9 Appendix list

Appendix 2.1

Growth media (3% glucose) under different inorganic phophorus concentrations

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For 1 litre of MS media with 3% Glucose

	Pi+ (5 mM)*	**MS**	**Pi-**
Bottle 1 (Glucose)			
Glucose 6% W/v	30g	30g	30g
Water	500 ml	500 ml	500 ml
Bottle 2 (Salt solutions)			
MS salts including vitamins (Duchefa) 4.4 g/L	---	4.4 g	---
Micronutrients (Stock 10X) (Sigma)	100 ml	---	100ml
Macronutrients stock		---	
a. NH4NO3 (100X)	10 ml (or 1.65 g/L)		10 ml (or 1.65 g/L)
b. CaCl2 anhydrous (100X)	10 ml (or 332.02 mg/L)		10 ml (or 332.02 mg/L)
c. MgSO4 (100X)	10 ml (or 180.54 mg/L)		10 ml (or 180.54 mg/L)
d. KNO3 (100X)	10 ml (or 1.9 g/L)		10 ml (or 1.9 g/L)
KH2PO4	680 mg	----	----
Vitamin mix (Sigma)	103.1 mg	---	103.1 mg
NAA (0.5 mg/L) (Stock 10 mg/ml)	50 microlitre	50 microlitre	50 microlitre
Kinetin (0.05 mg/L) (Stock 1 mg/ml)	50 microlitre	50 microlitre	50 microlitre
Water	Adjust total vol to 500 ml	Adjust total vol to 500 ml	Adjust total vol to 500 ml
Adjust pH	5.8	5.8	5.8

Autoclave Bottle 1 and Bottle 2 separately

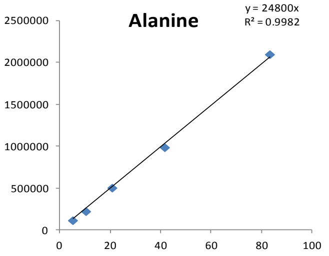
*** Alternatively make Pi+ medium (5 mM) by adding 510 mg KH2PO4 to MS**

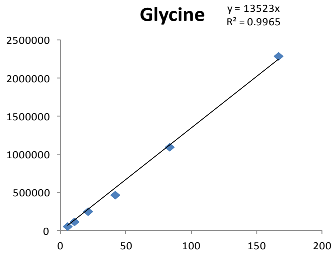
Macronutrients Stock (For 10X)

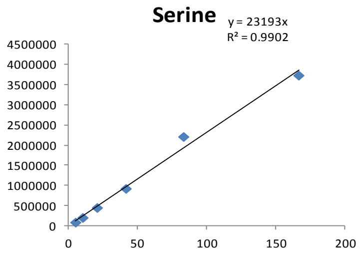
		100X
Ammonium Nitrate (NH4NO3)	16.5 g/L	16.5 g/100ml
Calcium chloride anhydrous	3.322 g/L	3.322g/100ml
Magnesium sulfate (MgSO4)	1.807 g/L	1.807g/100ml
Pottassium nitrate (KNO3)	19 g/L	19g/100ml

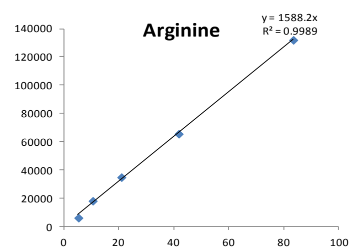
Appendix 2.2
Standard curves of amino acids and organic acids from GC-MS

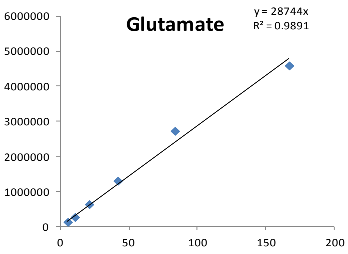
The standard curves (in relation to Table 5.2b) and Chapter 2 (Section 2.7.7) are plotted from known amount (in ng) of reference compounds (x-axis) vs total ion counts of targeted ions (y-axis) from the GC-MS spectra

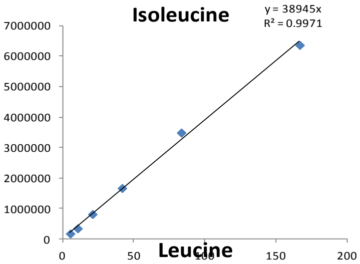


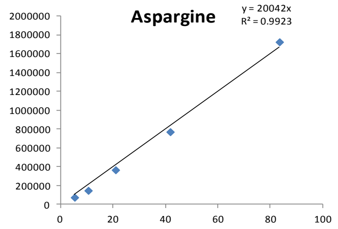


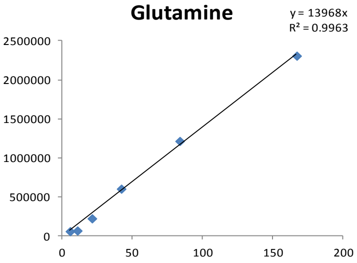


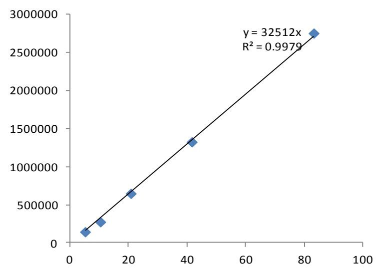


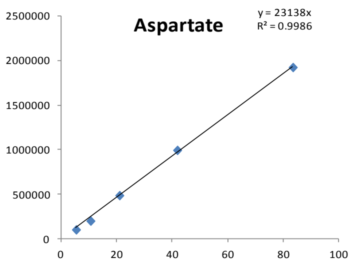


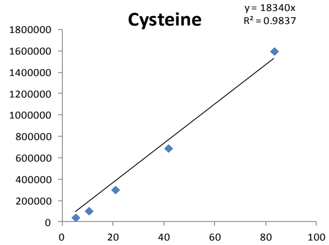


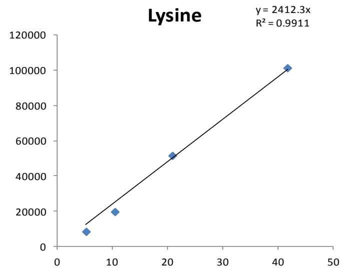


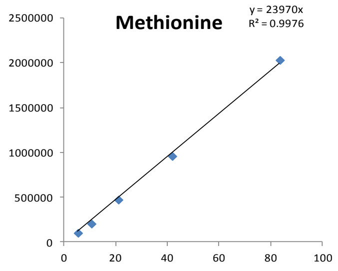


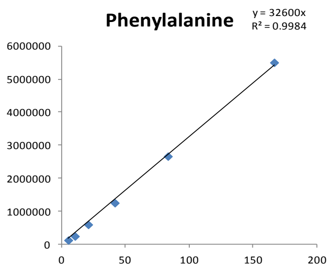


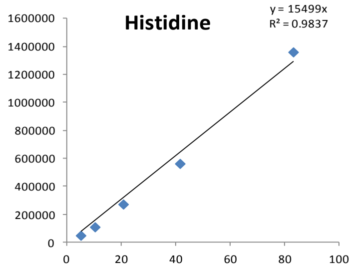


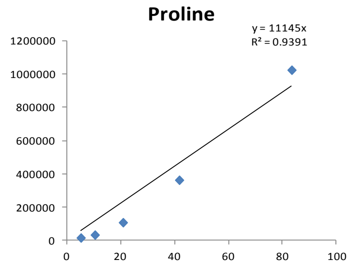


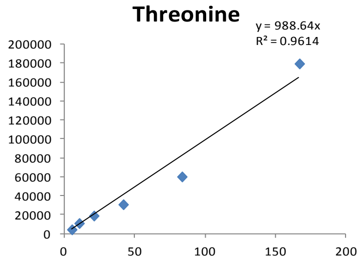


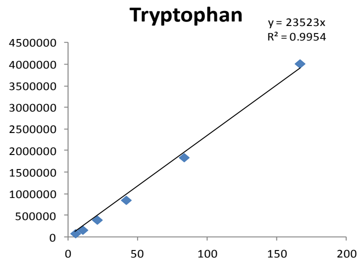


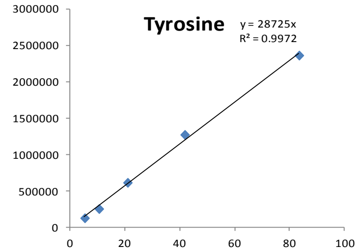


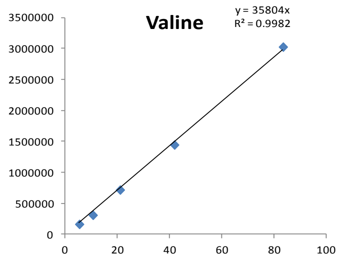


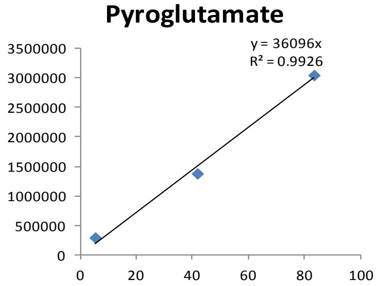

Proline

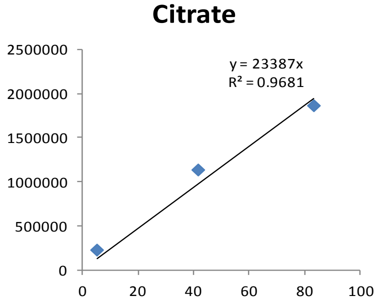

Threonine

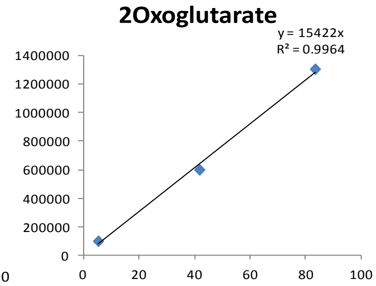

Tryptophan

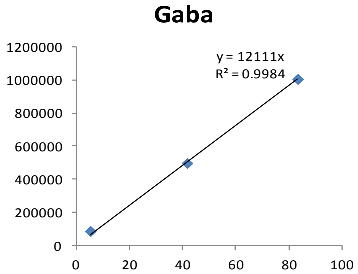

Tyrosine

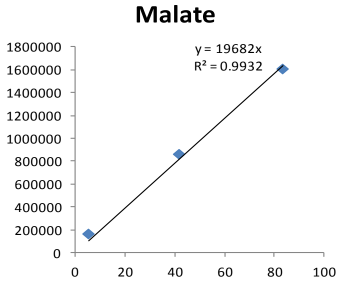

Valine

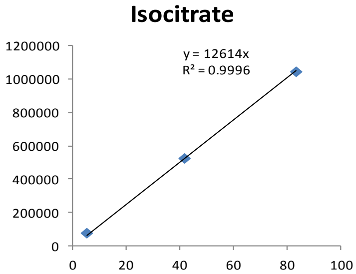

Pyroglutamate

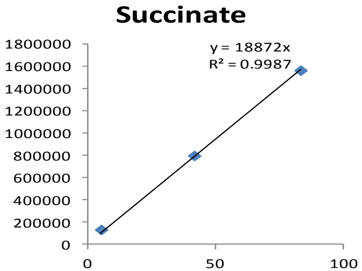

Citrate

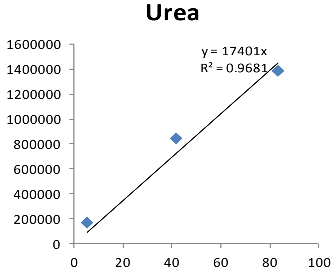

2Oxoglutarate

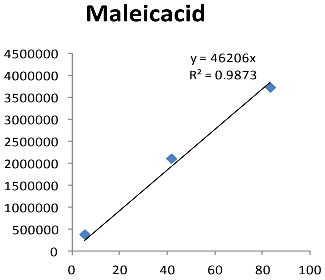

Gaba

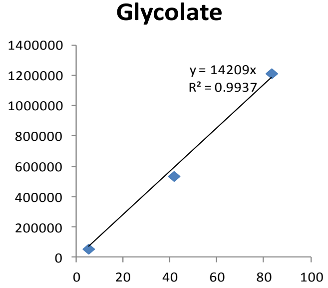

Malate


Isocitrate


Succinate


Urea


Maleicacid


Glycolate

Appendix 2.3

Linux code for Non-linearised confidence interval determination of free fluxes

Author Shyam Masakapalli
The program runs in conjunction with 13CFLUX

```
#!/bin/ksh
#need to install ksh for the if command to work with integers, KSH can be installed by command: sudo apt-get install ksh
#can check the version ksh by command: ksh --version

#############################################################Optimal Bestfit
sed 's/thaliana//g' $1 > original.ftbl                                  #'thaliana'is used as flux identifier whose
                                                                                  #Confidence is calculated
                                                                                  #$1 is the input ftbl model
#export PATH=$PATH:/home/shyam/Desktop/13CFLUX/FBINS.20050329            #path for 13CFLUX tool
Donlp2 original.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
grep Resi DON_OUT.txt > Residuum.txt
grep -v "infeasible" Residuum.txt > tmp.txt                              #remove lines containing infeasible solutions
mv tmp.txt Residuum.txt
cut -f2 Residuum.txt > 2.txt
sed '/^$/d' 2.txt > 3.txt
tail -1 3.txt > 4.txt
OptResid=$(tail -1 3.txt)
OptResiduum=`echo $OptResid | awk '{ printf "%.4f\n", $0}'`   #this will allow to over come any scientific
                                                              #notation to 4 decimal integer
                                                                         #useful when residuum is low for example
                                                                                  #9.28406e-05

echo "Optimal Resdiuum of actual best fit model is:                               $OptResid"
#Optimal or best fit Residuum
grep $OptResiduum -A 5000 *donlp2* > bestfit_original.txt          #Store bestfit residuum
cutoff=3.84                                                              #for 95% confidence limit Chi2 at 1 df
CutoffResiduum=$(dc -e "$OptResiduum $cutoff + p")                 #code for addition of non integers
echo "The cut off Resdiuum for 95% confidence limit is:                           $CutoffResiduum"


#############################Identify the optimal flux along with its identifier("thaliana")

grep 'thaliana' $1 > 5.txt
cut -f5 5.txt > 6.txt
thal=$(grep 'thaliana' 6.txt)                                            #gives the thaliana plus the number
#echo "The optimal flux with identifier    : $thal"
StartFreeflux=$(sed 's/thaliana//g' 6.txt)                               #gives the starting free flux value
echo "The starting free flux value is:                        $StartFreeflux"

#############################Formulate step size and replace one of the free flux with an increment/decrement
#For step size to be 10th of the flux value
if [ "$StartFreeflux" -lt 0.1 ]
then
        stepindex=1                                                #for small fluxes < 0.1 starting step size is 100% of flux
else
        stepindex=10                                                     #for larger fluxes > 0.1 starting step size is 10% of flux
fi
stepsize1=`echo $StartFreeflux $stepindex | awk '{ print $1/$2}'`  #calculates stepsize #next line to deal with any
                                                              #scientific notations

stepsize=$(echo $stepsize1 | sed 's/\([0-9]*\(\.[0-9]*\)\?\)[eE]+\?\(-\?[0-9]*\)/(\1*10^\3)/g;s/^/scale=9;/'| bc)

echo "######## Started iterations for confidence interval #######"
echo "######## Increments #######"
##################################First increment
ftblindex=1                                                        #index to store ftbl, Residuum and bestfit files
if [ "$StartFreeflux" -le 0 ]                                            #to deal with negative free fluxes and calculate new starting flux
then
        StartFreeflux=$((abs($StartFreeflux)))
        newflux=$(dc -e "_$StartFreeflux $stepsize + p")
#       echo "$newflux"
else
        newflux=$(dc -e "$StartFreeflux $stepsize + p")
#       echo "I am $newflux"
fi
echo "The constrained flux value is:                          $newflux"
sed 's/'$thal'/'$newflux'/g' $1 > increment$ftblindex.ftbl         #to replace the free flux with incremented value
Donlp2 increment$ftblindex.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
grep Resi DON_OUT.txt > Resinc$ftblindex.txt
grep -v "infeasible" Resinc$ftblindex.txt > tmp.txt
mv tmp.txt Resinc$ftblindex.txt
cut -f2 Resinc$ftblindex.txt > 2.txt
```

```
sed '/^$/d' 2.txt > 3.txt
tail -1 3.txt > 4.txt
Residuum1=$(tail -1 3.txt)
echo "The residuum after increment $ftblindex is:                    $Residuum1"          #Optimal or best fit Residuum
grep $Residuum1 -A 5000 *donlp2* > bestfit_inc$ftblindex.txt                                  #Store bestfit residuum

##########if conditional loop..if Residuum is greater then the step size is halved the index until Residuum reaches less than cutoff
##########else step size is doubled the index until Residuum gets higher than cutoff
if [ "$Residuum1" -gt "$CutoffResiduum" ]
then
        until [ "$Residuum1" -le "$CutoffResiduum" ]
        do
                echo "###############"
                ftblindex=$(($ftblindex+1))
                stepsize1=`echo $stepsize 2 | awk '{ print $1/$2}'`
                stepsize=$(echo $stepsize1 | sed 's/\([0-9]*\(\.[0-9]*\)\?\)[eE]+\?\(-\?[0-9]*\)/(\1*10^\3)/g;s/^/scale=9;/'| bc)
                if [ "$StartFreeflux" -le 0 ]
                then
                        StartFreeflux=$((abs($StartFreeflux)))
                        newflux=$(dc -e "_$StartFreeflux $stepsize + p")
#                       echo "$newflux"
                else
                        newflux=$(dc -e "$StartFreeflux $stepsize + p")
#                       echo "I am $newflux"
                fi
                echo "The constrained flux value is:             $newflux"
                sed 's/'$thal'/'$newflux'/g' $1 > increment$ftblindex.ftbl          #to replace the free flux with incremented value
                Donlp2 increment$ftblindex.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
                grep Resi DON_OUT.txt > Resinc$ftblindex.txt
                grep -v "infeasible" Resinc$ftblindex.txt > tmp.txt
                mv tmp.txt Resinc$ftblindex.txt
                cut -f2 Resinc$ftblindex.txt > 2.txt
                sed '/^$/d' 2.txt > 3.txt
                tail -1 3.txt > 4.txt
                Residuum1=$(tail -1 3.txt)
                if [ "$Residuum1" == "" ]; then
                        echo "The residuum after increment $ftblindex is:                           infeasible"
                        break
                else
                        echo "The residuum after increment $ftblindex is:                           $Residuum1"
        #Optimal or best fit Residuum
                fi
                grep $Residuum1 -A 5000 *donlp2* > bestfit_inc$ftblindex.txt              #Store bestfit residuum
        done

else
        if [ "$StartFreeflux" -lt 0.1 ]
        then
                stepindex=1
        else
                stepindex=10
        fi
#       stepindex=10
        stepsize=`echo $StartFreeflux $stepindex | awk '{ print $1/$2}'`
        until [ "$Residuum1" -ge "$CutoffResiduum" ]
        do
                echo "###############"
                ftblindex=$(($ftblindex+1))
                stepsize1=`echo $stepsize 2 | awk '{ print $1*$2}'`
                stepsize=$(echo $stepsize1 | sed 's/\([0-9]*\(\.[0-9]*\)\?\)[eE]+\?\(-\?[0-9]*\)/(\1*10^\3)/g;s/^/scale=9;/'| bc)
                if [ "$StartFreeflux" -le 0 ]
                then
                        StartFreeflux=$((abs($StartFreeflux)))
                        newflux=$(dc -e "_$StartFreeflux $stepsize + p")
#                       echo "$newflux"
                else
                        newflux=$(dc -e "$StartFreeflux $stepsize + p")
#                       echo "I am $newflux"
                fi
                echo "The constrained flux value is:             $newflux"
                sed 's/'$thal'/'$newflux'/g' $1 > increment$ftblindex.ftbl          #to replace the free flux with incremented or decremented
value
                Donlp2 increment$ftblindex.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
                grep Resi DON_OUT.txt > Resinc$ftblindex.txt
                grep -v "infeasible" Resinc$ftblindex.txt > tmp.txt
                mv tmp.txt Resinc$ftblindex.txt
                cut -f2 Resinc$ftblindex.txt > 2.txt
                sed '/^$/d' 2.txt > 3.txt
                tail -1 3.txt > 4.txt
                Residuum1=$(tail -1 3.txt)
```

```
                if [ "$Residuum1" == "" ]; then
                        echo "The residuum after increment $ftblindex is:                        infeasible"
                        break
                else
                        echo "The residuum after increment $ftblindex is:                        $Residuum1"
        #Optimal or best fit Residuum
                fi
                grep $Residuum1 -A 5000 *donlp2* > bestfit_inc$ftblindex.txt                     #Store bestfit residuum
        done
fi

#Restting the step index and step size
if [ "$StartFreeflux" -lt 0.1 ]
then
        stepindex=1
else
        stepindex=10
fi
#stepindex=10
stepsize1=`echo $StartFreeflux $stepindex | awk '{ print $1/$2}'`
stepsize=$(echo $stepsize1 | sed 's/\([0-9]*\(\.[0-9]*\)\?\)[eE]+\?\(-\?[0-9]*\)/(\1*10^\3)/g;s/^/scale=9;/'| bc)
echo "######## Decrements #######"
##############################################################First decrement

ftblindex=1                                                                              #reset index for storing
if [ "$StartFreeflux" -le 0 ]
then
        StartFreeflux=$((abs($StartFreeflux)))
        newflux=$(dc -e "_$StartFreeflux $stepsize - p")
#       echo "$newflux"
else
        newflux=$(dc -e "$StartFreeflux $stepsize - p")
#       echo "I am $newflux"
fi
echo "The constrained flux value is:                    $newflux"
sed 's/'$thal'/'$newflux'/g' $1 > decrement$ftblindex.ftbl                #to replace the free flux with incremented or decremented value
Donlp2 decrement$ftblindex.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
grep Resi DON_OUT.txt > Residec$ftblindex.txt
grep -v "infeasible" Residec$ftblindex.txt > tmp.txt
mv tmp.txt Residec$ftblindex.txt
cut -f2 Residec$ftblindex.txt > 2.txt
sed '/^$/d' 2.txt > 3.txt
tail -1 3.txt > 4.txt
Residuum2=$(tail -1 3.txt)
echo "The residuum after decrement $ftblindex is:                        $Residuum2"          #Optimal or best fit Residuum
grep $Residuum2 -A 5000 *donlp2* > bestfit_dec$ftblindex.txt                                #Store bestfit residuum

##########if conditional loop..if Residuum is greater then the step size is halved the index until Residuum reaches less than cutoff
##########else step size is doubled the index until Residuum gets higher than cutoff
if [ "$Residuum2" -gt "$CutoffResiduum" ]
then
        until [ "$Residuum2" -le "$CutoffResiduum" ]
        do
                echo "###############"
                ftblindex=$(($ftblindex+1))
                stepsize1=`echo $stepsize 2 | awk '{ print $1/$2}'`
                stepsize=$(echo $stepsize1 | sed 's/\([0-9]*\(\.[0-9]*\)\?\)[eE]+\?\(-\?[0-9]*\)/(\1*10^\3)/g;s/^/scale=9;/'| bc)
                if [ "$StartFreeflux" -le 0 ]
                then
                        StartFreeflux=$((abs($StartFreeflux)))
                        newflux=$(dc -e "_$StartFreeflux $stepsize - p")
                #       echo "$newflux"
                else
                        newflux=$(dc -e "$StartFreeflux $stepsize - p")
                #       echo "I am $newflux"
                fi
                echo "The constrained flux value is:                    $newflux"
                sed 's/'$thal'/'$newflux'/g' $1 > decrement$ftblindex.ftbl      #to replace the free flux with incremented or decremented value
                Donlp2 decrement$ftblindex.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
                grep Resi DON_OUT.txt > Residec$ftblindex.txt
                grep -v "infeasible" Residec$ftblindex.txt > tmp.txt
                mv tmp.txt Residec$ftblindex.txt
                cut -f2 Residec$ftblindex.txt > 2.txt
                sed '/^$/d' 2.txt > 3.txt
                tail -1 3.txt > 4.txt
                Residuum2=$(tail -1 3.txt)
                if [ "$Residuum2" == "" ]; then
                        echo "The residuum after decrement $ftblindex is:                        infeasible"
                        break
                else
```

```
                        echo "The residuum after decrement $ftblindex is:                               $Residuum2"
        #Optimal or best fit Residuum
                fi
                grep $Residuum2 -A 5000 *donlp2* > bestfit_dec$ftblindex.txt                            #Store bestfit residuum
        done

else

        if [ "$StartFreeflux" -lt 0.1 ]
        then
                stepindex=1
        else
                stepindex=10
        fi
        #stepindex=10
        stepsize=`echo $StartFreeflux $stepindex | awk '{ print $1/$2}'`
        until [ "$Residuum2" -ge "$CutoffResiduum" ]
        do
                echo "###############"
                ftblindex=$(($ftblindex+1))
                stepsize1=`echo $stepsize 2 | awk '{ print $1*$2}'`
                stepsize=$(echo $stepsize1 | sed 's/\([0-9]*\(\.[0-9]*\)\?\)[eE]+\?\(-\?[0-9]*\)/(\1*10^\3)/g;s/^/scale=9;/'| bc)
                if [ "$StartFreeflux" -le 0 ]
                then
                        StartFreeflux=$((abs($StartFreeflux)))
                        newflux=$(dc -e "_$StartFreeflux $stepsize - p")
                #       echo "$newflux"
                else
                        newflux=$(dc -e "$StartFreeflux $stepsize - p")
                #       echo "I am $newflux"
                fi
                echo "The constrained flux value is:                    $newflux"
                sed 's/'$thal'/'$newflux'/g' $1 > decrement$ftblindex.ftbl      #to replace the free flux with incremented or decremented value
                Donlp2 decrement$ftblindex.ftbl -a 0.00001 -m 0 -bootstrap -logAllF > DON_OUT.txt
                grep Resi DON_OUT.txt > Residec$ftblindex.txt
                grep -v "infeasible" Residec$ftblindex.txt > tmp.txt
                mv tmp.txt Residec$ftblindex.txt
                cut -f2 Residec$ftblindex.txt > 2.txt
                sed '/^$/d' 2.txt > 3.txt
                tail -1 3.txt > 4.txt
                Residuum2=$(tail -1 3.txt)
                if [ "$Residuum2" == "" ]; then
                        echo "The residuum after decrement $ftblindex is:                               infeasible"
                        break
                else
                        echo "The residuum after decrement $ftblindex is:                               $Residuum2"
        #Optimal or best fit Residuum
                fi
                grep $Residuum2 -A 5000 *donlp2* > bestfit_dec$ftblindex.txt                            #Store bestfit residuum
        done
fi

rm 2.txt 3.txt 4.txt 5.txt 6.txt *.ftbl.flx *.m DON_OUT.txt out.fimprove.donlp2.txt out.residuumscanner.txt *.mes *.pro
```

Appendix 2.4
Detailed instructions to use the Monte Carlo simulations along with other linux tool (Feasible infeasible residuum extractor)

In practise Monte Carlo simulations are run multiple times (hundreds to thousands), and each simulation results in a unique solution of flux estimates and corresponding residuum (Squared sum of error between the measured and predicted isotopomer abundances). It is observed that the solutions fall into two major categories, feasible and infeasibles. Here, a tool (FeasInf_Residuum_extractor) written in Linux shell programming is discussed which can be used to obtain the Residuums and infeasibles of all the simulations.

Make executable tool - Feasible infeasible residuum extractor: Paste the below mentioned code into gedit/ notepad and save the file as “FeasInf_Residuum_Extractor” and make this file executable by typing “chmod +x FeasInf_Residuum_Extractor” in Linux terminal.

#Code started

```
#File needed "Residuum.txt" obtained from the DON_OUT.txt file from 13CFLUX (version 20050329)
cat Residuum.txt|sed '$aResiduum:	best filter resetMonte'> 1.txt
cut -d: -f2,2 1.txt > 2.txt
grep for -n -v 2.txt >3.txt
grep best -B 1 3.txt > 4.txt
grep : 4.txt > 5.txt
sed '/with/{n;d}' 5.txt > 6.txt
cut -f2 6.txt > 7.txt
sed '1d' 7.txt > 8.txt
sed 's/best filter resetMonte/infeasible/g' 8.txt > Residuals_output.txt
rm -f 1.txt 2.txt 3.txt 4.txt 5.txt 6.txt 7.txt 8.txt
```

#code ended

Step 1: Using *13CFLUX®*, run donlp2 along with bootstrap Monte Carlo with a chosen number of simulations (say 1000).

Command: Donlp2 “model file name”.ftbl -a 0.00001 –m “number of simulations” -bootstrap -logAllF > “output file name”.txt&watch “grep Resi “output file name”.txt|tail -20”

Example: Donlp2 PPP.ftbl -a 0.00001 –m 1000 -bootstrap -logAllF > DON_OUT.txt&watch “grep Resi DON_OUT.txt|tail -20”

Many output files are generated (The important ones are mentioned below):

i) *_sto (An FTBL file- with all the free flux solutions)
ii) out.fimprove.donlp2.txt (Complete solutions of all the simulations-Huge file)
iii) User defined output file e.g DON_OUT.txt (huge file)

Step 2: Collect the list of residuums of all the simulations by using grep command and store it by the file name “Residuum.txt”. The huge DON_OUT.txt file can be deleted.

Command: grep Resi DON_OUT.txt > Residuum.txt

Step 3: **C**opy the file “Residuum.txt” and paste in the folder containing the “FeasInf_Residuum_extractor”. In the terminal go to the directory/folder and run the following command

Command: **./FeasInf_Residuum_extractor**

It generates an output files: **Residuals_output.txt:** Contains the values of feasible residuums and infeasibles if any. The free flux estimates of each residuum can be obtained form the *-sto file in the same order. The outputs can be pasted and analysed in an MS excel or spreadsheet. The flux solutions can be sorted based on the residuums to identify a threshold for selecting best fits and also to discard the high residuum (poor fitting) and infeasible solutions. (Masakapalli et al., 2010)

Step 4: To collect the complete solutions of the best fits (i.e lowest residuums) use the follwing command in the folder which has Out.fimprove.donlp2.txt file
Command: grep "ResiduumValue" -A "Number of lines" *donlp2* > filename.txt (example: grep 353.052 –A 200 *donlp2* > 1.txt)

Appendix 3.1 PPP.FTBL model (Used in Chapter 3)

```
PROJECT
                NAME            VERSION         FORMAT          DATE            COMMENT
                PPPbase1.ftbl              1.0                  17/10/07        Shyam
                // File: 99%[1-13C]glucose (GLC1)
                //Cumonet - simulated meas used with 5%sd (NMR) and .01(MS)
NETWORK
                FLUX_NAME       EDUCT_1         EDUCT_2         PRODUCT_1       PRODUCT_2
// Glucose Input
                upt             GLC1                            Glc6P
                                #ABCDEF                         #ABCDEF
// Embden Meyerhof Pathway
                emp1            Glc6P                           Fru6P
                                #ABCDEF                         #ABCDEF
                emp2            Fru6P                           FruBP
                                #ABCDEF                         #ABCDEF
                emp3            FruBP                           GA3P            GA3P
                                #ABCDEF                         #CBA            #DEF
                emp4            GA3P                            PGA
                                #ABC                            #ABC
                emp5            PGA                             PEP
                                #ABC                            #ABC
                emp6            PEP                             PYR
                                #ABC                            #ABC
// Pentose Phosphate Pathway
                ppp1            Glc6P                           CO2             Rul5P
                                #ABCDEF                         #A              #BCDEF
                ppp2            Rul5P                           Xul5P
                                #ABCDE                          #ABCDE
                ppp3            Rul5P                           Rib5P
                                #ABCDE                          #ABCDE
                ppp4            Xul5P           Ery4P           GA3P            Fru6P
```

```
                        #ABCDE      #abcd       #CDE          #ABabcd
            ppp5        Xul5P       Rib5P       Sed7P         GA3P
                        #ABCDE      #abcde      #ABabcde      #CDE
            ppp6        GA3P        Sed7P       Ery4P         Fru6P
                        #ABC        #abcdefg    #defg         #abcABC
// CO2 output
            coOut       CO2                     CO2_out
                        #A                      #A
FLUXES
            NET
                        NAME        FCD         VALUE(F/C)    ED_WEIGHT     LOW(F)
                        upt         C                    1
                        emp1        F                  0.5
                        emp2        D
                        emp3        D
                        emp4        D
                        emp5        D
                        emp6        D
                        ppp1        D
                        ppp2        D
                        ppp3        D
                        ppp4        D
                        ppp5        D
                        ppp6        D
            XCH
                        NAME        FCD         VALUE(F/C)    ED_WEIGHT     LOW(F)
                        upt         D
                        emp1        C           0
                        emp2        C           0
                        emp3        C           0
                        emp4        C           0
                        emp5        C           0
                        emp6        D
                        ppp1        C           0
                        ppp2        F           0.8
```

```
                                ppp3          F             0.83932
                                ppp4          F             0.826289
                                ppp5          F             0.179947
                                ppp6          F             0.212767
                                coOut         D
EQUALITIES
                    NET
                                VALUE         FORMULA
                    XCH
                                VALUE         FORMULA
INEQUALITIES
                    NET
                                VALUE         COMP          FORMULA
                    XCH
                                VALUE         COMP          FORMULA
FLUX_MEASUREMENTS
                    FLUX_NAME   VALUE         DEVIATION
                    upt                    1          0.05
LABEL_INPUT
                    META_NAME   ISOTOPOMER    VALUE
                    GLC1        #000000               0.01                //
                                                                          // 99% percent labeled at position
                                #100000              0.935                1
                                #100001              0.011                // Naturally marked isos!!!
                                #100010              0.011                // Naturally marked isos!!!
                                #100100              0.011                // Naturally marked isos!!!
                                #101000              0.011                // Naturally marked isos!!!
                                #110000              0.011                // Naturally marked isos!!!
//                  GLC2        #000000               0.01                //
                                                                          // 99% percent labeled at position
//                              #010000              0.935                2
//                              #010001              0.011                // Naturally marked isos!!!
//                              #010010              0.011                // Naturally marked isos!!!
//                              #010100              0.011                // Naturally marked isos!!!
//                              #011000              0.011                // Naturally marked isos!!!
```

```
//                          #110000            0.011              // Naturally marked isos!!!
LABEL_MEASUREMENTS
               META_NAME    CUM_GROUP   VALUE          DEVIATION  CUM_CONSTRAINTS
//Measurements from 1-13C glucose fed
               Ery4P        C1234            0.10467     0.0052   #1xxx
                                             0.03555     0.0018   #x1xx
                                             0.01277     0.0006   #xx1x
                                             0.13156     0.0066   #xxx1
               GA3P         C123             0.05563     0.0028   #1xx
                                             0.01422     0.0007   #x1x
                                             0.23015     0.0115   #xx1
               PEP          C123             0.05563     0.0028   #1xx
                                             0.01422     0.0007   #x1x
                                             0.23015     0.0115   #xx1
               Rul5P        C12345           0.39152     0.0196   #1xxxx
                                             0.01954     0.0010   #x1xxx
                                             0.04681     0.0023   #xx1xx
                                             0.01359     0.0007   #xxx1x
                                             0.18681     0.0093   #xxxx1
//Measurements from 2-13C glucose fed
//             Ery4P        C1234            0.25294     0.01265  #1xxx
//                                           0.06949     0.00347  #x1xx
//                                           0.13428     0.00671  #xx1x
//                                           0.12301     0.00615  #xxx1
//             GA3P         C123             0.11731     0.00587  #1xx
//                                           0.23509     0.01175  #x1x
//                                           0.21460     0.01073  #xx1
//             PEP          C123             0.11731     0.00587  #1xx
//                                           0.23509     0.01175  #x1x
//                                           0.21460     0.01073  #xx1
//             Rul5P        C12345           0.55050     0.02753  #1xxxx
//                                           0.40462     0.02023  #x1xxx
//                                           0.09629     0.00481  #xx1xx
//                                           0.19077     0.00954  #xxx1x
//                                           0.17433     0.00872  #xxxx1
```

```
PEAK_MEASUREMENTS
                META_NAME   PEAK_NO      VALUE_S     VALUE_D-     VALUE_D+     VALUE_DD
MASS_SPECTROMETRY
                META_NAME   FRAGMENT     WEIGHT      VALUE        DEVIATION
//Measurements from 1-13C glucose fed
                PEP         1,2,3                0       0.7258         0.01
                                                 1      0.24869         0.01
                                                 2      0.02523         0.01
                                                 3      0.00028         0.01
//Measurements from 2-13C glucose fed
//              PEP         1,2,3                0      0.54486         0.01
//                                               1      0.34498         0.01
//                                               2      0.10848         0.01
//                                               3      0.00169         0.01
OPTIONS
                OPT_NAME    OPT_VALUE
```

Appendix 3.2
Elution times and fragment ions of TBDMS derivatised amino acids

Elution time	Amino acid	Derivative	Specific ions (m/z)					
13.476	Alanine	2TBDMS	158	232	260	317	302	
14.276	Glycine	2TBDMS	218	246	144	288	303	
16.705	Valine	2TBDMS	186	260	288	345		
17.798	Leucine	2TBDMS	200	274	302	344		
18.644	Isoleucine	2TBDMS	200	274	302	344		
19.640	Proline	2TBDMS	184	258	286			
24.708	Methionine	2TBDMS	218	292	320	302	362	
25.127	Serine	3TBDMS	288	362	390	302	432	
25.736	Threonine	3TBDMS	302	376	404	417		
27.532	Phenylalanine	2TBDMS	234	308	336	378	302	
28.973	Aspartate	3TBDMS	316	390	418	302	244	
30.056	Cysteine	3TBDMS	304	378	406			
31.573	Glutamate	3TBDMS	272	330	432	358	404	
32.172	Aspargine	3TBDMS	302	315	417	400		
33.820	Lysine	3TBDMS	329	431	488	302	473	
34.682	Glutamine	3TBDMS	329	357	431			
35.936	Arginine	3TBDMS	414	442	484	340		
37.780	Histidine	3TBDMS	196	338	413	440		
38.750	Tyrosine	3TBDMS	364	438	466	302		
39.639	Tryptophan	2TBDMS	302	461	489	347	375	273

Appendix 4.1
Metabolic model used in Chapter 4 for final flux determination (extracted from 13C-FLUX network definition)

PROJECT						
	NAME	VERSION	FORMAT	DATE	COMMENT	
	AtMFA	2.05	.ftbl	Jul-09	Author SKM	
NETWORK						
	FLUX_NAME	EDUCT_1	EDUCT_2	PRODUCT_1	PRODUCT_2	
// Metabolic input						
	upt	GLCext		G6Pc		
		#ABCDEF		#ABCDEF		
//Cytosolic hexose metabolism						
	chex1	G6Pc		F6Pc		
		#ABCDEF		#ABCDEF		
	chex2	F6Pc		TPc	TPc	//TPc includes cytosolic triose-3-P, xPGA and PEP
		#ABCDEF		#CBA	#DEF	
	chex3	TPc		PYRc		
		#ABC		#ABC		
//Plastidic hexose metabolism						
	phex1	G6Pp		F6Pp		
		#ABCDEF		#ABCDEF		
	phex2	F6Pp		TPp	TPp	//TPp includes plastidic triose-3-P, xPGA and PEP
		#ABCDEF		#CBA	#DEF	
	phex3	TPp		PYRp		
		#ABC		#ABC		
//Cytosolic pentose-P pathway						
	cppp1	G6Pc		CO2	P5Pp	//Incorporates uptake into plastid via xpt
		#ABCDEF		#A	#BCDEF	
//Plastid pentose-P pathway						
	pppp1	G6Pp		CO2	P5Pp	
		#ABCDEF		#A	#BCDEF	

	pppp2a	P5Pp	TKC2p	S7Pp		//Half Reaction
		#abcde	#AB	#ABabcde		
	pppp2b	E4Pp	TKC2p	F6Pp		//Half Reaction
		#abcd	#AB	#ABabcd		
	pppp2c	P5Pp		TPp	TKC2p	//Half Reaction
		#ABCDE		#CDE	#AB	
	pppp3a	S7Pp		E4Pp	TAC3p	//Half Reaction
		#ABCDEFG		#DEFG	#ABC	
	pppp3b	TPp	TAC3p	F6Pp		//Half Reaction
		#abc	#ABC	#ABCabc		
//Transporters/exchanges						
	gpt	G6Pc		G6Pp		
		#ABCDEF		#ABCDEF		
	tpt_ppt	TPp		TPc		//Plastid to cytosol direction for tpt+ppt
		#ABC		#ABC		
	cpex	PYRc		PYRp		
		#ABC		#ABC		
	cmex	PYRc		PYRm		
		#ABC		#ABC		
//TCA cycle						
	tca1	PYRm		CO2	AcCoA	
		#ABC		#A	#BC	
	tca2	AcCoA	MAL_OAA	CIT		//OAA and malate are in single uncompartmented pool
		#AB	#abcd	#dcbBAa		
	tca3	CIT		CO2	AKG	//Includes citrate and isocitrate
		#ABCDEF		#F	#ABCDE	
	tca4	AKG		CO2	FUM	//Includes flux via succinylCoA and GABA shunt
		#ABCDE		#A	#BCDE	
	tca5a	FUM		MAL_OAA		
		#ABCD		#ABCD		
	tca5b	FUM		MAL_OAA		

		#ABCD		#DCBA		
//Anaplerotic reactions						
	ana1	TPc	CO2	MAL_OAA		
		#ABC	#a	#ABCa		
	ana2	MAL_OAA		CO2	PYRm	
		#ABCD		#D	#ABC	
	ana3	MAL_OAA		PYRp	CO2	
		#ABCD		#ABC	#D	
//Biosynthetic outputs						
	gsuc	G6Pc		GSUC		
		#ABCDEF		#ABCDEF		
	sucgOUT	GSUC		G6Peff		
		#ABCDEF		#ABCDEF		
	fsuc	F6Pc		FSUC		
		#ABCDEF		#ABCDEF		
	sucfOUT	FSUC		F6Peff		
		#ABCDEF		#ABCDEF		
	stsp	G6Pp		STA		
		#ABCDEF		#ABCDEF		
	starchOUT	STA		STAeff		
		#ABCDEF		#ABCDEF		
	cellwallhOUT	G6Pc		WALL		//Hexosyl units of cell wall polysaccharides
		#ABCDEF		#ABCDEF		
	pentan	G6Pc		PENTAN	CO2	
		#ABCDEF		#ABCDE	#F	
	cellwallpOUT	PENTAN		PENTANeff		//Pentosyl units of cell wall polysaccharides
		#ABCDE		#ABCDE		
	adh	PYRc		EtOH	CO2	
		#ABC		#BC	#A	
	ethanolOUT	EtOH		EtOH_out		
		#AB		#AB		
	co2	CO2		CO2eff		

		#A		#A		
//Lipid metabolism						
	glycerolOUT	TPc		G3P		//Glycerol backbone of glycerolipids
		#ABC		#ABC		
	pdhp	PYRp		CO2	AcCoAp	
		#ABC		#A	#BC	
	lipidOUT	AcCoAp		AcCoAeff		//Fatty acid components of acyl-lipids
		#AB		#AB		
//Organic acid accumulation						
	citOUT	CIT		CITeff		
		#ABCDEF		#ABCDEF		
	malOUT	MAL_OAA		MAL_OAAeff		
		#ABCD		#ABCD		
	succOUT	FUM		FUMeff		
		#ABCD		#ABCD		
//Amino acid metabolism						
	glu	AKG		GLU		
		#ABCDE		#ABCDE		
	gluOUT	GLU		GLUeff		
		#ABCDE		#ABCDE		
	asp	MAL_OAA		ASP		
		#ABCD		#ABCD		
	aspOUT	ASP		ASPeff		
		#ABCD		#ABCD		
	arg	AKG	CO2	ARG		
		#ABCDE	#a	#ABCDEa		
	argOUT	ARG		ARGeff		
		#ABCDEF		#ABCDEF		
	asp_arg	ASP		FUM		//Reaction linked to transfer of -N from Asp to Arg
		#ABCD		#ABCD		
	ser	TPp		SER		

		#ABC		#ABC		
	cys	SER		CYS		
		#ABC		#ABC		
	cysOUT	CYS		CYSeff		
		#ABC		#ABC		
	gly	SER		GLY	CX	
		#ABC		#AB	#C	
	glyOUT	GLY		GLYeff		
		#AB		#AB		
	cxeff	CX		CXeff		
		#A		#A		
	ala	PYRc		ALA		
		#ABC		#ABC		
	alaOUT	ALA		ALAeff		
		#ABC		#ABC		
	leu1	PYRp	PYRp	ISOVAL	CO2	
		#ABC	#abc	#abBCc	#A	
	leu2	ISOVAL	AcCoAp	LEU	CO2	
		#ABCDE	#ab	#abBCDE	#A	
	leuOUT	LEU		LEUeff		
		#ABCDEF		#ABCDEF		
	val	ISOVAL		VAL		
		#ABCDE		#ABCDE		
	valOUT	VAL		VALeff		
		#ABCDE		#ABCDE		
	met	ASP	CX	MET		
		#ABCD	#a	#ABCDa		
	metOUT	MET		METeff		
		#ABCDE		#ABCDE		
	thr	ASP		THR		
		#ABCD		#ABCD		
	thrOUT	THR		THReff		
		#ABCD		#ABCD		
	ile	PYRp	THR	ILE	CO2	

		#ABC	#abcd	#abBcdC	#A	
	ileOUT	ILE		ILEeff		
		#ABCDEF		#ABCDEF		
	aro1	E4Pp	TPp	ARO		
		#ABCD	#abc	#abcABCD		
	aro2	E4Pp	TPp	ARO		
		#ABCD	#abc	#abDCBAc		
	phe_tyr	ARO	TPp	PHE_TYR	CO2	//Combines flux to Phe and Tyr
		#ABCDEFG	#abc	#abcBCDEFG	#A	
	pheOUT	PHE_TYR		PHE_TYReff		
		#ABCDEFGHI		#ABCDEFGHI		
	pro	GLU		PRO		
		#ABCDE		#ABCDE		
	proOUT	PRO		PROeff		
		#ABCDE		#ABCDE		
	lys	MAL_OAA	PYRp	LYS	CO2	
		#ABCD	#abc	#ABCDcb	#a	
	lys1	MAL_OAA	PYRp	LYS	CO2	
		#ABCD	#abc	#abcDCB	#A	
	lysOUT	LYS		LYSeff		
		#ABCDEF		#ABCDEF		
	his	P5Pp	CX	HIS		
		#ABCDE	#a	#aEDCBA		
	hisOUT	HIS		HISeff		
		#ABCDEF		#ABCDEF		
//For Tryptophan						
	trp2ca	P5Pp		TPp	CCa	
		#ABCDE		#CDE	#AB	
	trpaOUT	CCa		CCaeff		//For 2C fragment
		#AB		#AB		
	trp2cb	TPp		CO2	CCb	
		#ABC		#A	#BC	
	trpbOUT	CCb		CCbeff		//For 2C fragment
		#AB		#AB		

	trpcOUT	SER		SEReff		//Combines Trp (3C fragment) and Ser production
		#ABC		#ABC		
	trpdOUT	E4Pp		E4Ppeff		//For 4C fragment
		#ABCD		#ABCD		
EQUALITIES						
	NET					
		VALUE	**FORMULA**			
		0	tca5a-tca5b			
		0	gsuc-fsuc			
		0	aro1-aro2			
		0	asp_arg-arg			
		0	lys-lys1			
	XCH					
		VALUE	**FORMULA**			
		0	tca5a-tca5b			
		0	chex3			
		0	phex2			
		0	phex3			
		0	cppp1			
		0	pppp1			
		0	cmex			
		0	cpex			
		0	adh			
		0	stsp			
		0	pdhp			
		0	ana1			
		0	ana2			
		0	ana3			
		0	tca1			
		0	tca2			
		0	tca3			
		0	asp			
		0	arg			

		0	ser			
		0	cys			
		0	gly			
		0	ala			
		0	aro1			
		0	aro2			
		0	leu1			
		0	leu2			
		0	thr			
		0	ile			
		0	val			
		0	met			
		0	phe_tyr			
		0	pro			
		0	lys			
		0	his			
		0	trp2ca			
		0	trp2cb			
INEQUALITIES						
	NET					
		VALUE	**COMP**	**FORMULA**		
		0	<=	chex3		
		0	<=	phex2		
		0	<=	phex3		
		0	<=	cppp1		
		0	<=	pppp1		
		0	<=	cmex		
		0	<=	cpex		
		0	<=	adh		
		0	<=	stsp		
		0	<=	pdhp		
		0	<=	ana1		
		0	<=	ana2		

		0	<=	ana3		
		0	<=	tca1		
		0	<=	tca2		
		0	<=	tca3		
		0	<=	asp		
		0	<=	arg		
		0	<=	ser		
		0	<=	cys		
		0	<=	gly		
		0	<=	ala		
		0	<=	aro1		
		0	<=	aro2		
		0	<=	leu1		
		0	<=	leu2		
		0	<=	thr		
		0	<=	ile		
		0	<=	val		
		0	<=	met		
		0	<=	phe_tyr		
		0	<=	pro		
		0	<=	lys		
		0	<=	his		
		0	<=	trp2ca		
		0	<=	trp2cb		
LABEL_INPUT //Select one of the following groups and adjust glucose input name accordingly						
	META_NAME	**ISOTOPOMER**	**VALUE**			
//Either	GLCext	#000000	0.010			
		#100000	0.935	// 99% labelled at 1st position		
		#100001	0.011	//Due to natural abundance of 13C		
		#100010	0.011	//Due to natural abundance of 13C		
		#100100	0.011	//Due to natural abundance of 13C		
		#101000	0.011	//Due to natural abundance of 13C		
		#110000	0.011	//Due to natural abundance of 13C		

//Or	GLCext_2	#000000	0.010	
		#010000	0.935	// 99% labelled at 2nd position
		#010001	0.011	//Due to natural abundance of 13C
		#010010	0.011	//Due to natural abundance of 13C
		#010100	0.011	//Due to natural abundance of 13C
		#011000	0.011	//Due to natural abundance of 13C
		#110000	0.011	//Due to natural abundance of 13C
//Or	GLCext_3	#000000	0.840	
		#111111	0.100	//10% labelled at every position
		#010000	0.010	//Due to natural abundance of 13C
		#100000	0.010	//Due to natural abundance of 13C
		#000010	0.010	//Due to natural abundance of 13C
		#000100	0.010	//Due to natural abundance of 13C
		#001000	0.010	//Due to natural abundance of 13C
		#000001	0.010	//Due to natural abundance of 13C

Appendix 4.2
^{13}C NMR data of metabolites from independently labelled cell suspension cultures of *Arabidopsis thaliana* (Chapter 4)

Key to identification of data sets

Heading	Labelled substrate	Replicate no	Total no of isotopomer measurements
1C1	99% [1-13C]glucose	1	114
1C2	99% [1-13C]glucose	2	113
2C1	99% [2-13C]glucose	1	102
2C2	99% [2-13C]glucose	2	107
UC1	10% [U-13C]glucose	1	134
UC2	10% [U-13C]glucose	2	134
Total			**704**

1C1

Metabolite	Groups	Positional isotopomers	Measured	SD	Predicted
AKG	x1Gaba1	#x010x+#x111x	40.21	6.03	41.10
		#x110x+#x011x	32.60	4.89	32.65
		#x111x	8.15	1.63	7.79
	x1Gaba2	#xx010	67.00	10.05	65.37
		#xx110	25.30	3.80	26.36
		#x10xx	61.18	9.18	59.36
		#x11xx	21.81	3.27	22.01
ALA	x1Ala1	#x01	183.63	18.36	213.86
		#x11	11.69	1.17	3.03
ARG	x1Arg1	#xxxxx1	43.96	2.20	39.66
		#x110xx+#x011xx	26.51	1.33	28.40
		#x010xx	28.64	1.43	28.98
ASP	x1Asp1	#xx11	29.19	1.46	29.10
		#xx01	74.15	3.71	74.39
	x1Asp2	#110x	19.12	0.96	18.88
		#011x	40.34	2.02	43.63
		#010x	118.28	5.91	108.55
	x1Asp3	#x011	26.64	1.33	24.36
		#x110	48.55	2.43	49.79
		#x010	130.06	6.50	136.54
CIT	x1Cit1	#x110x0+#x011x0	121.25	18.19	117.93
		#x010x0+#x111x0+#x111x0	172.44	25.87	176.92
	x1Cit2	#xx0xx1	143.87	21.58	144.64
		#xx1xx1	54.14	8.12	53.85
	x1Cit3	#11xxxx+#xxx11x	58.99	8.85	61.76
		#10xxxx+#xxx01x	167.59	25.14	158.91
	x1Cit4	#010xxx+#xx010x	629.31	94.40	607.31
		#011xxx+#xx110x	227.25	34.09	234.67
FSUC	x1Sucf1	#xxxx01	82.55	12.38	91.39
		#xxxx11	1.87	0.37	1.31

	x1Sucf2	#110xxx+#011xxx	7.10	1.06	5.25
		#010xxx	7.24	1.09	8.43
	x1Sucf3	#xx110x+#xx011x	2.03	0.30	1.56
		#xx010x	15.09	2.26	17.41
	x1Sucf4	#11xxxx	7.25	1.09	5.95
		#10xxxx	391.93	58.79	442.79
	x1Sucf5	#x010xx	25.20	3.78	25.22
		#x110xx+#x011xx	2.02	0.40	2.02
FUM	x1Fumr1	#11xx+#xx11	9.11	1.37	10.44
		#01xx+#xx10	73.11	10.97	57.62
	x1Fumr2	#11xx+#xx11	5.54	0.83	6.46
		#10xx+#xx01	23.28	3.49	17.04
GLU	x1Glu1	#xxx11	5.58	0.30	5.59
		#xxx01	14.71	0.74	14.68
	x1Glu2	#110xx	23.62	1.18	23.51
		#011xx	46.92	2.35	48.06
		#010xx	134.56	6.73	131.78
	x1Glu3	#xx011	8.42	0.42	7.08
		#xx110	62.43	3.12	66.82
		#xx010	156.96	7.85	165.72
	x1Glu4	#x111x	25.64	1.28	19.80
		#x110x+#x011x	75.69	3.78	83.02
		#x010x	79.49	3.97	84.70
GSUC	x1Sucg1	#xxxx01	92.65	13.90	109.90
		#xxxx11	2.29	0.34	1.57
	x1Sucg2	#10xxxx	271.02	40.65	249.42
		#11xxxx	3.00	0.60	3.35
	x1Sucg3	#010xxx	5.45	0.82	6.10
		#110xxx+#011xxx	4.56	0.68	3.82
	x1Sucg4	#xxx010	13.50	2.70	7.15
		#xxx011+#xxx110	1.79	0.36	2.16
	x1Sucg5	#x010xx	24.17	3.63	25.21
		#x011xx+#x110xx	2.21	0.44	2.02
ILE	x1Ile1	#xx110x+#xx011x	13.14	0.66	11.23
		#xx010x	40.72	2.04	45.24
	x1Ile2	#110xxx+#011xxx	7.88	0.39	8.15
		#010xxx	34.52	1.73	33.23
	x1Ile3	#xxx11x	5.34	0.27	5.69
		#xxx01x	15.69	0.78	14.55
LEU	x1Leu1	#11xxxx	6.04	0.30	5.57
		#10xxxx	13.84	0.69	14.78
	x1Leu2	#110xxx	7.50	0.38	7.07
		#011xxx	9.18	0.46	9.11
		#010xxx	133.40	6.67	141.04
	x1Leu3	#x110xx+#x011xx	6.16	0.31	6.25
		#x010xx	10.64	0.53	10.48
	x1Leu4	#xxx01x	133.67	6.68	137.73
		#xxx0x1	140.40	7.02	135.86
LYS	x1Lys1	#xxxx11	20.70	1.04	19.07

		#xxxx01	44.27	2.21	47.24
	x1Lys2	#011xxx	21.44	1.07	21.92
		#010xxx	56.56	2.83	55.22
	x1Lys3	#x110xx+#x011xx	33.26	1.66	32.50
		#x010xx	83.91	4.20	85.75
	x1Lys4	#xxx110+#xxx011	32.11	1.61	32.73
		#xxx010	90.64	4.53	88.82
	x1Lys5	#xx110x+#xx011x	25.30	1.27	25.29
		#xx010x	27.37	1.37	27.38
MET	x1Met1	#xx01x	15.76	0.79	12.38
		#xxxx1	25.54	1.28	29.29
PHE_TYR	x1Phe_Tyr	#110xxxxxx+#011xxxxxx	2.74	0.41	2.88
		#010xxxxxx	9.24	1.39	8.71
PRO	x1Pro2	#110xx	17.28	1.72	12.61
		#011xx	26.13	2.61	25.77
		#010xx	59.88	5.98	70.66
SER	x1Ser1	#x01	93.78	4.69	86.42
		#010	5.10	0.26	5.46
STA	x1Starch	#10xxxx	55.75	17.92	37.49
		#010xxx	1.24	0.32	1.49
		#x010xx	4.01	1.05	4.50
		#xx010x	3.03	0.80	2.60
		#xxx010	1.20	0.32	1.18
		#xxxx01	22.97	6.03	20.25
THR	x1Thr1	#11xx	10.22	0.51	9.80
		#10xx	25.36	1.27	26.33
	x1Thr2	#x110+#x011	24.54	1.23	25.20
		#x010	47.76	2.39	46.40
	x1Thr3	#x11x	25.54	1.28	24.57
		#010x	49.31	2.47	51.05
	x1Thr4	#xx11	13.26	0.66	11.00
		#xx01	24.94	1.25	28.12
VAL	x1Val1	#010xx	14.77	0.74	13.26
		#xx0x1	81.66	4.08	87.11
		#xx01x	86.60	4.33	88.31

1C2					
AKG	y1Gaba1	#x010x	81.90	12.29	66.66
		#x111x	13.44	2.02	15.58
		#x110x+#x011x	67.62	10.14	65.33
	y1Gaba2	#xx110	40.74	8.52	51.35
		#xx011	7.40	1.11	5.44
		#xx010	124.28	18.64	127.37
	y1Gaba3	#x10xx	135.52	20.33	133.57
		#x11xx	48.84	7.33	49.53
ALA	y1Ala1	#011	4.58	0.23	4.75
		#010	14.59	0.73	14.01
ARG	y1Arg1	#xxxxx1	54.71	2.74	45.85
		#xxx01x	9.00	0.45	10.09

	y1Arg2	#x110xx+#x011xx	42.09	2.10	42.98
		#x010xx	44.84	2.24	43.85
ASP	y1Asp1	#xx11	30.16	1.51	30.97
		#xx01	81.52	4.08	79.19
	y1Asp2	#110x	22.38	1.12	22.17
		#011x	47.59	2.38	51.24
		#010x	138.50	6.93	127.47
	y1Asp3	#x011	26.64	1.33	26.07
		#x110	52.04	2.60	53.28
		#x010	146.62	7.33	146.11
CIT	y1Cit1	#x110x0+#x011x0	256.19	38.43	308.92
		#x010x1	80.82	12.12	55.27
		#x010x0	328.63	49.29	317.80
	y1Cit2	#xx0xx1	172.64	25.90	173.57
		#xx1xx1	64.97	9.75	64.61
	y1Cit3	#11xxxx+#xxx11x	43.04	6.46	43.81
		#10xxxx+#xxx01x	114.87	17.23	112.73
	y1Cit4	#010xxx+#xx010x	1581.60	237.24	1477.07
		#011xxx+#xx110x	550.40	82.56	570.76
		#110xxx+#xx011x	147.00	22.05	150.36
FSUC	y1Sucf1	#xxxx01	149.60	22.44	175.15
		#xxxx11	3.50	0.53	2.50
	y1Sucf2	#110xxx+#011xxx	10.88	2.18	6.54
		#010xxx	9.38	1.41	10.51
	y1Sucf3	#xx110x+#xx011x	2.80	0.42	2.15
		#xx010x	20.70	3.11	23.92
	y1Sucf4	#xxx010	11.40	1.71	6.92
		#xxx110+#xxx011	1.30	0.40	2.11
	y1Sucf5	#x010xx	31.24	4.69	27.28
		#x110xx+#x011xx	1.98	0.30	2.18
	y1Sucf6	#11xxxx	5.82	1.16	6.55
		#10xxxx	579.60	112.37	487.37
FUM	y1Fum1	#10xx+#xx01	44.46	6.67	39.83
		#11xx+#xx11	13.91	2.09	15.11
GLU	y1Glu1	#xxx11	8.49	0.42	7.76
		#xxx01	18.94	0.95	20.37
	y1Glu2	#110xx	28.46	1.42	28.39
		#011xx	54.90	2.75	58.02
		#010xx	169.50	8.48	159.11
	y1Glu3	#xx011	5.66	0.28	6.90
		#xx110	75.26	3.76	65.10
		#xx010	200.32	10.02	161.46
	y1Glu4	#x010x	100.54	5.03	99.70
		#x110x+#x011x	90.44	4.52	97.72
		#x111x	25.52	1.28	23.31
GSUC	y1Sucg1	#xxxx01	132.62	19.89	151.23
		#x010xx+#xxx011+#xxx110	34.00	5.10	27.20
	y1Sucg2	#010xxx	9.00	1.35	10.56
		#110xxx+#011xxx	9.30	1.40	6.61

	y1Sucg3	#xxx010	35.90	5.39	15.83
		#xxx011+#xxx110	3.60	0.72	4.78
	y1Sucg4	#x010xx+#xxx011+#xxx110	34.00	5.10	38.10
		#x011xx+#x110xx	4.68	0.94	2.76
	y1Sucg5	#10xxxx	558.56	83.78	534.45
		#11xxxx	6.72	1.34	7.18
ILE	y1Ile1	#110xxx	9.50	0.48	9.96
		#010xxx	58.21	2.91	55.14
	y1Ile2	#xx110x+#xx011x	14.42	0.72	14.57
		#xx010x	59.34	2.97	58.69
	y1Ile3	#xx1xx1	4.99	0.25	4.70
		#xx0xx1	88.98	4.45	93.66
	y1Ile4	#xxx11x	8.26	0.41	8.99
		#xxx01x	25.84	1.29	23.00
LEU	y1Leu1	#11xxxx	5.20	0.26	5.71
		#10xxxx	17.31	0.87	15.17
	y1Leu2	#110xxx	6.82	0.34	7.89
		#011xxx	10.75	0.54	10.16
		#010xxx	186.37	9.32	157.38
	y1Leu3	#x110xx+#x011xx	8.41	0.42	8.70
		#x010xx	15.16	0.76	14.58
	y1Leu4	#xxx11x	8.84	0.44	8.92
		#xxx01x	179.60	8.98	177.92
	y1Leu5	#xxx1x1	9.90	0.50	10.67
		#xxx0x1	181.71	9.09	165.28
LYS	y1Lys1	#011xxx	25.42	1.27	25.59
		#010xxx	64.90	3.25	64.46
	y1Lys2	#xxxx11	22.97	1.15	23.01
		#xxxx01	57.12	2.86	57.01
	y1Lys3	#x110xx+#x011xx	48.50	2.43	45.93
		#x010xx	115.66	5.78	121.17
	y1Lys4	#xxx110+#xxx011	44.90	2.25	44.66
		#xxx010	120.53	6.03	121.18
	y1Lys5	#xx110x+#xx011x	32.84	1.64	33.73
		#xx010x	37.60	1.88	36.52
SER	y1Ser1	#x01	134.10	6.71	123.86
		#010	7.33	0.37	7.82
STA	y1Starch	#010xxx	69.39	10.41	73.96
		#x010xx	187.81	28.17	222.57
		#xx010x	141.19	21.18	128.82
		#xxx010	72.81	10.92	58.49
		#xxxx01	1060.14	159.02	1002.35
THR	y1Thr1	#11xx	13.36	0.67	13.13
		#10xx	34.68	1.73	35.26
THR	y1Thr2	#x110+#x011	34.75	1.74	34.97
		#x010	64.81	3.24	64.39
	y1Thr3	#x11x	25.90	1.30	27.04
		#010x	58.98	2.95	56.17
VAL	y1Val1	#xx1x1	9.10	0.46	8.68

		#xx0x1	129.07	6.45	134.42
	y1Val2	#xx11x	7.70	0.39	7.00
		#xx01x	130.00	6.50	139.69

2C1					
AKG_2	x2Gaba1	#xx110	21.01	3.15	23.94
		#xx010	159.58	23.94	127.88
	x2Gaba2	#x011x+#x110x	46.01	6.90	49.27
		#x010x+#x111x+#x111x	271.08	40.66	248.66
ALA_2	x2Ala1	#11x	7.30	0.37	8.22
		#10x	19.61	0.98	16.38
	x2Ala2	#110	7.12	0.36	8.43
		#011	4.94	0.25	3.56
		#010	136.85	6.84	134.53
	x2Ala3	#x11	5.19	0.26	4.29
		#x01	27.57	1.38	31.06
ARG_2	x2Arg2	#xxx01x	60.75	3.04	58.80
		#x010xx	20.10	1.01	22.43
		#xxxxx1	31.77	1.59	28.30
ASP_2	x2Asp1	#xx11	7.40	0.37	6.21
		#xx01	84.61	4.23	94.81
	x2Asp2	#110x	6.06	0.30	5.61
		#011x	5.74	0.29	5.55
		#010x	53.35	2.67	58.29
	x2Asp3	#x110+#x011	11.98	0.60	12.39
		#x010	59.56	2.98	57.40
CIT_2	x2Cit1	#xx1xx1	10.34	1.55	8.58
		#xx0xx1	108.56	16.28	122.19
	x2Cit2	#x010x1	16.39	2.46	11.21
		#x110x0+#x011x0	20.10	3.02	23.25
		#x010x0	112.61	16.89	116.43
	x2Cit3	#110xxx+#xx011x	32.38	4.86	33.17
		#011xxx+#xx110x	38.15	5.72	39.68
		#010xxx+#xx010x	306.72	46.01	284.76
FSUC_2	x2Sucf1	#xxxx11	12.31	1.85	13.53
		#xxxx01	122.29	18.34	107.21
	x2Sucf2	#11xxxx	27.03	4.05	28.37
		#10xxxx	184.58	27.69	174.43
	x2Sucf3	#x110xx+#x011xx	59.65	8.95	38.89
		#x010xx	50.09	7.51	59.62
	x2Sucf4	#xx110x+#xx011x	45.44	6.82	36.76
		#xx010x	58.11	8.72	66.01
FUM_2	x2Fum1	#11xx+#xx11	7.40	1.11	8.59
		#10xx+#xx01	178.42	26.76	134.16
	x2Fum2	#110x+#x011	47.23	7.08	49.01
		#010x+#x010	497.02	74.55	476.70
GLU_2	x2Glu1	#xxx11	7.66	0.39	6.28
		#xxx01	170.30	8.52	192.40
	x2Glu2	#xx011	3.81	0.19	3.89

		#xx110	5.82	0.29	5.47
		#xx010	28.25	1.41	29.21
	x2Glu3	#x110x+#x011x	11.81	0.59	11.22
		#x010x	53.10	2.66	55.51
GLY_2	x2Gly1	#11	12.10	0.61	12.04
		#01	113.94	5.70	114.51
GSUC_2	x2Sucg1	#xxxx01	91.38	13.71	79.81
		#xxxx11	9.13	1.37	10.05
	x2Sucg2	#11xxxx	12.13	0.61	12.06
		#10xxxx	70.51	10.58	73.96
	x2Sucg3	#x110xx+#x011xx	103.70	15.56	48.63
		#x010xx+#x111xx	89.92	13.49	77.50
		#xxx011+#xxx110	29.13	4.37	37.46
ILE_2	x2Ile1	#110xxx+#011xxx	6.87	0.34	7.16
		#010xxx	12.56	0.63	11.97
	x2Ile2	#x110x0+#x011x0+#x010x1	15.94	0.80	17.05
		#x010x0	45.07	2.25	41.45
	x2Ile3	#xx110x+#xx011x	10.37	0.52	9.10
		#xx010x	13.66	0.68	14.98
	x2Ile4	#xx0xx1	11.81	0.59	11.42
		#xxx01x	25.94	1.30	26.75
LEU_2	x2Leu1	#011xxx+#110xxx	10.32	0.52	10.97
		#010xxx	18.81	0.94	17.47
	x2Leu2	#x111xx	6.04	0.60	4.09
		#x110xx+#x011xx	43.50	2.18	44.84
		#x010xx	71.72	3.59	73.39
	x2Leu3	#xx1100+#xx011x+#xx01x1	50.06	2.50	50.37
		#xx0100	66.99	3.35	66.56
	x2Leu4	#xxx11x	7.62	0.76	7.76
		#xxx01x	25.85	2.58	31.20
	x2Leu5	#xxx1x1	12.42	0.62	10.75
		#xxx0x1	19.46	0.97	21.51
LYS_2	x2Lys1	#xxxx01	72.27	3.61	69.12
		#x010xx	25.96	1.30	27.00
	x2Lys2	#xxx110+#xxx011	9.36	0.47	8.25
		#xxx010	25.65	1.28	28.06
	x2Lys3	#xx110x+#xx011x	12.67	0.63	9.80
		#xx010x	48.07	2.40	55.43
MET_2	x2Met1	#x010x	11.86	0.59	9.08
		#xxxx1	7.85	0.39	9.07
PRO_2	x2Pro1	#010xx	24.21	2.42	24.28
		#x010x	28.03	2.80	27.79
		#xxx01	72.40	7.24	72.83
SER_2	x2Ser1	#x11	13.48	1.34	3.51
		#x01	28.41	1.42	29.73
	x2Ser2	#110	4.96	0.50	6.85
		#011	8.34	0.84	2.56
		#010	73.79	3.69	67.58
STA_2	x2Starch1	#10xxxx	22.40	3.36	27.12

		#x010xx	16.79	2.52	14.42
		#010xxx	113.70	17.06	95.59
	x2Starch2	#xxx010	40.89	6.13	39.91
		#xxxx01	11.19	1.68	11.45
THR_2	x2Thr1	#x010	20.62	1.03	20.18
		#10xx	38.28	1.91	35.83
		#xx01	34.36	1.72	36.96
VAL_2	x2Val	#x1100+#x011x+#x01x1	46.47	2.32	42.39
		#x0100	52.11	2.61	56.02

2C2					
AKG_2	y2Gaba1	#xx010	2.14	0.32	1.29
		#xx110+#xx011	0.35	0.05	0.41
	y2Gaba2	#x010x	3.98	0.60	3.52
		#x110x+#x011x	0.65	0.10	0.71
	y2Gaba3	#x10xx	3.71	0.56	3.60
		#x11xx	0.39	0.06	0.40
ALA_2	y2Ala1	#11x	22.44	1.12	21.79
		#10x	42.27	2.11	43.43
	y2Ala2	#110	19.14	0.96	16.53
		#011	5.84	0.29	6.97
		#010	305.28	15.26	263.73
	y2Ala4	#x11	6.76	0.34	7.50
		#x01	63.12	3.16	54.28
ARG_2	y2Arg1	#xxxxx1	68.51	6.85	67.51
		#xxx01x	138.33	13.83	140.29
ASP_2	y2Asp1	#xx01	198.82	9.94	177.86
		#xx11	10.70	0.54	11.64
	y2Asp2	#110x	11.30	0.57	10.05
		#011x	8.44	0.42	9.95
		#010x	120.57	6.03	104.44
	y2Asp3	#x011	13.46	0.67	12.51
		#x010	110.97	5.55	117.89
CIT_2	y2Cit1	#x110x0+#x011x0	2.96	0.44	3.10
		#x010x1	2.20	0.33	1.50
		#x010x0	13.57	2.04	15.54
	y2Cit2	#xx0xx1	17.70	2.65	21.00
		#xx1xx1	2.16	0.32	1.47
	y2Cit3	#11xxxx+#xxx11x	2.47	0.37	2.52
		#10xxxx+#xxx01x	56.94	8.54	55.83
	y2Cit4	#010xxx+#xx010x	19.16	2.87	16.78
		#011xxx+#xx110x	2.13	0.32	2.34
		#110xxx+#xx011x	1.95	0.29	1.95
FSUC_2	y2Sucf1	#10xxxx	3.40	0.51	3.42
		#11xxxx	0.56	0.08	0.56
	y2Sucf2	#xxxx01	1.71	0.26	1.69
		#xxxx11	0.21	0.03	0.21
	y2Sucf3	#110xxx+#011xxx	1.40	0.21	1.57
		#010xxx	26.57	3.98	22.18

	y2Sucf4	#xxx010	4.84	0.73	4.90
		#xxx110+#xxx011	0.47	0.07	0.46
	y2Sucf5	#x010xx	1.82	0.27	2.15
		#x110xx+#x011xx	2.02	0.30	1.40
FUM_2	y2Fum1	#10xx+#xx01	10.04	1.51	9.93
		#11xx+#xx11	0.63	0.09	0.64
	y2Fum2	#11xx+#xx11	0.38	0.06	0.41
		#01xx+#xx10	4.23	0.63	3.90
GLU_2	y2Glu1	#xxx01	367.21	18.36	312.85
		#xxx11	9.16	0.46	10.21
	y2Glu2	#xx010	69.22	3.46	57.49
		#xx110	9.88	0.49	10.76
		#xx011	7.36	0.37	7.66
	y2Glu3	#x010x	128.71	6.44	120.79
		#x110x+#x011x	23.15	1.16	24.42
	y2Gly1	#11	22.98	2.29	23.90
		#10	52.51	5.25	50.20
	y2Gly2	#11	26.64	2.66	26.58
		#01	252.17	25.21	252.78
GSUC_2	y2Sucg1	#xxxx01	0.73	0.11	0.78
		#xxxx11	0.11	0.02	0.10
	y2Sucg2	#010xxx	13.90	2.09	14.28
		#110xxx+#011xxx	1.04	0.16	1.01
	y2Sucg3	#11xxxx	0.54	0.11	0.57
		#10xxxx	3.59	0.54	3.48
	y2Sucg4	#xxx010+#x110xx+#x011xx	5.22	0.78	5.74
		#xxx011+#xxx110	0.55	0.08	0.49
	y2Sucg5	#x010xx+#xxx011+#xxx110	2.11	0.42	1.83
		#x011xx+#x110xx	0.75	0.11	0.79
ILE_2	y2Ile1	#110xxx+#011xxx	15.94	0.80	17.03
		#010xxx	30.90	1.55	28.46
	y2Ile2	#x110x0+#x011x0+#x010x1	32.31	1.62	36.81
		#x010x0	111.39	5.57	89.49
	y2Ile3	#xx110x+#xx011x	19.96	1.00	19.51
		#xx010x	31.42	1.57	32.10
	y2Ile4	#xx1xx1	3.08	0.15	3.40
		#xx0xx1	29.03	1.45	26.43
		#xxx01x	64.49	3.22	61.92
LEU_2	y2Leu1	#10xxxx	268.70	13.44	206.40
		#11xxxx	4.90	0.50	7.33
	y2Leu2	#011xxx+#110xxx	22.00	1.10	24.74
		#010xxx	47.37	2.37	39.38
	y2Leu3	#x110xx+#x011xx	106.36	5.32	107.51
		#x010xx	177.90	8.90	175.94
	y2Leu4	#xxx11x	7.62	0.76	4.01
		#xxx01x	61.09	3.05	60.35
	y2Leu5	#xxx1x1	20.96	1.05	21.97
		#xxx0x1	46.44	2.32	43.97
LYS_2	y2Lys1	#xxx110+#xxx011	14.74	0.74	15.75

		#xxx010	58.15	2.91	53.55
	y2Lys2	#xx110x+#xx011x	17.21	0.86	18.61
		#xx010x	116.55	5.83	105.19
SER_2	y2Ser1	#110	17.76	0.89	18.16
		#010	183.49	9.17	179.18
STA_2	y2Starch1	#010xxx	13.08	1.96	12.36
		#10xxxx	4.19	0.63	3.51
		#x010xx	2.12	0.32	1.86
		#xx010x	0.92	0.14	1.01
		#xxx010	5.65	0.85	6.70
		#xxxx01	1.98	0.30	1.92
THR_2	y2Thr1	#11xx	6.70	0.34	6.43
		#10xx	88.24	4.41	91.49
	y2Thr2	#x110+#x011	9.70	0.49	10.10
		#x010	50.45	2.52	46.79
		#xx01	83.63	4.18	85.71
VAL_2	y2Val1	#x1100+#x011x+#x01x1	89.38	4.47	91.05
		#x0100	122.69	6.13	120.31
	y2Val2	#xx0x1	40.73	4.08	28.41
		#xx01x	32.05	3.20	37.75

UC1					
AKG_3	xuGaba1	#xx110+#xx011	6.26	0.94	6.88
		#xx010	2.72	0.41	2.38
	xuGaba2	#x010x	5.64	0.85	5.81
		#x110x+#x011x	2.81	0.42	2.72
	xuGaba3	#x10xx	6.34	0.95	6.91
		#x11xx	2.67	0.40	2.38
ALA_3	xuAla1	#11x	26.66	1.33	25.14
		#10x	12.54	0.63	13.19
ALA_3	xuAla2	#010	7.87	0.39	7.25
		#011	5.62	0.28	6.32
		#111	27.27	1.36	25.30
	xuAla3	#x11	31.06	1.55	33.27
		#x01	8.98	0.45	8.23
ARG_3	xuArg1	#xxx11x	13.56	0.68	14.70
		#xxx01x	5.93	0.30	5.32
	xuArg2	#x110xx+#x011xx	6.44	0.32	5.75
		#x010xx	11.29	0.56	12.28
ASP_3	xuAsp1	#xx11	20.40	1.02	20.73
		#xx01	25.28	1.26	24.85
	xuAsp2	#11xx	28.58	1.43	29.97
		#10xx	33.17	1.66	31.39
	xuAsp3	#110x	14.86	0.74	15.91
		#011x	5.76	0.29	5.38
		#010x	18.06	0.90	17.79
	xuAsp4	#x011	18.42	0.92	20.59
		#x110	11.04	0.55	8.94
		#x010	22.47	1.12	22.96

CIT_3	xuCit1	#x110x0+#x011x0	8.06	1.21	4.11
		#x010x0	11.75	1.76	9.63
		#x010x1	6.60	0.99	8.61
	xuCit2	#xx0xx1	31.58	4.74	19.55
		#xx1xx1	15.59	2.34	18.66
	xuCit3	#11xxxx+#xxx11x	61.97	9.30	60.76
		#10xxxx+#xxx01x	40.68	6.10	41.44
	xuCit4	#010xxx+#xx010x	28.65	4.30	31.26
		#011xxx+#xx110x	10.94	1.64	9.07
		#110xxx+#xx011x	47.07	7.06	49.96
		#111xxx+#xx111x	9.39	1.41	9.17
FSUC_3	xuSucf1	#11xxxx	30.28	4.54	32.76
		#10xxxx	9.36	1.40	8.45
	xuSucf2	#xx010x	9.44	1.42	8.81
		#xx110x+#xx011x	14.00	2.10	14.82
	xuSucf3	#xxx111	25.02	3.75	31.12
		#xxx010	9.90	1.49	7.05
		#xxx110+#xxx011	6.31	0.95	5.59
	xuSucf4	#xxxx01	5.44	0.82	5.78
		#xxxx11	30.00	4.50	26.58
	xuSucf5	#x010xx	16.54	2.48	8.42
		#x110xx+#x011xx	8.51	1.28	10.28
FUM_3	xuFum1	#11xx+#xx11	11.60	1.74	10.49
		#01xx+#xx10	10.63	1.59	11.48
	xuFum2	#10xx+#xx01	12.93	1.94	13.85
		#11xx+#xx11	13.80	2.07	12.65
GLU_3	xuGlu1	#11xxx	22.54	1.13	23.44
		#10xxx	29.36	1.47	28.09
	xuGlu2	#110xx	22.76	1.14	25.04
		#011xx	11.40	0.57	10.88
		#010xx	30.05	1.50	27.92
	xuGlu3	#xx110+#xx011	33.52	1.68	32.76
		#xx010	11.10	0.56	11.35
	xuGlu4	#x110x+#x011x	15.22	0.76	14.84
		#x010x	30.93	1.55	31.67
GLY_3	xuGly1	#10	19.31	0.97	15.06
		#11	17.78	0.89	20.42
	xuGly2	#11	19.02	0.95	21.18
		#01	18.37	0.92	15.62
GSUC_3	xuSucg1	#11xxxx	49.19	7.38	51.16
		#10xxxx	13.80	2.07	13.20
	xuSucg2	#xxxx01	3.52	0.53	4.11
		#xxxx11	27.00	4.05	19.90
	xuSucg3	#xx010x	6.19	0.93	6.04
		#xx011x+#xx110x	9.88	1.48	10.11
	xuSucg4	#xxx010	9.18	1.38	6.06
		#xxx011+#xxx110	5.96	0.89	4.79
		#x010xx	19.11	2.87	11.79
		#x011xx+#x110xx	9.95	1.49	14.23

ILE_3	xuIle1	#110xxx+#011xxx	5.50	0.28	5.83
		#010xxx	5.78	0.29	5.40
	xuIle2	#x110x0+#x011x0+#x010x1	11.00	0.55	11.40
		#x010x0	4.36	0.22	4.18
	xuIle3	#xx110x+#xx011x	8.14	0.41	8.25
		#xx010x	8.73	0.44	8.61
	xuIle4	#xx1xx1	10.24	0.51	8.45
		#xx0xx1	2.96	0.15	3.35
	xuIle5	#xxx11x	4.62	0.23	4.98
		#xxx01x	6.60	0.33	5.97
LEU_3	xuLeu1	#11xxxx	22.92	1.15	20.68
		#10xxxx	7.59	0.38	8.21
	xuLeu2	#011xxx+#110xxx	21.72	1.09	20.53
		#010xxx	7.40	0.37	7.76
	xuLeu3	#x110xx+#x011xx	6.60	0.33	6.73
		#x010xx	27.48	1.37	26.94
	xuLeu4	#xxx11x	21.78	1.09	21.93
		#xxx01x	8.76	0.44	8.70
	xuLeu5	#xxx1x1	4.32	0.22	3.87
		#xxx0x1	28.59	1.43	30.98
LYS_3	xuLys1	#xxx110+#xxx011	18.16	0.91	19.25
		#xxx010	11.20	0.56	10.44
	xuLys2	#xx110x+#xx011x	11.40	0.57	12.28
		#xx010x	14.07	0.70	12.80
MET_3	xuMet1	#xx01x	10.24	0.51	9.57
		#x010x	6.50	0.33	6.89
PRO_3	xuPro1	#xxx11	13.66	0.68	12.70
		#xxx01	4.32	0.22	4.60
SER_3	xuSer1	#11x	14.52	0.73	14.48
		#10x	10.65	0.53	10.68
STA_3	xuStarcha1	#10xxxx	2.35	0.35	2.26
		#11xxxx	6.04	0.91	6.26
	xuStarcha2	#010xxx	3.30	0.50	3.01
		#110xxx+#011xxx	3.40	0.51	3.65
	xuStarcha3	#x010xx	5.00	0.75	4.09
		#x110xx+#x011xx	2.94	0.44	3.32
	xuStarcha4	#xx010x	2.59	0.39	2.56
		#xx110x+#xx011x	4.09	0.61	4.14
	xuStarcha5	#xxx010	1.98	0.30	1.77
		#xxx011+#xxx110	1.41	0.21	1.53
	xuStarcha6	#xxxx01	1.27	0.19	1.36
		#xxxx11	6.55	0.98	6.04
	xuStarchb1	#10xxxx	3.25	0.49	3.23
		#11xxxx	8.90	1.34	8.95
	xuStarchb2	#010xxx	4.91	0.74	4.74
		#110xxx+#011xxx	5.59	0.84	5.77
	xuStarchb3	#x010xx+#xxx011+#xxx110	8.57	1.29	6.72
		#x110xx+#x011xx	3.53	0.53	4.05
	xuStarchb4	#xx010x	4.06	0.61	3.57

		#xx110x+#xx011x	5.27	0.79	5.78
	xuStarchb6	#xxxx01	2.03	0.30	2.00
		#xxxx11	8.82	1.32	8.93
THR_3	xuThr1	#11xx	9.30	0.47	9.13
		#10xx	9.41	0.47	9.57
	xuThr2	#x110+#x011	9.44	0.47	10.16
		#x010	8.68	0.43	7.90
	xuThr3	#xx11	7.34	0.37	7.61
		#xx01	9.51	0.48	9.13

UC2					
AKG_3	xuGaba1	#xx110+#xx011	6.26	0.94	6.88
		#xx010	2.72	0.41	2.38
	xuGaba2	#x010x	5.64	0.85	5.81
		#x110x+#x011x	2.81	0.42	2.72
	xuGaba3	#x10xx	6.34	0.95	6.91
		#x11xx	2.67	0.40	2.38
ALA_3	xuAla1	#11x	26.66	1.33	25.14
		#10x	12.54	0.63	13.19
ALA_3	xuAla2	#010	7.87	0.39	7.25
		#011	5.62	0.28	6.32
		#111	27.27	1.36	25.30
	xuAla3	#x11	31.06	1.55	33.27
		#x01	8.98	0.45	8.23
ARG_3	xuArg1	#xxx11x	13.56	0.68	14.70
		#xxx01x	5.93	0.30	5.32
	xuArg2	#x110xx+#x011xx	6.44	0.32	5.75
		#x010xx	11.29	0.56	12.28
ASP_3	xuAsp1	#xx11	20.40	1.02	20.73
		#xx01	25.28	1.26	24.85
	xuAsp2	#11xx	28.58	1.43	29.97
		#10xx	33.17	1.66	31.39
	xuAsp3	#110x	14.86	0.74	15.91
		#011x	5.76	0.29	5.38
		#010x	18.06	0.90	17.79
	xuAsp4	#x011	18.42	0.92	20.59
		#x110	11.04	0.55	8.94
		#x010	22.47	1.12	22.96
CIT_3	xuCit1	#x110x0+#x011x0	8.06	1.21	4.11
		#x010x0	11.75	1.76	9.63
		#x010x1	6.60	0.99	8.61
	xuCit2	#xx0xx1	31.58	4.74	19.55
		#xx1xx1	15.59	2.34	18.66
	xuCit3	#11xxxx+#xxx11x	61.97	9.30	60.76
		#10xxxx+#xxx01x	40.68	6.10	41.44
	xuCit4	#010xxx+#xx010x	28.65	4.30	31.26
		#011xxx+#xx110x	10.94	1.64	9.07
		#110xxx+#xx011x	47.07	7.06	49.96
		#111xxx+#xx111x	9.39	1.41	9.17

FSUC_3	xuSucf1	#11xxxx	30.28	4.54	32.76
		#10xxxx	9.36	1.40	8.45
	xuSucf2	#xx010x	9.44	1.42	8.81
		#xx110x+#xx011x	14.00	2.10	14.82
	xuSucf3	#xxx111	25.02	3.75	31.12
		#xxx010	9.90	1.49	7.05
		#xxx110+#xxx011	6.31	0.95	5.59
	xuSucf4	#xxxx01	5.44	0.82	5.78
		#xxxx11	30.00	4.50	26.58
	xuSucf5	#x010xx	16.54	2.48	8.42
		#x110xx+#x011xx	8.51	1.28	10.28
FUM_3	xuFum1	#11xx+#xx11	11.60	1.74	10.49
		#01xx+#xx10	10.63	1.59	11.48
	xuFum2	#10xx+#xx01	12.93	1.94	13.85
		#11xx+#xx11	13.80	2.07	12.65
GLU_3	xuGlu1	#11xxx	22.54	1.13	23.44
		#10xxx	29.36	1.47	28.09
	xuGlu2	#110xx	22.76	1.14	25.04
		#011xx	11.40	0.57	10.88
		#010xx	30.05	1.50	27.92
	xuGlu3	#xx110+#xx011	33.52	1.68	32.76
		#xx010	11.10	0.56	11.35
	xuGlu4	#x110x+#x011x	15.22	0.76	14.84
		#x010x	30.93	1.55	31.67
GLY_3	xuGly1	#10	19.31	0.97	15.06
		#11	17.78	0.89	20.42
	xuGly2	#11	19.02	0.95	21.18
		#01	18.37	0.92	15.62
GSUC_3	xuSucg1	#11xxxx	49.19	7.38	51.16
		#10xxxx	13.80	2.07	13.20
	xuSucg2	#xxxx01	3.52	0.53	4.11
		#xxxx11	27.00	4.05	19.90
	xuSucg3	#xx010x	6.19	0.93	6.04
		#xx011x+#xx110x	9.88	1.48	10.11
	xuSucg4	#xxx010	9.18	1.38	6.06
		#xxx011+#xxx110	5.96	0.89	4.79
		#x010xx	19.11	2.87	11.79
		#x011xx+#x110xx	9.95	1.49	14.23
ILE_3	xuIle1	#110xxx+#011xxx	5.50	0.28	5.83
		#010xxx	5.78	0.29	5.40
	xuIle2	#x110x0+#x011x0+#x010x1	11.00	0.55	11.40
		#x010x0	4.36	0.22	4.18
	xuIle3	#xx110x+#xx011x	8.14	0.41	8.25
		#xx010x	8.73	0.44	8.61
	xuIle4	#xx1xx1	10.24	0.51	8.45
		#xx0xx1	2.96	0.15	3.35
	xuIle5	#xxx11x	4.62	0.23	4.98
		#xxx01x	6.60	0.33	5.97
LEU_3	xuLeu1	#11xxxx	22.92	1.15	20.68

		#10xxxx	7.59	0.38	8.21
	xuLeu2	#011xxx+#110xxx	21.72	1.09	20.53
		#010xxx	7.40	0.37	7.76
	xuLeu3	#x110xx+#x011xx	6.60	0.33	6.73
		#x010xx	27.48	1.37	26.94
	xuLeu4	#xxx11x	21.78	1.09	21.93
		#xxx01x	8.76	0.44	8.70
	xuLeu5	#xxx1x1	4.32	0.22	3.87
		#xxx0x1	28.59	1.43	30.98
LYS_3	xuLys1	#xxx110+#xxx011	18.16	0.91	19.25
		#xxx010	11.20	0.56	10.44
	xuLys2	#xx110x+#xx011x	11.40	0.57	12.28
		#xx010x	14.07	0.70	12.80
MET_3	xuMet1	#xx01x	10.24	0.51	9.57
		#x010x	6.50	0.33	6.89
PRO_3	xuPro1	#xxx11	13.66	0.68	12.70
		#xxx01	4.32	0.22	4.60
SER_3	xuSer1	#11x	14.52	0.73	14.48
		#10x	10.65	0.53	10.68
STA_3	xuStarcha1	#10xxxx	2.35	0.35	2.26
		#11xxxx	6.04	0.91	6.26
	xuStarcha2	#010xxx	3.30	0.50	3.01
		#110xxx+#011xxx	3.40	0.51	3.65
	xuStarcha3	#x010xx	5.00	0.75	4.09
		#x110xx+#x011xx	2.94	0.44	3.32
	xuStarcha4	#xx010x	2.59	0.39	2.56
		#xx110x+#xx011x	4.09	0.61	4.14
	xuStarcha5	#xxx010	1.98	0.30	1.77
		#xxx011+#xxx110	1.41	0.21	1.53
	xuStarcha6	#xxxx01	1.27	0.19	1.36
		#xxxx11	6.55	0.98	6.04
	xuStarchb1	#10xxxx	3.25	0.49	3.23
		#11xxxx	8.90	1.34	8.95
	xuStarchb2	#010xxx	4.91	0.74	4.74
		#110xxx+#011xxx	5.59	0.84	5.77
	xuStarchb3	#x010xx+#xxx011+#xxx110	8.57	1.29	6.72
		#x110xx+#x011xx	3.53	0.53	4.05
	xuStarchb4	#xx010x	4.06	0.61	3.57
		#xx110x+#xx011x	5.27	0.79	5.78
	xuStarchb6	#xxxx01	2.03	0.30	2.00
		#xxxx11	8.82	1.32	8.93
THR_3	xuThr1	#11xx	9.30	0.47	9.13
		#10xx	9.41	0.47	9.57
	xuThr2	#x110+#x011	9.44	0.47	10.16
		#x010	8.68	0.43	7.90
	xuThr3	#xx11	7.34	0.37	7.61
		#xx01	9.51	0.48	9.13

Appendix 5.1A : ^{13}C NMR measurements of metabolites derived from *Arabidopsis* suspension grown on normal MS medium fed with 99%[1-^{13}C]glucose or 99%[2-^{13}C]glucose (Chapter 5)

Metabolite Source	Metabolite name used in the model	Carbon atom subgroups	Peak area	sd	Cumomer
MS [1-^{13}C]glucose_Replica 1					
Citrate	CIT	C6	7.625	0.948	#xx1xx1
			30.664	2.243	#xx0xx1
		C1C5	44.028	2.23	#10xxxx+#xxx01x
			20.118	1.592	#11xxxx+#xxx11x
		C3	36.192	2.259	#x010x0
			30.314	1.447	#x110x0+#x011x0
			3.864	0.376	#x010x1
		C2	125.96	4.317	#010xxx+#xx010x
			51.401	2.259	#011xxx+#xx110x
			8.92	0.755	#110xxx+#xx011x
Malate	OAA	malC1	34.798	1.643	#10xx
			10.284	0.727	#11xx
		malC2	63.521	2.477	#010x
			23.196	1.281	#011x
			8.935	0.682	#110x
		malC3	22.203	1.035	#x011+#x110
			43.483	2.339	#x010
		malC4	34.942	1.67	#xx01
			14.724	1.074	#xx11
Glutamate/ glutamine	GLU	gluc23	38.491	2.603	#010xx
			20.564	1.42	#x010x
		gluC4	27.682	2.074	#xx010
			10.202	0.802	#xx110
		gluC3	20.564	1.42	#x010x
			16.99	1.295	#x110x+#x011x
		glnC4	34.378	1.574	#xx010
			14.91	0.984	#xx110
		glnC3	18.863	1.188	#x010x
			17.527	1.203	#x110x+#x011x
		glnC23	33.838	2.052	#010xx
			18.863	1.188	#x010x
GABA	GABA	C2	4.116	0.403	#011x
			12.694	1.29	#010x
		c3	4.838	0.528	#x010
			3.929	0.482	#x110+#x011
Alanine	ALA	C3C1	96.593	3.997	#x01
			7.014	0.779	#10x
Sucrose	FSUC	fructopyrC1C6b	87.43	3.212	#10xxxx
			20.776	1.188	#xxxx01
		sucFC1C6b	11.928	1.196	#10xxxx

			2.89	0.745	#xxxx01
Starch	STA	C1C6alpha	47.676	1.532	#10xxxx
			16.88	0.788	#xxxx01
MS [1-^{13}C]glucose_Replica 2					
Citrate	CIT	C6	18.108	1.169	#xx1xx1
			42.355	1.896	#xx0xx1
		C1C5	61.467	2.83	#10xxxx+#xxx01x
			29.422	2.01	#11xxxx+#xxx11x
		C3	52.351	2.123	#x010x0
			47.266	2.054	#x110x0+#x011x0
			8.998	0.735	#x010x1
		C2	175.863	5.725	#010xxx+#xx010x
			74.591	2.996	#011xxx+#xx110x
			15.18	1.111	#110xxx+#xx011x
Malate	OAA	malC1	34.044	1.598	#10xx
			16.728	1.161	#11xx
		malC2	62.409	2.436	#010x
			25.216	1.346	#011x
			10.318	0.793	#110x
		malC3	10.603	0.81	#x011
			25.004	1.37	#x110
			61.285	2.397	#x010
		malC4	35.593	1.706	#xx01
			16.94	1.236	#xx11
Glutamate/ glutamine	GLU	gluc2	24.624	3.127	#011xx
			90.46	6.096	#010xx
		gluc4	76.04	3.796	#xx010
			35.315	2.68	#xx110
		gluC3	60.185	2.807	#x010x
			53.212	2.664	#x110x+#x011x
		glnC1	47.892	2.426	#10xxx
			18.962	1.465	#11xxx
		glnC4	50.103	2.077	#xx010
			25.172	1.468	#xx110
		glnC3	29.582	1.621	#x010x
			27.985	1.633	#x110x+#x011x
GABA	GABA	C2	13.954	1.922	#011x
			19.46	1.546	#010x
		C3	6.877	0.634	#x010
			5.001	0.507	#x110+#x011
Aspartate	ASP	C3	7.738	0.693	#x010
			4.854	0.805	#x110+#x011
Sucrose	FSUC	fructopyrC1C6b	191.095	6.105	#10xxxx
			47.254	2.147	#xxxx01
		sucFC1C6b	44.4	2.064	#10xxxx
			14.758	1.652	#xxxx01
Starch	STA	C1C6beta	157.185	7.088	#10xxxx

			51.619	4.562	#xxxx01
		C1C6alpha	95.289	5.122	#10xxxx
			27.31	2.965	#xxxx01
MS [1-^{13}C]glucose_Replica 3					
Citrate	CIT	C6	9.805	0.759	#xx1xx1
			25.722	1.272	#xx0xx1
		C1C5	33.477	1.855	#10xxxx+#xxx01x
			12.056	1.118	#11xxxx+#xxx11x
		C2	112.173	3.983	#010xxx+#xx010x
			45.191	2.098	#011xxx+#xx110x
			7.203	0.672	#110xxx+#xx011x
Malate	OAA	malC1	25.247	1.326	#10xx
			11.023	0.889	#11xx
		malC2	47.982	1.996	#010x
			18.416	1.102	#011x
			6.167	0.545	#110x
		malC3	47.771	2.032	#x010
			19.104	1.182	#x110
			9.295	0.849	#x011
		malC4	25.791	1.326	#xx01
			9.551	0.758	#xx11
Glutamate/ glutamine	GLU	gluC3	43.598	2.183	#x010x
			38.749	2.099	#x110x+#x011x
		glnC1	32.849	1.781	#10xxx
			12.215	1.089	#11xxx
		glnC4	58.464	2.332	#xx010
			23.959	1.353	#xx110
		glnC3	25.751	1.495	#x010x
			19.876	1.253	#x110x+#x011x
		glnC21	64.138	3.228	#010xx
			32.849	1.781	#10xxx
GABA	GABA	C4	8.974	0.864	#xx01
			2.05	0.312	#xx11
		C2	15.741	0.944	#010x
			8.77	0.845	#011x
		C3C4	6.591	0.714	#x010
			8.974	0.864	#xx01
Sucrose	FSUC	fructopyrC1C6b	126.654	4.386	#10xxxx
			30.091	1.562	#xxxx01
		sucFC1C6b	45.839	2.168	#10xxxx
			13.283	1.411	#xxxx01
Starch	STA	C1C6beta	90.119	3.928	#10xxxx
			29.287	2.522	#xxxx01
		C1C6alpha	53.459	2.784	#10xxxx
			16.378	1.8	#xxxx01
MS [2-^{13}C]glucose_Replica 1					
Citrate	CIT_2	C2C4	38.933	1.873	#010xxx+#xx010x

			3.854	0.525	#011xxx+#xx110x
Malate	OAA_2	malC23	29.074	1.413	#010x
			26.07	1.295	#x010
Glutamate/ glutamine	GLU_2	gluC3	29.924	1.698	#x010x
			5.532	0.747	#x110x+#x011x
		glnC3	17.078	1.107	#x010x
			3.898	0.622	#x110x+#x011x
Starch	STA_2	C1C6beta	18.345	1.423	#10xxxx
			9.34	1.273	#xxxx01
		C1C6alpha	11.142	1.081	#10xxxx
			5.263	0.936	#xxxx01
		C2C5beta	92.668	3.915	#010xxx
			26.998	1.745	#xxx010
		C2C5alpha	54.811	2.747	#010xxx
			16.263	1.339	#xxx010
MS [2-^{13}C]glucose_Replica 2					
Citrate	CIT_2	C6	124.443	4.805	#xx0xx1
			10.444	1.136	#xx1xx1
		C2C4	116.69	4.612	#010xxx+#xx010x
			10.251	0.988	#011xxx+#xx110x
			8.578	0.924	#110xxx+#xx011x
		C1C5	408.666	12.949	#10xxxx+#xxx01x
			15.933	1.493	#11xxxx+#xxx11x
Malate	OAA_2	malC3	5.571	0.78	#x011
			7.693	1.1	#x110
			63.164	2.697	#x010
		malC2	51.131	2.125	#010x
			14.718	1.081	#011x+#110x
GABA	GABA_2	C3C4	12.617	1.137	#xx01
			11.162	1.018	#x010
		C3	11.162	1.018	#x010
			2.46	0.751	#x110+#x011
Glutamate/ glutamine	GLU_2	gluC4	14.948	1.077	#xx010
			3.429	0.795	#xx110
			2.314	0.622	#xx011
		gluC3	47.898	2.715	#x010x
			8.325	1.281	#x110x+#x011x
		glnC4	18.612	1.26	#xx010
			2.161	0.582	#xx110
			1.97	0.517	#xx011
		glnC3	28.348	1.736	#x010x
			6.012	1.051	#x110x+#x011x
Sucrose	FSUC_2	SucroseF2F5	48.379	2.42	#010xxx
			8.949	0.831	#xxx010
Fructose	F6P_2	bFruC2C5	79.78	3	#010xxx
			19.813	1.238	#xxx010
Starch	STA_2	C1C6beta	10.907	1.175	#10xxxx

			4.827	0.986	#xxxx01
		C1C6alpha	6.422	0.863	#10xxxx
			2.579	0.788	#xxxx01
		C2C5beta	53.946	2.827	#010xxx
			15.009	1.261	#xxx010
		C2C5alpha	31.347	2.007	#010xxx
			10.537	1.15	#xxx010
MS [2-13C]glucose_Replica 3					
Citrate	CIT_2	C6	73.815	3.143	#xx0xx1
			3.195	0.445	#xx1xx1
		C2C4	68.657	3.106	#010xxx+#xx010x
			10.152	0.966	#011xxx+#xx110x+#110xxx+#xx011x
Malate	OAA_2	malC14	70.187	2.98	#10xx
			72.187	3.169	#xx01
		malC3	34.436	1.753	#x010
			2.757	0.506	#x110
			2.907	0.499	#x011
		malC2	42.168	2.094	#010x
			5.01	0.746	#011x
			3.526	0.609	#110x
Glutamate/ glutamine	GLU_2	C4	10.732	0.881	#xx010
			1.774	0.449	#xx110
		C3	44.605	2.604	#x010x
			6.121	0.95	#x110x+#x011x
		glnC4	6.174	0.68	#xx010
			1.024	0.262	#xx110
		glnC3	20.925	1.466	#x010x
			2.642	0.521	#x110x+#x011x
Sucrose	GSUC_2	C5C2	6.176	0.78	#xxx010
			31.349	2.278	#010xxx
Fructose	F6P_2	bFruC2C5	52.793	2.236	#010xxx
			13.584	1.017	#xxx010
Starch	STA_2	C1C6beta	14.941	1.44	#10xxxx
			6.87	1.211	#xxxx01
		C1C6alpha	9.124	1.193	#10xxxx
			3.537	0.79	#xxxx01
		C2C5beta	80.745	3.83	#010xxx
			21.557	1.69	#xxx010
		C2C5alpha	48.434	2.771	#010xxx
			14.068	1.406	#xxx010

Appendix 5.1B : Mass isotopomer measurements of metabolites derived from *Arabidopsis* suspension grown on normal MS medium fed with either 99%[1-^{13}C]glucose, 99%[2-^{13}C]glucose or 20%[^{13}C$_6$]glucose (Chapter 5)

Metabolite	Metabolite name used in the model	Carbon atoms	Mass (m+)	[1-^{13}C]glucose			[2-^{13}C]glucose			[^{13}C$_6$]glucose			Max error
				Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	sd
Alanine	ALA	1,2,3	0	0.598	0.593	0.593	0.529	0.53	0.528	0.741	0.736	0.741	0.01
			1	0.383	0.387	0.387	0.43	0.431	0.431	0.074	0.076	0.074	0.01
			2	0.019	0.019	0.02	0.041	0.039	0.04	0.038	0.04	0.038	0.01
			3	0.001	0	0	0	0	0	0.147	0.148	0.147	0.01
		2,3	0	0.618	0.615	0.615	0.564	0.562	0.562	0.779	0.775	0.778	0.01
			1	0.375	0.377	0.377	0.429	0.432	0.432	0.052	0.053	0.051	0.01
			2	0.007	0.008	0.008	0.006	0.006	0.005	0.169	0.173	0.171	0.01
Glycine	GLYeff	1,2	0	0.947	0.941	0.947	0.675	0.685	0.679	0.794	0.792	0.798	0.014
			1	0.053	0.058	0.055	0.304	0.299	0.308	0.109	0.091	0.095	0.01
			2	-0.001	0.001	-0.002	0.021	0.016	0.013	0.097	0.116	0.107	0.01
		1,2	0	0.94	0.947	0.949	0.681	0.676	0.676	0.789	0.794	0.794	0.01
			1	0.06	0.053	0.051	0.304	0.308	0.308	0.105	0.091	0.097	0.01
			2	0.001	0	0	0.015	0.016	0.016	0.105	0.114	0.11	0.01
		2	0	0.982	0.983	0.983	0.726	0.726	0.727	0.843	0.839	0.842	0.01
			1	0.018	0.017	0.017	0.274	0.274	0.273	0.157	0.161	0.158	0.01
Valine	VAL	1,2,3,4,5	0	0.349	0.34	0.346	0.278	0.285	0.288	0.563		0.563	0.012
			1	0.476	0.476	0.475	0.493	0.487	0.486	0.11		0.113	0.012
			2	0.163	0.167	0.165	0.208	0.207	0.205	0.162		0.162	0.012
			3	0.012	0.016	0.014	0.022	0.022	0.02	0.129		0.125	0.012
			4	0	0.001	0.001	0	0	0	0.015		0.015	0.012
			5	0	0	-0.001	-0.001	0	0	0.021		0.022	0.012
		2,3,4,5	0	0.372	0.362	0.362	0.309	0.313	0.318	0.591		0.593	0.012
			1	0.469	0.472	0.475	0.503	0.499	0.495	0.102		0.102	0.012
			2	0.15	0.157	0.152	0.182	0.183	0.18	0.261		0.258	0.012
			3	0.009	0.01	0.011	0.006	0.006	0.006	0.021		0.021	0.012
			4	0	-0.001	0	-0.001	0	0	0.025		0.026	0.012
Leucine	LEU	2,3,4,5,6	0	0.235	0.227	0.231	0.276	0.279	0.285	0.477		0.48	0.017

			1	0.453	0.451	0.455	0.483	0.48	0.477	0.189		0.188	0.017
			2	0.252	0.258	0.253	0.212	0.213	0.21	0.24		0.239	0.017
			3	0.056	0.059	0.057	0.026	0.026	0.025	0.063		0.062	0.017
			4	0.004	0.004	0.004	0.003	0.003	0.003	0.026		0.026	0.017
			5	0	0	0	0	0	0	0.005		0.005	0.017
Serine	SEReff	1,2,3	0	0.705	0.709	0.712	0.602	0.609	0.602	0.696	0.693	0.709	0.01
			1	0.284	0.28	0.281	0.353	0.343	0.352	0.17	0.155	0.158	0.01
			2	0.011	0.012	0.006	0.046	0.049	0.046	0.084	0.087	0.08	0.01
			3	0	0	0.002	-0.001	-0.001	0	0.051	0.065	0.052	0.01
		1,2,3	0	0.718	0.712	0.716	0.607	0.607	0.606	0.699	0.693	0.704	0.01
			1	0.278	0.281	0.279	0.349	0.348	0.35	0.165	0.156	0.157	0.01
			2	0.008	0.009	0.008	0.044	0.046	0.044	0.084	0.088	0.085	0.01
			3	-0.005	-0.002	-0.002	0	0	0	0.053	0.063	0.055	0.01
		2,3	0	0.733	0.731	0.734	0.639	0.64	0.64	0.736	0.727	0.739	0.01
			1	0.266	0.268	0.265	0.339	0.337	0.337	0.197	0.195	0.192	0.01
			2	0	0.001	0.001	0.021	0.022	0.023	0.067	0.078	0.069	0.01
		2,3	0	0.733	0.732	0.735	0.639	0.641	0.642	0.74	0.728	0.741	0.01
			1	0.264	0.265	0.262	0.338	0.335	0.334	0.193	0.193	0.191	0.01
			2	0.003	0.003	0.004	0.023	0.023	0.023	0.066	0.078	0.069	0.01
Threonine	THR	1,2,3,4	0	0.372	0.356	0.372	0.408	0.421	0.426	0.542	0.55	0.561	0.02
			1	0.477	0.473	0.46	0.485	0.475	0.464	0.235	0.223	0.222	0.02
			2	0.15	0.171	0.157	0.109	0.11	0.119	0.149	0.152	0.145	0.02
			3	0.012	0.011	0.019	0.007	0.002	-0.003	0.061	0.064	0.063	0.02
			4	-0.011	-0.011	-0.007	-0.008	-0.008	-0.005	0.012	0.01	0.008	0.02
		2,3,4	0	0.451	0.44	0.458	0.559	0.575	0.569	0.618	0.624	0.619	0.01
			1	0.425	0.43	0.417	0.403	0.376	0.389	0.235	0.226	0.228	0.01
			2	0.125	0.117	0.121	0.041	0.052	0.043	0.109	0.115	0.12	0.01
			3	-0.001	0.012	0.004	-0.003	-0.003	-0.001	0.038	0.035	0.033	0.01
Phenylalanine	PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.269	0.262	0.266	0.144	0.153	0.157	0.373	0.367	0.381	0.011
			1	0.449	0.449	0.451	0.403	0.396	0.394	0.145	0.14	0.139	0.011
			2	0.23	0.235	0.229	0.309	0.307	0.305	0.138	0.141	0.137	0.011
			3	0.047	0.049	0.048	0.115	0.115	0.115	0.172	0.176	0.173	0.011
			4	0.004	0.003	0.004	0.025	0.025	0.024	0.084	0.086	0.082	0.011
			5	0.001	0.001	0.001	0.004	0.003	0.004	0.043	0.044	0.043	0.011

			6	0	0	0	0	0.001	0.001	0.028	0.028	0.028	0.011
			7	0	0.001	0.001	0	0.001	0.001	0.011	0.012	0.011	0.011
			8	0	0	0	0	0	0	0.003	0.003	0.003	0.011
			9	0	0	0	0	0	0	0.002	0.002	0.001	0.011
		2,3,4,5,6,7,8,9	0	0.277	0.273	0.275	0.154	0.164	0.166	0.393	0.386	0.397	0.011
			1	0.453	0.452	0.453	0.418	0.411	0.41	0.135	0.131	0.133	0.011
			2	0.223	0.227	0.225	0.307	0.304	0.302	0.215	0.22	0.216	0.011
			3	0.044	0.045	0.043	0.104	0.103	0.102	0.115	0.114	0.112	0.011
			4	0.002	0.003	0.003	0.017	0.018	0.019	0.082	0.086	0.08	0.011
			5	0	0	0.001	0.001	0.001	0.002	0.034	0.035	0.035	0.011
			6	0	0	0	0	0	0	0.022	0.023	0.021	0.011
			7	0	0	0	0	0	0	0.003	0.004	0.004	0.011
			8	0	0	0	0	0	0	0.002	0.003	0.003	0.011
		1,2	0	0.961	0.962	0.965	0.572	0.575	0.578	0.762	0.754	0.766	0.01
			1	0.039	0.038	0.036	0.413	0.41	0.408	0.08	0.085	0.077	0.01
			2	0	0	-0.001	0.015	0.014	0.014	0.158	0.162	0.157	0.01
Aspartate	ASP	1,2,3,4	0	0.366	0.366	0.368	0.424	0.434	0.431	0.552		0.566	0.01
			1	0.45	0.441	0.44	0.459	0.453	0.456	0.226		0.214	0.01
			2	0.161	0.172	0.171	0.112	0.108	0.109	0.148		0.146	0.01
			3	0.021	0.021	0.023	0.005	0.005	0.003	0.06		0.061	0.01
			4	0.001	0	-0.002	-0.001	0	0.002	0.014		0.013	0.01
		1,2,3,4	0	0.37	0.369	0.367	0.425	0.438	0.433	0.555		0.558	0.01
			1	0.443	0.442	0.448	0.46	0.449	0.453	0.226		0.223	0.01
			2	0.163	0.165	0.162	0.11	0.107	0.109	0.144		0.143	0.01
			3	0.023	0.023	0.022	0.005	0.006	0.005	0.062		0.061	0.01
			4	0	0	0	0	0	0	0.014		0.014	0.01
		2,3,4	0	0.437	0.431	0.432	0.556	0.568	0.562	0.618		0.622	0.01
			1	0.434	0.437	0.439	0.396	0.384	0.39	0.233		0.23	0.01
			2	0.119	0.123	0.12	0.048	0.048	0.048	0.115		0.113	0.01
			3	0.009	0.009	0.008	0	0	0	0.035		0.035	0.01
		2,3,4	0	0.447	0.442	0.443	0.565	0.574	0.569	0.624		0.625	0.018
			1	0.421	0.424	0.425	0.379	0.372	0.377	0.227		0.225	0.018
			2	0.117	0.119	0.117	0.048	0.047	0.048	0.109		0.111	0.018
			3	0.015	0.015	0.014	0.007	0.007	0.007	0.04		0.039	0.018

		1,2	0	0.622	0.62	0.62	0.656	0.662	0.661	0.732		0.734	0.011
			1	0.344	0.344	0.344	0.335	0.33	0.331	0.16		0.156	0.011
			2	0.035	0.035	0.036	0.009	0.009	0.008	0.108		0.11	0.011
Glutamate	GLU	1,2,3,4,5	0	0.274	0.272	0.273	0.323	0.33	0.328	0.487		0.485	0.01
			1	0.434	0.433	0.435	0.463	0.459	0.46	0.213		0.216	0.01
			2	0.233	0.235	0.233	0.19	0.187	0.188	0.205		0.205	0.01
			3	0.053	0.056	0.054	0.023	0.023	0.023	0.071		0.067	0.01
			4	0.005	0.005	0.005	0.001	0	0	0.02		0.022	0.01
			5	0	0	0	0	0	0	0.005		0.005	0.01
		1,2,3,4,5	0									0.489	0.01
			1									0.211	0.01
			2									0.205	0.01
			3									0.07	0.01
			4									0.019	0.01
			5									0.006	0.01
		2,3,4,5	0				0.416	0.414	0.418			0.543	0.01
			1				0.463	0.463	0.461			0.227	0.01
			2				0.118	0.118	0.116			0.181	0.01
			3				0.005	0.005	0.005			0.039	0.01
			4				-0.001	0	-0.001			0.009	0.01
		2,3,4,5	0	0.317	0.315	0.319		0.419		0.541	0.541	0.542	0.012
			1	0.454	0.454	0.455		0.461		0.226	0.225	0.227	0.012
			2	0.199	0.201	0.198		0.116		0.18	0.181	0.18	0.012
			3	0.03	0.031	0.029		0.005		0.042	0.041	0.042	0.012
			4	0	-0.001	-0.001		0		0.01	0.012	0.009	0.012
Isoleucine	ILE	2,3,4,5,6	0	0.259	0.257	0.256	0.288	0.296	0.298	0.478	0.474	0.485	0.013
			1	0.463	0.46	0.465	0.494	0.489	0.488	0.211	0.211	0.208	0.013
			2	0.223	0.226	0.225	0.192	0.189	0.189	0.218	0.22	0.215	0.013
			3	0.05	0.051	0.049	0.025	0.024	0.024	0.068	0.069	0.067	0.013
			4	0.005	0.005	0.005	0.001	0.002	0.001	0.019	0.02	0.02	0.013
			5	0	0	0	0	0	0	0.005	0.006	0.005	0.013
Methionine	METeff	1,2,3,4,5	0	0.411	0.412	0.412	0.505	0.512	0.51	0.565	0.565	0.57	0.01
			1	0.367	0.366	0.369	0.37	0.368	0.364	0.243	0.237	0.238	0.01
			2	0.176	0.176	0.174	0.115	0.108	0.112	0.117	0.121	0.117	0.01

			3	0.04	0.042	0.04	0.009	0.012	0.013	0.057	0.058	0.056	0.01
			4	0.006	0.004	0.004	0	0	0	0.017	0.017	0.016	0.01
			5	0	0	0	0	0	0.001	0.002	0.002	0.003	0.01
		2,3,4,5	0	0.451	0.449	0.45	0.598	0.604	0.603	0.608	0.606	0.611	0.01
			1	0.372	0.371	0.372	0.333	0.331	0.33	0.253	0.25	0.25	0.01
			2	0.149	0.151	0.15	0.065	0.062	0.064	0.1	0.102	0.099	0.01
			3	0.027	0.028	0.026	0.004	0.003	0.004	0.035	0.038	0.037	0.01
			4	0.001	0.001	0.002	0	0	0	0.005	0.005	0.004	0.01
		2,3,4,5	0	0.457	0.456	0.457	0.6	0.606	0.607	0.614	0.607	0.615	0.011
			1	0.371	0.371	0.373	0.334	0.327	0.328	0.251	0.25	0.247	0.011
			2	0.149	0.15	0.148	0.065	0.063	0.064	0.099	0.101	0.1	0.011
			3	0.024	0.025	0.023	0.003	0.004	0.002	0.033	0.037	0.035	0.011
			4	-0.001	-0.001	-0.001	-0.001	0	-0.002	0.002	0.005	0.003	0.011
Lysine	LYS	1,2,3,4,5,6	0	0.281	0.278	0.278	0.289	0.298	0.299		0.445		0.01
			1	0.418	0.414	0.422	0.44	0.439	0.434		0.211		0.01
			2	0.235	0.238	0.234	0.228	0.221	0.224		0.175		0.01
			3	0.062	0.062	0.061	0.04	0.04	0.042		0.112		0.01
			4	0.007	0.007	0.005	0.005	0.003	0.003		0.04		0.01
			5	0	0.001	0.001	-0.001	0	-0.001		0.015		0.01
			6	-0.002	0	-0.001	-0.001	0	0		0.004		0.01
		2,3,4,5,6	0	0.303	0.299	0.299	0.338	0.34	0.344		0.476		0.01
			1	0.441	0.438	0.445	0.472	0.456	0.46		0.218		0.01
			2	0.222	0.222	0.22	0.183	0.183	0.181		0.208		0.01
			3	0.044	0.048	0.045	0.019	0.023	0.023		0.073		0.01
			4	-0.002	-0.001	0	-0.005	0	-0.002		0.02		0.01
			5	-0.009	-0.006	-0.008	-0.009	-0.002	-0.005		0.004		0.01
Arginine	ARGeff	1,2,3,4,5,6	0	0.402	0.399	0.396	0.422	0.429	0.428	0.522	0.519	0.535	0.01
			1	0.342	0.34	0.342	0.362	0.361	0.365	0.227	0.222	0.217	0.01
			2	0.194	0.193	0.2	0.176	0.17	0.169	0.153	0.159	0.156	0.01
			3	0.058	0.059	0.052	0.038	0.037	0.035	0.07	0.072	0.066	0.01
			4	0.008	0.01	0.011	0.005	0.002	0.003	0.022	0.019	0.025	0.01
			5	0	-0.002	0.001	-0.002	0	0.001	0.007	0.007	0.004	0.01
			6	-0.003	0	-0.002	-0.002	0	-0.001	-0.001	0.001	-0.004	0.01
Histidine	HISeff	1,2,3,4,5,6	0	0.545	0.532	0.537	0.332	0.338	0.339	0.592	0.584	0.587	0.01

			1	0.342	0.339	0.337	0.42	0.408	0.41	0.179	0.167	0.172	0.01
			2	0.1	0.11	0.117	0.207	0.213	0.213	0.083	0.096	0.092	0.01
			3	0.013	0.018	0.015	0.041	0.037	0.037	0.092	0.089	0.088	0.01
			4	0	0.001	0.001	0.003	0.004	-0.001	0.029	0.029	0.028	0.01
			5	0.001	0.001	-0.003	0	0	0.004	0.025	0.03	0.024	0.01
			6	-0.003	-0.001	-0.003	-0.003	-0.001	-0.002	0	0.006	0.009	0.01
		1,2,3,4,5,6	0	0.538	0.531	0.533	0.332	0.336	0.339	0.585	0.582	0.592	0.012
			1	0.331	0.328	0.333	0.413	0.407	0.407	0.173	0.169	0.166	0.012
			2	0.112	0.118	0.114	0.21	0.21	0.209	0.096	0.099	0.097	0.012
			3	0.018	0.02	0.019	0.041	0.042	0.042	0.084	0.088	0.086	0.012
			4	0.001	0.001	0.002	0.005	0.004	0.003	0.029	0.028	0.027	0.012
			5	0	0.001	0	0	0	0	0.027	0.03	0.027	0.012
			6	0	0	0	0	0	0	0.006	0.005	0.005	0.012
		2,3,4,5,6	0	0.645	0.635	0.64	0.344	0.35	0.352	0.586	0.583	0.591	0.022
			1	0.293	0.289	0.29	0.426	0.42	0.42	0.18	0.175	0.176	0.022
			2	0.051	0.056	0.05	0.194	0.192	0.193	0.146	0.153	0.147	0.022
			3	0.011	0.014	0.013	0.031	0.03	0.031	0.049	0.048	0.047	0.022
			4	0.003	0.006	0.005	0.005	0.005	0.005	0.032	0.035	0.032	0.022
			5	-0.002	0.001	0.001	0	0.002	0.001	0.006	0.007	0.007	0.022
Fructose	F6P	4,5,6	0	0.816	0.816	0.819	0.815	0.785	0.785	0.775	0.767	0.771	0.01
			1	0.191	0.188	0.18	0.183	0.207	0.211	0.038	0.04	0.04	0.01
			2	-0.001	0.001	0.002	0.008	0.011	0.01	0.015	0.019	0.018	0.01
			3	-0.007	-0.005	-0.001	-0.005	-0.003	-0.005	0.172	0.174	0.171	0.01
		1,2,3,4	0	0.233	0.231	0.228		0.176	0.184	0.69	0.692	0.686	0.011
			1	0.74	0.746	0.75		0.785	0.778	0.117	0.112	0.117	0.011
			2	0.027	0.023	0.028		0.046	0.042	0.022	0.024	0.024	0.011
			3	0.002	0.001	-0.003		-0.004	-0.001	0.064	0.057	0.062	0.011
			4	-0.002	-0.001	-0.003		-0.003	-0.002	0.107	0.115	0.11	0.011
Fructose	F6P	4,5,6	0	0.821	0.817	0.828	0.817	0.787	0.789	0.779	0.772	0.771	0.013
			1	0.19	0.189	0.182	0.183	0.212	0.213	0.036	0.036	0.038	0.01
			2	-0.002	0	-0.003	0.007	0.009	0.008	0.013	0.016	0.016	0.01
			3	-0.009	-0.006	-0.007	-0.007	-0.008	-0.01	0.173	0.176	0.175	0.01
Succinate	SUCC	1,2,3,4	0	0.311	0.321	0.329	0.448	0.435	0.436	0.549	0.566	0.549	0.011
			1	0.437	0.427	0.425	0.44	0.447	0.447	0.225	0.221	0.226	0.011

			2	0.215	0.214	0.21	0.107	0.114	0.112	0.17	0.165	0.171	0.011
			3	0.036	0.036	0.036	0.005	0.005	0.004	0.044	0.039	0.043	0.011
			4	0.001	0.002	0	0	-0.001	0	0.011	0.009	0.01	0.011
Malate	OAA	1,2,3,4	0	0.351	0.345	0.352	0.431	0.432	0.435	0.553	0.55	0.552	0.01
			1	0.439	0.438	0.436	0.453	0.448	0.451	0.232	0.226	0.231	0.01
			2	0.182	0.191	0.184	0.111	0.11	0.112	0.141	0.15	0.145	0.01
			3	0.028	0.027	0.027	0.004	0.007	0.003	0.06	0.06	0.057	0.01
			4	-0.001	-0.001	0	0.001	0.003	0	0.014	0.014	0.015	0.01
		1,2,3,4	0	0.355	0.348	0.352	0.436	0.437	0.436	0.556	0.555	0.556	0.01
			1	0.437	0.437	0.436	0.452	0.449	0.451	0.23	0.227	0.228	0.01
			2	0.18	0.186	0.183	0.108	0.108	0.108	0.143	0.146	0.144	0.01
			3	0.027	0.028	0.028	0.005	0.006	0.005	0.059	0.059	0.059	0.01
			4	0.001	0.001	0.001	0	-0.001	0	0.013	0.013	0.013	0.01
Citrate	CIT	1,2,3,4,5,6	0	0.226	0.216	0.221	0.255	0.256	0.257	0.43	0.43	0.425	0.01
			1	0.399	0.397	0.399	0.439	0.438	0.439	0.226	0.216	0.223	0.01
			2	0.275	0.28	0.276	0.25	0.249	0.249	0.208	0.215	0.212	0.01
			3	0.088	0.093	0.09	0.053	0.054	0.052	0.092	0.092	0.093	0.01
			4	0.012	0.014	0.014	0.003	0.003	0.003	0.033	0.036	0.035	0.01
			5	0	0	0	-0.001	0	0	0.009	0.01	0.01	0.01
			6	0	0	0	0	0	0	0.002	0.002	0.002	0.01
Cell Wall	G6P	3,4,5	0	0.965	0.964	0.967	0.82	0.818	0.815	0.718	0.727	0.714	0.01
			1	0.037	0.037	0.036	0.169	0.169	0.174	0.098	0.092	0.1	0.01
			2	-0.002	-0.001	-0.003	0.012	0.013	0.011	0.057	0.054	0.061	0.01
			3	0	0	0	0	-0.001	-0.001	0.128	0.127	0.125	0.01
Cell Wall	PENTAN	3,4,5	0	0.966	0.966	0.964	0.827	0.824	0.815	0.725	0.72	0.716	0.01
			1	0.038	0.04	0.037	0.162	0.167	0.172	0.095	0.094	0.099	0.01
			2	-0.004	-0.005	-0.001	0.012	0.008	0.013	0.056	0.055	0.058	0.01
			3	0	-0.002	0	-0.001	0	0	0.124	0.13	0.128	0.01
Cell Wall	PENTAN	3,4,5	0	0.971	0.965	0.967		0.819	0.819	0.721	0.724	0.717	0.01
			1	0.034	0.04	0.038		0.173	0.177	0.098	0.093	0.097	0.01
			2	-0.004	-0.002	-0.003		0.013	0.007	0.057	0.052	0.057	0.01
			3	-0.001	-0.004	-0.002		-0.005	-0.003	0.124	0.131	0.129	0.01
Starch	STA	3,4,5,6	0	0.785	0.77	0.776	0.701	0.707	0.727	0.693	0.71	0.683	0.01
			1	0.203	0.22	0.213	0.253	0.25	0.232	0.118	0.099	0.118	0.01

			2	0.011	0.01	0.009	0.043	0.04	0.037	0.019	0.015	0.019	0.01
			3	0.001	0	0.001	0.003	0.003	0.003	0.07	0.056	0.071	0.01
			4	0	0	0	0	0	0.001	0.101	0.12	0.109	0.01
Starch	STA	3,4,5,6	0	0.793	0.767	0.775	0.695	0.713	0.726	0.69	0.709	0.684	0.01
			1	0.202	0.222	0.216	0.257	0.251	0.234	0.119	0.096	0.12	0.01
			2	0.009	0.011	0.01	0.045	0.038	0.037	0.019	0.013	0.017	0.01
			3	-0.002	0	-0.001	0.002	0	0.002	0.071	0.055	0.071	0.01
			4	-0.001	0.001	0	0.001	-0.002	0.001	0.102	0.126	0.108	0.01
Cell Wall	G6P	3,4,5,6	0	0.814	0.814	0.814	0.786	0.776	0.772	0.704	0.708	0.7	0.01
			1	0.177	0.177	0.177	0.189	0.201	0.202	0.101	0.095	0.104	0.01
			2	0.009	0.008	0.009	0.023	0.022	0.025	0.016	0.015	0.017	0.01
			3	0	0	0.001	0.002	0.001	0.001	0.059	0.055	0.062	0.01
			4	0	0	0	0	0	0	0.119	0.127	0.117	0.01
CellWall	G6P	3,4,5,6	0	0.819	0.818	0.822	0.792	0.78	0.774	0.711		0.704	0.01
			1	0.175	0.175	0.173	0.186	0.197	0.203	0.098		0.101	0.01
			2	0.005	0.006	0.005	0.021	0.022	0.022	0.013		0.015	0.01
			3	0	0	-0.001	0.001	0.001	0.001	0.057		0.06	0.01
			4	0	0	0	0	0	0	0.121		0.12	0.01
CellWall	G6P	3,4,5,6	0	0.818	0.818	0.822	0.798	0.779	0.772	0.712		0.706	0.01
			1	0.174	0.175	0.17	0.179	0.196	0.202	0.096		0.1	0.01
			2	0.008	0.007	0.008	0.021	0.023	0.024	0.014		0.015	0.01
			3	0	0	0	0.002	0.002	0.002	0.058		0.059	0.01
			4	0	0	0	0	0.001	0	0.12		0.12	0.01
Sucrose	GSUC	1,2,3,4,5,6	0	0.177	0.17	0.164	0.123	0.126	0.128	0.657			0.02
			1	0.699	0.706	0.716	0.703	0.709	0.703	0.079			0.02
			2	0.115	0.114	0.111	0.152	0.144	0.148	0.035			0.02
			3	0.007	0.007	0.007	0.02	0.018	0.019	0.1			0.02
			4	0.001	0.001	0.001	0	0.001	0.001	0.015			0.02
			5	0.001	0.001	0.001	0.001	0.001	0.001	0.013			0.02
			6	0	0	0	0	0	0	0.101			0.02

Appendix 5.1C : ^{13}C NMR measurements of metabolites derived from *Arabidopsis* suspension grown on N40 (nitrate only) medium fed with 99%[1-^{13}C]glucose or 99%[2-^{13}C]glucose (Chapter 5)

Metabolite	Metabolite name used in the model	Carbon atom subgroups	Peak area	sd	Cumomer
N40 [1-^{13}C]glucose_Replica 1					
Citrate	CIT	C6a	40.057	2.046	#xx1xx1
			99.016	3.67	#xx0xx1
		C1C5a	105.858	4.054	#10xxxx+#xxx01x
			39.947	2.144	#11xxxx+#xxx11x
		C2C4a	272.211	9.433	#010xxx+#xx010x
			119.518	5.506	#011xxx+#xx110x+#110xxx+#xx011x+#111xxx+#xx111x
Malate	OAA	C1a	79.425	3.365	#10xx
			31.726	2.404	#11xx
		C2a	186.048	7.796	#010x
			64.527	2.846	#011x
			34.484	1.817	#110x
		C3a	185.067	8.024	#x010
			7.556	1.117	#x111
			61.406	2.844	#x110
			27.592	1.68	#x011
Glutamate/ Glutamine	GLU	C1a	5.759	0.614	#10xxx
			3.111	0.58	#11xxx
		C2a	11.937	1.15	#010xx
			5.067	0.864	#011xx
		C4a	16.079	1.095	#xx010
			7.764	0.875	#xx110
		C4agln	40.104	2.046	#xx010
			12.161	2.485	#xx110+#xx011
		C3agln	9.213	0.841	#x010x
			8.436	0.862	#x110x+#x011x
	GABA	C2a	6.05	0.598	#010x
			1.527	0.284	#011x+#110x
	FSUC	fructopyrC1 C6b	376.6	11.693	#10xxxx
			71.358	3.084	#xxxx01
		sucFC1C6b	324.015	10.559	#10xxxx
			60.284	3.523	#xxxx01
	STA	C1C6beta	201.662	5.063	#10xxxx
			53.281	3.31	#xxxx01
		C1C6alpha	120.139	4.897	#10xxxx

			29.264	2.204	#xxxx01
N40 [1-13C]glucose_Replica 2					
	CIT	C6a	28.07	1.738	#xx1xx1
			76.855	3.205	#xx0xx1
		C1C5b	101.679	4.364	#10xxxx+#xxx01x
			34.88	2.301	#11xxxx+#xxx11x
		C3b	58.746	2.319	#x010x0
			44.806	1.907	#x110x0+#x011x0
			8.899	0.687	#x010x1
	OAA	C1a	111.965	4.215	#10xx
			37.892	2.049	#11xx
		C4	120.899	4.611	#xx01
			42.802	2.365	#xx11
		C2	203.305	6.805	#010x
			11.871	1.118	#111x
			66.512	2.989	#011x
			29.759	1.702	#110x
		C3	136.566	4.567	#x010
			7.257	0.63	#x111
			49.137	2.249	#x110
			18.047	1.034	#x011
	GLU	C4a	14.006	1.089	#xx010
			9.197	1.156	#xx110
		C4agln	38.184	1.99	#xx010
			6.721	1.373	#xx110+#xx011
		C3agln	7.918	0.875	#x010x
			8.312	1.085	#x110x+#x011x
	GABA	C2a	5.984	0.671	#010x
			3.425	0.691	#011x+#110x
	FSUC	fructopyrC1C6b	470.009	13.944	#10xxxx
			87.012	3.581	#xxxx01
		sucFC1C6b	230.686	7.91	#10xxxx
			40.165	2.946	#xxxx01
	STA	C1C6beta	269.495	9.472	#10xxxx
			67.271	4.091	#xxxx01
		C1C6alpha	157.346	6.208	#10xxxx
			37.422	2.759	#xxxx01
N40 [1-13C]glucose_Replica 3					
	CIT	C6a	21.559	1.598	#xx1xx1
			48.641	2.26	#xx0xx1
		C1C5b	66.842	3.275	#10xxxx+#xxx01x
			21.699	1.767	#11xxxx+#xxx11x
		C3b	22.347	1.301	#x110x0+#x011x0

			21.773	2.332	#x010x0
		C2C4a	185.706	6.075	#010xxx+#xx010x
			81.388	3.452	#011xxx+#xx110x+#110xxx+#xx011x+#111xxx+#xx111x
	OAA	C1a	68.638	2.603	#10xx
			24.028	1.322	#11xx
		C4	74.045	2.874	#xx01
			25.803	1.47	#xx11
		C2	125.738	5.387	#010x
			6.882	1.164	#111x
			41.894	1.94	#011x
			18.496	1.104	#110x
		C3	84.23	3.681	#x010
			4.407	0.468	#x111
			25.536	1.201	#x110
			12.232	0.749	#x011
	GLU	C4a	8.487	0.697	#xx010
			3.413	0.491	#xx110
		C3agln	5.685	1.157	#x010x
			3.52	0.884	#x110x+#x011x
	GABA	C2a	3.582	0.421	#010x
			1.074	0.273	#011x+#110x
	FSUC	fructopyrC1 C6b	235.694	7.394	#10xxxx
			44.156	2.008	#xxxx01
		sucFC1C6b	315.714	9.812	#10xxxx
			61.272	3.075	#xxxx01
	STA	C1C6beta	251.745	9.59	#10xxxx
			68.992	4.851	#xxxx01
		C1C6alpha	146.84	6.418	#10xxxx
			36.792	3.249	#xxxx01
N40 [2-13C]glucose_Replica 1					
	CIT_2	C6a	45.588	1.873	#xx0xx1
			3.514	0.338	#xx1xx1
		C1C5b	146.672	6.206	#10xxxx+#xxx01x
			9.147	1.005	#11xxxx+#xxx11x
		C2C4a	86.41	3.346	#010xxx+#xx010x
			10.156	0.838	#011xxx+#xx110x
	OAA_2	C1a	83.796	2.934	#10xx
			4.665	0.457	#11xx
		C4	87.826	3.109	#xx01
			8.349	0.817	#xx11
		C2	94.481	3.472	#010x
			9.163	0.781	#011x

			9.958	0.92	#110x
		C3	80.264	3.014	#x010
			7.427	0.668	#x110
			6.837	0.64	#x011
	FSUC_2	SucroseF2F5	258.45	8.209	#010xxx
			46.955	3.269	#xxx010
	GSUC_2	C5C2	41.934	2.013	#xxx010
			264.984	8.59	#010xxx
	STA_2	C1beta	4.02	0.827	#11xxxx
			54.219	3.234	#10xxxx
		C1625beta	54.219	3.234	#10xxxx
			23.754	2.346	#xxxx01
			271.744	10.225	#010xxx
			63.546	3.348	#xxx010
		C1625alpha	31.519	2.324	#10xxxx
			12.961	1.65	#xxxx01
			162.433	6.866	#010xxx
			38.613	2.531	#xxx010
N40 [2-13C]glucose_Replica 2					
	CIT_2	C6a	82.798	3.513	#xx0xx1
			8.773	0.91	#xx1xx1
		C1C5b	173.139	5.759	#10xxxx+#xxx01x
			8.985	1.008	#11xxxx+#xxx11x
		C2C4a	95.883	4.425	#010xxx+#xx010x
			11.443	1.32	#011xxx+#xx110x
		C3b	4.721	1.048	#x010x1
			12.328	1.985	#x110x0+#x011x0
			63.725	4.225	#x010x0
	OAA_2	C1a	162.299	5.777	#10xx
			9.841	0.988	#11xx
		C4	169.475	7.997	#xx01
			13.399	1.278	#xx11
		C2	131.597	5.011	#010x
			17.048	1.359	#011x
			17.937	1.726	#110x
		C3	72.382	2.79	#x010
			8.534	0.824	#x110
			6.989	0.704	#x011
	GLU_2	C4C3	2.792	0.386	#xx010
			3.597	0.458	#x010x
	ALA_2	C2C3	2.451	0.349	#x01
			10.42	0.87	#010
	FSUC_2	SucroseF2F	231.263	7.447	#010xxx

		5			
			48.648	3.597	#xxx010
	GSUC_2	C5C2	37.127	1.889	#xxx010
			236.832	8.043	#010xxx
	STA_2	C1625beta	48.953	2.566	#10xxxx
			19.35	1.63	#xxxx01
			238.694	8.051	#010xxx
			58.658	2.803	#xxx010
		C1625alpha	28.648	1.799	#10xxxx
			11.63	1.203	#xxxx01
			142.88	5.365	#010xxx
			38.065	2.195	#xxx010
N40 [2-13C]glucose_Replica 3					
	CIT_2	C6a	71.804	2.801	#xx0xx1
			6.973	0.694	#xx1xx1
		C1C5b	218.534	6.994	#10xxxx+#xxx01x
			7.272	0.706	#11xxxx+#xxx11x
		C2C4a	78.811	8.896	#010xxx+#xx010x
			18.334	6.578	#011xxx+#xx110x+#110xxx+#xx011x+#111xxx+#xx111x
	OAA_2	C1a	105.38	3.783	#10xx
			6.404	0.656	#11xx
		C4	111.774	4.1	#xx01
			7.262	0.895	#xx11
		C2	82.624	3.17	#010x
			8.822	0.833	#011x
			9.713	0.887	#110x
		C3	69.728	2.722	#x010
			6.442	0.642	#x110
			6.126	0.613	#x011
	GSUC_2	C5C2	29.758	1.406	#xxx010
			170.027	5.695	#010xxx
	STA_2	C1625beta	46.04	2.627	#10xxxx
			18.25	1.687	#xxxx01
			213.14	7.584	#010xxx
			56.653	2.981	#xxx010
		C1625alpha	26.78	1.844	#10xxxx
			10.52	1.246	#xxxx01
			133.842	5.379	#010xxx
			36.582	2.337	#xxx010

Appendix 5.1D : Mass isotopomer measurements of metabolites derived from *Arabidopsis* suspension grown on N40 medium (nitrate only) fed with either 99%[1-^{13}C]glucose, 99%[2-^{13}C]glucose or 20%[$^{13}C_6$]glucose (Chapter 5)

Metabolite	Metabolite name used in the model	Carbon atoms	Mass (m+)	[1-^{13}C]glucose fed			[2-^{13}C]glucose fed			[$^{13}C_6$]glucose fed			Max error
				Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	sd
Alanine	ALA	1,2,3	0	0.639	0.642	0.641	0.535	0.514	0.522	0.674	0.713	0.715	0.01
			1	0.344	0.338	0.339	0.426	0.434	0.427	0.165	0.103	0.106	0.01
			2	0.017	0.019	0.019	0.043	0.056	0.049	0.058	0.06	0.057	0.01
			3	0	0.001	0.001	-0.003	-0.003	0.002	0.103	0.124	0.123	0.01
		1,2,3	0	0.62	0.624	0.622	0.541	0.537	0.537	0.694	0.725	0.725	0.01
			1	0.36	0.356	0.357	0.409	0.414	0.414	0.153	0.098	0.094	0.01
			2	0.019	0.02	0.02	0.049	0.048	0.048	0.042	0.042	0.044	0.01
			3	0.001	0.001	0.001	0.001	0.001	0	0.11	0.135	0.137	0.01
		2,3	0	0.65	0.65	0.651	0.58	0.574	0.576	0.737	0.765	0.77	0.011
			1	0.342	0.342	0.341	0.413	0.421	0.417	0.132	0.075	0.066	0.011
			2	0.008	0.009	0.008	0.007	0.005	0.006	0.131	0.16	0.164	0.011
Glycine	GLYeff	1,2	0	0.939	0.938	0.935	0.706	0.692	0.702	0.761	0.783	0.779	0.014
			1	0.062	0.062	0.066	0.281	0.288	0.281	0.155	0.125	0.123	0.011
			2	-0.001	0	-0.001	0.014	0.019	0.016	0.084	0.092	0.098	0.011
		1,2	0	0.935	0.937	0.935	0.701	0.699	0.701	0.771	0.784	0.787	0.011
			1	0.064	0.063	0.065	0.281	0.282	0.281	0.151	0.124	0.122	0.011
			2	0	0	0	0.018	0.018	0.018	0.078	0.091	0.092	0.011
		2	0	0.983	0.985	0.985	0.759	0.752	0.755	0.829	0.841	0.845	0.012
			1	0.017	0.015	0.015	0.241	0.248	0.245	0.171	0.159	0.155	0.012
Valine	VAL	1,2,3,4,5	0	0.38	0.382	0.384	0.294	0.283	0.295	0.503	0.526	0.553	0.011
			1	0.463	0.463	0.46	0.481	0.487	0.481	0.194	0.132	0.121	0.011
			2	0.145	0.143	0.143	0.201	0.205	0.201	0.17	0.175	0.167	0.011
			3	0.012	0.011	0.012	0.024	0.025	0.023	0.104	0.127	0.123	0.011
			4	0.001	0.001	0	0.001	0	0	0.012	0.016	0.015	0.011
			5	0	0	0	0	0	-0.001	0.016	0.023	0.021	0.011
		2,3,4,5	0	0.411	0.412	0.414	0.335	0.325	0.335	0.542	0.562	0.59	0.013

			1	0.452	0.452	0.449	0.489	0.493	0.487	0.183	0.123	0.108	0.013
			2	0.13	0.129	0.13	0.172	0.176	0.172	0.237	0.267	0.257	0.013
			3	0.007	0.007	0.008	0.005	0.005	0.006	0.018	0.022	0.02	0.013
			4	0	0	0	-0.001	0	0	0.021	0.026	0.025	0.013
		2,3,4,5	0	0.423	0.425	0.427	0.35	0.34	0.352	0.551	0.572	0.597	0.021
			1	0.432	0.432	0.43	0.467	0.473	0.465	0.171	0.114	0.1	0.021
			2	0.127	0.124	0.124	0.166	0.169	0.166	0.232	0.258	0.25	0.021
			3	0.017	0.017	0.018	0.016	0.017	0.016	0.026	0.03	0.029	0.021
			4	0.001	0.001	0.001	0.001	0.001	0.001	0.02	0.027	0.025	0.021
Leucine	LEU	2,3,4,5,6	0	0.272	0.272	0.277	0.288	0.279	0.292	0.441	0.441	0.471	0.018
			1	0.448	0.454	0.452	0.472	0.477	0.469	0.249	0.216	0.195	0.018
			2	0.23	0.227	0.224	0.209	0.213	0.208	0.231	0.248	0.241	0.018
			3	0.046	0.044	0.044	0.028	0.028	0.028	0.054	0.064	0.062	0.018
			4	0.003	0.003	0.003	0.003	0.003	0.003	0.021	0.026	0.026	0.018
			5	0	0	0	0	0	0	0.004	0.005	0.005	0.018
Proline	GLU	2,3,4,5	0	0.359	0.364	0.369	0.415	0.412	0.42	0.519	0.53	0.537	0.013
			1	0.447	0.447	0.447	0.46	0.464	0.456	0.277	0.241	0.233	0.013
			2	0.171	0.167	0.162	0.119	0.119	0.117	0.165	0.179	0.18	0.013
			3	0.023	0.022	0.021	0.006	0.005	0.007	0.031	0.039	0.039	0.013
			4	0	0	0.001	0	-0.001	0	0.008	0.011	0.011	0.013
		2,3,4,5	0	0.347	0.332	0.333	0.385	0.383	0.386	0.501	0.517	0.526	0.045
			1	0.493	0.488	0.481	0.492	0.502	0.489	0.293	0.251	0.242	0.031
			2	0.175	0.176	0.174	0.126	0.124	0.126	0.177	0.192	0.193	0.027
			3	0.004	0.013	0.017	0.002	-0.001	0.003	0.028	0.036	0.035	0.034
			4	-0.019	-0.009	-0.005	-0.005	-0.008	-0.004	0.002	0.004	0.004	0.036
Serine	SEReff	1,2,3	0	0.747	0.748	0.752	0.626	0.622	0.618	0.682	0.696	0.693	0.02
			1	0.245	0.245	0.24	0.324	0.328	0.332	0.212	0.179	0.179	0.02
			2	0.008	0.009	0.01	0.05	0.047	0.049	0.071	0.08	0.081	0.02
			3	-0.001	-0.002	-0.001	0	0.003	0.001	0.036	0.045	0.047	0.02
		1,2,3	0	0.755	0.755	0.752	0.62	0.616	0.619	0.686	0.695	0.692	0.02
			1	0.246	0.243	0.242	0.328	0.333	0.33	0.203	0.182	0.185	0.02
			2	0.005	0.007	0.009	0.051	0.05	0.051	0.076	0.079	0.081	0.02
			3	-0.007	-0.005	-0.003	0.002	0.001	0	0.035	0.044	0.042	0.02
		2,3	0	0.779	0.781	0.783	0.66	0.653	0.656	0.729	0.737	0.737	0.02

			1	0.221	0.218	0.216	0.315	0.32	0.316	0.221	0.205	0.205	0.02
			2	0	0.001	0.001	0.025	0.027	0.028	0.05	0.058	0.058	0.02
		2,3	0	0.779	0.78	0.783	0.661	0.657	0.659	0.73	0.737	0.74	0.02
			1	0.219	0.217	0.215	0.311	0.315	0.313	0.219	0.205	0.203	0.02
			2	0.002	0.003	0.002	0.028	0.028	0.028	0.051	0.058	0.057	0.02
Threonine	THR	2,3,4	0	0.478	0.489	0.489	0.57	0.565	0.552	0.597	0.622	0.601	0.02
			1	0.416	0.414	0.413	0.39	0.374	0.382	0.28	0.239	0.248	0.02
			2	0.097	0.094	0.094	0.041	0.059	0.053	0.102	0.106	0.115	0.02
			3	0.009	0.003	0.004	-0.001	0.002	0.013	0.022	0.034	0.036	0.02
Phenylalanine	PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.302	0.307	0.309	0.17	0.16	0.168	0.333	0.363	0.37	0.013
			1	0.44	0.44	0.441	0.392	0.397	0.391	0.198	0.154	0.148	0.013
			2	0.21	0.206	0.205	0.294	0.297	0.296	0.171	0.148	0.144	0.013
			3	0.041	0.04	0.04	0.113	0.117	0.113	0.158	0.169	0.169	0.013
			4	0.004	0.003	0.003	0.026	0.025	0.026	0.071	0.082	0.084	0.013
			5	0.002	0.001	0.001	0.005	0.005	0.004	0.035	0.041	0.041	0.013
			6	0	0.001	0	0.001	0.001	0.001	0.021	0.026	0.027	0.013
			7	0	0.001	0	0.001	-0.001	0	0.009	0.011	0.012	0.013
			8	0	0.001	0	0	0	0	0.003	0.003	0.003	0.013
			9	0	0	0	0	0	0	0.001	0.002	0.002	0.013
		2,3,4,5,6,7,8,9	0	0.31	0.314	0.316	0.183	0.174	0.178	0.357	0.378	0.39	0.012
			1	0.445	0.447	0.445	0.407	0.409	0.406	0.193	0.148	0.141	0.012
			2	0.204	0.2	0.2	0.291	0.299	0.298	0.229	0.223	0.218	0.012
			3	0.037	0.037	0.036	0.099	0.1	0.098	0.108	0.112	0.11	0.012
			4	0.003	0.002	0.003	0.018	0.018	0.018	0.067	0.079	0.08	0.012
			5	0	0	0	0.002	0.001	0.002	0.026	0.033	0.034	0.012
			6	0	0	0	0	-0.001	0	0.016	0.021	0.021	0.012
			7	0	0	0	0	0	0	0.003	0.003	0.004	0.012
			8	0	0	0	0	-0.001	0	0.001	0.002	0.002	0.012
		2,3,4,5,6,7,8,9	0	0.308	0.314	0.317	0.182	0.173	0.18	0.355	0.379	0.388	0.011
			1	0.443	0.443	0.442	0.408	0.413	0.406	0.19	0.148	0.142	0.011
			2	0.206	0.201	0.201	0.293	0.297	0.294	0.231	0.222	0.218	0.011
			3	0.039	0.037	0.036	0.09	0.092	0.091	0.091	0.091	0.091	0.011
			4	0.003	0.003	0.003	0.019	0.019	0.019	0.066	0.079	0.08	0.011
			5	0	0	0	0.001	0.001	0.001	0.027	0.033	0.033	0.011

			6	0	0	0	-0.001	-0.001	0	0.017	0.021	0.021	0.011
			7	0	0	0	-0.001	-0.001	-0.001	0.003	0.003	0.003	0.011
			8	0	0	0	-0.001	-0.001	0	0.001	0.002	0.002	0.011
		1,2	0	0.961	0.961	0.958	0.609	0.602	0.604	0.728	0.751	0.757	0.01
			1	0.04	0.04	0.043	0.374	0.384	0.378	0.148	0.103	0.095	0.01
			2	-0.001	-0.001	-0.001	0.017	0.015	0.018	0.123	0.147	0.148	0.01
Aspartate	ASP	1,2,3,4	0	0.419	0.407	0.406	0.441	0.44	0.444	0.539	0.545	0.563	0.02
			1	0.421	0.431	0.431	0.446	0.445	0.44	0.278	0.235	0.221	0.02
			2	0.143	0.145	0.143	0.107	0.11	0.109	0.126	0.147	0.144	0.02
			3	0.017	0.016	0.017	0.007	0.005	0.006	0.042	0.059	0.058	0.02
			4	0	0.001	0.003	-0.001	0	0	0.015	0.013	0.014	0.02
		1,2,3,4	0	0.413	0.407	0.406	0.438	0.439	0.439	0.535	0.547	0.556	0.02
			1	0.425	0.433	0.431	0.445	0.445	0.444	0.273	0.237	0.23	0.02
			2	0.143	0.143	0.145	0.11	0.109	0.11	0.133	0.143	0.141	0.02
			3	0.018	0.017	0.018	0.006	0.007	0.007	0.048	0.06	0.059	0.02
			4	0	0	0.001	0	0	0	0.01	0.013	0.013	0.02
		2,3,4	0	0.481	0.477	0.475	0.564	0.565	0.564	0.612	0.615	0.62	0.02
			1	0.41	0.414	0.415	0.386	0.382	0.385	0.265	0.239	0.234	0.02
			2	0.102	0.101	0.102	0.051	0.052	0.052	0.097	0.112	0.112	0.02
			3	0.007	0.007	0.007	-0.001	0	0	0.025	0.034	0.034	0.02
		2,3,4	0	0.49	0.484	0.484	0.57	0.572	0.572	0.62	0.619	0.63	0.02
			1	0.395	0.403	0.401	0.373	0.373	0.369	0.252	0.232	0.223	0.02
			2	0.101	0.099	0.1	0.051	0.049	0.052	0.096	0.11	0.109	0.02
			3	0.014	0.014	0.015	0.007	0.007	0.007	0.032	0.039	0.039	0.02
		1,2	0	0.656	0.652	0.65	0.667	0.668	0.667	0.721	0.725	0.733	0.02
			1	0.314	0.318	0.318	0.322	0.321	0.321	0.195	0.17	0.163	0.02
			2	0.031	0.03	0.032	0.011	0.01	0.012	0.084	0.105	0.104	0.02
Glutamate	GLU	1,2,3,4,5	0	0.301	0.302	0.299	0.329	0.32	0.325	0.451	0.46	0.478	0.02
			1	0.431	0.439	0.439	0.461	0.465	0.461	0.275	0.23	0.219	0.02
			2	0.218	0.21	0.211	0.186	0.19	0.188	0.194	0.212	0.21	0.02
			3	0.046	0.044	0.047	0.025	0.023	0.026	0.063	0.073	0.067	0.02
			4	0.003	0.005	0.006	0.001	0.001	-0.001	0.016	0.02	0.022	0.02
			5	0	0	-0.001	-0.001	0	0	0.001	0.006	0.005	0.02
		1,2,3,4,5	0	0.307	0.307	0.305	0.327	0.324	0.328	0.454	0.466	0.479	0.02

			1	0.431	0.434	0.433	0.46	0.461	0.459	0.267	0.229	0.222	0.02
			2	0.212	0.21	0.212	0.187	0.19	0.188	0.198	0.208	0.205	0.02
			3	0.046	0.045	0.046	0.025	0.025	0.024	0.061	0.071	0.069	0.02
			4	0.004	0.004	0.004	0.001	0.001	0	0.016	0.02	0.019	0.02
			5	0	0	0	0	0	0	0.004	0.006	0.005	0.02
		2,3,4,5	0	0.344	0.343	0.343	0.415	0.409	0.412	0.513	0.514	0.532	0.02
			1	0.448	0.455	0.451	0.461	0.467	0.463	0.281	0.247	0.234	0.02
			2	0.181	0.178	0.18	0.121	0.121	0.122	0.169	0.184	0.184	0.02
			3	0.027	0.024	0.025	0.003	0.005	0.006	0.032	0.044	0.041	0.02
			4	0	0.001	0.001	-0.001	-0.002	-0.002	0.005	0.011	0.009	0.02
		2,3,4,5	0	0.356	0.354	0.354	0.42	0.415	0.416	0.514	0.527	0.536	0.02
			1	0.446	0.449	0.447	0.457	0.46	0.458	0.278	0.243	0.234	0.02
			2	0.177	0.175	0.176	0.119	0.12	0.12	0.166	0.182	0.18	0.02
			3	0.023	0.023	0.024	0.006	0.006	0.007	0.034	0.041	0.04	0.02
			4	-0.002	-0.001	-0.001	-0.002	-0.001	0	0.008	0.008	0.01	0.02
Isoleucine	ILE	2,3,4,5,6	0	0.299	0.298	0.302	0.297	0.289	0.298	0.445	0.463	0.475	0.014
			1	0.458	0.462	0.461	0.491	0.496	0.49	0.267	0.223	0.212	0.014
			2	0.199	0.197	0.194	0.185	0.189	0.186	0.212	0.223	0.222	0.014
			3	0.04	0.039	0.038	0.025	0.025	0.025	0.057	0.066	0.067	0.014
			4	0.004	0.004	0.004	0.001	0.001	0.001	0.015	0.019	0.02	0.014
			5	0	0	0	0	0	0	0.004	0.005	0.005	0.014
Methionine	METeff	1,2,3,4,5	0								0.566	0.587	0.01
			1								0.249	0.23	0.01
			2								0.117	0.116	0.01
			3								0.046	0.053	0.01
			4								0.018	0.01	0.01
			5								0.005	0.004	0.01
		1,2,3,4,5	0	0.474	0.47	0.477	0.532	0.522	0.532	0.575	0.578	0.581	0.011
			1	0.345	0.349	0.346	0.345	0.353	0.344	0.258	0.24	0.239	0.01
			2	0.145	0.147	0.143	0.107	0.111	0.108	0.111	0.113	0.11	0.01
			3	0.032	0.032	0.03	0.011	0.012	0.014	0.044	0.052	0.051	0.01
			4	0.003	0.002	0.002	-0.001	0.001	0.001	0.011	0.015	0.016	0.01
			5	0.001	0	0	0.005	0.001	0	0.001	0.003	0.003	0.01
		2,3,4,5	0	0.509	0.509	0.516	0.608	0.605	0.61	0.624	0.62	0.622	0.01

			1	0.347	0.349	0.348	0.323	0.323	0.318	0.26	0.249	0.247	0.01
			2	0.122	0.122	0.117	0.065	0.067	0.068	0.085	0.094	0.095	0.01
			3	0.021	0.019	0.018	0.004	0.005	0.004	0.028	0.033	0.033	0.01
			4	0.001	0.001	0.001	0	0	0	0.004	0.004	0.004	0.01
Lysine	LYS	1,2,3,4,5,6	0	0.287	0.278	0.276	0.27	0.259	0.266	0.421	0.423	0.441	0.01
			1	0.428	0.437	0.438	0.454	0.458	0.457	0.253	0.225	0.221	0.01
			2	0.226	0.227	0.227	0.227	0.237	0.234	0.181	0.185	0.174	0.01
			3	0.05	0.052	0.053	0.044	0.043	0.04	0.104	0.112	0.111	0.01
			4	0.007	0.005	0.005	0.006	0.004	0.004	0.026	0.039	0.039	0.01
			5	0.001	0	0.001	-0.001	0	0.001	0.013	0.013	0.01	0.01
			6	0	0	0	0	-0.001	-0.002	0.002	0.003	0.004	0.01
		2,3,4,5,6	0	0.294		0.281		0.303			0.44	0.476	0.011
			1	0.46		0.463		0.498			0.239	0.225	0.01
			2	0.212		0.211		0.197			0.222	0.223	0.01
			3	0.041		0.043		0.019			0.073	0.068	0.01
			4	-0.001		0.003		-0.006			0.02	0.011	0.01
			5	-0.005		-0.002		-0.011			0.005	-0.002	0.01
Arginine	ARGeff	1,2,3,4,5,6	0	0.473	0.468	0.465	0.475	0.47	0.481	0.543	0.555	0.565	0.01
			1	0.312	0.314	0.319	0.333	0.338	0.334	0.233	0.216	0.21	0.01
			2	0.167	0.167	0.167	0.16	0.155	0.151	0.149	0.143	0.137	0.01
			3	0.047	0.044	0.044	0.026	0.034	0.034	0.059	0.062	0.066	0.01
			4	0.004	0.007	0.006	0.005	0.005	0.003	0.016	0.018	0.019	0.01
			5	-0.001	0	-0.001	0.001	0	0	0.003	0.005	0.005	0.01
			6	-0.003	0	0	-0.002	-0.001	-0.003	-0.003	-0.001	-0.002	0.01
Histidine	HISeff	1,2,3,4,5,6	0	0.591	0.589	0.584	0.391	0.381	0.379	0.583	0.592	0.603	0.01
			1	0.308	0.299	0.305	0.391	0.388	0.376	0.208	0.176	0.18	0.01
			2	0.091	0.096	0.091	0.181	0.195	0.205	0.104	0.096	0.085	0.01
			3	0.013	0.015	0.018	0.042	0.034	0.04	0.072	0.079	0.083	0.01
			4	0	0	0.001	0.002	0.008	0.002	0.014	0.025	0.022	0.01
			5	0	0.001	0	-0.003	-0.001	0.002	0.026	0.026	0.024	0.01
			6	-0.003	0	0	-0.005	-0.005	-0.004	-0.006	0.006	0.002	0.01
		1,2,3,4,5,6	0	0.586	0.589	0.587	0.385	0.377	0.385	0.568	0.599	0.614	0.011
			1	0.302	0.301	0.302	0.376	0.38	0.375	0.206	0.169	0.16	0.011
			2	0.096	0.094	0.095	0.192	0.198	0.196	0.114	0.097	0.095	0.011

			3	0.014	0.015	0.015	0.042	0.041	0.039	0.071	0.079	0.077	0.011
			4	0.002	0	0.001	0.004	0.003	0.005	0.02	0.026	0.024	0.011
			5	0	0.001	0	0.001	0	0	0.019	0.025	0.025	0.011
			6	0	0	0	0	0.001	0	0.004	0.005	0.005	0.011
		2,3,4,5,6	0	0.684	0.686	0.681	0.395	0.39	0.403	0.574	0.602	0.606	0.018
			1	0.258	0.252	0.254	0.39	0.396	0.388	0.213	0.174	0.172	0.018
			2	0.045	0.046	0.048	0.178	0.178	0.174	0.141	0.143	0.139	0.018
			3	0.01	0.012	0.012	0.028	0.035	0.031	0.046	0.049	0.047	0.018
			4	0.004	0.004	0.004	0.006	0.005	0.004	0.022	0.026	0.028	0.018
			5	-0.001	0	0.001	0.002	-0.003	0	0.005	0.006	0.008	0.018
Fructose	F6P	4,5,6	0	0.844	0.849	0.846	0.828	0.831	0.814	0.771	0.774	0.768	0.01
			1	0.154	0.148	0.153	0.165	0.165	0.178	0.039	0.038	0.041	0.01
			2	0.002	0.003	0.002	0.012	0.01	0.012	0.017	0.016	0.019	0.01
			3	0	-0.001	-0.001	-0.005	-0.006	-0.005	0.173	0.172	0.172	0.01
		1,2,3,4	0	0.223	0.221	0.227	0.154	0.146	0.157	0.697	0.706	0.693	0.011
			1	0.751	0.758	0.749	0.804	0.813	0.801	0.106	0.098	0.107	0.011
			2	0.03	0.026	0.027	0.052	0.044	0.051	0.025	0.022	0.032	0.011
			3	-0.002	-0.003	-0.001	-0.006	0.003	-0.004	0.053	0.055	0.054	0.011
			4	-0.002	-0.002	-0.002	-0.004	-0.005	-0.004	0.119	0.119	0.114	0.011
Fructose	F6P	4,5,6	0	0.842	0.851	0.854	0.831	0.836	0.82	0.772	0.778	0.773	0.016
			1	0.159	0.151	0.156	0.168	0.166	0.182	0.037	0.035	0.037	0.01
			2	0.002	0	-0.003	0.008	0.007	0.009	0.015	0.011	0.015	0.01
			3	-0.002	-0.003	-0.007	-0.007	-0.008	-0.011	0.176	0.176	0.175	0.011
Succinate	SUCC	1,2,3,4	0	0.342	0.354	0.349	0.45	0.447	0.453	0.542	0.541	0.545	0.02
			1	0.434	0.43	0.435	0.422	0.427	0.432	0.229	0.229	0.229	0.02
			2	0.194	0.188	0.187	0.119	0.118	0.106	0.177	0.176	0.173	0.02
			3	0.03	0.027	0.028	0.014	0.008	0.011	0.042	0.043	0.042	0.02
			4	0.001	0.001	0.001	-0.005	0	-0.002	0.01	0.012	0.01	0.02
Malate	OAA	1,2,3,4	0	0.384	0.392	0.392	0.438	0.44	0.436	0.552	0.552	0.549	0.01
			1	0.429	0.429	0.428	0.436	0.438	0.444	0.228	0.23	0.23	0.01
			2	0.163	0.157	0.158	0.122	0.117	0.11	0.146	0.144	0.147	0.01
			3	0.024	0.021	0.02	0.005	0.005	0.015	0.061	0.062	0.06	0.01
			4	0	0.001	0.001	-0.001	0	-0.005	0.014	0.013	0.014	0.01
		1,2,3,4	0	0.385	0.393	0.391	0.441	0.434	0.437	0.555	0.556	0.55	0.01

			1	0.43	0.428	0.429	0.434	0.443	0.442	0.229	0.228	0.231	0.01
			2	0.162	0.157	0.158	0.118	0.115	0.115	0.142	0.141	0.143	0.01
			3	0.022	0.021	0.022	0.007	0.007	0.007	0.06	0.061	0.061	0.01
			4	0	0	0.001	0	0	0	0.013	0.014	0.014	0.01
Citrate	CIT	1,2,3,4,5,6	0	0.249	0.257	0.253	0.267	0.266	0.267	0.419	0.419	0.416	0.01
			1	0.406	0.409	0.407	0.436	0.435	0.436	0.236	0.234	0.236	0.01
			2	0.257	0.251	0.253	0.241	0.244	0.24	0.206	0.209	0.208	0.01
			3	0.077	0.072	0.076	0.053	0.051	0.054	0.095	0.094	0.095	0.01
			4	0.01	0.01	0.009	0.003	0.003	0.003	0.033	0.034	0.034	0.01
			5	0	0.001	0.001	0	0	-0.001	0.009	0.009	0.009	0.01
			6	0	0	0	0	0	0	0.002	0.002	0.002	0.01
Cellwall	G6P	3,4,5	0	0.96	0.965	0.977	0.861	0.824	0.821	0.731	0.731	0.703	0.012
			1	0.041	0.037	0.036	0.14	0.162	0.177	0.09	0.098	0.099	0.01
			2	-0.002	-0.002	-0.008	0.005	0.015	0.008	0.051	0.05	0.058	0.01
			3	0.001	0	-0.006	-0.006	-0.001	-0.005	0.128	0.121	0.14	0.01
Cellwall	PENTAN	3,4,5	0	0.964	0.96	0.964	0.834	0.831	0.828	0.721	0.725	0.724	0.01
			1	0.038	0.041	0.04	0.155	0.154	0.159	0.092	0.091	0.095	0.01
			2	-0.003	-0.001	-0.003	0.012	0.014	0.013	0.054	0.053	0.053	0.01
			3	0	0	0	-0.001	0	0	0.133	0.131	0.128	0.01
Cellwall	PENTAN	3,4,5	0	0.977	0.968	0.973	0.835	0.83	0.845	0.724	0.721	0.723	0.011
			1	0.033	0.035	0.034	0.156	0.16	0.156	0.092	0.094	0.096	0.01
			2	-0.005	-0.001	-0.004	0.013	0.01	0.006	0.051	0.055	0.054	0.01
			3	-0.005	-0.002	-0.003	-0.003	0	-0.007	0.133	0.131	0.127	0.01
Starch	STA	3,4,5,6	0	0.808	0.811	0.811	0.745	0.745	0.749	0.695	0.694	0.694	0.01
			1	0.183	0.181	0.18	0.214	0.214	0.21	0.112	0.109	0.114	0.01
			2	0.008	0.008	0.009	0.038	0.038	0.037	0.018	0.017	0.019	0.01
			3	0	0	0	0.003	0.003	0.003	0.064	0.063	0.065	0.01
			4	0	0	0	0	0	0	0.112	0.117	0.108	0.01
Starch	STA	3,4,5,6	0	0.807	0.808	0.81	0.744	0.744	0.75	0.695	0.692	0.695	0.01
			1	0.182	0.181	0.181	0.212	0.212	0.209	0.112	0.11	0.114	0.01
			2	0.01	0.01	0.009	0.04	0.04	0.038	0.018	0.019	0.019	0.01
			3	0	0	0	0.004	0.003	0.003	0.064	0.063	0.065	0.01
			4	0	0	0	0	0	0	0.111	0.116	0.108	0.01
Wall	G6P	3,4,5,6	0	0.839	0.844	0.842	0.801	0.803	0.795	0.715	0.715	0.71	0.01

			1	0.155	0.15	0.153	0.172	0.172	0.178	0.091	0.091	0.097	0.01
			2	0.006	0.006	0.006	0.025	0.024	0.026	0.013	0.013	0.014	0.01
			3	0	0	-0.001	0.002	0.001	0.001	0.052	0.052	0.054	0.01
			4	0	0	0	0	0	0	0.129	0.129	0.125	0.01
Wall	G6P	3,4,5,6	0	0.839	0.842	0.842	0.8	0.801	0.795	0.713	0.716	0.709	0.01
			1	0.154	0.151	0.15	0.173	0.172	0.178	0.093	0.091	0.096	0.01
			2	0.007	0.006	0.007	0.025	0.025	0.025	0.015	0.014	0.015	0.01
			3	0.001	0	0	0.003	0.002	0.001	0.052	0.051	0.054	0.01
			4	0	0	0	0	0	0	0.128	0.128	0.125	0.01
Sucrose	GSUC	1,2,3,4,5,6	0		0.18		0.147	0.12	0.125	0.59	0.678	0.666	0.02
			1		0.717		0.717	0.744	0.727	0.127	0.074	0.08	0.02
			2		0.096		0.115	0.115	0.125	0.046	0.03	0.033	0.02
			3		0.007		0.017	0.017	0.019	0.078	0.074	0.081	0.02
			4		0		0.002	0.002	0.003	0.015	0.014	0.015	0.02
			5		0.001		0.001	0.001	0.002	0.016	0.014	0.014	0.02
			6		0		0	0	0	0.128	0.116	0.111	0.02

Appendix 5.2
Metabolic Network of *Arabidopsis* cell suspension culture (Used in Chapters 5 and 6).

	FLUX_NAME	**EDUCT_1**	**EDUCT_2**	**PRODUCT_1**	**PRODUCT_2**	**Comments about the reaction**
//Subnetwork 1						
// Mixture Input						
	Vupt1	GLC_1 #ABCDEF		GLCext #ABCDEF		//Glucose uptake for [1-13C]
	Vupt0	GLC_0 #ABCDEF		GLCext #ABCDEF		//glucose uptake for unlabelled glucose
// uptake						
	upt	GLCext #ABCDEF		G6P #ABCDEF		//Net glucose uptake (set to 1)
	Vco2in	CO2ex #A		CO2 #A		//CO2 in natural abundance
	Vcxin	Cxex #A		CX #A		//Methylene Tetrahydrofolate in (1-Carbon) natural abundance
//Cytosol						
	chex1	G6P #ABCDEF		F6P #ABCDEF		Cytosolic phosphoglucose isomerase
	chex2	F6P #ABCDEF		DHAP #CBA	TP #DEF	Cytosolic Fru-6-P → triose-P/PEP interconversion
	chex3	TP #ABC		PYRc #ABC		Cytosolic pyruvate kinase
//plastid //Also Cytosol-Plastid exchange						
	phex1	G6Pp #ABCDEF		F6Pp #ABCDEF		Plastidic phosphoglucose isomerase

	phex2	F6Pp #ABCDEF		TPp #CBA	TPp #DEF	Plastidic Fru-6-P → triose-P/PEP interconversion
	phex3	TPp #ABC		PYRp #ABC		Plastidic pyruvate kinase
//Cytosolic pentose-P pathway						
	cppp1	G6P #ABCDEF		CO2 #A	P5Pp #BCDEF	Cytosolic pentose phosphate pathway - oxidative steps
//plastid pentose-P pathway //Half Reactions used						
	pppp1	G6Pp #ABCDEF		CO2 #A	P5Pp #BCDEF	Plastidic pentose phosphate pathway - oxidative steps
	pppp2a	P5Pp #abcde	TKC2p #AB	S7Pp #ABabcde		Plastidic transketolase - C7/C5 conversion
	pppp2b	E4Pp #abcd	TKC2p #AB	F6Pp #ABabcd		Plastidic transketolase - C6/C4 conversion
	pppp2c	P5Pp #ABCDE		TPp #CDE	TKC2p #AB	Plastidic transketolase - C5/C3 conversion
	pppp3a	S7Pp #ABCDEFG		E4Pp #DEFG	TAC3p #ABC	Plastidic transaldolase - C7/C4 conversion
	pppp3b	TPp #abc	TAC3p #ABC	F6Pp #ABCabc		Plastidic transaldolase - C6/C3 conversion
//Cytosol-plastid exchange						
	cmex	PYRc #ABC		PYRm #ABC		Pyruvate uptake by mitochondria
	cpex	PYRc		PYRp		Pyruvate uptake by plastids

		#ABC		#ABC		
	gpt	G6P		G6Pp		Plastidic Glc-6-P/Pi translocator
		#ABCDEF		#ABCDEF		
	tpt	TP		TPp		Plastidic triose-P/Pi & PEP/Pi translocators
		#ABC		#ABC		
// TCA cycle modified (Malate OAA single pool)						
	tca1	PYRm		CO2	AcCoA	Mitochondrial pyruvate dehydrogenase
		#ABC		#A	#BC	
	tca2	AcCoA	OAA	CIT		Citrate synthase
		#AB	#abcd	#dcbBAa		
	tca3	CIT		CO2	AKG	Aconitase/isocitrate dehydrogenase
		#ABCDEF		#F	#ABCDE	
	tca4	AKG		CO2	SUCC	2-oxoglutarate → Succinate
		#ABCDE		#A	#BCDE	
	tca5	SUCC		FUM		Succinate → fumarate convertion
		#ABCD		#ABCD		
	tca6a	FUM		OAA		Fumarase //Malate and OAA are considered single pool, malate dehydrogenase (mdh) exchanged fast Fumarase (randomisation)
		#ABCD		#ABCD		
	tca6b	FUM		OAA		
		#ABCD		#DCBA		
//Anaplerotic						
	ana1	TP	CO2	OAA		PEP carboxylase
		#ABC	#a	#ABCa		
	ana2	OAA		CO2	PYRm	Mitochodrial malic enzyme
		#ABCD		#D	#ABC	
	ana3	OAA		PYRp	CO2	Plastidic malic enzyme
		#ABCD		#ABC	#D	
//Other intermediary reactions						
	tpi	DHAP		TP		triosephoshate isomerase

		#ABC		#ABC		
	pdhp	PYRp #ABC		CO2 #A	AcCoAp #BC	Plastidic pyruvate dehydrogenase
	Vthrox	THR #ABCD		GLY #AB	AcCoA #CD	Threonine aldolase..acetaldehyde ends in AcCoA
	Vgly	SER #ABC		GLY #AB	CX #C	Serine to Glycine
	Vgly1	GLY #AB		CO2 #A	CX #B	Glycine decarboxylase
// Fatty acid, glycerol and alcohol synthesis						
	Vfas1	AcCoAp #AB		AcCoAeff #AB		Fatty acid OUT
	Vfas2	DHAP #ABC		G3P #ABC		Glycerol OUT
	Vadh	PYRc #ABC		EtOH #BC	CO2 #A	
	Vadheff	EtOH #AB		EtOH_out #AB		Alcohol dehrdrogenase
//Sugars Storage						
	Vgsuc	G6P #ABCDEF		GSUC #ABCDEF		Sucrose_glucosyl synthesis
	Vgsuceff	GSUC #ABCDEF		G6Peff #ABCDEF		
	Vfsuc	F6P #ABCDEF		FSUC #ABCDEF		Sucrose_fructosyl synthesis
	Vfsuceff	FSUC #ABCDEF		F6Peff #ABCDEF		
	Vstsp	G6Pp #ABCDEF		STA #ABCDEF		Starch synthesis

	Vsta	STA #ABCDEF		STAeff #ABCDEF		
	Vwall	G6P #ABCDEF		WALL #ABCDEF		Cell wall biosynthesis
	Vpentan	G6P #ABCDEF		PENTAN #ABCDE	CO2 #F	
	Vpentaneff	PENTAN #ABCDE		PENTANeff #ABCDE		
//CO2 and MTHF out						
	Vco2out	CO2 #A		CO2eff #A		//CO2 out
	Vcxout	CX #A		CXeff #A		//Methylene Tetrahydrofolate out
//TCA cycle efflux						
	VcitOUT	CIT #ABCDEF		CITeff #ABCDEF		//Citrate storage
	VsuccOUT	SUCC #ABCD		SUCCeff #ABCD		//Succinate storage
	VmalOUT	OAA #ABCD		MALeff #ABCD		//Malate storage
	Vgabaeff	AKG #ABCDE		GABA #EDCB	CO2 #A	//Gaba storage
	VgabaOUT	GABA #ABCD		GABAeff #ABCD		
//Amino acid metabolism and outputs						
	Vglu	AKG #ABCDE		GLU #ABCDE		
	Vglueff	GLU #ABCDE		GLUeff #ABCDE		//Glutamate+Glutamine+Proline OUT
	Vasp	OAA		ASP		

		#ABCD		#ABCD		
	Vaspeff	ASP		ASPeff		//Aspartate OUT
		#ABCD		#ABCD		
	Varg	AKG	CO2	ARG		
		#ABCDE	#a	#ABCDEa		
	Vargeff	ARG		ARGeff		//Arginine OUT
		#ABCDEF		#ABCDEF		
	Vasp_arg	ASP		FUM		
		#ABCD		#ABCD		
	Vser	TPp		SER		
		#ABC		#ABC		
	Vcys	SER		CYS		
		#ABC		#ABC		
	Vcyseff	CYS		CYSeff		//Cystine OUT
		#ABC		#ABC		
	Vglyeff	GLY		GLYeff		//Glycine OUT
		#AB		#AB		
	Vala	PYRc		ALA		
		#ABC		#ABC		
	Valaeff	ALA		ALAeff		//Alanine OUT
		#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		//Leucine OUT

		#ABCDEF		#ABCDEF		
	Vval	ISOVAL		VAL		
		#ABCDE		#ABCDE		
	Vvaleff	VAL		VALeff		//Valine OUT
		#ABCDE		#ABCDE		
	Vmet	ASP	CX	MET		
		#ABCD	#a	#ABCDa		
	Vmeteff	MET		METeff		//Methionine OUT
		#ABCDE		#ABCDE		
	Vthr	ASP		THR		
		#ABCD		#ABCD		
	Vthreff	THR		THReff		//Threonine OUT
		#ABCD		#ABCD		
	Vile	PYRp	THR	ILE	CO2	
		#ABC	#abcd	#abBcdC	#A	
	Vileeff	ILE		ILEeff		//Isoleucine OUT
		#ABCDEF		#ABCDEF		
	Vphe_tyr	ARO	TPp	PHE_TYR	CO2	
		#ABCDEFG	#abc	#abcBCDEFG	#A	
	Vphe_tyreff	PHE_TYR		PHE_TYReff		//Phenylalanine and Tyrosine OUT
		#ABCDEFGHI		#ABCDEFGHI		
	Vlys	OAA	PYRp	LYS	CO2	
		#ABCD	#abc	#ABCDcb	#a	
	Vlys1	OAA	PYRp	LYS	CO2	
		#ABCD	#abc	#abcDCB	#A	
	Vlyseff	LYS		LYSeff		//Lysine OUT
		#ABCDEF		#ABCDEF		
	Vhis	P5Pp	CX	HIS		
		#ABCDE	#a	#EDCBAa		
	Vhiseff	HIS		HISeff		//Histidine OUT

		#ABCDEF		#ABCDEF		
//For Tryptophan-reactions split to minimize						
	Vtrp2ca	P5Pp		TPp	CCa	
		#ABCDE		#CDE	#AB	
	Vtrp2caeff	CCa		CCaeff		//Typrtophan 2C out
		#AB		#AB		
	Vtrp2cb	TPp		CO2	CCb	
		#ABC		#A	#BC	
	Vtrp2cbeff	CCb		CCbeff		//Typrtophan 2C out
		#AB		#AB		
	Vtrp3c_sereff	SER		SEReff		//Tryptophan + Serine OUT
		#ABC		#ABC		
	Vtrp4c	E4Pp		E4Ppeff		//Typrtophan 4C out
		#ABCD		#ABCD		
//Additional proxy reactions (See text for explanation)						
	Vserin	AA3Cex		SEReff		//Serine in (natural abudance)
		#ABC		#ABC		
	Vserprotout	SEReff		SERProt		
		#ABC		#ABC		
	Vglyin	AA2Cex		GLYeff		//Glycine in
		#AB		#AB		
	Vglyprotout	GLYeff		GLYProt		
		#AB		#AB		
	Vargin	AA6Cex		ARGeff		//Arginine in
		#ABCDEF		#ABCDEF		
	Vargprotout	ARGeff		ARGProt		
		#ABCDEF		#ABCDEF		
	Vmetin	AA5Cex		METeff		//Methionine in
		#ABCDE		#ABCDE		
	Vmetprotout	METeff		METProt		

		#ABCDE		#ABCDE		
	Vhisin	AA6Cex		HISeff		//Histidine in
		#ABCDEF		#ABCDEF		
	Vhisprotout	HISeff		HISProt		
		#ABCDEF		#ABCDEF		
Subnetwork_2						
// Mixture Input						
	V2upt2	GLC_2		GLCext_2		
		#ABCDEF		#ABCDEF		
	V2upt0	GLC_0		GLCext_2		
		#ABCDEF		#ABCDEF		
	V2g	GLCext_2		G6P_2		//GLCext uptake-- 99% [2-13C]glucose
		#ABCDEF		#ABCDEF		
Note: Rest all reactions same as subnetwork 1 above, All fluxes start with prefix V2 and all metabolites end with suffix _2						
Subnetwork_3						
// Mixture Input						
	V3uptU	GLC_U		GLCext_3		//GLCext uptake-- 20% [U-13C]glucose
		#ABCDEF		#ABCDEF		
	V3upt0	GLC_0		GLCext_3		
		#ABCDEF		#ABCDEF		
	V3g	GLCext_3		G6P_3		
		#ABCDEF		#ABCDEF		
Rest all reactions same as subnetwork 1 above, All fluxes start with prefix V3 and all metabolites end with suffix _3						

Appendix 5.3A

Comprehensive list of model reactions tested while model construction of *Arabidopsis thaliana* suspension culture. The starting model used was from Masakapalli et al., 2010.

Reactions	Observation	Comment	Accepted or Rejected
Glucose uptake -for labeled and unlabelled	Improves fit, accounts for carryover of unlabelled glucose	Reliable	Accepted
Introduce unlabelled CO_2 uptake, as urea is partially labeled implying cells reassimilate $^{13}CO_2$ and naturally labeled CO_2	Influenced residuum in many models and ARG	Poorly determined, but improved residuums	Accepted
TMHF(Cx) uptake-unlabelled	Influenced residuum related to Gly, SER, His, Met	Reliable	Accepted
Full model-cytosolic and plastid PPP	Slight decrease of residuum	-	Rejected based on no biochemical evidence
PEP and TP as separate pools TP→PEP TPp→PEPp TP→TPp (transporter) PEP→PEPp (transporter)	No net effect on Residuum	Inversely related, having no reliability. Can pool them into single TP pool	Rejected. TP and PEP formulated as single pool of Triose phosphate (TP and TPp)
PEPc XCH to account PEPCK reaction	No influence, consistently Zero flux in all models	Reliable	Accepted
Thr DC reaction(NET and XCH) Vthrox THR→GLY+AcCoA	No influence, consistently Zero or very small NET and XCH[0-1] flux in all models	Reliable	Accepted, hoping it may influence Gly measurements
Gly DC (GLY→ CX+CO2)	Influences the residuum	Reliable	Accepted
GLY→SER XCH	Improves fit	Reliable	Accepted
MAL →OAA XCH (mdh)	XCH 0.99	Reliable	Pooled
MAL pools in cytosol and mitochondria	No influence, XCH 0.99	Can't use Malate measurements	Rejected
TriosePIsomerase NET and XCH cytosolic TP → G3P	Improves fit	Reliable	Included
Cytosolic Ile Leu (in MS)	No effect on residuum, PyrT decreases	--	Not included as known to be plastidic
SER,GLY with Raw meas	Improves fit	Way to deal Cx	Accepted
SER GLY MET HIS ARG with Raw meas	Improves fit	Way to deal Cx	Accepted
Fum1 and Fum2 as independent reactions	No net influence	Poorly determined because reciprocal	Rejected, and assumed to randomize equally

Malic enzymes: cytosolic, plastidic and mitochondrial including XCH	No influence, all minimal fluxes	Reliable	Retained mitochondrial and plsatidial for further simulations
SERXch in NoAAOx	Decreases residuum, but active in 13C Feeding studies/ photorespiration		Not included
AA recycling reactions	Influences substantially in all models, SER →PYR	Reliable	Accepted Additional feeding experiments with [2 ^{13}C]glycine conducted to validate
NoAA recycling model (See Table S7b)	Passes Chi2 , slightly higher Residuum	Reliable flux estimates similar to model with AA recycling.	Accepted
Unlabelled pools into organic acids	No effect, implies at isotopic steady state		Rejected

Appendix 5.3B. List of Amino acid recycling reactions tested in the models (Chapters 5 and 6)

//Amino acid recycling reactions in FTBL format

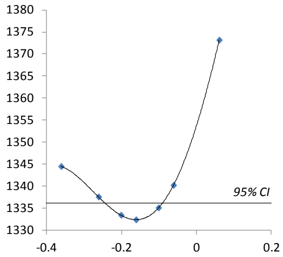
Flux	Substrate1	Substrate2	Product1	Product2	Comment
Vthrox	THR		GLY	AcCoA	//Threonine aldolase. acetaldehyde ends in AcCoA
	#ABCD		#AB	#CD	
Vserox	SER		PYRc		//Serine dehydratase/serine racemase. also includes CYS to PYR
	#ABC		#ABC		also includes the 3 carbons from tryptophan via alanine (SER-->ALA-->PYR)
Vtrpox1	CCa		CO2	CO2	//Tryptophan (2C unit –see full model)
	#AB		#A	#B	
Vtrpox2a	CCb	E4Pp	CO2	DEGtrp	//Tryptophan (2C unit –see full model)
	#AB	#CDEF	#A	#BFEDC	
Vtrpox2b	DEGtrp		AACoA	CO2	
	#ABCDE		#ABCD	#E	
Vlysox1	LYS		CO2	DEGlys	//Lysine
	#ABCDEF		#A	#BCDEF	
Vlysox2	DEGlys		CO2	AACoA	
	#ABCDE		#E	#ABCD	
Vphe_tyrox1	PHE_TYR		FUM	DEGaro	//Phenyalanine tyrosine
	#ABCDEFGHI		#DEFG	#ABCIH	
Vphe_tyrox2	PHE_TYR		FUM	DEGaro	
	#ABCDEFGHI		#DIHG	#ABCEF	
Vphe_tyrox3	DEGaro		CO2	AACoA	//Acetoacetyl Coa
	#ABCDE		#A	#BCDE	
Vleuox1	LEU		CO2	DEGleu	//Leucine
	#ABCDEF		#A	#BCDEF	
Vleuox2	DEGleu	CO2	AcCoA	AACoA	
	#ABCDE	#F	#AB	#FCDE	
Vaacoaox	AACoA		AcCoA	AcCoA	//AcetoacetylCoA ----> AcCoA AcCoA
	#ABCD		#AB	#CD	
Vhisox	HIS		GLU	CX	//Histidine
	#ABCDEF		#ABCDE	#F	
Vmetox1	MET		AKB	CH3	//Methionine
	#ABCDE		#ABCD	#E	
Vmetox2	AKB		PropCoA	CO2	
	#ABCD		#BCD	#A	
Vileox1	ILE		DEGile	CO2	//Isoleucine
	#ABCDEF		#BCDEF	#A	
Vileox2	DEGile		PropCoA	AcCoA	

	#ABCDE		#ABE	#CD	
Vvalox1	VAL		DEGval	CO2	//Valine
	#ABCDE		#BCDE	#A	
Vvalox2	DEGval		PropCoA	CO2	
	#ABCD		#ABC	#D	
Vpropcoaox	PropCoA	CO2	SUCC		//PropionylCoA--->SuccCoA
	#ABC	#D	#ABCD		
Vch3out	CH3		CH3eff		
	#A		#A		

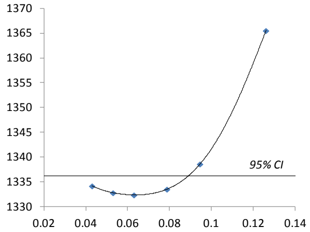
Appendix 5.4

Non linear statistical analysis of free fluxes of MS and N40 models. The plots are flux (x axis) vs the residuum (y axis). Fluxes that were undeterminable or negligible are not presented.

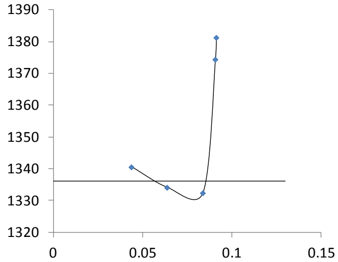
A. Net fluxes of MS



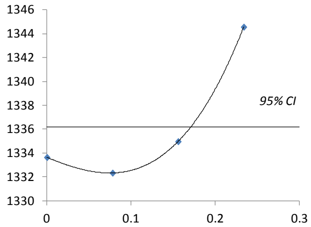
chex1



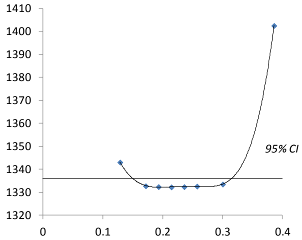
ana2



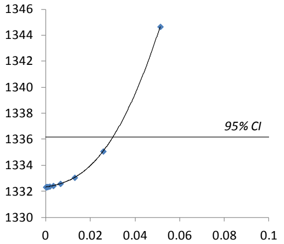
chex3



cppp1

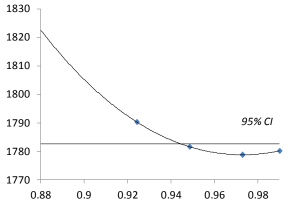


pppp1

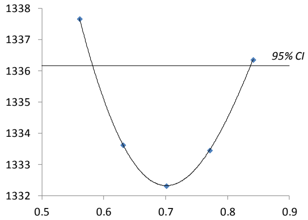


cpex

B. Exchange (XCH[0-1]) fluxes of MS



chex1



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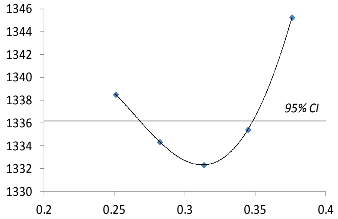
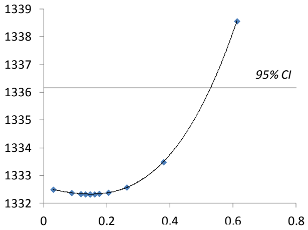
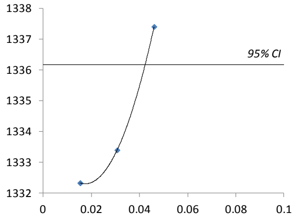


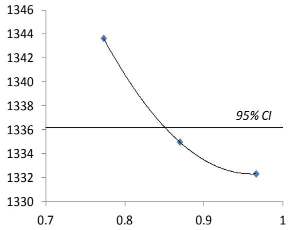
chex2



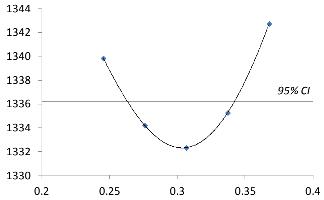
tpt/ppt



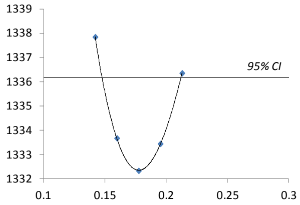
ana1



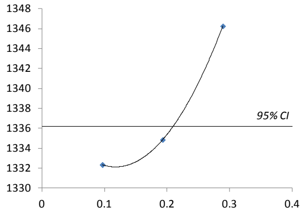
tca6



pppp2a

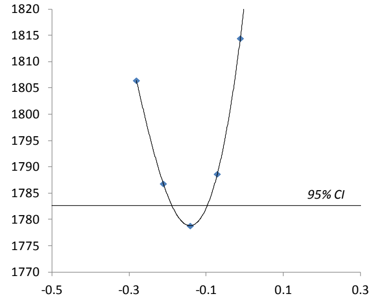


pppp2b



pppp3b

C. Net fluxes of N40



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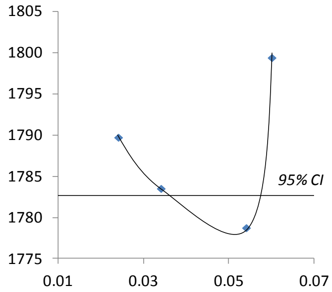
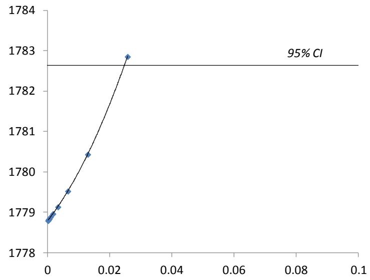
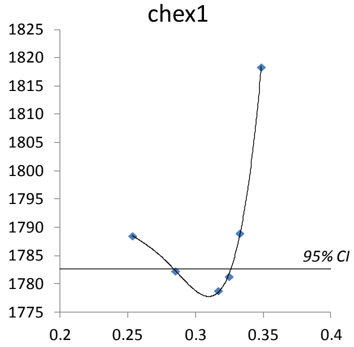


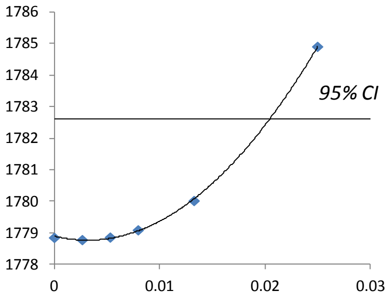
phex3



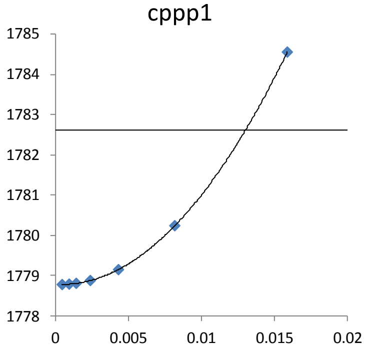
cppp1



pppp1

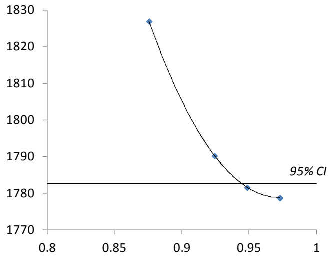


cpex



ana2

D. Exchange (XCH[0-1]) fluxes of N40



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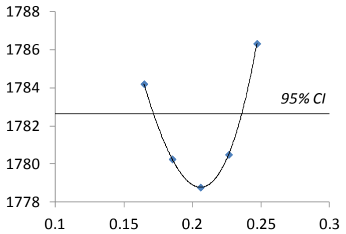
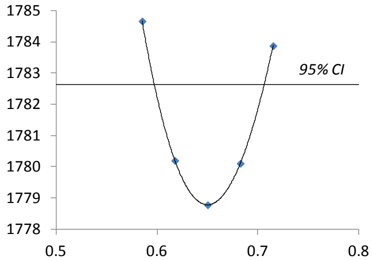
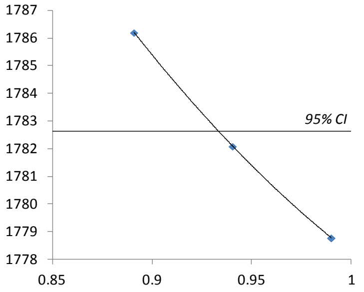


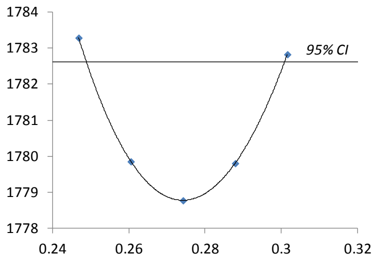
chex2



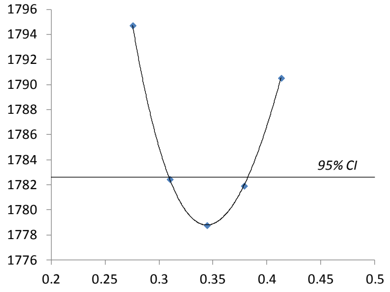
phex1



tca6



pppp2a



pppp2b

Appendix 6.1A

^{13}C NMR measurements of metabolites derived from *Arabidopsis* suspension grown on Pi- medium fed with either 99%[1-^{13}C]glucose , 99%[2-^{13}C]glucose or 20% [$^{13}C_6$]glucose (Chapter 6)

Metabolite	Metabolite name used in the model	Carbon atom sub-groups	Peak area	sd	Cumomer
//Pi-[1-^{13}C]glucose_Replica 1					
Alanine	ALA	C12aala	8.343	0.733	#10x
			2.26	0.614	#010
		C3aala	71.481	2.694	#x01
			0.166	2.694	#x11
Aspartate	ASP	C4aasn	2.375	0.385	#xx11
			7.142	0.68	#xx01
		C2aasp	5.326	0.576	#010x
			3.08	0.602	#110x+#011x
		C4aasp	6.724	0.818	#xx11
			23.898	1.972	#xx01
		C3aasp	1.987	0.314	#x011+#x110
			4.952	0.485	#x010
Citrate	CIT	C15acit	16.225	0.679	#10xxxx+#xxx01x
			6.225	0.496	#11xxxx+#xxx11x
		C24acit	38.346	2.314	#010xxx+#xx010x
			20.765	1.086	#110xxx+#xx011x+#011xxx+#xx110x
		C3acit	2.992	0.472	#x111x0
			17.303	1.12	#x110x0+#x011x0
			2.4	0.43	#x010x1
			17.45	1.805	#x010x0+#x111x0
		C6acit	3.78	0.353	#xx1xx1
			10.96	0.69	#xx0xx1
GABA	GABA	C2agaba	38.391	1.679	#010x
			20.889	1.167	#110x+#011x
		C3agaba	28.196	1.562	#x010
			31.976	1.68	#x110+#x011+#x111
Glutamate/glutamine	GLU	C3aglu	21.434	1.269	#x010x
			20.964	1.248	#x110x+#x011x
		C4aglu	34.405	1.678	#xx010
			16.73	1.123	#xx110
		C1agln	57.085	5.02	#11xxx
			134.82	5.538	#10xxx
		C3agln	206.33	6.94	#x010x
			171.277	5.823	#x110x+#x011x
		C4agln	303.199	9.71	#xx010
			129.936	4.962	#xx110
Glycine	GLY	C1gly	2.591	0.391	#10
			0	0.391	#11
Lysine	LYS	C3alys	7.058	0.715	#x010xx

			3.645	0.608	#x110xx+#x011xx
Malate	OAA	C1amal	3.712	0.418	#10xx
			1.644	0.336	#11xx
		C2amal	6.34	0.63	#010x
			2.98	0.512	#110x+#111x
			3.044	0.916	#011x
		C3amal	6.162	0.553	#x010
			1.848	0.277	#x110
Valine	VAL	C45aval	3.465	0.437	#xx01x
			3.342	0.404	#xx0x1
Sucrose	FSUC	C16afsuc	48.755	2.341	#10xxxx
			18.085	1.216	#xxxx01
Sucrose	GSUC	C6agsuc	17.733	1.317	#10xxxx
			0.001	1.317	#11xxxx
Starch	STA	StaA	0.087	0.009	#10xxxx
			0.06	0.012	#xxxx01
// Pi- [1-^{13}C]glucose_Replica2					
Alanine	ALA	C12bala	3.668	0.387	#10x
			1.196	0.412	#010
		C3bala	45.742	1.912	#x01
			0.251	0.139	#x11
Aspartate	ASP	C4basn	2.471	0.382	#xx11
			5.946	0.574	#xx01
		C2basp	4.792	0.543	#010x
			2.908	0.525	#110x+#011x
		C4basp	4.224	0.603	#xx11
			14.577	1.176	#xx01
Citrate	CIT	C3bcit	1.78	0.689	#x111x0
			13.694	3.118	#x110x0+#x011x0
			1.296	0.814	#x010x1
			17.146	3.444	#x010x0
		C6bcit	7.298	0.661	#xx1xx1
			15.15	0.939	#xx0xx1
GABA	GABA	C2bgaba	27.357	1.274	#010x
			15.433	0.996	#110x+#011x
		C3bgaba	18.26	1.146	#x010
			17.704	1.15	#x110+#x011
Glutamate/glutamine	GLU	C3bglu	18.242	1.082	#x010x
			17.732	1.115	#x110x+#x011x
		C4bglu	13.954	0.935	#xx110
			28.685	1.382	#xx010
		C1bgln	51.52	4.828	#11xxx
			107.636	7.838	#10xxx
		C3bgln	146.058	4.966	#x010x
			130.891	4.591	#x110x+#x011x
		C4bgln	192.15	6.116	#xx010
			88.667	4.571	#xx110
Glycine	GLY	C1bgly	2.045	0.414	#10
			0.001	0.414	#11

Lysine	LYS	C3blys	3.421	0.431	#x010xx
			2.412	0.53	#x110xx+#x011xx
Malate	OAA	C1bmal	4.537	0.459	#10xx
			1.762	0.299	#11xx
		C2bmal	9.218	0.696	#010x
			1.741	0.32	#110x+#111x
			3.369	0.433	#011x
		C3bmal	8.475	0.632	#x010
			2.949	0.412	#x110
			1.256	0.269	#x011
		C4bmal	2.233	0.384	#xx11
			7.508	0.815	#xx01
Valine	VAL	C35bval	2.754	0.35	#xx01x
			2.776	0.347	#xx0x1
Sucrose	FSUC	C16afsuc	48.807	2.256	#10xxxx
			16.913	1.138	#xxxx01
Sucrose	GSUC	C6agsuc	15.696	1.122	#10xxxx
			0.001	1.122	#11xxxx
Starch	STA	StaB	0.156	0.012	#10xxxx
			0.051	0.009	#xxxx01
//Pi- [1-^{13}C]glucose_Replica3					
Alanine	ALA	C12cala	5.52	0.571	#10x
			3.191	0.88	#010
		C3cala	70.593	2.909	#x01
			0.72	0.199	#x11
Aspartate	ASP	C2casn	14.283	1.174	#010x
			7.842	0.933	#110x+#011x
		C2casp	8.381	0.822	#010x
			4.642	0.687	#110x+#011x
Citrate	CIT	C15ccit	31.565	1.758	#10xxxx+#xxx01x
			13.387	1.169	#11xxxx+#xxx11x
		C24ccit	97.934	3.694	#010xxx+#xx010x
			7.896	0.79	#110xxx+#xx011x
			41.506	2.054	#011xxx+#xx110x
		C3ccit	3.493	1.266	#x111x0
			26.138	2.324	#x110x0+#x011x0
			5.081	1.076	#x010x1
			28.584	2.269	#x010x0
		C6ccit	11.629	0.873	#xx1xx1
			23.24	1.223	#xx0xx1
GABA	GABA	C2cgaba	7.56	0.675	#010x
			3.056	0.4	#011x
		C3cgaba	25.119	1.451	#x010
			4.408	0.708	#x111
			23.1	1.427	#x110+#x011
Glutamate/glutamine	GLU	C3cglu	27.298	1.689	#x010x
			22.29	1.411	#x110x+#x011x
		C4cglu	19.926	1.341	#xx110
			42.435	1.993	#xx010

		C3cgln	215.947	8.092	#x010x
			167.907	6.438	#x110x+#x011x
		C4cgln	338.322	11.005	#xx010
			137.409	5.561	#xx110
Glycine	GLY	C1cgly	2.222	0.323	#10
			0.001	0.323	#11
Lysine	LYS	C3clys	7.02	0.594	#x010xx
			3.84	1.073	#x110xx+#x011xx
Malate	OAA	C1cmal	8.315	0.676	#10xx
			5.199	0.724	#11xx
		C2cmal	16.613	1.15	#010x
			5.859	0.716	#011x
		C3cmal	15.76	1.014	#x010
			5.752	0.65	#x110
			1.359	0.221	#x011
		C4cmal	4.248	0.651	#xx11
			9.366	0.831	#xx01
Valine	VAL	C3cmal	4.584	0.553	#xx01x
			5.064	0.603	#xx0x1
Sucrose	FSUC	C16afsuc	89.193	3.701	#10xxxx
			25.488	1.689	#xxxx01
Sucrose	GSUC	C6agsuc	28.358	1.818	#10xxxx
			0.001	1.818	#11xxxx
Starch	STA	StaC	0.156	0.012	#10xxxx
			0.051	0.009	#xxxx01
// Pi- [2-^{13}C]glucose_Replica1					
Alanine	ALA_2	C2dala	74.216	2.879	#010
			4.668	0.601	#011+#110+#111
		C1dala	3.061	0.784	#11x
			3.395	0.362	#10x
		C3dala	7.82	0.626	#x01
			1.297	0.289	#x11
Aspartate	ASP_2	C23dasp	1.776	0.269	#010x
			1.558	0.25	#x010
Citrate	CIT_2	C15dcit	65.457	2.584	#10xxxx+#xxx01x
			1.912	0.363	#11xxxx+#xxx11x
		C24dcit	15.505	1.045	#010xxx+#xx010x
			1.604	0.329	#110xxx+#xx011x+#011xxx+#xx110x
GABA	GABA_2	C3dgaba	6.462	0.492	#x010
			0.536	0.174	#x110+#x011
Glutamate/glutamine	GLU_2	C4dglu	3.946	0.375	#xx010
			1.078	0.415	#xx110
			0.493	0.147	#xx011
		C2dgln	100.827	3.845	#010xx
			6.044	0.641	#110xx
			4.257	0.539	#011xx
		C3dglu	100.912	3.689	#x010x

			8.378	0.776	#x110x+#x011x
		C4dglu	44.486	2.036	#xx010
			4.972	0.604	#xx011
			4.549	0.559	#xx110
Glycine	GLY_2	C2dgly	27.538	1.471	#01
			0.89	1.471	#11
Malate	OAA_2	C1dmal	6.832	0.612	#10xx
			1.857	0.376	#11xx
		C14dmal	6.55	0.586	#xx01
			6.832	0.612	#10xx
Sucrose	GSUC_2	C25dgsuc	52.432	2.385	#010xxx
			17.266	1.071	#xxx010
Sucrose	FSUC_2	C25dfsuc	33.96	2.952	#010xxx
			16.691	2.062	#xxx010
Starch	STA_2	StaA_beta	0.029	0.006	#xxx010+#x010xx
			0.072	0.008	#010xxx
//Pi- [2-^{13}C]glucose_Replica2					
Alanine	ALA_2	C2eala	53.597	2.161	#010
			3.112	0.362	#011+#110+#111
		C3eala	5.485	0.474	#x01
			0.522	0.385	#x11
Citrate	CIT_2	C24ecit	15.088	0.944	#010xxx+#xx010x
			0.843	0.232	#110xxx+#xx011x
			1.139	0.23	#011xxx+#xx110x
GABA	GABA_2	C14egaba	20.162	1.097	#10xx
			5.66	0.513	#xx01
		C3egaba	5.489	0.446	#x010
			1.546	0.406	#x110+#x011
Glutamate/glutamine	GLU_2	C4eglu	6.007	0.557	#xx010
			0.556	0.169	#xx110
			0.467	0.146	#xx011
		C2eglu	94.222	3.798	#010xx
			5.473	0.696	#110xx
			3.867	0.51	#011xx
		C4egln	49.789	2.358	#xx010
			5.342	0.736	#xx011
			5.172	0.625	#xx110
Glycine	GLY_2	C2egly	18.855	1.107	#01
			0.512	1.107	#11
Malate	OAA_2	C3emal	4.065	0.399	#x010
			0.211	0.065	#x011+#x110
		C14emal	7.038	0.587	#xx01
			8.181	0.649	#10xx
Sucrose	FSUC_2	C25dfsuc	52.767	4.02	#010xxx
			22.86	2.488	#xxx010
Starch	STA_2	StaB_beta	0.055	0.008	#xxx010+#x010xx
			0.11	0.009	#010xxx
//Pi- [2-^{13}C]glucose_Replica3					
Alanine	ALA_2	C2fala	66.32	2.567	#010

			4.642	0.496	#011+#110+#111
		C3fala	8.494	0.609	#x01
			1.165	0.468	#x11
Aspartate	ASP_2	C23	1.995	0.308	#010x
			1.751	0.263	#x010
Citrate	CIT_2	C15	56.891	2.246	#10xxxx+#xxx01x
			0.691	0.247	#11xxxx+#xxx11x
		C24fcit	14.707	0.964	#010xxx+#xx010x
			1.061	0.204	#110xxx+#xx011x+#011xxx+#xx110x
		C36fcit	1.76	0.319	#x010x0
			3.597	0.426	#xx0xx1
GABA	GABA_2	C3fgaba	7.497	0.624	#x010
			1.524	0.481	#x110+#x011
Glutamate/glutamine	GLU_2	C2fglu	102.91	3.84	#010xx
			7.637	0.711	#110xx
			4.68	0.489	#011xx
		C3fgln	102.376	3.668	#x010x
			12.66	1.437	#x110x+#x011x
		C4fglu	44.844	1.968	#xx010
			5.699	0.653	#xx011
			6.225	0.646	#xx110
Glycine	GLY_2	C2fgly	22.435	1.245	#01
			0.782	1.245	#11
Malate	OAA_2	C1fmal	1.419	0.32	#11xx
			6.156	0.527	#10xx
		C14fmal	6.423	0.57	#xx01
			6.156	0.527	#10xx
Sucrose	GSUC_2	C25dgsuc	64.833	2.733	#010xxx
			20.12	1.142	#xxx010
Sucrose	FSUC_2	C25dfsuc	64.768	2.589	#010xxx
			21.891	1.264	#xxx010
Starch	STA_2	StaC_beta	0.042	0.008	#xxx010+#x010xx
			0.107	0.011	#010xxx
// Pi- $[^{13}C_6]$glucose_Replica 1					
Alanine	ALA_3	C2gala	21.315	0.951	#010+#011+#110
			43.763	1.752	#111
		C1gala	15.03	0.801	#11x
			5.216	0.373	#10x
Glycine	GLY_3	C1ggly	2.748	0.418	#10
			6.159	0.638	#11
// Pi- $[^{13}C_6]$glucose_Replica 2					
Alanine	ALA_3	C2hala	14.469	0.78	#010+#011+#110
			27.653	1.37	#111
		C1hala	8.983	0.566	#11x
			4.197	0.329	#10x
		C3hala	4.428	0.3	#x01
			32.99	1.32	#x11
// Pi- $[^{13}C_6]$glucose_Replica 3					

Alanine	ALA_3	C2iala	11.594	0.606	#010+#011+#110
			23.491	1.174	#111
		C1iala	7.943	0.568	#11x
			3.68	0.329	#10x
		C3hala	3.335	0.241	#x01
			25.627	1.073	#x11
Malate	OAA_3	C1imal	1.274	0.139	#10xx
			1.628	0.171	#11xx

Appendix 6.1B : ^{13}C NMR measurements of metabolites derived from *Arabidopsis* suspension grown on MS medium fed with either 99%[1-^{13}C]glucose or 99%[2-^{13}C]glucose (Chapter 6)

Metabolite	Metabolite name used in the model	Carbon atom subgroups	Peak area	sd	Cumomer
//MS [1-^{13}C]glucose_Replica 1					
Starch	STA	StaA	0.4542	0.027	#10xxxx
			0.1321	0.017	#xxxx01
Alanine	ALA	C1a	0.437	0.126	#11x
			11.174	0.806	#10x
		C2a	5.452	0.644	#010
			1.559	0.336	#011
		C3a	134.185	4.513	#x01
			1.3	0.469	#x11
Citrate	CIT	C1C5a	24.858	1.606	#10xxxx+#xxx01x
			9.926	1.057	#11xxxx+#xxx11x
		C6a	6.769	0.616	#xx1xx1
			20.328	1.289	#xx0xx1
		nosubCITa	24.858	1.606	#10xxxx+#xxx01x
			21.332	1.445	#x010x0
			20.328	1.289	#xx0xx1
GABA	GABA	C24a	6.158	0.547	#010x
			7.365	0.747	#xx01
		C3a	7.248	0.636	#x010
			4.934	0.498	#x110+#x011
Glutamate/glutamine	GLU	C1a	6.097	0.632	#11xxx
			14.299	0.938	#10xxx
		C3a	14.733	0.82	#x010x
			10.641	2.735	#x110x+#x011x
		C1a	36.226	1.732	#10xxx
			14.023	1.037	#11xxx
		C2a	62.831	2.617	#010xx
			7.233	0.659	#110xx
			20.212	1.24	#011xx
		C3a	48.067	2.088	#x010x
			38.288	1.803	#x110x+#x011x
Glycine	GLY	C1a	0.492	0.169	#10
			0.01	0.169	#11

Malate	OAA	C1a	13.493	0.83	#10xx
			4.463	0.46	#11xx
		C2a	24.597	1.237	#010x
			2.645	0.316	#110x
		//	1.342	0.203	#111x
			8.316	0.661	#011x
		C3a	26	1.332	#x010
			9.198	0.752	#x110
			3.613	0.456	#x011
		C4a	17.143	1.152	#xx01
			5.885	0.644	#xx11
		nonsubOAA	13.493	0.83	#10xx
			24.597	1.237	#010x
			24	1.233	#x010
Serine	SER	C3a	24.492	1.213	#x01
			0.01	0.853	#x11
Succinate	SUCC	C1C4a	2.904	0.51	#10xx+#xx01
			1.008	0.226	#11xx+#xx11
Sucrose	GSUC	Ca	0.464	0.08	#xxx010
			7.546	0.687	#xxxx01
Sucrose	FSUC	C16a1	38.328	1.93	#10xxxx
			10.068	0.884	#xxxx01
		C16a2	80.71	3.124	#10xxxx
			17.604	1.034	#xxxx01
		C16a3	23.947	1.303	#10xxxx
			5.223	0.763	#xxxx01
			1.29	0.3	#xx010x
//MS [1-^{13}C]glucose_Replica 2					
Starch	STA	StaB	0.3023	0.021	#10xxxx
			0.0942	0.013	#xxxx01
Alanine	ALA	C1b	0.316	0.07	#11x
			8.567	0.68	#10x
		C2b	3.197	0.491	#011
			7.053	0.637	#010
		C3b	115.249	3.913	#x01
			1.841	0.254	#x11
Citrate	CIT	C1C5b	24.969	1.363	#10xxxx+#xxx01x
			9.168	0.81	#11xxxx+#xxx11x
		C2C4b	84.365	3.158	#010xxx+#xx010x
			6.361	0.664	#110xxx+#xx011x
			31.554	1.6	#011xxx+#xx110x
		C6b	5.336	0.451	#xx1xx1
			12.811	0.695	#xx0xx1
		no subCITb	24.969	1.363	#10xxxx+#xxx01x
			84.365	3.158	#010xxx+#xx010x
			23.394	1.198	#x010x0
GABA	GABA	C2b	3.607	0.392	#010x
			1.363	0.244	#011x
		C3b	8.47	0.676	#x010

			8.112	0.74	#x110+#x011
		C4b	12.89	0.924	#xx01
			4.631	0.566	#xx11
		nosubGAGAb	8.47	0.676	#x010
			12.89	0.924	#xx01
Glutamate/glutamine	GLU	C2b	21.534	1.197	#010xx
			2.98	0.435	#110xx
			8.595	0.805	#011xx
		C3b	15.976	0.985	#x010x
			15.074	1.027	#x110x+#x011x
		C4b	28.098	1.374	#xx010
			11.917	0.883	#xx110
		C1b	19.389	1.183	#10xxx
			8.218	0.791	#11xxx
		C2b	35.007	1.643	#010xx
			6.001	0.647	#110xx
			13.661	1.024	#011xx
		C3b	23.708	1.216	#x010x
			25.197	1.497	#x110x+#x011x
		C4b	35.829	1.702	#xx010
			14.46	1.143	#xx110
Glycine	GLY	C1b	3.156	0.464	#10
			0.01	0.464	#11
Malate	OAA	C1b	11.138	0.626	#10xx
			4.523	0.411	#11xx
		C2b	33.471	1.601	#010x
			4.531	0.5	#110x
			12.555	0.934	#011x
		C3b	34.126	1.552	#x010
			12.311	0.863	#x110
			5.023	0.525	#x011
		C4b	17.683	1.04	#xx01
			6.768	0.634	#xx11
		NosubOAAb	33.471	1.601	#010x
			34.126	1.552	#x010
Serine	SER	C3b	22.156	1.132	#x01
			0.01	0.893	#x11
Succinate	SUCC	C1C4b	4.455	0.371	#10xx+#xx01
			1.257	0.221	#11xx+#xx11
Valine	VAL	C4b	1.304	0.25	#xx01x
			1.367	0.249	#xx0x1
Sucrose	GSUC	Cb	1.068	0.279	#x010xx
			10.203	0.908	#xxxx01
Sucrose	FSUC	C16b1	35.269	1.794	#10xxxx
			10.955	1.027	#xxxx01
			0.88	0.23	#xx010x
		C16b2	84.178	3.173	#10xxxx

			21.348	1.226	#xxxx01
		C16b3	27.03	1.419	#10xxxx
			6.855	0.924	#xxxx01
//MS [1-^{13}C]glucose_Replica 3					
Starch	STA	StaC	0.4258	0.028	#10xxxx
			0.1262	0.016	#xxxx01
Alanine	ALA	C1c	1.605	0.396	#11x
			12.499	0.944	#10x
		C2c	8.184	0.668	#010
			3.436	0.479	#011
			0.682	0.145	#110
		C3c	143.979	4.707	#x01
			2.566	0.431	#x11
Citrate	CIT	C1C5c	25.103	1.377	#10xxxx+#xxx01x
			9.697	0.85	#11xxxx+#xxx11x
		C2C4c	83.552	3.145	#010xxx+#xx010x
			6.272	0.648	#110xxx+#xx011x
			33.153	1.663	#011xxx+#xx110x
		C6c	8.377	0.679	#xx1xx1
			18.697	1	#xx0xx1
		nosubCITc	25.103	1.377	#10xxxx+#xxx01x
			83.552	3.145	#010xxx+#xx010x
			23.273	1.187	#x010x0
			18.697	1	#xx0xx1
GABA	GABA	C2c	15.447	0.871	#010x
			6.809	0.6	#011x
		C3c	9.35	0.712	#x010
			9.07	0.774	#x110+#x011
		C4c	13.933	0.974	#xx01
			5.425	0.664	#xx11
		nosubGABAc	9.35	0.712	#x010
			13.933	0.974	#xx01
Glutamate/glutamine	GLU	C2c	23.377	1.258	#010xx
			3.449	0.428	#110xx
			10.027	0.85	#011xx
		C3c	17.363	0.996	#x010x
			15.594	0.965	#x110x+#x011x
		C4c	31.002	1.473	#xx010
			13.672	0.951	#xx110
		C1c	29.441	1.501	#10xxx
			11.961	0.888	#11xxx
		C2c	55.01	2.261	#010xx
			9.559	0.826	#110xx
			21.721	1.344	#011xx
		C3c	40.968	1.873	#x010x
			35.833	1.751	#x110x+#x011x
Glycine	GLY	C1c	3.412	0.467	#10

			0.01	0.467	#11
Malate	OAA	C1c	13.516	0.796	#10xx
			6.316	0.593	#11xx
		C2c	19.097	0.96	#010x
			2.382	0.284	#110x
			7.484	0.58	#011x
		C3c	28.276	1.362	#x010
			10.101	0.734	#x110
			4.326	0.472	#x011
		C4c	14.856	0.932	#xx01
			6.281	0.661	#xx11
		NosubOAAc	13.516	0.796	#10xx
			28.276	1.362	#x010
Serine	SER	C3c	27.683	1.309	#x01
			0.01	0.862	#x11
Succinate	SUCC	C1C4c	2.978	0.369	#10xx+#xx01
			1.351	0.296	#11xx+#xx11
Valine	VAL	C4c	1.645	0.307	#xx01x
			1.627	0.274	#xx0x1
Sucrose	GSUC	Cc	0.517	0.139	#x010xx
			10.868	0.995	#xxxx01
Sucrose	FSUC	C16c1	37.759	1.932	#10xxxx
			11.102	1.044	#xxxx01
		C16c2	91.964	3.413	#10xxxx
			23.589	1.305	#xxxx01
		C16c3	29.165	1.5	#10xxxx
			7.481	0.953	#xxxx01
//MS [2-^{13}C]glucose_Replica 1					
Starch	STA_2	StaA_beta	0.0466	0.008	#10xxxx
			0.0626	0.008	#xxx010+#x010xx
			0.2086	0.016	#010xxx
		StaA_alpha	0.1726	0.017	#010xxx+#xxx010
			0.0353	0.008	#10xxxx
Alanine	ALA_2	C2d	140.469	4.708	#010
			3.997	0.468	#110
		C1d	5.437	0.628	#11x
			14.498	0.945	#10x
		C3d	22.549	1.225	#x01
			1.922	0.693	#x11
		NosubALAd	140.469	4.708	#010
			14.498	0.945	#10x
			22.549	1.225	#x01
Citrate	CIT_2	C1C5d	111.188	3.803	#10xxxx+#xxx01x
			2.988	0.41	#11xxxx+#xxx11x
		C2C4d	35.402	1.741	#010xxx+#xx010x
			2.443	0.435	#110xxx+#xx011x
			2.488	0.385	#011xxx+#xx110x
		C3d	23.002	1.204	#x010x0
			3.622	0.376	#x110x0+#x011x0

			1.468	0.197	#x010x1
		C6d	2.118	0.322	#xx1xx1
			34.567	1.567	#xx0xx1
		NoSubCITd	111.188	3.803	#10xxxx+#xxx01x
			35.402	1.741	#010xxx+#xx010x
			23.002	1.204	#x010x0
			35.567	1.567	#xx0xx1
GABA	GABA_2	C2d	3.923	0.42	#010x
			8.323	0.832	#xx01
		C3d	7.738	0.637	#x010
			1.03	0.259	#x110+#x011
Glutamate/glutamine	GLU_2	C2d	11.864	0.914	#010xx
			6.078	0.542	#xx010
		C3d	11.831	0.806	#x010x
			2.298	0.509	#x110x+#x011x
		C2d	23.393	1.414	#010xx
			1.648	0.393	#110xx
			0.928	0.239	#011xx
		C3d	23.566	1.428	#x010x
			3.97	0.768	#x110x+#x011x
		C4d	10.746	0.916	#xx010
			0.927	0.267	#xx110
			1.768	0.406	#xx110
		Cdglu	11.864	0.914	#010xx
			11.831	0.806	#x010x
		Cdgln	23.393	1.414	#010xx
			23.566	1.428	#x010x
			10.746	0.916	#xx010
Glycine	GLY_2	C2d	16.005	1.058	#01
			1.025	0.168	#11
		C1d	1.46	0.39	#10
			0.01	0.39	#11
Malate	OAA_2	C1d	32.977	1.487	#10xx
			1.218	0.313	#11xx
		C3d	19.395	1.069	#x010
			0.658	0.154	#x110
			0.76	0.163	#x011
		C4d	34.053	1.563	#xx01
			1.41	0.275	#xx11
		NosubMALd	32.977	1.487	#10xx
			19.395	1.069	#x010
			34.053	1.563	#xx01
Succinate	SUCC_2	C1C4d	10.361	0.646	#10xx+#xx01
			5.952	0.537	#01xx+#xx10
Sucrose	GSUC_2	Cd	10.1	0.773	#xxx010
			39.174	1.916	#010xxx
			1.629	0.33	#xxxx01
Sucrose	FSUC_2	Cd	1.695	0.317	#10xxxx

			24.227	1.137	#010xxx
			0.755	0.192	#110xxx+#011xxx
//MS [2-^{13}C]glucose_Replica 2					
Starch	STA_2	StaB_beta	0.0588	0.01	#10xxxx
			0.1017	0.014	#xxx010+#x010xx
			0.2572	0.021	#010xxx
		StaB_alpha	0.2234	0.021	#010xxx+#xxx010
			0.0445	0.01	#10xxxx
Alanine	ALA_2	C2e	127.347	4.225	#010
			3.265	0.36	#110
		C3e	13.583	0.763	#x01
			1.41	0.304	#x11
		NosubALAe	127.347	4.225	#010
			12.726	0.92	#10x
Citrate	CIT_2	C1C5e	102.983	3.508	#10xxxx+#xxx01x
			4.118	1.85	#11xxxx+#xxx11x
		C2C4e	21.446	1.028	#010xxx+#xx010x
			1.41	0.225	#110xxx+#xx011x
			1.562	0.219	#011xxx+#xx110x
		C3e	21.193	1.12	#x010x0
			3.841	0.388	#x110x0+#x011x0
			1.985	0.294	#x010x1
		C6e	2.577	0.345	#xx1xx1
			33.313	1.505	#xx0xx1
		NoSubCITe	102.983	3.508	#10xxxx+#xxx01x
			21.193	1.12	#x010x0
			33.313	1.505	#xx0xx1
GABA	GABA_2	C3e	7.254	0.614	#x010
			1.005	0.263	#x110+#x011
Glutamate/glutamine	GLU_2	C4e	3.852	0.354	#xx010
			0.434	0.139	#xx110
			0.395	0.12	#xx011
		C2e	19.361	1.265	#010xx
			1.035	0.248	#110xx
			0.94	0.25	#011xx
		C4e	9.251	0.798	#xx010
			0.88	0.226	#xx110
			1.755	0.616	#xx110
		Ceglu	10.76	0.832	#010xx
			3.852	0.354	#xx010
		Cegln	19.361	1.265	#010xx
			9.251	0.798	#xx010
Glycine	GLY_2	C2e	10.758	0.769	#01
			0.745	0.25	#11
Malate	OAA_2	C1e	25.769	1.194	#10xx
			1.42	0.282	#11xx
		C3e	15.123	0.816	#x010
			0.706	0.136	#x110

			1.026	0.194	#x011
		C4e	26.275	1.247	#xx01
			0.964	0.182	#xx11
		NosubMALe	25.769	1.194	#10xx
			15.123	0.816	#x010
			26.275	1.247	#xx01
Succinate	SUCC_2	C1C4e	10.077	0.604	#10xx+#xx01
			3.719	0.324	#01xx+#xx10
Sucrose	GSUC_2	Ce	8.539	0.637	#xxx010
			35.811	1.726	#010xxx
			1.053	0.199	#xxxx01
Sucrose	FSUC_2	Ce	2.112	0.358	#10xxxx
			23.071	1.079	#010xxx
			1.243	0.287	#110xxx+#011xxx
//MS [2-^{13}C]glucose_Replica 3					
Starch	STA_2	StaC_beta	0.0749	0.014	#10xxxx
			0.0889	0.012	#xxx010+#x010xx
			0.2413	0.02	#010xxx
		StaC_alpha	0.2083	0.02	#010xxx+#xxx010
			0.0385	0.01	#10xxxx
Alanine	ALA_2	C2f	143.533	4.644	#010
			3.779	0.404	#110
		C1f	6.707	0.828	#11x
			15.231	0.97	#10x
		C3f	22.987	1.164	#x01
			1.981	0.312	#x11
		NosubALAf	143.533	4.644	#010
			15.231	0.97	#10x
			22.987	1.164	#x01
Citrate	CIT_2	C1C5f	70.31	2.385	#10xxxx+#xxx01x
			2.301	0.296	#11xxxx+#xxx11x
		C2C4f	31.715	1.508	#010xxx+#xx010x
			2.232	0.338	#110xxx+#xx011x
		C3f	21.302	1.099	#x010x0
			3.22	0.33	#x110x0+#x011x0
		C6f	2.304	0.353	#xx1xx1
			32.729	1.467	#xx0xx1
		NoSubCITf	31.715	1.508	#010xxx+#xx010x
			21.302	1.099	#x010x0
			32.729	1.467	#xx0xx1
GABA	GABA_2	C2f	3.569	0.35	#010x
			0.235	0.155	#011x
			7.012	0.679	#xx01
		C3f	6.914	0.564	#x010
			0.866	0.254	#x110+#x011
Glutamate/glutamine	GLU_2	C2f	11.458	0.82	#010xx
			0.767	0.213	#011xx
		C3f	12.111	0.81	#x010x

			1.61	0.325	#x110x+#x011x
		C4f	6.029	0.503	#xx010
			0.878	0.278	#xx110
			0.535	0.17	#xx011
		C2f	22.632	1.325	#010xx
			2.182	0.446	#110xx
			1.001	0.211	#011xx
		C3f	22.531	1.395	#x010x
			4.523	0.779	#x110x+#x011x
		C4f	10.988	0.886	#xx010
			2.555	1.105	#xx110
		Cfglu	11.458	0.82	#010xx
			12.111	0.81	#x010x
			6.029	0.503	#xx010
		Cfgln	22.632	1.325	#010xx
			22.531	1.395	#x010x
			10.988	0.886	#xx010
Glycine	GLY_2	C2f	14.448	0.894	#01
			0.896	0.234	#11
Malate	OAA_2	C1f	27.601	1.247	#10xx
			1.427	0.392	#11xx
		C3f	16.526	0.878	#x010
			1.353	0.26	#x110+#x011
		C4f	28.857	1.331	#xx01
			0.917	0.191	#xx11
		NosubMALf	27.601	1.247	#10xx
			20.523	1.128	#010x
			16.526	0.878	#x010
			28.857	1.331	#xx01
Succinate	SUCC_2	C1C4f	8.85	0.558	#10xx+#xx01
			4.551	0.413	#01xx+#xx10
Sucrose	GSUC_2	Cf	9.451	0.689	#xxx010
			37.034	1.73	#010xxx
			1.731	0.302	#xxxx01
Sucrose	FSUC_2	Cf	1.756	0.541	#10xxxx
			35.914	1.643	#010xxx
			0.986	0.238	#110xxx+#011xxx

Appendix 6.1C : ^{13}C NMR measurements of metabolites derived from *Arabidopsis* suspension grown on Pi+ medium fed with either 99%[1-^{13}C]glucose or 99%[2-^{13}C]glucose (Chapter 6)

Metabolite	**Metabolite name used in the model**	**Carbon atom subgroups**	**Peak area**	**sd**	**Cumomer**
//Pi+ [1-^{13}C]glucose_Replica 1					
	ALA	C2	3.792	0.438	#010
			0.839	0.39	#011
		C1	0.905	0.467	#11x

			5.645	0.498	#10x
		C3	62.222	2.367	#x01
			0.814	0.31	#x11
	CIT	C1C5	17.498	1.042	#10xxxx+#xxx01x
			5.986	0.64	#11xxxx+#xxx11x
		C2C4	19.858	1.96	#011xxx+#xx110x+#110xxx+#xx011x
			57.328	2.288	#010xxx+#xx010x
		C3	15.475	0.856	#x010x0
			12.28	0.82	#x110x0+#x011x0
	GABA	C3	4.597	0.458	#x010
			2.918	0.367	#x110+#x011
		C4	2.163	0.789	#xx11
			7.468	0.659	#xx01
	GLU	C5	4.981	0.507	#xxx11
			14.118	0.809	#xxx01
		C2	10.621	0.746	#010xx
			0.908	0.186	#110xx
			2.762	0.408	#011xx
		C3	7.247	0.591	#x010x
			5.546	0.56	#x110x+#x011x
		C4	4.859	0.568	#xx110
			14.034	0.858	#xx010
		C2	7.881	0.623	#010xx
			0.76	0.167	#110xx
			1.65	0.279	#011xx
		C3	3.93	0.422	#x010x
			3.37	0.436	#x110x+#x011x
		C4	10.308	0.853	#xx010
			3.489	0.61	#xx110
	OAA	C1	20.198	1.01	#10xx
			5.407	0.479	#11xx
		C2	37.156	1.727	#010x
			4.383	0.514	#110x
			10.768	0.854	#011x
		C3	39.842	1.702	#x010
			10.157	0.746	#x110
			5.018	0.5	#x011
		C4	6.825	0.602	#xx11
			22.237	1.134	#xx01
	VAL	C45	2.709	0.397	#xx01x
			2.212	0.335	#xx0x1
	FSUC	C16	32.583	1.683	#10xxxx
			5.2	0.634	#xxxx01
	STA	StaA	0.16	0.015	#10xxxx
			0.057	0.012	#xxxx01
//Pi+ [1-^{13}C]glucose_Replica 2					
	ALA	C2	5.654	0.852	#010
			1.884	1.026	#011

			8.305	0.736	#10x
		C23	85.549	3.436	#x01
			5.654	0.852	#010
	CIT	C24	22.427	2.193	#011xxx+#xx110x+#110xxx+#xx011x
			59.716	3.168	#010xxx+#xx010x
	GABA	C3	6.812	0.768	#x010
			5.881	0.832	#x110+#x011
	GLU	C1	5.15	0.85	#11xxx
			9.374	0.773	#10xxx
		C2	13.918	1.064	#010xx
			2.039	0.711	#110xx
			3.319	1.011	#011xx
		C3	9.257	0.703	#x010x
			6.835	0.622	#x110x+#x011x
		C1	1.238	0.344	#11xxx
			6.636	0.615	#10xxx
		C2	12.798	1.074	#010xx
			4.62	0.711	#110xx+#011xx
		C3	8.746	0.775	#x010x
			1.603	0.747	#x111x
			7.416	0.758	#x110x+#x011x
		C4	12.663	0.815	#xx010
			5.386	1.347	#xx110
	OAA	C2	37.795	1.677	#010x
			4.105	0.412	#110x
			9.863	0.743	#011x
		C3	41.078	2.593	#x010
			10.843	0.839	#x110
			5.548	0.584	#x011
		C4	7.6	0.706	#xx11
			22.943	1.268	#xx01
	THR	C3	0.553	0.103	#x110
			1.494	0.172	#x010
			0.461	0.093	#x110
	VAL	C25	3.348	0.392	#xx01x
			3.697	0.417	#xx0x1
	STA	StaB	0.214	0.018	#10xxxx
			0.049	0.009	#xxxx01
//Pi+ [1-^{13}C]glucose_Replica 3					
	ALA	C2	6.247	0.666	#010
			2.049	0.87	#011
		C1	0.646	0.388	#11x
			9.636	0.703	#10x
		C3	95.26	3.375	#x01
			1.345	0.435	#x11
	CIT	C15	19.656	1.154	#10xxxx+#xxx01x
			5.918	0.633	#11xxxx+#xxx11x

		C24	22.879	2.179	#011xxx+#xx110x+#110xxx+#xx011x
			61.125	3.287	#010xxx+#xx010x
		C3	16.738	2.017	#x010x0
			13.406	1.268	#x110x0+#x011x0
			1.364	0.307	#x010x1
	GABA	C3	6.391	0.621	#x010
			5.099	1.295	#x110+#x011
		C4	2.482	1.006	#xx11
			10.656	1.167	#xx01
	GLU	C5	4.861	0.448	#xxx11
			15.895	0.899	#xxx01
		C1	3.504	0.463	#11xxx
			9.776	0.718	#10xxx
		C2	16.612	1.052	#010xx
			1.975	0.386	#110xx
			5.217	0.608	#011xx
		C3	11.327	0.736	#x010x
			9.034	0.699	#x110x+#x011x
		C2	14.334	0.929	#010xx
			1.553	0.297	#110xx
			2.659	0.321	#011xx
		C3	9.794	0.734	#x010x
			0.858	0.195	#x111x
			7.469	0.68	#x110x+#x011x
	OAA	C1	21.089	0.998	#10xx
			6.134	0.506	#11xx
		C2	41.942	1.716	#010x
			5.134	0.471	#110x
			11.911	0.772	#011x
		C3	45.207	1.803	#x010
			11.798	0.765	#x110
			6.011	0.519	#x011
	THR	C3	0.278	0.056	#x110
			1.99	0.237	#x010
			0.278	0.077	#x110
	VAL	C45	3.981	0.4	#xx01x
			4.292	0.435	#xx0x1
	FSUC	C16	81.044	3.166	#10xxxx
			15.856	1.146	#xxxx01
	STA	StaC	0.207	0.018	#10xxxx
			0.076	0.013	#xxxx01
//Pi+ [2-^{13}C]glucose_Replica 1					
	ALA_2	C2	69.139	2.665	#010
			3.549	0.493	#011+#110
		C1	2.849	0.346	#11x
			9.281	0.693	#10x
		C3	14.167	0.9	#x01
			1.05	0.232	#x11

	ASP_2	C23	0.599	0.162	#010x
			0.593	0.161	#x010
	CIT_2	C15	61.736	2.41	#10xxxx+#xxx01x
			1.994	0.35	#11xxxx+#xxx11x
		C24	22.612	1.276	#010xxx+#xx010x
			2.802	0.663	#110xxx+#xx011x+#011xxx+#xx110x
		C3	15.494	0.948	#x010x0
			4.366	0.4	#x110x0+#x011x0+#x010x1
	GABA_2	C24	1.343	0.215	#010x
			3.441	0.48	#xx01
		C34	4.423	0.499	#x010
			3.441	0.48	#xx01
			0.195	0.056	#x110+#x011
	GLU_2	C3	8.238	0.657	#x010x
			1.247	0.324	#x110x+#x011x
		C3	6.596	0.655	#x010x
			1.007	0.28	#x110x+#x011x
		C24	2.522	0.455	#xx010
			0.987	0.264	#xx110+#xx011
			5.554	0.632	#010xx
	OAA_2	C1	31.838	1.483	#10xx
			1.318	0.497	#11xx
		C2	19.33	1.009	#010x
			1.176	0.229	#110x
			1.196	0.191	#011x
		C3	15.398	0.801	#x010
			2.469	0.563	#x110
			1.184	0.214	#x011
		C4	33.263	1.566	#xx01
			1.798	0.306	#xx11
	SUCC_2	C14	75.779	3.481	#10xx+#xx01
			2.505	0.636	#11xx+#xx11
	FSUC_2	C25	8.619	0.808	#xxx010
			42.37	1.932	#010xxx
			1.48	0.382	#110xxx+#011xxx
	GSUC_2	C25	46.843	2.213	#010xxx
			8.126	0.654	#xxx010
	STA_2	StaA_beta	0.032	0.008	#10xxxx
			0.038	0.009	#xxx010+#x010xx
			0.075	0.009	#010xxx
		StaA_alpha	0.07	0.01	#010xxx+#xxx010
			0.013	0.004	#10xxxx
//Pi+ [2-^{13}C]glucose_Replica 2					
	ALA_2	C2	46.567	2.063	#010
			1.527	0.463	#011+#110
		C1	7.773	0.814	#10x
			2.528	1.228	#11x

		C3	9.69	0.863	#x01
			1.166	0.325	#x11
	CIT_2	C15	95.569	3.545	#10xxxx+#xxx01x
			4.123	1.4	#11xxxx+#xxx11x
		C24	23.313	1.218	#010xxx+#xx010x
			2.815	0.5	#110xxx+#xx011x
			2.668	0.386	#011xxx+#xx110x
		C3	16.556	0.978	#x010x0
			5.08	0.529	#x110x0+#x011x0+#x010x1
		C6	3.674	1.246	#xx1xx1
			30.064	1.554	#xx0xx1
	GABA_2	C24	1.544	0.276	#010x
			3.854	0.572	#xx01
		C3	3.626	0.473	#x010
			0.626	0.293	#x110+#x011
	GLU_2	C4	3.881	0.487	#xx010
			0.718	0.28	#xx110
			0.315	0.199	#xx011
		C14	3.289	0.536	#10xxx
			1.148	0.333	#xx010
	OAA_2	C1	41.428	1.848	#10xx
			1.544	0.548	#11xx
		C23	40.293	1.895	#010x
			30.731	1.49	#x010
		C4	44.138	2.022	#xx01
			3.064	0.639	#xx11
	SUCC_2	C14	85.218	3.067	#10xx+#xx01
			3.986	0.544	#11xx+#xx11
	FSUC_2	C25	20.191	1.13	#010xxx
			6.687	0.939	#xxx010
	GSUC_2	C25	21.805	1.268	#010xxx
			4.436	0.605	#xxx010
	STA_2	StaB_beta	0.032	0.008	#xxx010+#x010xx
			0.046	0.007	#010xxx
//Pi+ [2-^{13}C]glucose_Replica 3					
	ALA_2	C2	75.978	2.829	#010
			2.986	0.345	#011+#110
		C1	30.295	2.582	#10x
			4.791	1.1	#11x
		C3	19.439	1.129	#x01
			2.251	0.675	#x11
	CIT_2	C15	3.542	1.118	#11xxxx+#xxx11x
			55.297	2.197	#10xxxx+#xxx01x
		C24	20.328	1.149	#010xxx+#xx010x
			2.443	0.534	#110xxx+#xx011x+#011xxx+#xx110x
		C3	15.281	0.956	#x010x0
			6.098	1.095	#x110x0+#x011x0+#x

					010x1
	GABA_2	C24	2.399	0.294	#010x
			5.67	0.687	#xx01
		C3	5.575	0.586	#x010
			0.797	0.205	#x110+#x011
	GLU_2	C3	12.304	0.831	#x010x
			1.694	0.459	#x110x+#x011x
		C4	11.842	0.957	#xx010
			2.33	0.48	#xx011+#xx110
	OAA_2	C1	43.05	1.763	#10xx
			3.058	0.729	#11xx
		C2	39.331	1.712	#010x
			5.134	0.629	#110x+#011x
		C3	31.542	1.384	#x010
			3.582	0.392	#x110+#x011
		C4	45.525	1.906	#xx01
			3.277	0.824	#xx11
	SUCC_2	C14	36.584	1.493	#10xx+#xx01
			1.62	0.309	#11xx+#xx11
	FSUC_2	C25	17.336	1.692	#xxx010
			113.666	4.054	#010xxx
	GSUC_2	C25	111.54	4.091	#010xxx
			15.221	0.882	#xxx010
	STA_2	StaC_beta	0.072	0.011	#10xxxx
			0.089	0.011	#xxx010+#x010xx
			0.268	0.019	#010xxx
			0.037	0.01	#xxxx01
	STA_2	StaC_alpha	0.238	0.02	#010xxx+#xxx010
			0.041	0.008	#10xxxx

Appendix 6.1D

Mass isotopomer measurements of metabolites derived from *Arabidopsis* suspension grown on different phosphate levels (Pi-, MS and Pi+) fed with either 99%[1-^{13}C]glucose, 99%[2-^{13}C]glucose or 20%[$^{13}C_6$]glucose (Chapter 6).

Mass isotopomer datasets of Pi-

Metabolite name used in the model	Carbon Atoms	Mass (m+)	[1-^{13}C]glucose			[2-^{13}C]glucose			[$^{13}C_6$]glucose		
			Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3
ALA	1,2,3	0	0.568	0.567	0.582	0.535	0.545	0.542	0.734	0.72	0.717
		1	0.411	0.407	0.4	0.437	0.419	0.422	0.082	0.097	0.1
		2	0.021	0.025	0.023	0.028	0.036	0.035	0.046	0.054	0.054
		3	0	0	-0.004	0	0	0	0.139	0.128	0.129
	2,3	0	0.589	0.59	0.598	0.56	0.572	0.565	0.78	0.774	0.772
		1	0.406	0.403	0.394	0.435	0.422	0.43	0.044	0.054	0.056
		2	0.005	0.007	0.008	0.005	0.005	0.006	0.176	0.172	0.173
GLY	1,2	0	0.936	0.937	0.941	0.637	0.652	0.648	0.777	0.773	0.772
		1	0.063	0.064	0.061	0.345	0.328	0.331	0.105	0.116	0.116
		2	0.001	-0.001	-0.002	0.017	0.02	0.021	0.118	0.111	0.112
	2	0	0.972	0.972	0.973	0.675	0.692	0.685	0.829	0.829	0.828
		1	0.028	0.028	0.027	0.325	0.308	0.315	0.171	0.171	0.172
SER	1,2,3	0	0.647	0.658	0.668	0.583	0.587	0.584	0.658	0.651	0.648
		1	0.337	0.325	0.317	0.375	0.367	0.369	0.2	0.211	0.211
		2	0.017	0.016	0.016	0.042	0.046	0.047	0.104	0.103	0.105
		3	-0.001	0	-0.001	0.001	0	0.001	0.038	0.036	0.036
	2,3	0	0.67	0.68	0.69	0.615	0.62	0.619	0.704	0.697	0.697
		1	0.325	0.315	0.306	0.363	0.355	0.358	0.245	0.253	0.251
		2	0.005	0.005	0.003	0.022	0.025	0.023	0.052	0.05	0.052
	2,3	0	0.669	0.681	0.692	0.616	0.623	0.62	0.703	0.699	0.699
		1	0.324	0.314	0.3	0.36	0.353	0.355	0.243	0.252	0.25
		2	0.007	0.005	0.007	0.024	0.024	0.025	0.053	0.049	0.051
GABA	1,2,3,4	0	0.236	0.256	0.27	0.47	0.493	0.451	0.526	0.531	0.536

		1	0.415	0.432	0.424	0.429	0.42	0.398	0.25	0.256	0.257
		2	0.284	0.259	0.259	0.09	0.079	0.125	0.166	0.159	0.155
		3	0.063	0.053	0.051	0.012	0.008	0.025	0.05	0.047	0.045
		4	0.001	0	-0.002	0	0.001	0.001	0.008	0.007	0.007
F6P	4,5,6	0	0.767	0.779	0.792	0.75	0.771	0.759	0.763	0.757	0.756
		1	0.233	0.224	0.21	0.246	0.225	0.237	0.051	0.054	0.054
		2	0.007	0.003	0.005	0.011	0.011	0.012	0.027	0.026	0.025
		3	-0.007	-0.006	-0.007	-0.007	-0.007	-0.007	0.159	0.163	0.165
	1,2,3,4	0	0.306	0.289	0.275	0.247	0.22	0.238	0.653	0.658	0.67
		1	0.658	0.687	0.693	0.705	0.723	0.715	0.144	0.143	0.133
		2	0.039	0.032	0.043	0.049	0.061	0.048	0.043	0.043	0.043
		3	0.001	-0.006	-0.01	0	0	0.001	0.077	0.058	0.055
		4	-0.004	-0.003	-0.002	-0.002	-0.004	-0.002	0.083	0.097	0.099
GSUC	1,2,3,4,5,6	0	0.207	0.194	0.191	0.158	0.145	0.153		0.618	0.614
		1	0.646	0.664	0.672	0.654	0.673	0.661		0.109	0.109
		2	0.136	0.131	0.125	0.165	0.157	0.161		0.06	0.061
		3	0.011	0.01	0.01	0.02	0.022	0.022		0.098	0.095
		4	0.001	0.001	0.002	0.002	0.002	0.002		0.02	0.021
		5	0	0	0.001	0.001	0.001	0.001		0.013	0.013
		6	0	0	0	0	0	0		0.083	0.088
STA	3,4,5,6	0	0.775	0.762	0.758		0.688	0.697		0.67	0.659
		1	0.219	0.231	0.234		0.275	0.27		0.14	0.141
		2	0.012	0.013	0.015		0.041	0.038		0.029	0.029
		3	-0.003	-0.003	-0.004		0	-0.001		0.072	0.074
		4	-0.004	-0.004	-0.004		-0.003	-0.004		0.089	0.096
STA	3,4,5,6	0	0.768	0.755	0.757		0.69	0.692		0.667	0.659
		1	0.221	0.235	0.231		0.269	0.271		0.14	0.142
		2	0.015	0.015	0.016		0.044	0.04		0.031	0.032
		3	-0.001	-0.002	-0.001		0	0		0.073	0.072
		4	-0.003	-0.003	-0.003		-0.003	-0.003		0.088	0.095
OAA	1,2,3,4	0	0.321	0.336	0.351	0.44	0.46	0.458	0.549	0.553	0.551
		1	0.433	0.434	0.435	0.434	0.439	0.441	0.237	0.23	0.234
		2	0.209	0.197	0.186	0.099	0.096	0.096	0.146	0.144	0.145
		3	0.037	0.033	0.029	0.022	0.004	0.004	0.056	0.06	0.058

		4	0.001	0.001	0	0.004	0	0	0.011	0.014	0.012
CIT	1,2,3,4,5,6	0	0.202	0.211	0.211		0.292	0.29	0.424	0.43	0.427
		1	0.371	0.379	0.39		0.438	0.438	0.228	0.222	0.225
		2	0.294	0.286	0.285		0.226	0.228	0.213	0.21	0.211
		3	0.115	0.106	0.1		0.041	0.041	0.09	0.092	0.091
		4	0.018	0.018	0.014		0.004	0.002	0.033	0.034	0.034
		5	0	0	0		0	0	0.01	0.009	0.01
		6	0	0	0		0	0	0.001	0.002	0.002
G6P	3,4,5,6	0	0.769	0.774	0.788	0.736	0.755	0.773	0.68	0.688	0.674
		1	0.238	0.23	0.213	0.257	0.239	0.218	0.125	0.116	0.129
		2	0.007	0.008	0.009	0.019	0.02	0.021	0.016	0.02	0.027
		3	0.01	0.005	0.004	0.005	0.006	0.006	0.074	0.062	0.063
		4	0.01	0.006	0.007	0.008	0.007	0.006	0.105	0.114	0.106
G6P_3									0.667	0.674	
									0.136	0.129	
ALA	1,2,3	0	0.578	0.578	0.581	0.532	0.532	0.534	0.739	0.719	0.715
		1	0.401	0.399	0.395	0.438	0.433	0.43	0.079	0.099	0.103
		2	0.02	0.023	0.023	0.03	0.035	0.035	0.044	0.055	0.058
		3	0	0.001	0.001	0.001	0	0	0.138	0.127	0.124
	2,3	0	0.594	0.596	0.603	0.552	0.554	0.556	0.782	0.773	0.773
		1	0.401	0.398	0.392	0.443	0.44	0.437	0.044	0.054	0.057
		2	0.005	0.005	0.005	0.006	0.006	0.006	0.173	0.172	0.17
GLYeff	1,2	0	0.95	0.948	0.948	0.729	0.732	0.733	0.831	0.825	0.825
		1	0.049	0.051	0.052	0.26	0.254	0.254	0.079	0.09	0.09
		2	0.001	0.001	0	0.011	0.014	0.013	0.09	0.085	0.085
	2	0	0.977	0.977	0.977	0.762	0.766	0.768	0.871	0.87	0.87
		1	0.023	0.023	0.023	0.238	0.234	0.232	0.129	0.13	0.13
VAL	1,2,3,4,5	0	0.35	0.357	0.356	0.292	0.283	0.297	0.569	0.566	0.553
		1	0.471	0.468	0.471	0.49	0.497	0.494	0.098	0.108	0.114
		2	0.167	0.167	0.161	0.202	0.207	0.201	0.17	0.175	0.173
		3	0.012	0.008	0.011	0.016	0.014	0.013	0.129	0.118	0.121
		4	0	-0.001	0.001	0	0	-0.002	0.013	0.013	0.017
		5	0	0	0	0	-0.001	-0.003	0.023	0.02	0.021
	2,3,4,5	0	0.358	0.366	0.361	0.299	0.292	0.303	0.601	0.598	0.596

		1	0.478	0.476	0.482	0.509	0.518	0.509	0.079	0.089	0.09
		2	0.158	0.153	0.151	0.191	0.185	0.184	0.275	0.268	0.269
		3	0.006	0.006	0.006	0.002	0.005	0.004	0.015	0.018	0.02
		4	0	0	0	0	0	0	0.029	0.026	0.025
GLU	2,3,4,5	0	0.295	0.289	0.291	0.468	0.444	0.451	0.545	0.533	0.529
		1	0.441	0.449	0.457	0.45	0.464	0.455	0.242	0.247	0.246
		2	0.224	0.222	0.215	0.08	0.091	0.089	0.161	0.169	0.172
		3	0.041	0.04	0.036	0.003	0.002	0.005	0.043	0.044	0.044
		4	0	0.001	0	0	-0.001	0	0.008	0.008	0.009
	2,3,4,5	0	0.291	0.281	0.28	0.465	0.439	0.447	0.546	0.531	0.528
		1	0.446	0.456	0.466	0.454	0.468	0.462	0.238	0.244	0.244
		2	0.226	0.226	0.222	0.082	0.091	0.091	0.166	0.174	0.178
		3	0.039	0.038	0.035	0.001	0.003	0.003	0.044	0.043	0.043
		4	-0.002	-0.001	-0.002	-0.002	-0.002	-0.002	0.007	0.007	0.007
METeff	1,2,3,4,5	0	0.574	0.581	0.581	0.686	0.673	0.679	0.684	0.684	0.688
		1	0.273	0.272	0.274	0.261	0.267	0.262	0.193	0.192	0.188
		2	0.118	0.115	0.114	0.049	0.056	0.054	0.08	0.079	0.078
		3	0.03	0.028	0.026	0.003	0.003	0.004	0.034	0.033	0.033
		4	0.002	0.002	0.002	0	-0.001	0	0.008	0.008	0.008
		5	0.002	0.002	0.002	0.002	0.002	0.001	0.002	0.003	0.005
	2,3,4,5	0	0.607	0.615	0.615	0.767	0.753	0.755	0.715	0.716	0.721
		1	0.273	0.271	0.274	0.208	0.216	0.216	0.197	0.195	0.193
		2	0.099	0.095	0.092	0.023	0.027	0.027	0.065	0.064	0.063
		3	0.018	0.017	0.016	0	0.001	0.001	0.019	0.02	0.02
		4	0.003	0.003	0.003	0.002	0.003	0.002	0.004	0.004	0.004
	2,3,4,5	0	0.61	0.616	0.618	0.764	0.754	0.755	0.717	0.718	0.723
		1	0.273	0.27	0.272	0.209	0.218	0.215	0.197	0.196	0.192
		2	0.099	0.095	0.093	0.026	0.028	0.029	0.065	0.065	0.064
		3	0.018	0.017	0.016	0.001	0.001	0.002	0.019	0.02	0.02
		4	0	0.001	0	0	-0.001	0	0.001	0.002	0.002
SEReff	1,2,3	0	0.723	0.728	0.732	0.675	0.673	0.676	0.733	0.728	0.726
		1	0.266	0.26	0.257	0.299	0.297	0.294	0.156	0.166	0.167
		2	0.011	0.011	0.011	0.026	0.03	0.03	0.078	0.077	0.077
		3	0	0	0	0	0	0	0.033	0.029	0.029

	2,3	0	0.742	0.747	0.753	0.701	0.705	0.705	0.768	0.765	0.765
		1	0.255	0.25	0.245	0.286	0.282	0.281	0.19	0.195	0.195
		2	0.003	0.003	0.003	0.013	0.014	0.014	0.042	0.04	0.039
	2,3	0	0.741	0.746	0.753	0.703	0.705	0.706	0.768	0.766	0.767
		1	0.255	0.25	0.243	0.282	0.28	0.279	0.19	0.194	0.193
		2	0.004	0.005	0.004	0.014	0.015	0.015	0.043	0.04	0.04
THR	1,2,3,4	0	0.322	0.329	0.345	0.461	0.457	0.467	0.538	0.549	0.557
		1	0.445	0.445	0.451	0.458	0.457	0.451	0.243	0.238	0.229
		2	0.203	0.197	0.182	0.081	0.086	0.083	0.153	0.148	0.149
		3	0.032	0.031	0.027	-0.001	0.002	0.002	0.056	0.054	0.056
		4	-0.002	-0.002	-0.005	0.001	-0.002	-0.003	0.01	0.012	0.009
	2,3,4	0	0.391	0.402	0.413	0.623	0.603	0.614	0.598	0.615	0.621
		1	0.446	0.441	0.439	0.347	0.364	0.353	0.257	0.245	0.238
		2	0.148	0.146	0.134	0.031	0.032	0.033	0.119	0.111	0.113
		3	0.015	0.011	0.013	0	0	0	0.027	0.028	0.028
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.295	0.292	0.271	0.186	0.152	0.158	0.41	0.366	0.354
		1	0.396	0.401	0.415	0.375	0.389	0.386	0.139	0.153	0.154
		2	0.24	0.238	0.244	0.303	0.315	0.312	0.137	0.152	0.156
		3	0.062	0.062	0.062	0.113	0.118	0.118	0.162	0.166	0.167
		4	0.006	0.007	0.007	0.02	0.023	0.023	0.074	0.082	0.084
		5	0.001	0.001	0.001	0.002	0.003	0.003	0.04	0.041	0.043
		6	0	0	0	0.001	0.001	0	0.024	0.025	0.026
		7	0	0	0	0	-0.001	-0.001	0.009	0.01	0.01
		8	0	0	0	0	0	0	0.003	0.003	0.003
		9	0	0	0	0	0	0	0.001	0.001	0.002
	2,3,4,5,6,7,8,9	0	0.3	0.298	0.275	0.192	0.155	0.164	0.423	0.388	0.379
		1	0.403	0.407	0.426	0.388	0.407	0.406	0.137	0.145	0.147
		2	0.234	0.234	0.236	0.3	0.311	0.307	0.202	0.217	0.218
		3	0.056	0.055	0.057	0.104	0.107	0.105	0.111	0.114	0.116
		4	0.005	0.005	0.005	0.015	0.017	0.017	0.071	0.078	0.08
		5	0	0	0	0.001	0.002	0.002	0.033	0.034	0.034
		6	0	0	0.001	0	0	0	0.017	0.019	0.02
		7	0	0	0	-0.001	0	0	0.004	0.004	0.003
		8	0	0	0	0	0	0	0.002	0.002	0.003

					0.278	0.191			0.425	0.387	0.38
					0.418	0.387			0.134	0.144	0.144
					0.239	0.3			0.204	0.217	0.221
					0.058	0.104			0.112	0.116	0.116
					0.006	0.017			0.07	0.077	0.08
					0.001	0.001			0.033	0.034	0.034
					0	0			0.017	0.019	0.019
					0	0			0.003	0.004	0.004
					0	0			0.002	0.002	0.002
	1,2	0	0.961	0.957	0.954	0.586	0.576	0.58	0.771	0.747	0.739
		1	0.04	0.043	0.049	0.397	0.404	0.4	0.091	0.117	0.123
		2	-0.002	0	-0.002	0.017	0.02	0.021	0.137	0.137	0.138
ASP	1,2,3,4	0	0.3	0.301	0.312	0.467	0.462	0.464	0.544	0.542	0.544
		1	0.442	0.448	0.449	0.453	0.452	0.45	0.242	0.244	0.243
		2	0.217	0.212	0.205	0.077	0.083	0.082	0.149	0.15	0.148
		3	0.041	0.039	0.035	0.003	0.004	0.004	0.056	0.054	0.055
		4	0.001	0	0	0	0	0	0.01	0.009	0.01
	2,3,4	0	0.367	0.369	0.378	0.629	0.617	0.618	0.606	0.605	0.609
		1	0.449	0.451	0.451	0.341	0.348	0.348	0.254	0.255	0.252
		2	0.165	0.162	0.155	0.03	0.034	0.033	0.115	0.114	0.112
		3	0.019	0.018	0.016	0	0	0.001	0.025	0.025	0.027
	2,3,4	0	0.386	0.387	0.398	0.637	0.624	0.626	0.615	0.615	0.617
		1	0.432	0.434	0.433	0.325	0.334	0.332	0.243	0.242	0.241
		2	0.158	0.154	0.147	0.03	0.034	0.034	0.11	0.111	0.11
		3	0.024	0.024	0.022	0.008	0.008	0.008	0.031	0.032	0.032
GLU	1,2,3,4,5	0	0.226	0.229	0.236	0.356	0.353	0.355	0.48	0.478	0.48
		1	0.418	0.42	0.429	0.469	0.47	0.466	0.225	0.229	0.228
		2	0.269	0.267	0.258	0.16	0.161	0.163	0.204	0.204	0.203
		3	0.078	0.076	0.069	0.015	0.016	0.016	0.067	0.066	0.067
		4	0.009	0.008	0.007	0	0.001	0	0.02	0.019	0.019
		5	0	0	0	0	0	0	0.004	0.004	0.004
	2,3,4,5	0	0.276	0.279	0.286	0.466	0.464	0.462	0.536	0.533	0.535
		1	0.443	0.445	0.45	0.452	0.451	0.451	0.247	0.248	0.246
		2	0.234	0.234	0.225	0.079	0.082	0.085	0.161	0.164	0.168

		3	0.046	0.043	0.039	0.002	0.003	0.003	0.049	0.045	0.046
		4	0.001	-0.001	-0.001	0	-0.001	-0.001	0.007	0.009	0.006
	2,3,4,5	0	0.274	0.277	0.287	0.466	0.461	0.464	0.537	0.534	0.536
		1	0.443	0.447	0.451	0.453	0.451	0.448	0.244	0.246	0.244
		2	0.237	0.233	0.223	0.078	0.085	0.084	0.165	0.167	0.168
		3	0.046	0.043	0.039	0.003	0.003	0.004	0.047	0.045	0.044
		4	0.001	0	0	0	0	0	0.008	0.008	0.008
LYS	1,2,3,4,5,6	0	0.213	0.23		0.299	0.288	0.306	0.413	0.436	0.452
		1	0.409	0.41		0.474	0.476	0.467	0.224	0.219	0.215
		2	0.276	0.27		0.208	0.212	0.199	0.19	0.186	0.18
		3	0.093	0.084		0.025	0.028	0.03	0.121	0.114	0.107
		4	0.011	0.009		0.001	0.005	-0.001	0.038	0.034	0.038
		5	-0.002	0.008		-0.003	-0.005	-0.002	0.013	0.011	0.006
		6	0	-0.011		-0.003	-0.004	0.002	0	-0.001	0.002
HISeff	1,2,3,4,5,6	0	0.649	0.654	0.651	0.603	0.587	0.595	0.725	0.725	0.723
		1	0.231	0.227	0.232	0.264	0.267	0.263	0.123	0.126	0.128
		2	0.1	0.1	0.098	0.12	0.126	0.121	0.068	0.068	0.067
		3	0.021	0.018	0.017	0.014	0.02	0.019	0.056	0.052	0.054
		4	0	0.001	0.001	0.001	0	0	0.015	0.016	0.016
		5	0	0	0	0	0	0.001	0.011	0.011	0.011
		6	0	0	0	-0.002	0.001	0	0.002	0.002	0.002
	2,3,4,5,6	0	0.713	0.714	0.714	0.607	0.595	0.602	0.724	0.723	0.724
		1	0.219	0.219	0.223	0.259	0.267	0.264	0.127	0.133	0.131
		2	0.054	0.054	0.049	0.11	0.115	0.107	0.098	0.095	0.096
		3	0.011	0.01	0.011	0.019	0.019	0.022	0.034	0.032	0.033
		4	0.002	0.002	0.003	0.004	0.003	0.003	0.014	0.014	0.013
		5	0.001	0.001	0.001	0.001	0.001	0.001	0.003	0.003	0.003
	1,2	0	0.833	0.832	0.834	0.806	0.806	0.809	0.888	0.884	0.887
		1	0.167	0.167	0.165	0.194	0.19	0.189	0.031	0.037	0.038
		2	0	0.001	0.001	0	0.004	0.003	0.081	0.079	0.075
PHE_TYR	2,3,4,5,6,7,8,9	0	0.252	0.273	0.28				0.371	0.39	0.392
		1	0.432	0.429	0.433				0.139	0.141	0.139
		2	0.262	0.256	0.249				0.232	0.228	0.225
		3	0.063	0.061	0.057				0.127	0.117	0.118

		4	0.005	0.004	0.003				0.079	0.079	0.078
		5	-0.002	-0.003	-0.003				0.034	0.032	0.033
		6	-0.004	-0.008	-0.005				0.017	0.015	0.017
		7	-0.004	-0.005	-0.007				0	0.001	0.001
		8	-0.005	-0.006	-0.007				-0.001	-0.003	-0.002
ARGeff	1,2,3,4,5,6	0	0.616	0.624	0.622	0.66	0.651	0.662	0.694	0.701	0.709
		1	0.222	0.219	0.227	0.238	0.244	0.24	0.156	0.158	0.155
		2	0.116	0.115	0.115	0.091	0.09	0.087	0.101	0.09	0.09
		3	0.04	0.039	0.034	0.013	0.019	0.018	0.037	0.039	0.037
		4	0.009	0.006	0.006	0.002	0.004	0.002	0.014	0.015	0.013
		5	0	0.001	-0.002	-0.002	-0.01	-0.009	0.003	0.003	0.001
		6	-0.004	-0.004	-0.003	-0.001	0.001	0.001	-0.005	-0.005	-0.005
	2,3,4,5,6	0	0.627	0.64	0.64	0.684	0.676	0.688	0.698	0.707	0.708
		1	0.213	0.214	0.218	0.23	0.229	0.229	0.162	0.158	0.157
		2	0.112	0.105	0.101	0.064	0.065	0.064	0.088	0.084	0.085
		3	0.036	0.031	0.031	0.012	0.017	0.01	0.034	0.035	0.031
		4	0.006	0.005	0.005	0.005	0.005	0.004	0.01	0.009	0.012
		5	0.006	0.004	0.005	0.006	0.007	0.005	0.007	0.006	0.006
Mass isotopomer datasets of MS											
Metabolite name used in the model	**Carbon Atoms**	**Mass (m+)**	**[1-^{13}C]glucose**			**[2-^{13}C]glucose**			**[$^{13}C_6$]glucose**		
			Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3
ALA	1,2,3	0	0.593	0.59	0.588	0.539	0.541	0.538	0.744	0.751	0.743
		1	0.387	0.391	0.391	0.429	0.428	0.431	0.072	0.068	0.07
		2	0.02	0.018	0.019	0.031	0.031	0.031	0.036	0.034	0.034
		3	0.001	0.001	0.001	0	0	0	0.149	0.147	0.153
	2,3	0	0.61	0.606	0.606	0.565	0.568	0.565	0.776	0.783	0.776
		1	0.382	0.386	0.386	0.431	0.428	0.43	0.052	0.047	0.051
		2	0.008	0.008	0.008	0.004	0.004	0.004	0.172	0.169	0.174
GLY	1,2	0	0.943	0.942	0.946	0.627	0.627	0.63	0.766	0.773	0.767

		1	0.055	0.059	0.055	0.358	0.358	0.354	0.103	0.099	0.103
		2	0.002	-0.001	-0.001	0.015	0.016	0.016	0.131	0.128	0.13
	2	0	0.981	0.98	0.979	0.678	0.677	0.684	0.817	0.817	0.818
		1	0.019	0.02	0.021	0.322	0.323	0.316	0.183	0.183	0.182
SER	1,2,3	0	0.667	0.655	0.66	0.552	0.556	0.553	0.664	0.669	0.662
		1	0.324	0.331	0.328	0.4	0.396	0.398	0.176	0.171	0.178
		2	0.01	0.014	0.013	0.047	0.048	0.048	0.098	0.095	0.098
		3	-0.001	-0.001	-0.001	0.001	0.001	0.001	0.062	0.065	0.062
	2,3	0	0.693	0.679	0.681	0.593	0.593	0.59	0.701	0.706	0.701
		1	0.304	0.319	0.317	0.382	0.382	0.386	0.225	0.216	0.225
		2	0.003	0.002	0.002	0.025	0.025	0.023	0.075	0.079	0.074
	2,3	0	0.689	0.679	0.68	0.592	0.595	0.592	0.702	0.708	0.702
		1	0.308	0.318	0.316	0.382	0.379	0.383	0.224	0.214	0.224
		2	0.003	0.003	0.004	0.026	0.025	0.025	0.073	0.078	0.074
GABA	1,2,3,4	0	0.299	0.29	0.3	0.429	0.419	0.435	0.521	0.535	0.536
		1	0.443	0.452	0.442	0.447	0.454	0.456	0.245	0.232	0.233
		2	0.224	0.222	0.219	0.115	0.115	0.107	0.173	0.178	0.174
		3	0.038	0.033	0.039	0.008	0.012	0.004	0.05	0.044	0.048
		4	-0.004	0.002	-0.001	0	0.001	-0.001	0.01	0.011	0.009
	1,2,3,4	0	0.305	0.297	0.305	0.435	0.43	0.436	0.535	0.534	0.537
		1	0.44	0.443	0.437	0.449	0.449	0.448	0.234	0.233	0.233
		2	0.216	0.222	0.22	0.109	0.113	0.111	0.174	0.178	0.174
		3	0.037	0.037	0.038	0.006	0.008	0.006	0.047	0.045	0.046
		4	0.001	0	0	0	0	0	0.01	0.011	0.01
F6P	4,5,6	0	0.83	0.813	0.812	0.785	0.788	0.788	0.78	0.775	0.776
		1	0.179	0.194	0.196	0.215	0.212	0.211	0.036	0.036	0.035
		2	-0.002	0	-0.001	0.007	0.007	0.008	0.011	0.011	0.011
		3	-0.007	-0.007	-0.006	-0.008	-0.007	-0.007	0.173	0.178	0.178
	1,2,3,4	0	0.273	0.258	0.258	0.207	0.202	0.198	0.689	0.701	0.701
		1	0.703	0.719	0.714	0.755	0.755	0.766	0.119	0.105	0.109
		2	0.027	0.027	0.032	0.044	0.045	0.041	0.019	0.019	0.02
		3	0	-0.003	-0.002	-0.003	0.001	-0.001	0.058	0.061	0.056
		4	-0.003	-0.001	-0.001	-0.004	-0.003	-0.004	0.115	0.115	0.113
F6P	4,5,6	0	0.832	0.817	0.813	0.786	0.788	0.787	0.776	0.776	0.776

		1	0.181	0.194	0.195	0.215	0.213	0.214	0.037	0.037	0.038
		2	-0.004	-0.004	0	0.009	0.007	0.007	0.013	0.01	0.01
		3	-0.009	-0.008	-0.008	-0.009	-0.008	-0.008	0.174	0.178	0.177
SUCC	1,2,3,4	0	0.324	0.318	0.315	0.439	0.439	0.437	0.54	0.545	0.537
		1	0.429	0.439	0.434	0.448	0.448	0.451	0.233	0.227	0.233
		2	0.209	0.209	0.213	0.107	0.108	0.108	0.171	0.173	0.174
		3	0.036	0.034	0.037	0.005	0.005	0.005	0.045	0.044	0.046
		4	0.001	0	0.001	0	0	0	0.01	0.011	0.01
OAA	1,2,3,4	0	0.355	0.356	0.345	0.447	0.447	0.446	0.543	0.554	0.54
		1	0.434	0.433	0.435	0.443	0.442	0.443	0.237	0.228	0.238
		2	0.182	0.182	0.19	0.105	0.106	0.105	0.148	0.145	0.149
		3	0.029	0.027	0.03	0.005	0.005	0.005	0.058	0.06	0.06
		4	0	0.002	0.001	0	0	0	0.013	0.014	0.014
CIT	1,2,3,4,5,6	0	0.224	0.225	0.215	0.268	0.268	0.265	0.413	0.424	0.405
		1	0.399	0.399	0.396	0.438	0.437	0.439	0.23	0.227	0.229
		2	0.275	0.274	0.279	0.242	0.241	0.244	0.215	0.212	0.216
		3	0.089	0.088	0.096	0.049	0.052	0.049	0.095	0.092	0.099
		4	0.013	0.013	0.012	0.004	0.003	0.003	0.036	0.035	0.038
		5	-0.001	0.001	0	0	0	-0.001	0.01	0.008	0.01
		6	0	0	0	0	0	0	0.002	0.002	0.002
G6P	3,4,5,6	0	0.838	0.834	0.828	0.786	0.789	0.787	0.72	0.715	0.01
		1	0.172	0.172	0.177	0.201	0.198	0.202	0.092	0.091	0.01
		2	0	0.003	0.003	0.019	0.02	0.018	0.009	0.007	0.01
		3	-0.005	-0.004	-0.004	-0.002	-0.002	-0.003	0.053	0.053	0.01
		4	-0.006	-0.004	-0.004	-0.004	-0.004	-0.004	0.127	0.134	0.01
ALA	1,2,3	0	0.609	0.605	0.602	0.545	0.539	0.537	0.748	0.74	0.744
		1	0.373	0.377	0.38	0.418	0.422	0.425	0.069	0.071	0.071
		2	0.017	0.017	0.017	0.037	0.038	0.038	0.035	0.035	0.035
		3	0.001	0.001	0.001	0	0.001	0.001	0.148	0.153	0.15
	2,3	0	0.626	0.621	0.619	0.572	0.567	0.566	0.779	0.773	0.776
		1	0.366	0.371	0.373	0.424	0.428	0.429	0.051	0.051	0.052
		2	0.008	0.008	0.008	0.005	0.005	0.005	0.17	0.175	0.172
GLYeff	1,2	0	0.952	0.947	0.95	0.679	0.677	0.676	0.791	0.789	0.79
		1	0.047	0.053	0.05	0.306	0.308	0.308	0.098	0.095	0.096

		2	0	0	0	0.015	0.015	0.016	0.111	0.116	0.113
	2	0	0.985	0.985	0.985	0.73	0.729	0.727	0.841	0.838	0.84
		1	0.015	0.015	0.015	0.27	0.271	0.273	0.159	0.162	0.16
VAL	1,2,3,4,5	0	0.377	0.363	0.367	0.313	0.302	0.294	0.576	0.555	0.572
		1	0.46	0.472	0.464	0.478	0.486	0.487	0.105	0.112	0.105
		2	0.151	0.154	0.156	0.19	0.194	0.2	0.159	0.164	0.16
		3	0.012	0.012	0.013	0.019	0.017	0.019	0.126	0.132	0.128
		4	0.001	0	0	0	0	0	0.013	0.014	0.014
		5	-0.001	-0.001	0	0	0	0	0.021	0.022	0.022
	2,3,4,5	0	0.392	0.38	0.383	0.34	0.33	0.324	0.604	0.584	0.596
		1	0.46	0.469	0.464	0.487	0.493	0.498	0.096	0.103	0.099
		2	0.14	0.144	0.144	0.169	0.172	0.173	0.254	0.265	0.259
		3	0.008	0.008	0.009	0.005	0.005	0.004	0.02	0.022	0.02
		4	0	0	0	0	0	0	0.025	0.026	0.026
	2,3,4,5	0	0.408	0.396	0.4	0.362	0.349	0.343	0.612	0.594	0.606
		1	0.433	0.444	0.438	0.458	0.467	0.469	0.089	0.094	0.089
		2	0.137	0.14	0.141	0.162	0.165	0.169	0.245	0.256	0.25
		3	0.019	0.019	0.02	0.017	0.017	0.017	0.03	0.03	0.03
		4	0.001	0.001	0.002	0.002	0.002	0.002	0.025	0.026	0.026
LEU	2,3,4,5,6	0	0.272	0.253	0.259	0.319	0.305	0.297	0.494	0.469	0.485
		1	0.437	0.446	0.44	0.46	0.469	0.473	0.183	0.191	0.186
		2	0.236	0.243	0.242	0.196	0.199	0.203	0.231	0.242	0.235
		3	0.051	0.053	0.054	0.023	0.024	0.024	0.062	0.065	0.063
		4	0.004	0.004	0.004	0.002	0.002	0.003	0.026	0.027	0.026
		5	0	0	0	0	0	0	0.005	0.005	0.005
ILE	2,3,4,5,6	0	0.288	0.264	0.275	0.319	0.304	0.295	0.485	0.461	0.478
		1	0.451	0.46	0.455	0.474	0.483	0.487	0.206	0.214	0.207
		2	0.209	0.219	0.216	0.179	0.185	0.19	0.213	0.223	0.216
		3	0.044	0.047	0.047	0.023	0.023	0.024	0.068	0.073	0.069
		4	0.004	0.005	0.005	0.001	0.001	0.001	0.02	0.021	0.02
		5	0.004	0.004	0.003	0.003	0.003	0.003	0.009	0.009	0.009
GLU	2,3,4,5	0	0.334	0.322	0.323	0.427	0.412	0.407	0.538	0.522	0.535
		1	0.457	0.465	0.461	0.457	0.466	0.471	0.229	0.232	0.228
		2	0.183	0.188	0.189	0.112	0.117	0.118	0.181	0.192	0.184

		3	0.025	0.025	0.026	0.005	0.005	0.005	0.041	0.043	0.042
		4	0.001	0	0	-0.001	0	-0.001	0.01	0.011	0.011
	2,3,4,5	0	0.33	0.318	0.319	0.424	0.41	0.403	0.54	0.522	0.535
		1	0.463	0.469	0.466	0.461	0.472	0.476	0.224	0.23	0.226
		2	0.185	0.188	0.19	0.112	0.116	0.118	0.184	0.194	0.187
		3	0.024	0.025	0.025	0.004	0.004	0.004	0.041	0.043	0.042
		4	-0.001	-0.001	-0.001	-0.001	-0.002	-0.002	0.01	0.011	0.01
METeff	1,2,3,4,5	0	0.426	0.411	0.416	0.522	0.51	0.506	0.559	0.546	0.557
		1	0.362	0.368	0.368	0.362	0.369	0.371	0.243	0.247	0.244
		2	0.169	0.175	0.172	0.105	0.11	0.111	0.119	0.125	0.12
		3	0.038	0.041	0.04	0.011	0.011	0.011	0.058	0.061	0.059
		4	0.003	0.004	0.003	0	0	0.001	0.018	0.019	0.018
		5	0.001	0.001	0.001	0.001	0	0.001	0.003	0.003	0.003
	2,3,4,5	0	0.462	0.448	0.454	0.61	0.602	0.596	0.598	0.589	0.596
		1	0.368	0.371	0.371	0.324	0.33	0.333	0.254	0.257	0.255
		2	0.143	0.149	0.147	0.061	0.062	0.064	0.101	0.104	0.103
		3	0.023	0.027	0.025	0.002	0.002	0.003	0.039	0.04	0.037
		4	0.004	0.004	0.004	0.003	0.003	0.004	0.008	0.009	0.009
	2,3,4,5	0	0.469	0.453	0.459	0.612	0.605	0.599	0.601	0.592	0.599
		1	0.367	0.373	0.369	0.323	0.329	0.332	0.255	0.258	0.255
		2	0.14	0.147	0.146	0.061	0.062	0.064	0.103	0.107	0.105
		3	0.024	0.026	0.026	0.004	0.004	0.004	0.037	0.039	0.037
		4	0	0.001	0.001	0	0	0	0.004	0.005	0.004
SEReff	1,2,3	0	0.716	0.71	0.711	0.612	0.608	0.607	0.703	0.703	0.703
		1	0.276	0.281	0.28	0.345	0.348	0.35	0.157	0.151	0.156
		2	0.009	0.01	0.009	0.043	0.043	0.043	0.082	0.081	0.082
		3	-0.001	-0.001	0	0.001	0.001	0.001	0.058	0.065	0.059
	2,3	0	0.739	0.733	0.731	0.649	0.646	0.645	0.74	0.738	0.739
		1	0.261	0.267	0.268	0.331	0.334	0.336	0.191	0.186	0.19
		2	0	0	0.001	0.02	0.02	0.019	0.069	0.076	0.071
	2,3	0	0.736	0.731	0.731	0.649	0.646	0.644	0.742	0.741	0.739
		1	0.261	0.268	0.267	0.33	0.332	0.335	0.19	0.184	0.19
		2	0.002	0.002	0.002	0.021	0.021	0.021	0.068	0.076	0.071
THR	1,2,3,4	0	0.382	0.375	0.379	0.441	0.426	0.429	0.551	0.539	0.553

		1	0.449	0.456	0.451	0.451	0.462	0.464	0.228	0.231	0.222
		2	0.153	0.154	0.157	0.104	0.106	0.107	0.148	0.148	0.146
		3	0.015	0.018	0.017	0.005	0.006	0.003	0.059	0.066	0.065
		4	0	-0.003	-0.004	-0.001	0	-0.003	0.014	0.015	0.014
	2,3,4	0	0.448	0.432	0.437	0.564	0.556	0.556	0.614	0.602	0.613
		1	0.439	0.444	0.439	0.389	0.395	0.397	0.237	0.239	0.235
		2	0.105	0.115	0.116	0.049	0.048	0.048	0.114	0.121	0.116
		3	0.007	0.009	0.008	-0.002	0	-0.002	0.035	0.038	0.035
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.318	0.303	0.305	0.207	0.192	0.182	0.377	0.384	0.383
		1	0.43	0.437	0.434	0.381	0.39	0.391	0.141	0.139	0.141
		2	0.207	0.214	0.213	0.283	0.286	0.293	0.135	0.135	0.134
		3	0.041	0.042	0.043	0.104	0.107	0.108	0.18	0.175	0.177
		4	0.003	0.003	0.003	0.022	0.022	0.022	0.08	0.082	0.081
		5	0	0	0	0.003	0.003	0.003	0.043	0.042	0.043
		6	0.001	0	0	0	0	0	0.028	0.027	0.027
		7	0	0	0	0	0	0	0.01	0.01	0.011
		8	0	0	0	0	0	0	0.004	0.003	0.003
		9	0	0	0	0	0	0	0.002	0.002	0.002
	2,3,4,5,6,7,8,9	0	0.325	0.311	0.312	0.216	0.202	0.193	0.394	0.399	0.399
		1	0.431	0.438	0.436	0.396	0.403	0.405	0.136	0.133	0.136
		2	0.204	0.208	0.21	0.278	0.285	0.289	0.214	0.214	0.21
		3	0.038	0.04	0.04	0.093	0.093	0.096	0.117	0.113	0.115
		4	0.002	0.003	0.003	0.016	0.016	0.017	0.077	0.079	0.078
		5	0	0	0	0.001	0.001	0.001	0.036	0.035	0.036
		6	0	0	0	0	0	0	0.02	0.021	0.02
		7	0	0	0	0	0	-0.001	0.004	0.004	0.004
		8	0	0	0	0	0	0	0.002	0.002	0.002
	2,3,4,5,6,7,8,9	0	0.325	0.312	0.313	0.218	0.204	0.196	0.396	0.401	0.397
		1	0.428	0.434	0.433	0.392	0.4	0.402	0.136	0.133	0.135
		2	0.204	0.209	0.21	0.278	0.283	0.287	0.212	0.212	0.211
		3	0.039	0.041	0.041	0.094	0.094	0.096	0.117	0.112	0.117
		4	0.003	0.003	0.003	0.017	0.017	0.017	0.077	0.08	0.078
		5	0	0	0	0.002	0.002	0.002	0.036	0.035	0.036
		6	0	0	0	0	0	0	0.02	0.021	0.02

		7	0	0	0	0	0	0	0.004	0.004	0.004
		8	0	0	0	0	0	0	0.002	0.002	0.002
	1,2	0	0.969	0.968	0.968	0.611	0.604	0.598	0.763	0.769	0.772
		1	0.032	0.034	0.032	0.378	0.385	0.391	0.075	0.072	0.07
		2	-0.001	-0.002	0	0.011	0.012	0.011	0.162	0.159	0.158
ASP	1,2,3,4	0	0.384	0.374	0.37	0.444	0.437	0.432	0.55	0.541	0.552
		1	0.438	0.443	0.443	0.445	0.451	0.452	0.227	0.227	0.226
		2	0.157	0.16	0.165	0.105	0.106	0.109	0.145	0.148	0.144
		3	0.021	0.022	0.022	0.006	0.005	0.006	0.063	0.068	0.064
		4	0	0.001	0	0	0	0	0.014	0.016	0.014
	2,3,4	0	0.447	0.438	0.438	0.572	0.566	0.563	0.613	0.604	0.612
		1	0.431	0.436	0.435	0.38	0.385	0.388	0.237	0.237	0.237
		2	0.113	0.117	0.117	0.047	0.048	0.049	0.116	0.12	0.117
		3	0.008	0.009	0.009	0	0.001	0.001	0.034	0.039	0.034
	2,3,4	0	0.463	0.455	0.452	0.582	0.576	0.572	0.62	0.612	0.62
		1	0.412	0.416	0.418	0.364	0.37	0.373	0.228	0.229	0.227
		2	0.11	0.113	0.115	0.047	0.047	0.048	0.113	0.117	0.114
		3	0.015	0.015	0.016	0.007	0.007	0.007	0.039	0.042	0.04
	1,2	0	0.634	0.63	0.626	0.665	0.661	0.658	0.732	0.718	0.73
		1	0.332	0.335	0.337	0.325	0.329	0.331	0.156	0.164	0.157
		2	0.034	0.035	0.037	0.01	0.01	0.011	0.112	0.118	0.113
GLU	1,2,3,4,5	0	0.285	0.272	0.275	0.332	0.325	0.321	0.481	0.469	0.479
		1	0.435	0.441	0.437	0.462	0.467	0.467	0.216	0.217	0.216
		2	0.225	0.231	0.23	0.183	0.185	0.188	0.207	0.213	0.207
		3	0.051	0.052	0.053	0.022	0.023	0.023	0.071	0.074	0.072
		4	0.004	0.004	0.005	0.001	0	0.001	0.02	0.021	0.021
		5	0	0	0	0	0	0	0.005	0.006	0.006
	2,3,4,5	0	0.336	0.325	0.324	0.431	0.423	0.419	0.539	0.529	0.536
		1	0.444	0.453	0.45	0.452	0.459	0.46	0.228	0.229	0.227
		2	0.192	0.195	0.197	0.113	0.113	0.115	0.179	0.187	0.182
		3	0.028	0.028	0.03	0.004	0.005	0.006	0.043	0.044	0.044
		4	0	0	0	0.001	0	0	0.011	0.012	0.011
	2,3,4,5	0	0.334	0.326	0.323	0.43	0.422	0.419	0.54	0.529	0.536
		1	0.447	0.452	0.451	0.453	0.458	0.461	0.227	0.228	0.228

		2	0.191	0.192	0.196	0.112	0.114	0.114	0.178	0.187	0.182
		3	0.028	0.029	0.03	0.006	0.006	0.006	0.044	0.044	0.044
		4	0.001	0.001	0.001	0	0	0	0.011	0.012	0.011
LYS	1,2,3,4,5,6	0	0.252	0.23	0.238	0.27	0.257	0.245	0.443	0.41	0.435
		1	0.436	0.452	0.444	0.457	0.468	0.472	0.211	0.223	0.214
		2	0.238	0.247	0.247	0.226	0.235	0.237	0.172	0.185	0.181
		3	0.063	0.062	0.062	0.043	0.043	0.043	0.119	0.122	0.115
		4	0.006	0.009	0.008	0.003	0.001	0.003	0.038	0.039	0.039
		5	0.008	0	0.001	0.001	0	0.001	0.014	0.014	0.014
		6	-0.002	0	0	-0.001	-0.004	0	0.003	0.006	0.003
HISeff	1,2,3,4,5,6	0	0.56	0.553	0.556	0.355	0.343	0.333	0.591	0.583	0.591
		1	0.324	0.332	0.328	0.409	0.418	0.421	0.169	0.172	0.171
		2	0.1	0.1	0.102	0.196	0.199	0.205	0.093	0.092	0.092
		3	0.015	0.013	0.014	0.037	0.037	0.037	0.087	0.087	0.086
		4	0.002	0.001	0	0.003	0.003	0.004	0.027	0.028	0.028
		5	-0.001	0	0	-0.001	0	0	0.028	0.032	0.028
		6	0	0	0	0	0	0	0.005	0.006	0.005
	2,3,4,5,6	0	0.664	0.667	0.664	0.368	0.351	0.345	0.596	0.58	0.59
		1	0.275	0.274	0.279	0.417	0.428	0.427	0.171	0.181	0.175
		2	0.047	0.044	0.046	0.18	0.185	0.192	0.145	0.15	0.146
		3	0.01	0.011	0.008	0.03	0.03	0.03	0.05	0.048	0.05
		4	0.002	0.002	0.003	0.004	0.004	0.004	0.031	0.033	0.032
		5	0.001	0.001	0.001	0.001	0.002	0.002	0.008	0.008	0.007
	1,2	0	0.792	0.788	0.788	0.737	0.737	0.735	0.837	0.828	0.829
		1	0.207	0.213	0.21	0.261	0.262	0.265	0.039	0.04	0.044
		2	0.001	-0.001	0.002	0.002	0	0	0.124	0.132	0.127
PHE_TYR	2,3,4,5,6,7,8,9	0	0.303	0.285	0.289	0.188	0.175	0.166	0.394	0.383	0.392
		1	0.446	0.458	0.454	0.411	0.419	0.419	0.134	0.133	0.134
		2	0.216	0.226	0.221	0.295	0.3	0.302	0.219	0.225	0.219
		3	0.042	0.044	0.044	0.1	0.1	0.102	0.117	0.118	0.116
		4	0.003	0.001	0.002	0.016	0.017	0.018	0.079	0.084	0.081
		5	-0.001	-0.002	-0.002	0	0	0	0.035	0.035	0.036
		6	-0.002	-0.003	-0.002	-0.002	-0.002	-0.001	0.02	0.021	0.02
		7	-0.002	-0.004	-0.004	-0.004	-0.004	-0.002	0.002	0.002	0.002

		8	-0.003	-0.004	-0.003	-0.004	-0.004	-0.003	0	0	0
ARGeff	1,2,3,4,5,6	0	0.401	0.39	0.397	0.431	0.418	0.413	0.516	0.502	0.513
		1	0.348	0.349	0.344	0.367	0.372	0.368	0.223	0.225	0.221
		2	0.187	0.194	0.196	0.161	0.171	0.178	0.154	0.164	0.162
		3	0.054	0.056	0.051	0.034	0.035	0.036	0.074	0.076	0.071
		4	0.007	0.008	0.009	0.004	0.002	0.003	0.024	0.023	0.022
		5	0.002	0.002	0.003	0.002	0.002	0.001	0.008	0.008	0.009
		6	0	0	-0.001	0	0	0	0.001	0.001	0.001
	2,3,4,5,6	0	0.427	0.415	0.418	0.485	0.473	0.47	0.555	0.529	0.54
		1	0.349	0.361	0.357	0.361	0.368	0.365	0.227	0.24	0.231
		2	0.169	0.175	0.171	0.123	0.128	0.129	0.144	0.151	0.151
		3	0.04	0.038	0.04	0.019	0.018	0.024	0.054	0.057	0.053
		4	0.008	0.005	0.007	0.005	0.005	0.004	0.013	0.015	0.018
		5	0.007	0.006	0.007	0.007	0.007	0.007	0.007	0.007	0.007
Mass isotopomer datasets of Pi+											
Metabolite name used in the model	**Carbon Atoms**	**Mass (m+)**	**[1-^{13}C]glucose**			**[2-^{13}C]glucose**			**[$^{13}C_6$]glucose**		
			Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3	Replica 1	Replica 2	Replica 3
ALA	1,2,3	0	0.628	0.624	0.624	0.557	0.548	0.563	0.737	0.737	0.734
		1	0.356	0.359	0.357	0.401	0.407	0.391	0.084	0.081	0.084
		2	0.015	0.018	0.018	0.041	0.044	0.045	0.04	0.038	0.041
		3	0	0	0.001	0.001	0.002	0.001	0.14	0.144	0.142
	2,3	0	0.646	0.645	0.646	0.585	0.578	0.6	0.774	0.774	0.771
		1	0.347	0.349	0.348	0.408	0.412	0.394	0.064	0.061	0.065
		2	0.006	0.006	0.007	0.007	0.01	0.007	0.162	0.166	0.164
GLY	1,2	0	0.912	0.909	0.913	0.634	0.627	0.65	0.745	0.738	0.744
		1	0.088	0.089	0.084	0.343	0.348	0.328	0.139	0.148	0.137
		2	-0.001	0.002	0.003	0.023	0.025	0.022	0.117	0.114	0.119
	2	0	0.976	0.976	0.976	0.697	0.699	0.717	0.81	0.815	0.814
		1	0.024	0.024	0.024	0.303	0.301	0.283	0.19	0.185	0.186
SER	1,2,3	0	0.685	0.678	0.678	0.571	0.569	0.581	0.667	0.663	0.669

		1	0.302	0.307	0.308	0.376	0.375	0.367	0.174	0.181	0.171
		2	0.014	0.016	0.014	0.051	0.053	0.053	0.084	0.087	0.085
		3	-0.001	-0.001	0	0.001	0.002	-0.001	0.075	0.07	0.074
	2,3	0	0.718	0.707	0.712	0.616	0.619	0.62	0.713	0.709	0.715
		1	0.281	0.29	0.288	0.364	0.358	0.358	0.195	0.203	0.194
		2	0.001	0.003	0.001	0.021	0.023	0.022	0.092	0.088	0.091
	2,3	0	0.716	0.709	0.711	0.618	0.621	0.623	0.715	0.713	0.715
		1	0.281	0.288	0.285	0.359	0.357	0.353	0.194	0.199	0.193
		2	0.003	0.003	0.003	0.023	0.022	0.024	0.091	0.088	0.092
GABA	1,2,3,4	0	0.362	0.353	0.356	0.415	0.429	0.428	0.533	0.538	0.544
		1	0.438	0.445	0.435	0.405	0.45	0.438	0.232	0.235	0.228
		2	0.178	0.182	0.187	0.146	0.122	0.126	0.183	0.176	0.171
		3	0.022	0.02	0.022	0.03	0.002	0.01	0.043	0.04	0.044
		4	0	-0.001	0	0.005	-0.003	-0.002	0.009	0.01	0.012
	1,2,3,4	0	0.36	0.356	0.353	0.436	0.434	0.433	0.535	0.537	0.541
		1	0.438	0.441	0.443	0.444	0.443	0.434	0.234	0.233	0.225
		2	0.178	0.179	0.18	0.115	0.118	0.123	0.177	0.176	0.181
		3	0.024	0.023	0.024	0.006	0.007	0.01	0.043	0.044	0.041
		4	0	0	0	-0.001	-0.001	0	0.011	0.01	0.012
F6P	4,5,6	0	0.886	0.869	0.865	0.856	0.874	0.838	0.777	0.777	0.778
		1	0.126	0.142	0.144	0.147	0.129	0.161	0.036	0.036	0.035
		2	-0.005	-0.003	-0.002	0.006	0.005	0.009	0.01	0.01	0.01
		3	-0.007	-0.007	-0.007	-0.009	-0.008	-0.008	0.177	0.177	0.177
F6P	4,5,6	0	0.89	0.871	0.866	0.855	0.877	0.84	0.775	0.778	0.781
		1	0.124	0.14	0.144	0.148	0.128	0.161	0.036	0.035	0.034
		2	-0.005	-0.003	-0.002	0.005	0.004	0.007	0.01	0.009	0.008
		3	-0.009	-0.008	-0.008	-0.008	-0.009	-0.008	0.179	0.177	0.177
GSUC	1,2,3,4,5,6	0	0.19	0.203	0.191	0.129	0.138	0.121	0.669	0.663	0.671
		1	0.711	0.703	0.715	0.726	0.727	0.738	0.082	0.085	0.081
		2	0.094	0.088	0.089	0.122	0.13	0.12	0.033	0.036	0.032
		3	0.005	0.005	0.004	0.02	0.016	0.019	0.074	0.078	0.076
		4	0	0.001	0.001	0.002	-0.006	0.002	0.016	0.017	0.015
		5	0	0.001	0.001	0.001	-0.005	0.001	0.012	0.012	0.012
		6	0	0	0	0	0	0	0.113	0.109	0.114

STA	3,4,5,6	0	0.829	0.808	0.806	0.754	0.773	0.727	0.685	0.692	0.697
		1	0.173	0.193	0.195	0.212	0.196	0.232	0.118	0.122	0.112
		2	0.004	0.005	0.006	0.037	0.033	0.042	0.016	0.016	0.013
		3	-0.003	-0.003	-0.002	0.001	0.001	0.001	0.071	0.072	0.068
		4	-0.003	-0.004	-0.004	-0.003	-0.003	-0.003	0.11	0.098	0.109
	3,4,5,6	0	0.825	0.805	0.797	0.747	0.771	0.72	0.682	0.689	0.7
		1	0.172	0.191	0.198	0.214	0.194	0.233	0.121	0.122	0.111
		2	0.009	0.01	0.01	0.042	0.033	0.047	0.016	0.018	0.013
		3	-0.003	-0.003	-0.002	-0.001	0.005	0.002	0.072	0.072	0.067
		4	-0.003	-0.003	-0.003	-0.002	-0.003	-0.002	0.109	0.099	0.108
SUCC	1,2,3,4	0	0.379	0.371	0.364	0.431	0.438	0.439	0.53	0.527	0.541
		1	0.434	0.436	0.439	0.444	0.442	0.436	0.23	0.23	0.223
		2	0.166	0.17	0.173	0.119	0.115	0.117	0.185	0.186	0.183
		3	0.02	0.022	0.023	0.006	0.006	0.007	0.042	0.045	0.04
		4	0	0.001	0.001	0	0	0	0.012	0.013	0.012
OAA	1,2,3,4	0	0.427	0.423	0.418	0.459	0.462	0.457	0.552	0.551	0.557
		1	0.419	0.422	0.423	0.429	0.427	0.427	0.233	0.234	0.226
		2	0.138	0.138	0.141	0.106	0.106	0.108	0.138	0.139	0.137
		3	0.016	0.017	0.017	0.006	0.005	0.008	0.062	0.062	0.064
		4	0.001	0.001	0.001	0	0	0	0.015	0.014	0.016
CIT	1,2,3,4,5,6	0	0.279	0.278	0.274	0.289	0.289	0.295	0.423	0.419	0.431
		1	0.412	0.414	0.416	0.437	0.432	0.428	0.24	0.231	0.226
		2	0.236	0.238	0.237	0.223	0.23	0.222	0.204	0.211	0.209
		3	0.065	0.063	0.065	0.047	0.046	0.051	0.09	0.095	0.089
		4	0.007	0.006	0.007	0.004	0.003	0.006	0.033	0.032	0.034
		5	0	0	0	0	0	-0.002	0.008	0.01	0.008
		6	0	0	0	0	0	0.001	0.002	0.002	0.003
G6P	3,4,5,6	0	0.882	0.87	0.876	0.836	0.85	0.814	0.722	0.727	0.728
		1	0.124	0.136	0.132	0.153	0.142	0.168	0.083	0.084	0.082
		2	0.001	0	-0.001	0.015	0.013	0.023	0.007	0.008	0.008
		3	-0.004	-0.004	-0.004	-0.001	-0.001	-0.002	0.048	0.048	0.046
		4	-0.004	-0.003	-0.004	-0.003	-0.004	-0.003	0.14	0.133	0.137
G6P	3,4,5,6	0	0.877	0.871	0.871	0.837	0.848	0.82	0.724		0.728
		1	0.13	0.135	0.136	0.152	0.142	0.165	0.084		0.082

		2	0	0.001	0.001	0.016	0.015	0.019	0.008		0.007
		3	-0.004	-0.003	-0.004				0.047		0.047
		4	-0.004	-0.004	-0.004				0.138		0.136
ALA	1,2,3	0	0.633	0.635	0.635	0.556	0.555	0.554	0.743	0.747	0.743
		1	0.352	0.349	0.35	0.401	0.4	0.401	0.073	0.072	0.072
		2	0.014	0.015	0.015	0.042	0.044	0.044	0.035	0.034	0.035
		3	0.001	0	0	0.001	0.001	0.001	0.149	0.146	0.149
	2,3	0	0.65	0.652	0.652	0.585	0.586	0.586	0.777	0.781	0.777
		1	0.344	0.341	0.342	0.41	0.409	0.408	0.053	0.052	0.053
		2	0.006	0.006	0.006	0.005	0.005	0.006	0.17	0.167	0.17
GLYeff	1,2	0	0.928	0.928	0.929	0.673	0.67	0.678	0.769	0.77	0.773
		1	0.071	0.072	0.071	0.307	0.309	0.303	0.125	0.131	0.118
		2	0.001	0.001	0.001	0.02	0.02	0.019	0.106	0.098	0.11
	2	0	0.986	0.986	0.987	0.738	0.736	0.737	0.833	0.837	0.833
		1	0.014	0.014	0.013	0.262	0.264	0.263	0.167	0.163	0.167
VAL	1,2,3,4,5	0	0.393	0.402	0.403	0.318	0.314	0.32	0.571	0.588	0.568
		1	0.46	0.455	0.452	0.474	0.475	0.471	0.104	0.099	0.109
		2	0.137	0.136	0.136	0.188	0.19	0.189	0.158	0.154	0.159
		3	0.01	0.008	0.009	0.019	0.021	0.02	0.13	0.125	0.128
		4	0	0	0	0	0	0	0.014	0.012	0.014
		5	0	0	0	0	0	0	0.023	0.022	0.022
	2,3,4,5	0	0.408	0.416	0.421	0.343	0.341	0.349	0.596	0.611	0.595
		1	0.456	0.45	0.447	0.486	0.488	0.483	0.097	0.092	0.1
		2	0.129	0.127	0.128	0.166	0.167	0.162	0.26	0.253	0.258
		3	0.007	0.006	0.004	0.005	0.005	0.005	0.02	0.019	0.021
		4	0	0	0	0	0	0	0.026	0.025	0.026
	2,3,4,5	0	0.422	0.43	0.434	0.362	0.359	0.366	0.604	0.618	0.604
		1	0.433	0.428	0.425	0.461	0.464	0.458	0.089	0.083	0.092
		2	0.126	0.125	0.125	0.159	0.159	0.157	0.252	0.245	0.249
		3	0.017	0.017	0.017	0.016	0.016	0.017	0.029	0.028	0.03
		4	0.002	0	0	0.001	0.002	0.002	0.026	0.025	0.026
LEU	2,3,4,5,6	0	0.273	0.284	0.291	0.315	0.311	0.322	0.484	0.504	0.48
		1	0.443	0.438	0.433	0.464	0.467	0.459	0.189	0.178	0.19
		2	0.232	0.227	0.226	0.194	0.196	0.193	0.233	0.226	0.234

		3	0.048	0.047	0.047	0.024	0.023	0.024	0.063	0.061	0.065
		4	0.003	0.003	0.003	0.002	0.002	0.002	0.026	0.025	0.026
		5	0	0	0	0	0	0	0.005	0.005	0.005
ILE	2,3,4,5,6	0	0.291	0.303	0.311	0.327	0.323	0.333	0.48	0.501	0.481
		1	0.447	0.44	0.434	0.465	0.468	0.461	0.21	0.203	0.21
		2	0.211	0.207	0.205	0.18	0.181	0.179	0.211	0.204	0.212
		3	0.044	0.043	0.043	0.023	0.024	0.023	0.07	0.066	0.07
		4	0.004	0.004	0.004	0.001	0.001	0.001	0.02	0.019	0.021
		5	0.002	0.003	0.003	0.003	0.002	0.002	0.008	0.008	0.007
GLU	2,3,4,5	0	0.367	0.378	0.38	0.442	0.442	0.438	0.547	0.567	0.548
		1	0.443	0.436	0.434	0.442	0.443	0.444	0.221	0.212	0.22
		2	0.17	0.167	0.166	0.111	0.111	0.114	0.18	0.17	0.18
		3	0.021	0.02	0.02	0.005	0.004	0.005	0.04	0.039	0.04
		4	-0.001	-0.001	0	0	-0.001	0	0.012	0.011	0.011
	2,3,4,5	0	0.361	0.372	0.375	0.439	0.437	0.435	0.55	0.567	0.547
		1	0.447	0.441	0.437	0.447	0.449	0.448	0.218	0.211	0.218
		2	0.172	0.168	0.167	0.111	0.111	0.113	0.182	0.173	0.183
		3	0.021	0.02	0.021	0.004	0.004	0.005	0.04	0.038	0.04
		4	-0.001	-0.001	0	-0.001	-0.001	-0.001	0.011	0.01	0.011
METeff	1,2,3,4,5	0	0.396	0.405	0.409	0.486	0.485	0.486	0.53	0.541	0.531
		1	0.382	0.376	0.375	0.383	0.383	0.382	0.254	0.251	0.252
		2	0.179	0.176	0.174	0.118	0.117	0.118	0.128	0.123	0.129
		3	0.039	0.039	0.039	0.013	0.013	0.013	0.065	0.062	0.064
		4	0.004	0.004	0.003	0	0	0	0.02	0.019	0.02
		5	0.001	0.001	0	0.001	0	0.001	0.003	0.004	0.004
	2,3,4,5	0	0.437	0.444	0.448	0.578	0.577	0.578	0.571	0.583	0.575
		1	0.384	0.38	0.377	0.345	0.347	0.344	0.267	0.261	0.264
		2	0.149	0.148	0.145	0.07	0.07	0.07	0.111	0.106	0.11
		3	0.024	0.024	0.024	0.004	0.004	0.004	0.042	0.039	0.042
		4	0.005	0.004	0.006	0.003	0.003	0.004	0.01	0.01	0.009
	2,3,4,5	0	0.44	0.448	0.452	0.579	0.579	0.578	0.575	0.588	0.575
		1	0.382	0.38	0.377	0.345	0.345	0.344	0.268	0.261	0.265
		2	0.151	0.148	0.146	0.072	0.071	0.072	0.113	0.108	0.112
		3	0.026	0.024	0.024	0.005	0.005	0.005	0.04	0.038	0.042

		4	0.001	0	0.001	0	0	0	0.004	0.004	0.006
SEReff	1,2,3	0	0.723	0.722	0.722	0.605	0.602	0.609	0.693	0.693	0.694
		1	0.266	0.267	0.266	0.344	0.345	0.341	0.163	0.169	0.16
		2	0.011	0.011	0.012	0.049	0.051	0.049	0.078	0.077	0.078
		3	0	0	0	0.002	0.001	0.001	0.067	0.061	0.068
	2,3	0	0.755	0.753	0.754	0.65	0.649	0.65	0.736	0.738	0.736
		1	0.244	0.246	0.246	0.329	0.33	0.33	0.184	0.188	0.183
		2	0.001	0	0	0.021	0.021	0.02	0.08	0.074	0.081
	2,3	0	0.752	0.752	0.752	0.651	0.649	0.649	0.736	0.738	0.736
		1	0.245	0.245	0.246	0.328	0.329	0.33	0.183	0.188	0.183
		2	0.002	0.003	0.002	0.022	0.022	0.021	0.081	0.075	0.081
THR	1,2,3,4	0	0.412	0.419	0.423	0.458	0.457	0.456	0.563	0.574	0.563
		1	0.434	0.427	0.423	0.436	0.436	0.434	0.222	0.217	0.218
		2	0.14	0.14	0.139	0.103	0.103	0.105	0.137	0.133	0.139
		3	0.015	0.014	0.016	0.004	0.005	0.004	0.064	0.061	0.064
		4	-0.001	-0.001	0	-0.001	-0.001	0	0.014	0.014	0.015
	2,3,4	0	0.477	0.487	0.488	0.578	0.58	0.575	0.622	0.634	0.626
		1	0.417	0.409	0.408	0.373	0.372	0.377	0.229	0.224	0.225
		2	0.101	0.098	0.097	0.049	0.048	0.047	0.114	0.109	0.113
		3	0.006	0.006	0.007	0	0	0.001	0.035	0.033	0.036
PHE_TYR	1,2,3,4,5,6,7,8,9	0	0.316	0.32	0.326	0.188	0.186	0.19	0.384	0.403	0.386
		1	0.447	0.442	0.439	0.402	0.401	0.4	0.14	0.139	0.137
		2	0.2	0.199	0.197	0.283	0.283	0.282	0.133	0.129	0.133
		3	0.036	0.037	0.035	0.102	0.103	0.102	0.172	0.166	0.172
		4	0.003	0.003	0.003	0.023	0.022	0.023	0.084	0.082	0.085
		5	0	0	0	0.003	0.003	0.003	0.043	0.04	0.042
		6	-0.001	0	0	0	0.001	0	0.028	0.026	0.028
		7	0	0	0	0	0	0	0.011	0.011	0.011
		8	0	0	0	0	0	0	0.003	0.003	0.003
		9	0	0	0	0	0	0	0.002	0.002	0.002
	2,3,4,5,6,7,8,9	0	0.322	0.328	0.335	0.202	0.199	0.203	0.4	0.419	0.403
		1	0.447	0.443	0.438	0.415	0.417	0.416	0.134	0.134	0.132
		2	0.195	0.193	0.191	0.276	0.276	0.275	0.211	0.203	0.211
		3	0.034	0.033	0.034	0.089	0.089	0.088	0.11	0.105	0.11

		4	0.002	0.002	0.002	0.016	0.017	0.017	0.083	0.079	0.083
		5	0	0	0	0.001	0.002	0.001	0.034	0.033	0.034
		6	0	0	0	0	0	0	0.023	0.021	0.022
		7	0	0	0	0	0	0	0.004	0.003	0.004
		8	0	0	0	0	0	0	0.002	0.002	0.002
	2,3,4,5,6,7,8,9	0	0.323	0.329	0.334	0.203	0.2	0.204	0.401	0.419	0.402
		1	0.443	0.44	0.435	0.413	0.415	0.413	0.133	0.133	0.132
		2	0.195	0.193	0.192	0.275	0.276	0.275	0.211	0.203	0.211
		3	0.035	0.035	0.034	0.089	0.09	0.089	0.11	0.106	0.109
		4	0.003	0.003	0.003	0.017	0.017	0.017	0.082	0.078	0.082
		5	0.001	0.001	0.002	0.002	0.002	0.002	0.034	0.033	0.035
		6	0	0	0	0	0	0	0.022	0.022	0.023
		7	0	0	0	0	0	0	0.004	0.004	0.004
		8	0	0	0	0	0	0	0.002	0.002	0.002
	1,2	0	0.966	0.965	0.966	0.602	0.6	0.602	0.769	0.776	0.769
		1	0.035	0.036	0.035	0.385	0.386	0.385	0.07	0.072	0.071
		2	-0.001	-0.001	-0.001	0.013	0.014	0.013	0.161	0.153	0.16
ASP	1,2,3,4	0	0.425	0.437	0.433	0.467	0.464	0.469	0.569	0.581	0.563
		1	0.417	0.412	0.412	0.422	0.424	0.422	0.217	0.215	0.216
		2	0.14	0.134	0.138	0.105	0.105	0.103	0.136	0.13	0.139
		3	0.018	0.016	0.017	0.007	0.007	0.006	0.063	0.061	0.066
		4	0.001	0	0.001	0	0	0	0.015	0.014	0.016
	2,3,4	0	0.486	0.498	0.494	0.584	0.582	0.585	0.629	0.638	0.62
		1	0.404	0.398	0.4	0.366	0.366	0.365	0.225	0.222	0.227
		2	0.101	0.096	0.1	0.05	0.051	0.049	0.111	0.108	0.116
		3	0.009	0.007	0.007	0	0.001	0.001	0.034	0.032	0.037
	2,3,4	0	0.497	0.508	0.504	0.59	0.588	0.59	0.633	0.644	0.628
		1	0.392	0.386	0.386	0.354	0.356	0.356	0.219	0.214	0.219
		2	0.099	0.094	0.097	0.049	0.049	0.048	0.11	0.105	0.112
		3	0.013	0.012	0.013	0.007	0.007	0.006	0.038	0.037	0.042
	1,2	0	0.671	0.681	0.676	0.677	0.675	0.681	0.741	0.749	0.734
		1	0.299	0.292	0.295	0.312	0.314	0.309	0.149	0.146	0.154
		2	0.03	0.027	0.03	0.011	0.011	0.01	0.11	0.105	0.113
GLU	1,2,3,4,5	0	0.329	0.339	0.339	0.359	0.356	0.363	0.498	0.506	0.491

		1	0.421	0.419	0.417	0.441	0.442	0.438	0.209	0.208	0.206
		2	0.203	0.199	0.2	0.176	0.177	0.176	0.198	0.193	0.202
		3	0.043	0.04	0.042	0.023	0.024	0.022	0.069	0.067	0.073
		4	0.003	0.003	0.003	0.001	0.001	0.001	0.02	0.02	0.021
		5	0	0	0	0	0	0	0.006	0.005	0.006
	2,3,4,5	0	0.383	0.393	0.392	0.451	0.449	0.454	0.556	0.564	0.548
		1	0.427	0.425	0.421	0.431	0.434	0.429	0.215	0.213	0.216
		2	0.167	0.161	0.166	0.112	0.111	0.112	0.176	0.173	0.18
		3	0.023	0.02	0.021	0.006	0.007	0.005	0.042	0.039	0.043
		4	0	0.001	0	0	0	0	0.012	0.011	0.013
	2,3,4,5	0	0.38	0.389	0.387	0.449	0.446	0.451	0.555	0.564	0.548
		1	0.43	0.427	0.425	0.433	0.435	0.431	0.215	0.212	0.215
		2	0.168	0.163	0.165	0.112	0.113	0.112	0.178	0.172	0.181
		3	0.022	0.021	0.022	0.006	0.006	0.006	0.041	0.041	0.043
		4	0.001	0	0.001	0	0	0	0.011	0.011	0.012
LYS	1,2,3,4,5,6	0	0.274	0.298	0.296	0.294	0.287	0.303	0.451	0.472	0.436
		1	0.428	0.427	0.418	0.438	0.444	0.435	0.209	0.205	0.213
		2	0.233	0.221	0.224	0.219	0.218	0.215	0.17	0.161	0.175
		3	0.058	0.055	0.055	0.046	0.047	0.044	0.113	0.108	0.116
		4	0.007	0.005	0.007	0.002	0.004	0.003	0.039	0.037	0.042
		5	0	0.001	0	0.001	0	0	0.013	0.014	0.015
		6	-0.001	-0.006	0	0	0	0	0.005	0.004	0.004
HISeff	1,2,3,4,5,6	0	0.575	0.576	0.582	0.315	0.312	0.316	0.572	0.582	0.571
		1	0.331	0.331	0.326	0.448	0.45	0.445	0.186	0.182	0.185
		2	0.085	0.084	0.083	0.196	0.198	0.197	0.089	0.088	0.089
		3	0.01	0.009	0.008	0.038	0.038	0.039	0.082	0.079	0.081
		4	-0.001	0	0.001	0.002	0.002	0.004	0.029	0.029	0.031
		5	0	0	0	0	0	-0.001	0.036	0.033	0.036
		6	0	0	0	0	0	0	0.007	0.007	0.007
	2,3,4,5,6	0	0.679	0.678	0.682	0.325	0.321	0.327	0.568	0.584	0.57
		1	0.273	0.272	0.27	0.456	0.46	0.454	0.189	0.186	0.188
		2	0.036	0.037	0.035	0.181	0.181	0.181	0.143	0.137	0.141
		3	0.008	0.009	0.008	0.032	0.03	0.032	0.054	0.048	0.054
		4	0.003	0.003	0.003	0.004	0.005	0.005	0.037	0.036	0.038

		5	0	0.001	0.001	0.002	0.003	0.001	0.009	0.008	0.01
	1,2	0	0.811	0.814	0.818	0.761	0.756	0.751	0.816	0.827	0.818
		1	0.188	0.187	0.185	0.236	0.244	0.25	0.046	0.042	0.042
		2	0.001	-0.001	-0.003	0.002	0	-0.001	0.138	0.131	0.141
ARGeff	1,2,3,4,5,6	0	0.364	0.369	0.377	0.39	0.391	0.392	0.482	0.503	0.479
		1	0.36	0.361	0.357	0.382	0.379	0.381	0.23	0.222	0.232
		2	0.208	0.205	0.197	0.184	0.187	0.185	0.173	0.165	0.174
		3	0.057	0.054	0.059	0.038	0.039	0.035	0.08	0.075	0.079
		4	0.008	0.008	0.007	0.003	0.002	0.004	0.025	0.026	0.025
		5	0.003	0.003	0.002	0.002	0.001	0.002	0.009	0.008	0.009
		6	0.001	0.001	0.001	0	0.001	0.001	0.001	0.001	0.001
	2,3,4,5,6	0	0.396	0.394	0.409	0.452	0.449	0.456	0.514	0.534	0.514
		1	0.369	0.371	0.363	0.377	0.38	0.376	0.247	0.236	0.241
		2	0.182	0.177	0.176	0.137	0.138	0.134	0.154	0.156	0.16
		3	0.041	0.042	0.04	0.022	0.021	0.022	0.06	0.054	0.06
		4	0.005	0.009	0.006	0.004	0.004	0.004	0.016	0.014	0.017
		5	0.006	0.007	0.006	0.008	0.007	0.007	0.007	0.006	0.008