011 0.021
PHE_TYR_U   1,2    0      0.76  0.01
            1      0.106 0.01
            2      0.134 0.01
ASP_U 1,2,3,4      0      0.553 0.01
            1      0.223 0.01
            2      0.144 0.01
            3      0.064 0.01
            4      0.016 0.01
ASP_U 2,3,4 0      0.619 0.01
            1      0.227 0.01
            2      0.116 0.01
            3      0.038 0.01
ASP_U 1,2   0      0.724 0.013
            1      0.166 0.013
            2      0.11  0.013
GLU_U 1,2,3,4,5    0      0.481 0.012
            1      0.221 0.012
            2      0.195 0.012
            3      0.08  0.012
            4      0.023 0.012
            5      0     0.012
GLU_U 1,2,3,4,5    0      0.476 0.01
            1      0.22  0.01
            2      0.199 0.01
            3      0.076 0.01
            4      0.023 0.01
            5      0.006 0.01
GLU_U 1,2,3,4,5    0      0.475 0.01
            1      0.218 0.01
            2      0.204 0.01
            3      0.076 0.01
            4      0.021 0.01
            5      0.006 0.01
GLU_U 2,3,4,5      0      0.522 0.01
            1      0.223 0.01
            2      0.182 0.01
            3      0.059 0.01
            4      0.014 0.01
```

```
ASP_U 1,2   0     0.723 0.01
            1     0.163 0.01
            2     0.114 0.01
GLU_U 1,2,3,4,5   0     0.486 0.013
            1     0.21  0.013
            2     0.205 0.013
            3     0.074 0.013
            4     0.024 0.013
            5     0.002 0.013
GLU_U 1,2,3,4,5   0     0.474 0.01
            1     0.212 0.01
            2     0.208 0.01
            3     0.077 0.01
            4     0.022 0.01
            5     0.006 0.01
GLU_U 1,2,3,4,5   0     0.48  0.011
            1     0.21  0.011
            2     0.205 0.011
            3     0.076 0.011
            4     0.022 0.011
            5     0.007 0.011
GABA_U      1,2,3,4     0     0.532 0.019
            1     0.232 0.019
            2     0.182 0.019
            3     0.043 0.019
            4     0.012 0.019
ALA_U 1,2,3 0     0.709 0.01
            1     0.111 0.01
            2     0.055 0.01
            3     0.125 0.01
ALA_U 2,3   0     0.759 0.011
            1     0.083 0.011
            2     0.158 0.011
GLY_U 1,2   0     0.722 0.011
            1     0.173 0.011
            2     0.105 0.011
GLY_U 2     0     0.804 0.011
            1     0.196 0.011
VAL_U 1,2,3,4,5   0     0.565 0.01
            1     0.132 0.01
            2     0.152 0.01
            3     0.113 0.01
            4     0.016 0.01
            5     0.021 0.01
VAL_U 2,3,4,5     0     0.584 0.029
            1     0.111 0.029
            2     0.231 0.029
            3     0.049 0.029
            4     0.025 0.029
SER_U 1,2,3 0     0.677 0.01
            1     0.166 0.01
            2     0.072 0.01
            3     0.085 0.01
```

SER_U 1,2,3	0	0.66	0.011	
	1	0.176	0.011	
	2	0.077	0.011	
	3	0.087	0.011	
SER_U 2,3	0	0.713	0.01	
	1	0.18	0.01	
	2	0.108	0.01	
SER_U 2,3	0	0.722	0.011	
	1	0.174	0.011	
	2	0.104	0.011	
SER_U 1,2	0	0.743	0.013	
	1	0.134	0.013	
	2	0.123	0.013	
PHE_TYR_U	2,3,4,5,6,7,8,9	0	0.415	0.021
	1	0.145	0.021	
	2	0.199	0.021	
	3	0.115	0.021	
	4	0.066	0.021	
	5	0.032	0.021	
	6	0.012	0.021	
	7	-0.001		0.021
	8	0.016	0.021	
PHE_TYR_U	1,2	0	0.771	0.01
	1	0.099	0.01	
	2	0.13	0.01	
ASP_U 1,2,3,4	0	0.559	0.01	
	1	0.221	0.01	
	2	0.142	0.01	
	3	0.064	0.01	
	4	0.013	0.01	
ASP_U 2,3,4	0	0.628	0.01	
	1	0.225	0.01	
	2	0.111	0.01	
	3	0.037	0.01	
ASP_U 1,2	0	0.728	0.013	
	1	0.161	0.013	
	2	0.111	0.013	
GLU_U 1,2,3,4,5	0	0.465	0.012	
	1	0.224	0.012	
	2	0.226	0.012	
	3	0.058	0.012	
	4	0.023	0.012	
	5	0.004	0.012	
GLU_U 1,2,3,4,5	0	0.467	0.01	
	1	0.219	0.01	
	2	0.202	0.01	
	3	0.086	0.01	
	4	0.018	0.01	
	5	0.009	0.01	
GLU_U 1,2,3,4,5	0	0.478	0.01	
	1	0.214	0.01	
	2	0.203	0.01	
	3	0.077	0.01	

		4	0.02	0.01
		5	0.006	0.01
GLU_U	2,3,4,5	0	0.522	0.01
		1	0.223	0.01
		2	0.18	0.01
		3	0.061	0.01
		4	0.013	0.01
ASP_U	1,2	0	0.724	0.01
		1	0.16	0.01
		2	0.115	0.01
GLU_U	1,2,3,4,5	0	0.479	0.013
		1	0.207	0.013
		2	0.201	0.013
		3	0.066	0.013
		4	0.045	0.013
		5	0.001	0.013
GLU_U	1,2,3,4,5	0	0.481	0.01
		1	0.212	0.01
		2	0.205	0.01
		3	0.075	0.01
		4	0.022	0.01
		5	0.004	0.01
GLU_U	1,2,3,4,5	0	0.479	0.011
		1	0.21	0.011
		2	0.206	0.011
		3	0.075	0.011
		4	0.023	0.011
		5	0.007	0.011
GABA_U	1,2,3,4	0	0.529	0.019
		1	0.235	0.019
		2	0.182	0.019
		3	0.043	0.019
		4	0.011	0.019
FUM	1,2,3,4	0	0.356	0.023
		1	0.41	0.03
		2	0.194	0.022
		3	0.029	0.026
		4	0.011	0.028
OAA	1,2,3,4	0	0.37	0.011
		1	0.439	0.011
		2	0.167	0.011
		3	0.022	0.011
		4	0.003	0.011
OAA	1,2,3,4	0	0.372	0.01
		1	0.438	0.01
		2	0.167	0.01
		3	0.022	0.01
		4	0	0.01
CIT	1,2,3,4,5,6	0	0.233	0.01
		1	0.41	0.01
		2	0.269	0.01
		3	0.078	0.01
		4	0.009	0.01

```
            5     -0.001      0.01
            6     0     0.01
FUM   1,2,3,4     0     0.361 0.017
            1     0.416 0.017
            2     0.178 0.017
            3     0.033 0.017
            4     0.012 0.017
OAA   1,2,3,4     0     0.368 0.011
            1     0.438 0.011
            2     0.169 0.011
            3     0.025 0.011
            4     0     0.011
OAA   1,2,3,4     0     0.368 0.01
            1     0.436 0.01
            2     0.172 0.01
            3     0.023 0.01
            4     0     0.01
CIT   1,2,3,4,5,6 0     0.229 0.01
            1     0.408 0.01
            2     0.271 0.01
            3     0.083 0.01
            4     0.01  0.01
            5     0     0.01
            6     0     0.01
FUM   1,2,3,4     0     0.362 0.017
            1     0.419 0.017
            2     0.178 0.017
            3     0.031 0.017
            4     0.01  0.017
OAA   1,2,3,4     0     0.376 0.011
            1     0.431 0.011
            2     0.169 0.011
            3     0.024 0.011
            4     0.001 0.011
OAA   1,2,3,4     0     0.366 0.01
            1     0.439 0.01
            2     0.171 0.01
            3     0.023 0.01
            4     0     0.01
FUM_U 1,2,3,4     0     0.547 0.017
            1     0.226 0.017
            2     0.146 0.017
            3     0.065 0.017
            4     0.016 0.017
OAA_U 1,2,3,4     0     0.548 0.011
            1     0.228 0.011
            2     0.144 0.011
            3     0.063 0.011
            4     0.017 0.011
OAA_U 1,2,3,4     0     0.546 0.01
            1     0.226 0.01
            2     0.145 0.01
            3     0.067 0.01
```

```
            4      0.016 0.01
CIT_U 1,2,3,4,5,6 0      0.419 0.01
            1      0.219 0.01
            2      0.212 0.01
            3      0.098 0.01
            4      0.04  0.01
            5      0.01  0.01
            6      0.002 0.01
FUM_U 1,2,3,4      0     0.548 0.017
            1      0.227 0.017
            2      0.142 0.017
            3      0.066 0.017
            4      0.017 0.017
OAA_U 1,2,3,4      0     0.55  0.011
            1      0.224 0.011
            2      0.148 0.011
            3      0.064 0.011
            4      0.015 0.011
OAA_U 1,2,3,4      0     0.548 0.01
            1      0.224 0.01
            2      0.146 0.01
            3      0.065 0.01
            4      0.017 0.01
CIT_U 1,2,3,4,5,6 0      0.424 0.01
            1      0.217 0.01
            2      0.212 0.01
            3      0.096 0.01
            4      0.039 0.01
            5      0.01  0.01
            6      0.003 0.01
FUM_U 1,2,3,4      0     0.538 0.017
            1      0.217 0.017
            2      0.147 0.017
            3      0.059 0.017
            4      0.039 0.017
OAA_U 1,2,3,4      0     0.55  0.011
            1      0.222 0.011
            2      0.147 0.011
            3      0.067 0.011
            4      0.014 0.011
OAA_U 1,2,3,4      0     0.551 0.01
            1      0.223 0.01
            2      0.145 0.01
            3      0.066 0.01
            4      0.015 0.01
CIT_U 1,2,3,4,5,6 0      0.422 0.01
            1      0.216 0.01
            2      0.215 0.01
            3      0.095 0.01
            4      0.036 0.01
            5      0.014 0.01
            6      0.001 0.01
ALA   1,2,3 0      0.601 0.011
```

		1	0.377	0.011
		2	0.021	0.011
		3	0.001	0.011
ALA	2,3	0	0.62	0.011
		1	0.371	0.011
		2	0.008	0.011
GLYeff	1,2	0	0.904	0.01
		1	0.093	0.01
		2	0.003	0.01
GLYeff	1,2	0	0.905	0.01
		1	0.092	0.01
		2	0.003	0.01
GLYeff	2	0	0.964	0.01
		1	0.036	0.01
VAL	1,2,3,4,5	0	0.391	0.01
		1	0.454	0.01
		2	0.151	0.01
		3	0.013	0.01
		4	-0.003	0.01
		5	-0.006	0.01
VAL	1,2,3,4,5	0	0.361	0.01
		1	0.465	0.01
		2	0.162	0.01
		3	0.013	0.01
		4	0	0.01
		5	-0.001	0.01
VAL	2,3,4,5	0	0.376	0.01
		1	0.465	0.01
		2	0.151	0.01
		3	0.009	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.42	0.024
		1	0.419	0.024
		2	0.141	0.024
		3	0.018	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.231	0.02
		1	0.44	0.02
		2	0.26	0.02
		3	0.067	0.02
		4	0.005	0.02
		5	0	0.02
		6	-0.002	0.02
LEU	2,3,4,5,6	0	0.261	0.017
		1	0.427	0.017
		2	0.252	0.017
		3	0.057	0.017
		4	0.003	0.017
		5	0	0.017
ILE	2,3,4,5,6	0	0.262	0.01
		1	0.443	0.01
		2	0.237	0.01
		3	0.055	0.01

		4	0.003	0.01
		5	-0.001	0.01
ILE	2,3,4,5,6	0	0.272	0.02
		1	0.434	0.02
		2	0.233	0.02
		3	0.053	0.02
		4	0.006	0.02
		5	0.001	0.02
METeff	1,2,3,4,5	0	0.389	0.01
		1	0.383	0.01
		2	0.171	0.01
		3	0.05	0.01
		4	0.004	0.01
		5	0.003	0.01
METeff	1,2,3,4,5	0	0.39	0.01
		1	0.394	0.01
		2	0.172	0.01
		3	0.039	0.01
		4	0.003	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.431	0.013
		1	0.399	0.013
		2	0.146	0.013
		3	0.023	0.013
		4	0.001	0.013
METeff	2,3,4,5	0	0.432	0.011
		1	0.396	0.011
		2	0.147	0.011
		3	0.023	0.011
		4	0.002	0.011
SEReff	1,2,3	0	0.699	0.01
		1	0.288	0.01
		2	0.013	0.01
		3	0	0.01
SEReff	1,2,3	0	0.7	0.01
		1	0.288	0.01
		2	0.015	0.01
		3	-0.003	0.01
SEReff	2,3	0	0.726	0.01
		1	0.271	0.01
		2	0.003	0.01
SEReff	2,3	0	0.725	0.011
		1	0.27	0.011
		2	0.005	0.011
SEReff	1,2	0	0.925	0.018
		1	0.07	0.018
		2	0.005	0.018
THR	1,2,3,4	0	0.365	0.01
		1	0.453	0.01
		2	0.161	0.01
		3	0.02	0.01
		4	0.001	0.01
THR	2,3,4	0	0.441	0.01

```
            1      0.431 0.01
            2      0.12  0.01
            3      0.008 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.266 0.015
            1      0.418 0.015
            2      0.243 0.015
            3      0.064 0.015
            4      0.008 0.015
            5      0.001 0.015
            6      0      0.015
            7      0      0.015
            8      0      0.015
            9      0      0.015
PHE_TYR     2,3,4,5,6,7,8,9   0      0.272 0.018
            1      0.423 0.018
            2      0.241 0.018
            3      0.057 0.018
            4      0.006 0.018
            5      0      0.018
            6      0      0.018
            7      0      0.018
            8      0      0.018
PHE_TYR     2,3,4,5,6,7,8,9   0      0.271 0.019
            1      0.424 0.019
            2      0.239 0.019
            3      0.059 0.019
            4      0.006 0.019
            5      0      0.019
            6      0      0.019
            7      0      0.019
            8      0      0.019
PHE_TYR     1,2    0      0.945 0.01
            1      0.055 0.01
            2      0      0.01
ASP   1,2,3,4      0      0.374 0.011
            1      0.438 0.011
            2      0.163 0.011
            3      0.023 0.011
            4      0.001 0.011
ASP   1,2,3,4      0      0.375 0.011
            1      0.435 0.011
            2      0.167 0.011
            3      0.022 0.011
            4      0.001 0.011
ASP   2,3,4 0      0.439 0.01
            1      0.432 0.01
            2      0.119 0.01
            3      0.01  0.01
ASP   2,3,4 0      0.442 0.018
            1      0.425 0.018
            2      0.119 0.018
            3      0.014 0.018
ASP   1,2   0      0.628 0.011
```

		1	0.336	0.011
		2	0.035	0.011
CYS	1,2,3	0	0.702	0.018
		1	0.278	0.018
		2	0.017	0.018
		3	0.003	0.018
GLU	1,2,3,4,5	0	0.254	0.023
		1	0.448	0.023
		2	0.24	0.023
		3	0.05	0.023
		4	0.009	0.023
		5	-0.001	0.023
GLU	1,2,3,4,5	0	0.28	0.01
		1	0.426	0.01
		2	0.235	0.01
		3	0.054	0.01
		4	0.005	0.01
		5	0	0.01
GLU	1,2,3,4,5	0	0.28	0.011
		1	0.426	0.011
		2	0.235	0.011
		3	0.055	0.011
		4	0.004	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.317	0.01
		1	0.458	0.01
		2	0.205	0.01
		3	0.026	0.01
		4	-0.005	0.01
GLU	2,3,4,5	0	0.322	0.011
		1	0.449	0.011
		2	0.2	0.011
		3	0.029	0.011
		4	-0.001	0.011
LYS	1,2,3,4,5,6	0	0.242	0.01
		1	0.423	0.01
		2	0.252	0.01
		3	0.075	0.01
		4	0.009	0.01
		5	-0.001	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.243	0.01
		1	0.428	0.01
		2	0.259	0.01
		3	0.069	0.01
		4	0.006	0.01
		5	-0.001	0.01
		6	-0.003	0.01
LYS	2,3,4,5,6	0	0.255	0.01
		1	0.44	0.01
		2	0.245	0.01
		3	0.057	0.01
		4	0.003	0.01

```
            5     -0.001      0.01
ARGeff      1,2,3,4,5,6 0     0.305 0.01
            1     0.379 0.01
            2     0.242 0.01
            3     0.072 0.01
            4     0.009 0.01
            5     -0.002      0.01
            6     -0.005      0.01
ARGeff      2,3,4,5,6   0     0.341 0.01
            1     0.393 0.01
            2     0.214 0.01
            3     0.045 0.01
            4     0.006 0.01
            5     0     0.01
HISeff      1,2,3,4,5,6 0     0.423 0.013
            1     0.381 0.013
            2     0.162 0.013
            3     0.029 0.013
            4     0.003 0.013
            5     0.001 0.013
            6     0.001 0.013
HISeff      2,3,4,5,6   0     0.547 0.023
            1     0.361 0.023
            2     0.086 0.023
            3     0.011 0.023
            4     0.004 0.023
            5     -0.009      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.258 0.01
            1     0.419 0.01
            2     0.254 0.01
            3     0.061 0.01
            4     0.008 0.01
            5     0.001 0.01
            6     0.001 0.01
            7     -0.002      0.01
            8     0     0.01
            9     0     0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.275 0.023
            1     0.412 0.023
            2     0.237 0.023
            3     0.063 0.023
            4     0.007 0.023
            5     0.002 0.023
            6     0.001 0.023
            7     0     0.023
            8     0.001 0.023
            9     0.001 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.283 0.01
            1     0.419 0.01
            2     0.235 0.01
            3     0.057 0.01
            4     0.003 0.01
            5     0.001 0.01
```

		6	0	0.01
		7	0	0.01
		8	0.002	0.01
PHE_TYR	2,3,4,5,6,7,8,9	0	0.249	0.01
		1	0.437	0.01
		2	0.249	0.01
		3	0.061	0.01
		4	0.008	0.01
		5	0	0.01
		6	-0.001	0.01
		7	-0.001	0.01
		8	-0.001	0.01
PHE_TYR	1,2	0	0.945	0.01
		1	0.054	0.01
		2	0.001	0.01
GLU	1,2,3,4,5	0	0.294	0.01
		1	0.413	0.01
		2	0.235	0.01
		3	0.057	0.01
		4	0.003	0.01
		5	-0.002	0.01
GLU	2,3,4,5	0	0.324	0.011
		1	0.447	0.011
		2	0.199	0.011
		3	0.028	0.011
		4	0.001	0.011
GLU	2,3,4,5	0	0.309	0.011
		1	0.46	0.013
		2	0.206	0.01
		3	0.028	0.012
		4	-0.003	0.013
ALA	1,2,3	0	0.589	0.011
		1	0.384	0.011
		2	0.025	0.011
		3	0.001	0.011
ALA	2,3	0	0.61	0.011
		1	0.38	0.011
		2	0.01	0.011
GLYeff	1,2	0	0.907	0.01
		1	0.096	0.01
		2	-0.003	0.01
GLYeff	1,2	0	0.897	0.01
		1	0.1	0.01
		2	0.003	0.01
GLYeff	2	0	0.969	0.01
		1	0.031	0.01
VAL	1,2,3,4,5	0	0.368	0.01
		1	0.465	0.01
		2	0.16	0.01
		3	0.015	0.01
		4	-0.001	0.01
		5	-0.006	0.01
VAL	1,2,3,4,5	0	0.342	0.01

		1	0.47	0.01
		2	0.173	0.01
		3	0.018	0.01
		4	-0.001	0.01
		5	-0.001	0.01
VAL	2,3,4,5	0	0.356	0.01
		1	0.473	0.01
		2	0.161	0.01
		3	0.01	0.01
		4	0	0.01
VAL	2,3,4,5	0	0.399	0.024
		1	0.423	0.024
		2	0.153	0.024
		3	0.023	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.198	0.02
		1	0.448	0.02
		2	0.272	0.02
		3	0.08	0.02
		4	0.006	0.02
		5	-0.001	0.02
		6	-0.002	0.02
LEU	2,3,4,5,6	0	0.243	0.017
		1	0.43	0.017
		2	0.261	0.017
		3	0.062	0.017
		4	0.004	0.017
		5	0	0.017
ILE	2,3,4,5,6	0	0.254	0.01
		1	0.46	0.013
		2	0.244	0.01
		3	0.055	0.01
		4	-0.003	0.011
		5	-0.009	0.011
ILE	2,3,4,5,6	0	0.251	0.02
		1	0.441	0.02
		2	0.243	0.02
		3	0.059	0.02
		4	0.006	0.02
		5	0.001	0.02
METeff	1,2,3,4,5	0	0.38	0.01
		1	0.394	0.01
		2	0.185	0.01
		3	0.044	0.01
		4	-0.003	0.01
		5	-0.001	0.01
METeff	1,2,3,4,5	0	0.384	0.01
		1	0.397	0.01
		2	0.177	0.01
		3	0.038	0.01
		4	0.002	0.01
		5	0.003	0.01
METeff	2,3,4,5	0	0.42	0.013

		1	0.405	0.013
		2	0.152	0.013
		3	0.023	0.013
		4	0	0.013
METeff	2,3,4,5	0	0.422	0.011
		1	0.403	0.011
		2	0.151	0.011
		3	0.023	0.011
		4	0.001	0.011
SEReff	1,2,3	0	0.686	0.01
		1	0.295	0.01
		2	0.016	0.01
		3	0.003	0.01
SEReff	1,2,3	0	0.695	0.01
		1	0.299	0.01
		2	0.012	0.01
		3	-0.006	0.01
SEReff	2,3	0	0.722	0.01
		1	0.274	0.01
		2	0.004	0.01
SEReff	2,3	0	0.721	0.011
		1	0.274	0.011
		2	0.005	0.011
SEReff	1,2	0	0.913	0.018
		1	0.08	0.018
		2	0.007	0.018
THR	1,2,3,4	0	0.369	0.01
		1	0.436	0.01
		2	0.169	0.01
		3	0.031	0.01
		4	-0.004	0.01
THR	2,3,4	0	0.433	0.01
		1	0.438	0.01
		2	0.121	0.01
		3	0.008	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.25	0.015
		1	0.42	0.015
		2	0.254	0.015
		3	0.067	0.015
		4	0.008	0.015
		5	0.001	0.015
		6	0	0.015
		7	0	0.015
		8	0	0.015
		9	0	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.251	0.018
		1	0.431	0.018
		2	0.249	0.018
		3	0.062	0.018
		4	0.007	0.018
		5	0	0.018
		6	0	0.018
		7	0	0.018

```
            8     0     0.018
PHE_TYR     2,3,4,5,6,7,8,9   0     0.255 0.019
            1     0.428 0.019
            2     0.249 0.019
            3     0.062 0.019
            4     0.006 0.019
            5     0     0.019
            6     0     0.019
            7     0     0.019
            8     0     0.019
PHE_TYR     1,2   0     0.944 0.01
            1     0.056 0.01
            2     0     0.01
ASP   1,2,3,4     0     0.366 0.011
            1     0.438 0.011
            2     0.179 0.011
            3     0.021 0.011
            4     -0.004      0.011
ASP   1,2,3,4     0     0.362 0.011
            1     0.446 0.011
            2     0.169 0.011
            3     0.023 0.011
            4     0     0.011
ASP   2,3,4 0     0.429 0.01
            1     0.438 0.01
            2     0.122 0.01
            3     0.011 0.01
ASP   2,3,4 0     0.429 0.018
            1     0.432 0.018
            2     0.125 0.018
            3     0.014 0.018
ASP   1,2   0     0.621 0.011
            1     0.343 0.011
            2     0.035 0.011
CYS   1,2,3 0     0.671 0.018
            1     0.302 0.018
            2     0.044 0.018
            3     -0.017      0.018
GLU   1,2,3,4,5   0     0.242 0.023
            1     0.449 0.023
            2     0.252 0.023
            3     0.059 0.023
            4     -0.001      0.023
            5     -0.001      0.023
GLU   1,2,3,4,5   0     0.265 0.01
            1     0.437 0.01
            2     0.237 0.01
            3     0.058 0.01
            4     0.002 0.01
            5     0.001 0.01
GLU   1,2,3,4,5   0     0.265 0.011
            1     0.432 0.011
            2     0.241 0.011
```

```
		3	0.057	0.011
		4	0.005	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.3	0.01
		1	0.466	0.01
		2	0.215	0.01
		3	0.026	0.01
		4	-0.006		0.01
GLU	2,3,4,5	0	0.309	0.011
		1	0.454	0.011
		2	0.206	0.011
		3	0.031	0.011
		4	-0.001		0.011
LYS	1,2,3,4,5,6	0	0.228	0.01
		1	0.422	0.01
		2	0.268	0.01
		3	0.074	0.01
		4	0.009	0.01
		5	0	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.231	0.01
		1	0.436	0.01
		2	0.27	0.01
		3	0.073	0.01
		4	0.005	0.01
		5	-0.006		0.01
		6	-0.009		0.01
LYS	2,3,4,5,6	0	0.24	0.01
		1	0.443	0.01
		2	0.254	0.01
		3	0.058	0.01
		4	0.006	0.01
		5	-0.001		0.01
ARGeff		1,2,3,4,5,6	0	0.287	0.01
		1	0.386	0.011
		2	0.246	0.01
		3	0.079	0.01
		4	0.011	0.01
		5	-0.002		0.01
		6	-0.007		0.01
ARGeff		2,3,4,5,6	0	0.323	0.01
		1	0.407	0.011
		2	0.224	0.01
		3	0.049	0.01
		4	-0.004		0.01
		5	0	0.01
HISeff		1,2,3,4,5,6	0	0.406	0.013
		1	0.387	0.013
		2	0.17	0.013
		3	0.033	0.013
		4	0.003	0.013
		5	0.001	0.013
		6	0	0.013
```

```
HISeff      2,3,4,5,6   0      0.522 0.023
            1      0.371 0.023
            2      0.088 0.023
            3      0.017 0.023
            4      0.005 0.023
            5      -0.003      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.243 0.01
            1      0.431 0.01
            2      0.263 0.01
            3      0.058 0.01
            4      0.01  0.01
            5      0.001 0.01
            6      -0.006      0.01
            7      0     0.01
            8      0     0.01
            9      0     0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.258 0.023
            1      0.414 0.023
            2      0.249 0.023
            3      0.065 0.023
            4      0.007 0.023
            5      0.001 0.023
            6      0.001 0.023
            7      0     0.023
            8      0.003 0.023
            9      0.002 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0      0.267 0.01
            1      0.423 0.01
            2      0.244 0.01
            3      0.058 0.01
            4      0.007 0.01
            5      0     0.01
            6      0.001 0.01
            7      -0.001      0.01
            8      0.002 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0      0.242 0.01
            1      0.448 0.01
            2      0.254 0.01
            3      0.063 0.01
            4      0.007 0.01
            5      -0.001      0.01
            6      -0.003      0.01
            7      -0.005      0.01
            8      -0.005      0.01
PHE_TYR     1,2    0      0.946 0.01
            1      0.052 0.01
            2      0.002 0.01
GLU   1,2,3,4,5    0      0.273 0.01
            1      0.422 0.01
            2      0.244 0.01
            3      0.062 0.01
            4      0.001 0.01
            5      -0.002      0.01
```

GLU	2,3,4,5	0	0.308	0.011
		1	0.452	0.011
		2	0.208	0.011
		3	0.033	0.011
		4	0	0.011
GLU	2,3,4,5	0	0.293	0.011
		1	0.466	0.014
		2	0.214	0.01
		3	0.029	0.012
		4	-0.002	0.013
ALA	1,2,3	0	0.591	0.011
		1	0.386	0.011
		2	0.022	0.011
		3	0.001	0.011
ALA	2,3	0	0.61	0.011
		1	0.382	0.011
		2	0.007	0.011
GLYeff	1,2	0	0.898	0.01
		1	0.101	0.01
		2	0.001	0.01
GLYeff	1,2	0	0.899	0.01
		1	0.098	0.01
		2	0.003	0.01
GLYeff	2	0	0.97	0.01
		1	0.03	0.01
VAL	1,2,3,4,5	0	0.375	0.01
		1	0.464	0.01
		2	0.152	0.01
		3	0.017	0.01
		4	-0.002	0.01
		5	-0.006	0.01
VAL	1,2,3,4,5	0	0.348	0.01
		1	0.464	0.01
		2	0.173	0.01
		3	0.017	0.01
		4	0	0.01
		5	-0.001	0.01
VAL	2,3,4,5	0	0.364	0.01
		1	0.467	0.01
		2	0.16	0.01
		3	0.01	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.406	0.024
		1	0.422	0.024
		2	0.15	0.024
		3	0.021	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.223	0.02
		1	0.438	0.02
		2	0.264	0.02
		3	0.073	0.02
		4	0.005	0.02
		5	0	0.02

		6	-0.002	0.02
LEU	2,3,4,5,6	0	0.251	0.017
		1	0.425	0.017
		2	0.257	0.017
		3	0.063	0.017
		4	0.004	0.017
		5	0	0.017
ILE	2,3,4,5,6	0	0.255	0.01
		1	0.447	0.01
		2	0.245	0.01
		3	0.055	0.01
		4	0.002	0.01
		5	-0.005	0.01
ILE	2,3,4,5,6	0	0.262	0.02
		1	0.435	0.02
		2	0.239	0.02
		3	0.058	0.02
		4	0.006	0.02
		5	0	0.02
METeff	1,2,3,4,5	0	0.385	0.01
		1	0.397	0.01
		2	0.168	0.01
		3	0.039	0.01
		4	0.01	0.01
		5	0.001	0.01
METeff	1,2,3,4,5	0	0.383	0.01
		1	0.399	0.01
		2	0.176	0.01
		3	0.037	0.01
		4	0.002	0.01
		5	0.003	0.01
METeff	2,3,4,5	0	0.424	0.013
		1	0.401	0.013
		2	0.148	0.013
		3	0.025	0.013
		4	0.002	0.013
METeff	2,3,4,5	0	0.425	0.011
		1	0.398	0.011
		2	0.151	0.011
		3	0.025	0.011
		4	0.001	0.011
SEReff	1,2,3	0	0.688	0.01
		1	0.29	0.01
		2	0.02	0.01
		3	0.002	0.01
SEReff	1,2,3	0	0.692	0.01
		1	0.299	0.01
		2	0.014	0.01
		3	-0.005	0.01
SEReff	2,3	0	0.722	0.01
		1	0.275	0.01
		2	0.003	0.01
SEReff	2,3	0	0.722	0.011

```
            1      0.273 0.011
            2      0.005 0.011
SEReff      1,2    0      0.916 0.018
            1      0.078 0.018
            2      0.006 0.018
THR   1,2,3,4      0      0.372 0.01
            1      0.436 0.01
            2      0.171 0.01
            3      0.029 0.01
            4      -0.008      0.01
THR   2,3,4 0      0.428 0.01
            1      0.438 0.01
            2      0.124 0.01
            3      0.01  0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.257 0.015
            1      0.421 0.015
            2      0.249 0.015
            3      0.064 0.015
            4      0.009 0.015
            5      0.001 0.015
            6      0      0.015
            7      -0.001      0.015
            8      0      0.015
            9      0      0.015
PHE_TYR     2,3,4,5,6,7,8,9   0      0.256 0.018
            1      0.428 0.018
            2      0.248 0.018
            3      0.061 0.018
            4      0.008 0.018
            5      0      0.018
            6      0      0.018
            7      0      0.018
            8      0      0.018
PHE_TYR     2,3,4,5,6,7,8,9   0      0.261 0.019
            1      0.425 0.019
            2      0.248 0.019
            3      0.062 0.019
            4      0.005 0.019
            5      0      0.019
            6      0      0.019
            7      0      0.019
            8      0      0.019
PHE_TYR     1,2    0      0.947 0.01
            1      0.052 0.01
            2      0.001 0.01
ASP   1,2,3,4      0      0.358 0.011
            1      0.445 0.011
            2      0.173 0.011
            3      0.021 0.011
            4      0.002 0.011
ASP   1,2,3,4      0      0.362 0.011
            1      0.444 0.011
            2      0.171 0.011
```

		3	0.022	0.011	
		4	0.001	0.011	
ASP	2,3,4	0	0.429	0.01	
		1	0.437	0.01	
		2	0.122	0.01	
		3	0.012	0.01	
ASP	2,3,4	0	0.428	0.018	
		1	0.433	0.018	
		2	0.124	0.018	
		3	0.015	0.018	
ASP	1,2	0	0.619	0.011	
		1	0.344	0.011	
		2	0.036	0.011	
CYS	1,2,3	0	0.688	0.03	
		1	0.284	0.022	
		2	0.018	0.024	
		3	0.01	0.025	
GLU	1,2,3,4,5	0	0.246	0.023	
		1	0.46	0.023	
		2	0.25	0.023	
		3	0.058	0.023	
		4	-0.008	0.023	
		5	-0.007	0.023	
GLU	1,2,3,4,5	0	0.265	0.01	
		1	0.432	0.01	
		2	0.239	0.01	
		3	0.059	0.01	
		4	0.003	0.01	
		5	0.002	0.01	
GLU	1,2,3,4,5	0	0.265	0.011	
		1	0.429	0.011	
		2	0.243	0.011	
		3	0.058	0.011	
		4	0.005	0.011	
		5	0	0.011	
GLU	2,3,4,5	0	0.3	0.01	
		1	0.462	0.01	
		2	0.215	0.01	
		3	0.028	0.01	
		4	-0.005	0.01	
GLU	2,3,4,5	0	0.31	0.011	
		1	0.456	0.011	
		2	0.207	0.011	
		3	0.029	0.011	
		4	-0.003	0.011	
LYS	1,2,3,4,5,6	0	0.232	0.01	
		1	0.42	0.01	
		2	0.263	0.01	
		3	0.076	0.01	
		4	0.011	0.01	
		5	-0.001	0.01	
		6	-0.001	0.01	
LYS	1,2,3,4,5,6	0	0.236	0.01	

		1	0.424	0.01
		2	0.261	0.01
		3	0.074	0.01
		4	0.009	0.01
		5	-0.001	0.01
		6	-0.003	0.01
LYS	2,3,4,5,6	0	0.248	0.01
		1	0.44	0.01
		2	0.248	0.01
		3	0.061	0.01
		4	0.006	0.01
		5	-0.002	0.01
ARGeff	1,2,3,4,5,6	0	0.288	0.01
		1	0.383	0.01
		2	0.248	0.01
		3	0.078	0.01
		4	0.009	0.01
		5	-0.001	0.01
		6	-0.005	0.01
ARGeff	2,3,4,5,6	0	0.326	0.01
		1	0.402	0.01
		2	0.223	0.01
		3	0.047	0.01
		4	0.004	0.01
		5	-0.002	0.01
HISeff	1,2,3,4,5,6	0	0.409	0.013
		1	0.387	0.013
		2	0.17	0.013
		3	0.029	0.013
		4	0.004	0.013
		5	0	0.013
		6	0.001	0.013
HISeff	2,3,4,5,6	0	0.529	0.023
		1	0.37	0.023
		2	0.087	0.023
		3	0.011	0.023
		4	0.005	0.023
		5	-0.002	0.023
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.248	0.01
		1	0.415	0.01
		2	0.265	0.01
		3	0.063	0.01
		4	0.008	0.01
		5	0.002	0.01
		6	0	0.01
		7	-0.001	0.01
		8	0	0.01
		9	0	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.266	0.023
		1	0.411	0.023
		2	0.242	0.023
		3	0.063	0.023
		4	0.009	0.023

```
            5     0.001 0.023
            6     0.001 0.023
            7     0     0.023
            8     0.003 0.023
            9     0.003 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.269 0.01
            1     0.418 0.01
            2     0.239 0.01
            3     0.063 0.01
            4     0.007 0.01
            5     -0.001      0.01
            6     0.001 0.01
            7     0.001 0.01
            8     0.003 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0     0.248 0.01
            1     0.441 0.01
            2     0.249 0.01
            3     0.064 0.01
            4     0.006 0.01
            5     0     0.01
            6     -0.001      0.01
            7     -0.002      0.01
            8     -0.003      0.01
PHE_TYR     1,2   0     0.946 0.01
            1     0.053 0.01
            2     0.001 0.01
GLU   1,2,3,4,5   0     0.279 0.01
            1     0.416 0.01
            2     0.24  0.01
            3     0.06  0.01
            4     0.004 0.01
            5     0     0.01
GLU   2,3,4,5     0     0.31  0.011
            1     0.451 0.011
            2     0.207 0.011
            3     0.032 0.011
            4     0.001 0.011
GLU   2,3,4,5     0     0.295 0.01
            1     0.464 0.013
            2     0.215 0.01
            3     0.029 0.011
            4     -0.003      0.012
ALA_U 1,2,3 0     0.724 0.011
            1     0.095 0.011
            2     0.047 0.011
            3     0.135 0.011
ALA_U 2,3   0     0.771 0.011
            1     0.062 0.011
            2     0.168 0.011
GLYeff_U    1,2   0     0.737 0.01
            1     0.151 0.01
            2     0.112 0.01
GLYeff_U    1,2   0     0.742 0.01
```

```
            1     0.152 0.01
            2     0.106 0.01
GLYeff_U    2     0     0.817 0.01
            1     0.183 0.01
VAL_U 1,2,3,4,5   0     0.547 0.012
            1     0.141 0.01
            2     0.163 0.01
            3     0.114 0.01
            4     0.018 0.01
            5     0.017 0.01
VAL_U 1,2,3,4,5   0     0.554 0.01
            1     0.134 0.01
            2     0.159 0.01
            3     0.12  0.01
            4     0.014 0.01
            5     0.018 0.01
VAL_U 2,3,4,5     0     0.594 0.014
            1     0.114 0.01
            2     0.25  0.01
            3     0.021 0.01
            4     0.022 0.01
VAL_U 2,3,4,5     0     0.6   0.024
            1     0.106 0.024
            2     0.235 0.024
            3     0.036 0.024
            4     0.023 0.024
LEU_U 1,2,3,4,5,6 0     0.455 0.02
            1     0.14  0.02
            2     0.285 0.02
            3     0.057 0.02
            4     0.06  0.02
            5     0.002 0.02
            6     0.002 0.02
LEU_U 2,3,4,5,6   0     0.491 0.017
            1     0.196 0.017
            2     0.216 0.017
            3     0.066 0.017
            4     0.025 0.017
            5     0.005 0.017
ILE_U 2,3,4,5,6   0     0.487 0.01
            1     0.211 0.01
            2     0.21  0.01
            3     0.069 0.01
            4     0.019 0.01
            5     0.005 0.01
ILE_U 2,3,4,5,6   0     0.49  0.02
            1     0.208 0.02
            2     0.204 0.02
            3     0.072 0.02
            4     0.02  0.02
            5     0.006 0.02
METeff_U    1,2,3,4,5   0     0.5   0.01
            1     0.263 0.01
```

```
            2     0.128 0.01
            3     0.072 0.01
            4     0.028 0.01
            5     0.009 0.01
METeff_U    1,2,3,4,5   0     0.514 0.01
            1     0.261 0.01
            2     0.111 0.01
            3     0.079 0.01
            4     0.028 0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0     0.576 0.013
            1     0.255 0.013
            2     0.092 0.013
            3     0.064 0.013
            4     0.013 0.013
METeff_U    2,3,4,5     0     0.582 0.011
            1     0.25  0.011
            2     0.092 0.011
            3     0.066 0.011
            4     0.01  0.011
SEReff_U    1,2,3 0     0.68  0.01
            1     0.164 0.01
            2     0.077 0.01
            3     0.079 0.01
SEReff_U    1,2,3 0     0.682 0.01
            1     0.171 0.01
            2     0.075 0.01
            3     0.072 0.01
SEReff_U    2,3   0     0.726 0.01
            1     0.177 0.01
            2     0.097 0.01
SEReff_U    2,3   0     0.726 0.011
            1     0.173 0.011
            2     0.101 0.011
SEReff_U    1,2   0     0.749 0.018
            1     0.121 0.018
            2     0.13  0.018
THR_U 1,2,3,4     0     0.554 0.023
            1     0.207 0.016
            2     0.114 0.016
            3     0.099 0.017
            4     0.026 0.019
THR_U 2,3,4 0     0.612 0.01
            1     0.232 0.01
            2     0.127 0.01
            3     0.028 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.369 0.015
            1     0.158 0.015
            2     0.14  0.015
            3     0.166 0.015
            4     0.081 0.015
            5     0.044 0.015
            6     0.027 0.015
```

```
            7     0.01  0.015
            8     0.003 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.393 0.018
            1     0.152 0.018
            2     0.204 0.018
            3     0.118 0.018
            4     0.073 0.018
            5     0.037 0.018
            6     0.017 0.018
            7     0.004 0.018
            8     0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.39  0.019
            1     0.153 0.019
            2     0.203 0.019
            3     0.12  0.019
            4     0.074 0.019
            5     0.036 0.019
            6     0.018 0.019
            7     0.004 0.019
            8     0.002 0.019
PHE_TYR_U   1,2   0     0.759 0.01
            1     0.096 0.01
            2     0.145 0.01
ASP_U 1,2,3,4     0     0.557 0.011
            1     0.218 0.011
            2     0.147 0.011
            3     0.059 0.011
            4     0.019 0.011
ASP_U 1,2,3,4     0     0.558 0.011
            1     0.22  0.011
            2     0.143 0.011
            3     0.063 0.011
            4     0.016 0.011
ASP_U 2,3,4 0     0.622 0.01
            1     0.226 0.01
            2     0.113 0.01
            3     0.039 0.01
ASP_U 2,3,4 0     0.62  0.018
            1     0.222 0.018
            2     0.116 0.018
            3     0.042 0.018
ASP_U 1,2   0     0.732 0.011
            1     0.161 0.011
            2     0.107 0.011
CYS_U 1,2,3 0     0.666 0.023
            1     0.172 0.018
            2     0.06  0.018
            3     0.102 0.018
GLU_U 1,2,3,4,5   0     0.466 0.023
            1     0.242 0.023
            2     0.207 0.023
            3     0.069 0.023
```

```
            4     0.012 0.023
            5     0.004 0.023
GLU_U 1,2,3,4,5   0     0.483 0.01
            1     0.212 0.01
            2     0.2   0.01
            3     0.076 0.01
            4     0.022 0.01
            5     0.007 0.01
GLU_U 1,2,3,4,5   0     0.483 0.011
            1     0.212 0.011
            2     0.204 0.011
            3     0.074 0.011
            4     0.021 0.011
            5     0.006 0.011
GLU_U 2,3,4,5     0     0.529 0.01
            1     0.229 0.01
            2     0.192 0.01
            3     0.043 0.01
            4     0.007 0.01
GLU_U 2,3,4,5     0     0.538 0.011
            1     0.225 0.011
            2     0.187 0.011
            3     0.04  0.011
            4     0.01  0.011
LYS_U 1,2,3,4,5,6 0     0.449 0.01
            1     0.214 0.01
            2     0.171 0.01
            3     0.11  0.01
            4     0.038 0.01
            5     0.016 0.01
            6     0.002 0.01
LYS_U 1,2,3,4,5,6 0     0.447 0.01
            1     0.212 0.01
            2     0.172 0.01
            3     0.115 0.01
            4     0.038 0.01
            5     0.014 0.01
            6     0.003 0.01
LYS_U 2,3,4,5,6   0     0.478 0.01
            1     0.221 0.01
            2     0.203 0.01
            3     0.076 0.01
            4     0.018 0.01
            5     0.003 0.01
HISeff_U    1,2,3,4,5,6 0     0.498 0.013
            1     0.219 0.013
            2     0.114 0.013
            3     0.098 0.013
            4     0.041 0.013
            5     0.024 0.013
            6     0.005 0.013
HISeff_U    2,3,4,5,6   0     0.501 0.023
            1     0.226 0.023
```

```
            2     0.169 0.023
            3     0.07  0.023
            4     0.027 0.023
            5     0.007 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.365 0.01
            1     0.168 0.01
            2     0.138 0.01
            3     0.161 0.01
            4     0.083 0.01
            5     0.049 0.01
            6     0.027 0.01
            7     0.014 0.01
            8     0     0.01
            9     -0.006      0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.381 0.023
            1     0.157 0.023
            2     0.133 0.023
            3     0.156 0.023
            4     0.077 0.023
            5     0.043 0.023
            6     0.026 0.023
            7     0.016 0.023
            8     0.007 0.023
            9     0.003 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.39  0.01
            1     0.156 0.01
            2     0.2   0.01
            3     0.117 0.01
            4     0.073 0.01
            5     0.036 0.01
            6     0.016 0.01
            7     0.005 0.01
            8     0.007 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.376 0.01
            1     0.158 0.01
            2     0.218 0.01
            3     0.122 0.01
            4     0.073 0.01
            5     0.039 0.01
            6     0.015 0.01
            7     0     0.01
            8     -0.001      0.01
PHE_TYR_U   1,2   0     0.761 0.01
            1     0.095 0.01
            2     0.144 0.01
GLU_U 1,2,3,4,5   0     0.48  0.01
            1     0.211 0.01
            2     0.204 0.01
            3     0.076 0.01
            4     0.022 0.01
            5     0.007 0.01
GLU_U 2,3,4,5     0     0.541 0.011
            1     0.221 0.011
```

```
            2     0.184 0.011
            3     0.042 0.011
            4     0.012 0.011
GLU_U 2,3,4,5     0     0.532 0.016
            1     0.227 0.01
            2     0.19  0.01
            3     0.041 0.011
            4     0.01  0.012
ALA_U 1,2,3 0     0.725 0.011
            1     0.09  0.011
            2     0.045 0.011
            3     0.14  0.011
ALA_U 2,3   0     0.771 0.011
            1     0.06  0.011
            2     0.169 0.011
GLYeff_U    1,2   0     0.73  0.01
            1     0.158 0.01
            2     0.112 0.01
GLYeff_U    1,2   0     0.743 0.01
            1     0.149 0.01
            2     0.108 0.01
GLYeff_U    2     0     0.817 0.01
            1     0.183 0.01
VAL_U 1,2,3,4,5   0     0.547 0.011
            1     0.132 0.01
            2     0.166 0.01
            3     0.113 0.01
            4     0.02  0.01
            5     0.022 0.01
VAL_U 1,2,3,4,5   0     0.551 0.01
            1     0.13  0.01
            2     0.164 0.01
            3     0.123 0.01
            4     0.014 0.01
            5     0.019 0.01
VAL_U 2,3,4,5     0     0.585 0.013
            1     0.112 0.01
            2     0.259 0.01
            3     0.022 0.01
            4     0.022 0.01
VAL_U 2,3,4,5     0     0.594 0.024
            1     0.101 0.024
            2     0.243 0.024
            3     0.038 0.024
            4     0.024 0.024
LEU_U 1,2,3,4,5,6 0     0.447 0.02
            1     0.128 0.02
            2     0.297 0.02
            3     0.062 0.02
            4     0.06  0.02
            5     0.006 0.02
            6     0     0.02
LEU_U 2,3,4,5,6   0     0.476 0.017
```

		1	0.196	0.017
		2	0.227	0.017
		3	0.069	0.017
		4	0.026	0.017
		5	0.006	0.017
ILE_U	2,3,4,5,6	0	0.466	0.01
		1	0.219	0.01
		2	0.216	0.01
		3	0.072	0.01
		4	0.022	0.01
		5	0.006	0.01
ILE_U	2,3,4,5,6	0	0.472	0.02
		1	0.211	0.02
		2	0.213	0.02
		3	0.075	0.02
		4	0.022	0.02
		5	0.007	0.02
METeff_U	1,2,3,4,5	0	0.488	0.01
		1	0.277	0.01
		2	0.131	0.01
		3	0.072	0.01
		4	0.031	0.01
		5	0.001	0.01
METeff_U	1,2,3,4,5	0	0.505	0.01
		1	0.259	0.01
		2	0.12	0.01
		3	0.077	0.01
		4	0.03	0.01
		5	0.009	0.01
METeff_U	2,3,4,5	0	0.57	0.013
		1	0.254	0.013
		2	0.096	0.013
		3	0.068	0.013
		4	0.012	0.013
METeff_U	2,3,4,5	0	0.574	0.011
		1	0.252	0.011
		2	0.097	0.011
		3	0.067	0.011
		4	0.01	0.011
SEReff_U	1,2,3	0	0.677	0.01
		1	0.159	0.01
		2	0.076	0.01
		3	0.088	0.01
SEReff_U	1,2,3	0	0.675	0.01
		1	0.167	0.01
		2	0.077	0.01
		3	0.081	0.01
SEReff_U	2,3	0	0.722	0.01
		1	0.175	0.01
		2	0.103	0.01
SEReff_U	2,3	0	0.722	0.011
		1	0.175	0.011
		2	0.103	0.011

```
SEReff_U     1,2    0      0.748 0.018
             1      0.121 0.018
             2      0.131 0.018
THR_U 1,2,3,4       0      0.587 0.019
             1      0.204 0.012
             2      0.146 0.012
             3      0.063 0.013
             4      0      0.015
THR_U 2,3,4  0      0.618 0.01
             1      0.216 0.01
             2      0.135 0.01
             3      0.031 0.01
PHE_TYR_U    1,2,3,4,5,6,7,8,9 0      0.366 0.015
             1      0.16  0.015
             2      0.141 0.015
             3      0.168 0.015
             4      0.078 0.015
             5      0.045 0.015
             6      0.026 0.015
             7      0.011 0.015
             8      0.004 0.015
             9      0.001 0.015
PHE_TYR_U    2,3,4,5,6,7,8,9   0      0.379 0.018
             1      0.154 0.018
             2      0.209 0.018
             3      0.12  0.018
             4      0.076 0.018
             5      0.038 0.018
             6      0.017 0.018
             7      0.004 0.018
             8      0.002 0.018
PHE_TYR_U    2,3,4,5,6,7,8,9   0      0.382 0.019
             1      0.153 0.019
             2      0.208 0.019
             3      0.121 0.019
             4      0.074 0.019
             5      0.038 0.019
             6      0.018 0.019
             7      0.004 0.019
             8      0.002 0.019
PHE_TYR_U    1,2    0      0.756 0.01
             1      0.094 0.01
             2      0.15  0.01
ASP_U 1,2,3,4       0      0.55  0.011
             1      0.222 0.011
             2      0.152 0.011
             3      0.057 0.011
             4      0.019 0.011
ASP_U 1,2,3,4       0      0.552 0.011
             1      0.22  0.011
             2      0.148 0.011
             3      0.064 0.011
             4      0.017 0.011
```

ASP_U	2,3,4	0	0.614	0.01
		1	0.231	0.01
		2	0.116	0.01
		3	0.039	0.01
ASP_U	2,3,4	0	0.616	0.018
		1	0.226	0.018
		2	0.115	0.018
		3	0.042	0.018
ASP_U	1,2	0	0.73	0.011
		1	0.16	0.011
		2	0.11	0.011
GLU_U	1,2,3,4,5	0	0.459	0.023
		1	0.239	0.023
		2	0.214	0.023
		3	0.08	0.023
		4	0.013	0.023
		5	-0.004	0.023
GLU_U	1,2,3,4,5	0	0.477	0.01
		1	0.217	0.01
		2	0.203	0.01
		3	0.075	0.01
		4	0.023	0.01
		5	0.005	0.01
GLU_U	1,2,3,4,5	0	0.483	0.011
		1	0.21	0.011
		2	0.205	0.011
		3	0.075	0.011
		4	0.021	0.011
		5	0.007	0.011
GLU_U	2,3,4,5	0	0.531	0.01
		1	0.228	0.01
		2	0.195	0.01
		3	0.038	0.01
		4	0.009	0.01
GLU_U	2,3,4,5	0	0.532	0.011
		1	0.227	0.011
		2	0.187	0.011
		3	0.044	0.011
		4	0.01	0.011
LYS_U	1,2,3,4,5,6	0	0.424	0.01
		1	0.227	0.01
		2	0.174	0.01
		3	0.116	0.01
		4	0.037	0.01
		5	0.017	0.01
		6	0.005	0.01
LYS_U	1,2,3,4,5,6	0	0.426	0.01
		1	0.224	0.01
		2	0.178	0.01
		3	0.118	0.01
		4	0.038	0.01
		5	0.013	0.01
		6	0.003	0.01

```
LYS_U 2,3,4,5,6   0      0.466 0.01
            1      0.226 0.01
            2      0.214 0.01
            3      0.073 0.01
            4      0.02  0.01
            5      0.001 0.01
ARGeff_U    1,2,3,4,5,6 0      0.446 0.013
            1      0.254 0.01
            2      0.188 0.01
            3      0.091 0.01
            4      0.024 0.01
            5      0.004 0.01
            6      -0.006      0.01
ARGeff_U    2,3,4,5,6   0      0.492 0.021
            1      0.265 0.015
            2      0.178 0.014
            3      0.062 0.015
            4      0.007 0.016
            5      -0.004      0.017
HISeff_U    1,2,3,4,5,6 0      0.489 0.013
            1      0.23  0.013
            2      0.113 0.013
            3      0.095 0.013
            4      0.043 0.013
            5      0.023 0.013
            6      0.006 0.013
HISeff_U    2,3,4,5,6   0      0.493 0.023
            1      0.232 0.023
            2      0.168 0.023
            3      0.073 0.023
            4      0.026 0.023
            5      0.008 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.361 0.01
            1      0.15  0.01
            2      0.151 0.01
            3      0.173 0.01
            4      0.08  0.01
            5      0.044 0.01
            6      0.032 0.01
            7      0.008 0.01
            8      0.001 0.01
            9      0     0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.375 0.023
            1      0.16  0.023
            2      0.135 0.023
            3      0.166 0.023
            4      0.076 0.023
            5      0.046 0.023
            6      0.026 0.023
            7      0.011 0.023
            8      0.003 0.023
            9      0.002 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.389 0.01
```

```
            1     0.156 0.01
            2     0.2   0.01
            3     0.123 0.01
            4     0.072 0.01
            5     0.033 0.01
            6     0.02  0.01
            7     0.004 0.01
            8     0.002 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.372 0.01
            1     0.149 0.01
            2     0.226 0.01
            3     0.126 0.01
            4     0.075 0.01
            5     0.038 0.01
            6     0.018 0.01
            7     0     0.01
            8     -0.003      0.01
PHE_TYR_U   1,2   0     0.756 0.01
            1     0.093 0.01
            2     0.15  0.01
GLU_U 1,2,3,4,5   0     0.485 0.01
            1     0.204 0.01
            2     0.21  0.01
            3     0.077 0.01
            4     0.019 0.01
            5     0.005 0.01
GLU_U 2,3,4,5     0     0.535 0.011
            1     0.228 0.011
            2     0.183 0.011
            3     0.041 0.011
            4     0.013 0.011
GLU_U 2,3,4,5     0     0.529 0.02
            1     0.228 0.011
            2     0.191 0.011
            3     0.043 0.013
            4     0.009 0.015
ALA_U 1,2,3 0     0.727 0.011
            1     0.088 0.011
            2     0.043 0.011
            3     0.142 0.011
ALA_U 2,3   0     0.771 0.011
            1     0.058 0.011
            2     0.172 0.011
GLYeff_U    1,2   0     0.738 0.01
            1     0.152 0.01
            2     0.11  0.01
GLYeff_U    1,2   0     0.738 0.01
            1     0.154 0.01
            2     0.108 0.01
GLYeff_U    2     0     0.814 0.01
            1     0.186 0.01
VAL_U 1,2,3,4,5   0     0.545 0.01
            1     0.136 0.01
```

```
            2     0.165 0.01
            3     0.116 0.01
            4     0.018 0.01
            5     0.019 0.01
VAL_U 1,2,3,4,5   0     0.546 0.01
            1     0.128 0.01
            2     0.165 0.01
            3     0.124 0.01
            4     0.016 0.01
            5     0.021 0.01
VAL_U 2,3,4,5     0     0.578 0.01
            1     0.114 0.01
            2     0.261 0.01
            3     0.022 0.01
            4     0.025 0.01
VAL_U 2,3,4,5     0     0.599 0.024
            1     0.103 0.024
            2     0.241 0.024
            3     0.033 0.024
            4     0.024 0.024
LEU_U 1,2,3,4,5,6 0     0.43  0.02
            1     0.137 0.02
            2     0.312 0.02
            3     0.053 0.02
            4     0.06  0.02
            5     0.002 0.02
            6     0.005 0.02
LEU_U 2,3,4,5,6   0     0.47  0.017
            1     0.199 0.017
            2     0.23  0.017
            3     0.069 0.017
            4     0.026 0.017
            5     0.006 0.017
ILE_U 2,3,4,5,6   0     0.457 0.01
            1     0.224 0.01
            2     0.218 0.01
            3     0.075 0.01
            4     0.021 0.01
            5     0.006 0.01
ILE_U 2,3,4,5,6   0     0.464 0.02
            1     0.217 0.02
            2     0.215 0.02
            3     0.075 0.02
            4     0.022 0.02
            5     0.007 0.02
METeff_U    1,2,3,4,5   0     0.507 0.01
            1     0.243 0.01
            2     0.133 0.01
            3     0.078 0.01
            4     0.023 0.01
            5     0.016 0.01
METeff_U    1,2,3,4,5   0     0.501 0.01
            1     0.262 0.01
```

```
            2     0.121 0.01
            3     0.079 0.01
            4     0.03  0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0     0.572 0.013
            1     0.251 0.013
            2     0.099 0.013
            3     0.067 0.013
            4     0.011 0.013
METeff_U    2,3,4,5     0     0.573 0.011
            1     0.253 0.011
            2     0.098 0.011
            3     0.067 0.011
            4     0.009 0.011
SEReff_U    1,2,3 0     0.673 0.01
            1     0.167 0.01
            2     0.081 0.01
            3     0.079 0.01
SEReff_U    1,2,3 0     0.674 0.01
            1     0.168 0.01
            2     0.078 0.01
            3     0.08  0.01
SEReff_U    2,3   0     0.722 0.01
            1     0.177 0.01
            2     0.101 0.01
SEReff_U    2,3   0     0.721 0.011
            1     0.176 0.011
            2     0.103 0.011
SEReff_U    1,2   0     0.747 0.018
            1     0.122 0.018
            2     0.131 0.018
THR_U 1,2,3,4     0     0.553 0.01
            1     0.204 0.01
            2     0.151 0.01
            3     0.079 0.01
            4     0.013 0.01
THR_U 2,3,4 0     0.611 0.01
            1     0.232 0.01
            2     0.115 0.01
            3     0.041 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.36  0.015
            1     0.159 0.015
            2     0.141 0.015
            3     0.171 0.015
            4     0.081 0.015
            5     0.045 0.015
            6     0.027 0.015
            7     0.011 0.015
            8     0.003 0.015
            9     0.001 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.379 0.018
            1     0.153 0.018
            2     0.209 0.018
```

```
            3     0.122 0.018
            4     0.076 0.018
            5     0.037 0.018
            6     0.018 0.018
            7     0.004 0.018
            8     0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.378 0.019
            1     0.152 0.019
            2     0.211 0.019
            3     0.122 0.019
            4     0.076 0.019
            5     0.036 0.019
            6     0.018 0.019
            7     0.004 0.019
            8     0.002 0.019
PHE_TYR_U   1,2   0     0.755 0.01
            1     0.095 0.01
            2     0.15  0.01
ASP_U 1,2,3,4     0     0.547 0.011
            1     0.224 0.011
            2     0.149 0.011
            3     0.065 0.011
            4     0.015 0.011
ASP_U 1,2,3,4     0     0.546 0.011
            1     0.224 0.011
            2     0.148 0.011
            3     0.066 0.011
            4     0.016 0.011
ASP_U 2,3,4 0     0.61  0.01
            1     0.232 0.01
            2     0.118 0.01
            3     0.04  0.01
ASP_U 2,3,4 0     0.611 0.018
            1     0.227 0.018
            2     0.119 0.018
            3     0.042 0.018
ASP_U 1,2   0     0.726 0.011
            1     0.162 0.011
            2     0.113 0.011
CYS_U 1,2,3 0     0.691 0.018
            1     0.165 0.018
            2     0.072 0.018
            3     0.072 0.018
GLU_U 1,2,3,4,5   0     0.45  0.023
            1     0.223 0.023
            2     0.221 0.023
            3     0.073 0.023
            4     0.024 0.023
            5     0.009 0.023
GLU_U 1,2,3,4,5   0     0.478 0.01
            1     0.213 0.01
            2     0.208 0.01
            3     0.074 0.01
```

```
            4      0.024 0.01
            5      0.004 0.01
GLU_U 1,2,3,4,5    0      0.475 0.011
            1      0.214 0.011
            2      0.207 0.011
            3      0.076 0.011
            4      0.022 0.011
            5      0.006 0.011
GLU_U 2,3,4,5      0      0.525 0.01
            1      0.23  0.01
            2      0.195 0.01
            3      0.043 0.01
            4      0.007 0.01
GLU_U 2,3,4,5      0      0.528 0.011
            1      0.229 0.011
            2      0.187 0.011
            3      0.044 0.011
            4      0.012 0.011
LYS_U 1,2,3,4,5,6 0      0.421 0.01
            1      0.222 0.01
            2      0.182 0.01
            3      0.116 0.01
            4      0.041 0.01
            5      0.016 0.01
            6      0.003 0.01
LYS_U 1,2,3,4,5,6 0      0.416 0.01
            1      0.228 0.01
            2      0.182 0.01
            3      0.117 0.01
            4      0.04  0.01
            5      0.014 0.01
            6      0.003 0.01
LYS_U 2,3,4,5,6    0      0.444 0.01
            1      0.233 0.01
            2      0.219 0.01
            3      0.078 0.01
            4      0.022 0.01
            5      0.005 0.01
ARGeff_U    1,2,3,4,5,6 0      0.427 0.01
            1      0.257 0.01
            2      0.193 0.01
            3      0.091 0.01
            4      0.03  0.01
            5      0.006 0.01
            6      -0.004      0.01
ARGeff_U    2,3,4,5,6   0      0.471 0.01
            1      0.271 0.01
            2      0.176 0.01
            3      0.063 0.01
            4      0.016 0.01
            5      0.003 0.01
HISeff_U    1,2,3,4,5,6 0      0.483 0.013
            1      0.23  0.013
```

```
            2     0.114 0.013
            3     0.102 0.013
            4     0.042 0.013
            5     0.025 0.013
            6     0.005 0.013
HISeff_U    2,3,4,5,6   0     0.486 0.023
            1     0.236 0.023
            2     0.172 0.023
            3     0.068 0.023
            4     0.031 0.023
            5     0.008 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.341 0.01
            1     0.168 0.01
            2     0.141 0.01
            3     0.181 0.01
            4     0.084 0.01
            5     0.046 0.01
            6     0.025 0.01
            7     0.011 0.01
            8     0.005 0.01
            9     0     0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.367 0.023
            1     0.156 0.023
            2     0.142 0.023
            3     0.168 0.023
            4     0.079 0.023
            5     0.043 0.023
            6     0.027 0.023
            7     0.01  0.023
            8     0.005 0.023
            9     0.002 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.382 0.01
            1     0.15  0.01
            2     0.211 0.01
            3     0.118 0.01
            4     0.075 0.01
            5     0.037 0.01
            6     0.019 0.01
            7     0.004 0.01
            8     0.004 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.358 0.01
            1     0.153 0.01
            2     0.221 0.01
            3     0.127 0.01
            4     0.079 0.01
            5     0.038 0.01
            6     0.019 0.01
            7     0.003 0.01
            8     0.001 0.01
PHE_TYR_U   1,2   0     0.752 0.01
            1     0.095 0.01
            2     0.153 0.01
GLU_U 1,2,3,4,5   0     0.479 0.01
```

		1	0.206	0.01
		2	0.212	0.01
		3	0.075	0.01
		4	0.023	0.01
		5	0.005	0.01
GLU_U	2,3,4,5	0	0.528	0.011
		1	0.227	0.011
		2	0.188	0.011
		3	0.044	0.011
		4	0.013	0.011
GLU_U	2,3,4,5	0	0.528	0.018
		1	0.229	0.01
		2	0.193	0.01
		3	0.042	0.012
		4	0.009	0.014
STA	1,2	0	0.451	0.01
		1	0.557	0.01
		2	-0.009	0.01
STA	3,4,5,6	0	0.709	0.015
		1	0.264	0.015
		2	0.026	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.446	0.015
		1	0.555	0.016
		2	-0.001	0.02
STA	3,4,5,6	0	0.703	0.012
		1	0.267	0.012
		2	0.031	0.012
		3	-0.001	0.012
		4	0	0.012
STA	1,2	0	0.427	0.01
		1	0.58	0.01
		2	-0.007	0.01
STA	3,4,5,6	0	0.682	0.015
		1	0.285	0.015
		2	0.031	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.418	0.01
		1	0.59	0.011
		2	-0.008	0.013
STA	3,4,5,6	0	0.683	0.012
		1	0.286	0.012
		2	0.029	0.012
		3	0.001	0.012
		4	0.001	0.012
STA	1,2	0	0.447	0.01
		1	0.562	0.01
		2	-0.009	0.01
STA	3,4,5,6	0	0.693	0.015
		1	0.277	0.015
		2	0.029	0.015

		3	0.001	0.015	
		4	0	0.015	
STA	1,2	0	0.438	0.01	
		1	0.573	0.011	
		2	-0.011		0.013
STA	3,4,5,6	0	0.698	0.012	
		1	0.268	0.012	
		2	0.031	0.012	
		3	0.003	0.012	
		4	0	0.012	
STA_U	1,2	0	0.762	0.019	
		1	0.1	0.014	
		2	0.138	0.013	
STA_U	3,4,5,6	0	0.642	0.015	
		1	0.164	0.015	
		2	0.035	0.015	
		3	0.09	0.015	
		4	0.069	0.015	
STA_U	1,2	0	0.761	0.025	
		1	0.109	0.018	
		2	0.129	0.018	
STA_U	3,4,5,6	0	0.641	0.012	
		1	0.163	0.012	
		2	0.036	0.012	
		3	0.091	0.012	
		4	0.07	0.012	
STA_U	1,2	0	0.759	0.019	
		1	0.1	0.014	
		2	0.141	0.013	
STA_U	3,4,5,6	0	0.638	0.015	
		1	0.163	0.015	
		2	0.035	0.015	
		3	0.091	0.015	
		4	0.074	0.015	
STA_U	1,2	0	0.755	0.026	
		1	0.109	0.019	
		2	0.136	0.019	
STA_U	3,4,5,6	0	0.643	0.012	
		1	0.162	0.012	
		2	0.032	0.012	
		3	0.091	0.012	
		4	0.072	0.012	
STA_U	1,2	0	0.759	0.018	
		1	0.099	0.013	
		2	0.142	0.012	
STA_U	3,4,5,6	0	0.644	0.015	
		1	0.16	0.015	
		2	0.032	0.015	
		3	0.089	0.015	
		4	0.075	0.015	
STA_U	1,2	0	0.767	0.03	
		1	0.102	0.022	
		2	0.132	0.021	

STA_U	3,4,5,6	0	0.649	0.012
		1	0.156	0.012
		2	0.034	0.012
		3	0.087	0.012
		4	0.073	0.012
WALL	3,4,5,6	0	0.715	0.015
		1	0.257	0.015
		2	0.025	0.015
		3	0.001	0.015
		4	0.001	0.015
WALL	3,4,5,6	0	0.733	0.012
		1	0.243	0.012
		2	0.022	0.012
		3	0.001	0.012
		4	0.001	0.012
WALL	3,4,5,6	0	0.69	0.015
		1	0.279	0.015
		2	0.03	0.015
		3	0.001	0.015
		4	0	0.015
WALL	3,4,5,6	0	0.714	0.012
		1	0.261	0.012
		2	0.023	0.012
		3	0.001	0.012
		4	0.001	0.012
WALL	3,4,5,6	0	0.702	0.015
		1	0.269	0.015
		2	0.026	0.015
		3	0.002	0.015
		4	0	0.015
WALL	3,4,5,6	0	0.718	0.012
		1	0.256	0.012
		2	0.023	0.012
		3	0.001	0.012
		4	0.001	0.012
WALL_U	3,4,5,6	0	0.645	0.015
		1	0.159	0.015
		2	0.035	0.015
		3	0.089	0.015
		4	0.071	0.015
WALL_U	3,4,5,6	0	0.658	0.012
		1	0.149	0.012
		2	0.032	0.012
		3	0.079	0.012
		4	0.082	0.012
WALL_U	3,4,5,6	0	0.641	0.015
		1	0.157	0.015
		2	0.034	0.015
		3	0.089	0.015
		4	0.078	0.015
WALL_U	3,4,5,6	0	0.656	0.012
		1	0.148	0.012
		2	0.031	0.012

```
            3     0.081 0.012
            4     0.084 0.012
WALL_U      3,4,5,6     0     0.651 0.015
            1     0.155 0.015
            2     0.031 0.015
            3     0.087 0.015
            4     0.077 0.015
WALL_U      3,4,5,6     0     0.662 0.012
            1     0.142 0.012
            2     0.031 0.012
            3     0.081 0.012
            4     0.084 0.012
FSUC  4,5,6 0     0.753 0.014
            1     0.238 0.014
            2     0.01  0.014
            3     -0.001      0.014
FSUC  4,5,6 0     0.774 0.023
            1     0.233 0.011
            2     0.003 0.015
            3     -0.01 0.015
FSUC  1,2,3,4     0     0.352 0.013
            1     0.614 0.013
            2     0.037 0.013
            3     -0.001      0.013
            4     -0.002      0.013
FSUC  4,5,6 0     0.756 0.013
            1     0.235 0.013
            2     0.009 0.013
            3     -0.001      0.013
FSUC  4,5,6 0     0.756 0.027
            1     0.249 0.014
            2     0.004 0.018
            3     -0.009      0.019
FSUC  1,2,3,4     0     0.357 0.011
            1     0.613 0.011
            2     0.036 0.011
            3     -0.004      0.011
            4     -0.003      0.011
FSUC  4,5,6 0     0.738 0.014
            1     0.25  0.014
            2     0.013 0.014
            3     0     0.014
FSUC  4,5,6 0     0.759 0.021
            1     0.248 0.011
            2     0.004 0.014
            3     -0.011      0.014
FSUC  1,2,3,4     0     0.359 0.013
            1     0.603 0.013
            2     0.041 0.013
            3     -0.001      0.013
            4     -0.002      0.013
FSUC  4,5,6 0     0.741 0.013
            1     0.248 0.013
```

		2	0.012	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.745	0.025
		1	0.26	0.013
		2	0.005	0.017
		3	-0.009	0.018
FSUC	1,2,3,4	0	0.364	0.011
		1	0.606	0.011
		2	0.035	0.011
		3	-0.001	0.011
		4	-0.004	0.011
FSUC	4,5,6	0	0.74	0.014
		1	0.247	0.014
		2	0.013	0.014
		3	0	0.014
FSUC	4,5,6	0	0.762	0.022
		1	0.245	0.011
		2	0.003	0.014
		3	-0.01	0.015
FSUC	1,2,3,4	0	0.351	0.013
		1	0.613	0.013
		2	0.039	0.013
		3	-0.001	0.013
		4	-0.002	0.013
FSUC	4,5,6	0	0.744	0.013
		1	0.246	0.013
		2	0.011	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.747	0.026
		1	0.259	0.014
		2	0.004	0.018
		3	-0.01	0.019
FSUC	1,2,3,4	0	0.354	0.011
		1	0.617	0.011
		2	0.038	0.011
		3	-0.007	0.011
		4	-0.002	0.011
FSUC_U	4,5,6	0	0.748	0.014
		1	0.066	0.014
		2	0.03	0.014
		3	0.156	0.014
FSUC_U	4,5,6	0	0.77	0.015
		1	0.059	0.01
		2	0.022	0.01
		3	0.149	0.01
FSUC_U	1,2,3,4	0	0.622	0.013
		1	0.177	0.013
		2	0.065	0.013
		3	0.067	0.013
		4	0.07	0.013
FSUC_U	4,5,6	0	0.75	0.013
		1	0.065	0.013
		2	0.029	0.013

	3	0.156	0.013	
FSUC_U	4,5,6	0	0.766	0.018
	1	0.064	0.011	
	2	0.025	0.011	
	3	0.145	0.01	
FSUC_U	1,2,3,4	0	0.622	0.011
	1	0.177	0.011	
	2	0.064	0.011	
	3	0.066	0.011	
	4	0.07	0.011	
FSUC_U	4,5,6	0	0.753	0.014
	1	0.061	0.014	
	2	0.028	0.014	
	3	0.158	0.014	
FSUC_U	4,5,6	0	0.775	0.016
	1	0.055	0.01	
	2	0.02	0.01	
	3	0.151	0.01	
FSUC_U	1,2,3,4	0	0.627	0.013
	1	0.174	0.013	
	2	0.06	0.013	
	3	0.066	0.013	
	4	0.073	0.013	
FSUC_U	4,5,6	0	0.754	0.013
	1	0.061	0.013	
	2	0.028	0.013	
	3	0.157	0.013	
FSUC_U	4,5,6	0	0.77	0.02
	1	0.059	0.012	
	2	0.022	0.012	
	3	0.148	0.01	
FSUC_U	1,2,3,4	0	0.631	0.011
	1	0.17	0.011	
	2	0.062	0.011	
	3	0.066	0.011	
	4	0.07	0.011	
FSUC_U	4,5,6	0	0.755	0.014
	1	0.059	0.014	
	2	0.027	0.014	
	3	0.159	0.014	
FSUC_U	4,5,6	0	0.776	0.016
	1	0.052	0.01	
	2	0.02	0.01	
	3	0.152	0.01	
FSUC_U	1,2,3,4	0	0.633	0.013
	1	0.169	0.013	
	2	0.058	0.013	
	3	0.066	0.013	
	4	0.074	0.013	
FSUC_U	4,5,6	0	0.758	0.013
	1	0.057	0.013	
	2	0.027	0.013	
	3	0.158	0.013	

FSUC_U	4,5,6	0	0.772	0.02
		1	0.057	0.012
		2	0.022	0.012
		3	0.149	0.01
FSUC_U	1,2,3,4	0	0.638	0.011
		1	0.168	0.011
		2	0.059	0.011
		3	0.062	0.011
		4	0.073	0.011
PENTAN	5	0	0.994	0.01
		1	0.006	0.01
PENTAN	3,4,5	0	0.929	0.039
		1	0.089	0.02
		2	-0.007	0.02
		3	-0.011	0.021
PENTAN	3,4,5	0	0.926	0.01
		1	0.071	0.01
		2	0.003	0.01
		3	0	0.01
PENTAN	5	0	0.985	0.015
		1	0.015	0.015
PENTAN	5	0	0.997	0.01
		1	0.003	0.01
PENTAN	3,4,5	0	0.928	0.01
		1	0.067	0.01
		2	0.005	0.01
		3	0	0.01
WALL	3,4,5,6	0	0.724	0.011
		1	0.251	0.011
		2	0.024	0.011
		3	0.002	0.011
		4	0	0.011
WALL	3,4,5,6	0	0.737	0.012
		1	0.241	0.012
		2	0.022	0.012
		3	0	0.012
		4	0	0.012
PENTAN	5	0	0.991	0.01
		1	0.009	0.01
PENTAN	3,4,5	0	0.916	0.04
		1	0.099	0.02
		2	-0.005	0.021
		3	-0.01	0.022
PENTAN	3,4,5	0	0.922	0.01
		1	0.075	0.01
		2	0.002	0.01
		3	0	0.01
PENTAN	5	0	0.984	0.015
		1	0.016	0.015
PENTAN	3,4,5	0	0.918	0.034
		1	0.09	0.016
		2	0.004	0.018
		3	-0.012	0.018

PENTAN	3,4,5	0	0.94	0.01
		1	0.066	0.01
		2	-0.006	0.01
		3	0	0.01
PENTAN	5	0	0.992	0.01
		1	0.008	0.01
PENTAN	3,4,5	0	0.926	0.01
		1	0.075	0.01
		2	-0.002	0.01
		3	0.002	0.01
WALL	3,4,5,6	0	0.704	0.011
		1	0.267	0.011
		2	0.028	0.011
		3	0.001	0.011
		4	0.001	0.011
WALL	3,4,5,6	0	0.721	0.012
		1	0.256	0.012
		2	0.024	0.012
		3	0	0.012
		4	0	0.012
PENTAN	5	0	0.997	0.01
		1	0.003	0.01
PENTAN	3,4,5	0	0.932	0.041
		1	0.083	0.02
		2	-0.006	0.021
		3	-0.009	0.022
PENTAN	5	0	0.992	0.015
		1	0.008	0.015
PENTAN	3,4,5	0	0.929	0.028
		1	0.082	0.016
		2	-0.003	0.016
		3	-0.009	0.016
PENTAN	5	0	0.999	0.01
		1	0.001	0.01
WALL	3,4,5,6	0	0.724	0.012
		1	0.253	0.012
		2	0.022	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN_U	5	0	0.803	0.01
		1	0.197	0.01
PENTAN_U	3,4,5	0	0.657	0.02
		1	0.176	0.02
		2	0.087	0.02
		3	0.08	0.02
PENTAN_U	3,4,5	0	0.666	0.01
		1	0.162	0.01
		2	0.088	0.01
		3	0.083	0.01
PENTAN_U	5	0	0.804	0.015
		1	0.196	0.015
PENTAN_U	3,4,5	0	0.663	0.016
		1	0.17	0.016

	2	0.09	0.016		
	3	0.078	0.016		
PENTAN_U	3,4,5	0	0.659	0.01	
	1	0.17	0.01		
	2	0.087	0.01		
	3	0.085	0.01		
PENTAN_U	5	0	0.802	0.01	
	1	0.198	0.01		
PENTAN_U	3,4,5	0	0.662	0.01	
	1	0.164	0.01		
	2	0.091	0.01		
	3	0.084	0.01		
WALL_U	3,4,5,6		0	0.652	0.011
	1	0.15	0.011		
	2	0.034	0.011		
	3	0.084	0.011		
	4	0.08	0.011		
WALL_U	3,4,5,6		0	0.658	0.012
	1	0.146	0.012		
	2	0.031	0.012		
	3	0.08	0.012		
	4	0.085	0.012		
PENTAN_U	5	0	0.802	0.01	
	1	0.198	0.01		
PENTAN_U	3,4,5	0	0.66	0.02	
	1	0.172	0.02		
	2	0.085	0.02		
	3	0.083	0.02		
PENTAN_U	3,4,5	0	0.669	0.01	
	1	0.157	0.01		
	2	0.087	0.01		
	3	0.087	0.01		
PENTAN_U	5	0	0.799	0.015	
	1	0.201	0.015		
PENTAN_U	3,4,5	0	0.663	0.016	
	1	0.164	0.016		
	2	0.087	0.016		
	3	0.086	0.016		
PENTAN_U	3,4,5	0	0.664	0.012	
	1	0.167	0.01		
	2	0.089	0.01		
	3	0.079	0.01		
PENTAN_U	5	0	0.803	0.01	
	1	0.197	0.01		
PENTAN_U	3,4,5	0	0.671	0.01	
	1	0.156	0.01		
	2	0.086	0.01		
	3	0.087	0.01		
WALL_U	3,4,5,6		0	0.655	0.011
	1	0.153	0.011		
	2	0.029	0.011		
	3	0.08	0.011		
	4	0.084	0.011		

```
      WALL_U      3,4,5,6     0     0.659 0.012
                  1     0.145 0.012
                  2     0.029 0.012
                  3     0.08  0.012
                  4     0.087 0.012
      PENTAN_U    5     0     0.804 0.01
                  1     0.196 0.01
      PENTAN_U    3,4,5 0     0.662 0.02
                  1     0.171 0.02
                  2     0.083 0.02
                  3     0.084 0.02
      PENTAN_U    3,4,5 0     0.672 0.01
                  1     0.153 0.01
                  2     0.085 0.01
                  3     0.09  0.01
      PENTAN_U    5     0     0.805 0.015
                  1     0.195 0.015
      PENTAN_U    3,4,5 0     0.661 0.016
                  1     0.164 0.016
                  2     0.092 0.016
                  3     0.083 0.016
      PENTAN_U    3,4,5 0     0.676 0.01
                  1     0.145 0.01
                  2     0.089 0.01
                  3     0.09  0.01
      PENTAN_U    5     0     0.804 0.01
                  1     0.196 0.01
      PENTAN_U    3,4,5 0     0.672 0.01
                  1     0.155 0.01
                  2     0.086 0.01
                  3     0.087 0.01
      WALL_U      3,4,5,6     0     0.656 0.011
                  1     0.148 0.011
                  2     0.03  0.011
                  3     0.081 0.011
                  4     0.085 0.011
      WALL_U      3,4,5,6     0     0.663 0.012
                  1     0.142 0.012
                  2     0.028 0.012
                  3     0.079 0.012
                  4     0.088 0.012
```

Control line 6

```
MASS_SPECTROMETRY
      META_NAME   FRAGMENT    WEIGHT      VALUE DEVIATION
      ALA   1,2,3 0     0.589 0.01
                  1     0.387 0.01
                  2     0.023 0.01
                  3     0.001 0.01
      ALA   2,3   0     0.61  0.011
```

```
            1     0.381 0.011
            2     0.009 0.011
GLY   1,2   0     0.911 0.011
            1     0.087 0.011
            2     0.002 0.011
GLY   2     0     0.978 0.011
            1     0.022 0.011
VAL   1,2,3,4,5   0     0.377 0.01
            1     0.448 0.01
            2     0.16  0.01
            3     0.018 0.01
            4     -0.001      0.01
            5     -0.001      0.01
VAL   2,3,4,5     0     0.387 0.029
            1     0.436 0.029
            2     0.15  0.029
            3     0.025 0.029
            4     0.001 0.029
GLU   2,3,4,5     0     0.278 0.026
            1     0.43  0.026
            2     0.224 0.026
            3     0.053 0.026
            4     0.016 0.026
SER   1,2,3 0     0.678 0.01
            1     0.309 0.01
            2     0.01  0.01
            3     0.003 0.01
SER   1,2,3 0     0.681 0.011
            1     0.303 0.011
            2     0.015 0.011
            3     0.001 0.011
SER   2,3   0     0.7   0.011
            1     0.292 0.01
            2     0.008 0.011
SER   2,3   0     0.706 0.011
            1     0.285 0.011
            2     0.009 0.011
SER   1,2   0     0.942 0.013
            1     0.064 0.013
            2     -0.006      0.013
PHE_TYR     2,3,4,5,6,7,8,9   0     0.305 0.021
            1     0.446 0.021
            2     0.243 0.021
            3     0.05  0.021
            4     -0.004      0.021
            5     -0.011      0.021
            6     -0.012      0.021
            7     -0.012      0.021
            8     -0.006      0.021
ASP   1,2,3,4     0     0.38  0.01
            1     0.423 0.01
            2     0.18  0.01
            3     0.022 0.01
```

		4	-0.005		0.01
ASP	1,2,3,4		0	0.38	0.01
		1	0.438	0.01	
		2	0.161	0.01	
		3	0.021	0.01	
		4	0	0.01	
ASP	2,3,4	0	0.446	0.01	
		1	0.433	0.01	
		2	0.114	0.01	
		3	0.007	0.01	
ASP	1,2	0	0.627	0.013	
		1	0.338	0.013	
		2	0.035	0.013	
GLU	1,2,3,4,5		0	0.279	0.012
		1	0.425	0.012	
		2	0.235	0.012	
		3	0.05	0.012	
		4	0.021	0.012	
		5	-0.011		0.012
GLU	1,2,3,4,5		0	0.272	0.01
		1	0.431	0.01	
		2	0.232	0.01	
		3	0.053	0.01	
		4	0.01	0.01	
		5	0.003	0.01	
GLU	1,2,3,4,5		0	0.271	0.01
		1	0.431	0.01	
		2	0.239	0.01	
		3	0.056	0.01	
		4	0.004	0.01	
		5	0	0.01	
GLU	2,3,4,5		0	0.302	0.01
		1	0.445	0.01	
		2	0.218	0.01	
		3	0.033	0.01	
		4	0.003	0.01	
GLU	2,3,4,5		0	0.314	0.01
		1	0.445	0.01	
		2	0.204	0.01	
		3	0.032	0.01	
		4	0.005	0.01	
GLU	1,2,3,4,5		0	0.297	0.013
		1	0.429	0.013	
		2	0.229	0.013	
		3	0.048	0.013	
		4	0	0.013	
		5	-0.003		0.013
GLU	1,2,3,4,5		0	0.287	0.01
		1	0.429	0.01	
		2	0.23	0.01	
		3	0.051	0.01	
		4	0.004	0.01	
		5	-0.001		0.01

GLU	1,2,3,4,5	0	0.291	0.011
		1	0.431	0.011
		2	0.225	0.011
		3	0.048	0.011
		4	0.005	0.011
		5	0	0.011
GABA	1,2,3,4	0	0.328	0.019
		1	0.449	0.019
		2	0.201	0.019
		3	0.027	0.019
		4	-0.005	0.019
ALA	1,2,3	0	0.579	0.01
		1	0.391	0.01
		2	0.029	0.01
		3	0.001	0.01
ALA	2,3	0	0.603	0.011
		1	0.385	0.011
		2	0.012	0.011
GLY	1,2	0	0.914	0.011
		1	0.085	0.011
		2	0.002	0.011
GLY	2	0	0.978	0.011
		1	0.022	0.011
VAL	1,2,3,4,5	0	0.371	0.01
		1	0.447	0.01
		2	0.163	0.01
		3	0.017	0.01
		4	0.002	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.382	0.029
		1	0.441	0.029
		2	0.154	0.029
		3	0.021	0.029
		4	0.002	0.029
GLU	2,3,4,5	0	0.262	0.026
		1	0.421	0.026
		2	0.242	0.026
		3	0.065	0.026
		4	0.01	0.026
SER	1,2,3	0	0.674	0.01
		1	0.302	0.01
		2	0.017	0.01
		3	0.006	0.01
SER	1,2,3	0	0.67	0.011
		1	0.313	0.011
		2	0.017	0.011
		3	0.001	0.011
SER	2,3	0	0.7	0.012
		1	0.293	0.01
		2	0.007	0.012
SER	2,3	0	0.702	0.011
		1	0.291	0.011
		2	0.007	0.011

SER	1,2	0	0.937	0.013			
		1	0.064	0.013			
		2	-0.001		0.013		
THR	2,3,4	0	0.485	0.025			
		1	0.424	0.029			
		2	0.112	0.025			
		3	-0.021		0.03		
PHE_TYR		2,3,4,5,6,7,8,9			0	0.285	0.021
		1	0.431	0.021			
		2	0.247	0.021			
		3	0.054	0.021			
		4	0.002	0.021			
		5	-0.005		0.021		
		6	-0.006		0.021		
		7	-0.006		0.021		
		8	-0.002		0.021		
ASP	1,2,3,4		0	0.381	0.01		
		1	0.437	0.01			
		2	0.16	0.01			
		3	0.028	0.01			
		4	-0.007		0.01		
ASP	1,2,3,4		0	0.38	0.01		
		1	0.436	0.01			
		2	0.164	0.01			
		3	0.02	0.01			
		4	0	0.01			
ASP	2,3,4	0	0.443	0.01			
		1	0.439	0.01			
		2	0.113	0.01			
		3	0.006	0.01			
ASP	1,2	0	0.627	0.013			
		1	0.345	0.013			
		2	0.028	0.013			
GLU	1,2,3,4,5		0	0.277	0.012		
		1	0.433	0.012			
		2	0.243	0.012			
		3	0.047	0.012			
		4	0.005	0.012			
		5	-0.006		0.012		
GLU	1,2,3,4,5		0	0.274	0.01		
		1	0.423	0.01			
		2	0.234	0.01			
		3	0.058	0.01			
		4	0.009	0.01			
		5	0.003	0.01			
GLU	1,2,3,4,5		0	0.27	0.01		
		1	0.429	0.01			
		2	0.242	0.01			
		3	0.055	0.01			
		4	0.005	0.01			
		5	0	0.01			
GLU	2,3,4,5		0	0.302	0.01		
		1	0.44	0.01			

		2	0.222	0.01
		3	0.035	0.01
		4	0.001	0.01
GLU	2,3,4,5	0	0.314	0.01
		1	0.445	0.01
		2	0.206	0.01
		3	0.032	0.01
		4	0.003	0.01
GLU	1,2,3,4,5	0	0.296	0.013
		1	0.431	0.013
		2	0.235	0.013
		3	0.044	0.013
		4	-0.001	0.013
		5	-0.005	0.013
GLU	1,2,3,4,5	0	0.283	0.01
		1	0.429	0.01
		2	0.233	0.01
		3	0.053	0.01
		4	0.003	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.286	0.011
		1	0.427	0.011
		2	0.231	0.011
		3	0.051	0.011
		4	0.005	0.011
		5	0	0.011
GABA	1,2,3,4	0	0.322	0.019
		1	0.444	0.019
		2	0.205	0.019
		3	0.029	0.019
		4	0	0.019
ALA	1,2,3	0	0.583	0.01
		1	0.387	0.01
		2	0.028	0.01
		3	0.001	0.01
ALA	2,3	0	0.607	0.011
		1	0.381	0.011
		2	0.012	0.011
GLY	1,2	0	0.91	0.011
		1	0.087	0.011
		2	0.004	0.011
GLY	2	0	0.973	0.011
		1	0.027	0.011
VAL	1,2,3,4,5	0	0.374	0.01
		1	0.447	0.01
		2	0.166	0.01
		3	0.016	0.01
		4	0	0.01
		5	-0.002	0.01
VAL	2,3,4,5	0	0.384	0.029
		1	0.436	0.029
		2	0.151	0.029
		3	0.027	0.029

		4	0.001	0.029
GLU	2,3,4,5	0	0.294	0.026
		1	0.426	0.026
		2	0.226	0.026
		3	0.047	0.026
		4	0.007	0.026
SER	1,2,3	0	0.667	0.01
		1	0.307	0.01
		2	0.018	0.01
		3	0.008	0.01
SER	1,2,3	0	0.669	0.011
		1	0.312	0.011
		2	0.018	0.011
		3	0.001	0.011
SER	2,3	0	0.701	0.01
		1	0.292	0.01
		2	0.007	0.01
SER	2,3	0	0.701	0.011
		1	0.292	0.011
		2	0.007	0.011
SER	1,2	0	0.941	0.013
		1	0.061	0.013
		2	-0.002	0.013
THR	2,3,4	0	0.462	0.01
		1	0.427	0.011
		2	0.115	0.01
		3	-0.005	0.012
PHE_TYR	2,3,4,5,6,7,8,9	0	0.302	0.021
		1	0.454	0.021
		2	0.254	0.021
		3	0.047	0.021
		4	-0.007	0.021
		5	-0.012	0.021
		6	-0.015	0.021
		7	-0.014	0.021
		8	-0.009	0.021
ASP	1,2,3,4	0	0.383	0.01
		1	0.446	0.01
		2	0.153	0.01
		3	0.021	0.01
		4	-0.002	0.01
ASP	2,3,4	0	0.451	0.01
		1	0.42	0.01
		2	0.122	0.01
		3	0.007	0.01
ASP	1,2	0	0.629	0.013
		1	0.34	0.013
		2	0.031	0.013
GLU	1,2,3,4,5	0	0.284	0.012
		1	0.446	0.012
		2	0.205	0.012
		3	0.065	0.012
		4	0.002	0.012

		5	-0.003	0.012
GLU	1,2,3,4,5	0	0.28	0.01
		1	0.421	0.01
		2	0.238	0.01
		3	0.051	0.01
		4	0.009	0.01
		5	0	0.01
GLU	1,2,3,4,5	0	0.278	0.01
		1	0.428	0.01
		2	0.236	0.01
		3	0.054	0.01
		4	0.004	0.01
		5	0	0.01
GLU	2,3,4,5	0	0.313	0.01
		1	0.441	0.01
		2	0.215	0.01
		3	0.033	0.01
		4	-0.001	0.01
GLU	2,3,4,5	0	0.319	0.01
		1	0.445	0.01
		2	0.201	0.01
		3	0.031	0.01
		4	0.003	0.01
GLU	1,2,3,4,5	0	0.301	0.013
		1	0.433	0.013
		2	0.227	0.013
		3	0.045	0.013
		4	-0.003	0.013
		5	-0.003	0.013
GLU	1,2,3,4,5	0	0.289	0.01
		1	0.431	0.01
		2	0.229	0.01
		3	0.049	0.01
		4	0.003	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.291	0.011
		1	0.427	0.011
		2	0.229	0.011
		3	0.049	0.011
		4	0.004	0.011
		5	0	0.011
GABA	1,2,3,4	0	0.33	0.019
		1	0.443	0.019
		2	0.2	0.019
		3	0.026	0.019
		4	0	0.019
ALA_U	1,2,3	0	0.707	0.01
		1	0.101	0.01
		2	0.052	0.01
		3	0.14	0.01
ALA_U	2,3	0	0.753	0.011
		1	0.076	0.011
		2	0.171	0.011

```
GLY_U 1,2   0      0.726 0.011
            1      0.148 0.011
            2      0.126 0.011
GLY_U 2     0      0.798 0.011
            1      0.202 0.011
VAL_U 1,2,3,4,5   0      0.554 0.01
            1      0.124 0.01
            2      0.158 0.01
            3      0.124 0.01
            4      0.017 0.01
            5      0.022 0.01
VAL_U 2,3,4,5      0      0.577 0.029
            1      0.107 0.029
            2      0.253 0.029
            3      0.035 0.029
            4      0.028 0.029
GLU_U 2,3,4,5      0      0.461 0.026
            1      0.254 0.026
            2      0.203 0.026
            3      0.063 0.026
            4      0.019 0.026
SER_U 1,2,3 0      0.66  0.01
            1      0.161 0.01
            2      0.08  0.01
            3      0.1   0.01
SER_U 1,2,3 0      0.66  0.011
            1      0.163 0.011
            2      0.08  0.011
            3      0.098 0.011
SER_U 2,3   0      0.706 0.01
            1      0.175 0.01
            2      0.119 0.01
SER_U 2,3   0      0.709 0.011
            1      0.174 0.011
            2      0.118 0.011
SER_U 1,2   0      0.73  0.013
            1      0.122 0.013
            2      0.148 0.013
THR_U 2,3,4 0      0.631 0.026
            1      0.224 0.02
            2      0.114 0.021
            3      0.032 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.377 0.021
            1      0.149 0.021
            2      0.204 0.021
            3      0.121 0.021
            4      0.08  0.021
            5      0.038 0.021
            6      0.02  0.021
            7      0.004 0.021
            8      0.008 0.021
ASP_U 1,2,3,4      0      0.544 0.01
            1      0.216 0.01
```

	2	0.15	0.01
	3	0.073	0.01
	4	0.017	0.01
ASP_U 1,2,3,4	0	0.542	0.01
	1	0.22	0.01
	2	0.149	0.01
	3	0.071	0.01
	4	0.018	0.01
ASP_U 2,3,4	0	0.609	0.01
	1	0.227	0.01
	2	0.123	0.01
	3	0.041	0.01
ASP_U 1,2	0	0.708	0.013
	1	0.171	0.013
	2	0.121	0.013
GLU_U 1,2,3,4,5	0	0.457	0.012
	1	0.222	0.012
	2	0.212	0.012
	3	0.084	0.012
	4	0.019	0.012
	5	0.005	0.012
GLU_U 1,2,3,4,5	0	0.462	0.01
	1	0.213	0.01
	2	0.209	0.01
	3	0.086	0.01
	4	0.024	0.01
	5	0.007	0.01
GLU_U 1,2,3,4,5	0	0.461	0.01
	1	0.213	0.01
	2	0.209	0.01
	3	0.085	0.01
	4	0.024	0.01
	5	0.008	0.01
GLU_U 2,3,4,5	0	0.511	0.01
	1	0.231	0.01
	2	0.198	0.01
	3	0.045	0.01
	4	0.015	0.01
GLU_U 2,3,4,5	0	0.517	0.01
	1	0.222	0.01
	2	0.199	0.01
	3	0.047	0.01
	4	0.015	0.01
GLU_U 1,2,3,4,5	0	0.47	0.013
	1	0.209	0.013
	2	0.211	0.013
	3	0.081	0.013
	4	0.023	0.013
	5	0.006	0.013
GLU_U 1,2,3,4,5	0	0.459	0.01
	1	0.209	0.01
	2	0.213	0.01
	3	0.085	0.01

	4	0.025	0.01
	5	0.008	0.01
GLU_U 1,2,3,4,5	0	0.467	0.011
	1	0.207	0.011
	2	0.209	0.011
	3	0.083	0.011
	4	0.024	0.011
	5	0.008	0.011
GABA_U 1,2,3,4	0	0.521	0.019
	1	0.222	0.019
	2	0.198	0.019
	3	0.044	0.019
	4	0.015	0.019
ALA_U 1,2,3	0	0.712	0.01
	1	0.096	0.01
	2	0.048	0.01
	3	0.144	0.01
ALA_U 2,3	0	0.757	0.011
	1	0.071	0.011
	2	0.172	0.011
GLY_U 1,2	0	0.723	0.011
	1	0.151	0.011
	2	0.126	0.011
GLY_U 2	0	0.798	0.011
	1	0.202	0.011
VAL_U 1,2,3,4,5	0	0.551	0.01
	1	0.124	0.01
	2	0.162	0.01
	3	0.123	0.01
	4	0.017	0.01
	5	0.023	0.01
VAL_U 2,3,4,5	0	0.576	0.029
	1	0.105	0.029
	2	0.255	0.029
	3	0.035	0.029
	4	0.028	0.029
GLU_U 2,3,4,5	0	0.466	0.026
	1	0.252	0.026
	2	0.202	0.026
	3	0.062	0.026
	4	0.018	0.026
SER_U 1,2,3	0	0.661	0.01
	1	0.165	0.01
	2	0.075	0.01
	3	0.1	0.01
SER_U 1,2,3	0	0.66	0.011
	1	0.161	0.011
	2	0.08	0.011
	3	0.099	0.011
SER_U 2,3	0	0.707	0.01
	1	0.174	0.01
	2	0.119	0.01
SER_U 2,3	0	0.709	0.011

```
            1     0.174 0.011
            2     0.118 0.011
SER_U 1,2   0     0.737 0.013
            1     0.116 0.013
            2     0.147 0.013
THR_U 2,3,4 0     0.635 0.01
            1     0.22  0.01
            2     0.117 0.01
            3     0.028 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.386 0.021
            1     0.145 0.021
            2     0.209 0.021
            3     0.118 0.021
            4     0.078 0.021
            5     0.038 0.021
            6     0.02  0.021
            7     0.002 0.021
            8     0.006 0.021
ASP_U 1,2,3,4     0     0.552 0.01
            1     0.21  0.01
            2     0.156 0.01
            3     0.066 0.01
            4     0.016 0.01
ASP_U 1,2,3,4     0     0.547 0.01
            1     0.214 0.01
            2     0.153 0.01
            3     0.07  0.01
            4     0.016 0.01
ASP_U 2,3,4 0     0.613 0.01
            1     0.229 0.01
            2     0.117 0.01
            3     0.041 0.01
ASP_U 1,2   0     0.722 0.013
            1     0.161 0.013
            2     0.118 0.013
GLU_U 1,2,3,4,5   0     0.471 0.012
            1     0.218 0.012
            2     0.21  0.012
            3     0.074 0.012
            4     0.023 0.012
            5     0.003 0.012
GLU_U 1,2,3,4,5   0     0.465 0.01
            1     0.212 0.01
            2     0.209 0.01
            3     0.081 0.01
            4     0.023 0.01
            5     0.009 0.01
GLU_U 1,2,3,4,5   0     0.463 0.01
            1     0.212 0.01
            2     0.21  0.01
            3     0.083 0.01
            4     0.024 0.01
            5     0.008 0.01
```

```
GLU_U 2,3,4,5      0      0.511 0.01
            1      0.227 0.01
            2      0.201 0.01
            3      0.045 0.01
            4      0.017 0.01
GLU_U 2,3,4,5      0      0.517 0.01
            1      0.221 0.01
            2      0.198 0.01
            3      0.048 0.01
            4      0.015 0.01
GLU_U 1,2,3,4,5    0      0.477 0.013
            1      0.206 0.013
            2      0.212 0.013
            3      0.08  0.013
            4      0.023 0.013
            5      0.002 0.013
GLU_U 1,2,3,4,5    0      0.461 0.01
            1      0.208 0.01
            2      0.214 0.01
            3      0.084 0.01
            4      0.025 0.01
            5      0.008 0.01
GLU_U 1,2,3,4,5    0      0.468 0.011
            1      0.205 0.011
            2      0.211 0.011
            3      0.083 0.011
            4      0.024 0.011
            5      0.008 0.011
GABA_U      1,2,3,4      0      0.52  0.019
            1      0.222 0.019
            2      0.199 0.019
            3      0.045 0.019
            4      0.015 0.019
ALA_U 1,2,3 0      0.713 0.01
            1      0.096 0.01
            2      0.048 0.01
            3      0.143 0.01
ALA_U 2,3   0      0.756 0.011
            1      0.071 0.011
            2      0.172 0.011
GLY_U 1,2   0      0.723 0.011
            1      0.151 0.011
            2      0.127 0.011
GLY_U 2     0      0.8   0.011
            1      0.2   0.011
VAL_U 1,2,3,4,5    0      0.554 0.01
            1      0.122 0.01
            2      0.158 0.01
            3      0.125 0.01
            4      0.017 0.01
            5      0.023 0.01
VAL_U 2,3,4,5      0      0.576 0.029
            1      0.107 0.029
```

```
            2     0.254 0.029
            3     0.036 0.029
            4     0.028 0.029
GLU_U 2,3,4,5     0     0.471 0.026
            1     0.251 0.026
            2     0.197 0.026
            3     0.062 0.026
            4     0.019 0.026
SER_U 1,2,3 0     0.665 0.01
            1     0.152 0.01
            2     0.083 0.01
            3     0.101 0.01
SER_U 1,2,3 0     0.661 0.011
            1     0.161 0.011
            2     0.079 0.011
            3     0.099 0.011
SER_U 2,3   0     0.708 0.01
            1     0.171 0.01
            2     0.122 0.01
SER_U 2,3   0     0.712 0.011
            1     0.169 0.011
            2     0.119 0.011
SER_U 1,2   0     0.739 0.013
            1     0.117 0.013
            2     0.144 0.013
THR_U 2,3,4 0     0.618 0.01
            1     0.233 0.01
            2     0.106 0.01
            3     0.042 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.382 0.021
            1     0.148 0.021
            2     0.205 0.021
            3     0.12  0.021
            4     0.076 0.021
            5     0.037 0.021
            6     0.02  0.021
            7     0.004 0.021
            8     0.007 0.021
ASP_U 1,2,3,4     0     0.556 0.01
            1     0.215 0.01
            2     0.149 0.01
            3     0.068 0.01
            4     0.012 0.01
ASP_U 1,2,3,4     0     0.547 0.01
            1     0.216 0.01
            2     0.152 0.01
            3     0.07  0.01
            4     0.016 0.01
ASP_U 2,3,4 0     0.605 0.01
            1     0.23  0.01
            2     0.123 0.01
            3     0.042 0.01
ASP_U 1,2   0     0.719 0.013
```

		1	0.164	0.013	
		2	0.117	0.013	
GLU_U	1,2,3,4,5	0	0.468	0.012	
		1	0.22	0.012	
		2	0.205	0.012	
		3	0.079	0.012	
		4	0.026	0.012	
		5	0.002	0.012	
GLU_U	1,2,3,4,5	0	0.461	0.01	
		1	0.214	0.01	
		2	0.212	0.01	
		3	0.085	0.01	
		4	0.02	0.01	
		5	0.008	0.01	
GLU_U	1,2,3,4,5	0	0.462	0.01	
		1	0.213	0.01	
		2	0.211	0.01	
		3	0.083	0.01	
		4	0.024	0.01	
		5	0.008	0.01	
GLU_U	2,3,4,5	0	0.511	0.01	
		1	0.233	0.01	
		2	0.195	0.01	
		3	0.046	0.01	
		4	0.015	0.01	
GLU_U	2,3,4,5	0	0.517	0.01	
		1	0.223	0.01	
		2	0.198	0.01	
		3	0.048	0.01	
		4	0.015	0.01	
GLU_U	1,2,3,4,5	0	0.483	0.013	
		1	0.201	0.013	
		2	0.214	0.013	
		3	0.079	0.013	
		4	0.023	0.013	
		5	0.001	0.013	
GLU_U	1,2,3,4,5	0	0.462	0.01	
		1	0.208	0.01	
		2	0.214	0.01	
		3	0.084	0.01	
		4	0.025	0.01	
		5	0.008	0.01	
GLU_U	1,2,3,4,5	0	0.466	0.011	
		1	0.206	0.011	
		2	0.212	0.011	
		3	0.083	0.011	
		4	0.024	0.011	
		5	0.008	0.011	
GABA_U		1,2,3,4	0	0.521	0.019
		1	0.223	0.019	
		2	0.196	0.019	
		3	0.046	0.019	
		4	0.014	0.019	

FUM	1,2,3,4	0	0.391	0.017
		1	0.411	0.017
		2	0.154	0.017
		3	0.033	0.017
		4	0.01	0.017
OAA	1,2,3,4	0	0.372	0.011
		1	0.445	0.011
		2	0.157	0.011
		3	0.023	0.011
		4	0.003	0.011
OAA	1,2,3,4	0	0.379	0.01
		1	0.44	0.01
		2	0.16	0.01
		3	0.021	0.01
		4	0	0.01
CIT	1,2,3,4,5,6	0	0.238	0.01
		1	0.41	0.01
		2	0.265	0.01
		3	0.083	0.01
		4	0.003	0.01
		5	0	0.01
		6	0.001	0.01
FUM	1,2,3,4	0	0.377	0.017
		1	0.425	0.017
		2	0.163	0.017
		3	0.029	0.017
		4	0.005	0.017
OAA	1,2,3,4	0	0.376	0.011
		1	0.443	0.011
		2	0.158	0.011
		3	0.023	0.011
		4	0.001	0.011
OAA	1,2,3,4	0	0.38	0.01
		1	0.437	0.01
		2	0.161	0.01
		3	0.02	0.01
		4	0.001	0.01
CIT	1,2,3,4,5,6	0	0.235	0.01
		1	0.408	0.01
		2	0.269	0.01
		3	0.079	0.01
		4	0.01	0.01
		5	-0.001	0.01
		6	0.001	0.01
FUM	1,2,3,4	0	0.363	0.017
		1	0.442	0.017
		2	0.156	0.017
		3	0.03	0.017
		4	0.008	0.017
OAA	1,2,3,4	0	0.392	0.011
		1	0.428	0.011
		2	0.16	0.011
		3	0.022	0.011

	4	-0.003		0.011
OAA	1,2,3,4	0	0.386	0.01
	1	0.437	0.01	
	2	0.158	0.01	
	3	0.02	0.01	
	4	-0.001		0.01
CIT	1,2,3,4,5,6	0	0.241	0.01
	1	0.41	0.01	
	2	0.266	0.01	
	3	0.075	0.01	
	4	0.009	0.01	
	5	0	0.01	
	6	0	0.01	
FUM_U	1,2,3,4	0	0.534	0.017
	1	0.22	0.017	
	2	0.157	0.017	
	3	0.068	0.017	
	4	0.022	0.017	
OAA_U	1,2,3,4	0	0.542	0.011
	1	0.216	0.011	
	2	0.146	0.011	
	3	0.076	0.011	
	4	0.02	0.011	
OAA_U	1,2,3,4	0	0.542	0.01
	1	0.219	0.01	
	2	0.144	0.01	
	3	0.074	0.01	
	4	0.02	0.01	
CIT_U	1,2,3,4,5,6	0	0.409	0.01
	1	0.214	0.01	
	2	0.214	0.01	
	3	0.103	0.01	
	4	0.044	0.01	
	5	0.012	0.01	
	6	0.004	0.01	
FUM_U	1,2,3,4	0	0.532	0.017
	1	0.223	0.017	
	2	0.156	0.017	
	3	0.067	0.017	
	4	0.022	0.017	
OAA_U	1,2,3,4	0	0.546	0.011
	1	0.216	0.011	
	2	0.145	0.011	
	3	0.074	0.011	
	4	0.018	0.011	
OAA_U	1,2,3,4	0	0.542	0.01
	1	0.219	0.01	
	2	0.146	0.01	
	3	0.073	0.01	
	4	0.02	0.01	
CIT_U	1,2,3,4,5,6	0	0.411	0.01
	1	0.212	0.01	
	2	0.216	0.01	

```
            3     0.102 0.01
            4     0.043 0.01
            5     0.012 0.01
            6     0.003 0.01
FUM_U 1,2,3,4     0     0.526 0.017
            1     0.223 0.017
            2     0.158 0.017
            3     0.07  0.017
            4     0.023 0.017
OAA_U 1,2,3,4     0     0.547 0.011
            1     0.22  0.011
            2     0.139 0.011
            3     0.074 0.011
            4     0.02  0.011
OAA_U 1,2,3,4     0     0.543 0.01
            1     0.22  0.01
            2     0.146 0.01
            3     0.073 0.01
            4     0.02  0.01
CIT_U 1,2,3,4,5,6 0     0.409 0.01
            1     0.212 0.01
            2     0.215 0.01
            3     0.105 0.01
            4     0.044 0.01
            5     0.012 0.01
            6     0.003 0.01
ALA   1,2,3 0     0.6   0.011
            1     0.379 0.011
            2     0.019 0.011
            3     0.002 0.011
ALA   2,3   0     0.62  0.011
            1     0.372 0.011
            2     0.008 0.011
GLYeff      1,2   0     0.915 0.011
            1     0.09  0.01
            2     -0.005      0.01
GLYeff      1,2   0     0.906 0.01
            1     0.09  0.01
            2     0.005 0.01
GLYeff      2     0     0.969 0.01
            1     0.031 0.01
VAL   1,2,3,4,5   0     0.382 0.01
            1     0.464 0.01
            2     0.146 0.01
            3     0.017 0.01
            4     -0.004      0.01
            5     -0.006      0.01
VAL   1,2,3,4,5   0     0.365 0.01
            1     0.466 0.01
            2     0.161 0.01
            3     0.012 0.01
            4     -0.001      0.01
            5     -0.002      0.01
```

VAL	2,3,4,5	0	0.385	0.01
		1	0.459	0.01
		2	0.151	0.01
		3	0.007	0.01
		4	-0.002	0.01
VAL	2,3,4,5	0	0.398	0.024
		1	0.429	0.024
		2	0.148	0.024
		3	0.022	0.024
		4	0.002	0.024
LEU	1,2,3,4,5,6	0	0.236	0.02
		1	0.433	0.02
		2	0.259	0.02
		3	0.073	0.02
		4	0.001	0.02
		5	-0.001	0.02
		6	-0.002	0.02
LEU	1,2,3,4,5,6	0	0.223	0.012
		1	0.454	0.012
		2	0.257	0.012
		3	0.062	0.012
		4	0.004	0.012
		5	0	0.012
		6	0	0.012
LEU	2,3,4,5,6	0	0.261	0.017
		1	0.425	0.017
		2	0.252	0.017
		3	0.058	0.017
		4	0.003	0.017
		5	0	0.017
ILE	1,2,3,4,5,6	0	0.212	0.018
		1	0.441	0.018
		2	0.27	0.018
		3	0.074	0.018
		4	0.011	0.018
		5	-0.007	0.018
		6	-0.001	0.018
ILE	2,3,4,5,6	0	0.266	0.01
		1	0.438	0.01
		2	0.239	0.01
		3	0.055	0.01
		4	0.003	0.01
		5	-0.001	0.01
ILE	2,3,4,5,6	0	0.27	0.02
		1	0.433	0.02
		2	0.236	0.02
		3	0.055	0.02
		4	0.005	0.02
		5	0.001	0.02
GLU	2,3,4,5	0	0.332	0.019
		1	0.434	0.019
		2	0.2	0.019
		3	0.033	0.019

```
            4      0      0.019
METeff      1,2,3,4,5    0      0.359 0.01
            1      0.417 0.01
            2      0.178 0.01
            3      0.045 0.01
            4      -0.001       0.01
            5      0.001 0.01
METeff      1,2,3,4,5    0      0.37  0.01
            1      0.398 0.01
            2      0.183 0.01
            3      0.044 0.01
            4      0.003 0.01
            5      0.003 0.01
METeff      2,3,4,5      0      0.408 0.013
            1      0.41  0.013
            2      0.152 0.013
            3      0.028 0.013
            4      0.002 0.013
METeff      2,3,4,5      0      0.408 0.011
            1      0.407 0.011
            2      0.158 0.011
            3      0.026 0.011
            4      0.001 0.011
SEReff      1,2,3 0      0.697 0.01
            1      0.283 0.01
            2      0.021 0.01
            3      -0.001       0.01
SEReff      1,2,3 0      0.693 0.01
            1      0.298 0.01
            2      0.012 0.01
            3      -0.003       0.01
SEReff      2,3    0      0.72  0.01
            1      0.277 0.01
            2      0.003 0.01
SEReff      2,3    0      0.719 0.011
            1      0.277 0.011
            2      0.003 0.011
SEReff      1,2    0      0.931 0.018
            1      0.063 0.018
            2      0.005 0.018
THR   1,2,3,4      0      0.368 0.01
            1      0.447 0.01
            2      0.166 0.01
            3      0.019 0.01
            4      0      0.01
THR   2,3,4 0      0.436 0.01
            1      0.438 0.01
            2      0.119 0.01
            3      0.007 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.269 0.015
            1      0.428 0.015
            2      0.238 0.015
            3      0.057 0.015
```

		4	0.006	0.015
		5	0.001	0.015
		6	0	0.015
		7	-0.001	0.015
		8	0	0.015
		9	0	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.277	0.018
		1	0.429	0.018
		2	0.235	0.018
		3	0.054	0.018
		4	0.004	0.018
		5	0.001	0.018
		6	0	0.018
		7	0	0.018
		8	0	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.276	0.019
		1	0.431	0.019
		2	0.234	0.019
		3	0.053	0.019
		4	0.006	0.019
		5	0	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.953	0.01
		1	0.048	0.01
		2	0	0.01
ASP	1,2,3,4	0	0.373	0.011
		1	0.441	0.011
		2	0.162	0.011
		3	0.026	0.011
		4	-0.002	0.011
ASP	1,2,3,4	0	0.377	0.011
		1	0.436	0.011
		2	0.165	0.011
		3	0.022	0.011
		4	0	0.011
ASP	2,3,4	0	0.441	0.01
		1	0.432	0.01
		2	0.117	0.01
		3	0.01	0.01
ASP	2,3,4	0	0.44	0.018
		1	0.427	0.018
		2	0.119	0.018
		3	0.014	0.018
ASP	1,2	0	0.628	0.011
		1	0.337	0.011
		2	0.036	0.011
CYS	1,2,3	0	0.677	0.027
		1	0.289	0.02
		2	0.043	0.022
		3	-0.009	0.024
CYS	2,3	0	0.733	0.01

		1	0.276	0.01
		2	-0.009	0.01
GLU	1,2,3,4,5	0	0.266	0.023
		1	0.439	0.023
		2	0.248	0.023
		3	0.049	0.023
		4	0.001	0.023
		5	-0.003	0.023
GLU	1,2,3,4,5	0	0.283	0.01
		1	0.425	0.01
		2	0.231	0.01
		3	0.056	0.01
		4	0.005	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.28	0.011
		1	0.426	0.011
		2	0.236	0.011
		3	0.054	0.011
		4	0.004	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.322	0.01
		1	0.458	0.01
		2	0.203	0.01
		3	0.025	0.01
		4	-0.008	0.01
GLU	2,3,4,5	0	0.324	0.011
		1	0.449	0.011
		2	0.201	0.011
		3	0.028	0.011
		4	-0.002	0.011
LYS	1,2,3,4,5,6	0	0.245	0.01
		1	0.415	0.01
		2	0.259	0.01
		3	0.07	0.01
		4	0.009	0.01
		5	0	0.01
		6	0.001	0.01
LYS	1,2,3,4,5,6	0	0.249	0.01
		1	0.413	0.01
		2	0.265	0.01
		3	0.078	0.01
		4	-0.005	0.01
		5	0.004	0.01
		6	-0.004	0.01
LYS	1,2,3,4,5,6	0	0.255	0.01
		1	0.421	0.01
		2	0.263	0.01
		3	0.07	0.01
		4	0.003	0.01
		5	-0.005	0.01
		6	-0.007	0.01
LYS	2,3,4,5,6	0	0.276	0.01
		1	0.434	0.01

```
            2     0.239 0.01
            3     0.052 0.01
            4     0.003 0.01
            5     -0.004      0.01
ARGeff      1,2,3,4,5,6 0     0.282 0.01
            1     0.385 0.01
            2     0.245 0.01
            3     0.085 0.01
            4     0.015 0.01
            5     -0.004      0.01
            6     -0.008      0.01
ARGeff      2,3,4,5,6   0     0.309 0.014
            1     0.425 0.021
            2     0.227 0.014
            3     0.046 0.015
            4     -0.001      0.016
            5     -0.006      0.017
HISeff      1,2,3,4,5,6 0     0.414 0.011
            1     0.422 0.011
            2     0.142 0.011
            3     0.034 0.011
            4     -0.007      0.011
            5     -0.005      0.011
            6     0     0.011
HISeff      1,2,3,4,5,6 0     0.42  0.013
            1     0.388 0.013
            2     0.157 0.013
            3     0.032 0.013
            4     0.002 0.013
            5     0     0.013
            6     0.001 0.013
HISeff      2,3,4,5,6   0     0.528 0.023
            1     0.367 0.023
            2     0.089 0.023
            3     0.019 0.023
            4     0.005 0.023
            5     -0.007      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.272 0.01
            1     0.453 0.01
            2     0.225 0.01
            3     0.063 0.01
            4     0.001 0.01
            5     -0.004      0.01
            6     -0.004      0.01
            7     -0.001      0.01
            8     -0.001      0.01
            9     -0.002      0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.277 0.023
            1     0.418 0.023
            2     0.235 0.023
            3     0.057 0.023
            4     0.007 0.023
            5     0.001 0.023
```

		6	0.002	0.023
		7	0	0.023
		8	0.002	0.023
		9	0.002	0.023
PHE_TYR	2,3,4,5,6,7,8,9	0	0.285	0.01
		1	0.427	0.01
		2	0.229	0.01
		3	0.051	0.01
		4	0.008	0.01
		5	-0.001	0.01
		6	0	0.01
		7	-0.001	0.01
		8	0.002	0.01
PHE_TYR	2,3,4,5,6,7,8,9	0	0.279	0.01
		1	0.44	0.01
		2	0.24	0.01
		3	0.051	0.01
		4	0.004	0.01
		5	-0.002	0.01
		6	-0.003	0.01
		7	-0.004	0.01
		8	-0.004	0.01
PHE_TYR	1,2	0	0.952	0.01
		1	0.047	0.01
		2	0.001	0.01
GLU	1,2,3,4,5	0	0.285	0.01
		1	0.422	0.01
		2	0.24	0.01
		3	0.056	0.01
		4	0.002	0.01
		5	-0.004	0.01
GLU	2,3,4,5	0	0.322	0.011
		1	0.447	0.011
		2	0.2	0.011
		3	0.03	0.011
		4	0.002	0.011
GLU	2,3,4,5	0	0.302	0.013
		1	0.465	0.016
		2	0.209	0.011
		3	0.029	0.014
		4	-0.005	0.015
ALA	1,2,3	0	0.596	0.011
		1	0.381	0.011
		2	0.022	0.011
		3	0	0.011
ALA	2,3	0	0.618	0.011
		1	0.374	0.011
		2	0.008	0.011
GLYeff	1,2	0	0.917	0.01
		1	0.084	0.01
		2	-0.001	0.01
GLYeff	1,2	0	0.911	0.01
		1	0.086	0.01

		2	0.003	0.01
GLYeff		2	0	0.972	0.01
		1	0.028	0.01
VAL	1,2,3,4,5	0	0.381	0.01
		1	0.456	0.01
		2	0.156	0.01
		3	0.012	0.01
		4	0.001	0.01
		5	-0.005	0.01
VAL	1,2,3,4,5	0	0.362	0.01
		1	0.463	0.01
		2	0.164	0.01
		3	0.014	0.01
		4	-0.001	0.01
		5	-0.001	0.01
VAL	2,3,4,5	0	0.38	0.01
		1	0.462	0.01
		2	0.151	0.01
		3	0.009	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.404	0.024
		1	0.439	0.024
		2	0.15	0.024
		3	0.002	0.024
		4	0.004	0.024
LEU	1,2,3,4,5,6	0	0.239	0.02
		1	0.435	0.02
		2	0.253	0.02
		3	0.075	0.02
		4	0.001	0.02
		5	-0.001	0.02
		6	-0.002	0.02
LEU	1,2,3,4,5,6	0	0.221	0.012
		1	0.453	0.012
		2	0.258	0.012
		3	0.064	0.012
		4	0.004	0.012
		5	0	0.012
		6	0	0.012
LEU	2,3,4,5,6	0	0.259	0.017
		1	0.425	0.017
		2	0.253	0.017
		3	0.059	0.017
		4	0.003	0.017
		5	0	0.017
ILE	1,2,3,4,5,6	0	0.211	0.018
		1	0.428	0.018
		2	0.273	0.018
		3	0.084	0.018
		4	0.01	0.018
		5	-0.003	0.018
		6	-0.002	0.018
ILE	2,3,4,5,6	0	0.271	0.01

		1	0.443	0.01
		2	0.243	0.01
		3	0.051	0.01
		4	-0.001	0.01
		5	-0.008	0.01
ILE	2,3,4,5,6	0	0.27	0.02
		1	0.432	0.02
		2	0.236	0.02
		3	0.055	0.02
		4	0.006	0.02
		5	0	0.02
GLU	2,3,4,5	0	0.328	0.019
		1	0.433	0.019
		2	0.206	0.019
		3	0.031	0.019
		4	0.002	0.019
METeff	1,2,3,4,5	0	0.386	0.01
		1	0.378	0.01
		2	0.187	0.01
		3	0.039	0.01
		4	0.006	0.01
		5	0.003	0.01
METeff	1,2,3,4,5	0	0.372	0.01
		1	0.402	0.01
		2	0.181	0.01
		3	0.041	0.01
		4	0.002	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.409	0.013
		1	0.408	0.013
		2	0.157	0.013
		3	0.024	0.013
		4	0.002	0.013
METeff	2,3,4,5	0	0.412	0.011
		1	0.404	0.011
		2	0.156	0.011
		3	0.026	0.011
		4	0.002	0.011
SEReff	1,2,3	0	0.691	0.01
		1	0.291	0.01
		2	0.017	0.01
		3	0.001	0.01
SEReff	1,2,3	0	0.695	0.01
		1	0.301	0.01
		2	0.009	0.01
		3	-0.006	0.01
SEReff	2,3	0	0.718	0.01
		1	0.28	0.01
		2	0.002	0.01
SEReff	2,3	0	0.714	0.011
		1	0.281	0.011
		2	0.005	0.011
SEReff	1,2	0	0.924	0.018

		1	0.07	0.018
		2	0.006	0.018
THR	1,2,3,4	0	0.369	0.01
		1	0.442	0.01
		2	0.17	0.01
		3	0.02	0.01
		4	-0.001	0.01
THR	2,3,4	0	0.434	0.01
		1	0.435	0.01
		2	0.123	0.01
		3	0.008	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.268	0.015
		1	0.423	0.015
		2	0.239	0.015
		3	0.061	0.015
		4	0.006	0.015
		5	0.002	0.015
		6	0.001	0.015
		7	-0.001	0.015
		8	0	0.015
		9	0	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.275	0.018
		1	0.429	0.018
		2	0.236	0.018
		3	0.053	0.018
		4	0.006	0.018
		5	0	0.018
		6	0	0.018
		7	0	0.018
		8	0	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.273	0.019
		1	0.428	0.019
		2	0.238	0.019
		3	0.056	0.019
		4	0.005	0.019
		5	0	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.95	0.01
		1	0.048	0.01
		2	0.002	0.01
ASP	1,2,3,4	0	0.373	0.011
		1	0.437	0.011
		2	0.169	0.011
		3	0.023	0.011
		4	-0.001	0.011
ASP	1,2,3,4	0	0.376	0.011
		1	0.437	0.011
		2	0.166	0.011
		3	0.021	0.011
		4	0	0.011
ASP	2,3,4	0	0.443	0.01

		1	0.428	0.01
		2	0.119	0.01
		3	0.01	0.01
ASP	2,3,4	0	0.441	0.018
		1	0.428	0.018
		2	0.118	0.018
		3	0.014	0.018
ASP	1,2	0	0.628	0.011
		1	0.337	0.011
		2	0.035	0.011
CYS	1,2,3	0	0.68	0.028
		1	0.318	0.021
		2	0.027	0.022
		3	-0.025	0.025
CYS	2,3	0	0.702	0.01
		1	0.293	0.01
		2	0.005	0.01
GLU	1,2,3,4,5	0	0.256	0.023
		1	0.448	0.023
		2	0.244	0.023
		3	0.054	0.023
		4	0.004	0.023
		5	-0.006	0.023
GLU	1,2,3,4,5	0	0.278	0.01
		1	0.424	0.01
		2	0.241	0.01
		3	0.055	0.01
		4	0.003	0.01
		5	0	0.01
GLU	1,2,3,4,5	0	0.281	0.011
		1	0.424	0.011
		2	0.236	0.011
		3	0.056	0.011
		4	0.005	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.322	0.01
		1	0.456	0.01
		2	0.204	0.01
		3	0.025	0.01
		4	-0.007	0.01
GLU	2,3,4,5	0	0.324	0.011
		1	0.448	0.011
		2	0.202	0.011
		3	0.029	0.011
		4	-0.003	0.011
LYS	1,2,3,4,5,6	0	0.244	0.01
		1	0.421	0.01
		2	0.259	0.01
		3	0.067	0.01
		4	0.009	0.01
		5	0.001	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.245	0.01

		1	0.427	0.01
		2	0.262	0.01
		3	0.072	0.01
		4	0.007	0.01
		5	-0.008	0.01
		6	-0.005	0.01
LYS	1,2,3,4,5,6	0	0.245	0.01
		1	0.43	0.01
		2	0.257	0.01
		3	0.068	0.01
		4	0.008	0.01
		5	-0.003	0.01
		6	-0.005	0.01
LYS	2,3,4,5,6	0	0.274	0.01
		1	0.431	0.01
		2	0.242	0.01
		3	0.055	0.01
		4	0.002	0.01
		5	-0.005	0.01
ARGeff	1,2,3,4,5,6	0	0.276	0.013
		1	0.378	0.013
		2	0.234	0.013
		3	0.094	0.013
		4	0.028	0.013
		5	0	0.013
		6	-0.011	0.013
ARGeff	1,2,3,4,5,6	0	0.28	0.01
		1	0.386	0.01
		2	0.253	0.01
		3	0.082	0.01
		4	0.011	0.01
		5	-0.003	0.01
		6	-0.008	0.01
ARGeff	2,3,4,5,6	0	0.314	0.01
		1	0.41	0.01
		2	0.223	0.01
		3	0.048	0.01
		4	0.007	0.01
		5	-0.002	0.01
HISeff	1,2,3,4,5,6	0	0.411	0.011
		1	0.4	0.011
		2	0.171	0.011
		3	0.018	0.011
		4	0.003	0.011
		5	0	0.011
		6	-0.003	0.011
HISeff	1,2,3,4,5,6	0	0.409	0.013
		1	0.389	0.013
		2	0.169	0.013
		3	0.029	0.013
		4	0.002	0.013
		5	0.001	0.013
		6	0.001	0.013

```
HISeff      2,3,4,5,6   0      0.528 0.023
            1      0.368 0.023
            2      0.088 0.023
            3      0.014 0.023
            4      0.005 0.023
            5      -0.002      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.275 0.01
            1      0.419 0.01
            2      0.245 0.01
            3      0.058 0.01
            4      0.003 0.01
            5      0.004 0.01
            6      -0.002      0.01
            7      -0.001      0.01
            8      0      0.01
            9      0      0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.27  0.023
            1      0.419 0.023
            2      0.24  0.023
            3      0.057 0.023
            4      0.006 0.023
            5      0      0.023
            6      0.002 0.023
            7      0      0.023
            8      0.003 0.023
            9      0.003 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0      0.282 0.01
            1      0.423 0.01
            2      0.233 0.01
            3      0.053 0.01
            4      0.005 0.01
            5      0.001 0.01
            6      0      0.01
            7      0.001 0.01
            8      0.003 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0      0.281 0.01
            1      0.435 0.01
            2      0.237 0.01
            3      0.052 0.01
            4      0.007 0.01
            5      -0.002      0.01
            6      -0.003      0.01
            7      -0.004      0.01
            8      -0.004      0.01
PHE_TYR     1,2    0      0.949 0.01
            1      0.05  0.01
            2      0.001 0.01
GLU   1,2,3,4,5    0      0.283 0.01
            1      0.422 0.01
            2      0.236 0.01
            3      0.058 0.01
            4      0.004 0.01
            5      -0.003      0.01
```

GLU	2,3,4,5	0	0.321	0.011
		1	0.447	0.011
		2	0.203	0.011
		3	0.03	0.011
		4	-0.001	0.011
GLU	2,3,4,5	0	0.299	0.01
		1	0.46	0.01
		2	0.208	0.01
		3	0.033	0.01
		4	0	0.01
ALA	1,2,3	0	0.597	0.011
		1	0.382	0.011
		2	0.02	0.011
		3	0.001	0.011
ALA	2,3	0	0.618	0.011
		1	0.374	0.011
		2	0.008	0.011
GLYeff	1,2	0	0.903	0.01
		1	0.092	0.01
		2	0.005	0.01
GLYeff	1,2	0	0.905	0.01
		1	0.091	0.01
		2	0.003	0.01
GLYeff	2	0	0.97	0.01
		1	0.03	0.01
VAL	1,2,3,4,5	0	0.381	0.01
		1	0.463	0.01
		2	0.148	0.01
		3	0.016	0.01
		4	-0.001	0.01
		5	-0.006	0.01
VAL	1,2,3,4,5	0	0.362	0.01
		1	0.465	0.01
		2	0.163	0.01
		3	0.014	0.01
		4	-0.001	0.01
		5	-0.002	0.01
VAL	2,3,4,5	0	0.381	0.01
		1	0.46	0.01
		2	0.151	0.01
		3	0.009	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.397	0.024
		1	0.432	0.024
		2	0.149	0.024
		3	0.02	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.238	0.02
		1	0.44	0.02
		2	0.252	0.02
		3	0.07	0.02
		4	0.004	0.02
		5	0	0.02

		6	-0.002	0.02
LEU	1,2,3,4,5,6	0	0.219	0.012
		1	0.453	0.012
		2	0.261	0.012
		3	0.062	0.012
		4	0.004	0.012
		5	0	0.012
		6	0	0.012
LEU	2,3,4,5,6	0	0.256	0.017
		1	0.427	0.017
		2	0.254	0.017
		3	0.059	0.017
		4	0.003	0.017
		5	0	0.017
ILE	1,2,3,4,5,6	0	0.206	0.018
		1	0.446	0.018
		2	0.262	0.018
		3	0.084	0.018
		4	0.007	0.018
		5	-0.004	0.018
		6	-0.002	0.018
ILE	2,3,4,5,6	0	0.265	0.01
		1	0.443	0.01
		2	0.241	0.01
		3	0.053	0.01
		4	0.002	0.01
		5	-0.004	0.01
ILE	2,3,4,5,6	0	0.267	0.02
		1	0.433	0.02
		2	0.238	0.02
		3	0.056	0.02
		4	0.005	0.02
		5	0	0.02
GLU	2,3,4,5	0	0.338	0.019
		1	0.433	0.019
		2	0.2	0.019
		3	0.031	0.019
		4	-0.002	0.019
METeff	1,2,3,4,5	0	0.38	0.01
		1	0.391	0.01
		2	0.188	0.01
		3	0.035	0.01
		4	0.002	0.01
		5	0.003	0.01
METeff	1,2,3,4,5	0	0.371	0.01
		1	0.402	0.01
		2	0.181	0.01
		3	0.039	0.01
		4	0.005	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.408	0.013
		1	0.409	0.013
		2	0.155	0.013

```
            3     0.026 0.013
            4     0.002 0.013
METeff      2,3,4,5     0     0.411 0.011
            1     0.404 0.011
            2     0.157 0.011
            3     0.026 0.011
            4     0.001 0.011
SEReff      1,2,3 0     0.691 0.01
            1     0.296 0.01
            2     0.017 0.01
            3     -0.003      0.01
SEReff      1,2,3 0     0.693 0.01
            1     0.299 0.01
            2     0.012 0.01
            3     -0.004      0.01
SEReff      2,3   0     0.716 0.01
            1     0.282 0.01
            2     0.001 0.01
SEReff      2,3   0     0.717 0.011
            1     0.279 0.011
            2     0.004 0.011
SEReff      1,2   0     0.925 0.018
            1     0.07  0.018
            2     0.004 0.018
THR   1,2,3,4     0     0.364 0.01
            1     0.45  0.01
            2     0.168 0.01
            3     0.02  0.01
            4     -0.003      0.01
THR   2,3,4 0     0.436 0.01
            1     0.425 0.01
            2     0.13  0.01
            3     0.008 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.27  0.015
            1     0.424 0.015
            2     0.243 0.015
            3     0.056 0.015
            4     0.007 0.015
            5     0.001 0.015
            6     0     0.015
            7     0     0.015
            8     0     0.015
            9     0     0.015
PHE_TYR     2,3,4,5,6,7,8,9   0     0.276 0.018
            1     0.431 0.018
            2     0.236 0.018
            3     0.052 0.018
            4     0.005 0.018
            5     0     0.018
            6     0     0.018
            7     0     0.018
            8     0     0.018
PHE_TYR     2,3,4,5,6,7,8,9   0     0.275 0.019
```

		1	0.429	0.019
		2	0.236	0.019
		3	0.054	0.019
		4	0.005	0.019
		5	0.001	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.951	0.01
		1	0.048	0.01
		2	0.001	0.01
ASP	1,2,3,4	0	0.373	0.011
		1	0.441	0.011
		2	0.162	0.011
		3	0.025	0.011
		4	-0.001	0.011
ASP	1,2,3,4	0	0.374	0.011
		1	0.439	0.011
		2	0.166	0.011
		3	0.021	0.011
		4	0	0.011
ASP	2,3,4	0	0.44	0.01
		1	0.431	0.01
		2	0.119	0.01
		3	0.01	0.01
ASP	2,3,4	0	0.44	0.018
		1	0.428	0.018
		2	0.119	0.018
		3	0.014	0.018
ASP	1,2	0	0.629	0.011
		1	0.336	0.011
		2	0.035	0.011
CYS	1,2,3	0	0.691	0.018
		1	0.313	0.018
		2	0.011	0.018
		3	-0.014	0.018
CYS	2,3	0	0.699	0.01
		1	0.303	0.01
		2	-0.002	0.01
GLU	1,2,3,4,5	0	0.261	0.023
		1	0.442	0.023
		2	0.246	0.023
		3	0.052	0.023
		4	0.001	0.023
		5	-0.001	0.023
GLU	1,2,3,4,5	0	0.283	0.01
		1	0.426	0.01
		2	0.231	0.01
		3	0.057	0.01
		4	0.004	0.01
		5	0.001	0.01
GLU	1,2,3,4,5	0	0.28	0.011
		1	0.426	0.011

		2	0.235	0.011
		3	0.054	0.011
		4	0.005	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.319	0.01
		1	0.458	0.01
		2	0.206	0.01
		3	0.024	0.01
		4	-0.007	0.01
GLU	2,3,4,5	0	0.325	0.011
		1	0.45	0.011
		2	0.199	0.011
		3	0.028	0.011
		4	-0.002	0.011
LYS	1,2,3,4,5,6	0	0.242	0.01
		1	0.42	0.01
		2	0.258	0.01
		3	0.069	0.01
		4	0.012	0.01
		5	0.001	0.01
		6	-0.001	0.01
LYS	1,2,3,4,5,6	0	0.248	0.01
		1	0.419	0.01
		2	0.249	0.01
		3	0.079	0.01
		4	0.007	0.01
		5	-0.001	0.01
		6	-0.002	0.01
LYS	1,2,3,4,5,6	0	0.244	0.01
		1	0.426	0.01
		2	0.259	0.01
		3	0.07	0.01
		4	0.007	0.01
		5	-0.002	0.01
		6	-0.004	0.01
LYS	2,3,4,5,6	0	0.271	0.01
		1	0.432	0.01
		2	0.239	0.01
		3	0.056	0.01
		4	0.005	0.01
		5	-0.002	0.01
ARGeff	1,2,3,4,5,6	0	0.274	0.01
		1	0.392	0.01
		2	0.251	0.01
		3	0.077	0.01
		4	0.016	0.01
		5	-0.004	0.01
		6	-0.005	0.01
ARGeff	2,3,4,5,6	0	0.308	0.011
		1	0.424	0.016
		2	0.22	0.011
		3	0.046	0.011
		4	0.005	0.012

```
            5     -0.003      0.013
HISeff      1,2,3,4,5,6 0     0.406 0.011
            1     0.41  0.011
            2     0.163 0.011
            3     0.022 0.011
            4     -0.002      0.011
            5     0.004 0.011
            6     -0.004      0.011
HISeff      1,2,3,4,5,6 0     0.41  0.013
            1     0.395 0.013
            2     0.163 0.013
            3     0.031 0.013
            4     0     0.013
            5     0.001 0.013
            6     0.001 0.013
HISeff      2,3,4,5,6   0     0.532 0.023
            1     0.374 0.023
            2     0.084 0.023
            3     0.014 0.023
            4     0.005 0.023
            5     -0.007      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.263 0.01
            1     0.432 0.01
            2     0.242 0.01
            3     0.059 0.01
            4     0.007 0.01
            5     -0.002      0.01
            6     -0.002      0.01
            7     0     0.01
            8     0     0.01
            9     0     0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.271 0.023
            1     0.425 0.023
            2     0.234 0.023
            3     0.057 0.023
            4     0.007 0.023
            5     0     0.023
            6     0.002 0.023
            7     0     0.023
            8     0.001 0.023
            9     0.002 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.281 0.01
            1     0.428 0.01
            2     0.234 0.01
            3     0.05  0.01
            4     0.006 0.01
            5     -0.001      0.01
            6     0.001 0.01
            7     -0.001      0.01
            8     0.002 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0     0.28  0.01
            1     0.436 0.01
            2     0.238 0.01
```

		3	0.055	0.01
		4	0.004	0.01
		5	-0.002	0.01
		6	-0.003	0.01
		7	-0.004	0.01
		8	-0.004	0.01
PHE_TYR	1,2	0	0.95	0.01
		1	0.049	0.01
		2	0.002	0.01
GLU	1,2,3,4,5	0	0.289	0.01
		1	0.419	0.01
		2	0.238	0.01
		3	0.057	0.01
		4	0.001	0.01
		5	-0.003	0.01
GLU	2,3,4,5	0	0.32	0.011
		1	0.449	0.011
		2	0.2	0.011
		3	0.031	0.011
		4	0	0.011
GLU	2,3,4,5	0	0.299	0.01
		1	0.465	0.012
		2	0.21	0.01
		3	0.029	0.01
		4	-0.003	0.011
ALA_U	1,2,3	0	0.722	0.011
		1	0.085	0.011
		2	0.042	0.011
		3	0.151	0.011
ALA_U	2,3	0	0.764	0.011
		1	0.056	0.011
		2	0.18	0.011
VAL_U	1,2,3,4,5	0	0.54	0.01
		1	0.125	0.01
		2	0.167	0.01
		3	0.125	0.01
		4	0.019	0.01
		5	0.023	0.01
VAL_U	1,2,3,4,5	0	0.548	0.01
		1	0.116	0.01
		2	0.168	0.01
		3	0.129	0.01
		4	0.016	0.01
		5	0.023	0.01
VAL_U	2,3,4,5	0	0.582	0.01
		1	0.102	0.01
		2	0.265	0.01
		3	0.022	0.01
		4	0.029	0.01
VAL_U	2,3,4,5	0	0.588	0.024
		1	0.095	0.024
		2	0.257	0.024
		3	0.032	0.024

		4	0.028	0.024
LEU_U	1,2,3,4,5,6	0	0.44	0.02
		1	0.124	0.02
		2	0.305	0.02
		3	0.055	0.02
		4	0.07	0.02
		5	0.004	0.02
		6	0.003	0.02
LEU_U	1,2,3,4,5,6	0	0.438	0.012
		1	0.117	0.012
		2	0.319	0.012
		3	0.05	0.012
		4	0.067	0.012
		5	0.005	0.012
		6	0.005	0.012
LEU_U	2,3,4,5,6	0	0.469	0.017
		1	0.191	0.017
		2	0.231	0.017
		3	0.073	0.017
		4	0.029	0.017
		5	0.006	0.017
ILE_U	1,2,3,4,5,6	0	0.411	0.018
		1	0.205	0.018
		2	0.23	0.018
		3	0.101	0.018
		4	0.039	0.018
		5	0.011	0.018
		6	0.002	0.018
ILE_U	2,3,4,5,6	0	0.459	0.01
		1	0.213	0.01
		2	0.219	0.01
		3	0.08	0.01
		4	0.023	0.01
		5	0.006	0.01
ILE_U	2,3,4,5,6	0	0.464	0.02
		1	0.21	0.02
		2	0.216	0.02
		3	0.079	0.02
		4	0.024	0.02
		5	0.007	0.02
GLU_U	2,3,4,5	0	0.522	0.019
		1	0.23	0.019
		2	0.185	0.019
		3	0.047	0.019
		4	0.015	0.019
METeff_U	1,2,3,4,5	0	0.477	0.01
		1	0.268	0.01
		2	0.126	0.01
		3	0.079	0.01
		4	0.042	0.01
		5	0.009	0.01
METeff_U	1,2,3,4,5	0	0.488	0.01
		1	0.263	0.01

```
            2     0.126 0.01
            3     0.083 0.01
            4     0.033 0.01
            5     0.008 0.01
METeff_U    2,3,4,5     0     0.553 0.013
            1     0.255 0.013
            2     0.105 0.013
            3     0.074 0.013
            4     0.012 0.013
METeff_U    2,3,4,5     0     0.555 0.011
            1     0.257 0.011
            2     0.107 0.011
            3     0.071 0.011
            4     0.01  0.011
SEReff_U    1,2,3 0     0.68  0.01
            1     0.15  0.01
            2     0.077 0.01
            3     0.093 0.01
SEReff_U    1,2,3 0     0.677 0.01
            1     0.152 0.01
            2     0.077 0.01
            3     0.095 0.01
SEReff_U    2,3   0     0.716 0.01
            1     0.168 0.01
            2     0.116 0.01
SEReff_U    2,3   0     0.719 0.011
            1     0.165 0.011
            2     0.116 0.011
SEReff_U    1,2   0     0.743 0.018
            1     0.111 0.018
            2     0.146 0.018
THR_U 1,2,3,4     0     0.539 0.01
            1     0.222 0.01
            2     0.149 0.01
            3     0.07  0.01
            4     0.02  0.01
THR_U 2,3,4 0     0.601 0.01
            1     0.231 0.01
            2     0.125 0.01
            3     0.043 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.356 0.015
            1     0.153 0.015
            2     0.136 0.015
            3     0.173 0.015
            4     0.085 0.015
            5     0.047 0.015
            6     0.031 0.015
            7     0.012 0.015
            8     0.005 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.377 0.018
            1     0.143 0.018
            2     0.209 0.018
```

		3	0.119	0.018
		4	0.082	0.018
		5	0.039	0.018
		6	0.024	0.018
		7	0.005	0.018
		8	0.003	0.018
PHE_TYR_U	2,3,4,5,6,7,8,9	0	0.376	0.019
		1	0.145	0.019
		2	0.212	0.019
		3	0.121	0.019
		4	0.08	0.019
		5	0.039	0.019
		6	0.021	0.019
		7	0.003	0.019
		8	0.002	0.019
PHE_TYR_U	1,2	0	0.752	0.01
		1	0.089	0.01
		2	0.159	0.01
ASP_U	1,2,3,4	0	0.545	0.011
		1	0.215	0.011
		2	0.148	0.011
		3	0.073	0.011
		4	0.02	0.011
ASP_U	1,2,3,4	0	0.542	0.011
		1	0.22	0.011
		2	0.148	0.011
		3	0.071	0.011
		4	0.018	0.011
ASP_U	2,3,4	0	0.607	0.01
		1	0.227	0.01
		2	0.122	0.01
		3	0.043	0.01
ASP_U	2,3,4	0	0.607	0.018
		1	0.225	0.018
		2	0.121	0.018
		3	0.047	0.018
ASP_U	1,2	0	0.72	0.011
		1	0.161	0.011
		2	0.12	0.011
CYS_U	1,2,3	0	0.729	0.018
		1	0.117	0.018
		2	0.068	0.018
		3	0.085	0.018
CYS_U	2,3	0	0.74	0.01
		1	0.139	0.01
		2	0.12	0.01
GLU_U	1,2,3,4,5	0	0.469	0.023
		1	0.215	0.023
		2	0.212	0.023
		3	0.085	0.023
		4	0.022	0.023
		5	-0.004	0.023
GLU_U	1,2,3,4,5	0	0.467	0.01

		1	0.208	0.01
		2	0.212	0.01
		3	0.08	0.01
		4	0.025	0.01
		5	0.009	0.01
GLU_U	1,2,3,4,5	0	0.469	0.011
		1	0.208	0.011
		2	0.211	0.011
		3	0.08	0.011
		4	0.024	0.011
		5	0.008	0.011
GLU_U	2,3,4,5	0	0.519	0.01
		1	0.229	0.01
		2	0.197	0.01
		3	0.045	0.01
		4	0.01	0.01
GLU_U	2,3,4,5	0	0.523	0.011
		1	0.223	0.011
		2	0.194	0.011
		3	0.047	0.011
		4	0.013	0.011
LYS_U	1,2,3,4,5,6	0	0.426	0.01
		1	0.205	0.01
		2	0.185	0.01
		3	0.124	0.01
		4	0.041	0.01
		5	0.015	0.01
		6	0.005	0.01
LYS_U	1,2,3,4,5,6	0	0.417	0.01
		1	0.211	0.01
		2	0.196	0.01
		3	0.116	0.01
		4	0.046	0.01
		5	0.014	0.01
		6	0	0.01
LYS_U	1,2,3,4,5,6	0	0.419	0.01
		1	0.218	0.01
		2	0.181	0.01
		3	0.121	0.01
		4	0.044	0.01
		5	0.014	0.01
		6	0.004	0.01
LYS_U	2,3,4,5,6	0	0.459	0.01
		1	0.216	0.01
		2	0.218	0.01
		3	0.078	0.01
		4	0.023	0.01
		5	0.006	0.01
ARGeff_U	1,2,3,4,5,6	0	0.403	0.013
		1	0.248	0.013
		2	0.213	0.013
		3	0.101	0.013
		4	0.027	0.013

	5	0.011	0.013			
	6	-0.005		0.013		
ARGeff_U	1,2,3,4,5,6		0	0.416	0.01	
	1	0.253	0.01			
	2	0.194	0.01			
	3	0.1	0.01			
	4	0.033	0.01			
	5	0.007	0.01			
	6	-0.002		0.01		
ARGeff_U	2,3,4,5,6		0	0.452	0.01	
	1	0.273	0.01			
	2	0.179	0.01			
	3	0.074	0.01			
	4	0.016	0.01			
	5	0.006	0.01			
HISeff_U	1,2,3,4,5,6		0	0.458	0.011	
	1	0.233	0.011			
	2	0.115	0.011			
	3	0.097	0.011			
	4	0.034	0.011			
	5	0.06	0.011			
	6	0.003	0.011			
HISeff_U	1,2,3,4,5,6		0	0.468	0.013	
	1	0.227	0.013			
	2	0.119	0.013			
	3	0.103	0.013			
	4	0.044	0.013			
	5	0.032	0.013			
	6	0.008	0.013			
HISeff_U	2,3,4,5,6		0	0.494	0.015	
	1	0.248	0.014			
	2	0.166	0.014			
	3	0.066	0.014			
	4	0.022	0.014			
	5	0.003	0.014			
HISeff_U	2,3,4,5,6		0	0.471	0.023	
	1	0.241	0.023			
	2	0.174	0.023			
	3	0.071	0.023			
	4	0.035	0.023			
	5	0.008	0.023			
PHE_TYR_U	1,2,3,4,5,6,7,8,9			0	0.357	0.01
	1	0.149	0.01			
	2	0.137	0.01			
	3	0.173	0.01			
	4	0.087	0.01			
	5	0.05	0.01			
	6	0.03	0.01			
	7	0.012	0.01			
	8	0.003	0.01			
	9	0.001	0.01			
PHE_TYR_U	1,2,3,4,5,6,7,8,9			0	0.36	0.023
	1	0.151	0.023			

```
            2     0.138 0.023
            3     0.172 0.023
            4     0.082 0.023
            5     0.047 0.023
            6     0.029 0.023
            7     0.014 0.023
            8     0.004 0.023
            9     0.003 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.378 0.01
            1     0.146 0.01
            2     0.206 0.01
            3     0.117 0.01
            4     0.081 0.01
            5     0.038 0.01
            6     0.022 0.01
            7     0.005 0.01
            8     0.005 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.371 0.01
            1     0.145 0.01
            2     0.21  0.01
            3     0.124 0.01
            4     0.082 0.01
            5     0.042 0.01
            6     0.022 0.01
            7     0.004 0.01
            8     0.001 0.01
PHE_TYR_U   1,2   0     0.752 0.01
            1     0.09  0.01
            2     0.158 0.01
GLU_U 1,2,3,4,5   0     0.469 0.01
            1     0.208 0.01
            2     0.21  0.01
            3     0.08  0.01
            4     0.024 0.01
            5     0.009 0.01
GLU_U 2,3,4,5     0     0.521 0.011
            1     0.225 0.011
            2     0.192 0.011
            3     0.048 0.011
            4     0.014 0.011
GLU_U 2,3,4,5     0     0.515 0.018
            1     0.23  0.01
            2     0.199 0.01
            3     0.045 0.012
            4     0.01  0.014
ALA_U 1,2,3 0     0.723 0.011
            1     0.083 0.011
            2     0.04  0.011
            3     0.154 0.011
ALA_U 2,3   0     0.764 0.011
            1     0.055 0.011
            2     0.181 0.011
GLYeff_U    1,2   0     0.735 0.01
```

```
            1     0.139 0.01
            2     0.125 0.01
GLYeff_U    1,2   0     0.736 0.01
            1     0.139 0.01
            2     0.125 0.01
GLYeff_U    2     0     0.805 0.01
            1     0.195 0.01
VAL_U 1,2,3,4,5   0     0.541 0.01
            1     0.125 0.01
            2     0.168 0.01
            3     0.124 0.01
            4     0.019 0.01
            5     0.023 0.01
VAL_U 1,2,3,4,5   0     0.545 0.01
            1     0.116 0.01
            2     0.166 0.01
            3     0.132 0.01
            4     0.016 0.01
            5     0.025 0.01
VAL_U 2,3,4,5     0     0.579 0.01
            1     0.103 0.01
            2     0.267 0.01
            3     0.023 0.01
            4     0.029 0.01
VAL_U 2,3,4,5     0     0.589 0.024
            1     0.095 0.024
            2     0.257 0.024
            3     0.031 0.024
            4     0.028 0.024
LEU_U 1,2,3,4,5,6 0     0.431 0.02
            1     0.123 0.02
            2     0.31  0.02
            3     0.058 0.02
            4     0.066 0.02
            5     0.007 0.02
            6     0.006 0.02
LEU_U 1,2,3,4,5,6 0     0.436 0.012
            1     0.117 0.012
            2     0.32  0.012
            3     0.05  0.012
            4     0.067 0.012
            5     0.005 0.012
            6     0.005 0.012
LEU_U 2,3,4,5,6   0     0.466 0.017
            1     0.192 0.017
            2     0.234 0.017
            3     0.073 0.017
            4     0.029 0.017
            5     0.006 0.017
ILE_U 1,2,3,4,5,6 0     0.388 0.018
            1     0.214 0.018
            2     0.235 0.018
            3     0.102 0.018
```

```
            4     0.044 0.018
            5     0.014 0.018
            6     0.003 0.018
ILE_U 2,3,4,5,6   0     0.455 0.01
            1     0.216 0.01
            2     0.22  0.01
            3     0.079 0.01
            4     0.024 0.01
            5     0.007 0.01
ILE_U 2,3,4,5,6   0     0.46  0.02
            1     0.212 0.02
            2     0.217 0.02
            3     0.08  0.02
            4     0.024 0.02
            5     0.007 0.02
GLU_U 2,3,4,5     0     0.524 0.019
            1     0.224 0.019
            2     0.189 0.019
            3     0.047 0.019
            4     0.016 0.019
METeff_U    1,2,3,4,5   0     0.489 0.01
            1     0.259 0.01
            2     0.125 0.01
            3     0.078 0.01
            4     0.036 0.01
            5     0.013 0.01
METeff_U    1,2,3,4,5   0     0.491 0.01
            1     0.26  0.01
            2     0.126 0.01
            3     0.082 0.01
            4     0.033 0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0     0.559 0.013
            1     0.251 0.013
            2     0.107 0.013
            3     0.071 0.013
            4     0.011 0.013
METeff_U    2,3,4,5     0     0.561 0.011
            1     0.252 0.011
            2     0.106 0.011
            3     0.071 0.011
            4     0.011 0.011
SEReff_U    1,2,3 0     0.673 0.01
            1     0.153 0.01
            2     0.078 0.01
            3     0.096 0.01
SEReff_U    1,2,3 0     0.675 0.01
            1     0.153 0.01
            2     0.077 0.01
            3     0.096 0.01
SEReff_U    2,3   0     0.716 0.01
            1     0.166 0.01
            2     0.118 0.01
```

```
SEReff_U     2,3    0      0.717 0.011
             1      0.165 0.011
             2      0.118 0.011
SEReff_U     1,2    0      0.743 0.018
             1      0.11  0.018
             2      0.148 0.018
THR_U 1,2,3,4       0      0.537 0.01
             1      0.223 0.01
             2      0.153 0.01
             3      0.07  0.01
             4      0.017 0.01
THR_U 2,3,4 0       0.602 0.01
             1      0.231 0.01
             2      0.123 0.01
             3      0.044 0.01
PHE_TYR_U    1,2,3,4,5,6,7,8,9 0      0.357 0.015
             1      0.151 0.015
             2      0.137 0.015
             3      0.175 0.015
             4      0.085 0.015
             5      0.047 0.015
             6      0.03  0.015
             7      0.012 0.015
             8      0.004 0.015
             9      0.002 0.015
PHE_TYR_U    2,3,4,5,6,7,8,9   0      0.374 0.018
             1      0.146 0.018
             2      0.209 0.018
             3      0.12  0.018
             4      0.082 0.018
             5      0.039 0.018
             6      0.023 0.018
             7      0.005 0.018
             8      0.003 0.018
PHE_TYR_U    2,3,4,5,6,7,8,9   0      0.37  0.019
             1      0.143 0.019
             2      0.212 0.019
             3      0.122 0.019
             4      0.083 0.019
             5      0.04  0.019
             6      0.023 0.019
             7      0.005 0.019
             8      0.003 0.019
PHE_TYR_U    1,2    0      0.751 0.01
             1      0.088 0.01
             2      0.161 0.01
ASP_U 1,2,3,4       0      0.539 0.011
             1      0.218 0.011
             2      0.154 0.011
             3      0.072 0.011
             4      0.018 0.011
ASP_U 1,2,3,4       0      0.539 0.011
             1      0.221 0.011
```

```
            2     0.151 0.011
            3     0.07  0.011
            4     0.019 0.011
ASP_U 2,3,4 0     0.603 0.01
            1     0.23  0.01
            2     0.122 0.01
            3     0.044 0.01
ASP_U 2,3,4 0     0.601 0.018
            1     0.228 0.018
            2     0.123 0.018
            3     0.048 0.018
ASP_U 1,2   0     0.717 0.011
            1     0.163 0.011
            2     0.12  0.011
CYS_U 1,2,3 0     0.684 0.018
            1     0.145 0.018
            2     0.068 0.018
            3     0.103 0.018
CYS_U 2,3   0     0.73  0.01
            1     0.152 0.01
            2     0.117 0.01
GLU_U 1,2,3,4,5   0     0.454 0.023
            1     0.215 0.023
            2     0.22  0.023
            3     0.083 0.023
            4     0.024 0.023
            5     0.004 0.023
GLU_U 1,2,3,4,5   0     0.466 0.01
            1     0.21  0.01
            2     0.209 0.01
            3     0.084 0.01
            4     0.024 0.01
            5     0.007 0.01
GLU_U 1,2,3,4,5   0     0.465 0.011
            1     0.209 0.011
            2     0.212 0.011
            3     0.081 0.011
            4     0.024 0.011
            5     0.008 0.011
GLU_U 2,3,4,5     0     0.513 0.01
            1     0.23  0.01
            2     0.196 0.01
            3     0.048 0.01
            4     0.013 0.01
GLU_U 2,3,4,5     0     0.519 0.011
            1     0.225 0.011
            2     0.195 0.011
            3     0.048 0.011
            4     0.013 0.011
LYS_U 1,2,3,4,5,6 0     0.421 0.01
            1     0.213 0.01
            2     0.18  0.01
            3     0.122 0.01
```

```
            4     0.043 0.01
            5     0.016 0.01
            6     0.005 0.01
LYS_U 1,2,3,4,5,6 0     0.415 0.01
            1     0.214 0.01
            2     0.185 0.01
            3     0.12  0.01
            4     0.047 0.01
            5     0.014 0.01
            6     0.005 0.01
LYS_U 1,2,3,4,5,6 0     0.414 0.01
            1     0.219 0.01
            2     0.181 0.01
            3     0.122 0.01
            4     0.044 0.01
            5     0.016 0.01
            6     0.004 0.01
LYS_U 2,3,4,5,6   0     0.453 0.01
            1     0.217 0.01
            2     0.221 0.01
            3     0.079 0.01
            4     0.024 0.01
            5     0.006 0.01
ARGeff_U    1,2,3,4,5,6 0     0.417 0.013
            1     0.243 0.013
            2     0.194 0.013
            3     0.105 0.013
            4     0.03  0.013
            5     0.019 0.013
            6     -0.008      0.013
ARGeff_U    1,2,3,4,5,6 0     0.409 0.01
            1     0.25  0.01
            2     0.198 0.01
            3     0.101 0.01
            4     0.033 0.01
            5     0.009 0.01
            6     0     0.01
ARGeff_U    2,3,4,5,6   0     0.451 0.01
            1     0.265 0.01
            2     0.187 0.01
            3     0.074 0.01
            4     0.019 0.01
            5     0.005 0.01
HISeff_U    1,2,3,4,5,6 0     0.469 0.011
            1     0.237 0.011
            2     0.108 0.011
            3     0.106 0.011
            4     0.046 0.011
            5     0.028 0.011
            6     0.005 0.011
HISeff_U    1,2,3,4,5,6 0     0.465 0.013
            1     0.229 0.013
            2     0.117 0.013
```

```
            3      0.105 0.013
            4      0.047 0.013
            5      0.031 0.013
            6      0.007 0.013
HISeff_U    2,3,4,5,6   0      0.493 0.018
            1      0.243 0.014
            2      0.175 0.014
            3      0.066 0.014
            4      0.023 0.014
            5      0     0.015
HISeff_U    2,3,4,5,6   0      0.472 0.023
            1      0.237 0.023
            2      0.176 0.023
            3      0.071 0.023
            4      0.036 0.023
            5      0.008 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.35  0.01
            1      0.151 0.01
            2      0.144 0.01
            3      0.175 0.01
            4      0.085 0.01
            5      0.048 0.01
            6      0.03  0.01
            7      0.01  0.01
            8      0.004 0.01
            9      0.002 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.358 0.023
            1      0.15  0.023
            2      0.139 0.023
            3      0.171 0.023
            4      0.085 0.023
            5      0.049 0.023
            6      0.03  0.023
            7      0.012 0.023
            8      0.004 0.023
            9      0.002 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.377 0.01
            1      0.147 0.01
            2      0.208 0.01
            3      0.118 0.01
            4      0.08  0.01
            5      0.039 0.01
            6      0.022 0.01
            7      0.004 0.01
            8      0.004 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.371 0.01
            1      0.145 0.01
            2      0.212 0.01
            3      0.12  0.01
            4      0.083 0.01
            5      0.04  0.01
            6      0.022 0.01
            7      0.004 0.01
```

```
            8     0.002 0.01
PHE_TYR_U   1,2   0     0.748 0.01
            1     0.091 0.01
            2     0.161 0.01
GLU_U 1,2,3,4,5   0     0.47  0.01
            1     0.207 0.01
            2     0.213 0.01
            3     0.079 0.01
            4     0.024 0.01
            5     0.007 0.01
GLU_U 2,3,4,5     0     0.522 0.011
            1     0.225 0.011
            2     0.193 0.011
            3     0.047 0.011
            4     0.013 0.011
GLU_U 2,3,4,5     0     0.514 0.017
            1     0.23  0.01
            2     0.201 0.01
            3     0.045 0.012
            4     0.01  0.013
ALA_U 1,2,3 0     0.725 0.011
            1     0.081 0.011
            2     0.041 0.011
            3     0.153 0.011
ALA_U 2,3   0     0.764 0.011
            1     0.056 0.011
            2     0.181 0.011
GLYeff_U    1,2   0     0.725 0.01
            1     0.147 0.01
            2     0.128 0.01
GLYeff_U    1,2   0     0.735 0.01
            1     0.141 0.01
            2     0.124 0.01
GLYeff_U    2     0     0.807 0.01
            1     0.193 0.01
VAL_U 1,2,3,4,5   0     0.546 0.01
            1     0.126 0.01
            2     0.161 0.01
            3     0.125 0.01
            4     0.017 0.01
            5     0.025 0.01
VAL_U 1,2,3,4,5   0     0.551 0.01
            1     0.116 0.01
            2     0.165 0.01
            3     0.129 0.01
            4     0.016 0.01
            5     0.024 0.01
VAL_U 2,3,4,5     0     0.58  0.01
            1     0.102 0.01
            2     0.266 0.01
            3     0.024 0.01
            4     0.029 0.01
VAL_U 2,3,4,5     0     0.586 0.024
```

		1	0.095	0.024
		2	0.258	0.024
		3	0.032	0.024
		4	0.028	0.024
LEU_U	1,2,3,4,5,6	0	0.436	0.02
		1	0.123	0.02
		2	0.315	0.02
		3	0.052	0.02
		4	0.064	0.02
		5	0.007	0.02
		6	0.003	0.02
LEU_U	1,2,3,4,5,6	0	0.436	0.012
		1	0.119	0.012
		2	0.319	0.012
		3	0.05	0.012
		4	0.067	0.012
		5	0.005	0.012
		6	0.005	0.012
LEU_U	2,3,4,5,6	0	0.467	0.017
		1	0.192	0.017
		2	0.233	0.017
		3	0.073	0.017
		4	0.029	0.017
		5	0.006	0.017
ILE_U	1,2,3,4,5,6	0	0.396	0.018
		1	0.223	0.018
		2	0.227	0.018
		3	0.1	0.018
		4	0.043	0.018
		5	0.012	0.018
		6	-0.001	0.018
ILE_U	2,3,4,5,6	0	0.457	0.01
		1	0.218	0.01
		2	0.218	0.01
		3	0.078	0.01
		4	0.022	0.01
		5	0.007	0.01
ILE_U	2,3,4,5,6	0	0.461	0.02
		1	0.211	0.02
		2	0.217	0.02
		3	0.08	0.02
		4	0.024	0.02
		5	0.007	0.02
GLU_U	2,3,4,5	0	0.522	0.019
		1	0.226	0.019
		2	0.188	0.019
		3	0.047	0.019
		4	0.017	0.019
METeff_U	1,2,3,4,5	0	0.487	0.01
		1	0.252	0.01
		2	0.124	0.01
		3	0.08	0.01
		4	0.037	0.01

```
            5     0.02  0.01
METeff_U    1,2,3,4,5   0     0.486 0.01
            1     0.263 0.01
            2     0.128 0.01
            3     0.082 0.01
            4     0.032 0.01
            5     0.008 0.01
METeff_U    2,3,4,5     0     0.552 0.013
            1     0.257 0.013
            2     0.105 0.013
            3     0.072 0.013
            4     0.014 0.013
METeff_U    2,3,4,5     0     0.552 0.011
            1     0.257 0.011
            2     0.106 0.011
            3     0.073 0.011
            4     0.011 0.011
SEReff_U    1,2,3 0     0.68  0.01
            1     0.15  0.01
            2     0.074 0.01
            3     0.097 0.01
SEReff_U    1,2,3 0     0.675 0.01
            1     0.152 0.01
            2     0.077 0.01
            3     0.095 0.01
SEReff_U    2,3   0     0.717 0.01
            1     0.165 0.01
            2     0.118 0.01
SEReff_U    2,3   0     0.718 0.011
            1     0.165 0.011
            2     0.116 0.011
SEReff_U    1,2   0     0.742 0.018
            1     0.111 0.018
            2     0.146 0.018
THR_U 1,2,3,4     0     0.534 0.01
            1     0.229 0.01
            2     0.153 0.01
            3     0.069 0.01
            4     0.015 0.01
THR_U 2,3,4 0     0.604 0.01
            1     0.233 0.01
            2     0.123 0.01
            3     0.039 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.359 0.015
            1     0.149 0.015
            2     0.137 0.015
            3     0.175 0.015
            4     0.085 0.015
            5     0.047 0.015
            6     0.029 0.015
            7     0.012 0.015
            8     0.004 0.015
            9     0.002 0.015
```

```
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.376 0.018
            1      0.145 0.018
            2      0.209 0.018
            3      0.12  0.018
            4      0.08  0.018
            5      0.04  0.018
            6      0.022 0.018
            7      0.005 0.018
            8      0.003 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.372 0.019
            1      0.143 0.019
            2      0.212 0.019
            3      0.122 0.019
            4      0.082 0.019
            5      0.04  0.019
            6      0.022 0.019
            7      0.004 0.019
            8      0.002 0.019
PHE_TYR_U   1,2    0      0.75  0.01
            1      0.089 0.01
            2      0.161 0.01
ASP_U 1,2,3,4      0      0.54  0.011
            1      0.223 0.011
            2      0.154 0.011
            3      0.066 0.011
            4      0.018 0.011
ASP_U 1,2,3,4      0      0.54  0.011
            1      0.221 0.011
            2      0.15  0.011
            3      0.071 0.011
            4      0.018 0.011
ASP_U 2,3,4 0      0.604 0.01
            1      0.23  0.01
            2      0.122 0.01
            3      0.043 0.01
ASP_U 2,3,4 0      0.604 0.018
            1      0.227 0.018
            2      0.122 0.018
            3      0.047 0.018
ASP_U 1,2   0      0.719 0.011
            1      0.162 0.011
            2      0.119 0.011
CYS_U 1,2,3 0      0.66  0.018
            1      0.172 0.018
            2      0.061 0.018
            3      0.107 0.018
CYS_U 2,3   0      0.715 0.01
            1      0.161 0.01
            2      0.125 0.01
GLU_U 1,2,3,4,5    0      0.441 0.023
            1      0.229 0.023
            2      0.22  0.023
            3      0.078 0.023
```

		4	0.026	0.023
		5	0.007	0.023
GLU_U	1,2,3,4,5	0	0.471	0.01
		1	0.209	0.01
		2	0.208	0.01
		3	0.078	0.01
		4	0.027	0.01
		5	0.007	0.01
GLU_U	1,2,3,4,5	0	0.468	0.011
		1	0.208	0.011
		2	0.212	0.011
		3	0.082	0.011
		4	0.023	0.011
		5	0.008	0.011
GLU_U	2,3,4,5	0	0.517	0.01
		1	0.226	0.01
		2	0.2	0.01
		3	0.046	0.01
		4	0.01	0.01
GLU_U	2,3,4,5	0	0.522	0.011
		1	0.224	0.011
		2	0.194	0.011
		3	0.047	0.011
		4	0.013	0.011
LYS_U	1,2,3,4,5,6	0	0.422	0.01
		1	0.211	0.01
		2	0.183	0.01
		3	0.121	0.01
		4	0.04	0.01
		5	0.019	0.01
		6	0.004	0.01
LYS_U	1,2,3,4,5,6	0	0.421	0.01
		1	0.209	0.01
		2	0.185	0.01
		3	0.123	0.01
		4	0.046	0.01
		5	0.011	0.01
		6	0.005	0.01
LYS_U	1,2,3,4,5,6	0	0.418	0.01
		1	0.218	0.01
		2	0.178	0.01
		3	0.123	0.01
		4	0.045	0.01
		5	0.014	0.01
		6	0.004	0.01
LYS_U	2,3,4,5,6	0	0.457	0.01
		1	0.217	0.01
		2	0.217	0.01
		3	0.078	0.01
		4	0.024	0.01
		5	0.007	0.01
ARGeff_U	1,2,3,4,5,6	0	0.417	0.013
		1	0.263	0.013

```
            2     0.213 0.013
            3     0.078 0.013
            4     0.035 0.013
            5     0.009 0.013
            6     -0.013      0.013
ARGeff_U    1,2,3,4,5,6 0     0.414 0.01
            1     0.253 0.01
            2     0.198 0.01
            3     0.102 0.01
            4     0.036 0.01
            5     0.003 0.01
            6     -0.005      0.01
ARGeff_U    2,3,4,5,6   0     0.449 0.01
            1     0.271 0.01
            2     0.186 0.01
            3     0.069 0.01
            4     0.02  0.01
            5     0.004 0.01
HISeff_U    1,2,3,4,5,6 0     0.466 0.011
            1     0.244 0.011
            2     0.105 0.011
            3     0.107 0.011
            4     0.044 0.011
            5     0.03  0.011
            6     0.005 0.011
HISeff_U    1,2,3,4,5,6 0     0.468 0.013
            1     0.226 0.013
            2     0.12  0.013
            3     0.104 0.013
            4     0.046 0.013
            5     0.031 0.013
            6     0.007 0.013
HISeff_U    2,3,4,5,6   0     0.493 0.023
            1     0.263 0.017
            2     0.174 0.016
            3     0.053 0.017
            4     0.024 0.018
            5     -0.008      0.02
HISeff_U    2,3,4,5,6   0     0.47  0.023
            1     0.236 0.023
            2     0.175 0.023
            3     0.072 0.023
            4     0.036 0.023
            5     0.011 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.354 0.01
            1     0.152 0.01
            2     0.14  0.01
            3     0.172 0.01
            4     0.09  0.01
            5     0.044 0.01
            6     0.032 0.01
            7     0.009 0.01
            8     0.005 0.01
```

```
            9     0.001 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.357 0.023
            1     0.153 0.023
            2     0.135 0.023
            3     0.173 0.023
            4     0.085 0.023
            5     0.046 0.023
            6     0.03  0.023
            7     0.012 0.023
            8     0.005 0.023
            9     0.003 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.379 0.01
            1     0.144 0.01
            2     0.207 0.01
            3     0.118 0.01
            4     0.08  0.01
            5     0.039 0.01
            6     0.024 0.01
            7     0.005 0.01
            8     0.005 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.375 0.01
            1     0.145 0.01
            2     0.213 0.01
            3     0.119 0.01
            4     0.082 0.01
            5     0.039 0.01
            6     0.022 0.01
            7     0.004 0.01
            8     0.001 0.01
PHE_TYR_U   1,2   0     0.752 0.01
            1     0.088 0.01
            2     0.16  0.01
GLU_U 1,2,3,4,5   0     0.469 0.01
            1     0.207 0.01
            2     0.213 0.01
            3     0.078 0.01
            4     0.025 0.01
            5     0.009 0.01
GLU_U 2,3,4,5     0     0.521 0.011
            1     0.226 0.011
            2     0.194 0.011
            3     0.047 0.011
            4     0.013 0.011
GLU_U 2,3,4,5     0     0.514 0.018
            1     0.23  0.011
            2     0.2   0.011
            3     0.046 0.013
            4     0.01  0.014
STA   1,2   0     0.37  0.01
            1     0.634 0.01
            2     -0.004      0.01
STA   3,4,5,6     0     0.744 0.015
            1     0.237 0.015
```

		2	0.018	0.015
		3	0	0.015
		4	0.001	0.015
STA	1,2	0	0.36	0.011
		1	0.645	0.015
		2	-0.004	0.016
STA	3,4,5,6	0	0.745	0.012
		1	0.233	0.012
		2	0.021	0.012
		3	0.001	0.012
		4	0	0.012
STA	1,2	0	0.369	0.01
		1	0.636	0.01
		2	-0.005	0.01
STA	3,4,5,6	0	0.748	0.015
		1	0.233	0.015
		2	0.018	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.365	0.01
		1	0.639	0.01
		2	-0.004	0.01
STA	3,4,5,6	0	0.749	0.012
		1	0.233	0.012
		2	0.015	0.012
		3	0.001	0.012
		4	0.001	0.012
STA	1,2	0	0.378	0.01
		1	0.627	0.01
		2	-0.005	0.01
STA	3,4,5,6	0	0.755	0.015
		1	0.226	0.015
		2	0.018	0.015
		3	0.002	0.015
		4	-0.001	0.015
STA	1,2	0	0.362	0.01
		1	0.633	0.014
		2	0.005	0.015
STA	3,4,5,6	0	0.749	0.012
		1	0.23	0.012
		2	0.022	0.012
		3	-0.001	0.012
		4	0	0.012
STA_U	1,2	0	0.755	0.02
		1	0.093	0.015
		2	0.152	0.014
STA_U	3,4,5,6	0	0.659	0.015
		1	0.138	0.015
		2	0.025	0.015
		3	0.084	0.015
		4	0.094	0.015
STA_U	1,2	0	0.754	0.028
		1	0.098	0.021

		2	0.147	0.02	
STA_U	3,4,5,6	0	0.66	0.012	
		1	0.14	0.012	
		2	0.024	0.012	
		3	0.084	0.012	
		4	0.092	0.012	
STA_U	1,2	0	0.75	0.02	
		1	0.094	0.015	
		2	0.155	0.014	
STA_U	3,4,5,6	0	0.659	0.015	
		1	0.136	0.015	
		2	0.024	0.015	
		3	0.085	0.015	
		4	0.097	0.015	
STA_U	1,2	0	0.752	0.03	
		1	0.101	0.023	
		2	0.147	0.021	
STA_U	3,4,5,6	0	0.663	0.012	
		1	0.134	0.012	
		2	0.023	0.012	
		3	0.086	0.012	
		4	0.094	0.012	
STA_U	1,2	0	0.752	0.019	
		1	0.093	0.014	
		2	0.155	0.013	
STA_U	3,4,5,6	0	0.659	0.015	
		1	0.137	0.015	
		2	0.024	0.015	
		3	0.083	0.015	
		4	0.097	0.015	
STA_U	1,2	0	0.755	0.03	
		1	0.098	0.022	
		2	0.147	0.021	
STA_U	3,4,5,6	0	0.66	0.012	
		1	0.138	0.012	
		2	0.023	0.012	
		3	0.085	0.012	
		4	0.094	0.012	
WALL	3,4,5,6	0	0.749	0.015	
		1	0.233	0.015	
		2	0.017	0.015	
		3	0.002	0.015	
		4	0	0.015	
WALL	3,4,5,6	0	0.771	0.012	
		1	0.211	0.012	
		2	0.017	0.012	
		3	0	0.012	
		4	0.001	0.012	
WALL	3,4,5,6	0	0.74	0.015	
		1	0.24	0.015	
		2	0.02	0.015	
		3	0	0.015	
		4	0	0.015	

WALL	3,4,5,6	0	0.768	0.012
		1	0.214	0.012
		2	0.016	0.012
		3	0.001	0.012
		4	0	0.012
WALL	3,4,5,6	0	0.747	0.015
		1	0.236	0.015
		2	0.015	0.015
		3	0.002	0.015
		4	0	0.015
WALL	3,4,5,6	0	0.765	0.012
		1	0.217	0.012
		2	0.016	0.012
		3	0.002	0.012
		4	0.001	0.012
WALL_U	3,4,5,6	0	0.648	0.015
		1	0.138	0.015
		2	0.028	0.015
		3	0.083	0.015
		4	0.103	0.015
WALL_U	3,4,5,6	0	0.669	0.012
		1	0.127	0.012
		2	0.023	0.012
		3	0.072	0.012
		4	0.108	0.012
WALL_U	3,4,5,6	0	0.651	0.015
		1	0.136	0.015
		2	0.026	0.015
		3	0.083	0.015
		4	0.104	0.015
WALL_U	3,4,5,6	0	0.671	0.012
		1	0.126	0.012
		2	0.023	0.012
		3	0.073	0.012
		4	0.107	0.012
WALL_U	3,4,5,6	0	0.688	0.015
		1	0.128	0.015
		2	0.02	0.015
		3	0.073	0.015
		4	0.092	0.015
WALL_U	3,4,5,6	0	0.681	0.012
		1	0.121	0.012
		2	0.022	0.012
		3	0.073	0.012
		4	0.103	0.012
FSUC	4,5,6	0	0.796	0.014
		1	0.197	0.014
		2	0.008	0.014
		3	-0.001	0.014
FSUC	4,5,6	0	0.812	0.029
		1	0.195	0.014
		2	0.001	0.018
		3	-0.008	0.019

FSUC	1,2,3,4	0	0.271	0.013
		1	0.699	0.013
		2	0.032	0.013
		3	-0.001	0.013
		4	-0.002	0.013
FSUC	4,5,6	0	0.796	0.013
		1	0.197	0.013
		2	0.007	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.789	0.034
		1	0.216	0.017
		2	0.002	0.021
		3	-0.007	0.022
FSUC	1,2,3,4	0	0.271	0.011
		1	0.705	0.011
		2	0.032	0.011
		3	-0.007	0.011
		4	-0.001	0.011
FSUC	4,5,6	0	0.793	0.014
		1	0.201	0.014
		2	0.007	0.014
		3	0	0.014
FSUC	4,5,6	0	0.807	0.029
		1	0.199	0.014
		2	0.002	0.018
		3	-0.008	0.019
FSUC	1,2,3,4	0	0.273	0.013
		1	0.696	0.013
		2	0.034	0.013
		3	-0.002	0.013
		4	-0.002	0.013
FSUC	4,5,6	0	0.794	0.013
		1	0.2	0.013
		2	0.007	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.792	0.028
		1	0.218	0.014
		2	-0.001	0.018
		3	-0.009	0.019
FSUC	1,2,3,4	0	0.276	0.011
		1	0.698	0.011
		2	0.029	0.011
		3	-0.002	0.011
		4	-0.001	0.011
FSUC	4,5,6	0	0.796	0.014
		1	0.197	0.014
		2	0.007	0.014
		3	-0.001	0.014
FSUC	4,5,6	0	0.814	0.028
		1	0.195	0.014
		2	0	0.017
		3	-0.009	0.018
FSUC	1,2,3,4	0	0.272	0.013

		1	0.697	0.013
		2	0.035	0.013
		3	-0.002	0.013
		4	-0.002	0.013
FSUC	4,5,6	0	0.798	0.013
		1	0.199	0.013
		2	0.004	0.013
		3	0	0.013
FSUC	4,5,6	0	0.796	0.029
		1	0.215	0.014
		2	-0.001	0.018
		3	-0.01	0.019
FSUC	1,2,3,4	0	0.276	0.011
		1	0.703	0.011
		2	0.029	0.011
		3	-0.006	0.011
		4	-0.002	0.011
FSUC_U	4,5,6	0	0.756	0.014
		1	0.048	0.014
		2	0.021	0.014
		3	0.175	0.014
FSUC_U	4,5,6	0	0.779	0.015
		1	0.04	0.01
		2	0.013	0.01
		3	0.169	0.01
FSUC_U	1,2,3,4	0	0.655	0.013
		1	0.144	0.013
		2	0.045	0.013
		3	0.059	0.013
		4	0.097	0.013
FSUC_U	4,5,6	0	0.759	0.013
		1	0.047	0.013
		2	0.019	0.013
		3	0.174	0.013
FSUC_U	4,5,6	0	0.774	0.019
		1	0.045	0.011
		2	0.015	0.012
		3	0.166	0.01
FSUC_U	1,2,3,4	0	0.657	0.011
		1	0.144	0.011
		2	0.045	0.011
		3	0.059	0.011
		4	0.095	0.011
FSUC_U	4,5,6	0	0.758	0.014
		1	0.047	0.014
		2	0.02	0.014
		3	0.176	0.014
FSUC_U	4,5,6	0	0.779	0.017
		1	0.039	0.01
		2	0.012	0.011
		3	0.17	0.01
FSUC_U	1,2,3,4	0	0.656	0.013
		1	0.141	0.013

	2	0.045	0.013		
	3	0.058	0.013		
	4	0.101	0.013		
FSUC_U	4,5,6	0	0.758	0.013	
	1	0.047	0.013		
	2	0.02	0.013		
	3	0.175	0.013		
FSUC_U	4,5,6	0	0.775	0.02	
	1	0.043	0.012		
	2	0.013	0.013		
	3	0.169	0.01		
FSUC_U	1,2,3,4		0	0.661	0.011
	1	0.138	0.011		
	2	0.044	0.011		
	3	0.058	0.011		
	4	0.099	0.011		
FSUC_U	4,5,6	0	0.757	0.014	
	1	0.047	0.014		
	2	0.02	0.014		
	3	0.176	0.014		
FSUC_U	4,5,6	0	0.779	0.017	
	1	0.039	0.01		
	2	0.012	0.011		
	3	0.17	0.01		
FSUC_U	1,2,3,4		0	0.655	0.013
	1	0.143	0.013		
	2	0.043	0.013		
	3	0.058	0.013		
	4	0.101	0.013		
FSUC_U	4,5,6	0	0.761	0.013	
	1	0.047	0.013		
	2	0.017	0.013		
	3	0.175	0.013		
FSUC_U	4,5,6	0	0.777	0.02	
	1	0.042	0.012		
	2	0.014	0.012		
	3	0.167	0.01		
FSUC_U	1,2,3,4		0	0.658	0.011
	1	0.139	0.011		
	2	0.044	0.011		
	3	0.055	0.011		
	4	0.103	0.011		
PENTAN	5	0	0.999	0.01	
	1	0.001	0.01		
PENTAN	3,4,5	0	0.938	0.043	
	1	0.075	0.02		
	2	-0.004		0.022	
	3	-0.009		0.023	
PENTAN	3,4,5	0	0.94	0.01	
	1	0.058	0.01		
	2	0.002	0.01		
	3	0	0.01		
PENTAN	5	0	0.992	0.015	

		1	0.008	0.015
PENTAN	3,4,5	0	0.942	0.01
		1	0.064	0.01
		2	-0.008	0.01
		3	0.001	0.01
PENTAN	5	0	1	0.01
		1	0	0.01
PENTAN	3,4,5	0	0.944	0.01
		1	0.056	0.01
		2	0.002	0.01
		3	-0.002	0.01
WALL	3,4,5,6	0	0.768	0.011
		1	0.215	0.011
		2	0.014	0.011
		3	0.003	0.011
		4	0	0.011
WALL	3,4,5,6	0	0.776	0.012
		1	0.207	0.012
		2	0.016	0.012
		3	0.001	0.012
		4	0.001	0.012
PENTAN	5	0	0.997	0.01
		1	0.003	0.01
PENTAN	3,4,5	0	0.934	0.042
		1	0.08	0.02
		2	-0.004	0.022
		3	-0.009	0.022
PENTAN	3,4,5	0	0.937	0.01
		1	0.061	0.01
		2	0.002	0.01
		3	0	0.01
PENTAN	5	0	0.989	0.015
		1	0.011	0.015
PENTAN	3,4,5	0	0.94	0.038
		1	0.079	0.017
		2	0	0.02
		3	-0.019	0.021
PENTAN	3,4,5	0	0.957	0.011
		1	0.048	0.01
		2	-0.003	0.01
		3	-0.002	0.01
PENTAN	5	0	0.999	0.01
		1	0.001	0.01
PENTAN	3,4,5	0	0.943	0.01
		1	0.056	0.01
		2	0.001	0.01
		3	0.001	0.01
WALL	3,4,5,6	0	0.756	0.011
		1	0.225	0.011
		2	0.017	0.011
		3	0.001	0.011
		4	0.001	0.011
WALL	3,4,5,6	0	0.773	0.012

	1	0.211	0.012	
	2	0.015	0.012	
	3	0.001	0.012	
	4	0	0.012	
PENTAN	5	0	0.998	0.01
	1	0.002	0.01	
PENTAN	3,4,5	0	0.937	0.042
	1	0.078	0.02	
	2	-0.006		0.022
	3	-0.009		0.022
PENTAN	3,4,5	0	0.94	0.01
	1	0.059	0.01	
	2	0.001	0.01	
	3	0	0.01	
PENTAN	5	0	0.985	0.015
	1	0.015	0.015	
PENTAN	3,4,5	0	0.927	0.01
	1	0.072	0.01	
	2	-0.003		0.01
	3	0.003	0.01	
PENTAN	5	0	1	0.01
	1	0	0.01	
PENTAN	3,4,5	0	0.956	0.029
	1	0.075	0.029	
	2	-0.013		0.029
	3	-0.019		0.029
PENTAN	3,4,5	0	0.946	0.01
	1	0.057	0.01	
	2	-0.003		0.01
	3	0	0.01	
WALL	3,4,5,6	0	0.759	0.011
	1	0.22	0.011	
	2	0.016	0.011	
	3	0.004	0.011	
	4	0.001	0.011	
WALL	3,4,5,6	0	0.774	0.012
	1	0.212	0.012	
	2	0.014	0.012	
	3	0.001	0.012	
	4	0	0.012	
PENTAN_U	5	0	0.796	0.01
	1	0.204	0.01	
PENTAN_U	3,4,5	0	0.683	0.02
	1	0.136	0.02	
	2	0.071	0.02	
	3	0.11	0.02	
PENTAN_U	3,4,5	0	0.689	0.01
	1	0.126	0.01	
	2	0.074	0.01	
	3	0.111	0.01	
PENTAN_U	5	0	0.794	0.015
	1	0.206	0.015	
PENTAN_U	3,4,5	0	0.668	0.016

	1	0.141	0.016		
	2	0.084	0.016		
	3	0.106	0.016		
PENTAN_U	3,4,5	0	0.681	0.012	
	1	0.134	0.01		
	2	0.075	0.01		
	3	0.11	0.01		
PENTAN_U	5	0	0.796	0.01	
	1	0.204	0.01		
PENTAN_U	3,4,5	0	0.679	0.029	
	1	0.141	0.029		
	2	0.071	0.029		
	3	0.11	0.029		
PENTAN_U	3,4,5	0	0.686	0.01	
	1	0.126	0.01		
	2	0.073	0.01		
	3	0.114	0.01		
WALL_U	3,4,5,6		0	0.671	0.011
	1	0.132	0.011		
	2	0.023	0.011		
	3	0.074	0.011		
	4	0.1	0.011		
WALL_U	3,4,5,6		0	0.674	0.012
	1	0.124	0.012		
	2	0.023	0.012		
	3	0.072	0.012		
	4	0.108	0.012		
PENTAN_U	5	0	0.796	0.01	
	1	0.204	0.01		
PENTAN_U	3,4,5	0	0.682	0.02	
	1	0.135	0.02		
	2	0.07	0.02		
	3	0.112	0.02		
PENTAN_U	3,4,5	0	0.688	0.01	
	1	0.124	0.01		
	2	0.075	0.01		
	3	0.114	0.01		
PENTAN_U	5	0	0.798	0.015	
	1	0.202	0.015		
PENTAN_U	3,4,5	0	0.668	0.016	
	1	0.142	0.016		
	2	0.086	0.016		
	3	0.105	0.016		
PENTAN_U	3,4,5	0	0.689	0.01	
	1	0.134	0.01		
	2	0.08	0.01		
	3	0.097	0.01		
PENTAN_U	5	0	0.796	0.01	
	1	0.204	0.01		
PENTAN_U	3,4,5	0	0.677	0.029	
	1	0.141	0.029		
	2	0.072	0.029		
	3	0.109	0.029		

```
PENTAN_U     3,4,5 0     0.693 0.01
             1     0.123 0.01
             2     0.075 0.01
             3     0.109 0.01
WALL_U       3,4,5,6     0     0.66  0.011
             1     0.13  0.011
             2     0.028 0.011
             3     0.075 0.011
             4     0.107 0.011
WALL_U       3,4,5,6     0     0.674 0.012
             1     0.124 0.012
             2     0.02  0.012
             3     0.071 0.012
             4     0.111 0.012
PENTAN_U     5     0     0.796 0.01
             1     0.204 0.01
PENTAN_U     3,4,5 0     0.681 0.02
             1     0.135 0.02
             2     0.07  0.02
             3     0.114 0.02
PENTAN_U     3,4,5 0     0.689 0.01
             1     0.123 0.01
             2     0.073 0.01
             3     0.115 0.01
PENTAN_U     5     0     0.796 0.015
             1     0.204 0.015
PENTAN_U     3,4,5 0     0.691 0.019
             1     0.135 0.016
             2     0.076 0.016
             3     0.098 0.016
PENTAN_U     3,4,5 0     0.672 0.01
             1     0.132 0.01
             2     0.081 0.01
             3     0.114 0.01
PENTAN_U     5     0     0.795 0.01
             1     0.205 0.01
PENTAN_U     3,4,5 0     0.679 0.029
             1     0.141 0.029
             2     0.071 0.029
             3     0.11  0.029
PENTAN_U     3,4,5 0     0.684 0.011
             1     0.127 0.01
             2     0.073 0.01
             3     0.116 0.01
WALL_U       3,4,5,6     0     0.668 0.011
             1     0.133 0.011
             2     0.023 0.011
             3     0.073 0.011
             4     0.103 0.011
WALL_U       3,4,5,6     0     0.679 0.012
             1     0.119 0.012
             2     0.021 0.012
             3     0.07  0.012
```

```
            4      0.11  0.012
```

ATCS line 6

```
MASS_SPECTROMETRY
      META_NAME   FRAGMENT    WEIGHT      VALUE DEVIATION
      ALA   1,2,3 0      0.58  0.01
                  1      0.383 0.01
                  2      0.035 0.01
                  3      0.002 0.01
      ALA   2,3   0      0.607 0.011
                  1      0.377 0.011
                  2      0.016 0.011
      GLY   1,2   0      0.886 0.011
                  1      0.113 0.011
                  2      0.002 0.011
      GLY   2     0      0.97  0.011
                  1      0.03  0.011
      VAL   1,2,3,4,5    0     0.39  0.01
                  1      0.428 0.01
                  2      0.162 0.01
                  3      0.019 0.01
                  4      0.001 0.01
                  5      0     0.01
      VAL   2,3,4,5      0     0.406 0.01
                  1      0.437 0.01
                  2      0.148 0.01
                  3      0.009 0.01
                  4      -0.001      0.01
      VAL   2,3,4,5      0     0.402 0.029
                  1      0.426 0.029
                  2      0.147 0.029
                  3      0.023 0.029
                  4      0.002 0.029
      SER   1,2,3 0      0.681 0.01
                  1      0.302 0.01
                  2      0.019 0.01
                  3      -0.002      0.01
      SER   1,2,3 0      0.681 0.011
                  1      0.3   0.011
                  2      0.019 0.011
                  3      0     0.011
      SER   2,3   0      0.719 0.01
                  1      0.276 0.01
                  2      0.005 0.01
      SER   2,3   0      0.718 0.011
                  1      0.276 0.011
                  2      0.006 0.011
      SER   1,2   0      0.925 0.013
                  1      0.073 0.013
                  2      0.001 0.013
```

THR	2,3,4	0	0.483	0.014
		1	0.421	0.016
		2	0.104	0.014
		3	-0.008	0.017
PHE_TYR	2,3,4,5,6,7,8,9	0	0.311	0.021
		1	0.43	0.021
		2	0.233	0.021
		3	0.05	0.021
		4	-0.001	0.021
		5	-0.007	0.021
		6	-0.008	0.021
		7	-0.009	0.021
		8	0.003	0.021
ASP	1,2,3,4	0	0.375	0.01
		1	0.437	0.01
		2	0.167	0.01
		3	0.024	0.01
		4	-0.003	0.01
ASP	2,3,4	0	0.439	0.01
		1	0.429	0.01
		2	0.125	0.01
		3	0.006	0.01
ASP	1,2	0	0.615	0.013
		1	0.349	0.013
		2	0.035	0.013
GLU	1,2,3,4,5	0	0.286	0.012
		1	0.428	0.012
		2	0.235	0.012
		3	0.06	0.012
		4	0	0.012
		5	-0.009	0.012
GLU	1,2,3,4,5	0	0.271	0.01
		1	0.43	0.01
		2	0.233	0.01
		3	0.057	0.01
		4	0.008	0.01
		5	0.001	0.01
GLU	1,2,3,4,5	0	0.27	0.01
		1	0.426	0.01
		2	0.243	0.01
		3	0.057	0.01
		4	0.005	0.01
		5	-0.001	0.01
GLU	2,3,4,5	0	0.316	0.01
		1	0.442	0.01
		2	0.207	0.01
		3	0.033	0.01
		4	0.003	0.01
ASP	1,2,3,4	0	0.39	0.01
		1	0.431	0.01
		2	0.164	0.01
		3	0.018	0.01
		4	-0.003	0.01

GLU	1,2,3,4,5	0	0.287	0.013
		1	0.429	0.013
		2	0.236	0.013
		3	0.051	0.013
		4	0.001	0.013
		5	-0.004	0.013
GLU	1,2,3,4,5	0	0.274	0.01
		1	0.427	0.01
		2	0.239	0.01
		3	0.056	0.01
		4	0.004	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.279	0.011
		1	0.427	0.011
		2	0.236	0.011
		3	0.054	0.011
		4	0.004	0.011
		5	0	0.011
GABA	1,2,3,4	0	0.318	0.019
		1	0.444	0.019
		2	0.206	0.019
		3	0.031	0.019
		4	0	0.019
ALA	1,2,3	0	0.586	0.01
		1	0.382	0.01
		2	0.03	0.01
		3	0.001	0.01
ALA	2,3	0	0.612	0.011
		1	0.377	0.011
		2	0.011	0.011
GLY	1,2	0	0.881	0.011
		1	0.114	0.011
		2	0.004	0.011
GLY	2	0	0.973	0.011
		1	0.027	0.011
VAL	1,2,3,4,5	0	0.394	0.01
		1	0.427	0.01
		2	0.157	0.01
		3	0.02	0.01
		4	0.001	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.409	0.01
		1	0.431	0.01
		2	0.152	0.01
		3	0.01	0.01
		4	-0.002	0.01
VAL	2,3,4,5	0	0.405	0.029
		1	0.424	0.029
		2	0.147	0.029
		3	0.023	0.029
		4	0.001	0.029
SER	1,2,3	0	0.679	0.01
		1	0.298	0.01

		2	0.021	0.01
		3	0.002	0.01
SER	1,2,3	0	0.676	0.011
		1	0.303	0.011
		2	0.02	0.011
		3	0.001	0.011
SER	2,3	0	0.717	0.01
		1	0.278	0.01
		2	0.005	0.01
SER	2,3	0	0.719	0.011
		1	0.275	0.011
		2	0.005	0.011
SER	1,2	0	0.919	0.013
		1	0.078	0.013
		2	0.003	0.013
THR	2,3,4	0	0.467	0.01
		1	0.422	0.01
		2	0.109	0.01
		3	0.001	0.01
PHE_TYR	2,3,4,5,6,7,8,9	0	0.312	0.021
		1	0.432	0.021
		2	0.236	0.021
		3	0.051	0.021
		4	-0.003	0.021
		5	-0.01	0.021
		6	-0.012	0.021
		7	-0.012	0.021
		8	0.006	0.021
ASP	1,2,3,4	0	0.375	0.01
		1	0.436	0.01
		2	0.17	0.01
		3	0.02	0.01
		4	0	0.01
ASP	2,3,4	0	0.447	0.01
		1	0.424	0.01
		2	0.12	0.01
		3	0.01	0.01
ASP	1,2	0	0.624	0.013
		1	0.343	0.013
		2	0.032	0.013
GLU	1,2,3,4,5	0	0.28	0.012
		1	0.425	0.012
		2	0.248	0.012
		3	0.062	0.012
		4	-0.005	0.012
		5	-0.01	0.012
GLU	1,2,3,4,5	0	0.271	0.01
		1	0.435	0.01
		2	0.231	0.01
		3	0.059	0.01
		4	0.004	0.01
		5	0	0.01
GLU	1,2,3,4,5	0	0.266	0.01

		1	0.424	0.01
		2	0.246	0.01
		3	0.059	0.01
		4	0.004	0.01
		5	0	0.01
GLU	2,3,4,5	0	0.309	0.01
		1	0.441	0.01
		2	0.21	0.01
		3	0.035	0.01
		4	0.006	0.01
ASP	1,2,3,4	0	0.392	0.01
		1	0.43	0.01
		2	0.161	0.01
		3	0.02	0.01
		4	-0.003	0.01
GLU	1,2,3,4,5	0	0.286	0.013
		1	0.433	0.013
		2	0.239	0.013
		3	0.046	0.013
		4	0	0.013
		5	-0.004	0.013
GLU	1,2,3,4,5	0	0.275	0.01
		1	0.429	0.01
		2	0.238	0.01
		3	0.055	0.01
		4	0.004	0.01
		5	-0.002	0.01
GLU	1,2,3,4,5	0	0.278	0.011
		1	0.427	0.011
		2	0.236	0.011
		3	0.055	0.011
		4	0.004	0.011
		5	-0.001	0.011
GABA	1,2,3,4	0	0.309	0.019
		1	0.447	0.019
		2	0.21	0.019
		3	0.033	0.019
		4	0.001	0.019
ALA	1,2,3	0	0.582	0.01
		1	0.384	0.01
		2	0.033	0.01
		3	0.001	0.01
ALA	2,3	0	0.607	0.011
		1	0.377	0.011
		2	0.015	0.011
GLY	1,2	0	0.886	0.011
		1	0.113	0.011
		2	0.001	0.011
GLY	2	0	0.974	0.011
		1	0.026	0.011
VAL	1,2,3,4,5	0	0.383	0.01
		1	0.43	0.01
		2	0.164	0.01

```
		3	0.022	0.01
		4	0.002	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.398	0.01
		1	0.438	0.01
		2	0.154	0.01
		3	0.011	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.395	0.029
		1	0.43	0.029
		2	0.149	0.029
		3	0.025	0.029
		4	0.002	0.029
SER	1,2,3	0	0.684	0.01
		1	0.301	0.01
		2	0.014	0.01
		3	0.001	0.01
SER	1,2,3	0	0.678	0.011
		1	0.302	0.011
		2	0.019	0.011
		3	0.001	0.011
SER	2,3	0	0.721	0.01
		1	0.275	0.01
		2	0.004	0.01
SER	2,3	0	0.721	0.011
		1	0.275	0.011
		2	0.004	0.011
SER	1,2	0	0.927	0.013
		1	0.073	0.013
		2	0.001	0.013
THR	2,3,4	0	0.47	0.01
		1	0.425	0.01
		2	0.101	0.01
		3	0.003	0.01
PHE_TYR	2,3,4,5,6,7,8,9	0	0.312	0.021
		1	0.438	0.021
		2	0.236	0.021
		3	0.049	0.021
		4	-0.005	0.021
		5	-0.011	0.021
		6	-0.012	0.021
		7	-0.012	0.021
		8	0.005	0.021
ASP	1,2,3,4	0	0.373	0.01
		1	0.44	0.01
		2	0.166	0.01
		3	0.023	0.01
		4	-0.002	0.01
ASP	2,3,4	0	0.44	0.01
		1	0.439	0.01
		2	0.117	0.01
		3	0.005	0.01
ASP	1,2	0	0.628	0.013
```

		1	0.342	0.013
		2	0.031	0.013
GLU	1,2,3,4,5	0	0.291	0.012
		1	0.418	0.012
		2	0.233	0.012
		3	0.055	0.012
		4	0.006	0.012
		5	-0.003	0.012
GLU	1,2,3,4,5	0	0.269	0.01
		1	0.416	0.01
		2	0.236	0.01
		3	0.059	0.01
		4	0.013	0.01
		5	0.008	0.01
GLU	1,2,3,4,5	0	0.27	0.01
		1	0.424	0.01
		2	0.243	0.01
		3	0.059	0.01
		4	0.005	0.01
		5	-0.001	0.01
GLU	2,3,4,5	0	0.311	0.01
		1	0.443	0.01
		2	0.205	0.01
		3	0.035	0.01
		4	0.007	0.01
GLU	1,2,3,4,5	0	0.289	0.013
		1	0.431	0.014
		2	0.239	0.013
		3	0.048	0.013
		4	-0.003	0.013
		5	-0.004	0.013
GLU	1,2,3,4,5	0	0.274	0.01
		1	0.428	0.01
		2	0.24	0.01
		3	0.056	0.01
		4	0.004	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.276	0.011
		1	0.426	0.011
		2	0.238	0.011
		3	0.055	0.011
		4	0.004	0.011
		5	0	0.011
GABA	1,2,3,4	0	0.313	0.019
		1	0.446	0.019
		2	0.208	0.019
		3	0.032	0.019
		4	0.001	0.019
ALA_U	1,2,3	0	0.717	0.01
		1	0.101	0.01
		2	0.049	0.01
		3	0.133	0.01
ALA_U	2,3	0	0.766	0.011

```
            1     0.068 0.011
            2     0.167 0.011
GLY_U 1,2   0     0.712 0.011
            1     0.198 0.011
            2     0.09  0.011
GLY_U 2     0     0.81  0.011
            1     0.19  0.011
VAL_U 1,2,3,4,5   0     0.565 0.01
            1     0.137 0.01
            2     0.153 0.01
            3     0.11  0.01
            4     0.017 0.01
            5     0.018 0.01
VAL_U 2,3,4,5     0     0.592 0.01
            1     0.129 0.01
            2     0.234 0.01
            3     0.023 0.01
            4     0.023 0.01
VAL_U 2,3,4,5     0     0.591 0.029
            1     0.118 0.029
            2     0.234 0.029
            3     0.034 0.029
            4     0.024 0.029
SER_U 1,2,3 0     0.673 0.01
            1     0.166 0.01
            2     0.07  0.01
            3     0.091 0.01
SER_U 1,2,3 0     0.665 0.011
            1     0.172 0.011
            2     0.071 0.011
            3     0.092 0.011
SER_U 2,3   0     0.725 0.01
            1     0.157 0.01
            2     0.119 0.01
SER_U 2,3   0     0.726 0.011
            1     0.158 0.011
            2     0.116 0.011
SER_U 1,2   0     0.733 0.013
            1     0.139 0.013
            2     0.128 0.013
THR_U 2,3,4 0     0.629 0.01
            1     0.22  0.01
            2     0.117 0.01
            3     0.035 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.404 0.021
            1     0.153 0.021
            2     0.2   0.021
            3     0.113 0.021
            4     0.068 0.021
            5     0.033 0.021
            6     0.016 0.021
            7     0.002 0.021
            8     0.013 0.021
```

ASP_U 1,2,3,4	0	0.555	0.01
	1	0.221	0.01
	2	0.143	0.01
	3	0.066	0.01
	4	0.016	0.01
ASP_U 2,3,4	0	0.618	0.01
	1	0.227	0.01
	2	0.116	0.01
	3	0.039	0.01
ASP_U 1,2	0	0.727	0.013
	1	0.168	0.013
	2	0.105	0.013
GLU_U 1,2,3,4,5	0	0.481	0.014
	1	0.223	0.012
	2	0.199	0.012
	3	0.077	0.012
	4	0.023	0.012
	5	-0.003	0.012
GLU_U 1,2,3,4,5	0	0.471	0.01
	1	0.225	0.01
	2	0.204	0.01
	3	0.076	0.01
	4	0.018	0.01
	5	0.006	0.01
GLU_U 1,2,3,4,5	0	0.473	0.01
	1	0.22	0.01
	2	0.203	0.01
	3	0.076	0.01
	4	0.021	0.01
	5	0.006	0.01
GLU_U 2,3,4,5	0	0.527	0.01
	1	0.232	0.01
	2	0.184	0.01
	3	0.045	0.01
	4	0.012	0.01
ASP_U 1,2,3,4	0	0.556	0.01
	1	0.222	0.01
	2	0.144	0.01
	3	0.063	0.01
	4	0.015	0.01
GLU_U 1,2,3,4,5	0	0.477	0.013
	1	0.218	0.013
	2	0.207	0.013
	3	0.073	0.013
	4	0.021	0.013
	5	0.004	0.013
GLU_U 1,2,3,4,5	0	0.468	0.01
	1	0.219	0.01
	2	0.207	0.01
	3	0.077	0.01
	4	0.023	0.01
	5	0.006	0.01
GLU_U 1,2,3,4,5	0	0.475	0.011

	1	0.219	0.011
	2	0.202	0.011
	3	0.077	0.011
	4	0.02	0.011
	5	0.007	0.011
GABA_U 1,2,3,4	0	0.521	0.019
	1	0.244	0.019
	2	0.182	0.019
	3	0.042	0.019
	4	0.011	0.019
ALA_U 1,2,3	0	0.718	0.01
	1	0.1	0.01
	2	0.049	0.01
	3	0.133	0.01
ALA_U 2,3	0	0.766	0.011
	1	0.068	0.011
	2	0.166	0.011
GLY_U 1,2	0	0.708	0.011
	1	0.201	0.011
	2	0.091	0.011
GLY_U 2	0	0.809	0.011
	1	0.191	0.011
VAL_U 1,2,3,4,5	0	0.56	0.01
	1	0.142	0.01
	2	0.152	0.01
	3	0.11	0.01
	4	0.018	0.01
	5	0.017	0.01
VAL_U 2,3,4,5	0	0.583	0.01
	1	0.141	0.01
	2	0.229	0.01
	3	0.025	0.01
	4	0.022	0.01
VAL_U 2,3,4,5	0	0.587	0.029
	1	0.125	0.029
	2	0.23	0.029
	3	0.035	0.029
	4	0.023	0.029
SER_U 1,2,3	0	0.673	0.01
	1	0.164	0.01
	2	0.068	0.01
	3	0.095	0.01
SER_U 1,2,3	0	0.667	0.011
	1	0.17	0.011
	2	0.069	0.011
	3	0.094	0.011
SER_U 2,3	0	0.724	0.01
	1	0.156	0.01
	2	0.12	0.01
SER_U 2,3	0	0.725	0.011
	1	0.156	0.011
	2	0.119	0.011
SER_U 1,2	0	0.733	0.013

```
            1      0.139 0.013
            2      0.128 0.013
THR_U 2,3,4 0      0.63  0.01
            1      0.223 0.01
            2      0.102 0.01
            3      0.045 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.408 0.021
            1      0.154 0.021
            2      0.201 0.021
            3      0.113 0.021
            4      0.065 0.021
            5      0.031 0.021
            6      0.011 0.021
            7      -0.002      0.021
            8      0.018 0.021
ASP_U 1,2,3,4      0      0.554 0.01
            1      0.222 0.01
            2      0.142 0.01
            3      0.068 0.01
            4      0.014 0.01
ASP_U 2,3,4 0      0.618 0.01
            1      0.228 0.01
            2      0.116 0.01
            3      0.038 0.01
ASP_U 1,2   0      0.728 0.013
            1      0.166 0.013
            2      0.106 0.013
GLU_U 1,2,3,4,5   0      0.469 0.012
            1      0.227 0.012
            2      0.212 0.012
            3      0.068 0.012
            4      0.022 0.012
            5      0.003 0.012
GLU_U 1,2,3,4,5   0      0.466 0.01
            1      0.23  0.01
            2      0.198 0.01
            3      0.08  0.01
            4      0.022 0.01
            5      0.004 0.01
GLU_U 1,2,3,4,5   0      0.471 0.01
            1      0.222 0.01
            2      0.204 0.01
            3      0.077 0.01
            4      0.021 0.01
            5      0.006 0.01
GLU_U 2,3,4,5      0      0.526 0.01
            1      0.232 0.01
            2      0.182 0.01
            3      0.047 0.01
            4      0.012 0.01
ASP_U 1,2,3,4      0      0.558 0.01
            1      0.221 0.01
            2      0.142 0.01
```

```
            3     0.064 0.01
            4     0.015 0.01
GLU_U 1,2,3,4,5   0     0.486 0.013
            1     0.213 0.013
            2     0.208 0.013
            3     0.074 0.013
            4     0.019 0.013
            5     0     0.013
GLU_U 1,2,3,4,5   0     0.468 0.01
            1     0.219 0.01
            2     0.207 0.01
            3     0.078 0.01
            4     0.023 0.01
            5     0.006 0.01
GLU_U 1,2,3,4,5   0     0.475 0.011
            1     0.216 0.011
            2     0.203 0.011
            3     0.078 0.011
            4     0.022 0.011
            5     0.006 0.011
GABA_U      1,2,3,4     0     0.526 0.019
            1     0.238 0.019
            2     0.181 0.019
            3     0.045 0.019
            4     0.01  0.019
ALA_U 1,2,3 0     0.712 0.01
            1     0.107 0.01
            2     0.053 0.01
            3     0.128 0.01
ALA_U 2,3   0     0.763 0.011
            1     0.075 0.011
            2     0.162 0.011
GLY_U 1,2   0     0.711 0.011
            1     0.198 0.011
            2     0.091 0.011
GLY_U 2     0     0.809 0.011
            1     0.191 0.011
VAL_U 1,2,3,4,5   0     0.56  0.01
            1     0.144 0.01
            2     0.153 0.01
            3     0.111 0.01
            4     0.016 0.01
            5     0.017 0.01
VAL_U 2,3,4,5     0     0.58  0.01
            1     0.145 0.01
            2     0.226 0.01
            3     0.025 0.01
            4     0.024 0.01
VAL_U 2,3,4,5     0     0.587 0.029
            1     0.126 0.029
            2     0.229 0.029
            3     0.035 0.029
            4     0.023 0.029
```

```
SER_U 1,2,3 0      0.667 0.01
            1      0.171 0.01
            2      0.074 0.01
            3      0.088 0.01
SER_U 1,2,3 0      0.663 0.011
            1      0.174 0.011
            2      0.073 0.011
            3      0.089 0.011
SER_U 2,3   0      0.72  0.01
            1      0.164 0.01
            2      0.115 0.01
SER_U 2,3   0      0.724 0.011
            1      0.162 0.011
            2      0.114 0.011
SER_U 1,2   0      0.733 0.013
            1      0.142 0.013
            2      0.126 0.013
THR_U 2,3,4 0      0.628 0.01
            1      0.219 0.01
            2      0.116 0.01
            3      0.038 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.405 0.021
            1      0.153 0.021
            2      0.199 0.021
            3      0.115 0.021
            4      0.068 0.021
            5      0.032 0.021
            6      0.014 0.021
            7      -0.002      0.021
            8      0.017 0.021
ASP_U 1,2,3,4      0      0.551 0.01
            1      0.227 0.01
            2      0.144 0.01
            3      0.061 0.01
            4      0.017 0.01
ASP_U 2,3,4 0      0.616 0.01
            1      0.228 0.01
            2      0.118 0.01
            3      0.038 0.01
ASP_U 1,2   0      0.725 0.013
            1      0.167 0.013
            2      0.108 0.013
GLU_U 1,2,3,4,5    0      0.478 0.012
            1      0.23  0.012
            2      0.192 0.012
            3      0.08  0.012
            4      0.017 0.012
            5      0.004 0.012
GLU_U 1,2,3,4,5    0      0.466 0.01
            1      0.224 0.01
            2      0.204 0.01
            3      0.079 0.01
            4      0.02  0.01
```

		5	0.007	0.01
GLU_U	1,2,3,4,5	0	0.469	0.01
		1	0.223	0.01
		2	0.205	0.01
		3	0.076	0.01
		4	0.021	0.01
		5	0.006	0.01
GLU_U	2,3,4,5	0	0.525	0.01
		1	0.235	0.01
		2	0.181	0.01
		3	0.048	0.01
		4	0.011	0.01
ASP_U	1,2,3,4	0	0.59	0.028
		1	0.226	0.019
		2	0.139	0.019
		3	0.05	0.021
		4	-0.006	0.023
GLU_U	1,2,3,4,5	0	0.489	0.013
		1	0.212	0.013
		2	0.206	0.013
		3	0.072	0.013
		4	0.02	0.013
		5	0	0.013
GLU_U	1,2,3,4,5	0	0.465	0.01
		1	0.221	0.01
		2	0.207	0.01
		3	0.078	0.01
		4	0.022	0.01
		5	0.006	0.01
GLU_U	1,2,3,4,5	0	0.472	0.011
		1	0.219	0.011
		2	0.204	0.011
		3	0.077	0.011
		4	0.022	0.011
		5	0.006	0.011
GABA_U	1,2,3,4	0	0.526	0.019
		1	0.237	0.019
		2	0.181	0.019
		3	0.044	0.019
		4	0.011	0.019
FUM	1,2,3,4	0	0.361	0.017
		1	0.432	0.017
		2	0.172	0.017
		3	0.032	0.017
		4	0.004	0.017
OAA	1,2,3,4	0	0.363	0.011
		1	0.442	0.011
		2	0.169	0.011
		3	0.026	0.011
		4	0	0.011
OAA	1,2,3,4	0	0.368	0.01
		1	0.438	0.01
		2	0.172	0.01

		3	0.022	0.01
		4	0.001	0.01
CIT	1,2,3,4,5,6	0	0.233	0.01
		1	0.409	0.01
		2	0.265	0.01
		3	0.084	0.01
		4	0.011	0.01
		5	0	0.01
		6	-0.001	0.01
FUM	1,2,3,4	0	0.372	0.017
		1	0.434	0.017
		2	0.143	0.017
		3	0.04	0.017
		4	0.011	0.017
OAA	1,2,3,4	0	0.361	0.011
		1	0.447	0.011
		2	0.163	0.011
		3	0.023	0.011
		4	0.006	0.011
OAA	1,2,3,4	0	0.366	0.01
		1	0.439	0.01
		2	0.169	0.01
		3	0.026	0.01
		4	0	0.01
CIT	1,2,3,4,5,6	0	0.229	0.01
		1	0.405	0.01
		2	0.265	0.01
		3	0.092	0.01
		4	0.011	0.01
		5	-0.001	0.01
		6	0	0.01
FUM	1,2,3,4	0	0.374	0.017
		1	0.411	0.017
		2	0.17	0.017
		3	0.037	0.017
		4	0.008	0.017
OAA	1,2,3,4	0	0.368	0.011
		1	0.442	0.011
		2	0.168	0.011
		3	0.021	0.011
		4	0.001	0.011
OAA	1,2,3,4	0	0.369	0.01
		1	0.437	0.01
		2	0.17	0.01
		3	0.023	0.01
		4	0.001	0.01
CIT	1,2,3,4,5,6	0	0.229	0.01
		1	0.408	0.01
		2	0.268	0.01
		3	0.084	0.01
		4	0.009	0.01
		5	0.001	0.01
		6	0.001	0.01

FUM_U	1,2,3,4	0	0.544	0.017
		1	0.232	0.017
		2	0.135	0.017
		3	0.072	0.017
		4	0.016	0.017
OAA_U	1,2,3,4	0	0.549	0.011
		1	0.23	0.011
		2	0.144	0.011
		3	0.062	0.011
		4	0.015	0.011
OAA_U	1,2,3,4	0	0.546	0.01
		1	0.228	0.01
		2	0.145	0.01
		3	0.066	0.01
		4	0.015	0.01
CIT_U	1,2,3,4,5,6	0	0.414	0.01
		1	0.227	0.01
		2	0.212	0.01
		3	0.098	0.01
		4	0.036	0.01
		5	0.01	0.01
		6	0.003	0.01
FUM_U	1,2,3,4	0	0.54	0.017
		1	0.223	0.017
		2	0.156	0.017
		3	0.061	0.017
		4	0.02	0.017
OAA_U	1,2,3,4	0	0.543	0.011
		1	0.231	0.011
		2	0.15	0.011
		3	0.06	0.011
		4	0.015	0.011
OAA_U	1,2,3,4	0	0.547	0.01
		1	0.228	0.01
		2	0.144	0.01
		3	0.065	0.01
		4	0.016	0.01
CIT_U	1,2,3,4,5,6	0	0.413	0.01
		1	0.229	0.01
		2	0.211	0.01
		3	0.096	0.01
		4	0.04	0.01
		5	0.01	0.01
		6	0.002	0.01
FUM_U	1,2,3,4	0	0.537	0.017
		1	0.231	0.017
		2	0.158	0.017
		3	0.054	0.017
		4	0.02	0.017
OAA_U	1,2,3,4	0	0.544	0.011
		1	0.231	0.011
		2	0.148	0.011
		3	0.062	0.011

		4	0.015	0.011	
OAA_U	1,2,3,4	0	0.542	0.01	
		1	0.231	0.01	
		2	0.148	0.01	
		3	0.064	0.01	
		4	0.015	0.01	
CIT_U	1,2,3,4,5,6	0	0.414	0.01	
		1	0.227	0.01	
		2	0.211	0.01	
		3	0.097	0.01	
		4	0.039	0.01	
		5	0.01	0.01	
		6	0.002	0.01	
ALA	1,2,3	0	0.605	0.011	
		1	0.37	0.011	
		2	0.024	0.011	
		3	0.001	0.011	
ALA	2,3	0	0.628	0.011	
		1	0.364	0.011	
		2	0.008	0.011	
VAL	1,2,3,4,5	0	0.387	0.01	
		1	0.459	0.01	
		2	0.151	0.01	
		3	0.01	0.01	
		4	-0.002		0.01
		5	-0.005		0.01
VAL	1,2,3,4,5	0	0.374	0.01	
		1	0.454	0.01	
		2	0.158	0.01	
		3	0.015	0.01	
		4	0	0.01	
		5	-0.001		0.01
VAL	2,3,4,5	0	0.391	0.01	
		1	0.457	0.01	
		2	0.143	0.01	
		3	0.01	0.01	
		4	-0.001		0.01
VAL	2,3,4,5	0	0.421	0.024	
		1	0.418	0.024	
		2	0.139	0.024	
		3	0.02	0.024	
		4	0.002	0.024	
LEU	1,2,3,4,5,6	0	0.243	0.02	
		1	0.444	0.02	
		2	0.249	0.02	
		3	0.062	0.02	
		4	0.004	0.02	
		5	-0.001		0.02
		6	-0.002		0.02
LEU	2,3,4,5,6	0	0.27	0.017	
		1	0.43	0.017	
		2	0.243	0.017	
		3	0.054	0.017	

		4	0.003	0.017
		5	0	0.017
ILE	2,3,4,5,6	0	0.273	0.02
		1	0.433	0.02
		2	0.233	0.02
		3	0.056	0.02
		4	0.005	0.02
		5	0	0.02
METeff	1,2,3,4,5	0	0.399	0.01
		1	0.39	0.01
		2	0.169	0.01
		3	0.027	0.01
		4	0.01	0.01
		5	0.005	0.01
METeff	1,2,3,4,5	0	0.39	0.01
		1	0.389	0.01
		2	0.175	0.01
		3	0.039	0.01
		4	0.005	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.434	0.013
		1	0.398	0.013
		2	0.147	0.013
		3	0.021	0.013
		4	0	0.013
METeff	2,3,4,5	0	0.432	0.011
		1	0.393	0.011
		2	0.15	0.011
		3	0.024	0.011
		4	0.001	0.011
THR	1,2,3,4	0	0.363	0.01
		1	0.443	0.01
		2	0.173	0.01
		3	0.022	0.01
		4	0	0.01
THR	2,3,4	0	0.431	0.01
		1	0.442	0.01
		2	0.12	0.01
		3	0.007	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.278	0.015
		1	0.419	0.015
		2	0.231	0.015
		3	0.06	0.015
		4	0.008	0.015
		5	0.002	0.015
		6	0.002	0.015
		7	-0.001	0.015
		8	0.001	0.015
		9	0	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.284	0.018
		1	0.427	0.018
		2	0.227	0.018
		3	0.052	0.018

		4	0.006	0.018
		5	0.001	0.018
		6	0	0.018
		7	0.002	0.018
		8	0.001	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.287	0.019
		1	0.435	0.019
		2	0.227	0.019
		3	0.052	0.019
		4	0.005	0.019
		5	-0.001	0.019
		6	-0.002	0.019
		7	-0.001	0.019
		8	-0.001	0.019
PHE_TYR	1,2	0	0.944	0.01
		1	0.056	0.01
		2	0.001	0.01
ASP	1,2,3,4	0	0.385	0.011
		1	0.438	0.011
		2	0.166	0.011
		3	0.016	0.011
		4	-0.005	0.011
ASP	1,2,3,4	0	0.376	0.011
		1	0.438	0.011
		2	0.165	0.011
		3	0.022	0.011
		4	0	0.011
ASP	2,3,4	0	0.443	0.01
		1	0.429	0.01
		2	0.118	0.01
		3	0.009	0.01
ASP	2,3,4	0	0.447	0.018
		1	0.422	0.018
		2	0.118	0.018
		3	0.013	0.018
ASP	1,2	0	0.626	0.011
		1	0.338	0.011
		2	0.036	0.011
CYS	1,2,3	0	0.716	0.028
		1	0.275	0.019
		2	0.019	0.021
		3	-0.009	0.023
GLU	1,2,3,4,5	0	0.283	0.023
		1	0.43	0.023
		2	0.232	0.023
		3	0.055	0.023
		4	0.004	0.023
		5	-0.005	0.023
GLU	1,2,3,4,5	0	0.284	0.011
		1	0.425	0.011
		2	0.233	0.011
		3	0.054	0.011
		4	0.004	0.011

		5	0	0.011
GLU	2,3,4,5	0	0.342	0.025
		1	0.48	0.035
		2	0.202	0.025
		3	0.005	0.029
		4	-0.03	0.032
GLU	2,3,4,5	0	0.328	0.011
		1	0.456	0.011
		2	0.2	0.011
		3	0.024	0.011
		4	-0.008	0.011
LYS	1,2,3,4,5,6	0	0.245	0.01
		1	0.423	0.01
		2	0.254	0.01
		3	0.071	0.01
		4	0.007	0.01
		5	0.003	0.01
		6	-0.001	0.01
ARGeff	1,2,3,4,5,6	0	0.301	0.01
		1	0.377	0.01
		2	0.235	0.01
		3	0.077	0.01
		4	0.018	0.01
		5	0	0.01
		6	-0.007	0.01
HISeff	1,2,3,4,5,6	0	0.431	0.013
		1	0.377	0.013
		2	0.154	0.013
		3	0.031	0.013
		4	0	0.013
		5	0.002	0.013
		6	0.005	0.013
HISeff	2,3,4,5,6	0	0.532	0.023
		1	0.377	0.023
		2	0.088	0.023
		3	0.021	0.023
		4	0.001	0.023
		5	-0.02	0.023
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.279	0.01
		1	0.433	0.01
		2	0.231	0.01
		3	0.055	0.01
		4	0.005	0.01
		5	0	0.01
		6	-0.002	0.01
		7	-0.001	0.01
		8	0	0.01
		9	-0.001	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.286	0.023
		1	0.416	0.023
		2	0.23	0.023
		3	0.057	0.023
		4	0.006	0.023

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            5     0.002 0.023
            6     0.002 0.023
            7     0.001 0.023
            8     0     0.023
            9     0     0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.29  0.01
            1     0.429 0.01
            2     0.225 0.01
            3     0.049 0.01
            4     0.006 0.01
            5     0     0.01
            6     0     0.01
            7     -0.001      0.01
            8     0.003 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0     0.28  0.01
            1     0.428 0.01
            2     0.228 0.01
            3     0.055 0.01
            4     0.008 0.01
            5     0.006 0.01
            6     0     0.01
            7     -0.002      0.01
            8     -0.003      0.01
PHE_TYR     1,2   0     0.942 0.01
            1     0.056 0.01
            2     0.002 0.01
GLU   1,2,3,4,5   0     0.282 0.011
            1     0.412 0.015
            2     0.238 0.011
            3     0.07  0.011
            4     0.003 0.013
            5     -0.006      0.013
GLU   2,3,4,5     0     0.323 0.011
            1     0.453 0.011
            2     0.201 0.011
            3     0.025 0.011
            4     -0.003      0.011
GLU   2,3,4,5     0     0.311 0.015
            1     0.474 0.019
            2     0.206 0.013
            3     0.021 0.016
            4     -0.011      0.018
ALA   1,2,3 0     0.599 0.011
            1     0.374 0.011
            2     0.026 0.011
            3     0     0.011
ALA   2,3   0     0.624 0.011
            1     0.368 0.011
            2     0.008 0.011
GLYeff      1,2   0     0.894 0.01
            1     0.101 0.01
            2     0.006 0.01
GLYeff      1,2   0     0.89  0.01
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		1	0.107	0.01
		2	0.003	0.01
GLYeff	2	0	0.972	0.01
		1	0.028	0.01
VAL	1,2,3,4,5	0	0.384	0.01
		1	0.458	0.01
		2	0.153	0.01
		3	0.017	0.01
		4	-0.006	0.01
		5	-0.005	0.01
VAL	1,2,3,4,5	0	0.37	0.01
		1	0.453	0.01
		2	0.16	0.01
		3	0.017	0.01
		4	0	0.01
		5	-0.001	0.01
VAL	2,3,4,5	0	0.391	0.01
		1	0.456	0.01
		2	0.147	0.01
		3	0.008	0.01
		4	-0.002	0.01
VAL	2,3,4,5	0	0.427	0.024
		1	0.424	0.024
		2	0.142	0.024
		3	0.003	0.024
		4	0.003	0.024
LEU	1,2,3,4,5,6	0	0.249	0.02
		1	0.437	0.02
		2	0.241	0.02
		3	0.069	0.02
		4	0.008	0.02
		5	-0.001	0.02
		6	-0.002	0.02
LEU	2,3,4,5,6	0	0.273	0.017
		1	0.426	0.017
		2	0.241	0.017
		3	0.055	0.017
		4	0.004	0.017
		5	0	0.017
ILE	2,3,4,5,6	0	0.276	0.01
		1	0.443	0.01
		2	0.236	0.01
		3	0.051	0.01
		4	-0.001	0.01
		5	-0.006	0.01
ILE	2,3,4,5,6	0	0.28	0.02
		1	0.428	0.02
		2	0.23	0.02
		3	0.056	0.02
		4	0.005	0.02
		5	0	0.02
METeff	1,2,3,4,5	0	0.386	0.01
		1	0.393	0.01

		2	0.177	0.01
		3	0.038	0.01
		4	-0.001	0.01
		5	0.007	0.01
METeff	1,2,3,4,5	0	0.395	0.01
		1	0.389	0.01
		2	0.174	0.01
		3	0.038	0.01
		4	0.003	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.435	0.013
		1	0.393	0.013
		2	0.145	0.013
		3	0.025	0.013
		4	0.002	0.013
METeff	2,3,4,5	0	0.437	0.011
		1	0.39	0.011
		2	0.147	0.011
		3	0.025	0.011
		4	0.001	0.011
SEReff	1,2,3	0	0.699	0.01
		1	0.278	0.01
		2	0.024	0.01
		3	-0.001	0.01
SEReff	1,2,3	0	0.706	0.01
		1	0.284	0.01
		2	0.014	0.01
		3	-0.004	0.01
SEReff	2,3	0	0.738	0.01
		1	0.259	0.01
		2	0.004	0.01
SEReff	2,3	0	0.737	0.011
		1	0.259	0.011
		2	0.004	0.011
SEReff	1,2	0	0.915	0.018
		1	0.08	0.018
		2	0.006	0.018
THR	1,2,3,4	0	0.37	0.01
		1	0.439	0.01
		2	0.17	0.01
		3	0.021	0.01
		4	-0.001	0.01
THR	2,3,4	0	0.43	0.01
		1	0.439	0.01
		2	0.123	0.01
		3	0.008	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.276	0.015
		1	0.421	0.015
		2	0.232	0.015
		3	0.06	0.015
		4	0.008	0.015
		5	0.002	0.015
		6	0	0.015

		7	-0.001	0.015
		8	0.001	0.015
		9	0.001	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.285	0.018
		1	0.426	0.018
		2	0.228	0.018
		3	0.055	0.018
		4	0.006	0.018
		5	0	0.018
		6	0	0.018
		7	0	0.018
		8	0	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.286	0.019
		1	0.426	0.019
		2	0.228	0.019
		3	0.055	0.019
		4	0.006	0.019
		5	0	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.943	0.01
		1	0.055	0.01
		2	0.001	0.01
ASP	1,2,3,4	0	0.378	0.011
		1	0.434	0.011
		2	0.167	0.011
		3	0.018	0.011
		4	0.003	0.011
ASP	1,2,3,4	0	0.376	0.011
		1	0.435	0.011
		2	0.166	0.011
		3	0.022	0.011
		4	0.001	0.011
ASP	2,3,4	0	0.441	0.01
		1	0.428	0.01
		2	0.121	0.01
		3	0.009	0.01
ASP	2,3,4	0	0.442	0.018
		1	0.425	0.018
		2	0.12	0.018
		3	0.013	0.018
ASP	1,2	0	0.626	0.011
		1	0.338	0.011
		2	0.036	0.011
CYS	1,2,3	0	0.674	0.018
		1	0.305	0.018
		2	0.026	0.018
		3	-0.005	0.018
GLU	1,2,3,4,5	0	0.284	0.023
		1	0.435	0.023
		2	0.236	0.023
		3	0.057	0.023

		4	-0.004	0.023
		5	-0.009	0.023
GLU	1,2,3,4,5	0	0.285	0.011
		1	0.424	0.011
		2	0.232	0.011
		3	0.055	0.011
		4	0.005	0.011
		5	0	0.011
GLU	2,3,4,5	0	0.322	0.01
		1	0.453	0.01
		2	0.205	0.01
		3	0.025	0.01
		4	-0.005	0.01
GLU	2,3,4,5	0	0.325	0.011
		1	0.45	0.011
		2	0.2	0.011
		3	0.028	0.011
		4	-0.003	0.011
LYS	1,2,3,4,5,6	0	0.245	0.01
		1	0.423	0.01
		2	0.253	0.01
		3	0.072	0.01
		4	0.009	0.01
		5	-0.001	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.236	0.01
		1	0.421	0.01
		2	0.267	0.01
		3	0.075	0.01
		4	0.01	0.01
		5	-0.003	0.01
		6	-0.005	0.01
LYS	1,2,3,4,5,6	0	0.247	0.01
		1	0.424	0.01
		2	0.253	0.01
		3	0.073	0.01
		4	0.008	0.01
		5	-0.002	0.01
		6	-0.003	0.01
LYS	2,3,4,5,6	0	0.264	0.01
		1	0.437	0.01
		2	0.241	0.01
		3	0.057	0.01
		4	0.004	0.01
		5	-0.003	0.01
ARGeff	1,2,3,4,5,6	0	0.323	0.013
		1	0.372	0.013
		2	0.215	0.013
		3	0.061	0.013
		4	0.027	0.013
		5	-0.001	0.013
		6	0.002	0.013
ARGeff	1,2,3,4,5,6	0	0.31	0.01

```
            1     0.373 0.01
            2     0.237 0.01
            3     0.073 0.01
            4     0.011 0.01
            5     0     0.01
            6     -0.003      0.01
ARGeff      2,3,4,5,6   0     0.319 0.014
            1     0.417 0.021
            2     0.197 0.015
            3     0.05  0.015
            4     0.014 0.017
            5     0.004 0.017
HISeff      1,2,3,4,5,6 0     0.435 0.011
            1     0.378 0.011
            2     0.161 0.011
            3     0.026 0.011
            4     0.003 0.011
            5     -0.003      0.011
            6     -0.001      0.011
HISeff      1,2,3,4,5,6 0     0.428 0.013
            1     0.381 0.013
            2     0.158 0.013
            3     0.03  0.013
            4     0.002 0.013
            5     0.001 0.013
            6     0.001 0.013
HISeff      2,3,4,5,6   0     0.537 0.023
            1     0.361 0.023
            2     0.088 0.023
            3     0.013 0.023
            4     0.003 0.023
            5     -0.003      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.28  0.01
            1     0.42  0.01
            2     0.241 0.01
            3     0.052 0.01
            4     0.008 0.01
            5     0.002 0.01
            6     0     0.01
            7     -0.002      0.01
            8     0     0.01
            9     0     0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.286 0.023
            1     0.414 0.023
            2     0.227 0.023
            3     0.056 0.023
            4     0.008 0.023
            5     0.001 0.023
            6     0.002 0.023
            7     0     0.023
            8     0.003 0.023
            9     0.004 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.294 0.01
```

```
            1     0.419 0.01
            2     0.225 0.01
            3     0.053 0.01
            4     0.006 0.01
            5     0     0.01
            6     0.001 0.01
            7     0.001 0.01
            8     0.003 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0     0.285 0.01
            1     0.433 0.01
            2     0.225 0.01
            3     0.057 0.01
            4     0.006 0.01
            5     0     0.01
            6     -0.002      0.01
            7     -0.003      0.01
            8     -0.003      0.01
PHE_TYR     1,2   0     0.942 0.01
            1     0.057 0.01
            2     0.001 0.01
GLU   1,2,3,4,5   0     0.286 0.01
            1     0.421 0.01
            2     0.234 0.01
            3     0.057 0.01
            4     0.004 0.01
            5     -0.003      0.01
GLU   2,3,4,5     0     0.329 0.011
            1     0.443 0.011
            2     0.199 0.011
            3     0.03  0.011
            4     0     0.011
GLU   2,3,4,5     0     0.302 0.01
            1     0.457 0.01
            2     0.205 0.01
            3     0.034 0.01
            4     0.002 0.01
ALA   1,2,3 0     0.601 0.011
            1     0.373 0.011
            2     0.026 0.011
            3     0     0.011
ALA   2,3   0     0.621 0.011
            1     0.371 0.011
            2     0.008 0.011
GLYeff      1,2   0     0.871 0.01
            1     0.123 0.01
            2     0.006 0.01
GLYeff      1,2   0     0.879 0.01
            1     0.117 0.01
            2     0.004 0.01
GLYeff      2     0     0.969 0.01
            1     0.031 0.01
VAL   1,2,3,4,5   0     0.376 0.01
            1     0.463 0.01
```

		2	0.151	0.01
		3	0.02	0.01
		4	-0.005	0.01
		5	-0.005	0.01
VAL	1,2,3,4,5	0	0.364	0.01
		1	0.458	0.01
		2	0.163	0.01
		3	0.016	0.01
		4	0	0.01
		5	-0.001	0.01
VAL	2,3,4,5	0	0.385	0.01
		1	0.461	0.01
		2	0.145	0.01
		3	0.009	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.412	0.024
		1	0.422	0.024
		2	0.142	0.024
		3	0.023	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.234	0.02
		1	0.437	0.02
		2	0.263	0.02
		3	0.063	0.02
		4	0.003	0.02
		5	0.001	0.02
		6	-0.002	0.02
LEU	2,3,4,5,6	0	0.263	0.017
		1	0.431	0.017
		2	0.245	0.017
		3	0.057	0.017
		4	0.004	0.017
		5	0	0.017
ILE	2,3,4,5,6	0	0.26	0.01
		1	0.446	0.01
		2	0.239	0.01
		3	0.055	0.01
		4	0.003	0.01
		5	-0.003	0.01
ILE	2,3,4,5,6	0	0.267	0.02
		1	0.435	0.02
		2	0.236	0.02
		3	0.056	0.02
		4	0.006	0.02
		5	0.001	0.02
METeff	1,2,3,4,5	0	0.388	0.01
		1	0.389	0.01
		2	0.178	0.01
		3	0.035	0.01
		4	0	0.01
		5	0.009	0.01
METeff	1,2,3,4,5	0	0.387	0.01
		1	0.389	0.01

```
            2     0.179 0.01
            3     0.039 0.01
            4     0.002 0.01
            5     0.004 0.01
METeff      2,3,4,5     0     0.43  0.013
            1     0.393 0.013
            2     0.15  0.013
            3     0.025 0.013
            4     0.002 0.013
METeff      2,3,4,5     0     0.43  0.011
            1     0.393 0.011
            2     0.15  0.011
            3     0.027 0.011
            4     0.001 0.011
SEReff      1,2,3 0     0.7   0.01
            1     0.279 0.01
            2     0.021 0.01
            3     0     0.01
SEReff      1,2,3 0     0.704 0.01
            1     0.285 0.01
            2     0.015 0.01
            3     -0.004      0.01
SEReff      2,3   0     0.74  0.01
            1     0.259 0.01
            2     0.001 0.01
SEReff      2,3   0     0.739 0.011
            1     0.257 0.011
            2     0.004 0.011
SEReff      1,2   0     0.915 0.018
            1     0.081 0.018
            2     0.005 0.018
THR   1,2,3,4     0     0.359 0.01
            1     0.45  0.01
            2     0.17  0.01
            3     0.021 0.01
            4     0     0.01
THR   2,3,4 0     0.428 0.01
            1     0.436 0.01
            2     0.13  0.01
            3     0.006 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.273 0.015
            1     0.423 0.015
            2     0.233 0.015
            3     0.059 0.015
            4     0.008 0.015
            5     0.002 0.015
            6     0     0.015
            7     0     0.015
            8     0     0.015
            9     0     0.015
PHE_TYR     2,3,4,5,6,7,8,9   0     0.279 0.018
            1     0.431 0.018
            2     0.229 0.018
```

		3	0.054	0.018
		4	0.006	0.018
		5	0	0.018
		6	0	0.018
		7	0	0.018
		8	0	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.28	0.019
		1	0.433	0.019
		2	0.229	0.019
		3	0.054	0.019
		4	0.005	0.019
		5	0	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.943	0.01
		1	0.056	0.01
		2	0.001	0.01
ASP	1,2,3,4	0	0.374	0.011
		1	0.435	0.011
		2	0.17	0.011
		3	0.022	0.011
		4	-0.002	0.011
ASP	1,2,3,4	0	0.371	0.011
		1	0.439	0.011
		2	0.167	0.011
		3	0.023	0.011
		4	0	0.011
ASP	2,3,4	0	0.435	0.01
		1	0.432	0.01
		2	0.122	0.01
		3	0.01	0.01
ASP	2,3,4	0	0.437	0.018
		1	0.429	0.018
		2	0.119	0.018
		3	0.015	0.018
ASP	1,2	0	0.624	0.011
		1	0.341	0.011
		2	0.035	0.011
CYS	1,2,3	0	0.708	0.018
		1	0.272	0.018
		2	0.012	0.018
		3	0.008	0.018
GLU	1,2,3,4,5	0	0.273	0.023
		1	0.434	0.023
		2	0.234	0.023
		3	0.061	0.023
		4	0.003	0.023
		5	-0.005	0.023
GLU	1,2,3,4,5	0	0.281	0.011
		1	0.427	0.011
		2	0.233	0.011
		3	0.055	0.011

```
            4      0.004 0.011
            5      0     0.011
GLU   2,3,4,5      0     0.317 0.01
            1      0.457 0.01
            2      0.206 0.01
            3      0.025 0.01
            4      -0.005      0.01
GLU   2,3,4,5      0     0.322 0.011
            1      0.453 0.011
            2      0.2   0.011
            3      0.028 0.011
            4      -0.003      0.011
LYS   1,2,3,4,5,6 0      0.232 0.01
            1      0.422 0.01
            2      0.264 0.01
            3      0.073 0.01
            4      0.008 0.01
            5      0.001 0.01
            6      0.001 0.01
LYS   1,2,3,4,5,6 0      0.231 0.01
            1      0.422 0.01
            2      0.277 0.01
            3      0.069 0.01
            4      0.009 0.01
            5      -0.004      0.01
            6      -0.003      0.01
LYS   1,2,3,4,5,6 0      0.233 0.01
            1      0.428 0.01
            2      0.262 0.01
            3      0.075 0.01
            4      0.006 0.01
            5      -0.002      0.01
            6      -0.002      0.01
LYS   2,3,4,5,6   0      0.255 0.01
            1      0.444 0.01
            2      0.247 0.01
            3      0.056 0.01
            4      0.004 0.01
            5      -0.005      0.01
ARGeff      1,2,3,4,5,6 0      0.299 0.01
            1      0.378 0.01
            2      0.25  0.01
            3      0.072 0.01
            4      0.011 0.01
            5      -0.005      0.01
            6      -0.006      0.01
ARGeff      2,3,4,5,6   0      0.311 0.01
            1      0.426 0.01
            2      0.216 0.01
            3      0.056 0.01
            4      -0.001      0.01
            5      -0.008      0.01
HISeff      1,2,3,4,5,6 0      0.438 0.011
```

```
            1      0.385 0.011
            2      0.159 0.011
            3      0.025 0.011
            4      -0.001      0.011
            5      -0.005      0.011
            6      -0.001      0.011
HISeff      1,2,3,4,5,6 0      0.427 0.013
            1      0.382 0.013
            2      0.16  0.013
            3      0.029 0.013
            4      0.001 0.013
            5      0.001 0.013
            6      0     0.013
HISeff      2,3,4,5,6   0      0.527 0.023
            1      0.365 0.023
            2      0.089 0.023
            3      0.014 0.023
            4      0.006 0.023
            5      -0.001      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.27  0.01
            1      0.434 0.01
            2      0.236 0.01
            3      0.065 0.01
            4      -0.001      0.01
            5      0.002 0.01
            6      0     0.01
            7      -0.003      0.01
            8      -0.001      0.01
            9      -0.002      0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.278 0.023
            1      0.418 0.023
            2      0.232 0.023
            3      0.056 0.023
            4      0.008 0.023
            5      0.001 0.023
            6      0.002 0.023
            7      0     0.023
            8      0.002 0.023
            9      0.003 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0      0.289 0.01
            1      0.425 0.01
            2      0.229 0.01
            3      0.051 0.01
            4      0.005 0.01
            5      0.001 0.01
            6      0     0.01
            7      0     0.01
            8      0.002 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0      0.279 0.01
            1      0.441 0.01
            2      0.232 0.01
            3      0.056 0.01
            4      0.005 0.01
```

```
            5     -0.002      0.01
            6     -0.003      0.01
            7     -0.004      0.01
            8     -0.004      0.01
PHE_TYR     1,2   0     0.944 0.01
            1     0.054 0.01
            2     0.001 0.01
GLU   1,2,3,4,5   0     0.278 0.01
            1     0.419 0.01
            2     0.239 0.01
            3     0.061 0.01
            4     0.005 0.01
            5     -0.002      0.01
GLU   2,3,4,5     0     0.32  0.011
            1     0.448 0.011
            2     0.203 0.011
            3     0.029 0.011
            4     0     0.011
GLU   2,3,4,5     0     0.299 0.013
            1     0.469 0.015
            2     0.208 0.011
            3     0.029 0.013
            4     -0.004      0.015
ALA_U 1,2,3 0     0.72  0.011
            1     0.097 0.011
            2     0.046 0.011
            3     0.136 0.011
ALA_U 2,3   0     0.767 0.011
            1     0.066 0.011
            2     0.167 0.011
GLYeff_U    1,2   0     0.724 0.01
            1     0.19  0.01
            2     0.086 0.01
GLYeff_U    1,2   0     0.726 0.01
            1     0.187 0.01
            2     0.087 0.01
GLYeff_U    2     0     0.819 0.01
            1     0.181 0.01
VAL_U 1,2,3,4,5   0     0.533 0.01
            1     0.149 0.01
            2     0.167 0.01
            3     0.112 0.01
            4     0.017 0.01
            5     0.021 0.01
VAL_U 1,2,3,4,5   0     0.546 0.01
            1     0.133 0.01
            2     0.165 0.01
            3     0.119 0.01
            4     0.016 0.01
            5     0.021 0.01
VAL_U 2,3,4,5     0     0.583 0.01
            1     0.118 0.01
            2     0.251 0.01
```

	3	0.024	0.01	
	4	0.024	0.01	
VAL_U 2,3,4,5		0	0.598	0.024
	1	0.109	0.024	
	2	0.237	0.024	
	3	0.032	0.024	
	4	0.024	0.024	
LEU_U 1,2,3,4,5,6		0	0.438	0.02
	1	0.146	0.02	
	2	0.29	0.02	
	3	0.058	0.02	
	4	0.06	0.02	
	5	0.004	0.02	
	6	0.003	0.02	
LEU_U 2,3,4,5,6		0	0.477	0.017
	1	0.2	0.017	
	2	0.224	0.017	
	3	0.068	0.017	
	4	0.026	0.017	
	5	0.005	0.017	
ILE_U 2,3,4,5,6		0	0.462	0.01
	1	0.228	0.01	
	2	0.212	0.01	
	3	0.073	0.01	
	4	0.02	0.01	
	5	0.004	0.01	
ILE_U 2,3,4,5,6		0	0.472	0.02
	1	0.219	0.02	
	2	0.208	0.02	
	3	0.074	0.02	
	4	0.021	0.02	
	5	0.006	0.02	
METeff_U	1,2,3,4,5	0	0.501	0.01
	1	0.263	0.01	
	2	0.127	0.01	
	3	0.072	0.01	
	4	0.023	0.01	
	5	0.015	0.01	
METeff_U	1,2,3,4,5	0	0.505	0.01
	1	0.265	0.01	
	2	0.123	0.01	
	3	0.072	0.01	
	4	0.028	0.01	
	5	0.007	0.01	
METeff_U	2,3,4,5	0	0.571	0.013
	1	0.255	0.013	
	2	0.102	0.013	
	3	0.062	0.013	
	4	0.01	0.013	
METeff_U	2,3,4,5	0	0.575	0.011
	1	0.255	0.011	
	2	0.102	0.011	
	3	0.061	0.011	

```
            4     0.008 0.011
SEReff_U    1,2,3 0     0.685 0.01
            1     0.161 0.01
            2     0.069 0.01
            3     0.084 0.01
SEReff_U    1,2,3 0     0.687 0.01
            1     0.163 0.01
            2     0.065 0.01
            3     0.085 0.01
SEReff_U    2,3   0     0.733 0.01
            1     0.156 0.01
            2     0.111 0.01
SEReff_U    2,3   0     0.737 0.011
            1     0.154 0.011
            2     0.109 0.011
SEReff_U    1,2   0     0.746 0.018
            1     0.129 0.018
            2     0.125 0.018
THR_U 1,2,3,4     0     0.547 0.01
            1     0.231 0.01
            2     0.148 0.01
            3     0.062 0.01
            4     0.012 0.01
THR_U 2,3,4 0     0.612 0.01
            1     0.235 0.01
            2     0.116 0.01
            3     0.037 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.36  0.015
            1     0.164 0.015
            2     0.142 0.015
            3     0.167 0.015
            4     0.08  0.015
            5     0.045 0.015
            6     0.027 0.015
            7     0.01  0.015
            8     0.004 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.381 0.018
            1     0.156 0.018
            2     0.208 0.018
            3     0.118 0.018
            4     0.075 0.018
            5     0.036 0.018
            6     0.019 0.018
            7     0.004 0.018
            8     0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.38  0.019
            1     0.157 0.019
            2     0.209 0.019
            3     0.118 0.019
            4     0.075 0.019
            5     0.035 0.019
            6     0.019 0.019
```

	7	0.004	0.019
	8	0.002	0.019
PHE_TYR_U 1,2	0	0.753	0.01
	1	0.104	0.01
	2	0.143	0.01
ASP_U 1,2,3,4	0	0.547	0.011
	1	0.228	0.011
	2	0.143	0.011
	3	0.067	0.011
	4	0.014	0.011
ASP_U 1,2,3,4	0	0.544	0.011
	1	0.232	0.011
	2	0.146	0.011
	3	0.063	0.011
	4	0.016	0.011
ASP_U 2,3,4	0	0.609	0.01
	1	0.238	0.01
	2	0.117	0.01
	3	0.037	0.01
ASP_U 2,3,4	0	0.612	0.018
	1	0.232	0.018
	2	0.116	0.018
	3	0.04	0.018
ASP_U 1,2	0	0.725	0.011
	1	0.167	0.011
	2	0.108	0.011
CYS_U 1,2,3	0	0.712	0.018
	1	0.151	0.018
	2	0.05	0.018
	3	0.088	0.018
GLU_U 1,2,3,4,5	0	0.468	0.023
	1	0.222	0.023
	2	0.212	0.023
	3	0.073	0.023
	4	0.023	0.023
	5	0.003	0.023
GLU_U 1,2,3,4,5	0	0.474	0.011
	1	0.219	0.011
	2	0.206	0.011
	3	0.074	0.011
	4	0.021	0.011
	5	0.006	0.011
GLU_U 2,3,4,5	0	0.524	0.01
	1	0.239	0.01
	2	0.187	0.01
	3	0.042	0.01
	4	0.009	0.01
GLU_U 2,3,4,5	0	0.526	0.011
	1	0.235	0.011
	2	0.184	0.011
	3	0.044	0.011
	4	0.01	0.011
LYS_U 1,2,3,4,5,6	0	0.424	0.01

```
            1     0.227 0.01
            2     0.183 0.01
            3     0.109 0.01
            4     0.04  0.01
            5     0.014 0.01
            6     0.004 0.01
LYS_U 1,2,3,4,5,6 0     0.415 0.01
            1     0.217 0.01
            2     0.196 0.01
            3     0.114 0.01
            4     0.038 0.01
            5     0.018 0.01
            6     0.001 0.01
LYS_U 1,2,3,4,5,6 0     0.415 0.01
            1     0.233 0.01
            2     0.181 0.01
            3     0.114 0.01
            4     0.04  0.01
            5     0.013 0.01
            6     0.004 0.01
LYS_U 2,3,4,5,6   0     0.455 0.01
            1     0.231 0.01
            2     0.216 0.01
            3     0.075 0.01
            4     0.02  0.01
            5     0.004 0.01
ARGeff_U    1,2,3,4,5,6 0     0.454 0.015
            1     0.255 0.011
            2     0.19  0.01
            3     0.089 0.01
            4     0.018 0.011
            5     0.004 0.011
            6     -0.009      0.012
ARGeff_U    2,3,4,5,6   0     0.468 0.017
            1     0.279 0.014
            2     0.169 0.012
            3     0.07  0.013
            4     0.028 0.014
            5     -0.015      0.015
HISeff_U    1,2,3,4,5,6 0     0.491 0.011
            1     0.229 0.011
            2     0.089 0.011
            3     0.101 0.011
            4     0.035 0.011
            5     0.044 0.011
            6     0.01  0.011
HISeff_U    1,2,3,4,5,6 0     0.499 0.013
            1     0.225 0.013
            2     0.114 0.013
            3     0.095 0.013
            4     0.041 0.013
            5     0.023 0.013
            6     0.001 0.013
```

```
HISeff_U    2,3,4,5,6   0      0.508 0.014
            1      0.255 0.014
            2      0.159 0.014
            3      0.067 0.014
            4      0.006 0.014
            5      0.004 0.014
HISeff_U    2,3,4,5,6   0      0.5   0.023
            1      0.237 0.023
            2      0.165 0.023
            3      0.064 0.023
            4      0.028 0.023
            5      0.006 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.351 0.01
            1      0.167 0.01
            2      0.152 0.01
            3      0.164 0.01
            4      0.077 0.01
            5      0.045 0.01
            6      0.028 0.01
            7      0.012 0.01
            8      0.004 0.01
            9      0.001 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.371 0.023
            1      0.159 0.023
            2      0.144 0.023
            3      0.16  0.023
            4      0.078 0.023
            5      0.045 0.023
            6      0.026 0.023
            7      0.011 0.023
            8      0.005 0.023
            9      0.002 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.39  0.01
            1      0.154 0.01
            2      0.206 0.01
            3      0.117 0.01
            4      0.071 0.01
            5      0.036 0.01
            6      0.019 0.01
            7      0.004 0.01
            8      0.001 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.374 0.01
            1      0.16  0.01
            2      0.211 0.01
            3      0.12  0.01
            4      0.077 0.01
            5      0.036 0.01
            6      0.018 0.01
            7      0.003 0.01
            8      0.001 0.01
PHE_TYR_U   1,2    0      0.754 0.01
            1      0.102 0.01
            2      0.145 0.01
```

```
GLU_U 1,2,3,4,5   0     0.478 0.01
            1     0.218 0.01
            2     0.204 0.01
            3     0.074 0.01
            4     0.022 0.01
            5     0.004 0.01
GLU_U 2,3,4,5     0     0.53  0.011
            1     0.235 0.011
            2     0.179 0.011
            3     0.045 0.011
            4     0.011 0.011
GLU_U 2,3,4,5     0     0.525 0.016
            1     0.239 0.01
            2     0.186 0.01
            3     0.042 0.011
            4     0.008 0.012
ALA_U 1,2,3 0     0.722 0.011
            1     0.095 0.011
            2     0.046 0.011
            3     0.137 0.011
ALA_U 2,3   0     0.768 0.011
            1     0.062 0.011
            2     0.169 0.011
GLYeff_U    1,2   0     0.728 0.01
            1     0.186 0.01
            2     0.086 0.01
GLYeff_U    1,2   0     0.725 0.01
            1     0.192 0.01
            2     0.083 0.01
GLYeff_U    2     0     0.822 0.01
            1     0.178 0.01
VAL_U 1,2,3,4,5   0     0.537 0.01
            1     0.137 0.01
            2     0.177 0.01
            3     0.12  0.01
            4     0.011 0.01
            5     0.017 0.01
VAL_U 1,2,3,4,5   0     0.548 0.01
            1     0.136 0.01
            2     0.163 0.01
            3     0.118 0.01
            4     0.015 0.01
            5     0.019 0.01
VAL_U 2,3,4,5     0     0.584 0.01
            1     0.118 0.01
            2     0.252 0.01
            3     0.024 0.01
            4     0.022 0.01
VAL_U 2,3,4,5     0     0.589 0.024
            1     0.108 0.024
            2     0.242 0.024
            3     0.037 0.024
            4     0.024 0.024
```

```
LEU_U 1,2,3,4,5,6 0      0.442 0.02
            1     0.133 0.02
            2     0.297 0.02
            3     0.065 0.02
            4     0.055 0.02
            5     0.006 0.02
            6     0.001 0.02
LEU_U 2,3,4,5,6   0      0.476 0.017
            1     0.199 0.017
            2     0.225 0.017
            3     0.069 0.017
            4     0.025 0.017
            5     0.005 0.017
ILE_U 2,3,4,5,6   0      0.466 0.01
            1     0.223 0.01
            2     0.214 0.01
            3     0.072 0.01
            4     0.021 0.01
            5     0.005 0.01
ILE_U 2,3,4,5,6   0      0.468 0.02
            1     0.221 0.02
            2     0.208 0.02
            3     0.074 0.02
            4     0.022 0.02
            5     0.006 0.02
METeff_U    1,2,3,4,5   0      0.502 0.01
            1     0.245 0.01
            2     0.152 0.01
            3     0.077 0.01
            4     0.025 0.01
            5     0     0.01
METeff_U    1,2,3,4,5   0      0.504 0.01
            1     0.262 0.01
            2     0.122 0.01
            3     0.076 0.01
            4     0.028 0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0      0.567 0.013
            1     0.259 0.013
            2     0.103 0.013
            3     0.06  0.013
            4     0.01  0.013
METeff_U    2,3,4,5     0      0.569 0.011
            1     0.262 0.011
            2     0.097 0.011
            3     0.062 0.011
            4     0.009 0.011
SEReff_U    1,2,3 0      0.686 0.01
            1     0.161 0.01
            2     0.066 0.01
            3     0.087 0.01
SEReff_U    1,2,3 0      0.684 0.01
            1     0.163 0.01
```

```
            2     0.065 0.01
            3     0.088 0.01
SEReff_U    2,3   0     0.734 0.01
            1     0.156 0.01
            2     0.11  0.01
SEReff_U    2,3   0     0.738 0.011
            1     0.152 0.011
            2     0.11  0.011
SEReff_U    1,2   0     0.747 0.018
            1     0.13  0.018
            2     0.123 0.018
THR_U 1,2,3,4     0     0.538 0.01
            1     0.232 0.01
            2     0.149 0.01
            3     0.069 0.01
            4     0.012 0.01
THR_U 2,3,4 0     0.607 0.01
            1     0.241 0.01
            2     0.112 0.01
            3     0.04  0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.365 0.015
            1     0.16  0.015
            2     0.141 0.015
            3     0.167 0.015
            4     0.081 0.015
            5     0.043 0.015
            6     0.027 0.015
            7     0.01  0.015
            8     0.003 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.38  0.018
            1     0.155 0.018
            2     0.209 0.018
            3     0.117 0.018
            4     0.078 0.018
            5     0.037 0.018
            6     0.018 0.018
            7     0.004 0.018
            8     0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.383 0.019
            1     0.152 0.019
            2     0.208 0.019
            3     0.12  0.019
            4     0.076 0.019
            5     0.036 0.019
            6     0.02  0.019
            7     0.004 0.019
            8     0.002 0.019
PHE_TYR_U   1,2   0     0.753 0.01
            1     0.1   0.01
            2     0.147 0.01
ASP_U 1,2,3,4     0     0.544 0.011
            1     0.23  0.011
```

	2	0.145	0.011
	3	0.064	0.011
	4	0.016	0.011
ASP_U 1,2,3,4	0	0.549	0.011
	1	0.227	0.011
	2	0.146	0.011
	3	0.064	0.011
	4	0.015	0.011
ASP_U 2,3,4	0	0.613	0.01
	1	0.231	0.01
	2	0.117	0.01
	3	0.039	0.01
ASP_U 2,3,4	0	0.611	0.018
	1	0.233	0.018
	2	0.116	0.018
	3	0.04	0.018
ASP_U 1,2	0	0.726	0.011
	1	0.164	0.011
	2	0.111	0.011
GLU_U 1,2,3,4,5	0	0.475	0.023
	1	0.216	0.023
	2	0.207	0.023
	3	0.084	0.023
	4	0.02	0.023
	5	-0.002	0.023
GLU_U 1,2,3,4,5	0	0.477	0.011
	1	0.218	0.011
	2	0.203	0.011
	3	0.073	0.011
	4	0.022	0.011
	5	0.007	0.011
GLU_U 2,3,4,5	0	0.525	0.01
	1	0.236	0.01
	2	0.189	0.01
	3	0.043	0.01
	4	0.007	0.01
GLU_U 2,3,4,5	0	0.528	0.011
	1	0.234	0.011
	2	0.183	0.011
	3	0.045	0.011
	4	0.01	0.011
LYS_U 1,2,3,4,5,6	0	0.43	0.01
	1	0.221	0.01
	2	0.174	0.01
	3	0.114	0.01
	4	0.044	0.01
	5	0.012	0.01
	6	0.003	0.01
LYS_U 1,2,3,4,5,6	0	0.417	0.011
	1	0.23	0.01
	2	0.188	0.01
	3	0.122	0.01
	4	0.038	0.01

```
            5     0.009 0.01
            6     -0.003      0.01
LYS_U 1,2,3,4,5,6 0     0.425 0.01
            1     0.229 0.01
            2     0.179 0.01
            3     0.119 0.01
            4     0.035 0.01
            5     0.012 0.01
            6     0.002 0.01
LYS_U 2,3,4,5,6   0     0.456 0.01
            1     0.238 0.01
            2     0.215 0.01
            3     0.073 0.01
            4     0.017 0.01
            5     0.002 0.01
ARGeff_U    1,2,3,4,5,6 0     0.45  0.017
            1     0.256 0.013
            2     0.187 0.012
            3     0.083 0.011
            4     0.033 0.012
            5     0.002 0.013
            6     -0.011      0.014
HISeff_U    1,2,3,4,5,6 0     0.479 0.012
            1     0.234 0.011
            2     0.117 0.011
            3     0.089 0.011
            4     0.046 0.011
            5     0.026 0.011
            6     0.01  0.011
HISeff_U    1,2,3,4,5,6 0     0.491 0.013
            1     0.227 0.013
            2     0.11  0.013
            3     0.097 0.013
            4     0.042 0.013
            5     0.026 0.013
            6     0.007 0.013
HISeff_U    2,3,4,5,6   0     0.535 0.03
            1     0.242 0.02
            2     0.154 0.019
            3     0.062 0.02
            4     0.028 0.021
            5     -0.021      0.024
HISeff_U    2,3,4,5,6   0     0.5   0.023
            1     0.229 0.023
            2     0.165 0.023
            3     0.067 0.023
            4     0.028 0.023
            5     0.01  0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.359 0.01
            1     0.157 0.01
            2     0.157 0.01
            3     0.172 0.01
            4     0.072 0.01
```

	5	0.048	0.01	
	6	0.032	0.01	
	7	0.005	0.01	
	8	0.001	0.01	
	9	-0.001	0.01	
PHE_TYR_U	1,2,3,4,5,6,7,8,9	0	0.369	0.023
	1	0.161	0.023	
	2	0.136	0.023	
	3	0.164	0.023	
	4	0.079	0.023	
	5	0.044	0.023	
	6	0.029	0.023	
	7	0.012	0.023	
	8	0.005	0.023	
	9	0.002	0.023	
PHE_TYR_U	2,3,4,5,6,7,8,9	0	0.388	0.01
	1	0.147	0.01	
	2	0.21	0.01	
	3	0.114	0.01	
	4	0.076	0.01	
	5	0.037	0.01	
	6	0.019	0.01	
	7	0.004	0.01	
	8	0.006	0.01	
PHE_TYR_U	2,3,4,5,6,7,8,9	0	0.376	0.01
	1	0.156	0.01	
	2	0.214	0.01	
	3	0.118	0.01	
	4	0.075	0.01	
	5	0.039	0.01	
	6	0.019	0.01	
	7	0.003	0.01	
	8	0	0.01	
PHE_TYR_U	1,2	0	0.755	0.01
	1	0.098	0.01	
	2	0.147	0.01	
GLU_U	1,2,3,4,5	0	0.477	0.01
	1	0.216	0.01	
	2	0.206	0.01	
	3	0.074	0.01	
	4	0.02	0.01	
	5	0.006	0.01	
GLU_U	2,3,4,5	0	0.531	0.011
	1	0.233	0.011	
	2	0.181	0.011	
	3	0.045	0.011	
	4	0.01	0.011	
GLU_U	2,3,4,5	0	0.522	0.019
	1	0.238	0.011	
	2	0.188	0.011	
	3	0.043	0.013	
	4	0.009	0.014	
ALA_U	1,2,3	0	0.721	0.011

```
            1     0.096 0.011
            2     0.047 0.011
            3     0.136 0.011
ALA_U 2,3   0     0.769 0.011
            1     0.063 0.011
            2     0.168 0.011
GLYeff_U    1,2   0     0.732 0.01
            1     0.181 0.01
            2     0.087 0.01
GLYeff_U    1,2   0     0.727 0.01
            1     0.187 0.01
            2     0.087 0.01
GLYeff_U    2     0     0.82  0.01
            1     0.18  0.01
VAL_U 1,2,3,4,5   0     0.543 0.01
            1     0.14  0.01
            2     0.172 0.01
            3     0.117 0.01
            4     0.015 0.01
            5     0.013 0.01
VAL_U 1,2,3,4,5   0     0.547 0.01
            1     0.135 0.01
            2     0.163 0.01
            3     0.121 0.01
            4     0.016 0.01
            5     0.019 0.01
VAL_U 2,3,4,5     0     0.585 0.01
            1     0.119 0.01
            2     0.25  0.01
            3     0.023 0.01
            4     0.024 0.01
VAL_U 2,3,4,5     0     0.597 0.024
            1     0.11  0.024
            2     0.235 0.024
            3     0.035 0.024
            4     0.024 0.024
LEU_U 1,2,3,4,5,6 0     0.45  0.02
            1     0.135 0.02
            2     0.286 0.02
            3     0.064 0.02
            4     0.058 0.02
            5     0.005 0.02
            6     0.001 0.02
LEU_U 2,3,4,5,6   0     0.48  0.017
            1     0.199 0.017
            2     0.222 0.017
            3     0.069 0.017
            4     0.025 0.017
            5     0.005 0.017
ILE_U 2,3,4,5,6   0     0.467 0.01
            1     0.225 0.01
            2     0.21  0.01
            3     0.073 0.01
```

		4	0.02	0.01
		5	0.005	0.01
ILE_U	2,3,4,5,6	0	0.474	0.02
		1	0.218	0.02
		2	0.207	0.02
		3	0.073	0.02
		4	0.022	0.02
		5	0.006	0.02
METeff_U	1,2,3,4,5	0	0.503	0.01
		1	0.258	0.01
		2	0.111	0.01
		3	0.084	0.01
		4	0.034	0.01
		5	0.01	0.01
METeff_U	1,2,3,4,5	0	0.512	0.01
		1	0.258	0.01
		2	0.121	0.01
		3	0.074	0.01
		4	0.028	0.01
		5	0.008	0.01
METeff_U	2,3,4,5	0	0.571	0.013
		1	0.256	0.013
		2	0.101	0.013
		3	0.064	0.013
		4	0.009	0.013
METeff_U	2,3,4,5	0	0.584	0.011
		1	0.254	0.011
		2	0.098	0.011
		3	0.059	0.011
		4	0.004	0.011
SEReff_U	1,2,3	0	0.683	0.01
		1	0.161	0.01
		2	0.068	0.01
		3	0.088	0.01
SEReff_U	1,2,3	0	0.683	0.01
		1	0.164	0.01
		2	0.069	0.01
		3	0.085	0.01
SEReff_U	2,3	0	0.736	0.01
		1	0.155	0.01
		2	0.11	0.01
SEReff_U	2,3	0	0.736	0.011
		1	0.156	0.011
		2	0.108	0.011
SEReff_U	1,2	0	0.744	0.018
		1	0.132	0.018
		2	0.124	0.018
THR_U	1,2,3,4	0	0.543	0.01
		1	0.231	0.01
		2	0.152	0.01
		3	0.06	0.01
		4	0.014	0.01
THR_U	2,3,4	0	0.614	0.01

```
           1     0.235 0.01
           2     0.114 0.01
           3     0.037 0.01
PHE_TYR_U  1,2,3,4,5,6,7,8,9 0     0.365 0.015
           1     0.161 0.015
           2     0.141 0.015
           3     0.167 0.015
           4     0.081 0.015
           5     0.044 0.015
           6     0.027 0.015
           7     0.01  0.015
           8     0.003 0.015
           9     0.002 0.015
PHE_TYR_U  2,3,4,5,6,7,8,9   0     0.384 0.018
           1     0.152 0.018
           2     0.208 0.018
           3     0.118 0.018
           4     0.077 0.018
           5     0.035 0.018
           6     0.02  0.018
           7     0.004 0.018
           8     0.002 0.018
PHE_TYR_U  2,3,4,5,6,7,8,9   0     0.383 0.019
           1     0.154 0.019
           2     0.207 0.019
           3     0.119 0.019
           4     0.076 0.019
           5     0.036 0.019
           6     0.019 0.019
           7     0.004 0.019
           8     0.002 0.019
PHE_TYR_U  1,2   0     0.753 0.01
           1     0.102 0.01
           2     0.145 0.01
ASP_U 1,2,3,4    0     0.551 0.011
           1     0.227 0.011
           2     0.143 0.011
           3     0.065 0.011
           4     0.014 0.011
ASP_U 1,2,3,4    0     0.545 0.011
           1     0.229 0.011
           2     0.149 0.011
           3     0.062 0.011
           4     0.015 0.011
ASP_U 2,3,4 0    0.611 0.01
           1     0.238 0.01
           2     0.116 0.01
           3     0.034 0.01
ASP_U 2,3,4 0    0.61  0.018
           1     0.233 0.018
           2     0.116 0.018
           3     0.041 0.018
ASP_U 1,2   0    0.726 0.011
```

	1	0.164	0.011	
	2	0.11	0.011	
CYS_U 1,2,3	0	0.707	0.018	
	1	0.145	0.018	
	2	0.046	0.018	
	3	0.103	0.018	
GLU_U 1,2,3,4,5	0		0.462	0.023
	1	0.227	0.023	
	2	0.209	0.023	
	3	0.08	0.023	
	4	0.019	0.023	
	5	0.002	0.023	
GLU_U 1,2,3,4,5	0		0.476	0.011
	1	0.218	0.011	
	2	0.204	0.011	
	3	0.074	0.011	
	4	0.021	0.011	
	5	0.006	0.011	
GLU_U 2,3,4,5	0		0.526	0.01
	1	0.238	0.01	
	2	0.184	0.01	
	3	0.042	0.01	
	4	0.01	0.01	
GLU_U 2,3,4,5	0		0.528	0.011
	1	0.237	0.011	
	2	0.184	0.011	
	3	0.043	0.011	
	4	0.008	0.011	
LYS_U 1,2,3,4,5,6	0		0.431	0.01
	1	0.225	0.01	
	2	0.177	0.01	
	3	0.11	0.01	
	4	0.042	0.01	
	5	0.012	0.01	
	6	0.003	0.01	
LYS_U 1,2,3,4,5,6	0		0.417	0.01
	1	0.239	0.01	
	2	0.183	0.01	
	3	0.113	0.01	
	4	0.036	0.01	
	5	0.013	0.01	
	6	-0.001		0.01
LYS_U 1,2,3,4,5,6	0		0.421	0.01
	1	0.232	0.01	
	2	0.182	0.01	
	3	0.113	0.01	
	4	0.038	0.01	
	5	0.013	0.01	
	6	0.002	0.01	
LYS_U 2,3,4,5,6	0		0.462	0.01
	1	0.23	0.01	
	2	0.212	0.01	
	3	0.073	0.01	

```
            4     0.019 0.01
            5     0.003 0.01
ARGeff_U    1,2,3,4,5,6 0     0.458 0.019
            1     0.254 0.014
            2     0.189 0.013
            3     0.088 0.012
            4     0.024 0.013
            5     -0.001      0.014
            6     -0.012      0.015
ARGeff_U    2,3,4,5,6   0     0.48  0.01
            1     0.267 0.01
            2     0.172 0.01
            3     0.072 0.01
            4     0.013 0.01
            5     -0.004      0.01
HISeff_U    1,2,3,4,5,6 0     0.5   0.011
            1     0.216 0.011
            2     0.107 0.011
            3     0.099 0.011
            4     0.048 0.011
            5     0.031 0.011
            6     0     0.011
HISeff_U    1,2,3,4,5,6 0     0.498 0.013
            1     0.225 0.013
            2     0.11  0.013
            3     0.094 0.013
            4     0.041 0.013
            5     0.026 0.013
            6     0.005 0.013
HISeff_U    2,3,4,5,6   0     0.537 0.034
            1     0.247 0.023
            2     0.168 0.022
            3     0.054 0.023
            4     0.003 0.025
            5     -0.009      0.027
HISeff_U    2,3,4,5,6   0     0.504 0.023
            1     0.234 0.023
            2     0.166 0.023
            3     0.067 0.023
            4     0.027 0.023
            5     0.003 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.358 0.01
            1     0.159 0.01
            2     0.149 0.01
            3     0.166 0.01
            4     0.079 0.01
            5     0.049 0.01
            6     0.024 0.01
            7     0.013 0.01
            8     0     0.01
            9     0.002 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.369 0.023
            1     0.162 0.023
```

```
            2     0.137 0.023
            3     0.165 0.023
            4     0.077 0.023
            5     0.043 0.023
            6     0.028 0.023
            7     0.01  0.023
            8     0.006 0.023
            9     0.003 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.387 0.01
            1     0.155 0.01
            2     0.201 0.01
            3     0.112 0.01
            4     0.077 0.01
            5     0.038 0.01
            6     0.019 0.01
            7     0.004 0.01
            8     0.005 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.376 0.01
            1     0.157 0.01
            2     0.214 0.01
            3     0.117 0.01
            4     0.077 0.01
            5     0.037 0.01
            6     0.02  0.01
            7     0.003 0.01
            8     0     0.01
PHE_TYR_U   1,2   0     0.752 0.01
            1     0.101 0.01
            2     0.146 0.01
GLU_U 1,2,3,4,5   0     0.472 0.01
            1     0.214 0.01
            2     0.214 0.01
            3     0.072 0.01
            4     0.022 0.01
            5     0.006 0.01
GLU_U 2,3,4,5     0     0.531 0.011
            1     0.232 0.011
            2     0.181 0.011
            3     0.045 0.011
            4     0.012 0.011
GLU_U 2,3,4,5     0     0.525 0.02
            1     0.239 0.011
            2     0.186 0.011
            3     0.044 0.013
            4     0.007 0.014
STA   3,4,5,6     0     0.679 0.015
            1     0.287 0.015
            2     0.031 0.015
            3     0.003 0.015
            4     0     0.015
STA   3,4,5,6     0     0.684 0.012
            1     0.284 0.012
            2     0.029 0.012
```

	3	0.003	0.012	
	4	0	0.012	
STA	3,4,5,6	0	0.684	0.015
	1	0.284	0.015	
	2	0.03	0.015	
	3	0.002	0.015	
	4	0.001	0.015	
STA	3,4,5,6	0	0.699	0.012
	1	0.267	0.012	
	2	0.027	0.012	
	3	0.006	0.012	
	4	0.001	0.012	
STA_U	3,4,5,6	0	0.637	0.015
	1	0.17	0.015	
	2	0.036	0.015	
	3	0.089	0.015	
	4	0.068	0.015	
STA_U	3,4,5,6	0	0.641	0.012
	1	0.169	0.012	
	2	0.035	0.012	
	3	0.088	0.012	
	4	0.067	0.012	
STA_U	3,4,5,6	0	0.642	0.015
	1	0.163	0.015	
	2	0.034	0.015	
	3	0.089	0.015	
	4	0.071	0.015	
STA_U	3,4,5,6	0	0.646	0.012
	1	0.161	0.012	
	2	0.033	0.012	
	3	0.089	0.012	
	4	0.071	0.012	
STA_U	3,4,5,6	0	0.638	0.015
	1	0.166	0.015	
	2	0.037	0.015	
	3	0.09	0.015	
	4	0.069	0.015	
STA_U	3,4,5,6	0	0.642	0.012
	1	0.164	0.012	
	2	0.037	0.012	
	3	0.088	0.012	
	4	0.069	0.012	
WALL	3,4,5,6	0	0.753	0.012
	1	0.226	0.012	
	2	0.02	0.012	
	3	0.002	0.012	
	4	0	0.012	
WALL	3,4,5,6	0	0.739	0.012
	1	0.237	0.012	
	2	0.024	0.012	
	3	0	0.012	
	4	0	0.012	
WALL	3,4,5,6	0	0.753	0.012

		1	0.225	0.012
		2	0.021	0.012
		3	0.001	0.012
		4	0	0.012
WALL_U	3,4,5,6	0	0.667	0.012
		1	0.144	0.012
		2	0.029	0.012
		3	0.074	0.012
		4	0.087	0.012
WALL_U	3,4,5,6	0	0.671	0.012
		1	0.136	0.012
		2	0.027	0.012
		3	0.075	0.012
		4	0.091	0.012
WALL_U	3,4,5,6	0	0.668	0.012
		1	0.138	0.012
		2	0.032	0.012
		3	0.073	0.012
		4	0.089	0.012
FSUC	4,5,6	0	0.765	0.014
		1	0.224	0.014
		2	0.012	0.014
		3	-0.001	0.014
FSUC	4,5,6	0	0.784	0.024
		1	0.223	0.012
		2	0.004	0.015
		3	-0.011	0.016
FSUC	1,2,3,4	0	0.327	0.013
		1	0.635	0.013
		2	0.041	0.013
		3	-0.001	0.013
		4	-0.002	0.013
FSUC	4,5,6	0	0.771	0.013
		1	0.223	0.013
		2	0.008	0.013
		3	-0.002	0.013
FSUC	4,5,6	0	0.769	0.029
		1	0.239	0.015
		2	0.003	0.019
		3	-0.011	0.02
FSUC	1,2,3,4	0	0.33	0.011
		1	0.642	0.011
		2	0.042	0.011
		3	-0.01	0.011
		4	-0.004	0.011
FSUC	4,5,6	0	0.753	0.014
		1	0.236	0.014
		2	0.013	0.014
		3	-0.001	0.014
FSUC	4,5,6	0	0.771	0.025
		1	0.234	0.013
		2	0.005	0.016
		3	-0.01	0.017

FSUC	1,2,3,4	0	0.343	0.013
		1	0.616	0.013
		2	0.041	0.013
		3	0	0.013
		4	-0.001	0.013
FSUC	4,5,6	0	0.756	0.013
		1	0.235	0.013
		2	0.011	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.759	0.027
		1	0.248	0.014
		2	0.004	0.018
		3	-0.011	0.019
FSUC	1,2,3,4	0	0.343	0.011
		1	0.625	0.011
		2	0.043	0.011
		3	-0.008	0.011
		4	-0.003	0.011
FSUC	4,5,6	0	0.767	0.014
		1	0.222	0.014
		2	0.012	0.014
		3	-0.001	0.014
FSUC	4,5,6	0	0.787	0.023
		1	0.22	0.011
		2	0.003	0.015
		3	-0.01	0.015
FSUC	1,2,3,4	0	0.326	0.013
		1	0.637	0.013
		2	0.041	0.013
		3	-0.002	0.013
		4	-0.002	0.013
FSUC	4,5,6	0	0.767	0.013
		1	0.224	0.013
		2	0.011	0.013
		3	-0.001	0.013
FSUC	4,5,6	0	0.765	0.032
		1	0.237	0.016
		2	0.006	0.021
		3	-0.008	0.022
FSUC	1,2,3,4	0	0.328	0.011
		1	0.649	0.011
		2	0.033	0.011
		3	-0.007	0.011
		4	-0.002	0.011
FSUC_U	4,5,6	0	0.756	0.014
		1	0.065	0.014
		2	0.026	0.014
		3	0.154	0.014
FSUC_U	4,5,6	0	0.777	0.015
		1	0.058	0.01
		2	0.02	0.01
		3	0.145	0.01
FSUC_U	1,2,3,4	0	0.622	0.013

	1	0.188	0.013	
	2	0.064	0.013	
	3	0.057	0.013	
	4	0.07	0.013	
FSUC_U	4,5,6	0	0.753	0.013
	1	0.066	0.013	
	2	0.027	0.013	
	3	0.154	0.013	
FSUC_U	4,5,6	0	0.772	0.021
	1	0.063	0.012	
	2	0.022	0.013	
	3	0.143	0.011	
FSUC_U	1,2,3,4	0	0.623	0.011
	1	0.189	0.011	
	2	0.066	0.011	
	3	0.057	0.011	
	4	0.065	0.011	
FSUC_U	4,5,6	0	0.76	0.014
	1	0.057	0.014	
	2	0.026	0.014	
	3	0.158	0.014	
FSUC_U	4,5,6	0	0.782	0.015
	1	0.052	0.01	
	2	0.016	0.01	
	3	0.15	0.01	
FSUC_U	1,2,3,4	0	0.633	0.013
	1	0.172	0.013	
	2	0.062	0.013	
	3	0.058	0.013	
	4	0.075	0.013	
FSUC_U	4,5,6	0	0.759	0.013
	1	0.058	0.013	
	2	0.024	0.013	
	3	0.159	0.013	
FSUC_U	4,5,6	0	0.775	0.021
	1	0.055	0.012	
	2	0.021	0.013	
	3	0.149	0.011	
FSUC_U	1,2,3,4	0	0.64	0.011
	1	0.172	0.011	
	2	0.061	0.011	
	3	0.054	0.011	
	4	0.073	0.011	
FSUC_U	4,5,6	0	0.755	0.014
	1	0.059	0.014	
	2	0.028	0.014	
	3	0.157	0.014	
FSUC_U	4,5,6	0	0.779	0.016
	1	0.054	0.01	
	2	0.019	0.01	
	3	0.148	0.01	
FSUC_U	1,2,3,4	0	0.631	0.013
	1	0.171	0.013	

		2	0.065	0.013
		3	0.059	0.013
		4	0.074	0.013
FSUC_U	4,5,6	0	0.759	0.013
		1	0.059	0.013
		2	0.026	0.013
		3	0.156	0.013
FSUC_U	4,5,6	0	0.773	0.02
		1	0.058	0.012
		2	0.022	0.013
		3	0.147	0.011
FSUC_U	1,2,3,4	0	0.633	0.011
		1	0.176	0.011
		2	0.062	0.011
		3	0.057	0.011
		4	0.072	0.011
PENTAN	5	0	0.992	0.01
		1	0.008	0.01
PENTAN	3,4,5	0	0.921	0.041
		1	0.092	0.02
		2	-0.005	0.022
		3	-0.009	0.022
PENTAN	3,4,5	0	0.923	0.01
		1	0.074	0.01
		2	0.003	0.01
		3	0	0.01
PENTAN	5	0	0.984	0.015
		1	0.016	0.015
PENTAN	3,4,5	0	0.917	0.034
		1	0.096	0.016
		2	0.001	0.017
		3	-0.013	0.018
PENTAN	5	0	0.993	0.01
		1	0.007	0.01
PENTAN	3,4,5	0	0.92	0.032
		1	0.1	0.029
		2	-0.006	0.029
		3	-0.014	0.029
PENTAN	3,4,5	0	0.922	0.01
		1	0.075	0.01
		2	0.003	0.01
		3	0.001	0.01
WALL	3,4,5,6	0	0.731	0.011
		1	0.248	0.011
		2	0.02	0.011
		3	0.001	0.011
		4	0	0.011
WALL	3,4,5,6	0	0.756	0.012
		1	0.221	0.012
		2	0.022	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN	5	0	0.989	0.01

		1	0.011	0.01
PENTAN	3,4,5	0	0.922	0.035
		1	0.096	0.02
		2	-0.007	0.02
		3	-0.011	0.02
PENTAN	3,4,5	0	0.918	0.01
		1	0.08	0.01
		2	0.002	0.01
		3	0	0.01
PENTAN	5	0	0.983	0.015
		1	0.017	0.015
PENTAN	3,4,5	0	0.919	0.037
		1	0.095	0.017
		2	0	0.019
		3	-0.014	0.02
PENTAN	3,4,5	0	0.931	0.01
		1	0.083	0.01
		2	-0.009	0.01
		3	-0.004	0.01
PENTAN	5	0	0.989	0.01
		1	0.011	0.01
PENTAN	3,4,5	0	0.922	0.029
		1	0.102	0.029
		2	-0.009	0.029
		3	-0.016	0.029
PENTAN	3,4,5	0	0.915	0.01
		1	0.084	0.01
		2	0	0.01
		3	0	0.01
WALL	3,4,5,6	0	0.732	0.011
		1	0.244	0.011
		2	0.02	0.011
		3	0.004	0.011
		4	0.001	0.011
WALL	3,4,5,6	0	0.742	0.012
		1	0.233	0.012
		2	0.023	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN	5	0	0.991	0.01
		1	0.009	0.01
PENTAN	3,4,5	0	0.92	0.038
		1	0.094	0.02
		2	-0.005	0.02
		3	-0.009	0.021
PENTAN	3,4,5	0	0.922	0.01
		1	0.076	0.01
		2	0.003	0.01
		3	0	0.01
PENTAN	5	0	0.983	0.015
		1	0.017	0.015
PENTAN	3,4,5	0	0.913	0.029
		1	0.101	0.016

	2	-0.003		0.016
	3	-0.012		0.016
PENTAN	3,4,5	0	0.924	0.01
	1	0.079	0.01	
	2	0.001	0.01	
	3	-0.003		0.01
PENTAN	5	0	0.993	0.01
	1	0.007	0.01	
PENTAN	3,4,5	0	0.936	0.029
	1	0.093	0.029	
	2	-0.012		0.029
	3	-0.017		0.029
PENTAN	3,4,5	0	0.922	0.01
	1	0.075	0.01	
	2	0.001	0.01	
	3	0.001	0.01	
WALL	3,4,5,6	0	0.74	0.011
	1	0.236	0.011	
	2	0.023	0.011	
	3	0	0.011	
	4	0.001	0.011	
WALL	3,4,5,6	0	0.751	0.012
	1	0.227	0.012	
	2	0.021	0.012	
	3	0.001	0.012	
	4	0	0.012	
PENTAN_U	5	0	0.81	0.01
	1	0.19	0.01	
PENTAN_U	3,4,5	0	0.679	0.02
	1	0.156	0.02	
	2	0.077	0.02	
	3	0.089	0.02	
PENTAN_U	3,4,5	0	0.686	0.01
	1	0.143	0.01	
	2	0.079	0.01	
	3	0.092	0.01	
PENTAN_U	5	0	0.808	0.015
	1	0.192	0.015	
PENTAN_U	3,4,5	0	0.685	0.018
	1	0.157	0.016	
	2	0.082	0.016	
	3	0.076	0.016	
PENTAN_U	3,4,5	0	0.677	0.01
	1	0.15	0.01	
	2	0.076	0.01	
	3	0.097	0.01	
PENTAN_U	5	0	0.81	0.01
	1	0.19	0.01	
PENTAN_U	3,4,5	0	0.674	0.029
	1	0.167	0.029	
	2	0.076	0.029	
	3	0.082	0.029	
PENTAN_U	3,4,5	0	0.685	0.01

		1	0.148	0.01
		2	0.076	0.01
		3	0.091	0.01
WALL_U	3,4,5,6	0	0.666	0.011
		1	0.145	0.011
		2	0.027	0.011
		3	0.079	0.011
		4	0.082	0.011
WALL_U	3,4,5,6	0	0.672	0.012
		1	0.14	0.012
		2	0.027	0.012
		3	0.072	0.012
		4	0.089	0.012
PENTAN_U	5	0	0.803	0.01
		1	0.197	0.01
PENTAN_U	3,4,5	0	0.673	0.02
		1	0.157	0.02
		2	0.077	0.02
		3	0.093	0.02
PENTAN_U	3,4,5	0	0.683	0.01
		1	0.142	0.01
		2	0.08	0.01
		3	0.095	0.01
PENTAN_U	5	0	0.802	0.015
		1	0.198	0.015
PENTAN_U	3,4,5	0	0.661	0.019
		1	0.161	0.016
		2	0.089	0.016
		3	0.089	0.016
PENTAN_U	3,4,5	0	0.681	0.014
		1	0.148	0.01
		2	0.072	0.01
		3	0.099	0.01
PENTAN_U	5	0	0.802	0.01
		1	0.198	0.01
PENTAN_U	3,4,5	0	0.663	0.029
		1	0.165	0.029
		2	0.082	0.029
		3	0.091	0.029
PENTAN_U	3,4,5	0	0.678	0.01
		1	0.143	0.01
		2	0.084	0.01
		3	0.094	0.01
WALL_U	3,4,5,6	0	0.662	0.011
		1	0.141	0.011
		2	0.029	0.011
		3	0.08	0.011
		4	0.088	0.011
WALL_U	3,4,5,6	0	0.669	0.012
		1	0.135	0.012
		2	0.028	0.012
		3	0.074	0.012
		4	0.094	0.012

```
	PENTAN_U	5	0	0.802	0.01
			1	0.198	0.01
	PENTAN_U	3,4,5	0	0.672	0.02
			1	0.159	0.02
			2	0.078	0.02
			3	0.091	0.02
	PENTAN_U	3,4,5	0	0.68	0.01
			1	0.144	0.01
			2	0.081	0.01
			3	0.095	0.01
	PENTAN_U	5	0	0.805	0.015
			1	0.195	0.015
	PENTAN_U	3,4,5	0	0.661	0.017
			1	0.166	0.016
			2	0.087	0.016
			3	0.086	0.016
	PENTAN_U	3,4,5	0	0.68	0.01
			1	0.152	0.01
			2	0.08	0.01
			3	0.087	0.01
	PENTAN_U	5	0	0.803	0.01
			1	0.197	0.01
	PENTAN_U	3,4,5	0	0.664	0.029
			1	0.171	0.029
			2	0.078	0.029
			3	0.087	0.029
	PENTAN_U	3,4,5	0	0.677	0.011
			1	0.149	0.01
			2	0.083	0.01
			3	0.091	0.01
	WALL_U		3,4,5,6	0	0.66	0.011
			1	0.148	0.011
			2	0.029	0.011
			3	0.076	0.011
			4	0.087	0.011
	WALL_U		3,4,5,6	0	0.668	0.012
			1	0.137	0.012
			2	0.028	0.012
			3	0.074	0.012
			4	0.092	0.012
```

ATCS line 16

```
MASS_SPECTROMETRY
	META_NAME	FRAGMENT	WEIGHT		VALUE	DEVIATION
	GLY	2	0	0.96	0.011
			1	0.04	0.011
	VAL	1,2,3,4,5	0	0.372	0.01
			1	0.44	0.01
			2	0.17	0.01
			3	0.017	0.01
```

		4	0.002	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.373	0.029
		1	0.435	0.029
		2	0.155	0.029
		3	0.034	0.029
		4	0.003	0.029
SER	1,2,3	0	0.68	0.027
		1	0.281	0.02
		2	0.019	0.022
		3	0.02	0.023
SER	1,2,3	0	0.682	0.011
		1	0.299	0.011
		2	0.019	0.011
		3	0	0.011
SER	2,3	0	0.713	0.011
		1	0.27	0.011
		2	0.017	0.011
SER	1,2	0	0.931	0.016
		1	0.078	0.013
		2	-0.009	0.013
ASP	1,2,3,4	0	0.386	0.01
		1	0.459	0.014
		2	0.13	0.01
		3	0.025	0.011
		4	-0.001	0.012
ASP	1,2,3,4	0	0.381	0.01
		1	0.437	0.01
		2	0.162	0.01
		3	0.019	0.01
		4	0.001	0.01
ASP	2,3,4	0	0.443	0.01
		1	0.436	0.01
		2	0.12	0.01
		3	0.002	0.01
ASP	1,2	0	0.625	0.013
		1	0.338	0.013
		2	0.037	0.013
GLU	1,2,3,4,5	0	0.265	0.01
		1	0.431	0.01
		2	0.243	0.01
		3	0.057	0.01
		4	0.005	0.01
		5	-0.001	0.01
GLU	2,3,4,5	0	0.303	0.01
		1	0.445	0.01
		2	0.21	0.01
		3	0.034	0.01
		4	0.008	0.01
ASP	1,2,3,4	0	0.398	0.01
		1	0.437	0.01
		2	0.162	0.01
		3	0.012	0.01

		4	-0.009	0.01
GLU	1,2,3,4,5	0	0.28	0.013
		1	0.429	0.013
		2	0.236	0.013
		3	0.05	0.013
		4	0.003	0.013
		5	0.002	0.013
GLU	1,2,3,4,5	0	0.271	0.01
		1	0.431	0.01
		2	0.241	0.01
		3	0.055	0.01
		4	0.004	0.01
		5	-0.001	0.01
GLU	1,2,3,4,5	0	0.275	0.011
		1	0.43	0.011
		2	0.235	0.011
		3	0.056	0.011
		4	0.003	0.011
		5	0.001	0.011
GABA	1,2,3,4	0	0.318	0.019
		1	0.445	0.019
		2	0.209	0.019
		3	0.03	0.019
		4	-0.003	0.019
GLY	2	0	0.964	0.011
		1	0.036	0.011
VAL	1,2,3,4,5	0	0.392	0.01
		1	0.44	0.01
		2	0.16	0.01
		3	0.02	0.01
		4	-0.009	0.01
		5	-0.004	0.01
VAL	1,2,3,4,5	0	0.371	0.01
		1	0.438	0.01
		2	0.17	0.01
		3	0.02	0.01
		4	0.001	0.01
		5	0	0.01
VAL	2,3,4,5	0	0.38	0.029
		1	0.438	0.029
		2	0.154	0.029
		3	0.026	0.029
		4	0.002	0.029
SER	1,2,3	0	0.665	0.03
		1	0.3	0.023
		2	0.021	0.025
		3	0.014	0.027
SER	1,2,3	0	0.678	0.011
		1	0.3	0.011
		2	0.022	0.011
		3	-0.001	0.011
SER	2,3	0	0.717	0.011
		1	0.274	0.011

		2	0.009	0.011
SER	1,2	0	0.915	0.013
		1	0.089	0.013
		2	-0.004	0.013
ASP	1,2,3,4	0	0.388	0.014
		1	0.426	0.019
		2	0.164	0.014
		3	0.018	0.016
		4	0.004	0.017
ASP	1,2,3,4	0	0.385	0.01
		1	0.445	0.01
		2	0.154	0.01
		3	0.018	0.01
		4	-0.002	0.01
ASP	2,3,4	0	0.461	0.01
		1	0.427	0.01
		2	0.108	0.01
		3	0.004	0.01
ASP	1,2	0	0.636	0.013
		1	0.336	0.013
		2	0.028	0.013
GLU	1,2,3,4,5	0	0.267	0.01
		1	0.43	0.01
		2	0.244	0.01
		3	0.056	0.01
		4	0.004	0.01
		5	-0.001	0.01
GLU	2,3,4,5	0	0.308	0.01
		1	0.443	0.01
		2	0.205	0.01
		3	0.034	0.01
		4	0.009	0.01
ASP	1,2,3,4	0	0.426	0.026
		1	0.456	0.034
		2	0.15	0.024
		3	-0.003	0.029
		4	-0.029	0.031
GLU	1,2,3,4,5	0	0.285	0.013
		1	0.434	0.013
		2	0.232	0.013
		3	0.044	0.013
		4	0.001	0.013
		5	0.003	0.013
GLU	1,2,3,4,5	0	0.275	0.01
		1	0.43	0.01
		2	0.24	0.01
		3	0.053	0.01
		4	0.003	0.01
		5	-0.002	0.01
GLU	1,2,3,4,5	0	0.278	0.011
		1	0.429	0.011
		2	0.236	0.011
		3	0.053	0.011

		4	0.004	0.011	
		5	0	0.011	
GABA	1,2,3,4		0	0.319	0.019
		1	0.448	0.019	
		2	0.208	0.019	
		3	0.029	0.019	
		4	-0.004		0.019
GLY	2	0	0.967	0.011	
		1	0.033	0.011	
VAL	1,2,3,4,5		0	0.37	0.01
		1	0.447	0.01	
		2	0.164	0.01	
		3	0.021	0.01	
		4	0	0.01	
		5	-0.002		0.01
VAL	2,3,4,5		0	0.382	0.029
		1	0.435	0.029	
		2	0.152	0.029	
		3	0.029	0.029	
		4	0.001	0.029	
SER	1,2,3	0	0.678	0.01	
		1	0.303	0.01	
		2	0.014	0.01	
		3	0.006	0.01	
SER	1,2,3	0	0.673	0.011	
		1	0.302	0.011	
		2	0.022	0.011	
		3	0.003	0.011	
SER	2,3	0	0.718	0.011	
		1	0.274	0.011	
		2	0.009	0.011	
SER	1,2	0	0.925	0.018	
		1	0.084	0.013	
		2	-0.009		0.014
ASP	1,2,3,4		0	0.4	0.01
		1	0.436	0.01	
		2	0.149	0.01	
		3	0.019	0.01	
		4	-0.003		0.01
ASP	2,3,4	0	0.461	0.01	
		1	0.429	0.01	
		2	0.102	0.01	
		3	0.008	0.01	
ASP	1,2	0	0.64	0.013	
		1	0.333	0.013	
		2	0.027	0.013	
GLU	1,2,3,4,5		0	0.274	0.01
		1	0.434	0.01	
		2	0.236	0.01	
		3	0.052	0.01	
		4	0.004	0.01	
		5	-0.001		0.01
GLU	2,3,4,5		0	0.313	0.01

		1	0.447	0.01
		2	0.203	0.01
		3	0.031	0.01
		4	0.007	0.01
ASP	1,2,3,4	0	0.421	0.022
		1	0.458	0.029
		2	0.147	0.021
		3	-0.002	0.025
		4	-0.023	0.026
GLU	1,2,3,4,5	0	0.285	0.013
		1	0.434	0.013
		2	0.227	0.013
		3	0.045	0.013
		4	0	0.013
		5	0.01	0.013
GLU	1,2,3,4,5	0	0.279	0.01
		1	0.435	0.01
		2	0.235	0.01
		3	0.051	0.01
		4	0.002	0.01
		5	-0.002	0.01
GLU	1,2,3,4,5	0	0.279	0.011
		1	0.433	0.011
		2	0.234	0.011
		3	0.052	0.011
		4	0.003	0.011
		5	0.001	0.011
GABA	1,2,3,4	0	0.324	0.019
		1	0.447	0.019
		2	0.203	0.019
		3	0.028	0.019
		4	-0.002	0.019
GLY_U	2	0	0.801	0.011
		1	0.199	0.011
VAL_U	1,2,3,4,5	0	0.558	0.01
		1	0.139	0.01
		2	0.154	0.01
		3	0.116	0.01
		4	0.023	0.01
		5	0.01	0.01
VAL_U	1,2,3,4,5	0	0.548	0.01
		1	0.132	0.01
		2	0.16	0.01
		3	0.121	0.01
		4	0.019	0.01
		5	0.021	0.01
VAL_U	2,3,4,5	0	0.571	0.029
		1	0.116	0.029
		2	0.248	0.029
		3	0.037	0.029
		4	0.027	0.029
MET_U	2,3,4,5	0	0.519	0.026
		1	0.283	0.026

```
            2     0.119 0.026
            3     0.063 0.026
            4     0.015 0.026
SER_U 1,2,3 0     0.646 0.01
            1     0.176 0.01
            2     0.089 0.01
            3     0.089 0.01
SER_U 1,2,3 0     0.646 0.011
            1     0.185 0.011
            2     0.074 0.011
            3     0.095 0.011
SER_U 2,3   0     0.708 0.01
            1     0.173 0.01
            2     0.119 0.01
SER_U 2,3   0     0.715 0.011
            1     0.17  0.011
            2     0.115 0.011
SER_U 1,2   0     0.722 0.013
            1     0.15  0.013
            2     0.128 0.013
ASP_U 1,2,3,4     0     0.537 0.01
            1     0.22  0.01
            2     0.155 0.01
            3     0.071 0.01
            4     0.017 0.01
ASP_U 1,2,3,4     0     0.55  0.01
            1     0.216 0.01
            2     0.143 0.01
            3     0.074 0.01
            4     0.017 0.01
ASP_U 2,3,4 0     0.613 0.01
            1     0.219 0.01
            2     0.121 0.01
            3     0.046 0.01
ASP_U 1,2   0     0.716 0.013
            1     0.166 0.013
            2     0.118 0.013
GLU_U 1,2,3,4,5   0     0.465 0.01
            1     0.21  0.01
            2     0.211 0.01
            3     0.084 0.01
            4     0.023 0.01
            5     0.007 0.01
GLU_U 2,3,4,5     0     0.517 0.01
            1     0.223 0.01
            2     0.194 0.01
            3     0.052 0.01
            4     0.014 0.01
ASP_U 1,2,3,4     0     0.549 0.01
            1     0.217 0.01
            2     0.147 0.01
            3     0.069 0.01
            4     0.019 0.01
```

```
GLU_U 1,2,3,4,5   0     0.475 0.013
            1     0.211 0.013
            2     0.209 0.013
            3     0.082 0.013
            4     0.022 0.013
            5     0.001 0.013
GLU_U 1,2,3,4,5   0     0.461 0.01
            1     0.212 0.01
            2     0.213 0.01
            3     0.083 0.01
            4     0.025 0.01
            5     0.007 0.01
GLU_U 1,2,3,4,5   0     0.465 0.011
            1     0.212 0.011
            2     0.211 0.011
            3     0.08  0.011
            4     0.026 0.011
            5     0.006 0.011
GABA_U      1,2,3,4     0     0.52  0.019
            1     0.227 0.019
            2     0.194 0.019
            3     0.045 0.019
            4     0.014 0.019
GLY_U 2     0     0.832 0.011
            1     0.168 0.011
MET_U 2,3,4,5     0     0.529 0.026
            1     0.271 0.026
            2     0.115 0.026
            3     0.072 0.026
            4     0.013 0.026
SER_U 1,2,3 0     0.672 0.01
            1     0.182 0.01
            2     0.067 0.01
            3     0.079 0.01
SER_U 1,2,3 0     0.656 0.011
            1     0.184 0.011
            2     0.074 0.011
            3     0.086 0.011
SER_U 2,3   0     0.714 0.01
            1     0.176 0.01
            2     0.11  0.01
SER_U 2,3   0     0.717 0.011
            1     0.175 0.011
            2     0.108 0.011
SER_U 1,2   0     0.727 0.013
            1     0.148 0.013
            2     0.125 0.013
THR_U 2,3,4 0     0.634 0.01
            1     0.211 0.01
            2     0.11  0.01
            3     0.045 0.01
ASP_U 1,2,3,4     0     0.574 0.01
            1     0.204 0.01
```

```
            2     0.148 0.01
            3     0.061 0.01
            4     0.013 0.01
ASP_U 1,2,3,4     0     0.577 0.01
            1     0.203 0.01
            2     0.137 0.01
            3     0.066 0.01
            4     0.016 0.01
ASP_U 2,3,4 0     0.638 0.01
            1     0.21  0.01
            2     0.112 0.01
            3     0.04  0.01
ASP_U 1,2   0     0.732 0.013
            1     0.158 0.013
            2     0.11  0.013
GLU_U 2,3,4,5     0     0.553 0.01
            1     0.208 0.01
            2     0.184 0.01
            3     0.041 0.01
            4     0.013 0.01
ASP_U 1,2,3,4     0     0.555 0.01
            1     0.215 0.01
            2     0.144 0.01
            3     0.069 0.01
            4     0.016 0.01
GLU_U 1,2,3,4,5   0     0.47  0.013
            1     0.208 0.013
            2     0.221 0.013
            3     0.076 0.013
            4     0.021 0.013
            5     0.003 0.013
GLU_U 1,2,3,4,5   0     0.46  0.01
            1     0.21  0.01
            2     0.215 0.01
            3     0.084 0.01
            4     0.024 0.01
            5     0.008 0.01
GLU_U 1,2,3,4,5   0     0.465 0.011
            1     0.209 0.011
            2     0.211 0.011
            3     0.083 0.011
            4     0.023 0.011
            5     0.009 0.011
GABA_U      1,2,3,4     0     0.533 0.019
            1     0.216 0.019
            2     0.191 0.019
            3     0.045 0.019
            4     0.014 0.019
GLY_U 2     0     0.795 0.011
            1     0.205 0.011
VAL_U 1,2,3,4,5   0     0.549 0.01
            1     0.143 0.01
            2     0.159 0.01
```

```
            3     0.108 0.01
            4     0.022 0.01
            5     0.018 0.01
VAL_U 1,2,3,4,5   0     0.547 0.01
            1     0.133 0.01
            2     0.16  0.01
            3     0.121 0.01
            4     0.017 0.01
            5     0.022 0.01
VAL_U 2,3,4,5     0     0.574 0.029
            1     0.113 0.029
            2     0.25  0.029
            3     0.035 0.029
            4     0.028 0.029
MET_U 2,3,4,5     0     0.514 0.026
            1     0.282 0.026
            2     0.117 0.026
            3     0.074 0.026
            4     0.013 0.026
SER_U 1,2,3 0     0.642 0.01
            1     0.192 0.01
            2     0.077 0.01
            3     0.088 0.01
SER_U 1,2,3 0     0.64  0.011
            1     0.193 0.011
            2     0.077 0.011
            3     0.09  0.011
SER_U 2,3   0     0.703 0.01
            1     0.182 0.01
            2     0.115 0.01
SER_U 2,3   0     0.707 0.011
            1     0.178 0.011
            2     0.115 0.011
SER_U 1,2   0     0.718 0.013
            1     0.158 0.013
            2     0.124 0.013
THR_U 2,3,4 0     0.622 0.01
            1     0.219 0.01
            2     0.105 0.01
            3     0.054 0.01
ASP_U 1,2,3,4     0     0.56  0.01
            1     0.219 0.01
            2     0.137 0.01
            3     0.063 0.01
            4     0.021 0.01
ASP_U 1,2,3,4     0     0.555 0.01
            1     0.215 0.01
            2     0.141 0.01
            3     0.073 0.01
            4     0.016 0.01
ASP_U 2,3,4 0     0.62  0.01
            1     0.214 0.01
            2     0.123 0.01
```

		3	0.043	0.01
ASP_U	1,2	0	0.729	0.013
		1	0.16	0.013
		2	0.111	0.013
GLU_U	1,2,3,4,5	0	0.463	0.01
		1	0.212	0.01
		2	0.212	0.01
		3	0.084	0.01
		4	0.022	0.01
		5	0.007	0.01
GLU_U	2,3,4,5	0	0.521	0.01
		1	0.218	0.01
		2	0.199	0.01
		3	0.047	0.01
		4	0.015	0.01
ASP_U	1,2,3,4	0	0.591	0.029
		1	0.216	0.02
		2	0.137	0.02
		3	0.059	0.021
		4	-0.002	0.024
GLU_U	1,2,3,4,5	0	0.478	0.013
		1	0.205	0.013
		2	0.213	0.013
		3	0.08	0.013
		4	0.021	0.013
		5	0.003	0.013
GLU_U	1,2,3,4,5	0	0.461	0.01
		1	0.207	0.01
		2	0.214	0.01
		3	0.085	0.01
		4	0.025	0.01
		5	0.008	0.01
GLU_U	1,2,3,4,5	0	0.467	0.011
		1	0.205	0.011
		2	0.212	0.011
		3	0.083	0.011
		4	0.024	0.011
		5	0.008	0.011
GABA_U	1,2,3,4	0	0.523	0.019
		1	0.225	0.019
		2	0.193	0.019
		3	0.045	0.019
		4	0.014	0.019
OAA	1,2,3,4	0	0.366	0.011
		1	0.441	0.011
		2	0.167	0.011
		3	0.027	0.011
		4	-0.001	0.011
OAA	1,2,3,4	0	0.368	0.01
		1	0.441	0.01
		2	0.167	0.01
		3	0.023	0.01
		4	0	0.01

CIT	1,2,3,4,5,6	0	0.223	0.01
		1	0.409	0.01
		2	0.274	0.01
		3	0.084	0.01
		4	0.008	0.01
		5	0.002	0.01
		6	-0.001	0.01
FUM	1,2,3,4	0	0.395	0.02
		1	0.401	0.023
		2	0.152	0.017
		3	0.034	0.02
		4	0.018	0.021
OAA	1,2,3,4	0	0.374	0.011
		1	0.436	0.011
		2	0.173	0.011
		3	0.014	0.011
		4	0.003	0.011
OAA	1,2,3,4	0	0.377	0.01
		1	0.439	0.01
		2	0.164	0.01
		3	0.021	0.01
		4	-0.001	0.01
CIT	1,2,3,4,5,6	0	0.229	0.01
		1	0.407	0.01
		2	0.273	0.01
		3	0.081	0.01
		4	0.01	0.01
		5	0	0.01
		6	0	0.01
FUM	1,2,3,4	0	0.392	0.017
		1	0.413	0.017
		2	0.152	0.017
		3	0.027	0.017
		4	0.016	0.017
OAA	1,2,3,4	0	0.389	0.011
		1	0.436	0.011
		2	0.15	0.011
		3	0.023	0.011
		4	0.002	0.011
OAA	1,2,3,4	0	0.384	0.01
		1	0.439	0.01
		2	0.158	0.01
		3	0.018	0.01
		4	0	0.01
CIT	1,2,3,4,5,6	0	0.231	0.01
		1	0.414	0.01
		2	0.272	0.01
		3	0.072	0.01
		4	0.008	0.01
		5	0.002	0.01
		6	0	0.01
FUM_U	1,2,3,4	0	0.549	0.017
		1	0.201	0.017

		2	0.152	0.017	
		3	0.077	0.017	
		4	0.021	0.017	
OAA_U	1,2,3,4	0	0.536	0.011	
		1	0.222	0.011	
		2	0.151	0.011	
		3	0.074	0.011	
		4	0.017	0.011	
OAA_U	1,2,3,4	0	0.542	0.01	
		1	0.218	0.01	
		2	0.148	0.01	
		3	0.073	0.01	
		4	0.018	0.01	
CIT_U	1,2,3,4,5,6	0	0.41	0.01	
		1	0.209	0.01	
		2	0.219	0.01	
		3	0.107	0.01	
		4	0.039	0.01	
		5	0.014	0.01	
		6	0.003	0.01	
CIT_U	1,2,3,4,5,6	0	0.415	0.01	
		1	0.211	0.01	
		2	0.214	0.01	
		3	0.101	0.01	
		4	0.043	0.01	
		5	0.012	0.01	
		6	0.003	0.01	
FUM_U	1,2,3,4	0	0.554	0.017	
		1	0.213	0.017	
		2	0.123	0.017	
		3	0.082	0.017	
		4	0.028	0.017	
OAA_U	1,2,3,4	0	0.547	0.011	
		1	0.219	0.011	
		2	0.144	0.011	
		3	0.071	0.011	
		4	0.018	0.011	
OAA_U	1,2,3,4	0	0.542	0.01	
		1	0.219	0.01	
		2	0.146	0.01	
		3	0.074	0.01	
		4	0.018	0.01	
CIT_U	1,2,3,4,5,6	0	0.407	0.01	
		1	0.214	0.01	
		2	0.218	0.01	
		3	0.103	0.01	
		4	0.043	0.01	
		5	0.011	0.01	
		6	0.003	0.01	
ALA	1,2,3	0	0.598	0.011	
		1	0.374	0.011	
		2	0.026	0.011	
		3	0.001	0.011	

ALA	2,3	0	0.62	0.011
		1	0.37	0.011
		2	0.01	0.011
GLYeff	1,2	0	0.876	0.01
		1	0.121	0.01
		2	0.004	0.01
GLYeff	1,2	0	0.883	0.01
		1	0.114	0.01
		2	0.003	0.01
GLYeff	2	0	0.969	0.01
		1	0.031	0.01
VAL	1,2,3,4,5	0	0.389	0.01
		1	0.451	0.01
		2	0.151	0.01
		3	0.014	0.01
		4	-0.001	0.01
		5	-0.004	0.01
VAL	1,2,3,4,5	0	0.362	0.01
		1	0.459	0.01
		2	0.165	0.01
		3	0.016	0.01
		4	-0.001	0.01
		5	-0.002	0.01
VAL	2,3,4,5	0	0.383	0.01
		1	0.458	0.01
		2	0.15	0.01
		3	0.009	0.01
		4	0	0.01
VAL	2,3,4,5	0	0.408	0.024
		1	0.422	0.024
		2	0.147	0.024
		3	0.022	0.024
		4	0.001	0.024
LEU	1,2,3,4,5,6	0	0.25	0.02
		1	0.43	0.02
		2	0.251	0.02
		3	0.069	0.02
		4	0.005	0.02
		5	-0.003	0.02
		6	-0.003	0.02
LEU	1,2,3,4,5,6	0	0.232	0.012
		1	0.448	0.012
		2	0.253	0.012
		3	0.061	0.012
		4	0.005	0.012
		5	0.001	0.012
		6	0	0.012
LEU	2,3,4,5,6	0	0.271	0.017
		1	0.423	0.017
		2	0.246	0.017
		3	0.057	0.017
		4	0.004	0.017
		5	0	0.017

ILE	1,2,3,4,5,6	0	0.263	0.018
		1	0.422	0.018
		2	0.25	0.018
		3	0.066	0.018
		4	0.006	0.018
		5	-0.003	0.018
		6	-0.003	0.018
ILE	2,3,4,5,6	0	0.329	0.027
		1	0.452	0.037
		2	0.223	0.024
		3	0.037	0.026
		4	-0.016	0.029
		5	-0.024	0.031
ILE	2,3,4,5,6	0	0.315	0.02
		1	0.415	0.02
		2	0.216	0.02
		3	0.05	0.02
		4	0.004	0.02
		5	0	0.02
GLU	2,3,4,5	0	0.367	0.019
		1	0.425	0.019
		2	0.182	0.019
		3	0.027	0.019
		4	-0.001	0.019
METeff	1,2,3,4,5	0	0.39	0.01
		1	0.402	0.01
		2	0.176	0.01
		3	0.032	0.01
		4	0.001	0.01
		5	-0.001	0.01
METeff	1,2,3,4,5	0	0.387	0.01
		1	0.399	0.01
		2	0.171	0.01
		3	0.038	0.01
		4	0.002	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.426	0.013
		1	0.409	0.013
		2	0.143	0.013
		3	0.02	0.013
		4	0.002	0.013
METeff	2,3,4,5	0	0.425	0.011
		1	0.405	0.011
		2	0.146	0.011
		3	0.023	0.011
		4	0.001	0.011
SEReff	1,2,3	0	0.688	0.01
		1	0.298	0.01
		2	0.016	0.01
		3	-0.002	0.01
SEReff	1,2,3	0	0.7	0.01
		1	0.29	0.01
		2	0.014	0.01

```
            3      -0.004      0.01
SEReff      2,3    0      0.732 0.01
            1      0.264 0.01
            2      0.004 0.01
SEReff      2,3    0      0.732 0.011
            1      0.263 0.011
            2      0.005 0.011
SEReff      1,2    0      0.907 0.018
            1      0.087 0.018
            2      0.006 0.018
THR   1,2,3,4      0      0.394 0.01
            1      0.431 0.01
            2      0.158 0.01
            3      0.018 0.01
            4      -0.001      0.01
THR   2,3,4 0      0.471 0.01
            1      0.413 0.01
            2      0.108 0.01
            3      0.009 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.268 0.015
            1      0.413 0.015
            2      0.245 0.015
            3      0.062 0.015
            4      0.009 0.015
            5      0.001 0.015
            6      0.001 0.015
            7      0      0.015
            8      0      0.015
            9      0      0.015
PHE_TYR     2,3,4,5,6,7,8,9   0      0.278 0.018
            1      0.419 0.018
            2      0.236 0.018
            3      0.059 0.018
            4      0.008 0.018
            5      0      0.018
            6      0      0.018
            7      0      0.018
            8      0      0.018
PHE_TYR     2,3,4,5,6,7,8,9   0      0.278 0.019
            1      0.422 0.019
            2      0.233 0.019
            3      0.059 0.019
            4      0.007 0.019
            5      0.001 0.019
            6      0      0.019
            7      0      0.019
            8      0      0.019
PHE_TYR     1,2    0      0.942 0.01
            1      0.057 0.01
            2      0.001 0.01
ASP   1,2,3,4      0      0.407 0.011
            1      0.421 0.011
            2      0.154 0.011
```

		3	0.018	0.011
		4	0	0.011
ASP	1,2,3,4	0	0.403	0.011
		1	0.423	0.011
		2	0.153	0.011
		3	0.021	0.011
		4	0	0.011
ASP	2,3,4	0	0.464	0.01
		1	0.416	0.01
		2	0.112	0.01
		3	0.008	0.01
ASP	2,3,4	0	0.464	0.018
		1	0.414	0.018
		2	0.11	0.018
		3	0.012	0.018
ASP	1,2	0	0.648	0.011
		1	0.32	0.011
		2	0.032	0.011
CYS	1,2,3	0	0.7	0.02
		1	0.281	0.018
		2	0.022	0.018
		3	-0.003	0.018
CYS	2,3	0	0.735	0.012
		1	0.265	0.01
		2	0	0.011
GLU	1,2,3,4,5	0	0.287	0.023
		1	0.43	0.023
		2	0.237	0.023
		3	0.042	0.023
		4	0.005	0.023
		5	-0.002	0.023
GLU	2,3,4,5	0	0.341	0.01
		1	0.444	0.01
		2	0.199	0.01
		3	0.023	0.01
		4	-0.006	0.01
GLU	2,3,4,5	0	0.345	0.011
		1	0.435	0.011
		2	0.194	0.011
		3	0.027	0.011
		4	-0.001	0.011
LYS	1,2,3,4,5,6	0	0.288	0.01
		1	0.4	0.01
		2	0.243	0.01
		3	0.062	0.01
		4	0.005	0.01
		5	0.002	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.256	0.01
		1	0.427	0.01
		2	0.264	0.01
		3	0.065	0.01
		4	0.004	0.01

		5	-0.007	0.01
		6	-0.009	0.01
LYS	1,2,3,4,5,6	0	0.291	0.01
		1	0.424	0.013
		2	0.238	0.01
		3	0.06	0.01
		4	0.004	0.01
		5	-0.009	0.01
		6	-0.009	0.01
LYS	2,3,4,5,6	0	0.309	0.01
		1	0.421	0.01
		2	0.222	0.01
		3	0.048	0.01
		4	0.003	0.01
		5	-0.003	0.01
ARGeff	1,2,3,4,5,6	0	0.284	0.01
		1	0.385	0.01
		2	0.251	0.01
		3	0.074	0.01
		4	0.013	0.01
		5	-0.001	0.01
		6	-0.005	0.01
ARGeff	2,3,4,5,6	0	0.315	0.01
		1	0.415	0.01
		2	0.217	0.01
		3	0.059	0.01
		4	0.001	0.01
		5	-0.006	0.01
ARGeff	2,3,4,5,6	0	0.316	0.012
		1	0.418	0.017
		2	0.221	0.012
		3	0.051	0.012
		4	-0.001	0.013
		5	-0.005	0.014
HISeff	1,2,3,4,5,6	0	0.399	0.011
		1	0.399	0.011
		2	0.183	0.011
		3	0.023	0.011
		4	0.001	0.011
		5	-0.002	0.011
		6	-0.003	0.011
HISeff	1,2,3,4,5,6	0	0.395	0.013
		1	0.394	0.013
		2	0.173	0.013
		3	0.034	0.013
		4	0.004	0.013
		5	0	0.013
		6	0.002	0.013
HISeff	2,3,4,5,6	0	0.505	0.023
		1	0.377	0.023
		2	0.095	0.023
		3	0.015	0.023
		4	0.005	0.023

```
            5     0.003 0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.273 0.01
            1     0.424 0.01
            2     0.229 0.01
            3     0.067 0.01
            4     0.011 0.01
            5     -0.001      0.01
            6     0     0.01
            7     -0.002      0.01
            8     0     0.01
            9     -0.001      0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.277 0.023
            1     0.412 0.023
            2     0.238 0.023
            3     0.06  0.023
            4     0.008 0.023
            5     0.001 0.023
            6     0.001 0.023
            7     0     0.023
            8     0.002 0.023
            9     0.002 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0     0.285 0.01
            1     0.417 0.01
            2     0.232 0.01
            3     0.056 0.01
            4     0.006 0.01
            5     0.001 0.01
            6     0.001 0.01
            7     -0.001      0.01
            8     0.003 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0     0.283 0.01
            1     0.423 0.01
            2     0.233 0.01
            3     0.058 0.01
            4     0.007 0.01
            5     0.001 0.01
            6     -0.002      0.01
            7     -0.002      0.01
            8     -0.002      0.01
PHE_TYR     1,2   0     0.938 0.01
            1     0.06  0.01
            2     0.002 0.01
GLU   2,3,4,5     0     0.333 0.012
            1     0.449 0.015
            2     0.197 0.011
            3     0.024 0.013
            4     -0.003      0.014
ALA   1,2,3 0     0.601 0.011
            1     0.372 0.011
            2     0.025 0.011
            3     0.001 0.011
ALA   2,3   0     0.626 0.011
            1     0.365 0.011
```

	2	0.009	0.011	
GLYeff	1,2	0	0.901	0.01
	1	0.099	0.01	
	2	0	0.01	
GLYeff	1,2	0	0.899	0.01
	1	0.098	0.01	
	2	0.003	0.01	
GLYeff	2	0	0.975	0.01
	1	0.025	0.01	
VAL	1,2,3,4,5	0	0.393	0.01
	1	0.445	0.01	
	2	0.15	0.01	
	3	0.016	0.01	
	4	0.002	0.01	
	5	-0.006		0.01
VAL	1,2,3,4,5	0	0.371	0.01
	1	0.453	0.01	
	2	0.161	0.01	
	3	0.016	0.01	
	4	0	0.01	
	5	-0.001		0.01
VAL	2,3,4,5	0	0.391	0.01
	1	0.454	0.01	
	2	0.146	0.01	
	3	0.01	0.01	
	4	-0.001		0.01
VAL	2,3,4,5	0	0.422	0.024
	1	0.427	0.024	
	2	0.145	0.024	
	3	0.002	0.024	
	4	0.004	0.024	
LEU	1,2,3,4,5,6	0	0.262	0.02
	1	0.431	0.02	
	2	0.241	0.02	
	3	0.063	0.02	
	4	0.006	0.02	
	5	-0.002		0.02
	6	-0.002		0.02
LEU	1,2,3,4,5,6	0	0.243	0.012
	1	0.447	0.012	
	2	0.246	0.012	
	3	0.058	0.012	
	4	0.005	0.012	
	5	0	0.012	
	6	0	0.012	
LEU	2,3,4,5,6	0	0.282	0.017
	1	0.422	0.017	
	2	0.238	0.017	
	3	0.054	0.017	
	4	0.004	0.017	
	5	0	0.017	
ILE	1,2,3,4,5,6	0	0.27	0.018
	1	0.427	0.018	

		2	0.233	0.018
		3	0.067	0.018
		4	0.007	0.018
		5	-0.002	0.018
		6	-0.002	0.018
ILE	2,3,4,5,6	0	0.325	0.01
		1	0.427	0.01
		2	0.213	0.01
		3	0.042	0.01
		4	-0.001	0.01
		5	-0.006	0.01
ILE	2,3,4,5,6	0	0.327	0.02
		1	0.414	0.02
		2	0.208	0.02
		3	0.046	0.02
		4	0.004	0.02
		5	0.001	0.02
GLU	2,3,4,5	0	0.383	0.019
		1	0.422	0.019
		2	0.176	0.019
		3	0.024	0.019
		4	-0.006	0.019
METeff	1,2,3,4,5	0	0.404	0.01
		1	0.397	0.01
		2	0.168	0.01
		3	0.033	0.01
		4	0.004	0.01
		5	-0.007	0.01
METeff	1,2,3,4,5	0	0.392	0.01
		1	0.401	0.01
		2	0.17	0.01
		3	0.032	0.01
		4	0.003	0.01
		5	0.002	0.01
METeff	2,3,4,5	0	0.436	0.013
		1	0.404	0.013
		2	0.14	0.013
		3	0.02	0.013
		4	0	0.013
METeff	2,3,4,5	0	0.438	0.011
		1	0.4	0.011
		2	0.141	0.011
		3	0.02	0.011
		4	0.001	0.011
SEReff	1,2,3	0	0.697	0.01
		1	0.281	0.01
		2	0.018	0.01
		3	0.003	0.01
SEReff	1,2,3	0	0.705	0.01
		1	0.29	0.01
		2	0.012	0.01
		3	-0.007	0.01
SEReff	2,3	0	0.739	0.01

```
            1     0.259 0.01
            2     0.002 0.01
SEReff      2,3   0     0.736 0.011
            1     0.259 0.011
            2     0.005 0.011
SEReff      1,2   0     0.908 0.018
            1     0.084 0.018
            2     0.008 0.018
THR   1,2,3,4     0     0.409 0.01
            1     0.428 0.01
            2     0.146 0.01
            3     0.019 0.01
            4     -0.002      0.01
THR   2,3,4 0     0.487 0.01
            1     0.409 0.01
            2     0.096 0.01
            3     0.008 0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0     0.277 0.015
            1     0.417 0.015
            2     0.234 0.015
            3     0.061 0.015
            4     0.008 0.015
            5     0.002 0.015
            6     0     0.015
            7     -0.001      0.015
            8     0.001 0.015
            9     0     0.015
PHE_TYR     2,3,4,5,6,7,8,9   0     0.286 0.018
            1     0.422 0.018
            2     0.231 0.018
            3     0.055 0.018
            4     0.006 0.018
            5     0.001 0.018
            6     0     0.018
            7     0     0.018
            8     0     0.018
PHE_TYR     2,3,4,5,6,7,8,9   0     0.287 0.019
            1     0.421 0.019
            2     0.231 0.019
            3     0.056 0.019
            4     0.006 0.019
            5     0     0.019
            6     0     0.019
            7     0     0.019
            8     0     0.019
PHE_TYR     1,2   0     0.942 0.01
            1     0.057 0.01
            2     0.001 0.01
ASP   1,2,3,4     0     0.412 0.011
            1     0.419 0.011
            2     0.15  0.011
            3     0.015 0.011
            4     0.003 0.011
```

ASP	1,2,3,4	0	0.416	0.011
		1	0.42	0.011
		2	0.147	0.011
		3	0.017	0.011
		4	0	0.011
ASP	2,3,4	0	0.475	0.01
		1	0.413	0.01
		2	0.105	0.01
		3	0.008	0.01
ASP	2,3,4	0	0.476	0.018
		1	0.409	0.018
		2	0.105	0.018
		3	0.011	0.018
ASP	1,2	0	0.657	0.011
		1	0.312	0.011
		2	0.031	0.011
CYS	1,2,3	0	0.687	0.026
		1	0.288	0.019
		2	0.021	0.021
		3	0.003	0.022
GLU	1,2,3,4,5	0	0.31	0.023
		1	0.422	0.023
		2	0.219	0.023
		3	0.05	0.023
		4	0	0.023
		5	-0.001	0.023
GLU	2,3,4,5	0	0.351	0.01
		1	0.443	0.01
		2	0.19	0.01
		3	0.023	0.01
		4	-0.007	0.01
GLU	2,3,4,5	0	0.363	0.011
		1	0.435	0.011
		2	0.183	0.011
		3	0.023	0.011
		4	-0.004	0.011
LYS	1,2,3,4,5,6	0	0.294	0.01
		1	0.409	0.01
		2	0.232	0.01
		3	0.057	0.01
		4	0.008	0.01
		5	0	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.27	0.01
		1	0.414	0.01
		2	0.258	0.01
		3	0.065	0.01
		4	0.004	0.01
		5	-0.007	0.01
		6	-0.003	0.01
LYS	1,2,3,4,5,6	0	0.296	0.01
		1	0.415	0.01
		2	0.235	0.01

		3	0.057	0.01
		4	0.003	0.01
		5	-0.001	0.01
		6	-0.004	0.01
LYS	2,3,4,5,6	0	0.325	0.01
		1	0.42	0.01
		2	0.216	0.01
		3	0.043	0.01
		4	0.002	0.01
		5	-0.005	0.01
ARGeff	1,2,3,4,5,6	0	0.284	0.013
		1	0.394	0.013
		2	0.251	0.013
		3	0.059	0.013
		4	0.025	0.013
		5	-0.004	0.013
		6	-0.008	0.013
ARGeff	1,2,3,4,5,6	0	0.294	0.01
		1	0.388	0.01
		2	0.243	0.01
		3	0.069	0.01
		4	0.012	0.01
		5	-0.001	0.01
		6	-0.004	0.01
ARGeff	2,3,4,5,6	0	0.309	0.012
		1	0.395	0.017
		2	0.222	0.013
		3	0.058	0.013
		4	0.008	0.014
		5	0.008	0.015
ARGeff	2,3,4,5,6	0	0.326	0.01
		1	0.419	0.012
		2	0.211	0.01
		3	0.046	0.01
		4	0.003	0.01
		5	-0.004	0.01
HISeff	1,2,3,4,5,6	0	0.41	0.011
		1	0.409	0.011
		2	0.161	0.011
		3	0.026	0.011
		4	-0.001	0.011
		5	-0.001	0.011
		6	-0.003	0.011
HISeff	1,2,3,4,5,6	0	0.404	0.013
		1	0.394	0.013
		2	0.169	0.013
		3	0.029	0.013
		4	0.002	0.013
		5	0.002	0.013
		6	0.001	0.013
HISeff	2,3,4,5,6	0	0.52	0.023
		1	0.372	0.023
		2	0.092	0.023

```
		3	0.014	0.023
		4	0.003	0.023
		5	-0.002	0.023
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.281	0.01
		1	0.431	0.01
		2	0.237	0.01
		3	0.06	0.01
		4	0.004	0.01
		5	0	0.01
		6	-0.006	0.01
		7	-0.002	0.01
		8	-0.002	0.01
		9	-0.003	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.287	0.023
		1	0.41	0.023
		2	0.226	0.023
		3	0.06	0.023
		4	0.006	0.023
		5	0.002	0.023
		6	0	0.023
		7	0	0.023
		8	0.005	0.023
		9	0.004	0.023
PHE_TYR	2,3,4,5,6,7,8,9	0	0.289	0.01
		1	0.42	0.01
		2	0.226	0.01
		3	0.054	0.01
		4	0.005	0.01
		5	0.002	0.01
		6	0.001	0.01
		7	0.001	0.01
		8	0.004	0.01
PHE_TYR	2,3,4,5,6,7,8,9	0	0.293	0.01
		1	0.433	0.01
		2	0.228	0.01
		3	0.057	0.01
		4	0.004	0.01
		5	-0.002	0.01
		6	-0.003	0.01
		7	-0.004	0.01
		8	-0.005	0.01
PHE_TYR	1,2	0	0.942	0.01
		1	0.056	0.01
		2	0.002	0.01
GLU	2,3,4,5	0	0.346	0.01
		1	0.439	0.01
		2	0.186	0.01
		3	0.027	0.01
		4	0.002	0.01
ALA	1,2,3	0	0.601	0.011
		1	0.372	0.011
		2	0.025	0.011
		3	0.001	0.011
```

ALA	2,3	0	0.625	0.011
		1	0.367	0.011
		2	0.007	0.011
GLYeff	1,2	0	0.871	0.01
		1	0.128	0.01
		2	0.001	0.01
GLYeff	1,2	0	0.874	0.01
		1	0.122	0.01
		2	0.004	0.01
GLYeff	2	0	0.968	0.01
		1	0.032	0.01
VAL	1,2,3,4,5	0	0.397	0.01
		1	0.436	0.01
		2	0.16	0.01
		3	0.012	0.01
		4	-0.001	0.01
		5	-0.005	0.01
VAL	1,2,3,4,5	0	0.369	0.01
		1	0.458	0.01
		2	0.161	0.01
		3	0.015	0.01
		4	0	0.01
		5	-0.002	0.01
VAL	2,3,4,5	0	0.385	0.01
		1	0.456	0.01
		2	0.151	0.01
		3	0.009	0.01
		4	-0.001	0.01
VAL	2,3,4,5	0	0.406	0.024
		1	0.423	0.024
		2	0.147	0.024
		3	0.022	0.024
		4	0.002	0.024
LEU	1,2,3,4,5,6	0	0.244	0.02
		1	0.431	0.02
		2	0.243	0.02
		3	0.078	0.02
		4	0.006	0.02
		5	0	0.02
		6	-0.002	0.02
LEU	1,2,3,4,5,6	0	0.234	0.012
		1	0.447	0.012
		2	0.253	0.012
		3	0.061	0.012
		4	0.004	0.012
		5	0.001	0.012
		6	0	0.012
LEU	2,3,4,5,6	0	0.277	0.017
		1	0.421	0.017
		2	0.242	0.017
		3	0.056	0.017
		4	0.004	0.017
		5	0	0.017

```
ILE    1,2,3,4,5,6 0      0.239 0.018
             1      0.445 0.018
             2      0.253 0.018
             3      0.075 0.018
             4      0.004 0.018
             5      -0.009      0.018
             6      -0.005      0.018
ILE    2,3,4,5,6    0      0.313 0.01
             1      0.424 0.01
             2      0.216 0.01
             3      0.048 0.01
             4      0.001 0.01
             5      -0.003      0.01
ILE    2,3,4,5,6    0      0.318 0.02
             1      0.414 0.02
             2      0.214 0.02
             3      0.049 0.02
             4      0.004 0.02
             5      0.001 0.02
GLU    2,3,4,5      0      0.372 0.019
             1      0.422 0.019
             2      0.183 0.019
             3      0.022 0.019
             4      0      0.019
METeff       1,2,3,4,5   0      0.389 0.01
             1      0.403 0.01
             2      0.169 0.01
             3      0.031 0.01
             4      0.005 0.01
             5      0.003 0.01
METeff       2,3,4,5     0      0.427 0.013
             1      0.409 0.013
             2      0.141 0.013
             3      0.021 0.013
             4      0.002 0.013
METeff       2,3,4,5     0      0.428 0.011
             1      0.403 0.011
             2      0.145 0.011
             3      0.021 0.011
             4      0.002 0.011
SEReff       1,2,3 0      0.69  0.01
             1      0.291 0.01
             2      0.016 0.01
             3      0.004 0.01
SEReff       1,2,3 0      0.699 0.01
             1      0.29  0.01
             2      0.014 0.01
             3      -0.003      0.01
SEReff       2,3    0      0.736 0.01
             1      0.261 0.01
             2      0.003 0.01
SEReff       2,3    0      0.735 0.011
             1      0.261 0.011
```

		2	0.004	0.011
SEReff	1,2	0	0.908	0.018
		1	0.086	0.018
		2	0.006	0.018
THR	1,2,3,4	0	0.404	0.01
		1	0.428	0.01
		2	0.153	0.01
		3	0.017	0.01
		4	-0.002	0.01
THR	2,3,4	0	0.483	0.01
		1	0.404	0.01
		2	0.105	0.01
		3	0.009	0.01
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.275	0.015
		1	0.417	0.015
		2	0.234	0.015
		3	0.063	0.015
		4	0.008	0.015
		5	0.002	0.015
		6	0.001	0.015
		7	0.001	0.015
		8	0	0.015
		9	0	0.015
PHE_TYR	2,3,4,5,6,7,8,9	0	0.283	0.018
		1	0.424	0.018
		2	0.232	0.018
		3	0.054	0.018
		4	0.006	0.018
		5	0.001	0.018
		6	0	0.018
		7	0	0.018
		8	0	0.018
PHE_TYR	2,3,4,5,6,7,8,9	0	0.284	0.019
		1	0.424	0.019
		2	0.232	0.019
		3	0.056	0.019
		4	0.006	0.019
		5	0	0.019
		6	0	0.019
		7	0	0.019
		8	0	0.019
PHE_TYR	1,2	0	0.944	0.01
		1	0.056	0.01
		2	0.001	0.01
ASP	1,2,3,4	0	0.414	0.011
		1	0.418	0.011
		2	0.154	0.011
		3	0.014	0.011
		4	0.001	0.011
ASP	1,2,3,4	0	0.41	0.011
		1	0.421	0.011
		2	0.15	0.011
		3	0.018	0.011

		4	0	0.011
ASP	2,3,4	0	0.468	0.01
		1	0.418	0.01
		2	0.108	0.01
		3	0.006	0.01
ASP	2,3,4	0	0.47	0.018
		1	0.412	0.018
		2	0.106	0.018
		3	0.011	0.018
ASP	1,2	0	0.657	0.011
		1	0.314	0.011
		2	0.029	0.011
CYS	1,2,3	0	0.707	0.025
		1	0.271	0.018
		2	0.006	0.019
		3	0.016	0.02
GLU	1,2,3,4,5	0	0.3	0.023
		1	0.428	0.023
		2	0.229	0.023
		3	0.032	0.023
		4	0.009	0.023
		5	0.002	0.023
GLU	2,3,4,5	0	0.348	0.01
		1	0.445	0.01
		2	0.189	0.01
		3	0.023	0.01
		4	-0.006	0.01
GLU	2,3,4,5	0	0.36	0.011
		1	0.434	0.011
		2	0.187	0.011
		3	0.023	0.011
		4	-0.003	0.011
LYS	1,2,3,4,5,6	0	0.293	0.01
		1	0.402	0.01
		2	0.237	0.01
		3	0.062	0.01
		4	0.005	0.01
		5	0.001	0.01
		6	0	0.01
LYS	1,2,3,4,5,6	0	0.268	0.01
		1	0.416	0.01
		2	0.25	0.01
		3	0.071	0.01
		4	0.005	0.01
		5	-0.003	0.01
		6	-0.008	0.01
LYS	1,2,3,4,5,6	0	0.295	0.01
		1	0.414	0.01
		2	0.242	0.01
		3	0.058	0.01
		4	0.002	0.01
		5	-0.004	0.01
		6	-0.007	0.01

```
LYS   2,3,4,5,6    0     0.316 0.01
            1      0.423 0.01
            2      0.216 0.01
            3      0.048 0.01
            4      0.001 0.01
            5      -0.005      0.01
ARGeff      1,2,3,4,5,6 0      0.293 0.01
            1      0.401 0.016
            2      0.241 0.011
            3      0.072 0.01
            4      0.009 0.011
            5      -0.005      0.012
            6      -0.011      0.012
ARGeff      2,3,4,5,6   0      0.312 0.01
            1      0.424 0.01
            2      0.214 0.01
            3      0.056 0.01
            4      0.002 0.01
            5      -0.007      0.01
ARGeff      2,3,4,5,6   0      0.326 0.01
            1      0.416 0.013
            2      0.215 0.01
            3      0.043 0.01
            4      -0.001      0.01
            5      0     0.011
HISeff      1,2,3,4,5,6 0      0.405 0.011
            1      0.386 0.011
            2      0.176 0.011
            3      0.025 0.011
            4      -0.004      0.011
            5      0.004 0.011
            6      0.009 0.011
HISeff      1,2,3,4,5,6 0      0.402 0.013
            1      0.395 0.013
            2      0.168 0.013
            3      0.032 0.013
            4      0.002 0.013
            5      0.001 0.013
            6      0.001 0.013
HISeff      2,3,4,5,6   0      0.512 0.023
            1      0.382 0.023
            2      0.089 0.023
            3      0.016 0.023
            4      0.005 0.023
            5      -0.004      0.023
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.272 0.01
            1      0.437 0.01
            2      0.238 0.01
            3      0.057 0.01
            4      0.004 0.01
            5      0.002 0.01
            6      -0.005      0.01
            7      -0.002      0.01
```

```
            8     -0.001      0.01
            9     -0.002      0.01
PHE_TYR     1,2,3,4,5,6,7,8,9 0      0.283 0.023
            1     0.412 0.023
            2     0.23  0.023
            3     0.058 0.023
            4     0.009 0.023
            5     0.001 0.023
            6     0.001 0.023
            7     0     0.023
            8     0.003 0.023
            9     0.003 0.023
PHE_TYR     2,3,4,5,6,7,8,9   0      0.29  0.01
            1     0.42  0.01
            2     0.231 0.01
            3     0.052 0.01
            4     0.007 0.01
            5     0     0.01
            6     -0.001      0.01
            7     -0.001      0.01
            8     0.001 0.01
PHE_TYR     2,3,4,5,6,7,8,9   0      0.288 0.01
            1     0.435 0.01
            2     0.23  0.01
            3     0.055 0.01
            4     0.005 0.01
            5     -0.002      0.01
            6     -0.003      0.01
            7     -0.004      0.01
            8     -0.004      0.01
PHE_TYR     1,2   0     0.943 0.01
            1     0.055 0.01
            2     0.002 0.01
GLU   2,3,4,5     0     0.342 0.011
            1     0.447 0.013
            2     0.19  0.01
            3     0.024 0.011
            4     -0.003      0.012
ALA_U 1,2,3 0     0.723 0.011
            1     0.087 0.011
            2     0.045 0.011
            3     0.146 0.011
ALA_U 2,3   0     0.767 0.011
            1     0.06  0.011
            2     0.173 0.011
GLYeff_U    1,2   0     0.704 0.01
            1     0.186 0.01
            2     0.11  0.01
GLYeff_U    1,2   0     0.714 0.01
            1     0.183 0.01
            2     0.104 0.01
GLYeff_U    2     0     0.804 0.01
            1     0.196 0.01
```

VAL_U	1,2,3,4,5	0	0.54	0.01
		1	0.126	0.01
		2	0.167	0.01
		3	0.121	0.01
		4	0.023	0.01
		5	0.023	0.01
VAL_U	1,2,3,4,5	0	0.543	0.01
		1	0.125	0.01
		2	0.166	0.01
		3	0.127	0.01
		4	0.017	0.01
		5	0.022	0.01
VAL_U	2,3,4,5	0	0.578	0.011
		1	0.11	0.01
		2	0.262	0.01
		3	0.024	0.01
		4	0.027	0.01
VAL_U	2,3,4,5	0	0.585	0.024
		1	0.102	0.024
		2	0.251	0.024
		3	0.036	0.024
		4	0.027	0.024
LEU_U	1,2,3,4,5,6	0	0.437	0.02
		1	0.132	0.02
		2	0.299	0.02
		3	0.06	0.02
		4	0.06	0.02
		5	0.008	0.02
		6	0.004	0.02
LEU_U	1,2,3,4,5,6	0	0.434	0.012
		1	0.127	0.012
		2	0.312	0.012
		3	0.053	0.012
		4	0.064	0.012
		5	0.005	0.012
		6	0.005	0.012
LEU_U	2,3,4,5,6	0	0.467	0.017
		1	0.195	0.017
		2	0.231	0.017
		3	0.073	0.017
		4	0.028	0.017
		5	0.006	0.017
ILE_U	1,2,3,4,5,6	0	0.422	0.018
		1	0.214	0.018
		2	0.221	0.018
		3	0.094	0.018
		4	0.044	0.018
		5	0.009	0.018
		6	-0.003	0.018
ILE_U	2,3,4,5,6	0	0.475	0.01
		1	0.21	0.01
		2	0.211	0.01
		3	0.076	0.01

```
            4     0.022 0.01
            5     0.006 0.01
ILE_U 2,3,4,5,6   0     0.482 0.02
            1     0.206 0.02
            2     0.206 0.02
            3     0.077 0.02
            4     0.023 0.02
            5     0.007 0.02
GLU_U 2,3,4,5     0     0.537 0.019
            1     0.22  0.019
            2     0.177 0.019
            3     0.047 0.019
            4     0.018 0.019
METeff_U    1,2,3,4,5   0     0.479 0.01
            1     0.267 0.01
            2     0.125 0.01
            3     0.084 0.01
            4     0.031 0.01
            5     0.014 0.01
METeff_U    1,2,3,4,5   0     0.478 0.01
            1     0.272 0.01
            2     0.127 0.01
            3     0.082 0.01
            4     0.034 0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0     0.551 0.013
            1     0.258 0.013
            2     0.103 0.013
            3     0.074 0.013
            4     0.014 0.013
METeff_U    2,3,4,5     0     0.551 0.011
            1     0.258 0.011
            2     0.105 0.011
            3     0.074 0.011
            4     0.012 0.011
SEReff_U    1,2,3 0     0.659 0.01
            1     0.172 0.01
            2     0.079 0.01
            3     0.091 0.01
SEReff_U    1,2,3 0     0.668 0.01
            1     0.167 0.01
            2     0.074 0.01
            3     0.091 0.01
SEReff_U    2,3   0     0.715 0.01
            1     0.168 0.01
            2     0.117 0.01
SEReff_U    2,3   0     0.717 0.011
            1     0.167 0.011
            2     0.115 0.011
SEReff_U    1,2   0     0.734 0.018
            1     0.131 0.018
            2     0.135 0.018
THR_U 1,2,3,4     0     0.548 0.01
```

```
            1      0.218 0.01
            2      0.148 0.01
            3      0.072 0.01
            4      0.015 0.01
THR_U 2,3,4 0      0.623 0.01
            1      0.212 0.01
            2      0.118 0.01
            3      0.047 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.353 0.015
            1      0.161 0.015
            2      0.137 0.015
            3      0.172 0.015
            4      0.084 0.015
            5      0.048 0.015
            6      0.029 0.015
            7      0.012 0.015
            8      0.003 0.015
            9      0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.372 0.018
            1      0.149 0.018
            2      0.21  0.018
            3      0.122 0.018
            4      0.079 0.018
            5      0.039 0.018
            6      0.021 0.018
            7      0.005 0.018
            8      0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0      0.373 0.019
            1      0.149 0.019
            2      0.208 0.019
            3      0.123 0.019
            4      0.08  0.019
            5      0.039 0.019
            6      0.021 0.019
            7      0.005 0.019
            8      0.002 0.019
PHE_TYR_U   1,2   0      0.748 0.01
            1      0.097 0.01
            2      0.155 0.01
ASP_U 1,2,3,4      0      0.555 0.011
            1      0.216 0.011
            2      0.143 0.011
            3      0.069 0.011
            4      0.018 0.011
ASP_U 1,2,3,4      0      0.556 0.011
            1      0.215 0.011
            2      0.144 0.011
            3      0.067 0.011
            4      0.018 0.011
ASP_U 2,3,4 0      0.617 0.01
            1      0.224 0.01
            2      0.118 0.01
            3      0.041 0.01
```

ASP_U 2,3,4	0	0.613	0.018
	1	0.221	0.018
	2	0.12	0.018
	3	0.046	0.018
ASP_U 1,2	0	0.728	0.011
	1	0.159	0.011
	2	0.113	0.011
CYS_U 1,2,3	0	0.672	0.018
	1	0.153	0.018
	2	0.077	0.018
	3	0.098	0.018
CYS_U 2,3	0	0.721	0.013
	1	0.166	0.011
	2	0.113	0.011
GLU_U 1,2,3,4,5	0	0.475	0.023
	1	0.213	0.023
	2	0.213	0.023
	3	0.078	0.023
	4	0.022	0.023
	5	-0.001	0.023
GLU_U 2,3,4,5	0	0.533	0.01
	1	0.221	0.01
	2	0.195	0.01
	3	0.042	0.01
	4	0.009	0.01
GLU_U 2,3,4,5	0	0.537	0.011
	1	0.218	0.011
	2	0.189	0.011
	3	0.044	0.011
	4	0.012	0.011
LYS_U 1,2,3,4,5,6	0	0.44	0.01
	1	0.208	0.01
	2	0.174	0.01
	3	0.114	0.01
	4	0.042	0.01
	5	0.018	0.01
	6	0.004	0.01
LYS_U 1,2,3,4,5,6	0	0.43	0.01
	1	0.212	0.01
	2	0.184	0.01
	3	0.121	0.01
	4	0.041	0.01
	5	0.012	0.01
	6	-0.001	0.01
LYS_U 1,2,3,4,5,6	0	0.441	0.01
	1	0.21	0.01
	2	0.175	0.01
	3	0.116	0.01
	4	0.042	0.01
	5	0.014	0.01
	6	0.003	0.01
LYS_U 2,3,4,5,6	0	0.475	0.01
	1	0.213	0.01

```
            2      0.207 0.01
            3      0.078 0.01
            4      0.021 0.01
            5      0.006 0.01
ARGeff_U    1,2,3,4,5,6 0      0.426 0.013
            1      0.242 0.013
            2      0.224 0.013
            3      0.085 0.013
            4      0.04  0.013
            5      -0.007      0.013
            6      -0.01 0.013
ARGeff_U    1,2,3,4,5,6 0      0.416 0.01
            1      0.252 0.01
            2      0.194 0.01
            3      0.105 0.01
            4      0.033 0.01
            5      0.006 0.01
            6      -0.004      0.01
ARGeff_U    2,3,4,5,6   0      0.467 0.02
            1      0.277 0.015
            2      0.192 0.014
            3      0.064 0.014
            4      0.011 0.016
            5      -0.011      0.017
HISeff_U    1,2,3,4,5,6 0      0.465 0.011
            1      0.231 0.011
            2      0.133 0.011
            3      0.094 0.011
            4      0.045 0.011
            5      0.031 0.011
            6      0.001 0.011
HISeff_U    1,2,3,4,5,6 0      0.461 0.013
            1      0.234 0.013
            2      0.117 0.013
            3      0.108 0.013
            4      0.046 0.013
            5      0.027 0.013
            6      0.008 0.013
HISeff_U    2,3,4,5,6   0      0.509 0.029
            1      0.237 0.021
            2      0.177 0.02
            3      0.068 0.02
            4      0.014 0.023
            5      -0.005      0.024
HISeff_U    2,3,4,5,6   0      0.468 0.023
            1      0.238 0.023
            2      0.181 0.023
            3      0.073 0.023
            4      0.031 0.023
            5      0.009 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0      0.345 0.01
            1      0.165 0.01
            2      0.138 0.01
```

```
            3     0.175 0.01
            4     0.085 0.01
            5     0.049 0.01
            6     0.028 0.01
            7     0.009 0.01
            8     0.004 0.01
            9     0.001 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.355 0.023
            1     0.157 0.023
            2     0.141 0.023
            3     0.17  0.023
            4     0.081 0.023
            5     0.048 0.023
            6     0.028 0.023
            7     0.013 0.023
            8     0.004 0.023
            9     0.003 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.378 0.01
            1     0.15  0.01
            2     0.202 0.01
            3     0.123 0.01
            4     0.079 0.01
            5     0.038 0.01
            6     0.021 0.01
            7     0.004 0.01
            8     0.005 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.371 0.01
            1     0.15  0.01
            2     0.209 0.01
            3     0.126 0.01
            4     0.079 0.01
            5     0.041 0.01
            6     0.021 0.01
            7     0.003 0.01
            8     0.001 0.01
PHE_TYR_U   1,2   0     0.751 0.01
            1     0.093 0.01
            2     0.156 0.01
GLU_U 2,3,4,5     0     0.53  0.019
            1     0.223 0.011
            2     0.193 0.011
            3     0.043 0.013
            4     0.011 0.014
ALA_U 1,2,3 0     0.721 0.011
            1     0.09  0.011
            2     0.045 0.011
            3     0.143 0.011
ALA_U 2,3   0     0.765 0.011
            1     0.062 0.011
            2     0.172 0.011
GLYeff_U    1,2   0     0.708 0.01
            1     0.188 0.01
            2     0.104 0.01
```

```
GLYeff_U     1,2    0      0.713 0.01
             1      0.186 0.01
             2      0.101 0.01
GLYeff_U     2      0      0.806 0.01
             1      0.194 0.01
VAL_U 1,2,3,4,5     0      0.54  0.01
             1      0.139 0.01
             2      0.164 0.01
             3      0.118 0.01
             4      0.018 0.01
             5      0.021 0.01
VAL_U 1,2,3,4,5     0      0.539 0.01
             1      0.132 0.01
             2      0.165 0.01
             3      0.125 0.01
             4      0.017 0.01
             5      0.022 0.01
VAL_U 2,3,4,5       0      0.575 0.01
             1      0.118 0.01
             2      0.257 0.01
             3      0.025 0.01
             4      0.026 0.01
VAL_U 2,3,4,5       0      0.588 0.024
             1      0.108 0.024
             2      0.244 0.024
             3      0.034 0.024
             4      0.026 0.024
LEU_U 1,2,3,4,5,6 0      0.433 0.02
             1      0.143 0.02
             2      0.29  0.02
             3      0.061 0.02
             4      0.063 0.02
             5      0.006 0.02
             6      0.005 0.02
LEU_U 1,2,3,4,5,6 0      0.436 0.012
             1      0.132 0.012
             2      0.306 0.012
             3      0.054 0.012
             4      0.062 0.012
             5      0.005 0.012
             6      0.004 0.012
LEU_U 2,3,4,5,6     0      0.469 0.017
             1      0.198 0.017
             2      0.228 0.017
             3      0.072 0.017
             4      0.027 0.017
             5      0.006 0.017
ILE_U 1,2,3,4,5,6 0      0.415 0.018
             1      0.221 0.018
             2      0.214 0.018
             3      0.097 0.018
             4      0.038 0.018
             5      0.012 0.018
```

```
            6     0.003 0.018
ILE_U 2,3,4,5,6   0     0.483 0.01
            1     0.21  0.01
            2     0.205 0.01
            3     0.074 0.01
            4     0.022 0.01
            5     0.006 0.01
ILE_U 2,3,4,5,6   0     0.488 0.02
            1     0.205 0.02
            2     0.202 0.02
            3     0.075 0.02
            4     0.023 0.02
            5     0.007 0.02
GLU_U 2,3,4,5     0     0.541 0.019
            1     0.219 0.019
            2     0.183 0.019
            3     0.042 0.019
            4     0.015 0.019
METeff_U    1,2,3,4,5   0     0.488 0.01
            1     0.263 0.01
            2     0.121 0.01
            3     0.083 0.01
            4     0.032 0.01
            5     0.014 0.01
METeff_U    1,2,3,4,5   0     0.49  0.01
            1     0.262 0.01
            2     0.123 0.01
            3     0.084 0.01
            4     0.034 0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0     0.558 0.013
            1     0.253 0.013
            2     0.102 0.013
            3     0.075 0.013
            4     0.012 0.013
METeff_U    2,3,4,5     0     0.561 0.011
            1     0.254 0.011
            2     0.103 0.011
            3     0.071 0.011
            4     0.011 0.011
SEReff_U    1,2,3 0     0.66  0.01
            1     0.173 0.01
            2     0.076 0.01
            3     0.09  0.01
SEReff_U    1,2,3 0     0.663 0.01
            1     0.173 0.01
            2     0.077 0.01
            3     0.087 0.01
SEReff_U    2,3   0     0.711 0.01
            1     0.177 0.01
            2     0.111 0.01
SEReff_U    2,3   0     0.712 0.011
            1     0.177 0.011
```

```
            2     0.111 0.011
SEReff_U    1,2   0     0.73  0.018
            1     0.134 0.018
            2     0.136 0.018
THR_U 1,2,3,4     0     0.559 0.01
            1     0.216 0.01
            2     0.144 0.01
            3     0.065 0.01
            4     0.016 0.01
THR_U 2,3,4 0     0.626 0.01
            1     0.221 0.01
            2     0.11  0.01
            3     0.044 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.352 0.015
            1     0.159 0.015
            2     0.14  0.015
            3     0.171 0.015
            4     0.085 0.015
            5     0.047 0.015
            6     0.029 0.015
            7     0.011 0.015
            8     0.004 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.374 0.018
            1     0.153 0.018
            2     0.206 0.018
            3     0.121 0.018
            4     0.079 0.018
            5     0.039 0.018
            6     0.021 0.018
            7     0.005 0.018
            8     0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.373 0.019
            1     0.152 0.019
            2     0.209 0.019
            3     0.122 0.019
            4     0.078 0.019
            5     0.039 0.019
            6     0.021 0.019
            7     0.005 0.019
            8     0.002 0.019
PHE_TYR_U   1,2   0     0.749 0.01
            1     0.096 0.01
            2     0.155 0.01
ASP_U 1,2,3,4     0     0.561 0.011
            1     0.211 0.011
            2     0.146 0.011
            3     0.065 0.011
            4     0.017 0.011
ASP_U 1,2,3,4     0     0.558 0.011
            1     0.212 0.011
            2     0.144 0.011
            3     0.069 0.011
```

		4	0.018	0.011
ASP_U	2,3,4	0	0.622	0.01
		1	0.218	0.01
		2	0.117	0.01
		3	0.043	0.01
ASP_U	2,3,4	0	0.619	0.018
		1	0.218	0.018
		2	0.117	0.018
		3	0.047	0.018
ASP_U	1,2	0	0.729	0.011
		1	0.158	0.011
		2	0.113	0.011
CYS_U	2,3	0	0.731	0.01
		1	0.161	0.01
		2	0.107	0.01
GLU_U	1,2,3,4,5	0	0.469	0.023
		1	0.208	0.023
		2	0.211	0.023
		3	0.08	0.023
		4	0.024	0.023
		5	0.007	0.023
GLU_U	2,3,4,5	0	0.533	0.01
		1	0.219	0.01
		2	0.195	0.01
		3	0.042	0.01
		4	0.011	0.01
GLU_U	2,3,4,5	0	0.538	0.011
		1	0.217	0.011
		2	0.19	0.011
		3	0.043	0.011
		4	0.012	0.011
LYS_U	1,2,3,4,5,6	0	0.449	0.01
		1	0.209	0.01
		2	0.172	0.01
		3	0.11	0.01
		4	0.04	0.01
		5	0.016	0.01
		6	0.003	0.01
LYS_U	1,2,3,4,5,6	0	0.439	0.01
		1	0.214	0.01
		2	0.181	0.01
		3	0.112	0.01
		4	0.043	0.01
		5	0.012	0.01
		6	-0.001	0.01
LYS_U	1,2,3,4,5,6	0	0.441	0.01
		1	0.212	0.01
		2	0.175	0.01
		3	0.115	0.01
		4	0.039	0.01
		5	0.016	0.01
		6	0.003	0.01
LYS_U	2,3,4,5,6	0	0.478	0.01

	1	0.212	0.01		
	2	0.208	0.01		
	3	0.074	0.01		
	4	0.023	0.01		
	5	0.006	0.01		
ARGeff_U	1,2,3,4,5,6	0		0.412	0.013
	1	0.259	0.013		
	2	0.208	0.013		
	3	0.087	0.013		
	4	0.037	0.013		
	5	0.007	0.013		
	6	-0.01	0.013		
ARGeff_U	1,2,3,4,5,6	0		0.415	0.01
	1	0.251	0.01		
	2	0.199	0.01		
	3	0.096	0.01		
	4	0.033	0.01		
	5	0.009	0.01		
	6	-0.003		0.01	
ARGeff_U	2,3,4,5,6	0		0.443	0.01
	1	0.272	0.01		
	2	0.188	0.01		
	3	0.069	0.01		
	4	0.024	0.01		
	5	0.004	0.01		
ARGeff_U	2,3,4,5,6	0		0.455	0.01
	1	0.27	0.01		
	2	0.181	0.01		
	3	0.07	0.01		
	4	0.018	0.01		
	5	0.005	0.01		
HISeff_U	1,2,3,4,5,6	0		0.467	0.011
	1	0.225	0.011		
	2	0.123	0.011		
	3	0.097	0.011		
	4	0.045	0.011		
	5	0.032	0.011		
	6	0.011	0.011		
HISeff_U	1,2,3,4,5,6	0		0.465	0.013
	1	0.23	0.013		
	2	0.12	0.013		
	3	0.106	0.013		
	4	0.045	0.013		
	5	0.028	0.013		
	6	0.006	0.013		
HISeff_U	2,3,4,5,6	0		0.483	0.02
	1	0.252	0.015		
	2	0.182	0.014		
	3	0.059	0.015		
	4	0.028	0.016		
	5	-0.004		0.017	
HISeff_U	2,3,4,5,6	0		0.467	0.023
	1	0.243	0.023		

```
            2     0.178 0.023
            3     0.072 0.023
            4     0.032 0.023
            5     0.008 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.356 0.01
            1     0.155 0.01
            2     0.145 0.01
            3     0.169 0.01
            4     0.085 0.01
            5     0.048 0.01
            6     0.026 0.01
            7     0.013 0.01
            8     0.003 0.01
            9     0.001 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.359 0.023
            1     0.155 0.023
            2     0.14  0.023
            3     0.169 0.023
            4     0.083 0.023
            5     0.047 0.023
            6     0.029 0.023
            7     0.011 0.023
            8     0.005 0.023
            9     0.002 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.375 0.01
            1     0.151 0.01
            2     0.204 0.01
            3     0.122 0.01
            4     0.078 0.01
            5     0.038 0.01
            6     0.022 0.01
            7     0.005 0.01
            8     0.005 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.37  0.01
            1     0.151 0.01
            2     0.212 0.01
            3     0.122 0.01
            4     0.08  0.01
            5     0.038 0.01
            6     0.021 0.01
            7     0.004 0.01
            8     0.001 0.01
PHE_TYR_U   1,2   0     0.749 0.01
            1     0.098 0.01
            2     0.153 0.01
GLU_U 2,3,4,5     0     0.536 0.017
            1     0.218 0.01
            2     0.193 0.01
            3     0.042 0.012
            4     0.011 0.013
ALA_U 1,2,3 0     0.723 0.011
            1     0.089 0.011
            2     0.044 0.011
```

```
            3     0.144 0.011
ALA_U 2,3   0     0.767 0.011
            1     0.06  0.011
            2     0.173 0.011
GLYeff_U    2     0     0.806 0.01
            1     0.194 0.01
VAL_U 1,2,3,4,5   0     0.548 0.01
            1     0.126 0.01
            2     0.165 0.01
            3     0.121 0.01
            4     0.02  0.01
            5     0.02  0.01
VAL_U 1,2,3,4,5   0     0.547 0.01
            1     0.127 0.01
            2     0.164 0.01
            3     0.124 0.01
            4     0.017 0.01
            5     0.021 0.01
VAL_U 2,3,4,5     0     0.58  0.01
            1     0.113 0.01
            2     0.257 0.01
            3     0.024 0.01
            4     0.026 0.01
VAL_U 2,3,4,5     0     0.59  0.024
            1     0.104 0.024
            2     0.245 0.024
            3     0.034 0.024
            4     0.026 0.024
LEU_U 1,2,3,4,5,6 0     0.436 0.02
            1     0.138 0.02
            2     0.299 0.02
            3     0.055 0.02
            4     0.062 0.02
            5     0.007 0.02
            6     0.004 0.02
LEU_U 1,2,3,4,5,6 0     0.438 0.012
            1     0.132 0.012
            2     0.305 0.012
            3     0.053 0.012
            4     0.063 0.012
            5     0.005 0.012
            6     0.004 0.012
LEU_U 2,3,4,5,6   0     0.472 0.017
            1     0.197 0.017
            2     0.227 0.017
            3     0.071 0.017
            4     0.028 0.017
            5     0.006 0.017
ILE_U 1,2,3,4,5,6 0     0.427 0.018
            1     0.215 0.018
            2     0.211 0.018
            3     0.09  0.018
            4     0.043 0.018
```

```
            5     0.014 0.018
            6     0     0.018
ILE_U 2,3,4,5,6   0     0.488 0.01
            1     0.206 0.01
            2     0.202 0.01
            3     0.076 0.01
            4     0.022 0.01
            5     0.006 0.01
ILE_U 2,3,4,5,6   0     0.491 0.02
            1     0.202 0.02
            2     0.202 0.02
            3     0.075 0.02
            4     0.022 0.02
            5     0.007 0.02
GLU_U 2,3,4,5     0     0.546 0.019
            1     0.216 0.019
            2     0.178 0.019
            3     0.043 0.019
            4     0.015 0.019
METeff_U    1,2,3,4,5   0     0.469 0.012
            1     0.265 0.01
            2     0.128 0.01
            3     0.088 0.01
            4     0.034 0.01
            5     0.016 0.01
METeff_U    1,2,3,4,5   0     0.485 0.01
            1     0.264 0.01
            2     0.13  0.01
            3     0.082 0.01
            4     0.033 0.01
            5     0.007 0.01
METeff_U    2,3,4,5     0     0.552 0.013
            1     0.257 0.013
            2     0.105 0.013
            3     0.074 0.013
            4     0.013 0.013
METeff_U    2,3,4,5     0     0.555 0.011
            1     0.257 0.011
            2     0.105 0.011
            3     0.072 0.011
            4     0.01  0.011
SEReff_U    1,2,3 0     0.655 0.01
            1     0.178 0.01
            2     0.076 0.01
            3     0.091 0.01
SEReff_U    1,2,3 0     0.658 0.01
            1     0.179 0.01
            2     0.076 0.01
            3     0.087 0.01
SEReff_U    2,3   0     0.711 0.01
            1     0.175 0.01
            2     0.114 0.01
SEReff_U    2,3   0     0.714 0.011
```

```
            1     0.174 0.011
            2     0.112 0.011
SEReff_U    1,2   0     0.73  0.018
            1     0.14  0.018
            2     0.13  0.018
THR_U 1,2,3,4     0     0.56  0.01
            1     0.213 0.01
            2     0.138 0.01
            3     0.072 0.01
            4     0.016 0.01
THR_U 2,3,4 0     0.625 0.01
            1     0.216 0.01
            2     0.112 0.01
            3     0.047 0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.359 0.015
            1     0.159 0.015
            2     0.138 0.015
            3     0.171 0.015
            4     0.083 0.015
            5     0.045 0.015
            6     0.029 0.015
            7     0.011 0.015
            8     0.004 0.015
            9     0.002 0.015
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.378 0.018
            1     0.151 0.018
            2     0.206 0.018
            3     0.12  0.018
            4     0.079 0.018
            5     0.039 0.018
            6     0.02  0.018
            7     0.005 0.018
            8     0.002 0.018
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.379 0.019
            1     0.152 0.019
            2     0.206 0.019
            3     0.121 0.019
            4     0.078 0.019
            5     0.039 0.019
            6     0.021 0.019
            7     0.005 0.019
            8     0.002 0.019
PHE_TYR_U   1,2   0     0.754 0.01
            1     0.095 0.01
            2     0.152 0.01
ASP_U 1,2,3,4     0     0.554 0.011
            1     0.215 0.011
            2     0.145 0.011
            3     0.069 0.011
            4     0.016 0.011
ASP_U 1,2,3,4     0     0.562 0.011
            1     0.21  0.011
            2     0.142 0.011
```

	3	0.068	0.011
	4	0.018	0.011
ASP_U 2,3,4	0	0.624	0.01
	1	0.217	0.01
	2	0.114	0.01
	3	0.045	0.01
ASP_U 2,3,4	0	0.62	0.018
	1	0.216	0.018
	2	0.116	0.018
	3	0.048	0.018
ASP_U 1,2	0	0.729	0.011
	1	0.159	0.011
	2	0.112	0.011
CYS_U 1,2,3	0	0.688	0.018
	1	0.157	0.018
	2	0.076	0.018
	3	0.079	0.018
CYS_U 2,3	0	0.717	0.01
	1	0.168	0.01
	2	0.114	0.01
GLU_U 1,2,3,4,5	0	0.471	0.023
	1	0.223	0.023
	2	0.212	0.023
	3	0.075	0.023
	4	0.018	0.023
	5	0.001	0.023
GLU_U 2,3,4,5	0	0.538	0.01
	1	0.216	0.01
	2	0.194	0.01
	3	0.041	0.01
	4	0.011	0.01
GLU_U 2,3,4,5	0	0.54	0.011
	1	0.214	0.011
	2	0.19	0.011
	3	0.043	0.011
	4	0.013	0.011
LYS_U 1,2,3,4,5,6	0	0.449	0.01
	1	0.206	0.01
	2	0.17	0.01
	3	0.114	0.01
	4	0.041	0.01
	5	0.015	0.01
	6	0.004	0.01
LYS_U 1,2,3,4,5,6	0	0.431	0.01
	1	0.22	0.01
	2	0.178	0.01
	3	0.112	0.01
	4	0.036	0.01
	5	0.017	0.01
	6	0.005	0.01
LYS_U 1,2,3,4,5,6	0	0.442	0.01
	1	0.214	0.01
	2	0.172	0.01

		3	0.114	0.01
		4	0.04	0.01
		5	0.015	0.01
		6	0.004	0.01
LYS_U	2,3,4,5,6	0	0.484	0.01
		1	0.211	0.01
		2	0.206	0.01
		3	0.074	0.01
		4	0.021	0.01
		5	0.004	0.01
ARGeff_U	1,2,3,4,5,6	0	0.428	0.013
		1	0.253	0.013
		2	0.184	0.013
		3	0.106	0.013
		4	0.038	0.013
		5	0.002	0.013
		6	-0.012	0.013
ARGeff_U	1,2,3,4,5,6	0	0.419	0.01
		1	0.25	0.01
		2	0.196	0.01
		3	0.097	0.01
		4	0.029	0.01
		5	0.011	0.01
		6	-0.002	0.01
ARGeff_U	2,3,4,5,6	0	0.439	0.01
		1	0.273	0.01
		2	0.2	0.01
		3	0.067	0.01
		4	0.023	0.01
		5	-0.001	0.01
ARGeff_U	2,3,4,5,6	0	0.469	0.01
		1	0.265	0.01
		2	0.187	0.01
		3	0.067	0.01
		4	0.015	0.01
		5	-0.003	0.01
HISeff_U	1,2,3,4,5,6	0	0.467	0.011
		1	0.236	0.011
		2	0.111	0.011
		3	0.105	0.011
		4	0.038	0.011
		5	0.037	0.011
		6	0.006	0.011
HISeff_U	1,2,3,4,5,6	0	0.47	0.013
		1	0.232	0.013
		2	0.118	0.013
		3	0.104	0.013
		4	0.046	0.013
		5	0.026	0.013
		6	0.004	0.013
HISeff_U	2,3,4,5,6	0	0.499	0.021
		1	0.253	0.015
		2	0.166	0.014

```
            3     0.067 0.015
            4     0.018 0.016
            5     -0.004      0.017
HISeff_U    2,3,4,5,6   0     0.472 0.023
            1     0.241 0.023
            2     0.18  0.023
            3     0.073 0.023
            4     0.03  0.023
            5     0.004 0.023
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.354 0.01
            1     0.156 0.01
            2     0.145 0.01
            3     0.169 0.01
            4     0.082 0.01
            5     0.05  0.01
            6     0.03  0.01
            7     0.011 0.01
            8     0.004 0.01
            9     0     0.01
PHE_TYR_U   1,2,3,4,5,6,7,8,9 0     0.364 0.023
            1     0.158 0.023
            2     0.138 0.023
            3     0.167 0.023
            4     0.081 0.023
            5     0.045 0.023
            6     0.029 0.023
            7     0.011 0.023
            8     0.005 0.023
            9     0.003 0.023
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.379 0.01
            1     0.152 0.01
            2     0.209 0.01
            3     0.117 0.01
            4     0.08  0.01
            5     0.038 0.01
            6     0.02  0.01
            7     0.004 0.01
            8     0.001 0.01
PHE_TYR_U   2,3,4,5,6,7,8,9   0     0.371 0.01
            1     0.154 0.01
            2     0.209 0.01
            3     0.122 0.01
            4     0.081 0.01
            5     0.039 0.01
            6     0.019 0.01
            7     0.004 0.01
            8     0.002 0.01
PHE_TYR_U   1,2   0     0.751 0.01
            1     0.096 0.01
            2     0.153 0.01
GLU_U 2,3,4,5     0     0.54  0.019
            1     0.214 0.011
            2     0.193 0.011
```

		3	0.041	0.013
		4	0.012	0.014
STA	1,2	0	0.37	0.01
		1	0.633	0.01
		2	-0.003	0.01
STA	3,4,5,6	0	0.704	0.015
		1	0.265	0.015
		2	0.03	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.382	0.01
		1	0.618	0.014
		2	0	0.015
STA	3,4,5,6	0	0.715	0.012
		1	0.259	0.012
		2	0.026	0.012
		3	0	0.012
		4	0	0.012
STA	1,2	0	0.385	0.01
		1	0.619	0.01
		2	-0.004	0.01
STA	3,4,5,6	0	0.711	0.015
		1	0.26	0.015
		2	0.028	0.015
		3	0.001	0.015
		4	0	0.015
STA	1,2	0	0.397	0.01
		1	0.611	0.014
		2	-0.007	0.015
STA	3,4,5,6	0	0.713	0.012
		1	0.256	0.012
		2	0.029	0.012
		3	0.002	0.012
		4	0.001	0.012
STA	1,2	0	0.386	0.01
		1	0.619	0.01
		2	-0.005	0.01
STA	3,4,5,6	0	0.714	0.015
		1	0.259	0.015
		2	0.026	0.015
		3	0.001	0.015
		4	-0.001	0.015
STA	1,2	0	0.4	0.01
		1	0.602	0.011
		2	-0.003	0.012
STA	3,4,5,6	0	0.712	0.012
		1	0.259	0.012
		2	0.026	0.012
		3	0.002	0.012
		4	0.002	0.012
STA_U	1,2	0	0.741	0.018
		1	0.102	0.014
		2	0.157	0.013

STA_U	3,4,5,6	0	0.626	0.015
		1	0.159	0.015
		2	0.033	0.015
		3	0.093	0.015
		4	0.088	0.015
STA_U	1,2	0	0.75	0.027
		1	0.105	0.021
		2	0.145	0.02
STA_U	3,4,5,6	0	0.639	0.012
		1	0.153	0.012
		2	0.032	0.012
		3	0.09	0.012
		4	0.086	0.012
STA_U	1,2	0	0.742	0.017
		1	0.104	0.013
		2	0.154	0.012
STA_U	3,4,5,6	0	0.627	0.015
		1	0.16	0.015
		2	0.034	0.015
		3	0.093	0.015
		4	0.087	0.015
STA_U	1,2	0	0.749	0.027
		1	0.106	0.02
		2	0.144	0.019
STA_U	3,4,5,6	0	0.641	0.012
		1	0.154	0.012
		2	0.031	0.012
		3	0.09	0.012
		4	0.083	0.012
STA_U	1,2	0	0.761	0.017
		1	0.099	0.013
		2	0.139	0.012
STA_U	3,4,5,6	0	0.642	0.015
		1	0.164	0.015
		2	0.037	0.015
		3	0.089	0.015
		4	0.068	0.015
STA_U	1,2	0	0.755	0.028
		1	0.105	0.021
		2	0.14	0.02
STA_U	3,4,5,6	0	0.65	0.012
		1	0.152	0.012
		2	0.03	0.012
		3	0.088	0.012
		4	0.081	0.012
WALL	3,4,5,6	0	0.711	0.015
		1	0.26	0.015
		2	0.028	0.015
		3	0.001	0.015
		4	0	0.015
WALL	3,4,5,6	0	0.731	0.012
		1	0.244	0.012
		2	0.025	0.012

		3	0	0.012
		4	0	0.012
WALL	3,4,5,6	0	0.74	0.015
		1	0.236	0.015
		2	0.023	0.015
		3	0.001	0.015
		4	0	0.015
WALL	3,4,5,6	0	0.747	0.012
		1	0.23	0.012
		2	0.023	0.012
		3	-0.001	0.012
		4	0.002	0.012
WALL	3,4,5,6	0	0.719	0.015
		1	0.255	0.015
		2	0.025	0.015
		3	0.002	0.015
		4	0	0.015
WALL	3,4,5,6	0	0.736	0.012
		1	0.237	0.012
		2	0.024	0.012
		3	0.003	0.012
		4	0.001	0.012
WALL_U	3,4,5,6	0	0.64	0.015
		1	0.153	0.015
		2	0.03	0.015
		3	0.09	0.015
		4	0.087	0.015
WALL_U	3,4,5,6	0	0.653	0.012
		1	0.142	0.012
		2	0.029	0.012
		3	0.083	0.012
		4	0.093	0.012
WALL_U	3,4,5,6	0	0.633	0.015
		1	0.156	0.015
		2	0.031	0.015
		3	0.092	0.015
		4	0.088	0.015
WALL_U	3,4,5,6	0	0.649	0.012
		1	0.147	0.012
		2	0.029	0.012
		3	0.08	0.012
		4	0.094	0.012
WALL_U	3,4,5,6	0	0.646	0.015
		1	0.152	0.015
		2	0.03	0.015
		3	0.088	0.015
		4	0.084	0.015
WALL_U	3,4,5,6	0	0.659	0.012
		1	0.14	0.012
		2	0.029	0.012
		3	0.079	0.012
		4	0.093	0.012
FSUC	4,5,6	0	0.763	0.014

		1	0.225	0.014	
		2	0.011	0.014	
		3	0	0.014	
FSUC	4,5,6	0	0.782	0.025	
		1	0.223	0.013	
		2	0.004	0.016	
		3	-0.009		0.017
FSUC	1,2,3,	4	0	0.298	0.013
		1	0.664	0.013	
		2	0.039	0.013	
		3	0.001	0.013	
		4	-0.001		0.013
FSUC	4,5,6	0	0.766	0.013	
		1	0.224	0.013	
		2	0.011	0.013	
		3	0	0.013	
FSUC	4,5,6	0	0.768	0.027	
		1	0.238	0.014	
		2	0.004	0.017	
		3	-0.01	0.018	
FSUC	1,2,3,	4	0	0.302	0.011
		1	0.669	0.011	
		2	0.039	0.011	
		3	-0.005		0.011
		4	-0.004		0.011
FSUC	4,5,6	0	0.767	0.014	
		1	0.223	0.014	
		2	0.011	0.014	
		3	0	0.014	
FSUC	4,5,6	0	0.785	0.025	
		1	0.22	0.013	
		2	0.004	0.016	
		3	-0.009		0.017
FSUC	1,2,3,	4	0	0.296	0.013
		1	0.666	0.013	
		2	0.041	0.013	
		3	-0.001		0.013
		4	-0.002		0.013
FSUC	4,5,6	0	0.769	0.013	
		1	0.223	0.013	
		2	0.009	0.013	
		3	-0.001		0.013
FSUC	4,5,6	0	0.766	0.029	
		1	0.237	0.015	
		2	0.005	0.019	
		3	-0.008		0.02
FSUC	1,2,3,	4	0	0.298	0.011
		1	0.671	0.011	
		2	0.038	0.011	
		3	-0.003		0.011
		4	-0.004		0.011
FSUC	4,5,6	0	0.767	0.014	
		1	0.222	0.014	

```
            2     0.011 0.014
            3     0     0.014
FSUC  4,5,6 0     0.784 0.025
            1     0.223 0.012
            2     0.003 0.016
            3     -0.009      0.016
FSUC  1,2,3,4     0     0.3   0.013
            1     0.665 0.013
            2     0.038 0.013
            3     -0.003      0.013
            4     0     0.013
FSUC  4,5,6 0     0.768 0.013
            1     0.222 0.013
            2     0.011 0.013
            3     0     0.013
FSUC  4,5,6 0     0.764 0.03
            1     0.239 0.016
            2     0.004 0.02
            3     -0.007      0.021
FSUC  1,2,3,4     0     0.303 0.011
            1     0.668 0.011
            2     0.039 0.011
            3     -0.007      0.011
            4     -0.003      0.011
FSUC_U      4,5,6 0     0.747 0.014
            1     0.056 0.014
            2     0.025 0.014
            3     0.171 0.014
FSUC_U      4,5,6 0     0.767 0.016
            1     0.05  0.01
            2     0.018 0.011
            3     0.165 0.01
FSUC_U      1,2,3,4     0     0.626 0.013
            1     0.164 0.013
            2     0.062 0.013
            3     0.063 0.013
            4     0.085 0.013
FSUC_U      4,5,6 0     0.748 0.013
            1     0.056 0.013
            2     0.026 0.013
            3     0.17  0.013
FSUC_U      4,5,6 0     0.764 0.019
            1     0.054 0.011
            2     0.02  0.012
            3     0.162 0.01
FSUC_U      1,2,3,4     0     0.63  0.011
            1     0.165 0.011
            2     0.059 0.011
            3     0.062 0.011
            4     0.083 0.011
FSUC_U      4,5,6 0     0.747 0.014
            1     0.057 0.014
            2     0.026 0.014
```

	3	0.171	0.014	
FSUC_U	4,5,6	0	0.769	0.017
	1	0.049	0.01	
	2	0.018	0.011	
	3	0.164	0.01	
FSUC_U	1,2,3,4	0	0.624	0.013
	1	0.165	0.013	
	2	0.064	0.013	
	3	0.063	0.013	
	4	0.084	0.013	
FSUC_U	4,5,6	0	0.75	0.013
	1	0.055	0.013	
	2	0.025	0.013	
	3	0.17	0.013	
FSUC_U	4,5,6	0	0.764	0.02
	1	0.054	0.012	
	2	0.02	0.013	
	3	0.161	0.011	
FSUC_U	1,2,3,4	0	0.628	0.011
	1	0.166	0.011	
	2	0.059	0.011	
	3	0.061	0.011	
	4	0.085	0.011	
FSUC_U	4,5,6	0	0.749	0.014
	1	0.056	0.014	
	2	0.026	0.014	
	3	0.17	0.014	
FSUC_U	4,5,6	0	0.769	0.016
	1	0.05	0.01	
	2	0.019	0.01	
	3	0.163	0.01	
FSUC_U	1,2,3,4	0	0.622	0.013
	1	0.169	0.013	
	2	0.06	0.013	
	3	0.065	0.013	
	4	0.084	0.013	
FSUC_U	4,5,6	0	0.749	0.013
	1	0.057	0.013	
	2	0.025	0.013	
	3	0.169	0.013	
FSUC_U	4,5,6	0	0.766	0.019
	1	0.054	0.012	
	2	0.02	0.012	
	3	0.16	0.01	
FSUC_U	1,2,3,4	0	0.627	0.011
	1	0.166	0.011	
	2	0.062	0.011	
	3	0.063	0.011	
	4	0.082	0.011	
PENTAN	5	0	0.992	0.01
	1	0.008	0.01	
PENTAN	3,4,5	0	0.921	0.042
	1	0.092	0.02	

		2	-0.005	0.022
		3	-0.008	0.023
PENTAN	3,4,5	0	0.923	0.01
		1	0.076	0.01
		2	0.002	0.01
		3	-0.001	0.01
PENTAN	5	0	0.986	0.015
		1	0.014	0.015
PENTAN	3,4,5	0	0.914	0.03
		1	0.095	0.016
		2	-0.001	0.016
		3	-0.008	0.017
PENTAN	3,4,5	0	0.933	0.01
		1	0.075	0.01
		2	0.002	0.01
		3	-0.01	0.01
PENTAN	5	0	0.994	0.01
		1	0.006	0.01
PENTAN	3,4,5	0	0.934	0.029
		1	0.091	0.029
		2	-0.01	0.029
		3	-0.015	0.029
PENTAN	3,4,5	0	0.925	0.01
		1	0.075	0.01
		2	0	0.01
		3	0	0.01
WALL	3,4,5,6	0	0.743	0.011
		1	0.24	0.011
		2	0.022	0.011
		3	-0.004	0.011
		4	0	0.011
WALL	3,4,5,6	0	0.745	0.012
		1	0.233	0.012
		2	0.021	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN	5	0	0.991	0.01
		1	0.009	0.01
PENTAN	3,4,5	0	0.917	0.04
		1	0.095	0.02
		2	-0.004	0.021
		3	-0.008	0.022
PENTAN	3,4,5	0	0.925	0.01
		1	0.074	0.01
		2	0.001	0.01
		3	0	0.01
PENTAN	5	0	0.985	0.015
		1	0.015	0.015
PENTAN	3,4,5	0	0.922	0.034
		1	0.088	0.016
		2	0.005	0.017
		3	-0.015	0.018
PENTAN	3,4,5	0	0.928	0.01

		1	0.071	0.01
		2	0.003	0.01
		3	-0.003	0.01
PENTAN	5	0	0.993	0.01
		1	0.007	0.01
PENTAN	3,4,5	0	0.926	0.032
		1	0.092	0.029
		2	-0.006	0.029
		3	-0.012	0.029
PENTAN	3,4,5	0	0.925	0.01
		1	0.077	0.01
		2	-0.002	0.01
		3	0.001	0.01
WALL	3,4,5,6	0	0.746	0.011
		1	0.232	0.011
		2	0.018	0.011
		3	0.002	0.011
		4	0	0.011
WALL	3,4,5,6	0	0.748	0.012
		1	0.23	0.012
		2	0.021	0.012
		3	0.001	0.012
		4	0	0.012
PENTAN	5	0	0.992	0.01
		1	0.008	0.01
PENTAN	3,4,5	0	0.918	0.041
		1	0.094	0.02
		2	-0.004	0.022
		3	-0.007	0.022
PENTAN	3,4,5	0	0.923	0.01
		1	0.075	0.01
		2	0.002	0.01
		3	-0.001	0.01
PENTAN	5	0	0.985	0.015
		1	0.015	0.015
PENTAN	3,4,5	0	0.914	0.031
		1	0.095	0.016
		2	0	0.016
		3	-0.009	0.017
PENTAN	3,4,5	0	0.92	0.01
		1	0.076	0.01
		2	0.003	0.01
		3	0.001	0.01
PENTAN	5	0	0.993	0.01
		1	0.007	0.01
PENTAN	3,4,5	0	0.923	0.01
		1	0.075	0.01
		2	0.001	0.01
		3	0	0.01
WALL	3,4,5,6	0	0.728	0.011
		1	0.243	0.011
		2	0.026	0.011
		3	0.002	0.011

	4	0	0.011		
WALL 3,4,5,6	0	0.747	0.012		
	1	0.232	0.012		
	2	0.02	0.012		
	3	0.001	0.012		
	4	0	0.012		
PENTAN_U	5	0	0.795	0.01	
	1	0.205	0.01		
PENTAN_U	3,4,5	0	0.668	0.02	
	1	0.15	0.02		
	2	0.08	0.02		
	3	0.102	0.02		
PENTAN_U	3,4,5	0	0.675	0.01	
	1	0.138	0.01		
	2	0.082	0.01		
	3	0.104	0.01		
PENTAN_U	5	0	0.79	0.015	
	1	0.21	0.015		
PENTAN_U	3,4,5	0	0.679	0.029	
	1	0.142	0.017		
	2	0.083	0.018		
	3	0.097	0.018		
PENTAN_U	3,4,5	0	0.672	0.01	
	1	0.132	0.01		
	2	0.087	0.01		
	3	0.108	0.01		
PENTAN_U	5	0	0.794	0.01	
	1	0.206	0.01		
PENTAN_U	3,4,5	0	0.662	0.029	
	1	0.155	0.029		
	2	0.08	0.029		
	3	0.103	0.029		
PENTAN_U	3,4,5	0	0.673	0.01	
	1	0.137	0.01		
	2	0.083	0.01		
	3	0.107	0.01		
WALL_U	3,4,5,6		0	0.651	0.011
	1	0.144	0.011		
	2	0.03	0.011		
	3	0.076	0.011		
	4	0.099	0.011		
WALL_U	3,4,5,6		0	0.661	0.012
	1	0.134	0.012		
	2	0.026	0.012		
	3	0.076	0.012		
	4	0.103	0.012		
PENTAN_U	5	0	0.795	0.01	
	1	0.205	0.01		
PENTAN_U	3,4,5	0	0.669	0.02	
	1	0.151	0.02		
	2	0.078	0.02		
	3	0.102	0.02		
PENTAN_U	3,4,5	0	0.677	0.01	

	1	0.138	0.01		
	2	0.081	0.01		
	3	0.104	0.01		
PENTAN_U	5	0	0.796	0.015	
	1	0.204	0.015		
PENTAN_U	3,4,5	0	0.659	0.025	
	1	0.154	0.016		
	2	0.089	0.016		
	3	0.098	0.016		
PENTAN_U	3,4,5	0	0.668	0.01	
	1	0.138	0.01		
	2	0.087	0.01		
	3	0.107	0.01		
PENTAN_U	5	0	0.794	0.01	
	1	0.206	0.01		
PENTAN_U	3,4,5	0	0.664	0.029	
	1	0.154	0.029		
	2	0.081	0.029		
	3	0.101	0.029		
PENTAN_U	3,4,5	0	0.674	0.01	
	1	0.144	0.01		
	2	0.081	0.01		
	3	0.101	0.01		
WALL_U	3,4,5,6		0	0.658	0.011
	1	0.135	0.011		
	2	0.028	0.011		
	3	0.076	0.011		
	4	0.103	0.011		
WALL_U	3,4,5,6		0	0.66	0.012
	1	0.135	0.012		
	2	0.028	0.012		
	3	0.075	0.012		
	4	0.102	0.012		
PENTAN_U	5	0	0.792	0.01	
	1	0.208	0.01		
PENTAN_U	3,4,5	0	0.656	0.02	
	1	0.161	0.02		
	2	0.084	0.02		
	3	0.098	0.02		
PENTAN_U	3,4,5	0	0.664	0.01	
	1	0.148	0.01		
	2	0.087	0.01		
	3	0.101	0.01		
PENTAN_U	5	0	0.796	0.015	
	1	0.204	0.015		
PENTAN_U	3,4,5	0	0.649	0.019	
	1	0.164	0.016		
	2	0.095	0.016		
	3	0.092	0.016		
PENTAN_U	3,4,5	0	0.682	0.01	
	1	0.142	0.01		
	2	0.083	0.01		
	3	0.093	0.01		

PENTAN_U	5	0	0.794	0.01
	1	0.206	0.01	
PENTAN_U	3,4,5	0	0.657	0.029
	1	0.167	0.029	
	2	0.084	0.029	
	3	0.092	0.029	
PENTAN_U	3,4,5	0	0.664	0.011
	1	0.15	0.01	
	2	0.086	0.01	
	3	0.1	0.01	
WALL_U	3,4,5,6	0	0.655	0.011
	1	0.147	0.011	
	2	0.021	0.011	
	3	0.084	0.011	
	4	0.093	0.011	
WALL_U	3,4,5,6	0	0.659	0.012
	1	0.137	0.012	
	2	0.027	0.012	
	3	0.079	0.012	
	4	0.099	0.012	

Appendix 5.11. Coenzyme demand and supply reaction stoichiometries

Coenzyme demand

With the exception of the sterols, reaction stoichiometries were taken from Masakapalli et al., 2010. An additional four molecules of ATP was required for each peptide bond. The stoichiometries assume equal assimilation of NH_4^+ and NO_3^-.

Metabolite		Coenzyme requirement (mol (mol precursor)$^{-1}$) ATP	NADH	NADPH
Amino acids	Alanine	**1**	**0.5**	**2.5**
	Arginine	**9**	**0.5**	**8.5**
	Asparagine	**4**	**1**	**4**
	Aspartate	**4**	**1**	**4**
	Cysteine	**6**	**-0.5**	**6.5**
	Glutamate	**2**	**1**	**4**
	Glutamine	**2**	**1**	**4**
	Glycine	**1**	**0.5**	**2.5**
	Histidine	**7**	**-2**	**6**
	Isoleucine	**4**	**1**	**8**
	Leucine	**1**	**-0.5**	**3.5**
	Lysine	**4**	**1**	**7**
	Methionine	**10**	**-0.5**	**9.5**
	Phenylalanine	**2**	**0.5**	**3.5**
	Proline	**2**	**0.5**	**4.5**
	Pyroglutamate	**2**	**1**	**4**
	Serine	**1**	**0.5**	**2.5**
	Threonine	**3**	**0.5**	**4.5**
	Tryptophan	**5**	**0.5**	**3.5**
	Tyrosine	**2**	**-0.5**	**3.5**
	Valine	**1**	**0.5**	**2.5**
Cell wall	Hexosyl unit	**1**	**0**	**0**
	Pentosyl unit	**1**	**-2**	**0**
Ethanol		**0**	**1**	**0**
Lipids	Acyl chain	**1**	**1**	**1**
	Glycerol unit	**0**	**1**	**0**
Starch		**1**	**0**	**0**
Sterols	24-methylene cholesterol	**18**	**0**	**18**
	Δ5-avenasterol	**18**	**0**	**18**
	Campesterol	**18**	**0**	**19**
	Cholesterol	**18**	**0**	**20**
	Cycloartenol	**18**	**0**	**14**
	Fucosterol	**18**	**0**	**18**
	Sitosterol	**18**	**0**	**19**
	Stigmasterol	**18**	**0**	**20**
Sucrose		**1**	**0**	**0**

Coenzyme production

The table describes the supply of coenzymes by the reactions of central metabolism. This ignores synthesis of ATP by oxidative phosphorylation.

		Coenzyme production (mol (unit flux)$^{-1}$)		
Reaction	**Flux name**	**ATP**	**NADH**	**NADPH**
Cytosolic aldolase	Vald	-1	0	0
Cytosolic hexokinase	Vg	-1	0	0
Cytosolic oxidative pentose phosphate pathway	Vppp1	0	0	2
Cytosolic pyruvate kinase	Vpk	2	1	0
Mitochondrial Fumarase	Vfum1+2	0	1	0
Mitochondrial isocitrate dehydrogenase	Vicdh	0	1[a]/0[b]	0[a]/1[b]
Mitochondrial malic enzyme	Vme	1	0	0
Mitochondrial pyruvate dehydrogenase	Vpdh	0	1	0
Mitochondrial α-ketoglutarate dehydrogenase/succinyl-CoA synthetase	Vakgdh	0	1	0
Plastidial aldolase	Valdp	-1	0	0
Plastidial malic enzyme	Vmep	1	0	0
Plastidial oxidative pentose phosphate pathway	Vppp1_p	0	0	2
Plastidial pyruvate dehydrogenase	Vpdhp	0	1	0
Plastidial pyruvate kinase	Vpkp	2	1	0

[a]NAD^+-dependent isocitrate dehydrogenase.
[b]$NADP^+$-dependent isocitrate dehydrogenase.

Appendix 6.1. pBI121-*HMG1* expression vector sequence

The *HMG1* insert was confirmed by sequencing using primers pBI121-T-DNA-F, pBI121-ins-F, pBI121-ins-R, pBI121-ins-R2 and pBI121-T-DNA-R.

Bases	Feature
2371-2391	pBI121-T-DNA-F primer binding site
2454-2478	Right transfer DNA border
2519-2825	*Nopaline synthase* (*nos*) promoter
2838-3632	*nptII* (neomycin phosphotransferase II)
4022-4277	*nos* terminator
4974-5808	Cauliflower mosaic virus (CaMV) *35S* promoter
5739-5758	pBI121-ins-F primer binding site
5929-7707	*HMG1* (At1g76490/F15M4.1) coding sequence
5918-5937	At-HMG1-F primer binding site
6418-6436	ATG_At-tHMG1-F primer binding site
7700-7722	At-HMG1-R primer binding site (antiparallel sequence)
8107-8125	pBI121-ins-R primer binding site (antiparallel sequence)
8120-8372	*nos* terminator
8423-8443	pBI121-ins-R2 primer binding site (antiparallel sequence)
9014-9039	Left transfer DNA border
9136-9155	pBI121-T-DNA-R primer binding site (antiparallel sequence)

5' Base	Sequence
1	TGAGCGTCGCAAAGGCGCTCGGTCTTGCCTTGCTCGTCGGTGATGTACTTCACCAGCTCC
61	GCGAAGTCGCTCTTCTTGATGGAGCGCATGGGGACGTGCTTGGCAATCACGCGCACCCCC
121	CGGCCGTTTTAGCGGCTAAAAAAGTCATGGCTCTGCCCTCGGGCGGACCACGCCCATCAT
181	GACCTTGCCAAGCTCGTCCTGCTTCTCTTCGATCTTCGCCAGCAGGGCGAGGATCGTGGC
241	ATCACCGAACCGCGCCGTGCGCGGGTCGTCGGTGAGCCAGAGTTTCAGCAGGCCGCCCAG
301	GCGGCCCAGGTCGCCATTGATGCGGGCCAGCTCGCGGACGTGCTCATAGTCCACGACGCC
361	CGTGATTTTGTAGCCCTGGCCGACGGCCAGCAGGTAGGCCGACAGGCTCATGCCGGCCGC
421	CGCCGCCTTTTCCTCAATCGCTCTTCGTTCGTCTGGAAGGCAGTACACCTTGATAGGTGG
481	GCTGCCCTTCCTGGTTGGCTTGGTTTCATCAGCCATCCGCTTGCCCTCATCTGTTACGCC
541	GGCGGTAGCCGGCCAGCCTCGCAGAGCAGGATTCCCGTTGAGCACCGCCAGGTGCGAATA
601	AGGGACAGTGAAGAAGGAACACCCGCTCGCGGGTGGGCCTACTTCACCTATCCTGCCCGG
661	CTGACGCCGTTGGATACACCAAGGAAAGTCTACACGAACCCTTTGGCAAAATCCTGTATA
721	TCGTGCGAAAAAGGATGGATATACCGAAAAAATCGCTATAATGACCCCGAAGCAGGGTTA
781	TGCAGCGGAAAAGCGCCACGCTTCCCGAAGGGAGAAAGGCGGACAGGTATCCGGTAAGCG
841	GCAGGGTCGGAACAGGAGAGCGCACGAGGGAGCTTCCAGGGGGAAACGCCTGGTATCTTT
901	ATAGTCCTGTCGGGTTTCGCCACCTCTGACTTGAGCGTCGATTTTTGTGATGCTCGTCAG
961	GGGGGCGGAGCCTATGGAAAAACGCCAGCAACGCGGCCTTTTTACGGTTCCTGGCCTTTT
1021	GCTGGCCTTTTGCTCACATGTTCTTTCCTGCGTTATCCCCTGATTCTGTGGATAACCGTA
1081	TTACCGCCTTTGAGTGAGCTGATACCGCTCGCCGCAGCCGAACGACCGAGCGCAGCGAGT
1141	CAGTGAGCGAGGAAGCGGAAGAGCGCCAGAAGGCCGCCAGAGAGGCCGAGCGCGGCCGTG
1201	AGGCTTGGACGCTAGGGCAGGGCATGAAAAAGCCCGTAGCGGGCTGCTACGGGCGTCTGA
1261	CGCGGTGGAAAGGGGGAGGGGATGTTGTCTACATGGCTCTGCTGTAGTGAGTGGGTTGCG
1321	CTCCGGCAGCGGTCCTGATCAATCGTCACCCTTTCTCGGTCCTTCAACGTTCCTGACAAC
1381	GAGCCTCCTTTTCGCCAATCCATCGACAATCACCGCGAGTCCCTGCTCGAACGCTGCGTC
1441	CGGACCGGCTTCGTCGAAGGCGTCTATCGCGGCCCGCAACAGCGGCGAGAGCGGAGCCTG
1501	TTCAACGGTGCCGCCGCGCTCGCCGGCATCGCTGTCGCCGGCCTGCTCCTCAAGCACGGC
1561	CCCAACAGTGAAGTAGCTGATTGTCATCAGCGCATTGACGGCGTCCCCGGCCGAAAAACC

5' Base	Sequence
1621	CGCCTCGCAGAGGAAGCGAAGCTGCGCGTCGGCCGTTTCCATCTGCGGTGCGCCCGGTCG
1681	CGTGCCGGCATGGATGCGCGCGCCATCGCGGTAGGCGAGCAGCGCCTGCCTGAAGCTGCG
1741	GGCATTCCCGATCAGAAATGAGCGCCAGTCGTCGTCGGCTCTCGGCACCGAATGCGTATG
1801	ATTCTCCGCCAGCATGGCTTCGGCCAGTGCGTCGAGCAGCGCCCGCTTGTTCCTGAAGTG
1861	CCAGTAAAGCGCCGGCTGCTGAACCCCCAACCGTTCCGCCAGTTTGCGTGTCGTCAGACC
1921	GTCTACGCCGACCTCGTTCAACAGGTCCAGGGCGGCACGGATCACTGTATTCGGCTGCAA
1981	CTTTGTCATGCTTGACACTTTATCACTGATAAACATAATATGTCCACCAACTTATCAGTG
2041	ATAAAGAATCCGCGCGTTCAATCGGACCAGCGGAGGCTGGTCCGGAGGCCAGACGTGAAA
2101	CCCAACATACCCCTGATCGTAATTCTGAGCACTGTCGCGCTCGACGCTGTCGGCATCGGC
2161	CTGATTATGCCGGTGCTGCCGGGCCTCCTGCGCGATCTGGTTCACTCGAACGACGTCACC
2221	GCCCACTATGGCATTCTGCTGGCGCTGTATGCGTTGGTGCAATTTGCCTGCGCACCTGTG
2281	CTGGGCGCGCTGTCGGATCGTTTCGGGCGGCGGCCAATCTTGCTCGTCTCGCTGGCCGGC
2341	GCCAGATCTGGGGAACCCTGTGGTTGGCATGCACATACAAATGGACGAACGGATAAACCT
2401	TTTCACGCCCTTTTAAATATCCGATTATTCTAATAAACGCTCTTTTCTCTTAG**GTTTACC**
2461	**CGCCAATATATCCTGTCA**AACACTGATAGTTTAAACTGAAGGCGGGAAACGACAATCT**GA**
2521	**TCATGAGCGGAGAATTAAGGGAGTCACGTTATGACCCCCGCCGATGACGCGGGACAAGCC**
2581	**GTTTTACGTTTGGAACTGACAGAACCGCAACGTTGAAGGAGCCACTCAGCCGCGGGTTTC**
2641	**TGGAGTTTAATGAGCTAAGCACATACGTCAGAAACCATTATTGCGCGTTCAAAAGTCGCC**
2701	**TAAGGTCACTATCAGCTAGCAAATATTTCTTGTCAAAAATGCTCCACTGACGTTCCATAA**
2761	**ATTCCCCTCGGTATCCAATTAGAGTCTCATATTCACTCTCAATCCAAATAATCTGCACCG**
2821	**GATCT**GGATCGTTTCGC**ATGATTGAACAAGATGGATTGCACGCAGGTTCTCCGGCCGCTT**
2881	**GGGTGGAGAGGCTATTCGGCTATGACTGGGCACAACAGACAATCGGCTGCTCTGATGCCG**
2941	**CCGTGTTCCGGCTGTCAGCGCAGGGGCGCCCGGTTCTTTTTGTCAAGACCGACCTGTCCG**
3001	**GTGCCCTGAATGAACTGCAGGACGAGGCAGCGCGGCTATCGTGGCTGGCCACGACGGGCG**
3061	**TTCCTTGCGCAGCTGTGCTCGACGTTGTCACTGAAGCGGGAAGGGACTGGCTGCTATTGG**
3121	**GCGAAGTGCCGGGGCAGGATCTCCTGTCATCTCACCTTGCTCCTGCCGAGAAAGTATCCA**
3181	**TCATGGCTGATGCAATGCGGCGGCTGCATACGCTTGATCCGGCTACCTGCCCATTCGACC**
3241	**ACCAAGCGAAACATCGCATCGAGCGAGCACGTACTCGGATGGAAGCCGGTCTTGTCGATC**
3301	**AGGATGATCTGGACGAAGAGCATCAGGGGCTCGCGCCAGCCGAACTGTTCGCCAGGCTCA**
3361	**AGGCGCGCATGCCCGACGGCGATGATCTCGTCGTGACCCATGGCGATGCCTGCTTGCCGA**
3421	**ATATCATGGTGGAAAATGGCCGCTTTTCTGGATTCATCGACTGTGGCCGGCTGGGTGTGG**
3481	**CGGACCGCTATCAGGACATAGCGTTGGCTACCCGTGATATTGCTGAAGAGCTTGGCGGCG**
3541	**AATGGGCTGACCGCTTCCTCGTGCTTTACGGTATCGCCGCTCCCGATTCGCAGCGCATCG**
3601	**CCTTCTATCGCCTTCTTGACGAGTTCTTCTGA**GCGGGACTCTGGGGTTCGAAATGACCGA
3661	CCAAGCGACGCCCAACCTGCCATCACGAGATTTCGATTCCACCGCCGCCTTCTATGAAAG
3721	GTTGGGCTTCGGAATCGTTTTCCGGGACGCCGGCTGGATGATCCTCCAGCGCGGGGATCT
3781	CATGCTGGAGTTCTTCGCCCACGGGATCTCTGCGGAACAGGCGGTCGAAGGTGCCGATAT
3841	CATTACGACAGCAACGGCCGACAAGCACAACGCCACGATCCTGAGCGACAATATGATCGG
3901	GCCCGGCGTCCACATCAACGGCGTCGGCGGCGACTGCCCAGGCAAGACCGAGATGCACCG
3961	CGATATCTTGCTGCGTTCGGATATTTTCGTGGAGTTCCCGCCACAGACCCGGATGATCCC
4021	C**GATCGTTCAAACATTTGGCAATAAAGTTTCTTAAGATTGAATCCTGTTGCCGGTCTTGC**
4081	**GATGATTATCATATAATTTCTGTTGAATTACGTTAAGCATGTAATAATTAACATGTAATG**
4141	**CATGACGTTATTTATGAGATGGGTTTTTATGATTAGAGTCCCGCAATTATACATTTAATA**
4201	**CGCGATAGAAAACAAAATATAGCGCGCAAACTAGGATAAATTATCGCGCGCGGTGTCATC**
4261	**TATGTTACTAGATCGGG**CCTCCTGTCAATGCTGGCGGCGGCTCTGGTGGTGGTTCTGGTG
4321	GCGGCTCTGAGGGTGGTGGCTCTGAGGGTGGCGGTTCTGAGGGTGGCGGCTCTGAGGGAG
4381	GCGGTTCCGGTGGTGGCTCTGGTTCCGGTGATTTTGATTATGAAAAGATGGCAAACGCTA
4441	ATAAGGGGGCTATGACCGAAAATGCCGATGAAAACGCGCTACAGTCTGACGCTAAAGGCA
4501	AACTTGATTCTGTCGCTACTGATTACGGTGCTGCTATCGATGGTTTCATTGGTGACGTTT
4561	CCGGCCTTGCTAATGGTAATGGTGCTACTGGTGATTTTGCTGGCTCTAATTCCCAAATGG
4621	CTCAAGTCGGTGACGGTGATAATTCACCTTTAATGAATAATTTCCGTCAATATTTACCTT
4681	CCCTCCCTCAATCGGTTGAATGTCGCCCTTTTGTCTTTGGCCCAATACGCAAACCGCCTC
4741	TCCCCGCGCGTTGGCCGATTCATTAATGCAGCTGGCACGACAGGTTTCCCGACTGGAAAG
4801	CGGGCAGTGAGCGCAACGCAATTAATGTGAGTTAGCTCACTCATTAGGCACCCCAGGCTT
4861	TACACTTTATGCTTCCGGCTCGTATGTTGTGTGGAATTGTGAGCGGATAACAATTTCACA
4921	CAGGAAACAGCTATGACCATGATTACGCCAAGCTTGCATGCCTGCAGGTCCCCAGATTAG
4981	CCTTTTCAATTTCAGAAAGAATGCTAACCCACAGATGGTTAGAGAGGCTTACGCAGCAGG
5041	TCTCATCAAGACGATCTACCCGAGCAATAATCTCCAGGAAATCAAATACCTTCCCAAGAA
5101	GGTTAAAGATGCAGTCAAAAGATTCAGGACTAACTGCATCAAGAACACAGAGAAAGATAT

5' Base	Sequence
5161	ATTTCTCAAGATCAGAAGTACTATTCCAGTATGGACGATTCAAGGCTTGCTTCACAAACC
5221	AAGGCAAGTAATAGAGATTGGAGTCTCTAAAAAGGTAGTTCCCACTGAATCAA**AGGCCAT**
5281	**GGAGTCAAAGATTCAAATAGAGGACCTAACAGAACTCGCCGTAAAGACTGGCGAACAGTT**
5341	**CATACAGAGTCTCTTACGACTCAATGACAAGAAGAAAATCTTCGTCAACATGGTGGAGCA**
5401	**CGACACACTTGTCTACTCCAAAAATATCAAAGATACAGTCTCAGAAGACCAAAGGGCAAT**
5461	**TGAGACTTTTCAACAAAGGGTAATATCCGGAAACCTCCTCGGATTCCATTGCCCAGCTAT**
5521	**CTGTCACTTTATTGTGAAGATAGTGGAAAAGGAAGGTGGCTCCTACAAATGCCATCATTG**
5581	**CGATAAAGGAAAGGCCATCGTTGAAGATGCCTCTGCCGACAGTGGTCCCAAAGATGGACC**
5641	**CCCACCCACGAGGAGCATCGTGGAAAAAGAAGACGTTCCAACCACGTCTTCAAAGCAAGT**
5701	**GGATTGATGTGATATCTCCACTGACGTAAGGGATGACGCACAATCCCACTATCCTTCGCA**
5761	**AGACCCTTCCTCTATATAAGGAAGTTCATTTCATTTGGAGAGAACACG**GGGGACTCTAGA
5821	GGATCCTCTAGAGTCGACGGTATCGATAAGCTTGATATCGAATTCGGCTCCACCACCTCT
5881	CTCCTCTCTCCTCTCTCTCCCCCCTGGAGAGATTATTCATTCCCTCCA**ATGGATCTCCGT**
5941	**CGGAGGCCTCCTAAACCACCGGTTACCAACAACAACAACTCCAACGGATCTTTCCGTTCT**
6001	**TATCAGCCTCGCACTTCCGATGACGATCATCGTCGCCGGGCTACAACAATTGCTCCTCCA**
6061	**CCGAAAGCATCCGACGCGCTTCCTCTTCCGTTATATCTCACAAACGCCGTTTTCTTCACG**
6121	**CTCTTCTTCTCCGTCGCGTATTACCTCCTCCACCGGTGGCGTGACAAGATCCGTTACAAT**
6181	**ACGCCTCTTCACGTCGTCACTATCACAGAACTCGGCGCCATTATTGCTCTCATCGCTTCG**
6241	**TTTATCTATCTCCTAGGGTTTTTGGTATTGACTTTGTTCAGTCATTTATCTCACGTGCC**
6301	**TCTGGTGATGCTTGGGATCTCGCCGATACGATCGATGATGATGACCACCGCCTTGTCACG**
6361	**TGCTCTCCACCGACTCCGATCGTTTCCGTTGCTAAATTACCTAATCCGGAACCTATTGTT**
6421	**ACCGAATCGCTTCCTGAGGAAGACGAGGAGATTGTGAAATCGGTTATCGACGGAGTTATT**
6481	**CCATCGTACTCGCTTGAATCTCGTCTCGGTGATTGCAAAAGAGCGGCGTCGATTCGTCGT**
6541	**GAGGCGTTGCAGAGAGTCACCGGGAGATCGATTGAAGGGTTACCGTTGGATGGATTTGAT**
6601	**TATGAATCGATTTTGGGGCAATGCTGTGAGATGCCTGTTGGATACATTCAGATTCCTGTT**
6661	**GGGATTGCTGGTCCATTGTTGCTTGATGGTTATGAGTACTCTGTTCCTATGGCTACAACC**
6721	**GAAGGTTGTTTGGTTGCTAGCACTAACAGAGGCTGCAAGGCTATGTTTATCTCTGGTGGC**
6781	**GCCACCAGTACCGTTCTTAAGGACGGTATGACCCGAGCACCTGTTGTTCGGTTCGCTTCG**
6841	**GCGAGACGAGCTTCGGAGCTTAAGTTTTTCTTGGAGAATCCAGAGAACTTTGATACTTTG**
6901	**GCAGTAGTCTTCAACAGGTCGAGTAGATTTGCAAGACTGCAAAGTGTTAAATGCACAATC**
6961	**GCGGGGAAGAATGCTTATGTAAGGTTCTGTTGTAGTACTGGTGATGCTATGGGGATGAAT**
7021	**ATGGTTTCTAAAGGTGTGCAGAATGTTCTTGAGTATCTTACCGATGATTTCCCTGACATG**
7081	**GATGTGATTGGAATCTCTGGTAACTTCTGTTCGGACAAGAAACCTGCTGCTGTGAACTGG**
7141	**ATTGAGGGACGTGGTAAATCAGTTGTTTGCGAGGCTGTAATCAGAGGAGAGATCGTGAAC**
7201	**AAGGTCTTGAAAACGAGCGTGGCTGCTTTAGTCGAGCTCAACATGCTCAAGAACCTAGCT**
7261	**GGCTCTGCTGTTGCAGGCTCTCTAGGTGGATTCAACGCTCATGCCAGTAACATAGTGTCT**
7321	**GCTGTATTCATAGCTACTGGCCAAGATCCAGCTCAAAACGTGGAGAGTTCTCAATGCATC**
7381	**ACCATGATGGAAGCTATTAATGACGGCAAAGATATCCATATCTCAGTCACTATGCCATCT**
7441	**ATCGAGGTGGGGACAGTGGGAGGAGGAACACAGCTTGCATCTCAATCAGCGTGTTTAAAC**
7501	**CTGCTCGGAGTTAAAGGAGCAAGCACAGAGTCGCCGGGAATGAACGCAAGGAGGCTAGCG**
7561	**ACGATCGTAGCCGGAGCAGTTTTAGCTGGAGAGTTATCTTTAATGTCAGCAATTGCAGCT**
7621	**GGACAGCTTGTGAGAAGTCACATGAAATACAATAGATCCAGCCGAGACATCTCTGGAGCA**
7681	**ACGACAACGACAACAACAACAACATGA**TCTGAATCTGAATCATCATCCTCTCAAAGAAGG
7741	ACAACAATCCAAAACAAGGGCAGGCTTTTTACAACGCATTCACTCAAAACTCGCTGGTGG
7801	ACAGATTTTAGCCATGTGCGTATGCGTTTGCCCTTTTGTTAAATAAAAAAACTATTTGTT
7861	TTGTTTGTTTGACTTGATATCTTTTTTTGGGATTGAGGATTGAGAGAGATAGAGAGATTT
7921	TACAAACTTTCTCTCTTTCTCTCTTTCTCTCTTTCTCATGGATAATTCGTGTCTCTTTGA
7981	TTTGTCTAAGGTTTGTCTTTGTTTGTTAGGAAGTGGTCTATATGAACGAAAAATTTGTGT
8041	ATGGTGCAGTTGCGTTTGGGGACATTTTTGAGATTTTTTCAAAAAAAAAAAAAAAAAACC
8101	GAATTCCTCGAATTTCCCC**GATCGTTCAAACATTTGGCAATAAAGTTTCTTAAGATTGAA**
8161	**TCCTGTTGCCGGTCTTGCGATGATTATCATATAATTTCTGTTGAATTACGTTAAGCATGT**
8221	**AATAATTAACATGTAATGCATGACGTTATTTATGAGATGGGTTTTTATGATTAGAGTCCC**
8281	**GCAATTATACATTTAATACGCGATAGAAAACAAAATATAGCGCGCAAACTAGGATAAATT**
8341	**ATCGCGCGCGGTGTCATCTATGTTACTAGATC**GGGAATTCACTGGCCGTCGTTTTACAAC
8401	GTCGTGACTGGGAAAACCCTGGCGTTACCCAACTTAATCGCCTTGCAGCACATCCCCCTT
8461	TCGCCAGCTGGCGTAATAGCGAAGAGGCCCGCACCGATCGCCCTTCCCAACAGTTGCGCA
8521	GCCTGAATGGCGCCCGCTCCTTTCGCTTTCTTCCCTTCCTTTCTCGCCACGTTCGCCGGC
8581	TTTCCCCGTCAAGCTCTAAATCGGGGGCTCCCTTTAGGGTTCCGATTTAGTGCTTTACGG
8641	CACCTCGACCCCAAAAAACTTGATTTGGGTGATGGTTCACGTAGTGGGCCATCGCCCTGA

5' Base	Sequence
8701	TAGACGGTTTTTCGCCCTTTGACGTTGGAGTCCACGTTCTTTAATAGTGGACTCTTGTTC
8761	CAAACTGGAACAACACTCAACCCTATCTCGGGCTATTCTTTTGATTTATAAGGGATTTTG
8821	CCGATTTCGGAACCACCATCAAACAGGATTTTCGCCTGCTGGGGCAAACCAGCGTGGACC
8881	GCTTGCTGCAACTCTCTCAGGGCCAGGCGGTGAAGGGCAATCAGCTGTTGCCCGTCTCAC
8941	TGGTGAAAAGAAAAACCACCCCAGTACATTAAAAACGTCCGCAATGTGTTATTAAGTTGT
9001	CTAAGCGTCAATT**TGTTTACACCACAATATATCCTGCCA**CCAGCCAGCCAACAGCTCCCC
9061	GACCGGCAGCTCGGCACAAAATCACCACTCGATACAGGCAGCCCATCAGTCCGGGACGGC
9121	GTCAGCGGGAGAGCCGTTGTAAGGCGGCAGACTTTGCTCATGTTACCGATGCTATTCGGA
9181	AGAACGGCAACTAAGCTGCCGGGTTTGAAACACGGATGATCTCGCGGAGGGTAGCATGTT
9241	GATTGTAACGATGACAGAGCGTTGCTGCCTGTGATCAAATATCATCTCCCTCGCAGAGAT
9301	CCGAATTATCAGCCTTCTTATTCATTTCTCGCTTAACCGTGACAGGCTGTCGATCTTGAG
9361	AACTATGCCGACATAATAGGAAATCGCTGGATAAAGCCGCTGAGGAAGCTGAGTGGCGCT
9421	ATTTCTTTAGAAGTGAACGTTGACGATATCAACTCCCCTATCCATTGCTCACCGAATGGT
9481	ACAGGTCGGGGACCCGAAGTTCCGACTGTCGGCCTGATGCATCCCCGGCTGATCGACCCC
9541	AGATCTGGGGCTGAGAAAGCCCAGTAAGGAAACAACTGTAGGTTCGAGTCGCGAGATCCC
9601	CCGGAACCAAAGGAAGTAGGTTAAACCCGCTCCGATCAGGCCGAGCCACGCCAGGCCGAG
9661	AACATTGGTTCCTGTAGGCATCGGGATTGGCGGATCAAACACTAAAGCTACTGGAACGAG
9721	CAGAAGTCCTCCGGCCGCCAGTTGCCAGGCGGTAAAGGTGAGCAGAGGCACGGGAGGTTG
9781	CCACTTGCGGGTCAGCACGGTTCCGAACGCCATGGAAACCGCCCCCGCCAGGCCCGCTGC
9841	GACGCCGACAGGATCTAGCGCTGCGTTTGGTGTCAACACCAACAGCGCCACGCCCGCAGT
9901	TCCGCAAATAGCCCCCAGGACCGCCATCAATCGTATCGGGCTACCTAGCAGAGCGGCAGA
9961	GATGAACACGACCATCAGCGGCTGCACAGCGCCTACCGTCGCCGCGACCCCGCCCGGCAG
10021	GCGGTAGACCGAAATAAACAACAAGCTCCAGAATAGCGAAATATTAAGTGCGCCGAGGAT
10081	GAAGATGCGCATCCACCAGATTCCCGTTGGAATCTGTCGGACGATCATCACGAGCAATAA
10141	ACCCGCCGGCAACGCCCGCAGCAGCATACCGGCGACCCCTCGGCCTCGCTGTTCGGGCTC
10201	CACGAAAACGCCGGACAGATGCGCCTTGTGAGCGTCCTTGGGGCCGTCCTCCTGTTTGAA
10261	GACCGACAGCCCAATGATCTCGCCGTCGATGTAGGCGCCGAATGCCACGGCATCTCGCAA
10321	CCGTTCAGCGAACGCCTCCATGGGCTTTTTCTCCTCGTGCTCGTAAACGGACCCGAACAT
10381	CTCTGGAGCTTTCTTCAGGGCCGACAATCGGATCTCGCGGAAATCCTGCACGTCGGCCGC
10441	TCCAAGCCGTCGAATCTGAGCCTTAATCACAATTGTCAATTTTAATCCTCTGTTTATCGG
10501	CAGTTCGTAGAGCGCGCCGTGCGTCCCGAGCGATACTGAGCGAAGCAAGTGCGTCGAGCA
10561	GTGCCCGCTTGTTCCTGAAATGCCAGTAAAGCGCTGGCTGCTGAACCCCCAGCCGGAACT
10621	GACCCCACAAGGCCCTAGCGTTTGCAATGCACCAGGTCATCATTGACCCAGGCGTGTTCC
10681	ACCAGGCCGCTGCCTCGCAACTCTTCGCAGGCTTCGCCGACCTGCTCGCGCCACTTCTTC
10741	ACGCGGGTGGAATCCGATCCGCACATGAGGCGGAAGGTTTCCAGCTTGAGCGGGTACGGC
10801	TCCCGGTGCGAGCTGAAATAGTCGAACATCCGTCGGGCCGTCGGCGACAGCTTGCGGTAC
10861	TTCTCCCATATGAATTTCGTGTAGTGGTCGCCAGCAAACAGCACGACGATTTCCTCGTCG
10921	ATCAGGACCTGGCAACGGGACGTTTTCTTGCCACGGTCCAGGACGCGGAAGCGGTGCAGC
10981	AGCGACACCGATTCCAGGTGCCCAACGCGGTCGGACGTGAAGCCCATCGCCGTCGCCTGT
11041	AGGCGCGACAGGCATTCCTCGGCCTTCGTGTAATACCGGCCATTGATCGACCAGCCCAGG
11101	TCCTGGCAAAGCTCGTAGAACGTGAAGGTGATCGGCTCGCCGATAGGGGTGCGCTTCGCG
11161	TACTCCAACACCTGCTGCCACACCAGTTCGTCATCGTCGGCCCGCAGCTCGACGCCGGTG
11221	TAGGTGATCTTCACGTCCTTGTTGACGTGGAAAATGACCTTGTTTTGCAGCGCCTCGCGC
11281	GGGATTTTCTTGTTGCGCGTGGTGAACAGGGCAGAGCGGGCCGTGTCGTTTGGCATCGCT
11341	CGCATCGTGTCCGGCCACGGCGCAATATCGAACAAGGAAAGCTGCATTTCCTTGATCTGC
11401	TGCTTCGTGTGTTTCAGCAACGCGGCCTGCTTGGCCTCGCTGACCTGTTTTGCCAGGTCC
11461	TCGCCGGCGGTTTTTCGCTTCTTGGTCGTCATAGTTCCTCGCGTGTCGATGGTCATCGAC
11521	TTCGCCAAACCTGCCGCCTCCTGTTCGAGACGACGCGAACGCTCCACGGCGGCCGATGGC
11581	GCGGGCAGGGCAGGGGGAGCCAGTTGCACGCTGTCGCGCTCGATCTTGGCCGTAGCTTGC
11641	TGGACCATCGAGCCGACGGACTGGAAGGTTTCGCGGGGCGCACGCATGACGGTGCGGCTT
11701	GCGATGGTTTCGGCATCCTCGGCGGAAAACCCCGCGTCGATCAGTTCTTGCCTGTATGCC
11761	TTCCGGTCAAACGTCCGATTCATTCACCCTCCTTGCGGGATTGCCCCGACTCACGCCGGG
11821	GCAATGTGCCCTTATTCCTGATTTGACCCGCCTGGTGCCTTGGTGTCCAGATAATCCACC
11881	TTATCGGCAATGAAGTCGGTCCCGTAGACCGTCTGGCCGTCCTTCTCGTACTTGGTATTC
11941	CGAATCTTGCCCTGCACGAATACCAGCGACCCCTTGCCCAAATACTTGCCGTGGGCCTCG
12001	GCCTGAGAGCCAAAACACTTGATGCGGAAGAAGTCGGTGCGCTCCTGCTTGTCGCCGGCA
12061	TCGTTGCGCCACATCTAGGTACTAAAACAATTCATCCAGTAAAATATAATATTTTATTTT
12121	CTCCCAATCAGGCTTGATCCCCAGTAAGTCAAAAAATAGCTCGACATACTGTTCTTCCCC
12181	GATATCCTCCCTGATCGACCGGACGCAGAAGGCAATGTCATACCACTTGTCCGCCCTGCC

5' Base	Sequence
12241	GCTTCTCCCAAGATCAATAAAGCCACTTACTTTGCCATCTTTCACAAAGATGTTGCTGTC
12301	TCCCAGGTCGCCGTGGGAAAAGACAAGTTCCTCTTCGGGCTTTTCCGTCTTTAAAAAATC
12361	ATACAGCTCGCGCGGATCTTTAAATGGAGTGTCTTCTTCCCAGTTTTCGCAATCCACATC
12421	GGCCAGATCGTTATTCAGTAAGTAATCCAATTCGGCTAAGCGGCTGTCTAAGCTATTCGT
12481	ATAGGGACAATCCGATATGTCGATGGAGTGAAAGAGCCTGATGCACTCCGCATACAGCTC
12541	GATAATCTTTTCAGGGCTTTGTTCATCTTCATACTCTTCCGAGCAAAGGACGCCATCGGC
12601	CTCACTCATGAGCAGATTGCTCCAGCCATCATGCCGTTCAAAGTGCAGGACCTTTGGAAC
12661	AGGCAGCTTTCCTTCCAGCCATAGCATCATGTCCTTTTCCCGTTCCACATCATAGGTGGT
12721	CCCTTTATACCGGCTGTCCGTCATTTTTAAATATAGGTTTTCATTTTCTCCCACCAGCTT
12781	ATATACCTTAGCAGGAGACATTCCTTCCGTATCTTTTACGCAGCGGTATTTTTCGATCAG
12841	TTTTTTCAATTCCGGTGATATTCTCATTTTAGCCATTTATTATTTCCTTCCTCTTTTCTA
12901	CAGTATTTAAAGATACCCCAAGAAGCTAATTATAACAAGACGAACTCCAATTCACTGTTC
12961	CTTGCATTCTAAAACCTTAAATACCAGAAAACAGCTTTTTCAAAGTTGTTTTCAAAGTTG
13021	GCGTATAACATAGTATCGACGGAGCCGATTTTGAAACCACAATTATGGGTGATGCTGCCA
13081	ACTTACTGATTTAGTGTATGATGGTGTTTTTGAGGTGCTCCAGTGGCTTCTGTGTCTATC
13141	AGCTGTCCCTCCTGTTCAGCTACTGACGGGGTGGTGCGTAACGGCAAAAGCACCGCCGGA
13201	CATCAGCGCTATCTCTGCTCTCACTGCCGTAAAACATGGCAACTGCAGTTCACTTACACC
13261	GCTTCTCAACCCGGTACGCACCAGAAAATCATTGATATGGCCATGAATGGCGTTGGATGC
13321	CGGGCAACAGCCCGCATTATGGGCGTTGGCCTCAACACGATTTTACGTCACTTAAAAAAC
13381	TCAGGCCGCAGTCGGTAACCTCGCGCATACAGCCGGGCAGTGACGTCATCGTCTGCGCGG
13441	AAATGGACGAACAGTGGGGCTATGTCGGGGCTAAATCGCGCCAGCGCTGGCTGTTTTACG
13501	CGTATGACAGTCTCCGGAAGACGGTTGTTGCGCACGTATTCGGTGAACGCACTATGGCGA
13561	CGCTGGGGCGTCTTATGAGCCTGCTGTCACCCTTTGACGTGGTGATATGGATGACGGATG
13621	GCTGGCCGCTGTATGAATCCCGCCTGAAGGGAAAGCTGCACGTAATCAGCAAGCGATATA
13681	CGCAGCGAATTGAGCGGCATAACCTGAATCTGAGGCAGCACCTGGCACGGCTGGGACGGA
13741	AGTCGCTGTCGTTCTCAAAATCGGTGGAGCTGCATGACAAAGTCATCGGGCATTATCTGA
13801	ACATAAAACACTATCAATAAGTTGGAGTCATTACCCAATTATGATAGAATTTACAAGCTA
13861	TAAGGTTATTGTCCTGGGTTTCAAGCATTAGTCCATGCAAGTTTTTATGCTTTGCCCATT
13921	CTATAGATATATTGATAAGCGCGCTGCCTATGCCTTGCCCCCTGAAATCCTTACATACGG
13981	CGATATCTTCTATATAAAAGATATATTATCTTATCAGTATTGTCAATATATTCAAGGCAA
14041	TCTGCCTCCTCATCCTCTTCATCCTCTTCGTCTTGGTAGCTTTTTAAATATGGCGCTTCA
14101	TAGAGTAATTCTGTAAAGGTCCAATTCTCGTTTTCATACCTCGGTATAATCTTACCTATC
14161	ACCTCAAATGGTTCGCTGGGTTTATCGCACCCCCGAACACGAGCACGGCACCCGCGACCA
14221	CTATGCCAAGAATGCCCAAGGTAAAAATTGCCGGCCCCGCCATGAAGTCCGTGAATGCCC
14281	CGACGGCCGAAGTGAAGGGCAGGCCGCCACCCAGGCCGCCGCCCTCACTGCCCGGCACCT
14341	GGTCGCTGAATGTCGATGCCAGCACCTGCGGCACGTCAATGCTTCCGGGCGTCGCGCTCG
14401	GGCTGATCGCCCATCCCGTTACTGCCCCGATCCCGGCAATGGCAAGGACTGCCAGCGCTG
14461	CCATTTTTGGGGTGAGGCCGTTCGCGGCCGAGGGGCGCAGCCCCTGGGGGGATGGGAGGC
14521	CCGCGTTAGCGGGCCGGGAGGGTTCGAGAAGGGGGGGCACCCCCCTTCGGCGTGCGCGGT
14581	CACGCGCACAGGGCGCAGCCCTGGTTAAAAACAAGGTTTATAAATATTGGTTTAAAAGCA
14641	GGTTAAAAGACAGGTTAGCGGTGGCCGAAAAACGGGCGGAAACCCTTGCAAATGCTGGAT
14701	TTTCTGCCTGTGGACAGCCCCTCAAATGTCAATAGGTGCGCCCCTCATCTGTCAGCACTC
14761	TGCCCCTCAAGTGTCAAGGATCGCGCCCCTCATCTGTCAGTAGTCGCGCCCCTCAAGTGT
14821	CAATACCGCAGGGCACTTATCCCCAGGCTTGTCCACATCATCTGTGGGAAACTCGCGTAA
14881	AATCAGGCGTTTTCGCCGATTTGCGAGGCTGGCCAGCTCCACGTCGCCGGCCGAAATCGA
14941	GCCTGCCCCTCATCTGTCAACGCCGCGCCGGGTGAGTCGGCCCCTCAAGTGTCAACGTCC
15001	GCCCCTCATCTGTCAGTGAGGGCCAAGTTTTCCGCGAGGTATCCACAACGCCGGCGGCCG
15061	CGGTGTCTCGCACACGGCTTCGACGGCGTTTCTGGCGCGTTTGCAGGGCCATAGACGGCC
15121	GCCAGCCCAGCGGCGAGGGCAACCAGCCCGG

Appendix 6.2. pK7WG2-*mCherry* expression vector sequence

The *mCherry* insert was confirmed by sequencing using the primers p7WG2-ins-F and p7WG2-ins-R.

Bases	Feature
18-242	CaMV *35S* terminator
242-260	p7WG2-ins-R primer binding site
252-276	attB2 (Gateway recombination site)
291-313	mCherry-R primer binding site
291-1001	*mCherry*
984-1001	mCherry-F primer binding site (antiparallel sequence)
1016-1040	attB1 (Gateway recombination site)
1068-2094	CaMV *35S* promoter
1139-1160	p7WG2-ins-F primer binding site (antiparallel sequence)
2116-2315	Right transfer DNA border
7218-8467	*Sm/SpR* (Bacterial streptomycin/spectinomycin resistance cassette)
8473-8804	Left transfer DNA border
8827-9080	*nos* terminator
9120-9914	*nptII* (including *nos* promoter and terminator)
9927-10191	*nos* promoter

5' Base	Sequence
1	CGACGTCGCATGCCTGC**AGGTCACTGGATTTTGGTTTTAGGAATTAGAAATTTTATTGAT**
61	**AGAAGTATTTTACAAATACAAATACATACTAAGGGTTTCTTATATGCTCAACACATGAGC**
121	**GAAACCCTATAAGAACCCTAATTCCCTTATCTGGGAACTACTCACACATTATTCTGGAGA**
181	**AAATAGAGAGAGATAGATTTGTAGAGAGAGACTGGTGATTTTTGCGGACTCTAGCATGGC**
241	**CG**CGGGATATC**ACCACTTTGTACAAGAAAGCTGGGT**CGAATTCGCCCTTT**TTACTTGTAC**
301	**AGCTCGTCCATGCCGCCGGTGGAGTGGCGGCCCTCGGCGCGTTCGTACTGTTCCACGATG**
361	**GTGTAGTCCTCGTTGTGGGAGGTGATGTCCAACTTGATGTTGACGTTGTAGGCGCCGGGC**
421	**AGCTGCACGGGCTTCTTGGCCTTGTAGGTGGTCTTGACCTCAGCGTCGTAGTGGCCGCCG**
481	**TCCTTCAGCTTCAGCCTCTGCTTGATCTCGCCCTTCAGGGCGCCGTCCTCGGGGTACATC**
541	**CGCTCGGAGGAGGCCTCCCAGCCCATGGTCTTCTTCTGCATTACGGGGCCGTCGGAGGGG**
601	**AAGTTGGTGCCGCGCAGCTTCACCTTGTAGATGAACTCGCCGTCCTGCAGGGAGGAGTCC**
661	**TGGGTCACGGTCACCACGCCGCCGTCCTCGAAGTTCATCACGCGCTCCCACTTGAAGCCC**
721	**TCGGGGAAGGACAGCTTCAAGTAGTCGGGGATGTCGGCGGGGTGCTTCACGTAGGCCTTG**
781	**GAGCCGTACATGAACTGAGGGGACAGGATGTCCCAGGCGAAGGGCAGGGGGCCACCCTTG**
841	**GTCACCTTCAGCTTGGCGGTCTGGGTGCCCTCGTAGGGGCGGCCCTCGCCCTCGCCCTCG**
901	**ATCTCGAACTCGTGGCCGTTCACGGAGCCCTCCATGTGCACCTTGAAGCGCATGAACTCC**
961	**TTGATGATGGCCATGTTATCCTCCTCGCCCTTGCTCACCAT**AAGGGCGAATTCGG**AGCCT**
1021	**GCTTTTTTGTACAAACTTGT**GATATCACTAGTGCGGCCGCCTGCAGG**TCGACTAGAATAG**
1081	**TAAATTGTAATGTTGTTTGTTGTTTGTTTTGTTGTGGTATTGTTGTAAAAATACCGGAGT**
1141	**CCTCTCCAAATGAAATGAACTTCCTTATATAGAGGAAGGGTCTTGCGAAGGATAGTGGGA**
1201	**TTGTGCGTCATCCCTTACGTCAGTGGAGATATCACATCAATCCACTTGCTTTGAAGACGT**
1261	**GGTTGGAACGTCTTCTTTTTCCACGATGCTCCTCGTGGGTGGGGGTCCATCTTTGGGACC**
1321	**ACTGTCGGCAGAGGCATCTTGAACGATAGCCTTTCCTTTATCGCAATGATGGCATTTGTA**
1381	**GGTGCCACCTTCCTTTTCTACTGTCCTTTTGATGAAGTGACAGATAGCTGGGCAATGGAA**
1441	**TCCGAGGAGGTTTCCCGATATTACCCTTTGTTGAAAAGTCTCAATAGCCCTTTGGTCTTC**
1501	**TGAGACTGTATCTTTGATATTCTTGGAGTAGACGAGAGTGTCGTGCTCCACCATGTTGAC**
1561	**GAAGATTTTCTTCTTGTCATTGAGTCGTAAAAGACTCTGTATGAACTGTTCGCCAGTCTT**
1621	**CACGGCGAGTTCTGTTAGATCCTCGATCTGAATTTTTGACTCCATGGCCTTTGATTCAGT**

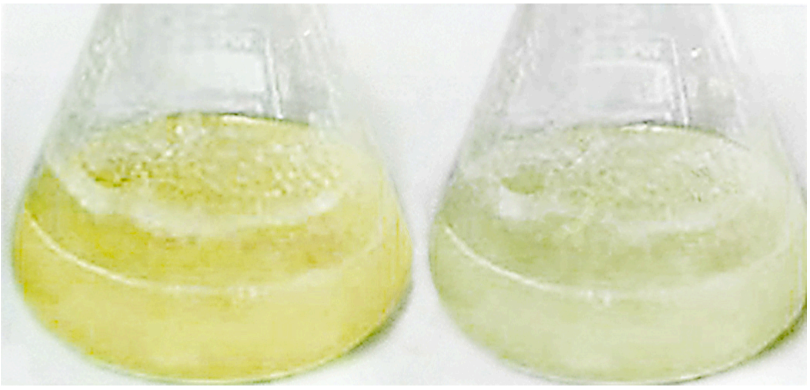
5' Base	Sequence
1681	**AGGAACTACTTTCTTAGAGACTCCAATCTCTATTACTTGCCTTGGTTTATGAAGCAAGCC**
1741	**TTGAATCGTCCATACTGGAATAGTACTTCTGATCTTGAGAAATATATCTTTCTCTGTGTT**
1801	**CTTGATGCAGTTAGTCCTGAATCTTTTGACTGCATCTTTAACCTTCTTGGGAAGGTATTT**
1861	**GATCTCCTGGAGATTATTACTCGGGTAGATCGTCTTGATGAGACCTGCCGCGTAGGCCTC**
1921	**TCTAACCATCTGTGGGTCAGCATTCTTTCTGAAATTGAAGAGGCTAATCTTCTCATTATC**
1981	**GGTGGTGAACATGGTATCGTCACCTTCTCCGTCGAACTTTCTTCCTAGATCGTAGAGATA**
2041	**GAGAAAGTCGTCCATGGTGATCTCCGGGGCAAAGGAGATCAGCTTGGCTCTAGT**CGACCA
2101	TATGGGAGAGCTCAA**GCTTAGCTTGAGCTTGGATCAGATTGTCGTTTCCCGCCTTCAGTT**
2161	**TAAACTATCAGTGTTTGACAGGATATATTGGCGGGTAAACCTAAGAGAAAAGAGCGTTTA**
2221	**TTAGAATAACGGATATTTAAAAGGGCGTGAAAAGGTTTATCCGTTCGTCCATTTGTATGT**
2281	**GCATGCCAACCACAGGGTTCCCCTCGGGATCAAAG**TACTTTGATCCAACCCCTCCGCTGC
2341	TATAGTGCAGTCGGCTTCTGACGTTCAGTGCAGCCGTCTTCTGAAAACGACATGTCGCAC
2401	AAGTCCTAAGTTACGCGACAGGCTGCCGCCCTGCCCTTTTCCTGGCGTTTTCTTGTCGCG
2461	TGTTTTAGTCGCATAAAGTAGAATACTTGCGACTAGAACCGGAGACATTACGCCATGAAC
2521	AAGAGCGCCGCCGCTGGCCTGCTGGGCTATGCCCGCGTCAGCACCGACGACCAGGACTTG
2581	ACCAACCAACGGGCCGAACTGCACGCGGCCGGCTGCACCAAGCTGTTTTCCGAGAAGATC
2641	ACCGGCACCAGGCGCGACCGCCCGGAGCTGGCCAGGATGCTTGACCACCTACGCCCTGGC
2701	GACGTTGTGACAGTGACCAGGCTAGACCGCCTGGCCCGCAGCACCCGCGACCTACTGGAC
2761	ATTGCCGAGCGCATCCAGGAGGCCGGCGCGGGCCTGCGTAGCCTGGCAGAGCCGTGGGCC
2821	GACACCACCACGCCGGCCGGCCGCATGGTGTTGACCGTGTTCGCCGGCATTGCCGAGTTC
2881	GAGCGTTCCCTAATCATCGACCGCACCCGGAGCGGGCGCGAGGCCGCCAAGGCCCGAGGC
2941	GTGAAGTTTGGCCCCCGCCCTACCCTCACCCCGGCACAGATCGCGCACGCCCGCGAGCTG
3001	ATCGACCAGGAAGGCCGCACCGTGAAAGAGGCGGCTGCACTGCTTGGCGTGCATCGCTCG
3061	ACCCTGTACCGCGCACTTGAGCGCAGCGAGGAAGTGACGCCCACCGAGGCCAGGCGGCGC
3121	GGTGCCTTCCGTGAGGACGCATTGACCGAGGCCGACGCCCTGGCGGCCGCCGAGAATGAA
3181	CGCCAAGAGGAACAAGCATGAAACCGCACCAGGACGGCCAGGACGAACCGTTTTTCATTA
3241	CCGAAGAGATCGAGGCGGAGATGATCGCGGCCGGGTACGTGTTCGAGCCGCCCGCGCACG
3301	TCTCAACCGTGCGGCTGCATGAAATCCTGGCCGGTTTGTCTGATGCCAAGCTGGCGGCCT
3361	GGCCGGCCAGCTTGGCCGCTGAAGAAACCGAGCGCCGCCGTCTAAAAAGGTGATGTGTAT
3421	TTGAGTAAAACAGCTTGCGTCATGCGGTCGCTGCGTATATGATGCGATGAGTAAATAAAC
3481	AAATACGCAAGGGGAACGCATGAAGGTTATCGCTGTACTTAACCAGAAAGGCGGGTCAGG
3541	CAAGACGACCATCGCAACCCATCTAGCCCGCGCCCTGCAACTCGCCGGGGCCGATGTTCT
3601	GTTAGTCGATTCCGATCCCCAGGGCAGTGCCCGCGATTGGGCGGCCGTGCGGGAAGATCA
3661	ACCGCTAACCGTTGTCGGCATCGACCGCCCGACGATTGACCGCGACGTGAAGGCCATCGG
3721	CCGGCGCGACTTCGTAGTGATCGACGGAGCGCCCCAGGCGGCGGACTTGGCTGTGTCCGC
3781	GATCAAGGCAGCCGACTTCGTGCTGATTCCGGTGCAGCCAAGCCCTTACGACATATGGGC
3841	CACCGCCGACCTGGTGGAGCTGGTTAAGCAGCGCATTGAGGTCACGGATGGAAGGCTACA
3901	AGCGGCCTTTGTCGTGTCGCGGGCGATCAAAGGCACGCGCATCGGCGGTGAGGTTGCCGA
3961	GGCGCTGGCCGGGTACGAGCTGCCCATTCTTGAGTCCCGTATCACGCAGCGCGTGAGCTA
4021	CCCAGGCACTGCCGCCGCCGGCACAACCGTTCTTGAATCAGAACCCGAGGGCGACGCTGC
4081	CCGCGAGGTCCAGGCGCTGGCCGCTGAAATTAAATCAAAACTCATTTGAGTTAATGAGGT
4141	AAAGAGAAAATGAGCAAAAGCACAAACACGCTAAGTGCCGGCCGTCCGAGCGCACGCAGC
4201	AGCAAGGCTGCAACGTTGGCCAGCCTGGCAGACACGCCAGCCATGAAGCGGGTCAACTTT
4261	CAGTTGCCGGCGGAGGATCACACCAAGCTGAAGATGTACGCGGTACGCCAAGGCAAGACC
4321	ATTACCGAGCTGCTATCTGAATACATCGCGCAGCTACCAGAGTAAATGAGCAAATGAATA
4381	AATGAGTAGATGAATTTTAGCGGCTAAAGGAGGCGGCATGGAAAATCAAGAACAACCAGG
4441	CACCGACGCCGTGGAATGCCCCATGTGTGGAGGAACGGGCGGTTGGCCAGGCGTAAGCGG
4501	CTGGGTTGTCTGCCGGCCCTGCAATGGCACTGGAACCCCCAAGCCCGAGGAATCGGCGTG
4561	ACGGTCGCAAACCATCCGGCCCGGTACAAATCGGCGCGGCGCTGGGTGATGACCTGGTGG
4621	AGAAGTTGAAGGCCGCGCAGGCCGCCCAGCGGCAACGCATCGAGGCAGAAGCACGCCCCG
4681	GTGAATCGTGGCAAGCGGCCGCTGATCGAATCCGCAAAGAATCCCGGCAACCGCCGGCAG
4741	CCGGTGCGCCGTCGATTAGGAAGCCGCCCAAGGGCGACGAGCAACCAGATTTTTTCGTTC
4801	CGATGCTCTATGACGTGGGCACCCGCGATAGTCGCAGCATCATGGACGTGGCCGTTTTCC
4861	GTCTGTCGAAGCGTGACCGACGAGCTGGCGAGGTGATCCGCTACGAGCTTCCAGACGGGC
4921	ACGTAGAGGTTTCCGCAGGGCCGGCCGGCATGGCCAGTGTGTGGGATTACGACCTGGTAC
4981	TGATGGCGGTTTCCCATCTAACCGAATCCATGAACCGATACCGGGAAGGGAAGGGAGACA
5041	AGCCCGGCCGCGTGTTCCGTCCACACGTTGCGGACGTACTCAAGTTCTGCCGGCGAGCCG
5101	ATGGCGGAAAGCAGAAAGACGACCTGGTAGAAACCTGCATTCGGTTAAACACCACGCACG
5161	TTGCCATGCAGCGTACGAAGAAGGCCAAGAACGGCCGCCTGGTGACGGTATCCGAGGGTG

5' Base	Sequence
5221	AAGCCTTGATTAGCCGCTACAAGATCGTAAAGAGCGAAACCGGGCGGCCGGAGTACATCG
5281	AGATCGAGCTAGCTGATTGGATGTACCGCGAGATCACAGAAGGCAAGAACCCGGACGTGC
5341	TGACGGTTCACCCCGATTACTTTTTGATCGATCCCGGCATCGGCCGTTTTCTCTACCGCC
5401	TGGCACGCCGCGCCGCAGGCAAGGCAGAAGCCAGATGGTTGTTCAAGACGATCTACGAAC
5461	GCAGTGGCAGCGCCGGAGAGTTCAAGAAGTTCTGTTTCACCGTGCGCAAGCTGATCGGGT
5521	CAAATGACCTGCCGGAGTACGATTTGAAGGAGGAGGCGGGGCAGGCTGGCCCGATCCTAG
5581	TCATGCGCTACCGCAACCTGATCGAGGGCGAAGCATCCGCCGGTTCCTAATGTACGGAGC
5641	AGATGCTAGGGCAAATTGCCCTAGCAGGGGAAAAAGGTCGAAAAGGTCTCTTTCCTGTGG
5701	ATAGCACGTACATTGGGAACCCAAAGCCGTACATTGGGAACCGGAACCCGTACATTGGGA
5761	ACCCAAAGCCGTACATTGGGAACCGGTCACACATGTAAGTGACTGATATAAAAGAGAAAA
5821	AAGGCGATTTTTCCGCCTAAAACTCTTTAAAACTTATTAAAACTCTTAAAACCCGCCTGG
5881	CCTGTGCATAACTGTCTGGCCAGCGCACAGCCGAAGAGCTGCAAAAAGCGCCTACCCTTC
5941	GGTCGCTGCGCTCCCTACGCCCCGCCGCTTCGCGTCGGCCTATCGCGGCCGCTGGCCGCT
6001	CAAAAATGGCTGGCCTACGGCCAGGCAATCTACCAGGGCGCGGACAAGCCGCGCCGTCGC
6061	CACTCGACCGCCGGCGCCCACATCAAGGCACCCTGCCTCGCGCGTTTCGGTGATGACGGT
6121	GAAAACCTCTGACACATGCAGCTCCCGGAGACGGTCACAGCTTGTCTGTAAGCGGATGCC
6181	GGGAGCAGACAAGCCCGTCAGGGCGCGTCAGCGGGTGTTGGCGGGTGTCGGGGCGCAGCC
6241	ATGACCCAGTCACGTAGCGATAGCGGAGTGTATACTGGCTTAACTATGCGGCATCAGAGC
6301	AGATTGTACTGAGAGTGCACCATATGCGGTGTGAAATACCGCACAGATGCGTAAGGAGAA
6361	AATACCGCATCAGGCGCTCTTCCGCTTCCTCGCTCACTGACTCGCTGCGCTCGGTCGTTC
6421	GGCTGCGGCGAGCGGTATCAGCTCACTCAAAGGCGGTAATACGGTTATCCACAGAATCAG
6481	GGGATAACGCAGGAAAGAACATGTGAGCAAAAGGCCAGCAAAAGGCCAGGAACCGTAAAA
6541	AGGCCGCGTTGCTGGCGTTTTTCCATAGGCTCCGCCCCCCTGACGAGCATCACAAAAATC
6601	GACGCTCAAGTCAGAGGTGGCGAAACCCGACAGGACTATAAAGATACCAGGCGTTTCCCC
6661	CTGGAAGCTCCCTCGTGCGCTCTCCTGTTCCGACCCTGCCGCTTACCGGATACCTGTCCG
6721	CCTTTCTCCCTTCGGGAAGCGTGGCGCTTTCTCATAGCTCACGCTGTAGGTATCTCAGTT
6781	CGGTGTAGGTCGTTCGCTCCAAGCTGGGCTGTGTGCACGAACCCCCCGTTCAGCCCGACC
6841	GCTGCGCCTTATCCGGTAACTATCGTCTTGAGTCCAACCCGGTAAGACACGACTTATCGC
6901	CACTGGCAGCAGCCACTGGTAACAGGATTAGCAGAGCGAGGTATGTAGGCGGTGCTACAG
6961	AGTTCTTGAAGTGGTGGCCTAACTACGGCTACACTAGAAGGACAGTATTTGGTATCTGCG
7021	CTCTGCTGAAGCCAGTTACCTTCGGAAAAAGAGTTGGTAGCTCTTGATCCGGCAAACAAA
7081	CCACCGCTGGTAGCGGTGGTTTTTTTGTTTGCAAGCAGCAGATTACGCGCAGAAAAAAAG
7141	GATCTCAAGAAGATCCTTTGATCTTTTCTACGGGGTCTGACGCTCAGTGGAACGAAAACT
7201	CACGTTAAGGGATTTTG**GTCATGCATGATATATCTCCCAATTTGTGTAGGGCTTATTATG**
7261	**CACGCTTAAAAATAATAAAAGCAGACTTGACCTGATAGTTTGGCTGTGAGCAATTATGTG**
7321	**CTTAGTGCATCTAATCGCTTGAGTTAACGCCGGCGAAGCGGCGTCGGCTTGAACGAATTT**
7381	**CTAGCTAGACATTATTTGCCGACTACCTTGGTGATCTCGCCTTTCACGTAGTGGACAAAT**
7441	**TCTTCCAACTGATCTGCGCGCGAGGCCAAGCGATCTTCTTCTTGTCCAAGATAAGCCTGT**
7501	**CTAGCTTCAAGTATGACGGGCTGATACTGGGCCGGCAGGCGCTCCATTGCCCAGTCGGCA**
7561	**GCGACATCCTTCGGCGCGATTTTGCCGGTTACTGCGCTGTACCAAATGCGGGACAACGTA**
7621	**AGCACTACATTTCGCTCATCGCCAGCCCAGTCGGGCGGCGAGTTCCATAGCGTTAAGGTT**
7681	**TCATTTAGCGCCTCAAATAGATCCTGTTCAGGAACCGGATCAAAGAGTTCCTCCGCCGCT**
7741	**GGACCTACCAAGGCAACGCTATGTTCTCTTGCTTTTGTCAGCAAGATAGCCAGATCAATG**
7801	**TCGATCGTGGCTGGCTCGAAGATACCTGCAAGAATGTCATTGCGCTGCCATTCTCCAAAT**
7861	**TGCAGTTCGCGCTTAGCTGGATAACGCCACGGAATGATGTCGTCGTGCACAACAATGGTG**
7921	**ACTTCTACAGCGCGGAGAATCTCGCTCTCTCCAGGGGAAGCCGAAGTTTCCAAAAGGTCG**
7981	**TTGATCAAAGCTCGCCGCGTTGTTTCATCAAGCCTTACGGTCACCGTAACCAGCAAATCA**
8041	**ATATCACTGTGTGGCTTCAGGCCGCCATCCACTGCGGAGCCGTACAAATGTACGGCCAGC**
8101	**AACGTCGGTTCGAGATGGCGCTCGATGACGCCAACTACCTCTGATAGTTGAGTCGATACT**
8161	**TCGGCGATCACCGCTTCCCCCATGATGTTTAACTTTGTTTTAGGGCGACTGCCCTGCTGC**
8221	**GTAACATCGTTGCTGCTCCATAACATCAAACATCGACCCACGGCGTAACGCGCTTGCTGC**
8281	**TTGGATGCCCGAGGCATAGACTGTACCCCAAAAAAACATGTCATAACAAGAAGCCATGAA**
8341	**AACCGCCACTGCGCCGTTACCACCGCTGCGTTCGGTCAAGGTTCTGGACCAGTTGCGTGA**
8401	**CGGCAGTTACGCTACTTGCATTACAGCTTACGAACCGAACGAGGCTTATGTCCACTGGGT**
8461	**TCGTGCC**CGAAT**TGATCACAGGCAGCAACGCTCTGTCATCGTTACAATCAACATGCTACC**
8521	**CTCCGCGAGATCATCCGTGTTTCAAACCCGGCAGCTTAGTTGCCGTTCTTCCGAATAGCA**
8581	**TCGGTAACATGAGCAAAGTCTGCCGCCTTACAACGGCTCTCCCGCTGACGCCGTCCCGGA**
8641	**CTGATGGGCTGCCTGTATCGAGTGGTGATTTTGTGCCGAGCTGCCGGTCGGGGAGCTGTT**
8701	**GGCTGGCTGGTGGCAGGATATATTGTGGTGTAAACAAATTGACGCTTAGACAACTTAATA**

5' Base	Sequence
8761	**ACACATTGCGGACGTTTTTAATGTACTGAATTAACGCCGAATTGA**ATTATCAGCTTGCAT
8821	GCCGGT**CGATCTAGTAACATAGATGACACCGCGCGCGATAATTTATCCTAGTTTGCGCGC**
8881	**TATATTTTGTTTTCTATCGCGTATTAAATGTATAATTGCGGGACTCTAATCATAAAAACC**
8941	**CATCTCATAAATAACGTCATGCATTACATGTTAATTATTACATGCTTAACGTAATTCAAC**
9001	**AGAAATTATATGATAATCATCGCAAGACCGGCAACAGGATTCAATCTTAAGAAACTTTAT**
9061	**TGCCAAATGTTTGAACGATC**TGCTTGACTCTAGCTAGAGTCCGAACCCCAGAGTCCCGC**T**
9121	**CAGAAGAACTCGTCAAGAAGGCGATAGAAGGCGATGCGCTGCGAATCGGGAGCGGCGATA**
9181	**CCGTAAAGCACGAGGAAGCGGTCAGCCCATTCGCCGCCAAGCTCTTCAGCAATATCACGG**
9241	**GTAGCCAACGCTATGTCCTGATAGCGGTCCGCCACACCCAGCCGGCCACAGTCGATGAAT**
9301	**CCAGAAAAGCGGCCATTTTCCACCATGATATTCGGCAAGCAGGCATCGCCGTGGGTCACG**
9361	**ACGAGATCCTCGCCGTCGGGCATCCGCGCCTTGAGCCTGGCGAACAGTTCGGCTGGCGCG**
9421	**AGCCCCTGATGCTCTTCGTCCAGATCATCCTGATCGACAAGACCGGCTTCCATCCGAGTA**
9481	**CGTGCTCGCTCGATGCGATGTTTCGCTTGGTGGTCGAATGGGCAGGTAGCCGGATCAAGC**
9541	**GTATGCAGCCGCCGCATTGCATCAGCCATGATGGATACTTTCTCGGCAGGAGCAAGGTGA**
9601	**GATGACAGGAGATCCTGCCCCGGCACTTCGCCCAATAGCAGCCAGTCCCTTCCCGCTTCA**
9661	**GTGACAACGTCGAGCACAGCTGCGCAAGGAACGCCCGTCGTGGCCAGCCACGATAGCCGC**
9721	**GCTGCCTCGTCTTGGAGTTCATTCAGGGCACCGGACAGGTCGGTCTTGACAAAAAGAACC**
9781	**GGGCGCCCCTGCGCTGACAGCCGGAACACGGCGGCATCAGAGCAGCCGATTGTCTGTTGT**
9841	**GCCCAGTCATAGCCGAATAGCCTCTCCACCCAAGCGGCCGGAGAACCTGCGTGCAATCCA**
9901	**TCTTGTTCAATCAT**GCCTCGATCGAGT**TGAGAGTGAATATGAGACTCTAATTGGATACCG**
9961	**AGGGGAATTTATGGAACGTCAGTGGAGCATTTTTGACAAGAAATATTTGCTAGCTGATAG**
10021	**TGACCTTAGGCGACTTTTGAACGCGCAATAATGGTTTCTGACGTATGTGCTTAGCTCATT**
10081	**AAACTCCAGAAACCCGCGGCTGAGTGGCTCCTTCAACGTTGCGGTTCTGTCAGTTCCAAA**
10141	**CGTAAAACGGCTTGTCCCGCGTCATCGGCGGGGGTCATAACGTGACTCCCTTAATTCTC**A
10201	TGTATGATAATTCGAGGGTACCCGGGGATCCTCTAGAGGGCC

Appendix 6.3. Culture appearance of *HMG1* and control BY-2 transgenic cell lines

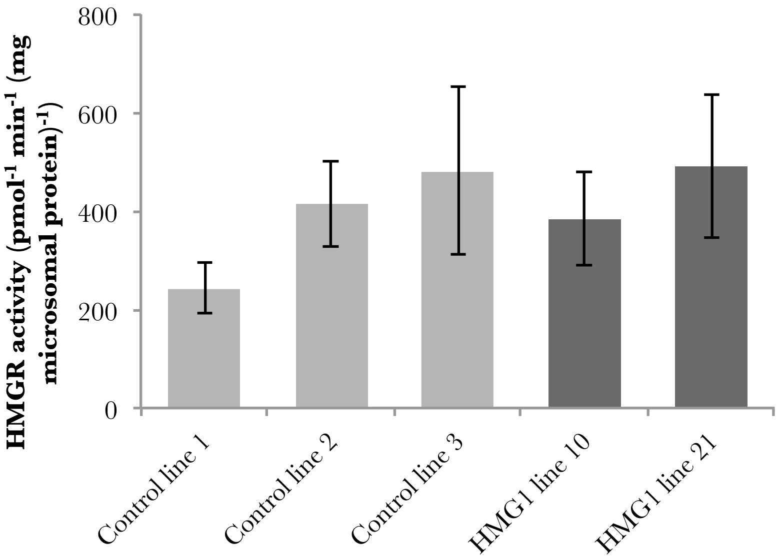
By seven days after subculture *HMG1* cultures became greyer than controls and stringy amalgamations of cells arose. Representative cultures of control line 1 and *HMG1* line 21 at seven days after subculture are shown. All control lines resembled control line 1 and *HMG1* line 10 resembled *HMG1* line 21 at this age.



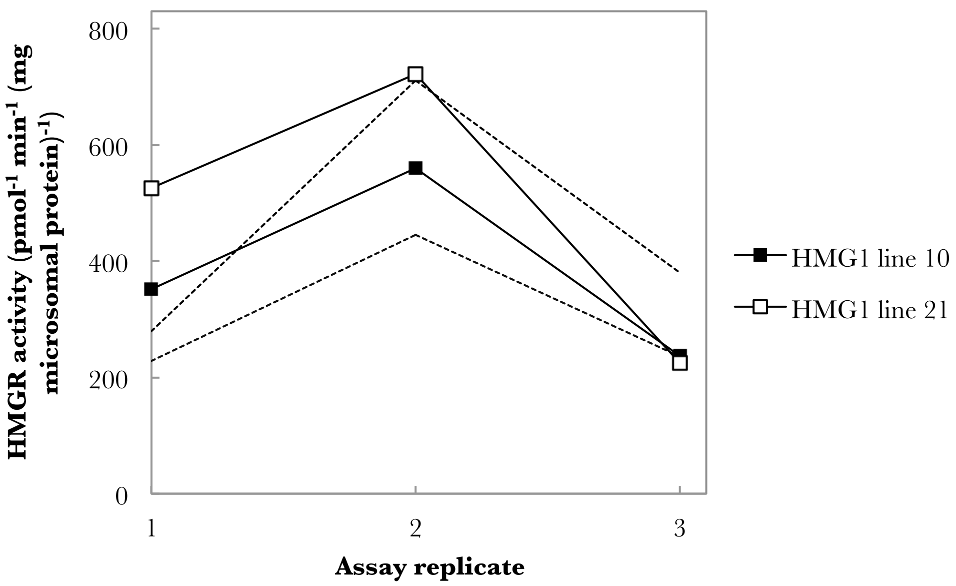
Control line 1 **_HMG1_ line 21**

Appendix 6.4. Absolute HMGR activity of transgenic *HMG1* and control BY-2 cell lines

HMGR activity in microsomal extracts from three biological replicates of each cell line were analysed following separate extractions and assays. There were no significant differences between any of the lines (student's *t* tests).



Absolute HMGR activity measurements of *HMG1* lines. Dashed lines indicated standard error of control measurements:



Appendix 6.5. pUB-*mCherry* expression vector sequence

Bases	Feature
5-637	*UBQ10* promoter
574-597	pUB-ins-F primer binding site
668-691	attB1 (Gateway recombination site)
706-723	mCherry-F primer binding site
706-1416	*mCherry*
1394-1416	mCherry-R primer binding site (antiparallel sequence)
1431-1455	attB2 (Gateway recombination site)
1515-1740	CaMV *35S* terminator
1518-1535	pUB-ins-R primer binding site (antiparallel sequence)
1794-2077	*nos* promoter
2098-2646	*Phosphinothricin N-acetyltransferase* (*ppt*)
2669-2922	*nos* terminator
2945-3276	Left transfer DNA border
9451-9655	Right transfer DNA border

5' Base	Sequence
1	TACC**CGACGAGTCAGTAATAAACGGCGTCAAAGTGGTTGCAGCCGGCACACACGAGTCGT**
61	**GTTTATCAACTCAAAGCACAAATACTTTTCCTCAACCTAAAAATAAGGCAATTAGCCAAA**
121	**AACAACTTTGCGTGTAAACAACGCTCAATACACGTGTCATTTTATTATTAGCTATTGCTT**
181	**CACCGCCTTAGCTTTCTCGTGACCTAGTCGTCCTCGTCTTTTCTTCTTCTTCTTCTATAA**
241	**AACAATACCCAAAGAGCTCTTCTTCTTCACAATTCAGATTTCAATTTCTCAAAATCTTAA**
301	**AAACTTTCTCTCAATTCTCTCTACCGTGATCAAGGTAAATTTCTGTGTTCCTTATTCTCT**
361	**CAAAATCTTCGATTTTGTTTTCGTTCGATCCCAATTTCGTATATGTTCTTTGGTTTAGAT**
421	**TCTGTTAATCTTAGATCGAAGACGATTTTCTGGGTTTGATCGTTAGATATCATCTTAATT**
481	**CTCGATTAGGGTTTCATAGATATCATCCGATTTGTTCAAATAATTTGAGTTTTGTCGAAT**
541	**AATTACTCTTCGATTTGTGATTTCTATCTAGATCTGGTGTTAGTTTCTAGTTTGTGCGAT**
601	**CGAATTTGTAGATTAATCTGAGTTTTTCTGATTAACA**CTCGAGTGCGGGATCCTCTAAGG
661	GCCCATC**CAAGTTTGTACAAAAAAGCAGGCT**CCGAATTCGCCCTT**ATGGTGAGCAAGGGC**
721	**GAGGAGGATAACATGGCCATCATCAAGGAGTTCATGCGCTTCAAGGTGCACATGGAGGGC**
781	**TCCGTGAACGGCCACGAGTTCGAGATCGAGGGCGAGGGCGAGGGCCGCCCCTACGAGGGC**
841	**ACCCAGACCGCCAAGCTGAAGGTGACCAAGGGTGGCCCCCTGCCCTTCGCCTGGGACATC**
901	**CTGTCCCCTCAGTTCATGTACGGCTCCAAGGCCTACGTGAAGCACCCCGCCGACATCCCC**
961	**GACTACTTGAAGCTGTCCTTCCCCGAGGGCTTCAAGTGGGAGCGCGTGATGAACTTCGAG**
1021	**GACGGCGGCGTGGTGACCGTGACCCAGGACTCCTCCCTGCAGGACGGCGAGTTCATCTAC**
1081	**AAGGTGAAGCTGCGCGGCACCAACTTCCCCTCCGACGGCCCCGTAATGCAGAAGAAGACC**
1141	**ATGGGCTGGGAGGCCTCCTCCGAGCGGATGTACCCCGAGGACGGCGCCCTGAAGGGCGAG**
1201	**ATCAAGCAGAGGCTGAAGCTGAAGGACGGCGGCCACTACGACGCTGAGGTCAAGACCACC**
1261	**TACAAGGCCAAGAAGCCCGTGCAGCTGCCCGGCGCCTACAACGTCAACATCAAGTTGGAC**
1321	**ATCACCTCCCACAACGAGGACTACACCATCGTGGAACAGTACGAACGCGCCGAGGGCCGC**
1381	**CACTCCACCGGCGGCATGGACGAGCTGTACAAGTAA**AAAGGGCGAATTCG**ACCCAGCTTT**
1441	**CTTGTACAAAGTGGT**GATGGGACGTCCGCGGAGATCTACGCGTGTCGACTCGAGATATCC
1501	AACTAGTTTATAAG**CGGCCATGCTAGAGTCCGCAAAAATCACCAGTCTCTCTCTACAAAT**
1561	**CTATCTCTCTCTATTTTTCTCCAGAATAATGTGTGAGTAGTTCCCAGATAAGGGAATTAG**
1621	**GGTTCTTATAGGGTTTCGCTCATGTGTTGAGCATATAAGAAACCCTTAGTATGTATTTGT**
1681	**ATTTGTAAAATACTTCTATCAATAAAATTTCTAATTCCTAAAACCAAAATCCAGTGACCT**
1741	GCAGGCATGCGACGTCGGGCCCTCTAGAGGATCCCCGGGTACCGCGAATTATC**GATCATG**
1801	**AGCGGAGAATTAAGGGAGTCACGTTATGACCCCCGCCGATGACGCGGGACAAGCCGTTTT**
1861	**ACGTTTGGAACTGACAGAACCGCAACGTTGAAGGAGCCACTGAGCCGCGGGTTTCTGGAG**
1921	**TTTAATGAGCTAAGCACATACGTCAGAAACCATTATTGCGCGTTCAAAAGTCGCCTAAGG**
1981	**TCACTATCAGCTAGCAAATATTTCTTGTCAAAAATGCTCCACTGACGTTCCATAAATTCC**

5' Base	Sequence
2041	**CCTCGGTATCCAATTAGAGTCTCATATTCACTCTCAA**CTCGATCGAGGGGATCTACC**ATG**
2101	**AGCCCAGAACGACGCCCGGCCGACATCCGCCGTGCCACCGAGGCGGACATGCCGGCGGTC**
2161	**TGCACCATCGTCAACCACTACATCGAGACAAGCACGGTCAACTTCCGTACCGAGCCGCAG**
2221	**GAACCGCAGGAGTGGACGGACGACCTCGTCCGTCTGCGGGAGCGCTATCCCTGGCTCGTC**
2281	**GCCGAGGTGGACGGCGAGGTCGCCGGCATCGCCTACGCGGGTCCCTGGAAGGCACGCAAC**
2341	**GCCTACGACTGGACGGCCGAGTCGACCGTGTACGTCTCCCCCCGCCACCAGCGGACGGGA**
2401	**CTGGGCTCCACGCTCTACACCCACCTGCTGAAGTCCCTGGAGGCACAGGGCTTCAAGAGC**
2461	**GTGGTCGCTGTCATCGGGCTGCCCAACGACCCGAGCGTGCGCATGCACGAGGCGCTCGGA**
2521	**TATGCCCCCCGCGGCATGCTGCGGGCGGCCGGCTTCAAGCACGGGAACTGGCATGACGTG**
2581	**GGTTTCTGGCAGCTGGACTTCAGCCTGCCGGTGCCGCCCCGTCCGGTCCTGCCCGTCACC**
2641	**GAAATC**TGATGACCCCTAGAGTCAAGCA**GATCGTTCAAACATTTGGCAATAAAGTTTCTT**
2701	**AAGATTGAATCCTGTTGCCGGTCTTGCGATGATTATCATATAATTTCTGTTGAATTACGT**
2761	**TAAGCATGTAATAATTAACATGTAATGCATGACGTTATTTATGAGATGGGTTTTTATGAT**
2821	**TAGAGTCCCGCAATTATACATTTAATACGCGATAGAAAACAAAATATAGCGCGCAAACTA**
2881	**GGATAAATTATCGCGCGCGGTGTCATCTATGTTACTAGATCG**ACCGGCATGCAAGCTGAT
2941	AATT**CAATTCGGCGTTAATTCAGTACATTAAAAACGTCCGCAATGTGTTATTAAGTTGTC**
3001	**TAAGCGTCAATTTGTTTACACCACAATATATCCTGCCACCAGCCAGCCAACAGCTCCCCG**
3061	**ACCGGCAGCTCGGCACAAAATCACCACTCGATACAGGCAGCCCATCAGTCCGGGACGGCG**
3121	**TCAGCGGGAGAGCCGTTGTAAGGCGGCAGACTTTGCTCATGTTACCGATGCTATTCGGAA**
3181	**GAACGGCAACTAAGCTGCCGGGTTTGAAACACGGATGATCTCGCGGAGGGTAGCATGTTG**
3241	**ATTGTAACGATGACAGAGCGTTGCTGCCTGTGATCA**ATTCGGGCACGAACCCAGTGGACA
3301	TAAGCCTGTTCGGTTCGTAAGCTGTAATGCAAGTAGCGTATGCGCTCACGCAACTGGTCC
3361	AGAACCTTGACCGAACGCAGCGGTGGTAACGGCGCAGTGGCGGTTTTCATGGCTTGTTAT
3421	GACTGTTTTTTTGGGGTACAGTCTATGCCTCGGGCATCCAAGCAGCAAGCGCGTTACGCC
3481	GTGGGTCGATGTTTGATGTTATGGAGCAGCAACGATGTTACGCAGCAGGGCAGTCGCCCT
3541	AAAACAAAGTTAAACATCATGGGGGAAGCGGTGATCGCCGAAGTATCGACTCAACTATCA
3601	GAGGTAGTTGGCGTCATCGAGCGCCATCTCGAACCGACGTTGCTGGCCGTACATTTGTAC
3661	GGCTCCGCAGTGGATGGCGGCCTGAAGCCACACAGTGATATTGATTTGCTGGTTACGGTG
3721	ACCGTAAGGCTTGATGAAACAACGCGGCGAGCTTTGATCAACGACCTTTTGGAAACTTCG
3781	GCTTCCCCTGGAGAGAGCGAGATTCTCCGCGCTGTAGAAGTCACCATTGTTGTGCACGAC
3841	GACATCATTCCGTGGCGTTATCCAGCTAAGCGCGAACTGCAATTTGGAGAATGGCAGCGC
3901	AATGACATTCTTGCAGGTATCTTCGAGCCAGCCACGATCGACATTGATCTGGCTATCTTG
3961	CTGACAAAAGCAAGAGAACATAGCGTTGCCTTGGTAGGTCCAGCGGCGGAGGAACTCTTT
4021	GATCCGGTTCCTGAACAGGATCTATTTGAGGCGCTAAATGAAACCTTAACGCTATGGAAC
4081	TCGCCGCCCGACTGGGCTGGCGATGAGCGAAATGTAGTGCTTACGTTGTCCCGCATTTGG
4141	TACAGCGCAGTAACCGGCAAAATCGCGCCGAAGGATGTCGCTGCCGACTGGGCAATGGAG
4201	CGCCTGCCGGCCCAGTATCAGCCCGTCATACTTGAAGCTAGACAGGCTTATCTTGGACAA
4261	GAAGAAGATCGCTTGGCCTCGCGCGCAGATCAGTTGGAAGAATTTGTCCACTACGTGAAA
4321	GGCGAGATCACCAAGGTAGTCGGCAAATAATGTCTAGCTAGAAATTCGTTCAAGCCGACG
4381	CCGCTTCGCGGCGCGGCTTAACTCAAGTCGTTAGATGCACTAAGCACATAATTGCTCACA
4441	GCCAAACTATCAGGTCAAGTCTGCTTTTATTATTTTTAAGCGTGCATAATAAGCCCTACA
4501	CAAATTGGGAGATATATCATGCATGACCAAAATCCCTTAACGTGAGTTTTCGTTCCACTG
4561	AGCGTCAGACCCCGTAGAAAAGATCAAAGGATCTTCTTGAGATCCTTTTTTTCTGCGCGT
4621	AATCTGCTGCTTGCAAACAAAAAAACCACCGCTACCAGCGGTGGTTTGTTTGCCGGATCA
4681	AGAGCTACCAACTCTTTTTCCGAAGGTAACTGGCTTCAGCAGAGCGCAGATACCAAATAC
4741	TGTCCTTCTAGTGTAGCCGTAGTTAGGCCACCACTTCAAGAACTCTGTAGCACCGCCTAC
4801	ATACCTCGCTCTGCTAATCCTGTTACCAGTGGCTGCTGCCAGTGGCGATAAGTCGTGTCT
4861	TACCGGGTTGGACTCAAGACGATAGTTACCGGATAAGGCGCAGCGGTCGGGCTGAACGGG
4921	GGGTTCGTGCACACAGCCCAGCTTGGAGCGAACGACCTACACCGAACTGAGATACCTACA
4981	GCGTGAGCTATGAGAAAGCGCCACGCTTCCCGAAGGGAGAAAGGCGGACAGGTATCCGGT
5041	AAGCGGCAGGGTCGGAACAGGAGAGCGCACGAGGGAGCTTCCAGGGGGAAACGCCTGGTA
5101	TCTTTATAGTCCTGTCGGGTTTCGCCACCTCTGACTTGAGCGTCGATTTTTGTGATGCTC
5161	GTCAGGGGGGCGGAGCCTATGGAAAAACGCCAGCAACGCGGCCTTTTTACGGTTCCTGGC
5221	CTTTTGCTGGCCTTTTGCTCACATGTTCTTTCCTGCGTTATCCCCTGATTCTGTGGATAA
5281	CCGTATTACCGCCTTTGAGTGAGCTGATACCGCTCGCCGCAGCCGAACGACCGAGCGCAG
5341	CGAGTCAGTGAGCGAGGAAGCGGAAGAGCGCCTGATGCGGTATTTTCTCCTTACGCATCT
5401	GTGCGGTATTTCACACCGCATATGGTGCACTCTCAGTACAATCTGCTCTGATGCCGCATA
5461	GTTAAGCCAGTATACACTCCGCTATCGCTACGTGACTGGGTCATGGCTGCGCCCCGACAC
5521	CCGCCAACACCCGCTGACGCGCCCTGACGGGCTTGTCTGCTCCCGGCATCCGCTTACAGA

5' Base	Sequence
5581	CAAGCTGTGACCGTCTCCGGGAGCTGCATGTGTCAGAGGTTTTCACCGTCATCACCGAAA
5641	CGCGCGAGGCAGGGTGCCTTGATGTGGGCGCCGGCGGTCGAGTGGCGACGGCGCGGCTTG
5701	TCCGCGCCCTGGTAGATTGCCTGGCCCTAGGCCAGCCATTTTTGAGCGGCCAGCGGCCGC
5761	GATAGGCCGACGCGAAGCGGCGGGGCGTAGGGAGCGCAGCGACCGAAGGGTAGGCGCTTT
5821	TTGCAGCTCTTCGGCTGTGCGCTGGCCAGACAGTTATGCACAGGCCAGGCGGGTTTTAAG
5881	AGTTTTAATAAGTTTTAAAGAGTTTTAGGCGGAAAAATCGCCTTTTTTCTCTTTTATATC
5941	AGTCACTTACATGTGTGACCGGTTCCCAATGTACGGCTTTGGGTTCCCAATGTACGGGTT
6001	CCGGTTCCCAATGTACGGCTTTGGGTTCCCAATGTACGTGCTATCCACAGGAAAGAGACC
6061	TTTTCGACCTTTTTCCCCTGCTAGGGCAATTTGCCCTAGCATCTGCTCCGTACATTAGGA
6121	ACCGGCGGATGCTTCGCCCTCGATCAGGTTGCGGTAGCGCATGACTAGGATCGGGCCAGC
6181	CTGCCCCGCCTCCTCCTTCAAATCGTACTCCGGCAGGTCATTTGACCCGATCAGCTTGCG
6241	CACGGTGAAACAGAACTTCTTGAACTCTCCGGCGCTGCCACTGCGTTCGTAGATCGTCTT
6301	GAACAACCATCTGGCTTCTGCCTTGCCTGCGGCGCGGCGTGCCAGGCGGTAGAGAAAACG
6361	GCCGATGCCGGGATCGATCAAAAAGTAATCGGGGTGAACCGTCAGCACGTCCGGGTTCTT
6421	GCCTTCTGTGATCTCGCGGTACATCCAATCAGCTAGCTCGATCTCGATGTACTCCGGCCG
6481	CCCGGTTTCGCTCTTTACGATCTTGTAGCGGCTAATCAAGGCTTCACCCTCGGATACCGT
6541	CACCAGGCGGCCGTTCTTGGCCTTCTTCGTACGCTGCATGGCAACGTGCGTGGTGTTTAA
6601	CCGAATGCAGGTTTCTACCAGGTCGTCTTTCTGCTTTCCGCCATCGGCTCGCCGGCAGAA
6661	CTTGAGTACGTCCGCAACGTGTGGACGGAACACGCGGCCGGGCTTGTCTCCCTTCCCTTC
6721	CCGGTATCGGTTCATGGATTCGGTTAGATGGGAAACCGCCATCAGTACCAGGTCGTAATC
6781	CCACACACTGGCCATGCCGGCCGGCCCTGCGGAAACCTCTACGTGCCCGTCTGGAAGCTC
6841	GTAGCGGATCACCTCGCCAGCTCGTCGGTCACGCTTCGACAGACGGAAAACGGCCACGTC
6901	CATGATGCTGCGACTATCGCGGGTGCCCACGTCATAGAGCATCGGAACGAAAAAATCTGG
6961	TTGCTCGTCGCCCTTGGGCGGCTTCCTAATCGACGGCGCACCGGCTGCCGGCGGTTGCCG
7021	GGATTCTTTGCGGATTCGATCAGCGGCCGCTTGCCACGATTCACCGGGGCGTGCTTCTGC
7081	CTCGATGCGTTGCCGCTGGGCGGCCTGCGCGGCCTTCAACTTCTCCACCAGGTCATCACC
7141	CAGCGCCGCGCCGATTTGTACCGGGCCGGATGGTTTGCGACCGTCACGCCGATTCCTCGG
7201	GCTTGGGGGTTCCAGTGCCATTGCAGGGCCGGCAGACAACCCAGCCGCTTACGCCTGGCC
7261	AACCGCCCGTTCCTCCACACATGGGGCATTCCACGGCGTCGGTGCCTGGTTGTTCTTGAT
7321	TTTCCATGCCGCCTCCTTTAGCCGCTAAAATTCATCTACTCATTTATTCATTTGCTCATT
7381	TACTCTGGTAGCTGCGCGATGTATTCAGATAGCAGCTCGGTAATGGTCTTGCCTTGGCGT
7441	ACCGCGTACATCTTCAGCTTGGTGTGATCCTCCGCCGGCAACTGAAAGTTGACCCGCTTC
7501	ATGGCTGGCGTGTCTGCCAGGCTGGCCAACGTTGCAGCCTTGCTGCTGCGTGCGCTCGGA
7561	CGGCCGGCACTTAGCGTGTTTGTGCTTTTGCTCATTTTCTCTTTACCTCATTAACTCAAA
7621	TGAGTTTTGATTTAATTTCAGCGGCCAGCGCCTGGACCTCGCGGGCAGCGTCGCCCTCGG
7681	GTTCTGATTCAAGAACGGTTGTGCCGGCGGCGGCAGTGCCTGGGTAGCTCACGCGCTGCG
7741	TGATACGGGACTCAAGAATGGGCAGCTCGTACCCGGCCAGCGCCTCGGCAACCTCACCGC
7801	CGATGCGCGTGCCTTTGATCGCCCGCGACACGACAAAGGCCGCTTGTAGCCTTCCATCCG
7861	TGACCTCAATGCGCTGCTTAACCAGCTCCACCAGGTCGGCGGTGGCCCATATGTCGTAAG
7921	GGCTTGGCTGCACCGGAATCAGCACGAAGTCGGCTGCCTTGATCGCGGACACAGCCAAGT
7981	CCGCCGCCTGGGGCGCTCCGTCGATCACTACGAAGTCGCGCCGGCCGATGGCCTTCACGT
8041	CGCGGTCAATCGTCGGGCGGTCGATGCCGACAACGGTTAGCGGTTGATCTTCCCGCACGG
8101	CCGCCCAATCGCGGGCACTGCCCTGGGGATCGGAATCGACTAACAGAACATCGGCCCCGG
8161	CGAGTTGCAGGGCGCGGGCTAGATGGGTTGCGATGGTCGTCTTGCCTGACCCGCCTTTCT
8221	GGTTAAGTACAGCGATAACCTTCATGCGTTCCCCTTGCGTATTTGTTTATTTACTCATCG
8281	CATCATATACGCAGCGACCGCATGACGCAAGCTGTTTTACTCAAATACACATCACCTTTT
8341	TAGACGGCGGCGCTCGGTTTCTTCAGCGGCCAAGCTGGCCGGCCAGGCCGCCAGCTTGGC
8401	ATCAGACAAACCGGCCAGGATTTCATGCAGCCGCACGGTTGAGACGTGCGCGGGCGGCTC
8461	GAACACGTACCCGGCCGCGATCATCTCCGCCTCGATCTCTTCGGTAATGAAAAACGGTTC
8521	GTCCTGGCCGTCCTGGTGCGGTTTCATGCTTGTTCCTCTTGGCGTTCATTCTCGGCGGCC
8581	GCCAGGGCGTCGGCCTCGGTCAATGCGTCCTCACGGAAGGCACCGCGCCGCCTGGCCTCG
8641	GTGGGCGTCACTTCCTCGCTGCGCTCAAGTGCGCGGTACAGGGTCGAGCGATGCACGCCA
8701	AGCAGTGCAGCCGCCTCTTTCACGGTGCGGCCTTCCTGGTCGATCAGCTCGCGGGCGTGC
8761	GCGATCTGTGCCGGGGTGAGGGTAGGGCGGGGGCCAAACTTCACGCCTCGGGCCTTGGCG
8821	GCCTCGCGCCCGCTCCGGGTGCGGTCGATGATTAGGGAACGCTCGAACTCGGCAATGCCG
8881	GCGAACACGGTCAACACCATGCGGCCGGCCGGCGTGGTGGTGTCGGCCCACGGCTCTGCC
8941	AGGCTACGCAGGCCCGCGCCGGCCTCCTGGATGCGCTCGGCAATGTCCAGTAGGTCGCGG
9001	GTGCTGCGGGCCAGGCGGTCTAGCCTGGTCACTGTCACAACGTCGCCAGGGCGTAGGTGG
9061	TCAAGCATCCTGGCCAGCTCCGGGCGGTCGCGCCTGGTGCCGGTGATCTTCTCGGAAAAC

5' Base	Sequence
9121	AGCTTGGTGCAGCCGGCCGCGTGCAGTTCGGCCCGTTGGTTGGTCAAGTCCTGGTCGTCG
9181	GTGCTGACGCGGGCATAGCCCAGCAGGCCAGCGGCGGCGCTCTTGTTCATGGCGTAATGT
9241	CTCCGGTTCTAGTCGCAAGTATTCTACTTTATGCGACTAAAACACGCGACAAGAAAACGC
9301	CAGGAAAAGGGCAGGGCGGCAGCCTGTCGCGTAACTTAGGACTTGTGCGACATGTCGTTT
9361	TCAGAAGACGGCTGCACTGAACGTCAGAAGCCGACTGCACTATAGCAGCGGAGGGGTTGG
9421	ATCAAAGTACTTTAAAGTACTTTAAAGTACTTTAAAGTAC**TTTGATCCCGAGGGGAACCC**
9481	**TGTGGTTGGCATGCACATACAAATGGACGAACGGATAAACCTTTTCACGCCCTTTTAAAT**
9541	**ATCCGTTATTCTAATAAACGCTCTTTTCTCTTAGGTTTACCCGCCAATATATCCTGTCAA**
9601	**ACACTGATAGTTTAAACTGAAGGCGGGAAACGACAATCTGATCCAAGCTCAAGCT**GCTCT
9661	AGCCAATACGCAAACCGCCTCTCCCCGCGCGTTGGCCGATTCATTAATGCAGCTGGCACG
9721	ACAGGTTTCCCGACTGGAAAGCGGGCAGTGAGCGCAACGCAATTAATGTGAGTTAGCTCA
9781	CTCATTAGGCACCCCAGGCTTTACACTTTATGCTTCCGGCTCGTATGTTGTGTGGAATTG
9841	TGAGCGGATAACAATTTCACACAGGAAACAGCTATGACCATGATTACGAATTCGAGCTCG
9901	G

Appendix 6.6. pUB-*HMG1* expression vector sequence

Bases	Feature
5-637	*UBQ10* promoter
574-597	pUB-ins-F primer binding site
668-691	attB1 (Gateway recombination site)
706-725	At-HMG1-F primer binding site
717-2495	*HMG1* (At1g76490/F15M4.1) coding sequence
2488-2510	At-HMG1-R primer binding site (antiparallel sequence)
2524-2548	attB2 (Gateway recombination site)
2608-2833	CaMV *35S* terminator
2611-2628	pUB-ins-R primer binding site (antiparallel sequence)
2887-3170	*nos* promoter
3191-3739	*ppt*
3761-4015	*nos* terminator
4038-4369	Left transfer DNA border
10544-10748	Right transfer DNA border

5' Base	Sequence
1	TACC**CGACGAGTCAGTAATAAACGGCGTCAAAGTGGTTGCAGCCGGCACACACGAGTCGT**
61	**GTTTATCAACTCAAAGCACAAATACTTTTCCTCAACCTAAAAATAAGGCAATTAGCCAAA**
121	**AACAACTTTGCGTGTAAACAACGCTCAATACACGTGTCATTTTATTATTAGCTATTGCTT**
181	**CACCGCCTTAGCTTTCTCGTGACCTAGTCGTCCTCGTCTTTTCTTCTTCTTCTTCTATAA**
241	**AACAATACCCAAAGAGCTCTTCTTCTTCACAATTCAGATTTCAATTTCTCAAAATCTTAA**
301	**AAACTTTCTCTCAATTCTCTCTACCGTGATCAAGGTAAATTTCTGTGTTCCTTATTCTCT**
361	**CAAAATCTTCGATTTTGTTTTCGTTCGATCCCAATTTCGTATATGTTCTTTGGTTTAGAT**
421	**TCTGTTAATCTTAGATCGAAGACGATTTTCTGGGTTTGATCGTTAGATATCATCTTAATT**
481	**CTCGATTAGGGTTTCATAGATATCATCCGATTTGTTCAAATAATTTGAGTTTTGTCGAAT**
541	**AATTACTCTTCGATTTGTGATTTCTATCTAGATCTGGTGTTAGTTTCTAGTTTGTGCGAT**
601	**CGAATTTGTAGATTAATCTGAGTTTTTCTGATTAACA**CTCGAGTGCGGGATCCTCTAAGG
661	GCCCATC**CAAGTTTGTACAAAAAAGCAGGCT**CCGAATTCGCCCTTCATTCCCTCCA**ATGG**
721	**ATCTCCGTCGGAGGCCTCCTAAACCACCGGTTACCAACAACAACAACTCCAACGGATCTT**
781	**TCCGTTCTTATCAGCCTCGCACTTCCGATGACGATCATCGTCGCCGGGCTACAACAATTG**
841	**CTCCTCCACCGAAAGCATCCGACGCGCTTCCTCTTCCGTTATATCTCACAAACGCCGTTT**
901	**TCTTCACGCTCTTCTTCTCCGTCGCGTATTACCTCCTCCACCGGTGGCGTGACAAGATCC**
961	**GTTACAATACGCCTCTTCACGTCGTCACTATCACAGAACTCGGCGCCATTATTGCTCTCA**
1021	**TCGCTTCGTTTATCTATCTCCTAGGGTTTTTTGGTATTGACTTTGTTCAGTCATTTATCT**
1081	**CACGTGCCTCTGGTGATGCTTGGGATCTCGCCGATACGATCGATGATGATGACCACCGCC**
1141	**TTGTCACGTGCTCTCCACCGACTCCGATCGTTTCCGTTGCTAAATTACCTAATCCGGAAC**
1201	**CTATTGTTACCGAATCGCTTCCTGAGGAAGACGAGGAGATTGTGAAATCGGTTATCGACG**
1261	**GAGTTATTCCATCGTACTCGCTTGAATCTCGTCTCGGTGATTGCAAAAGAGCGGCGTCGA**
1321	**TTCGTCGTGAGGCGTTGCAGAGAGTCACCGGGAGATCGATTGAAGGGTTACCGTTGGATG**
1381	**GATTTGATTATGAATCGATTTTGGGGCAATGCTGTGAGATGCCTGTTGGATACATTCAGA**
1441	**TTCCTGTTGGGATTGCTGGTCCATTGTTGCTTGATGGTTATGAGTACTCTGTTCCTATGG**
1501	**CTACAACCGAAGGTTGTTTGGTTGCTAGCACTAACAGAGGCTGCAAGGCTATGTTTATCT**
1561	**CTGGTGGCGCCACCAGTACCGTTCTTAAGGACGGTATGACCCGAGCACCTGTTGTTCGGT**
1621	**TCGCTTCGGCGAGACGAGCTTCGGAGCTTAAGTTTTTCTTGGAGAATCCAGAGAACTTTG**
1681	**ATACTTTGGCAGTAGTCTTCAACAGGTCGAGTAGATTTGCAAGACTGCAAAGTGTTAAAT**
1741	**GCACAATCGCGGGGAAGAATGCTTATGTAAGGTTCTGTTGTAGTACTGGTGATGCTATGG**
1801	**GGATGAATATGGTTTCTAAAGGTGTGCAGAATGTTCTTGAGTATCTTACCGATGATTTCC**
1861	**CTGACATGGATGTGATTGGAATCTCTGGTAACTTCTGTTCGGACAAGAAACCTGCTGCTG**
1921	**TGAACTGGATTGAGGGACGTGGTAAATCAGTTGTTTGCGAGGCTGTAATCAGAGGAGAGA**
1981	**TCGTGAACAAGGTCTTGAAAACGAGCGTGGCTGCTTTAGTCGAGCTCAACATGCTCAAGA**

5' Base	Sequence
2041	**ACCTAGCTGGCTCTGCTGTTGCAGGCTCTCTAGGTGGATTCAACGCTCATGCCAGTAACA**
2101	**TAGTGTCTGCTGTATTCATAGCTACTGGCCAAGATCCAGCTCAAAACGTGGAGAGTTCTC**
2161	**AATGCATCACCATGATGGAAGCTATTAATGACGGCAAAGATATCCATATCTCAGTCACTA**
2221	**TGCCATCTATCGAGGTGGGGACAGTGGGAGGAGGAACACAGCTTGCATCTCAATCAGCGT**
2281	**GTTTAAACCTGCTCGGAGTTAAAGGAGCAAGCACAGAGTCGCCGGGAATGAACGCAAGGA**
2341	**GGCTAGCGACGATCGTAGCCGGAGCAGTTTTAGCTGGAGAGTTATCTTTAATGTCAGCAA**
2401	**TTGCAGCTGGACAGCTTGTGAGAAGTCACATGAAATACAATAGATCCAGCCGAGACATCT**
2461	**CTGGAGCAACGACAACGACAACAACAACAACATGA**TCTGAATCTGAATCAAAGGGCGAAT
2521	TCG**ACCCAGCTTTCTTGTACAAAGTGGT**GATGGGACGTCCGCGGAGATCTACGCGTGTCG
2581	ACTCGAGATATCCAACTAGTTTATAAG**CGGCCATGCTAGAGTCCGCAAAAATCACCAGTC**
2641	**TCTCTCTACAAATCTATCTCTCTCTATTTTTCTCCAGAATAATGTGTGAGTAGTTCCCAG**
2701	**ATAAGGGAATTAGGGTTCTTATAGGGTTTCGCTCATGTGTTGAGCATATAAGAAACCCTT**
2761	**AGTATGTATTTGTATTTGTAAAATACTTCTATCAATAAAATTTCTAATTCCTAAAACCAA**
2821	**AATCCAGTGACCT**GCAGGCATGCGACGTCGGGCCCTCTAGAGGATCCCCGGGTACCGCGA
2881	ATTATC**GATCATGAGCGGAGAATTAAGGGAGTCACGTTATGACCCCCGCCGATGACGCGG**
2941	**GACAAGCCGTTTTACGTTTGGAACTGACAGAACCGCAACGTTGAAGGAGCCACTGAGCCG**
3001	**CGGGTTTCTGGAGTTTAATGAGCTAAGCACATACGTCAGAAACCATTATTGCGCGTTCAA**
3061	**AAGTCGCCTAAGGTCACTATCAGCTAGCAAATATTTCTTGTCAAAAATGCTCCACTGACG**
3121	**TTCCATAAATTCCCCTCGGTATCCAATTAGAGTCTCATATTCACTCTCAA**CTCGATCGAG
3181	GGGATCTACC**ATGAGCCCAGAACGACGCCCGGCCGACATCCGCCGTGCCACCGAGGCGGA**
3241	**CATGCCGGCGGTCTGCACCATCGTCAACCACTACATCGAGACAAGCACGGTCAACTTCCG**
3301	**TACCGAGCCGCAGGAACCGCAGGAGTGGACGGACGACCTCGTCCGTCTGCGGGAGCGCTA**
3361	**TCCCTGGCTCGTCGCCGAGGTGGACGGCGAGGTCGCCGGCATCGCCTACGCGGGTCCCTG**
3421	**GAAGGCACGCAACGCCTACGACTGGACGGCCGAGTCGACCGTGTACGTCTCCCCCCGCCA**
3481	**CCAGCGGACGGGACTGGGCTCCACGCTCTACACCCACCTGCTGAAGTCCCTGGAGGCACA**
3541	**GGGCTTCAAGAGCGTGGTCGCTGTCATCGGGCTGCCCAACGACCCGAGCGTGCGCATGCA**
3601	**CGAGGCGCTCGGATATGCCCCCCGCGGCATGCTGCGGGCGGCCGGCTTCAAGCACGGGAA**
3661	**CTGGCATGACGTGGGTTTCTGGCAGCTGGACTTCAGCCTGCCGGTGCCGCCCCGTCCGGT**
3721	**CCTGCCCGTCACCGAAATC**TGATGACCCCTAGAGTCAAGCA**GATCGTTCAAACATTTGGC**
3781	**AATAAAGTTTCTTAAGATTGAATCCTGTTGCCGGTCTTGCGATGATTATCATATAATTTC**
3841	**TGTTGAATTACGTTAAGCATGTAATAATTAACATGTAATGCATGACGTTATTTATGAGAT**
3901	**GGGTTTTTATGATTAGAGTCCCGCAATTATACATTTAATACGCGATAGAAAACAAAATAT**
3961	**AGCGCGCAAACTAGGATAAATTATCGCGCGCGGTGTCATCTATGTTACTAGATCG**ACCGG
4021	CATGCAAGCTGATAATT**CAATTCGGCGTTAATTCAGTACATTAAAAACGTCCGCAATGTG**
4081	**TTATTAAGTTGTCTAAGCGTCAATTTGTTTACACCACAATATATCCTGCCACCAGCCAGC**
4141	**CAACAGCTCCCCGACCGGCAGCTCGGCACAAAATCACCACTCGATACAGGCAGCCCATCA**
4201	**GTCCGGGACGGCGTCAGCGGGAGAGCCGTTGTAAGGCGGCAGACTTTGCTCATGTTACCG**
4261	**ATGCTATTCGGAAGAACGGCAACTAAGCTGCCGGGTTTGAAACACGGATGATCTCGCGGA**
4321	**GGGTAGCATGTTGATTGTAACGATGACAGAGCGTTGCTGCCTGTGATCA**ATTCGGGCACG
4381	AACCCAGTGGACATAAGCCTGTTCGGTTCGTAAGCTGTAATGCAAGTAGCGTATGCGCTC
4441	ACGCAACTGGTCCAGAACCTTGACCGAACGCAGCGGTGGTAACGGCGCAGTGGCGGTTTT
4501	CATGGCTTGTTATGACTGTTTTTTTGGGGTACAGTCTATGCCTCGGGCATCCAAGCAGCA
4561	AGCGCGTTACGCCGTGGGTCGATGTTTGATGTTATGGAGCAGCAACGATGTTACGCAGCA
4621	GGGCAGTCGCCCTAAAACAAAGTTAAACATCATGGGGGAAGCGGTGATCGCCGAAGTATC
4681	GACTCAACTATCAGAGGTAGTTGGCGTCATCGAGCGCCATCTCGAACCGACGTTGCTGGC
4741	CGTACATTTGTACGGCTCCGCAGTGGATGGCGGCCTGAAGCCACACAGTGATATTGATTT
4801	GCTGGTTACGGTGACCGTAAGGCTTGATGAAACAACGCGGCGAGCTTTGATCAACGACCT
4861	TTTGGAAACTTCGGCTTCCCCTGGAGAGAGCGAGATTCTCCGCGCTGTAGAAGTCACCAT
4921	TGTTGTGCACGACGACATCATTCCGTGGCGTTATCCAGCTAAGCGCGAACTGCAATTTGG
4981	AGAATGGCAGCGCAATGACATTCTTGCAGGTATCTTCGAGCCAGCCACGATCGACATTGA
5041	TCTGGCTATCTTGCTGACAAAAGCAAGAGAACATAGCGTTGCCTTGGTAGGTCCAGCGGC
5101	GGAGGAACTCTTTGATCCGGTTCCTGAACAGGATCTATTTGAGGCGCTAAATGAAACCTT
5161	AACGCTATGGAACTCGCCGCCCGACTGGGCTGGCGATGAGCGAAATGTAGTGCTTACGTT
5221	GTCCCGCATTTGGTACAGCGCAGTAACCGGCAAAATCGCGCCGAAGGATGTCGCTGCCGA
5281	CTGGGCAATGGAGCGCCTGCCGGCCCAGTATCAGCCCGTCATACTTGAAGCTAGACAGGC
5341	TTATCTTGGACAAGAAGAAGATCGCTTGGCCTCGCGCGCAGATCAGTTGGAAGAATTTGT
5401	CCACTACGTGAAAGGCGAGATCACCAAGGTAGTCGGCAAATAATGTCTAGCTAGAAATTC
5461	GTTCAAGCCGACGCCGCTTCGCGGCGCGGCTTAACTCAAGTCGTTAGATGCACTAAGCAC
5521	ATAATTGCTCACAGCCAAACTATCAGGTCAAGTCTGCTTTTATTATTTTTAAGCGTGCAT

5' Base	Sequence
5581	AATAAGCCCTACACAAATTGGGAGATATATCATGCATGACCAAAATCCCTTAACGTGAGT
5641	TTTCGTTCCACTGAGCGTCAGACCCCGTAGAAAAGATCAAAGGATCTTCTTGAGATCCTT
5701	TTTTTCTGCGCGTAATCTGCTGCTTGCAAACAAAAAAACCACCGCTACCAGCGGTGGTTT
5761	GTTTGCCGGATCAAGAGCTACCAACTCTTTTTCCGAAGGTAACTGGCTTCAGCAGAGCGC
5821	AGATACCAAATACTGTCCTTCTAGTGTAGCCGTAGTTAGGCCACCACTTCAAGAACTCTG
5881	TAGCACCGCCTACATACCTCGCTCTGCTAATCCTGTTACCAGTGGCTGCTGCCAGTGGCG
5941	ATAAGTCGTGTCTTACCGGGTTGGACTCAAGACGATAGTTACCGGATAAGGCGCAGCGGT
6001	CGGGCTGAACGGGGGGTTCGTGCACACAGCCCAGCTTGGAGCGAACGACCTACACCGAAC
6061	TGAGATACCTACAGCGTGAGCTATGAGAAAGCGCCACGCTTCCCGAAGGGAGAAAGGCGG
6121	ACAGGTATCCGGTAAGCGGCAGGGTCGGAACAGGAGAGCGCACGAGGGAGCTTCCAGGGG
6181	GAAACGCCTGGTATCTTTATAGTCCTGTCGGGTTTCGCCACCTCTGACTTGAGCGTCGAT
6241	TTTTGTGATGCTCGTCAGGGGGGCGGAGCCTATGGAAAAACGCCAGCAACGCGGCCTTTT
6301	TACGGTTCCTGGCCTTTTGCTGGCCTTTTGCTCACATGTTCTTTCCTGCGTTATCCCCTG
6361	ATTCTGTGGATAACCGTATTACCGCCTTTGAGTGAGCTGATACCGCTCGCCGCAGCCGAA
6421	CGACCGAGCGCAGCGAGTCAGTGAGCGAGGAAGCGGAAGAGCGCCTGATGCGGTATTTTC
6481	TCCTTACGCATCTGTGCGGTATTTCACACCGCATATGGTGCACTCTCAGTACAATCTGCT
6541	CTGATGCCGCATAGTTAAGCCAGTATACACTCCGCTATCGCTACGTGACTGGGTCATGGC
6601	TGCGCCCCGACACCCGCCAACACCCGCTGACGCGCCCTGACGGGCTTGTCTGCTCCCGGC
6661	ATCCGCTTACAGACAAGCTGTGACCGTCTCCGGGAGCTGCATGTGTCAGAGGTTTTCACC
6721	GTCATCACCGAAACGCGCGAGGCAGGGTGCCTTGATGTGGGCGCCGGCGGTCGAGTGGCG
6781	ACGGCGCGGCTTGTCCGCGCCCTGGTAGATTGCCTGGCCCTAGGCCAGCCATTTTTGAGC
6841	GGCCAGCGGCCGCGATAGGCCGACGCGAAGCGGCGGGGCGTAGGGAGCGCAGCGACCGAA
6901	GGGTAGGCGCTTTTTGCAGCTCTTCGGCTGTGCGCTGGCCAGACAGTTATGCACAGGCCA
6961	GGCGGGTTTTAAGAGTTTTAATAAGTTTTAAAGAGTTTTAGGCGGAAAAATCGCCTTTTT
7021	TCTCTTTTATATCAGTCACTTACATGTGTGACCGGTTCCCAATGTACGGCTTTGGGTTCC
7081	CAATGTACGGGTTCCGGTTCCCAATGTACGGCTTTGGGTTCCCAATGTACGTGCTATCCA
7141	CAGGAAAGAGACCTTTTCGACCTTTTTCCCCTGCTAGGGCAATTTGCCCTAGCATCTGCT
7201	CCGTACATTAGGAACCGGCGGATGCTTCGCCCTCGATCAGGTTGCGGTAGCGCATGACTA
7261	GGATCGGGCCAGCCTGCCCCGCCTCCTCCTTCAAATCGTACTCCGGCAGGTCATTTGACC
7321	CGATCAGCTTGCGCACGGTGAAACAGAACTTCTTGAACTCTCCGGCGCTGCCACTGCGTT
7381	CGTAGATCGTCTTGAACAACCATCTGGCTTCTGCCTTGCCTGCGGCGCGGCGTGCCAGGC
7441	GGTAGAGAAAACGGCCGATGCCGGGATCGATCAAAAAGTAATCGGGGTGAACCGTCAGCA
7501	CGTCCGGGTTCTTGCCTTCTGTGATCTCGCGGTACATCCAATCAGCTAGCTCGATCTCGA
7561	TGTACTCCGGCCGCCCGGTTTCGCTCTTTACGATCTTGTAGCGGCTAATCAAGGCTTCAC
7621	CCTCGGATACCGTCACCAGGCGGCCGTTCTTGGCCTTCTTCGTACGCTGCATGGCAACGT
7681	GCGTGGTGTTTAACCGAATGCAGGTTTCTACCAGGTCGTCTTTCTGCTTTCCGCCATCGG
7741	CTCGCCGGCAGAACTTGAGTACGTCCGCAACGTGTGGACGGAACACGCGGCCGGGCTTGT
7801	CTCCCTTCCCTTCCCGGTATCGGTTCATGGATTCGGTTAGATGGGAAACCGCCATCAGTA
7861	CCAGGTCGTAATCCCACACACTGGCCATGCCGGCCGGCCCTGCGGAAACCTCTACGTGCC
7921	CGTCTGGAAGCTCGTAGCGGATCACCTCGCCAGCTCGTCGGTCACGCTTCGACAGACGGA
7981	AAACGGCCACGTCCATGATGCTGCGACTATCGCGGGTGCCCACGTCATAGAGCATCGGAA
8041	CGAAAAAATCTGGTTGCTCGTCGCCCTTGGGCGGCTTCCTAATCGACGGCGCACCGGCTG
8101	CCGGCGGTTGCCGGGATTCTTTGCGGATTCGATCAGCGGCCGCTTGCCACGATTCACCGG
8161	GGCGTGCTTCTGCCTCGATGCGTTGCCGCTGGGCGGCCTGCGCGGCCTTCAACTTCTCCA
8221	CCAGGTCATCACCCAGCGCCGCGCCGATTTGTACCGGGCCGGATGGTTTGCGACCGTCAC
8281	GCCGATTCCTCGGGCTTGGGGGTTCCAGTGCCATTGCAGGGCCGGCAGACAACCCAGCCG
8341	CTTACGCCTGGCCAACCGCCCGTTCCTCCACACATGGGGCATTCCACGGCGTCGGTGCCT
8401	GGTTGTTCTTGATTTTCCATGCCGCCTCCTTTAGCCGCTAAAATTCATCTACTCATTTAT
8461	TCATTTGCTCATTTACTCTGGTAGCTGCGCGATGTATTCAGATAGCAGCTCGGTAATGGT
8521	CTTGCCTTGGCGTACCGCGTACATCTTCAGCTTGGTGTGATCCTCCGCCGGCAACTGAAA
8581	GTTGACCCGCTTCATGGCTGGCGTGTCTGCCAGGCTGGCCAACGTTGCAGCCTTGCTGCT
8641	GCGTGCGCTCGGACGGCCGGCACTTAGCGTGTTTGTGCTTTTGCTCATTTTCTCTTTACC
8701	TCATTAACTCAAATGAGTTTTGATTTAATTTCAGCGGCCAGCGCCTGGACCTCGCGGGCA
8761	GCGTCGCCCTCGGGTTCTGATTCAAGAACGGTTGTGCCGGCGGCGGCAGTGCCTGGGTAG
8821	CTCACGCGCTGCGTGATACGGGACTCAAGAATGGGCAGCTCGTACCCGGCCAGCGCCTCG
8881	GCAACCTCACCGCCGATGCGCGTGCCTTTGATCGCCCGCGACACGACAAAGGCCGCTTGT
8941	AGCCTTCCATCCGTGACCTCAATGCGCTGCTTAACCAGCTCCACCAGGTCGGCGGTGGCC
9001	CATATGTCGTAAGGGCTTGGCTGCACCGGAATCAGCACGAAGTCGGCTGCCTTGATCGCG
9061	GACACAGCCAAGTCCGCCGCCTGGGGCGCTCCGTCGATCACTACGAAGTCGCGCCGGCCG

5' Base	Sequence
9121	ATGGCCTTCACGTCGCGGTCAATCGTCGGGCGGTCGATGCCGACAACGGTTAGCGGTTGA
9181	TCTTCCCGCACGGCCGCCCAATCGCGGGCACTGCCCTGGGGATCGGAATCGACTAACAGA
9241	ACATCGGCCCCGGCGAGTTGCAGGGCGCGGGCTAGATGGGTTGCGATGGTCGTCTTGCCT
9301	GACCCGCCTTTCTGGTTAAGTACAGCGATAACCTTCATGCGTTCCCCTTGCGTATTTGTT
9361	TATTTACTCATCGCATCATATACGCAGCGACCGCATGACGCAAGCTGTTTTACTCAAATA
9421	CACATCACCTTTTTAGACGGCGGCGCTCGGTTTCTTCAGCGGCCAAGCTGGCCGGCCAGG
9481	CCGCCAGCTTGGCATCAGACAAACCGGCCAGGATTTCATGCAGCCGCACGGTTGAGACGT
9541	GCGCGGGCGGCTCGAACACGTACCCGGCCGCGATCATCTCCGCCTCGATCTCTTCGGTAA
9601	TGAAAAACGGTTCGTCCTGGCCGTCCTGGTGCGGTTTCATGCTTGTTCCTCTTGGCGTTC
9661	ATTCTCGGCGGCCGCCAGGGCGTCGGCCTCGGTCAATGCGTCCTCACGGAAGGCACCGCG
9721	CCGCCTGGCCTCGGTGGGCGTCACTTCCTCGCTGCGCTCAAGTGCGCGGTACAGGGTCGA
9781	GCGATGCACGCCAAGCAGTGCAGCCGCCTCTTTCACGGTGCGGCCTTCCTGGTCGATCAG
9841	CTCGCGGGCGTGCGCGATCTGTGCCGGGGTGAGGGTAGGGCGGGGGCCAAACTTCACGCC
9901	TCGGGCCTTGGCGGCCTCGCGCCCGCTCCGGGTGCGGTCGATGATTAGGGAACGCTCGAA
9961	CTCGGCAATGCCGGCGAACACGGTCAACACCATGCGGCCGGCCGGCGTGGTGGTGTCGGC
10021	CCACGGCTCTGCCAGGCTACGCAGGCCCGCGCCGGCCTCCTGGATGCGCTCGGCAATGTC
10081	CAGTAGGTCGCGGGTGCTGCGGGCCAGGCGGTCTAGCCTGGTCACTGTCACAACGTCGCC
10141	AGGGCGTAGGTGGTCAAGCATCCTGGCCAGCTCCGGGCGGTCGCGCCTGGTGCCGGTGAT
10201	CTTCTCGGAAAACAGCTTGGTGCAGCCGGCCGCGTGCAGTTCGGCCCGTTGGTTGGTCAA
10261	GTCCTGGTCGTCGGTGCTGACGCGGGCATAGCCCAGCAGGCCAGCGGCGGCGCTCTTGTT
10321	CATGGCGTAATGTCTCCGGTTCTAGTCGCAAGTATTCTACTTTATGCGACTAAAACACGC
10381	GACAAGAAAACGCCAGGAAAAGGGCAGGGCGGCAGCCTGTCGCGTAACTTAGGACTTGTG
10441	CGACATGTCGTTTTCAGAAGACGGCTGCACTGAACGTCAGAAGCCGACTGCACTATAGCA
10501	GCGGAGGGGTTGGATCAAAGTACTTTAAAGTACTTTAAAGTACTTTAAAGTAC**TTTGATC**
10561	**CCGAGGGGAACCCTGTGGTTGGCATGCACATACAAATGGACGAACGGATAAACCTTTTCA**
10621	**CGCCCTTTTAAATATCCGTTATTCTAATAAACGCTCTTTTCTCTTAGGTTTACCCGCCAA**
10681	**TATATCCTGTCAAACACTGATAGTTTAAACTGAAGGCGGGAAACGACAATCTGATCCAAG**
10741	**CTCAAGCT**GCTCTAGCCAATACGCAAACCGCCTCTCCCCGCGCGTTGGCCGATTCATTAA
10801	TGCAGCTGGCACGACAGGTTTCCCGACTGGAAAGCGGGCAGTGAGCGCAACGCAATTAAT
10861	GTGAGTTAGCTCACTCATTAGGCACCCCAGGCTTTACACTTTATGCTTCCGGCTCGTATG
10921	TTGTGTGGAATTGTGAGCGGATAACAATTTCACACAGGAAACAGCTATGACCATGATTAC
10981	GAATTCGAGCTCGG

Appendix 6.7. pUB-*tHMG1* expression vector sequence

Bases	Feature
5-637	*UBQ10* promoter
574-597	pUB-ins-F primer binding site
668-691	attB1 (Gateway recombination site)
706-726	Truncated_At-HMG1-F primer binding site
706-1998	N-terminal truncated *HMG1* (At1g76490/F15M4.1; *tHMG1*) coding sequence. (T→C synonymous mutation at 81 bp of *tHMG1* (786 bp of vector) is boxed.)
1991-2013	At-HMG1-R primer binding site (antiparallel sequence)
2027-2051	attB2 (Gateway recombination site)
2111-2336	CaMV *35S* terminator
2114-2131	pUB-ins-R primer binding site (antiparallel sequence)
2390-2673	*nos* promoter
2694-3243	*Phosphinothricin N-acetyltransferase*
3265-3518	*nos* terminator
3541-3872	Left transfer DNA border
10047-10251	Right transfer DNA border

5' Base	Sequence
1	TACC**CGACGAGTCAGTAATAAACGGCGTCAAAGTGGTTGCAGCCGGCACACACGAGTCGT**
61	**GTTTATCAACTCAAAGCACAAATACTTTTCCTCAACCTAAAAATAAGGCAATTAGCCAAA**
121	**AACAACTTTGCGTGTAAACAACGCTCAATACACGTGTCATTTTATTATTAGCTATTGCTT**
181	**CACCGCCTTAGCTTTCTCGTGACCTAGTCGTCCTCGTCTTTTCTTCTTCTTCTTCTATAA**
241	**AACAATACCCAAAGAGCTCTTCTTCTTCACAATTCAGATTTCAATTTCTCAAAATCTTAA**
301	**AAACTTTCTCTCAATTCTCTCTACCGTGATCAAGGTAAATTTCTGTGTTCCTTATTCTCT**
361	**CAAAATCTTCGATTTTGTTTTCGTTCGATCCCAATTTCGTATATGTTCTTTGGTTTAGAT**
421	**TCTGTTAATCTTAGATCGAAGACGATTTTCTGGGTTTGATCGTTAGATATCATCTTAATT**
481	**CTCGATTAGGGTTTCATAGATATCATCCGATTTGTTCAAATAATTTGAGTTTTGTCGAAT**
541	**AATTACTCTTCGATTTGTGATTTCTATCTAGATCTGGTGTTAGTTTCTAGTTTGTGCGAT**
601	**CGAATTTGTAGATTAATCTGAGTTTTTCTGATTAACA**CTCGAGTGCGGGATCCTCTAAGG
661	GCCCATC**CAAGTTTGTACAAAAAAGCAGGCT**CCGAATTCGCCCTT**ATGGTTACCGAATCG**
721	**CTTCCTGAGGAAGACGAGGAGATTGTGAAATCGGTTATCGACGGAGTTATTCCATCGTAC**
781	**TCGCTCGAATCTCGTCTCGGTGATTGCAAAAGAGCGGCGTCGATTCGTCGTGAGGCGTTG**
841	**CAGAGAGTCACCGGGAGATCGATTGAAGGGTTACCGTTGGATGGATTTGATTATGAATCG**
901	**ATTTTGGGGCAATGCTGTGAGATGCCTGTTGGATACATTCAGATTCCTGTTGGGATTGCT**
961	**GGTCCATTGTTGCTTGATGGTTATGAGTACTCTGTTCCTATGGCTACAACCGAAGGTTGT**
1021	**TTGGTTGCTAGCACTAACAGAGGCTGCAAGGCTATGTTTATCTCTGGTGGCGCCACCAGT**
1081	**ACCGTTCTTAAGGACGGTATGACCCGAGCACCTGTTGTTCGGTTCGCTTCGGCGAGACGA**
1141	**GCTTCGGAGCTTAAGTTTTTCTTGGAGAATCCAGAGAACTTTGATACTTTGGCAGTAGTC**
1201	**TTCAACAGGTCGAGTAGATTTGCAAGACTGCAAAGTGTTAAATGCACAATCGCGGGGAAG**
1261	**AATGCTTATGTAAGGTTCTGTTGTAGTACTGGTGATGCTATGGGGATGAATATGGTTTCT**
1321	**AAAGGTGTGCAGAATGTTCTTGAGTATCTTACCGATGATTTCCCTGACATGGATGTGATT**
1381	**GGAATCTCTGGTAACTTCTGTTCGGACAAGAAACCTGCTGCTGTGAACTGGATTGAGGGA**
1441	**CGTGGTAAATCAGTTGTTTGCGAGGCTGTAATCAGAGGAGAGATCGTGAACAAGGTCTTG**
1501	**AAAACGAGCGTGGCTGCTTTAGTCGAGCTCAACATGCTCAAGAACCTAGCTGGCTCTGCT**
1561	**GTTGCAGGCTCTCTAGGTGGATTCAACGCTCATGCCAGTAACATAGTGTCTGCTGTATTC**
1621	**ATAGCTACTGGCCAAGATCCAGCTCAAAACGTGGAGAGTTCTCAATGCATCACCATGATG**
1681	**GAAGCTATTAATGACGGCAAAGATATCCATATCTCAGTCACTATGCCATCTATCGAGGTG**
1741	**GGGACAGTGGGAGGAGGAACACAGCTTGCATCTCAATCAGCGTGTTTAAACCTGCTCGGA**
1801	**GTTAAAGGAGCAAGCACAGAGTCGCCGGGAATGAACGCAAGGAGGCTAGCGACGATCGTA**
1861	**GCCGGAGCAGTTTTAGCTGGAGAGTTATCTTTAATGTCAGCAATTGCAGCTGGACAGCTT**

5' Base	Sequence
1921	**GTGAGAAGTCACATGAAATACAATAGATCCAGCCGAGACATCTCTGGAGCAACGACAACG**
1981	**ACAACAACAACAACATGA**TCTGAATCTGAATCAAAGGGCGAATTCG**ACCCAGCTTTCTTG**
2041	**TACAAAGTGGT**GATGGGACGTCCGCGGAGATCTACGCGTGTCGACTCGAGATATCCAACT
2101	AGTTTATAAG**CGGCCATGCTAGAGTCCGCAAAAATCACCAGTCTCTCTCTACAAATCTAT**
2161	**CTCTCTCTATTTTTCTCCAGAATAATGTGTGAGTAGTTCCCAGATAAGGGAATTAGGGTT**
2221	**CTTATAGGGTTTCGCTCATGTGTTGAGCATATAAGAAACCCTTAGTATGTATTTGTATTT**
2281	**GTAAAATACTTCTATCAATAAAATTTCTAATTCCTAAAACCAAAATCCAGTGACCT**GCAG
2341	GCATGCGACGTCGGGCCCTCTAGAGGATCCCCGGGTACCGCGAATTATC**GATCATGAGCG**
2401	**GAGAATTAAGGGAGTCACGTTATGACCCCCGCCGATGACGCGGGACAAGCCGTTTTACGT**
2461	**TTGGAACTGACAGAACCGCAACGTTGAAGGAGCCACTGAGCCGCGGGTTTCTGGAGTTTA**
2521	**ATGAGCTAAGCACATACGTCAGAAACCATTATTGCGCGTTCAAAAGTCGCCTAAGGTCAC**
2581	**TATCAGCTAGCAAATATTTCTTGTCAAAAATGCTCCACTGACGTTCCATAAATTCCCCTC**
2641	**GGTATCCAATTAGAGTCTCATATTCACTCTCAA**CTCGATCGAGGGGATCTACC**ATGAGCC**
2701	**CAGAACGACGCCCGGCCGACATCCGCCGTGCCACCGAGGCGGACATGCCGGCGGTCTGCA**
2761	**CCATCGTCAACCACTACATCGAGACAAGCACGGTCAACTTCCGTACCGAGCCGCAGGAAC**
2821	**CGCAGGAGTGGACGGACGACCTCGTCCGTCTGCGGGAGCGCTATCCCTGGCTCGTCGCCG**
2881	**AGGTGGACGGCGAGGTCGCCGGCATCGCCTACGCGGGTCCCTGGAAGGCACGCAACGCCT**
2941	**ACGACTGGACGGCCGAGTCGACCGTGTACGTCTCCCCCCGCCACCAGCGGACGGGACTGG**
3001	**GCTCCACGCTCTACACCCACCTGCTGAAGTCCCTGGAGGCACAGGGCTTCAAGAGCGTGG**
3061	**TCGCTGTCATCGGGCTGCCCAACGACCCGAGCGTGCGCATGCACGAGGCGCTCGGATATG**
3121	**CCCCCCGCGGCATGCTGCGGGCGGCCGGCTTCAAGCACGGGAACTGGCATGACGTGGGTT**
3181	**TCTGGCAGCTGGACTTCAGCCTGCCGGTGCCGCCCCGTCCGGTCCTGCCCGTCACCGAAA**
3241	**TC**TGATGACCCCTAGAGTCAAGCA**GATCGTTCAAACATTTGGCAATAAAGTTTCTTAAGA**
3301	**TTGAATCCTGTTGCCGGTCTTGCGATGATTATCATATAATTTCTGTTGAATTACGTTAAG**
3361	**CATGTAATAATTAACATGTAATGCATGACGTTATTTATGAGATGGGTTTTTATGATTAGA**
3421	**GTCCCGCAATTATACATTTAATACGCGATAGAAAACAAAATATAGCGCGCAAACTAGGAT**
3481	**AAATTATCGCGCGCGGTGTCATCTATGTTACTAGATCG**ACCGGCATGCAAGCTGATAATT
3541	**CAATTCGGCGTTAATTCAGTACATTAAAAACGTCCGCAATGTGTTATTAAGTTGTCTAAG**
3601	**CGTCAATTTGTTTACACCACAATATATCCTGCCACCAGCCAGCCAACAGCTCCCCGACCG**
3661	**GCAGCTCGGCACAAAATCACCACTCGATACAGGCAGCCCATCAGTCCGGGACGGCGTCAG**
3721	**CGGGAGAGCCGTTGTAAGGCGGCAGACTTTGCTCATGTTACCGATGCTATTCGGAAGAAC**
3781	**GGCAACTAAGCTGCCGGGTTTGAAACACGGATGATCTCGCGGAGGGTAGCATGTTGATTG**
3841	**TAACGATGACAGAGCGTTGCTGCCTGTGATCA**ATTCGGGCACGAACCCAGTGGACATAAG
3901	CCTGTTCGGTTCGTAAGCTGTAATGCAAGTAGCGTATGCGCTCACGCAACTGGTCCAGAA
3961	CCTTGACCGAACGCAGCGGTGGTAACGGCGCAGTGGCGGTTTTCATGGCTTGTTATGACT
4021	GTTTTTTTGGGGTACAGTCTATGCCTCGGGCATCCAAGCAGCAAGCGCGTTACGCCGTGG
4081	GTCGATGTTTGATGTTATGGAGCAGCAACGATGTTACGCAGCAGGGCAGTCGCCCTAAAA
4141	CAAAGTTAAACATCATGGGGGAAGCGGTGATCGCCGAAGTATCGACTCAACTATCAGAGG
4201	TAGTTGGCGTCATCGAGCGCCATCTCGAACCGACGTTGCTGGCCGTACATTTGTACGGCT
4261	CCGCAGTGGATGGCGGCCTGAAGCCACACAGTGATATTGATTTGCTGGTTACGGTGACCG
4321	TAAGGCTTGATGAAACAACGCGGCGAGCTTTGATCAACGACCTTTTGGAAACTTCGGCTT
4381	CCCCTGGAGAGAGCGAGATTCTCCGCGCTGTAGAAGTCACCATTGTTGTGCACGACGACA
4441	TCATTCCGTGGCGTTATCCAGCTAAGCGCGAACTGCAATTTGGAGAATGGCAGCGCAATG
4501	ACATTCTTGCAGGTATCTTCGAGCCAGCCACGATCGACATTGATCTGGCTATCTTGCTGA
4561	CAAAAGCAAGAGAACATAGCGTTGCCTTGGTAGGTCCAGCGGCGGAGGAACTCTTTGATC
4621	CGGTTCCTGAACAGGATCTATTTGAGGCGCTAAATGAAACCTTAACGCTATGGAACTCGC
4681	CGCCCGACTGGGCTGGCGATGAGCGAAATGTAGTGCTTACGTTGTCCCGCATTTGGTACA
4741	GCGCAGTAACCGGCAAAATCGCGCCGAAGGATGTCGCTGCCGACTGGGCAATGGAGCGCC
4801	TGCCGGCCCAGTATCAGCCCGTCATACTTGAAGCTAGACAGGCTTATCTTGGACAAGAAG
4861	AAGATCGCTTGGCCTCGCGCGCAGATCAGTTGGAAGAATTTGTCCACTACGTGAAAGGCG
4921	AGATCACCAAGGTAGTCGGCAAATAATGTCTAGCTAGAAATTCGTTCAAGCCGACGCCGC
4981	TTCGCGGCGCGGCTTAACTCAAGTCGTTAGATGCACTAAGCACATAATTGCTCACAGCCA
5041	AACTATCAGGTCAAGTCTGCTTTTATTATTTTTAAGCGTGCATAATAAGCCCTACACAAA
5101	TTGGGAGATATATCATGCATGACCAAAATCCCTTAACGTGAGTTTTCGTTCCACTGAGCG
5161	TCAGACCCCGTAGAAAAGATCAAAGGATCTTCTTGAGATCCTTTTTTTCTGCGCGTAATC
5221	TGCTGCTTGCAAACAAAAAAACCACCGCTACCAGCGGTGGTTTGTTTGCCGGATCAAGAG
5281	CTACCAACTCTTTTTCCGAAGGTAACTGGCTTCAGCAGAGCGCAGATACCAAATACTGTC
5341	CTTCTAGTGTAGCCGTAGTTAGGCCACCACTTCAAGAACTCTGTAGCACCGCCTACATAC
5401	CTCGCTCTGCTAATCCTGTTACCAGTGGCTGCTGCCAGTGGCGATAAGTCGTGTCTTACC

5' Base	Sequence
5461	GGGTTGGACTCAAGACGATAGTTACCGGATAAGGCGCAGCGGTCGGGCTGAACGGGGGGT
5521	TCGTGCACACAGCCCAGCTTGGAGCGAACGACCTACACCGAACTGAGATACCTACAGCGT
5581	GAGCTATGAGAAAGCGCCACGCTTCCCGAAGGGAGAAAGGCGGACAGGTATCCGGTAAGC
5641	GGCAGGGTCGGAACAGGAGAGCGCACGAGGGAGCTTCCAGGGGGAAACGCCTGGTATCTT
5701	TATAGTCCTGTCGGGTTTCGCCACCTCTGACTTGAGCGTCGATTTTTGTGATGCTCGTCA
5761	GGGGGGCGGAGCCTATGGAAAAACGCCAGCAACGCGGCCTTTTTACGGTTCCTGGCCTTT
5821	TGCTGGCCTTTTGCTCACATGTTCTTTCCTGCGTTATCCCCTGATTCTGTGGATAACCGT
5881	ATTACCGCCTTTGAGTGAGCTGATACCGCTCGCCGCAGCCGAACGACCGAGCGCAGCGAG
5941	TCAGTGAGCGAGGAAGCGGAAGAGCGCCTGATGCGGTATTTTCTCCTTACGCATCTGTGC
6001	GGTATTTCACACCGCATATGGTGCACTCTCAGTACAATCTGCTCTGATGCCGCATAGTTA
6061	AGCCAGTATACACTCCGCTATCGCTACGTGACTGGGTCATGGCTGCGCCCCGACACCCGC
6121	CAACACCCGCTGACGCGCCCTGACGGGCTTGTCTGCTCCCGGCATCCGCTTACAGACAAG
6181	CTGTGACCGTCTCCGGGAGCTGCATGTGTCAGAGGTTTTCACCGTCATCACCGAAACGCG
6241	CGAGGCAGGGTGCCTTGATGTGGGCGCCGGCGGTCGAGTGGCGACGGCGCGGCTTGTCCG
6301	CGCCCTGGTAGATTGCCTGGCCCTAGGCCAGCCATTTTTGAGCGGCCAGCGGCCGCGATA
6361	GGCCGACGCGAAGCGGCGGGGCGTAGGGAGCGCAGCGACCGAAGGGTAGGCGCTTTTTGC
6421	AGCTCTTCGGCTGTGCGCTGGCCAGACAGTTATGCACAGGCCAGGCGGGTTTTAAGAGTT
6481	TTAATAAGTTTTAAAGAGTTTTAGGCGGAAAAATCGCCTTTTTTCTCTTTTATATCAGTC
6541	ACTTACATGTGTGACCGGTTCCCAATGTACGGCTTTGGGTTCCCAATGTACGGGTTCCGG
6601	TTCCCAATGTACGGCTTTGGGTTCCCAATGTACGTGCTATCCACAGGAAAGAGACCTTTT
6661	CGACCTTTTTCCCCTGCTAGGGCAATTTGCCCTAGCATCTGCTCCGTACATTAGGAACCG
6721	GCGGATGCTTCGCCCTCGATCAGGTTGCGGTAGCGCATGACTAGGATCGGGCCAGCCTGC
6781	CCCGCCTCCTCCTTCAAATCGTACTCCGGCAGGTCATTTGACCCGATCAGCTTGCGCACG
6841	GTGAAACAGAACTTCTTGAACTCTCCGGCGCTGCCACTGCGTTCGTAGATCGTCTTGAAC
6901	AACCATCTGGCTTCTGCCTTGCCTGCGGCGCGGCGTGCCAGGCGGTAGAGAAAACGGCCG
6961	ATGCCGGGATCGATCAAAAAGTAATCGGGGTGAACCGTCAGCACGTCCGGGTTCTTGCCT
7021	TCTGTGATCTCGCGGTACATCCAATCAGCTAGCTCGATCTCGATGTACTCCGGCCGCCCG
7081	GTTTCGCTCTTTACGATCTTGTAGCGGCTAATCAAGGCTTCACCCTCGGATACCGTCACC
7141	AGGCGGCCGTTCTTGGCCTTCTTCGTACGCTGCATGGCAACGTGCGTGGTGTTTAACCGA
7201	ATGCAGGTTTCTACCAGGTCGTCTTTCTGCTTTCCGCCATCGGCTCGCCGGCAGAACTTG
7261	AGTACGTCCGCAACGTGTGGACGGAACACGCGGCCGGGCTTGTCTCCCTTCCCTTCCCGG
7321	TATCGGTTCATGGATTCGGTTAGATGGGAAACCGCCATCAGTACCAGGTCGTAATCCCAC
7381	ACACTGGCCATGCCGGCCGGCCCTGCGGAAACCTCTACGTGCCCGTCTGGAAGCTCGTAG
7441	CGGATCACCTCGCCAGCTCGTCGGTCACGCTTCGACAGACGGAAAACGGCCACGTCCATG
7501	ATGCTGCGACTATCGCGGGTGCCCACGTCATAGAGCATCGGAACGAAAAAATCTGGTTGC
7561	TCGTCGCCCTTGGGCGGCTTCCTAATCGACGGCGCACCGGCTGCCGGCGGTTGCCGGGAT
7621	TCTTTGCGGATTCGATCAGCGGCCGCTTGCCACGATTCACCGGGGCGTGCTTCTGCCTCG
7681	ATGCGTTGCCGCTGGGCGGCCTGCGCGGCCTTCAACTTCTCCACCAGGTCATCACCCAGC
7741	GCCGCGCCGATTTGTACCGGGCCGGATGGTTTGCGACCGTCACGCCGATTCCTCGGGCTT
7801	GGGGGTTCCAGTGCCATTGCAGGGCCGGCAGACAACCCAGCCGCTTACGCCTGGCCAACC
7861	GCCCGTTCCTCCACACATGGGGCATTCCACGGCGTCGGTGCCTGGTTGTTCTTGATTTTC
7921	CATGCCGCCTCCTTTAGCCGCTAAAATTCATCTACTCATTTATTCATTTGCTCATTTACT
7981	CTGGTAGCTGCGCGATGTATTCAGATAGCAGCTCGGTAATGGTCTTGCCTTGGCGTACCG
8041	CGTACATCTTCAGCTTGGTGTGATCCTCCGCCGGCAACTGAAAGTTGACCCGCTTCATGG
8101	CTGGCGTGTCTGCCAGGCTGGCCAACGTTGCAGCCTTGCTGCTGCGTGCGCTCGGACGGC
8161	CGGCACTTAGCGTGTTTGTGCTTTTGCTCATTTTCTCTTTACCTCATTAACTCAAATGAG
8221	TTTTGATTTAATTTCAGCGGCCAGCGCCTGGACCTCGCGGGCAGCGTCGCCCTCGGGTTC
8281	TGATTCAAGAACGGTTGTGCCGGCGGCGGCAGTGCCTGGGTAGCTCACGCGCTGCGTGAT
8341	ACGGGACTCAAGAATGGGCAGCTCGTACCCGGCCAGCGCCTCGGCAACCTCACCGCCGAT
8401	GCGCGTGCCTTTGATCGCCCGCGACACGACAAAGGCCGCTTGTAGCCTTCCATCCGTGAC
8461	CTCAATGCGCTGCTTAACCAGCTCCACCAGGTCGGCGGTGGCCCATATGTCGTAAGGGCT
8521	TGGCTGCACCGGAATCAGCACGAAGTCGGCTGCCTTGATCGCGGACACAGCCAAGTCCGC
8581	CGCCTGGGGCGCTCCGTCGATCACTACGAAGTCGCGCCGGCCGATGGCCTTCACGTCGCG
8641	GTCAATCGTCGGGCGGTCGATGCCGACAACGGTTAGCGGTTGATCTTCCCGCACGGCCGC
8701	CCAATCGCGGGCACTGCCCTGGGGATCGGAATCGACTAACAGAACATCGGCCCCGGCGAG
8761	TTGCAGGGCGCGGGCTAGATGGGTTGCGATGGTCGTCTTGCCTGACCCGCCTTTCTGGTT
8821	AAGTACAGCGATAACCTTCATGCGTTCCCCTTGCGTATTTGTTTATTTACTCATCGCATC
8881	ATATACGCAGCGACCGCATGACGCAAGCTGTTTTACTCAAATACACATCACCTTTTTAGA
8941	CGGCGGCGCTCGGTTTCTTCAGCGGCCAAGCTGGCCGGCCAGGCCGCCAGCTTGGCATCA

5' Base	Sequence
9001	GACAAACCGGCCAGGATTTCATGCAGCCGCACGGTTGAGACGTGCGCGGGCGGCTCGAAC
9061	ACGTACCCGGCCGCGATCATCTCCGCCTCGATCTCTTCGGTAATGAAAAACGGTTCGTCC
9121	TGGCCGTCCTGGTGCGGTTTCATGCTTGTTCCTCTTGGCGTTCATTCTCGGCGGCCGCCA
9181	GGGCGTCGGCCTCGGTCAATGCGTCCTCACGGAAGGCACCGCGCCGCCTGGCCTCGGTGG
9241	GCGTCACTTCCTCGCTGCGCTCAAGTGCGCGGTACAGGGTCGAGCGATGCACGCCAAGCA
9301	GTGCAGCCGCCTCTTTCACGGTGCGGCCTTCCTGGTCGATCAGCTCGCGGGCGTGCGCGA
9361	TCTGTGCCGGGGTGAGGGTAGGGCGGGGGCCAAACTTCACGCCTCGGGCCTTGGCGGCCT
9421	CGCGCCCGCTCCGGGTGCGGTCGATGATTAGGGAACGCTCGAACTCGGCAATGCCGGCGA
9481	ACACGGTCAACACCATGCGGCCGGCCGGCGTGGTGGTGTCGGCCCACGGCTCTGCCAGGC
9541	TACGCAGGCCCGCGCCGGCCTCCTGGATGCGCTCGGCAATGTCCAGTAGGTCGCGGGTGC
9601	TGCGGGCCAGGCGGTCTAGCCTGGTCACTGTCACAACGTCGCCAGGGCGTAGGTGGTCAA
9661	GCATCCTGGCCAGCTCCGGGCGGTCGCGCCTGGTGCCGGTGATCTTCTCGGAAAACAGCT
9721	TGGTGCAGCCGGCCGCGTGCAGTTCGGCCCGTTGGTTGGTCAAGTCCTGGTCGTCGGTGC
9781	TGACGCGGGCATAGCCCAGCAGGCCAGCGGCGGCGCTCTTGTTCATGGCGTAATGTCTCC
9841	GGTTCTAGTCGCAAGTATTCTACTTTATGCGACTAAAACACGCGACAAGAAAACGCCAGG
9901	AAAAGGGCAGGGCGGCAGCCTGTCGCGTAACTTAGGACTTGTGCGACATGTCGTTTTCAG
9961	AAGACGGCTGCACTGAACGTCAGAAGCCGACTGCACTATAGCAGCGGAGGGGTTGGATCA
10021	AAGTACTTTAAAGTACTTTAAAGTACTTTAAAGTAC**TTTGATCCCGAGGGGAACCCTGTG**
10081	**GTTGGCATGCACATACAAATGGACGAACGGATAAACCTTTTCACGCCCTTTTAAATATCC**
10141	**GTTATTCTAATAAACGCTCTTTTCTCTTAGGTTTACCCGCCAATATATCCTGTCAAACAC**
10201	**TGATAGTTTAAACTGAAGGCGGGAAACGACAATCTGATCCAAGCTCAAGCT**GCTCTAGCC
10261	AATACGCAAACCGCCTCTCCCCGCGCGTTGGCCGATTCATTAATGCAGCTGGCACGACAG
10321	GTTTCCCGACTGGAAAGCGGGCAGTGAGCGCAACGCAATTAATGTGAGTTAGCTCACTCA
10381	TTAGGCACCCCAGGCTTTACACTTTATGCTTCCGGCTCGTATGTTGTGTGGAATTGTGAG
10441	CGGATAACAATTTCACACAGGAAACAGCTATGACCATGATTACGAATTCGAGCTCGG
10501	

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