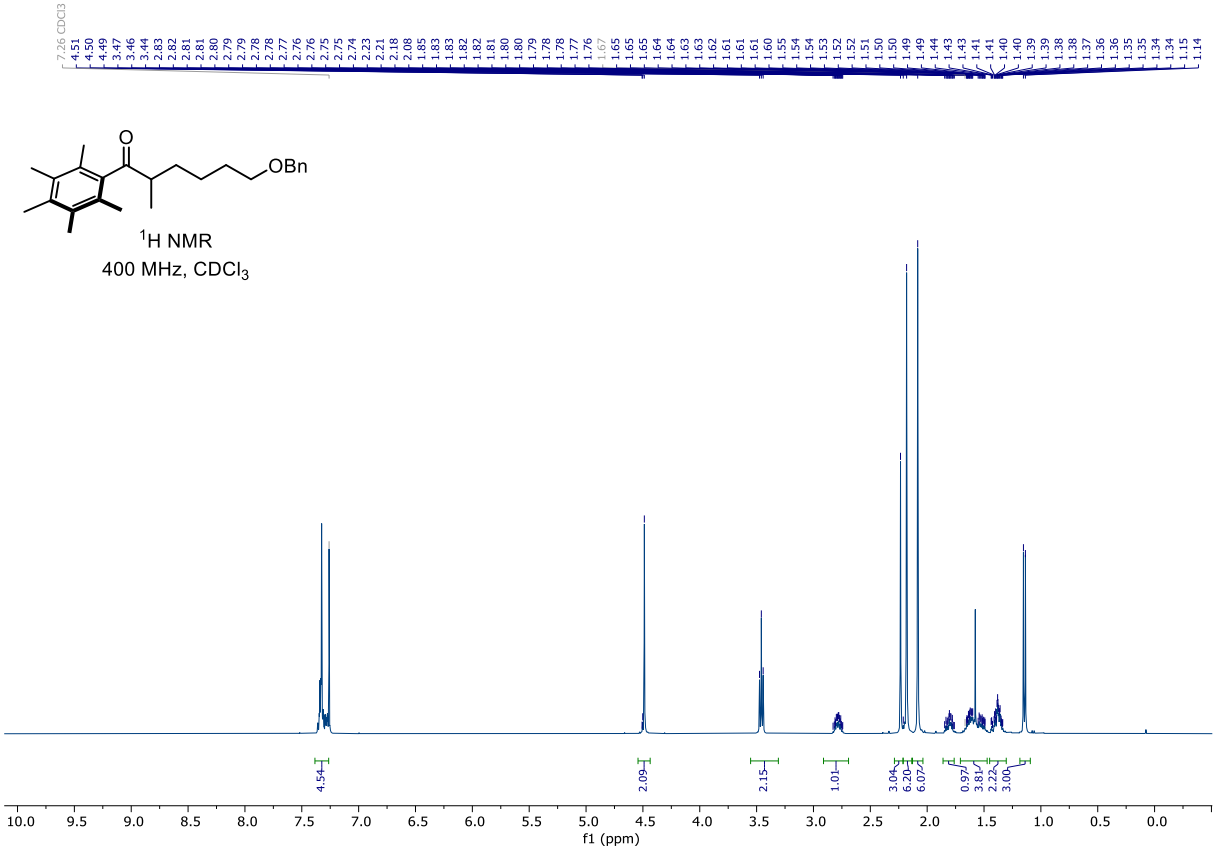
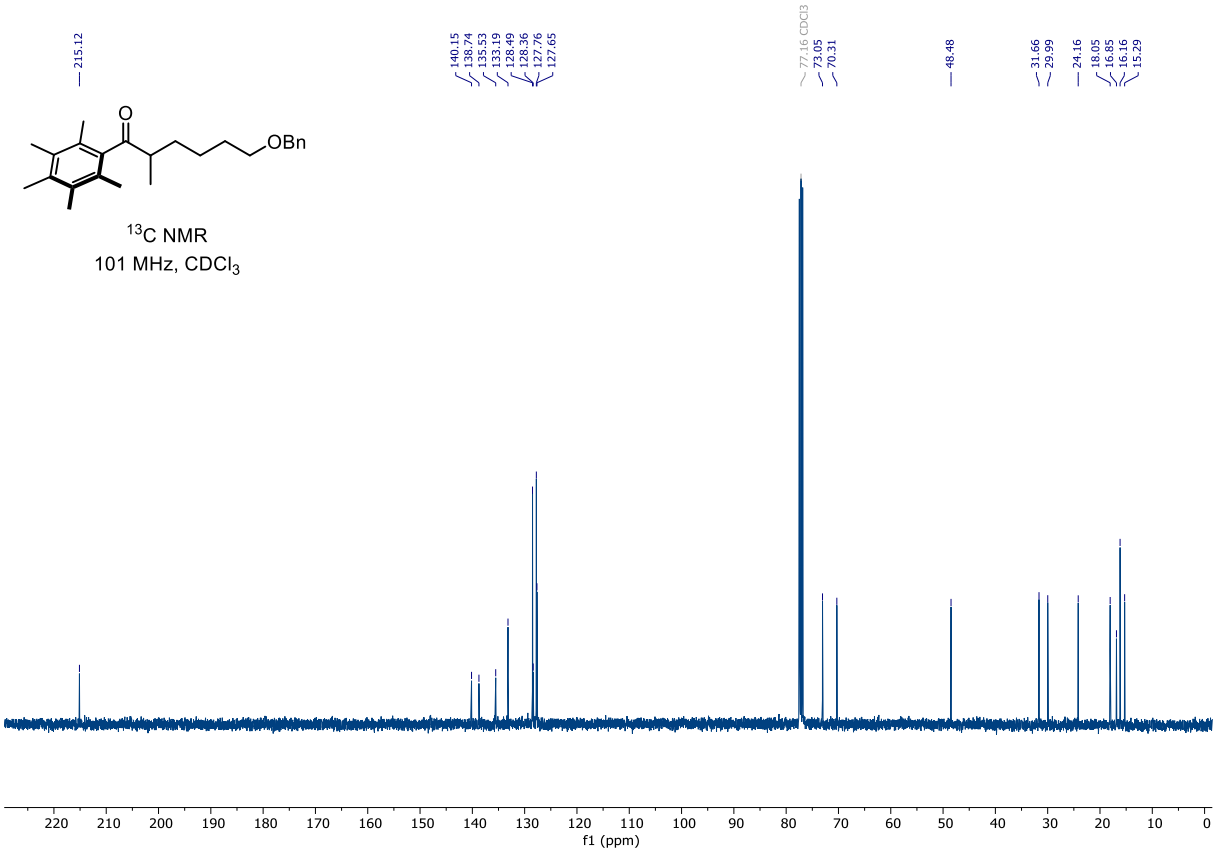
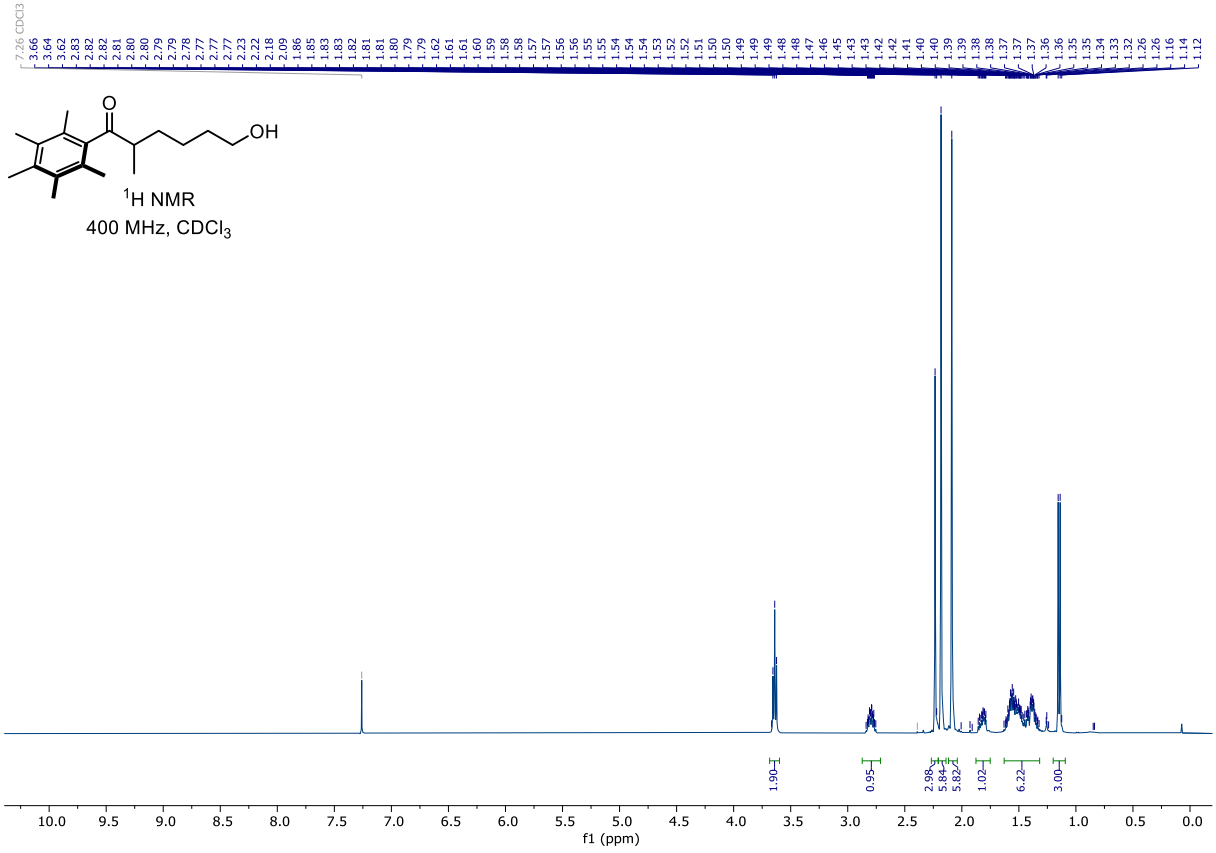
NMR Spectra of Novel Compounds

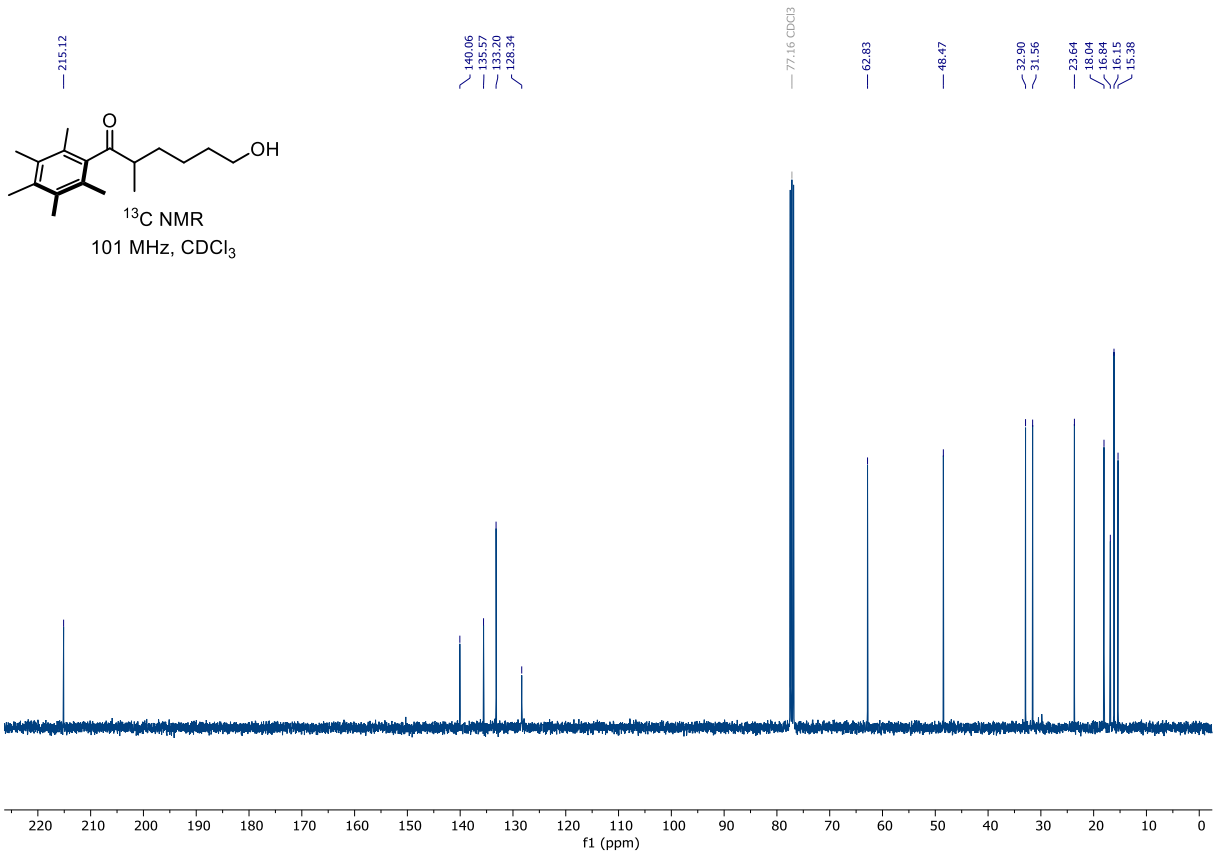
S2 6-(Benzyloxy)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one



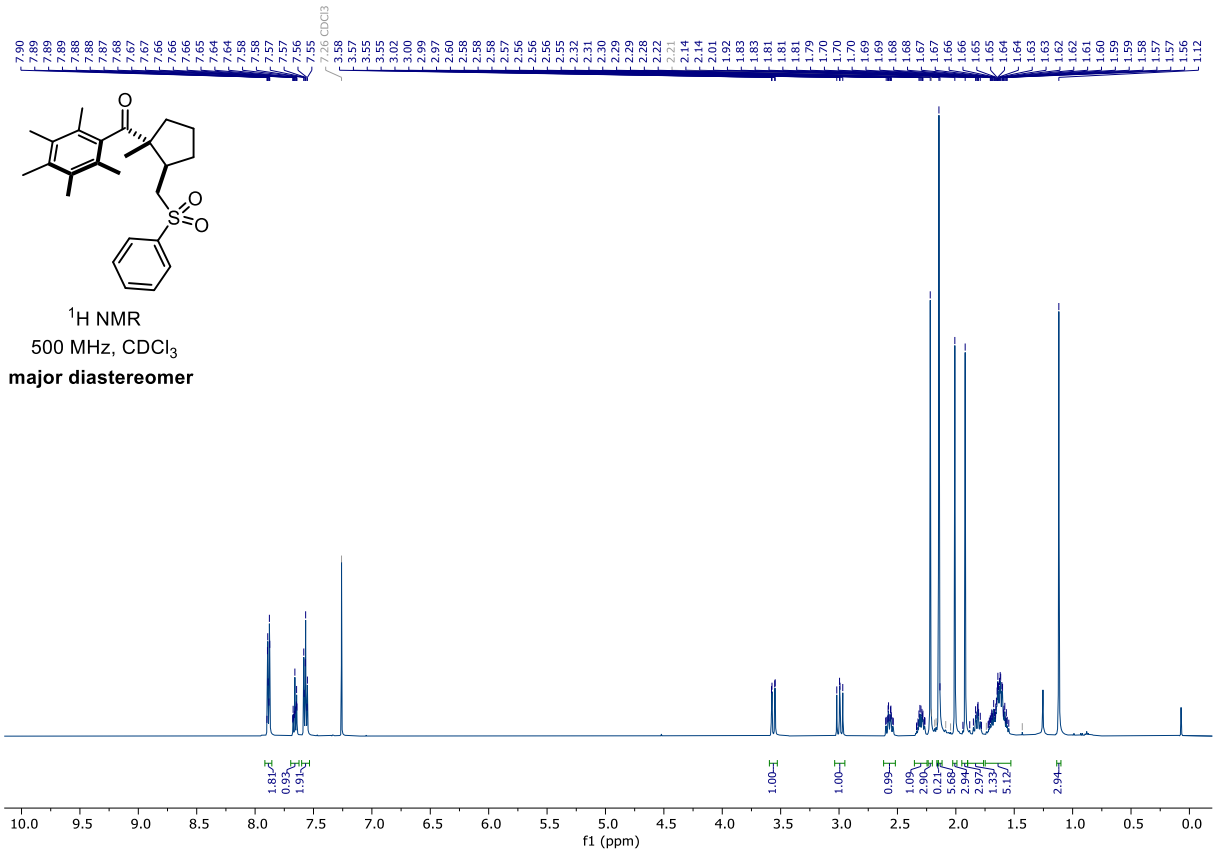


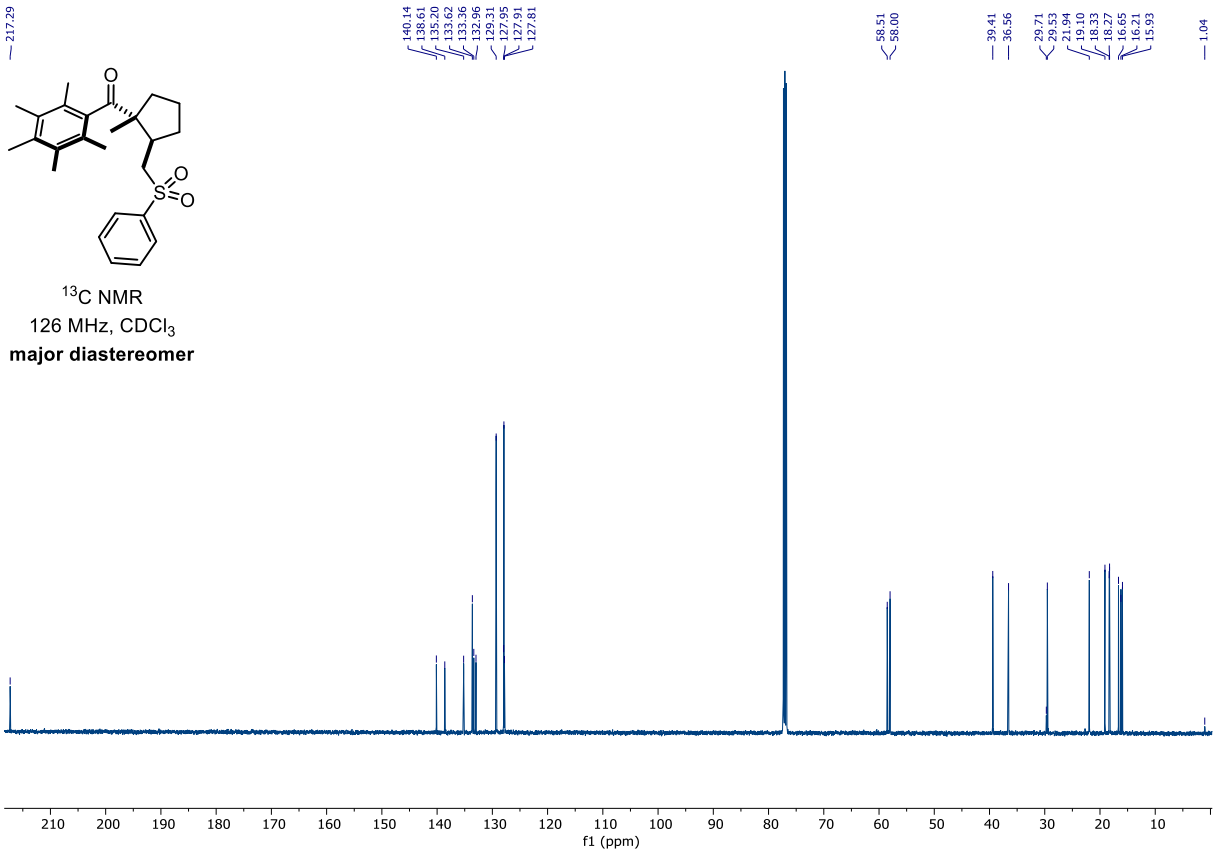
1a 6-Hydroxy-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one



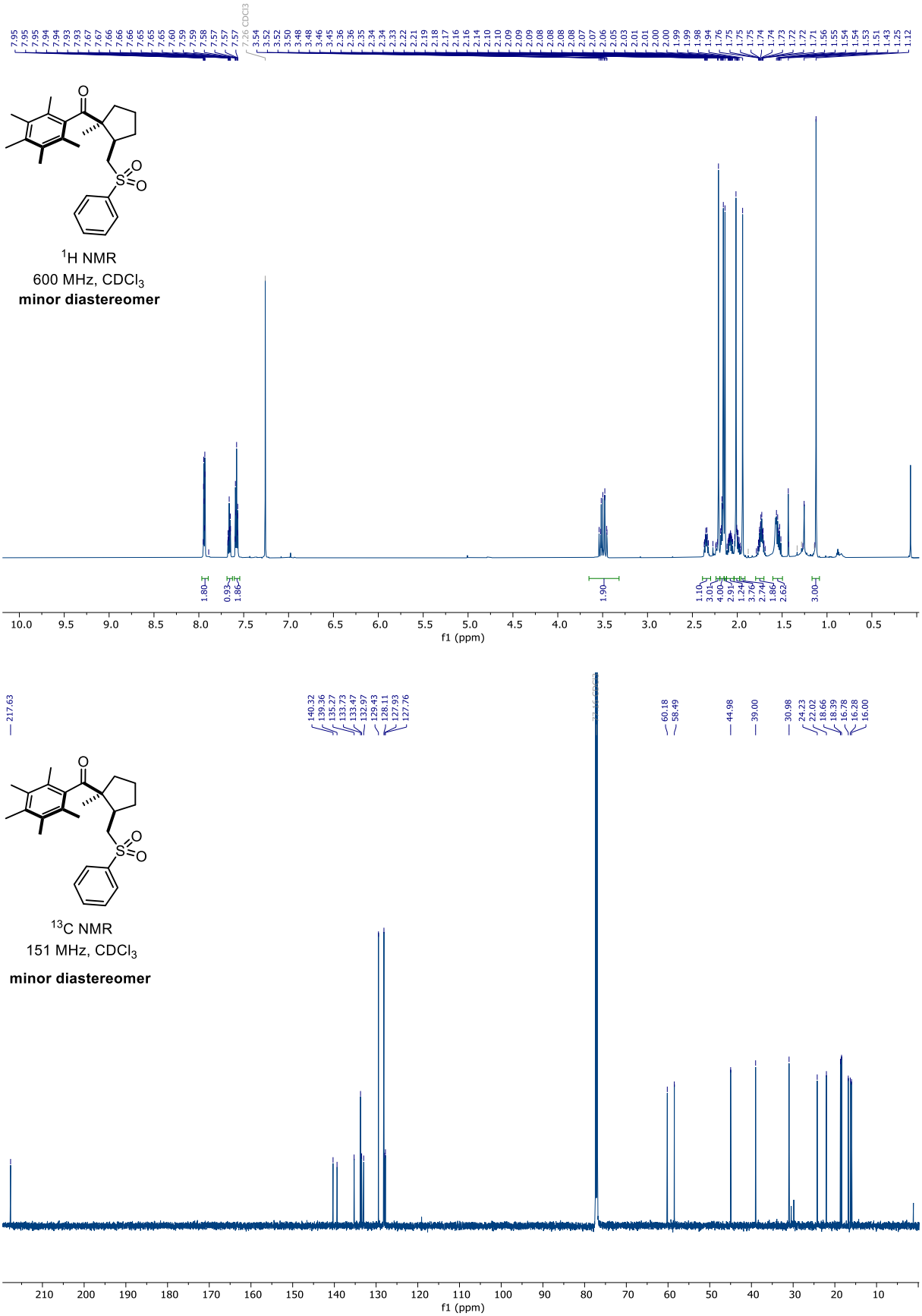


***trans*-3a ((1*RS*,2*RS*)-1-Methyl-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

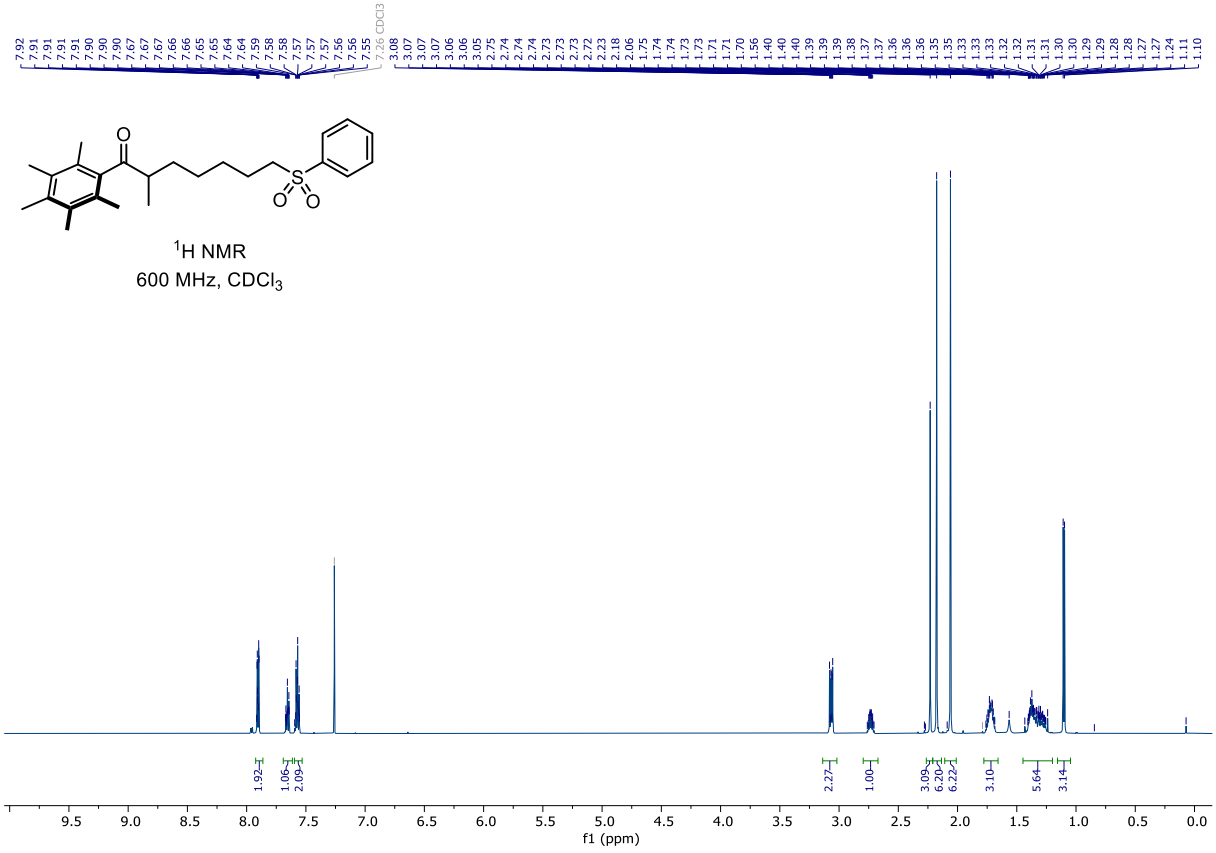


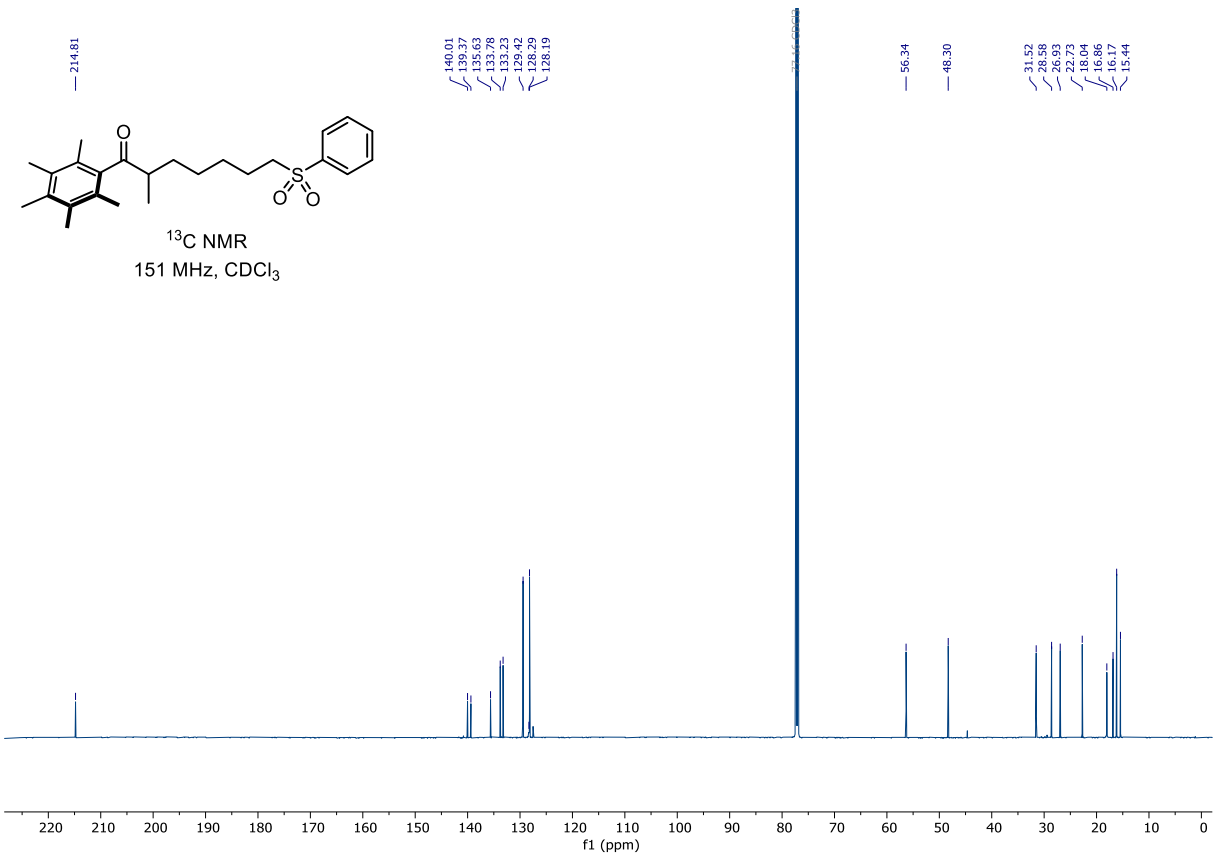


***cis*-3a ((1*SR*,2*RS*)-1-methyl-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

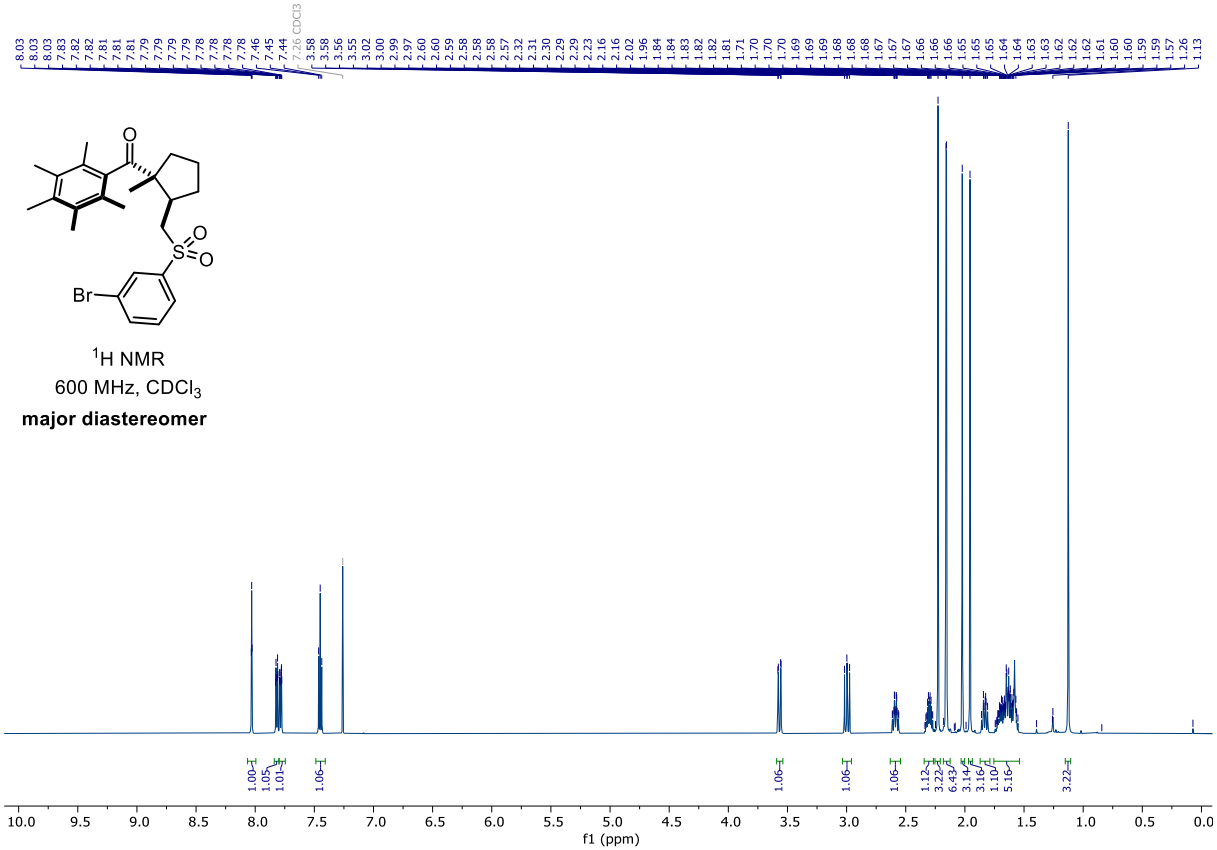


4 2-Methyl-1-(2,3,4,5,6-pentamethylphenyl)-7-(phenylsulfonyl)heptan-1-one

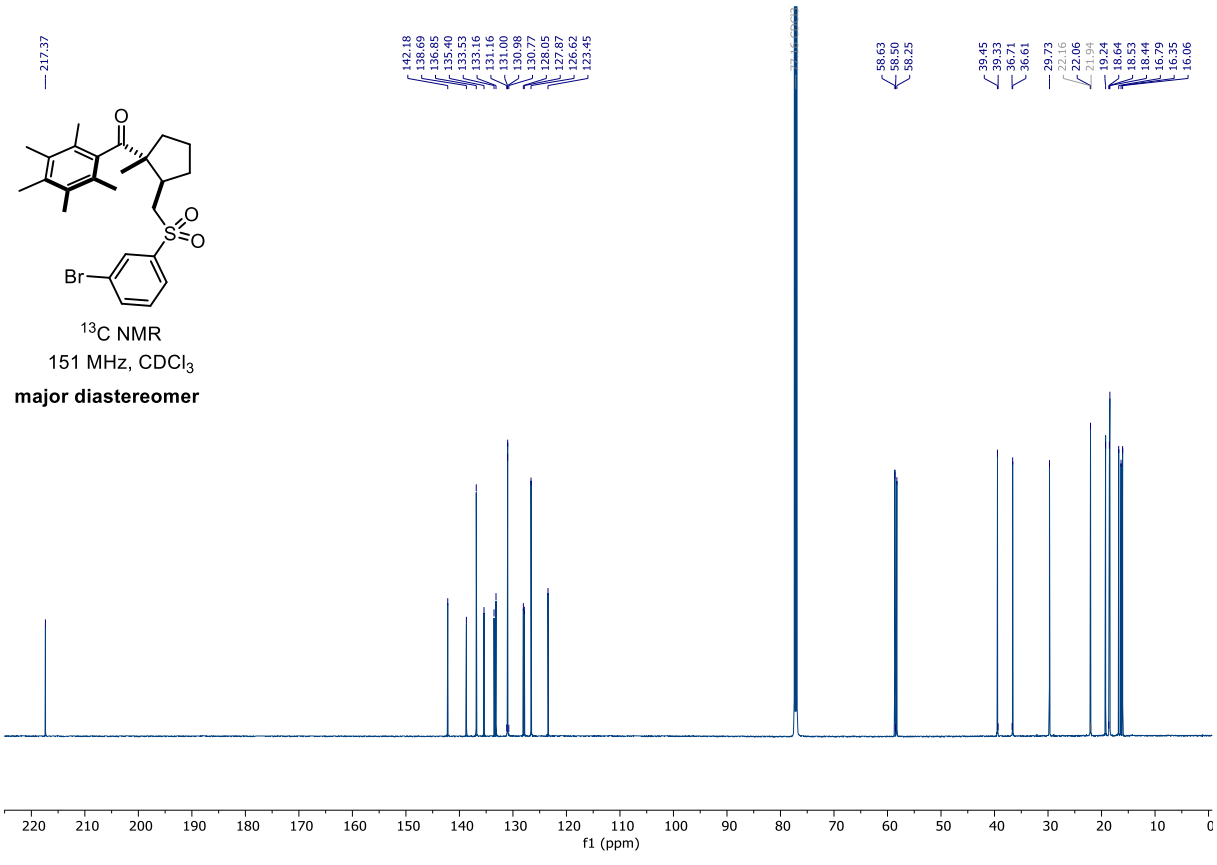




***trans*-3b ((1*RS*, 2*RS*)- 2-(((3-Bromophenyl)sulfonyl)methyl)-1-methylcyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

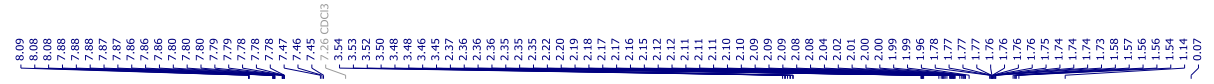


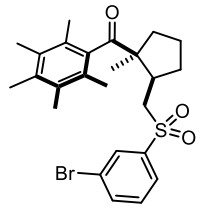
^{1}H NMR
600 MHz, $CDCl_3$
major diastereomer



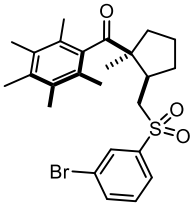
^{13}C NMR
151 MHz, $CDCl_3$
major diastereomer

***cis*-3b ((1*SR*, 2*RS*)- 2-(((3-Bromophenyl)sulfonyl)methyl)-1-methylcyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**



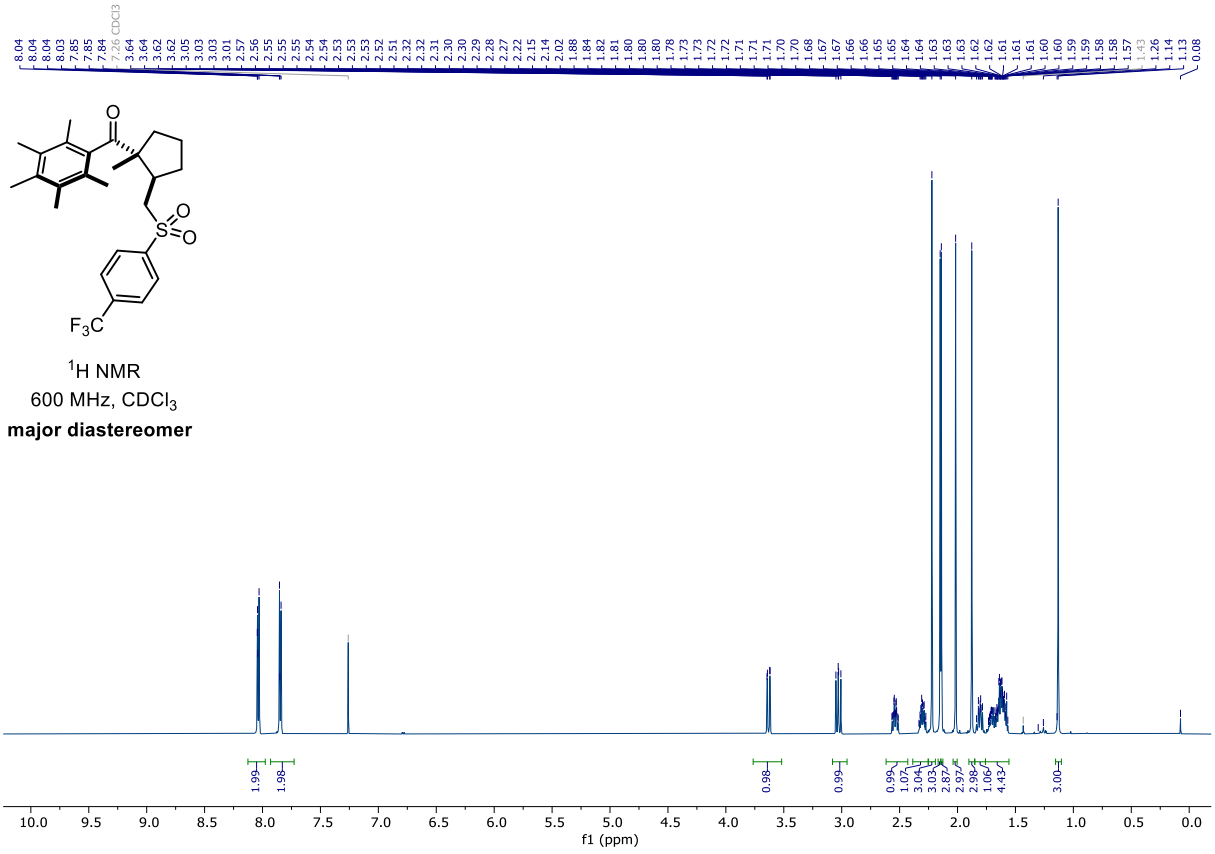


^{1}H NMR
600 MHz, $CDCl_3$
minor diastereomer

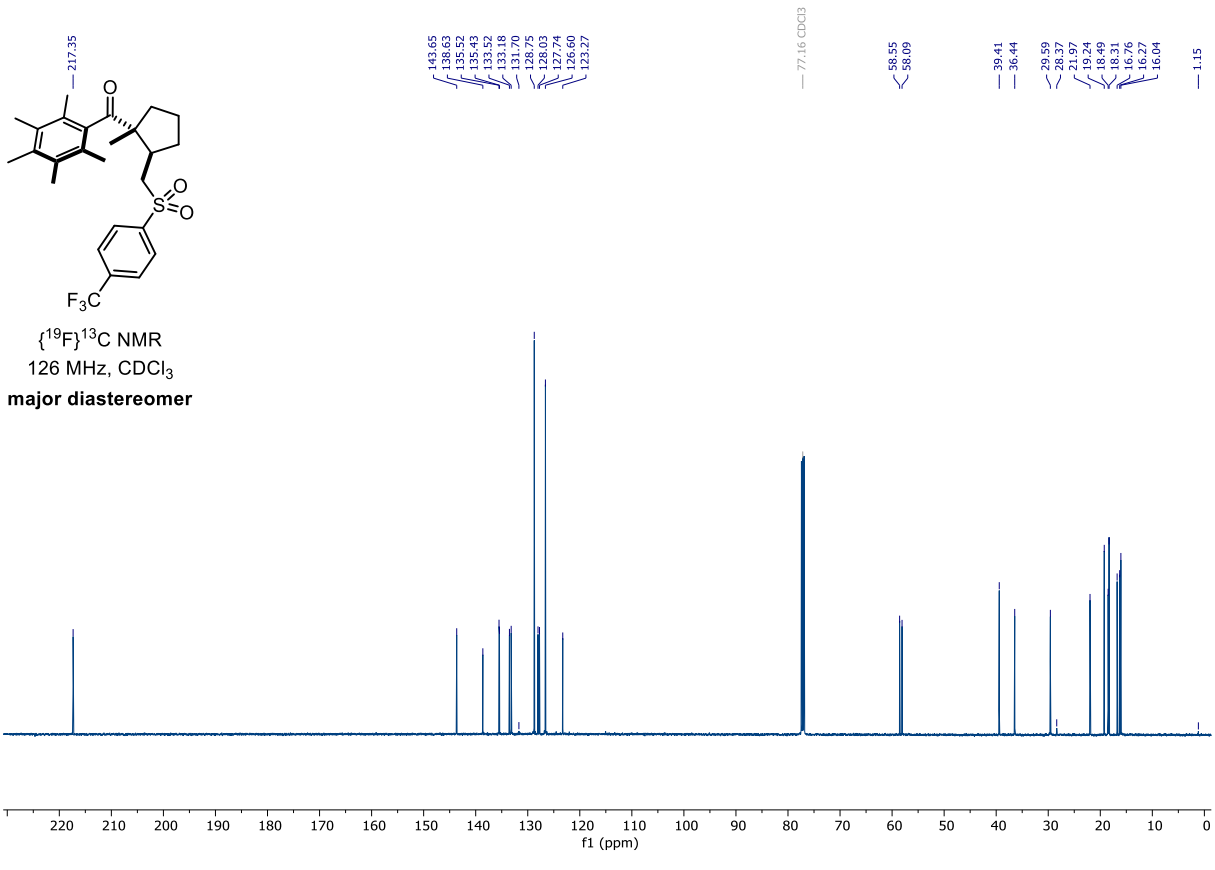


^{13}C NMR
151 MHz, $CDCl_3$
minor diastereomer

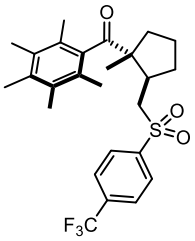
***trans*- 3c ((1*RS*,2*RS*)-1-Methyl-2-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**



^{1}H NMR
600 MHz, $CDCl_3$
major diastereomer



{^{19}F}^{13}C NMR
126 MHz, $CDCl_3$
major diastereomer

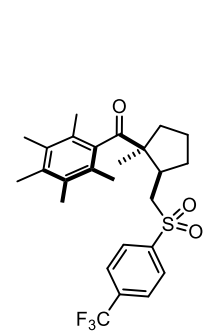


^{19}F NMR

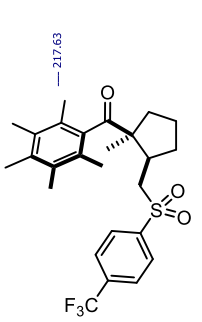
565 MHz, $CDCl_3$

major diastereomer

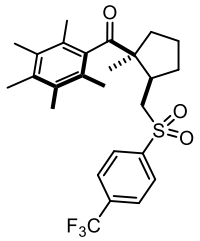
***cis*- 3c ((1*SR*,2*RS*)-1-Methyl-2-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**



^{1}H NMR
600 MHz, $CDCl_3$
minor diastereomer



^{13}C NMR
151 MHz, $CDCl_3$
minor diastereomer

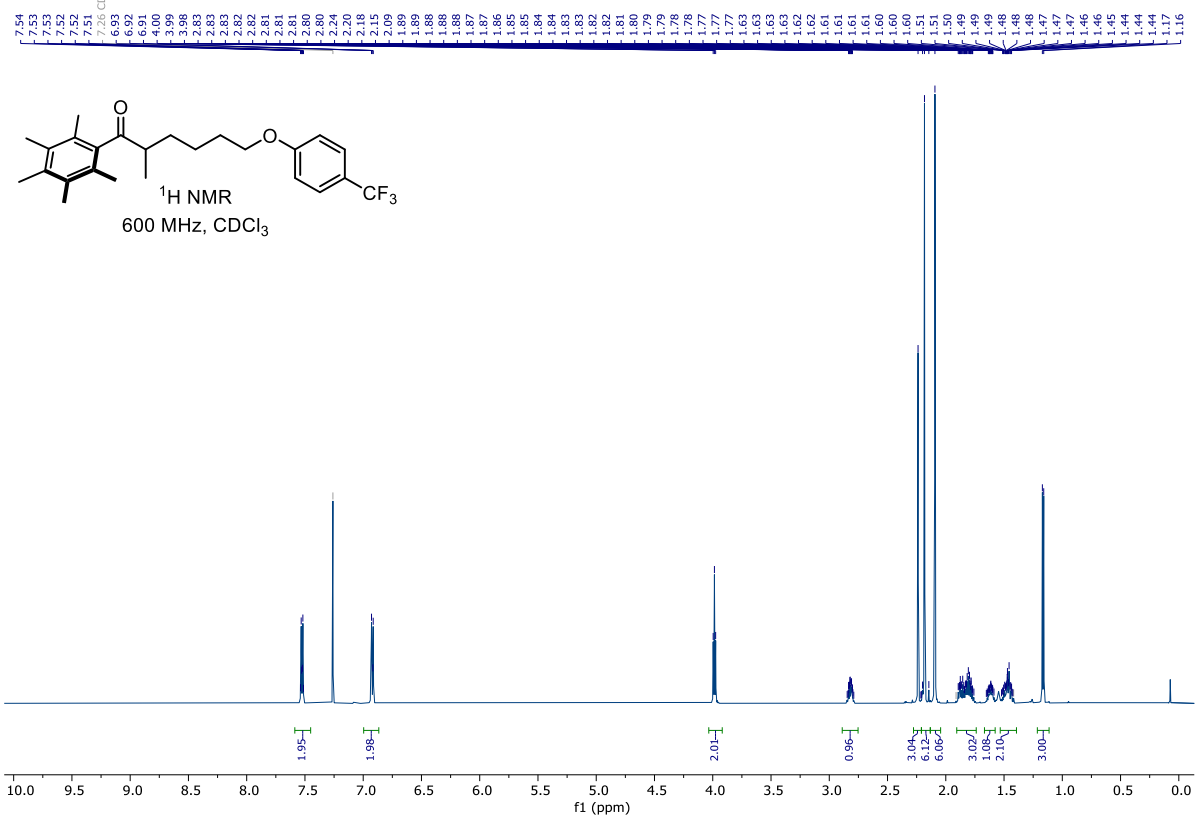


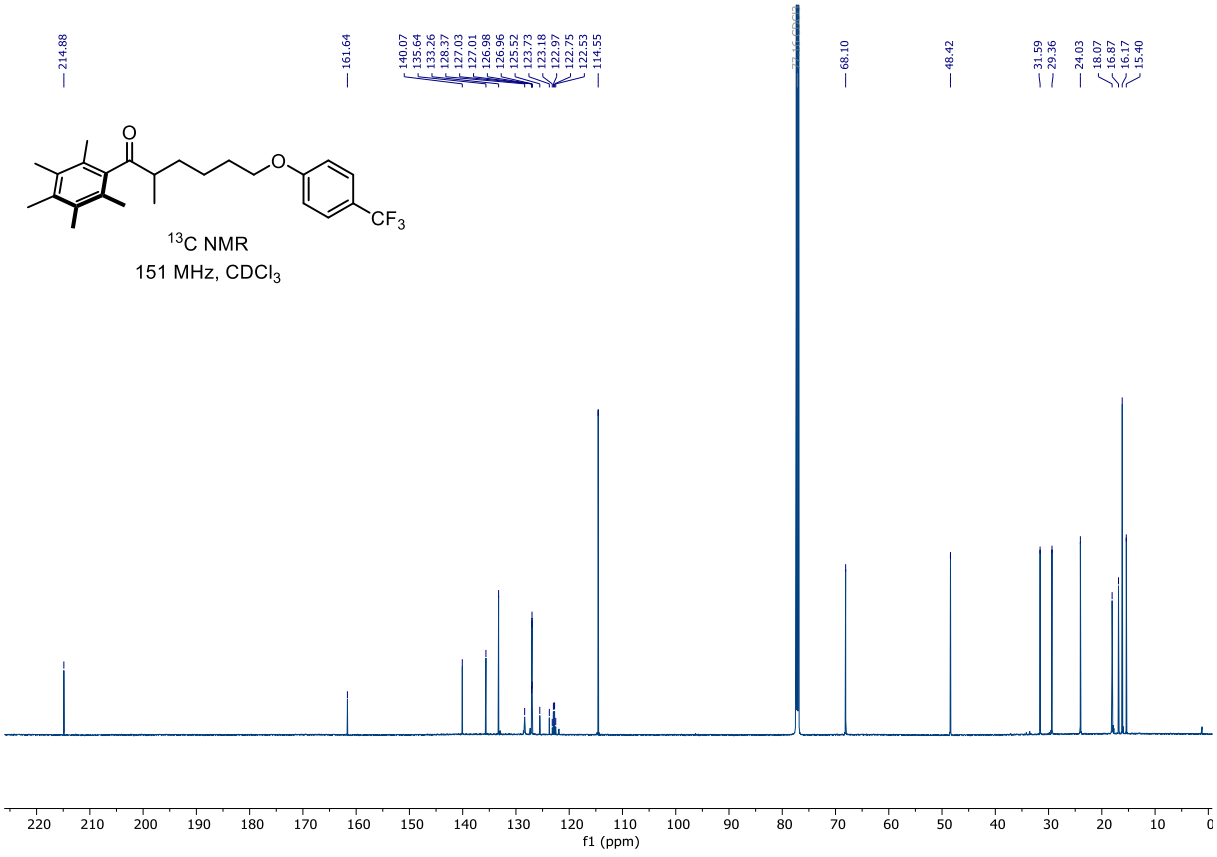
^{19}F NMR

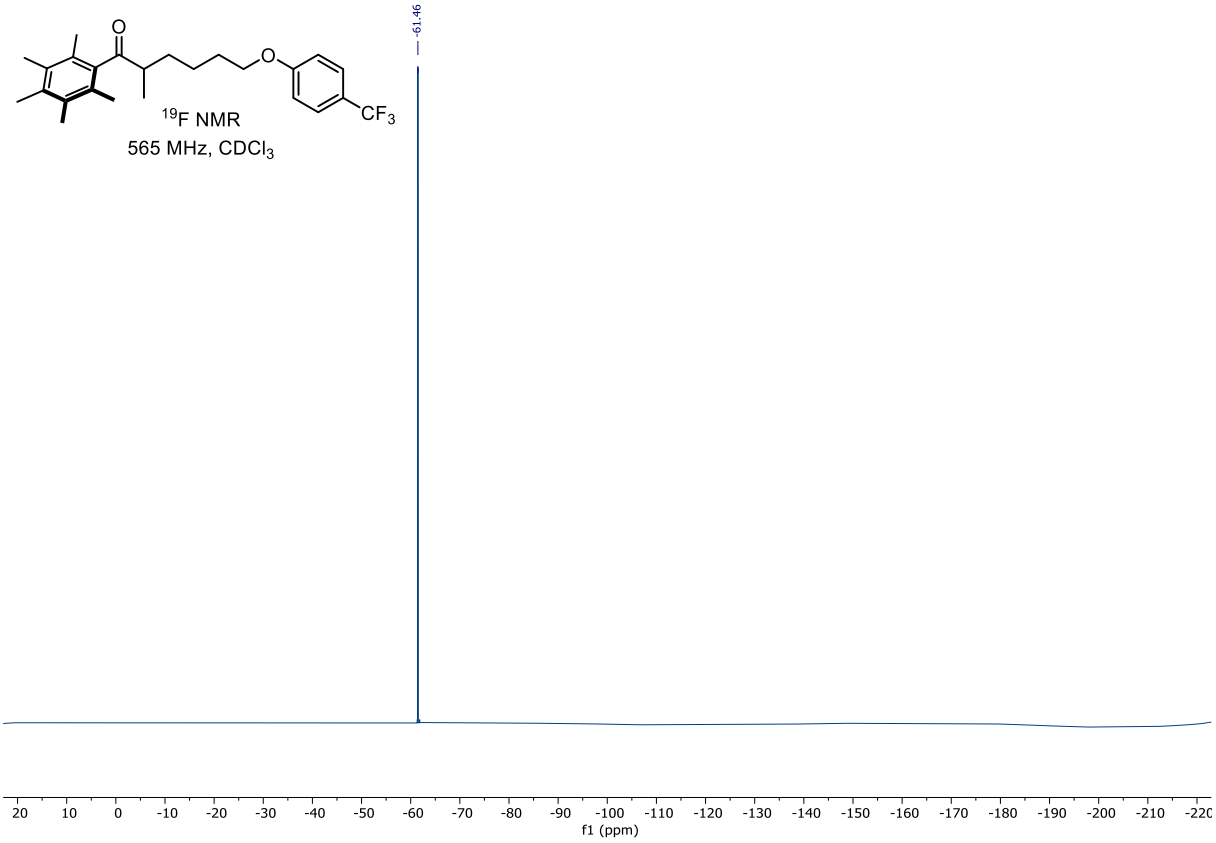
565 MHz, $CDCl_3$

minor diastereomer

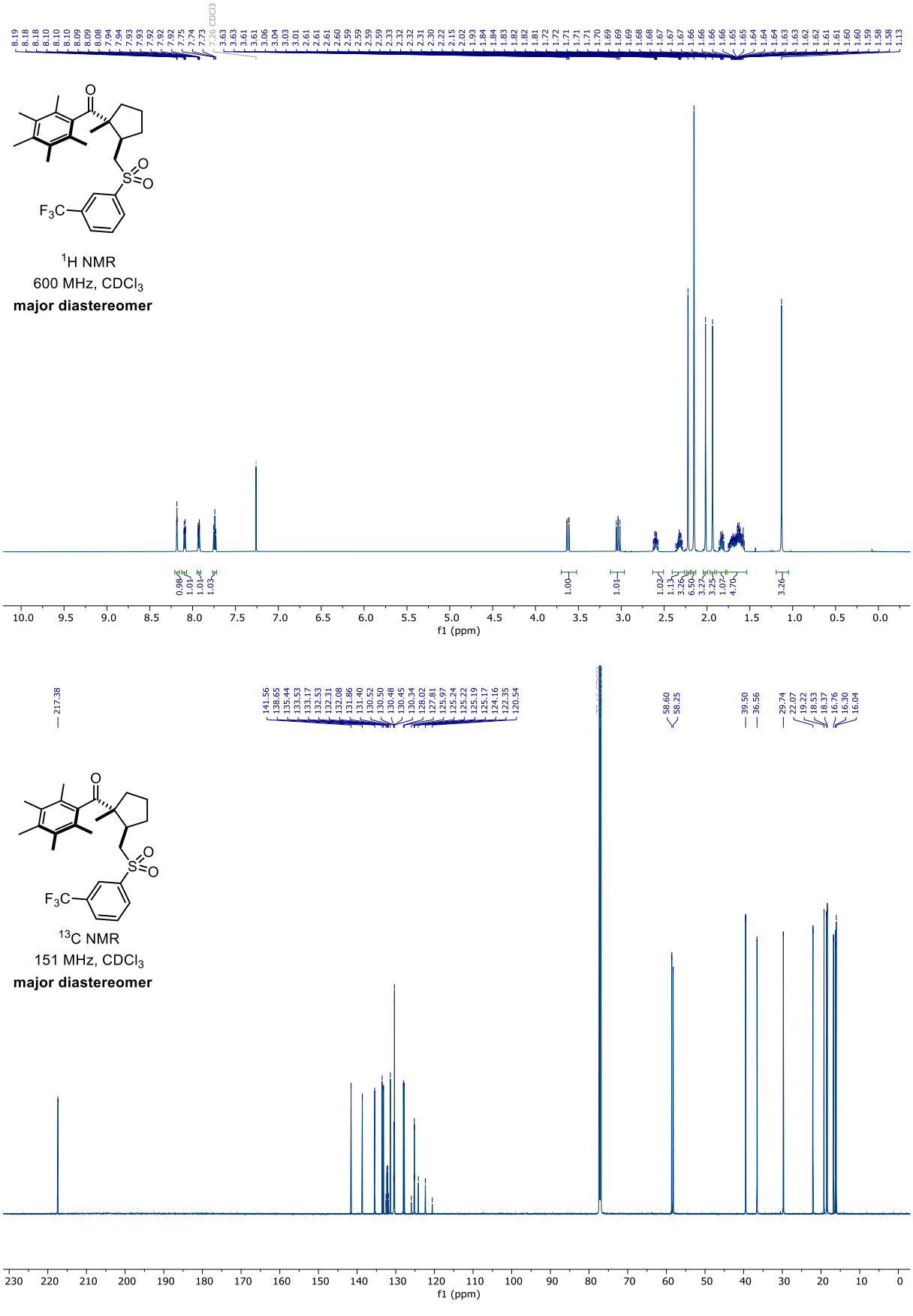
S4 2-Methyl-1-(2,3,4,5,6-pentamethylphenyl)-6-(4-(trifluoromethyl)phenoxy)hexan-1-one

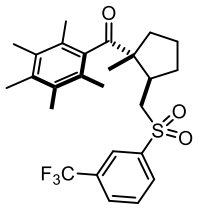





O
O
CF3
19F NMR
565 MHz, CDCl3
-61.46
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

***trans*-3d ((1*RS, 2RS*)-1-Methyl-2-(((3-(trifluoromethyl)phenyl)sulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**



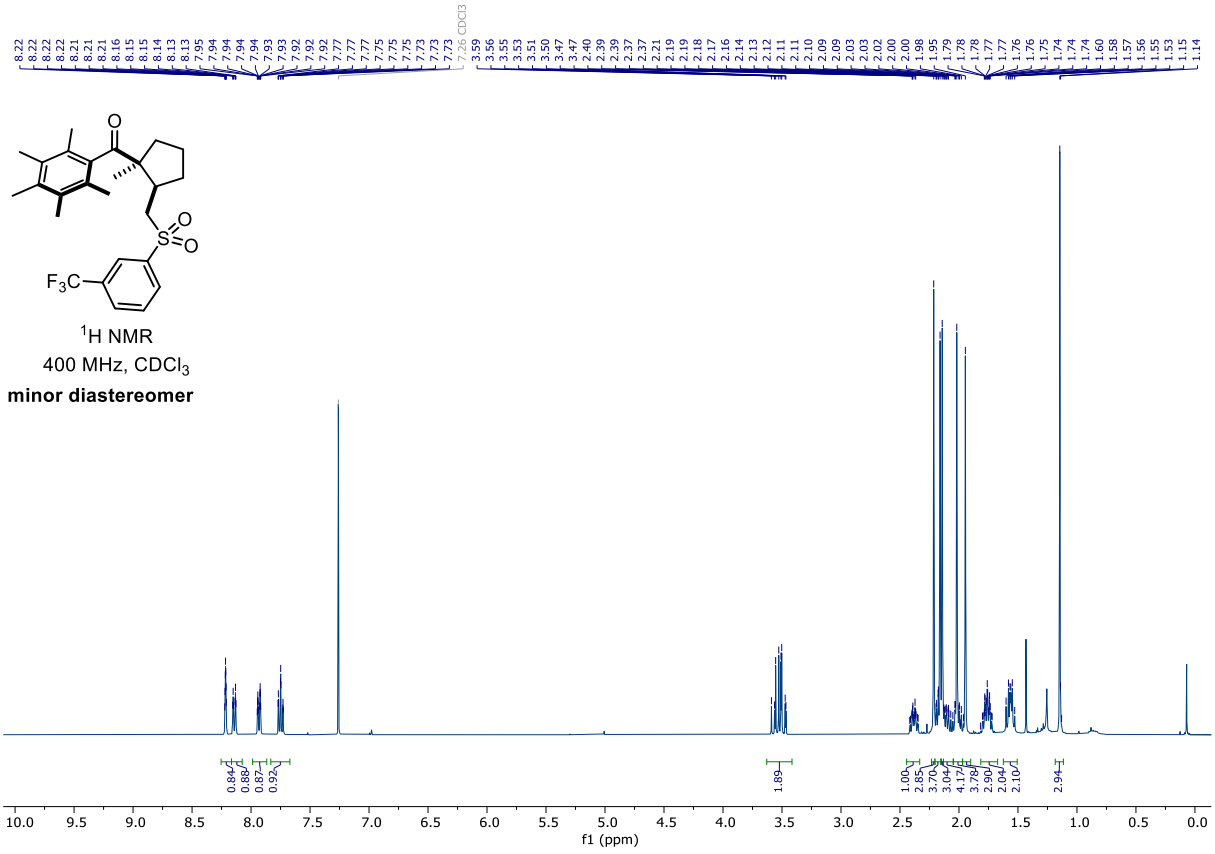


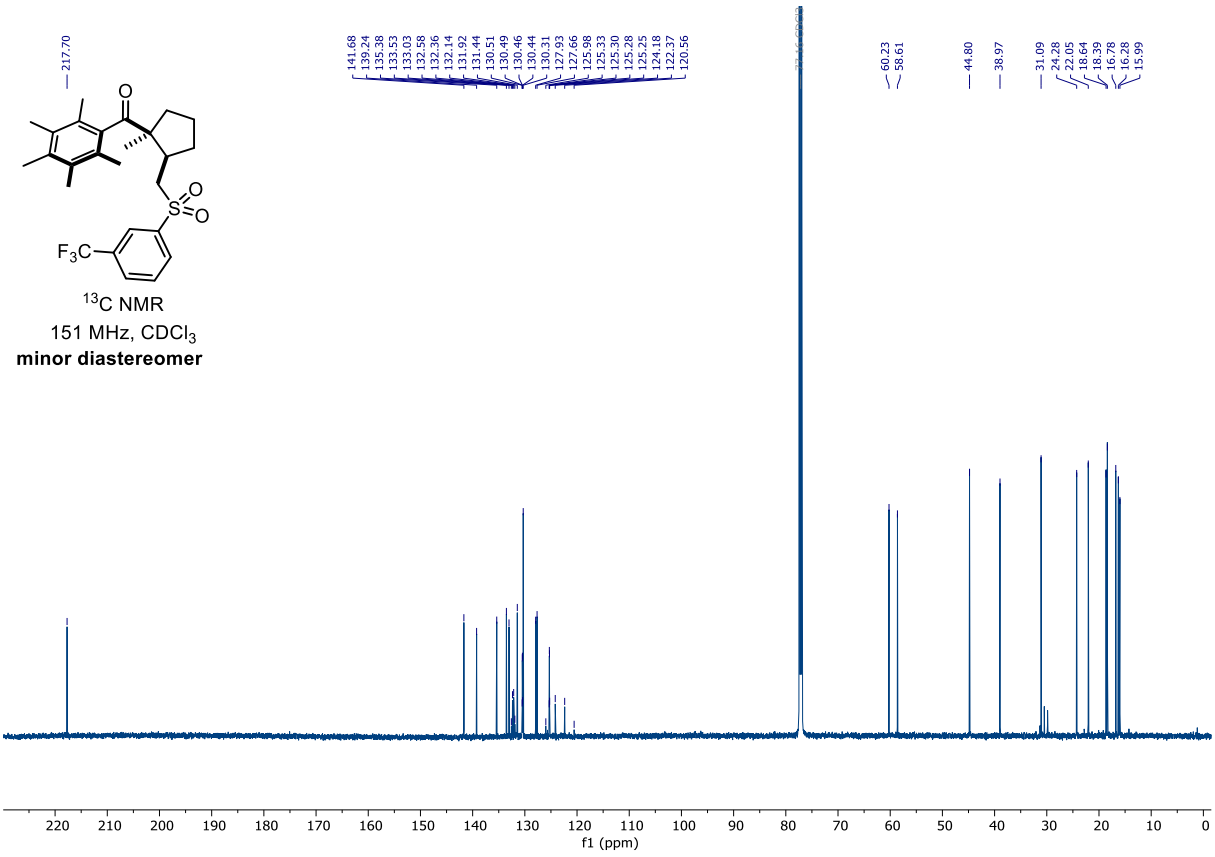
^{19}F NMR

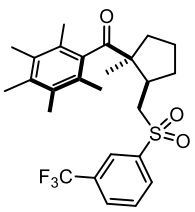
565 MHz, $CDCl_3$

major diastereomer

***cis*-3d (1*SR*, 2*RS*)-**
1-Methyl-2-(((3-(trifluoromethyl)phenyl)sulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone





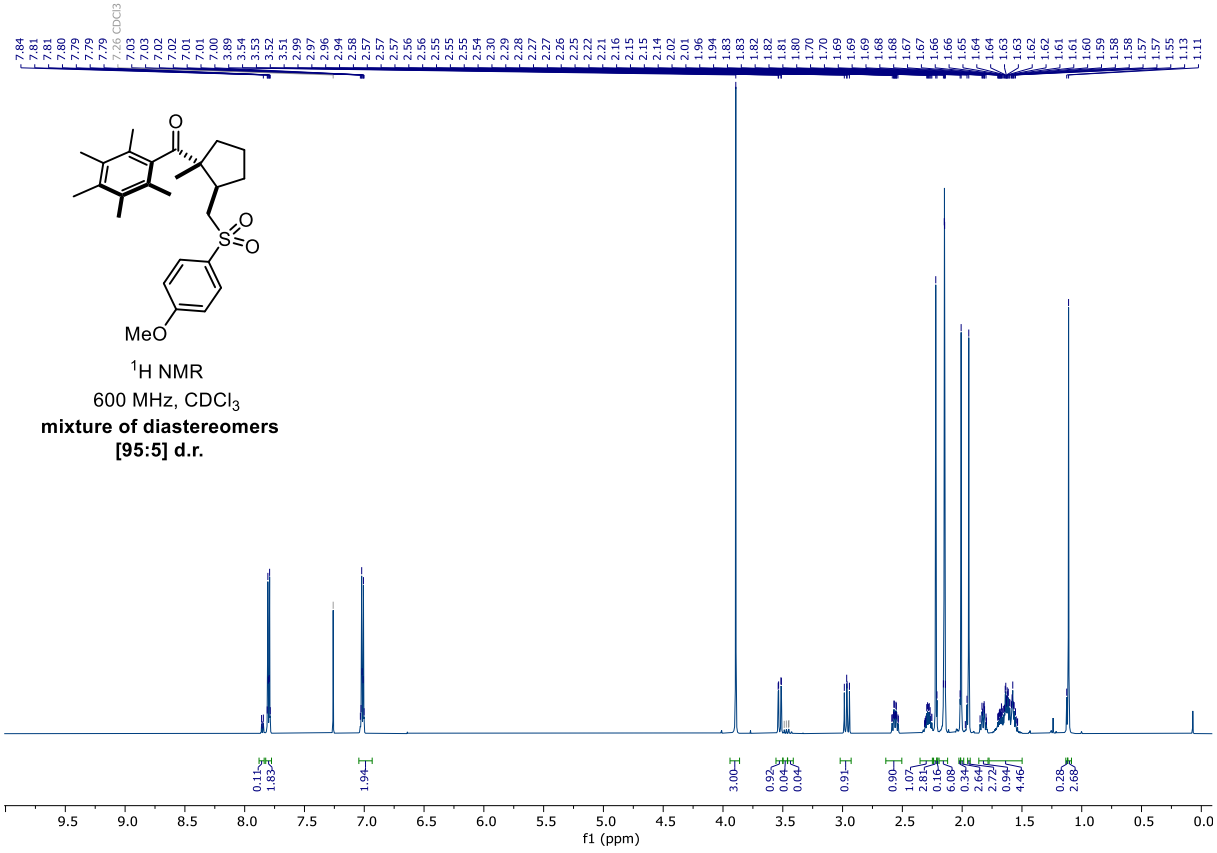


^{19}F NMR

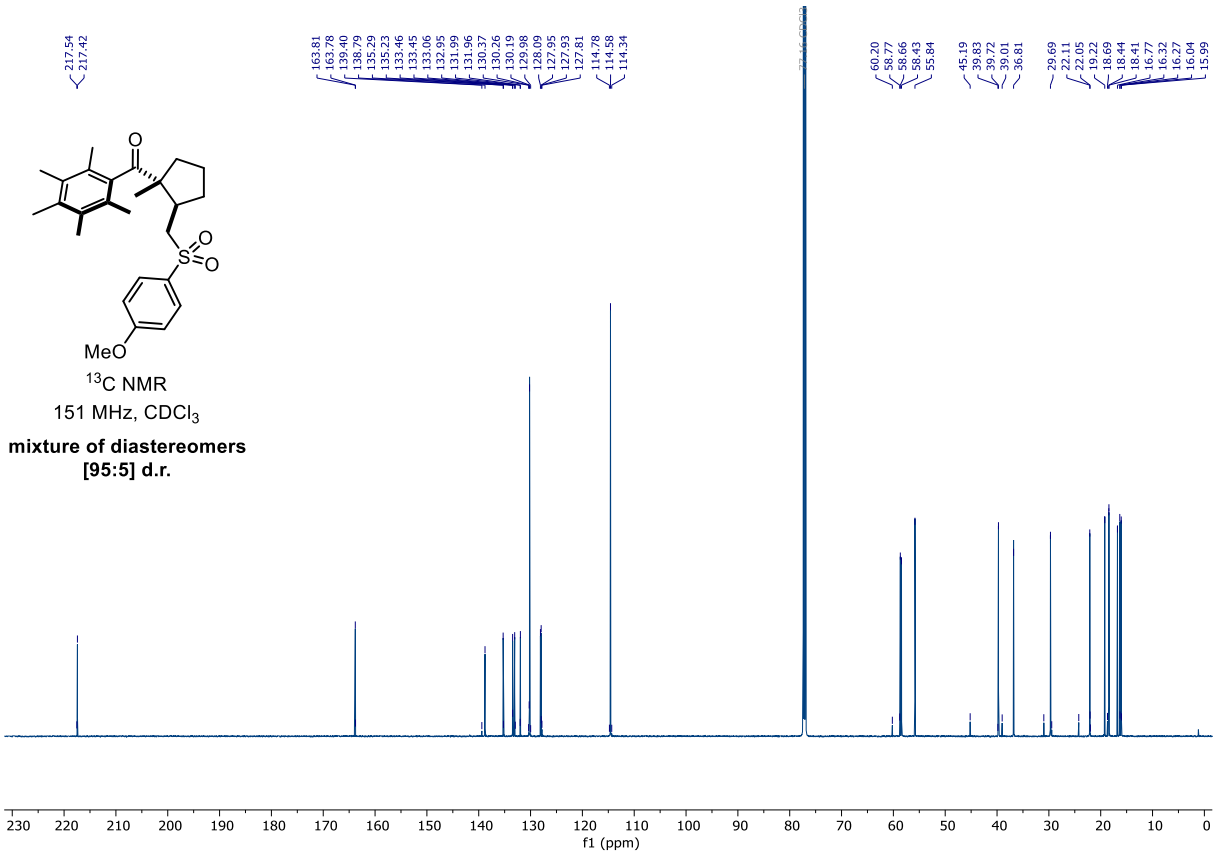
565 MHz, $CDCl_3$

minor diastereomer

3e (2-(((4-Methoxyphenyl)sulfonyl)methyl)-1-methylcyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone

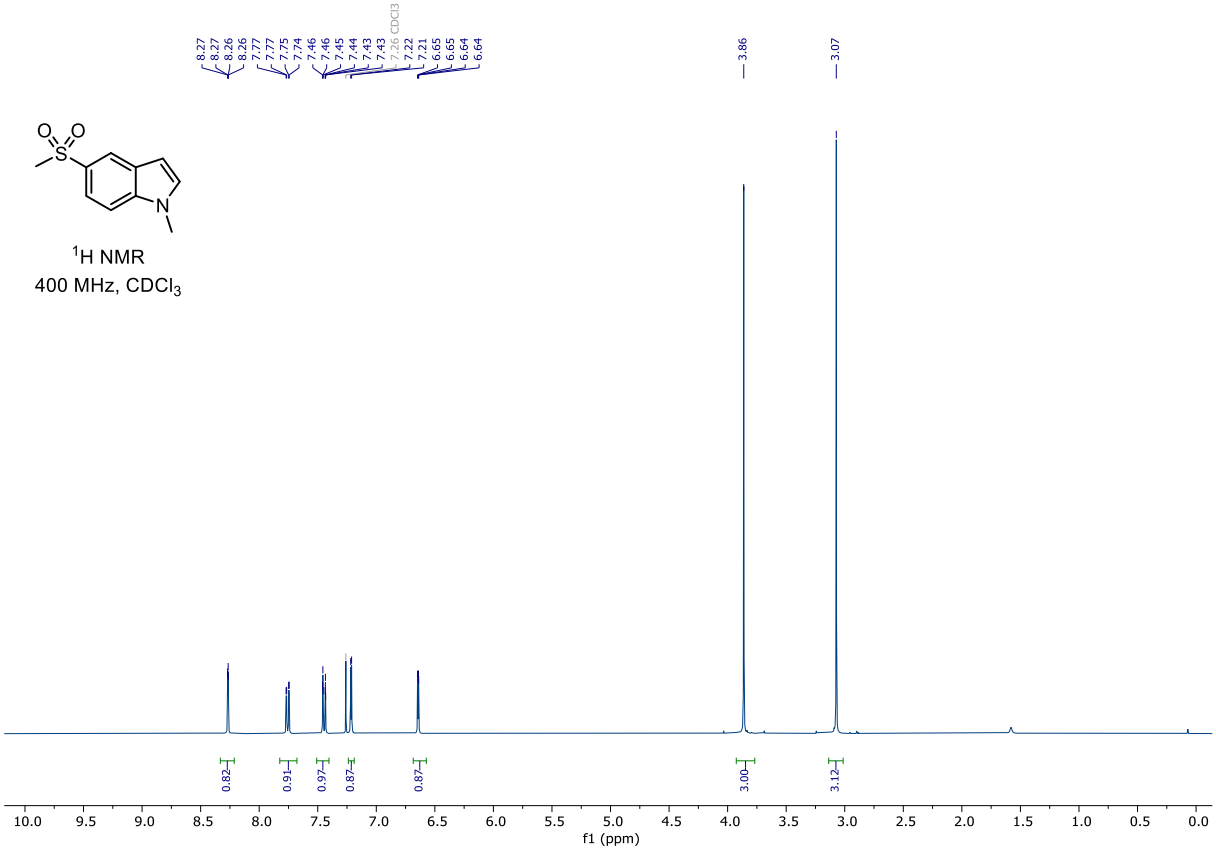


^{1}H NMR
600 MHz, $CDCl_3$
mixture of diastereomers
[95:5] d.r.

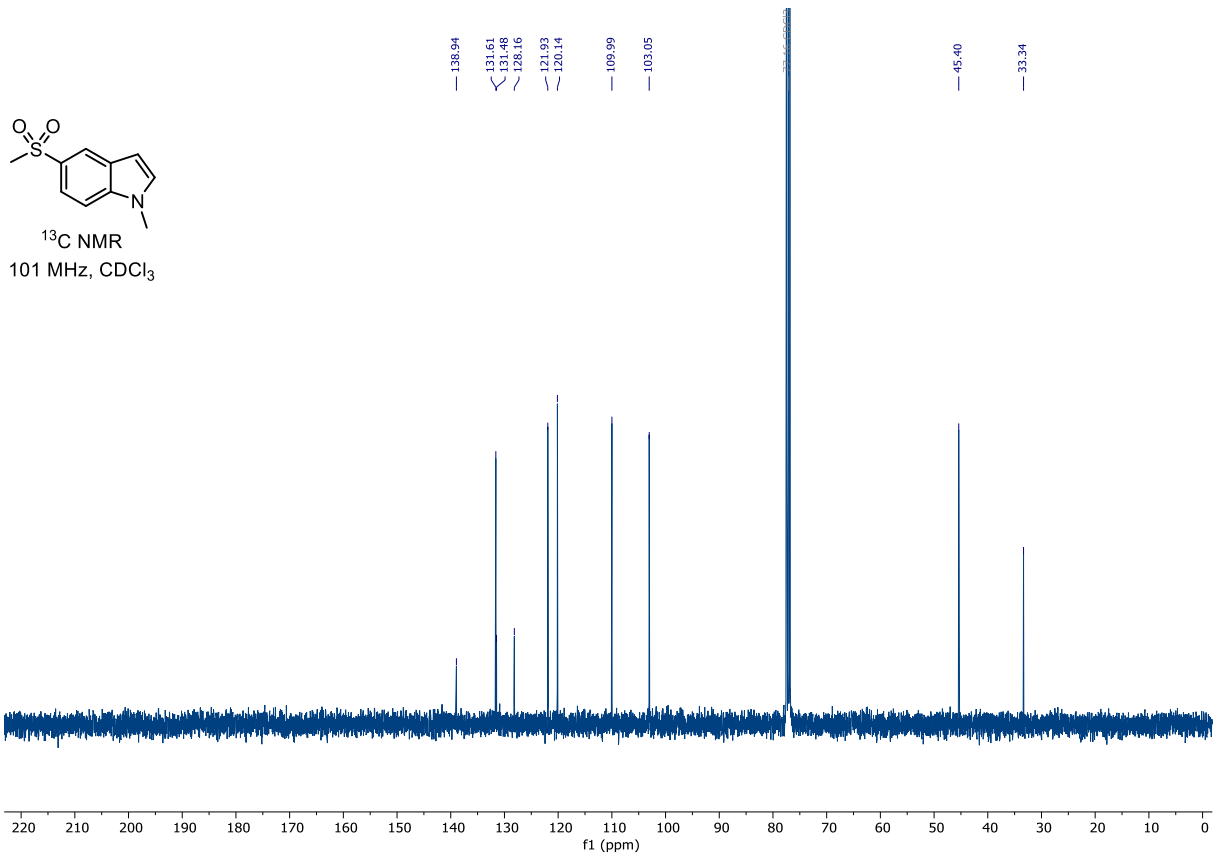


^{13}C NMR
151 MHz, $CDCl_3$
mixture of diastereomers
[95:5] d.r.

S7 1-Methyl-5-(methylsulfonyl)-1*H*-indole



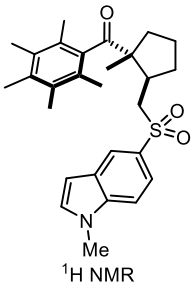
^{1}H NMR
400 MHz, $CDCl_3$



^{13}C NMR
101 MHz, $CDCl_3$

3f (1-Methyl-2-(((1-methyl-1*H*-indol-5-yl)sulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone



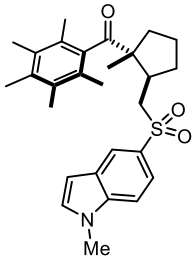


^{1}H NMR

600 MHz, $CDCl_3$

mixture of diastereomers

[94:6] d.r.



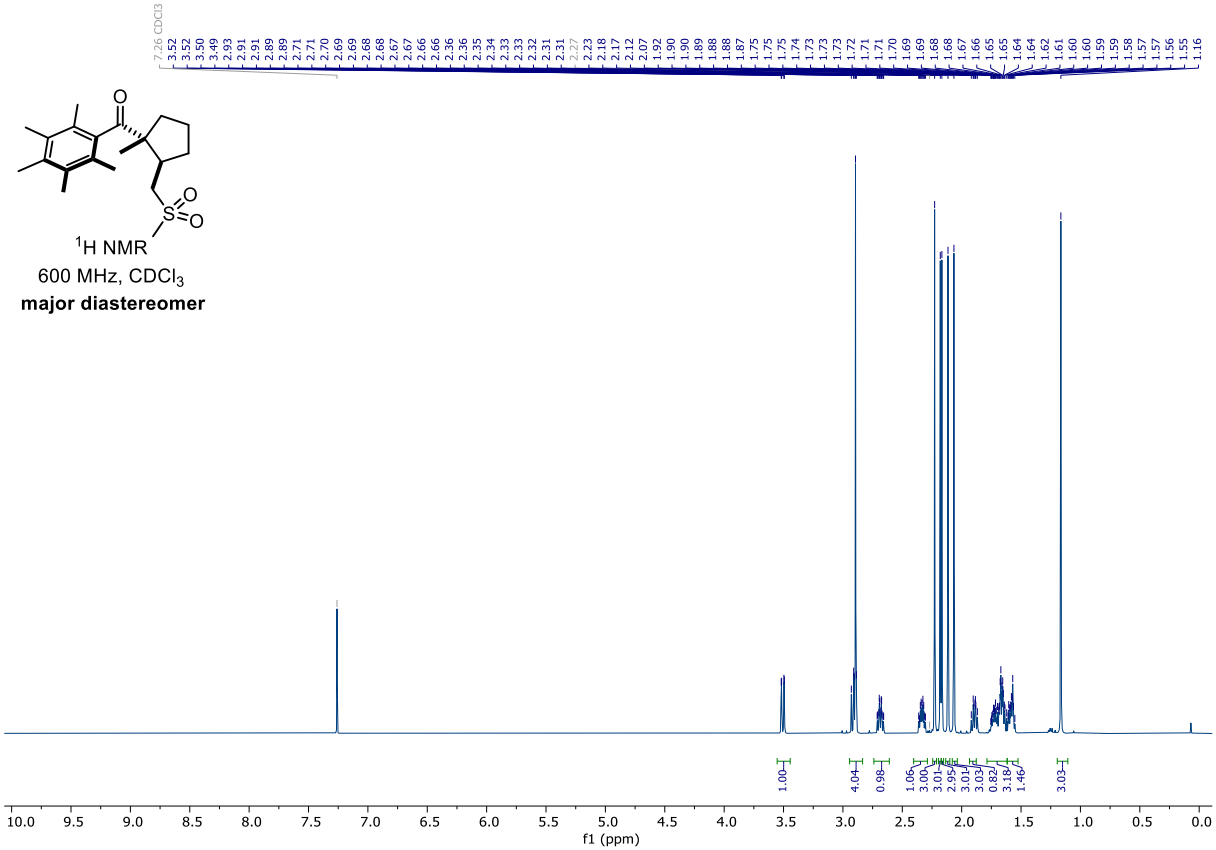
^{13}C NMR

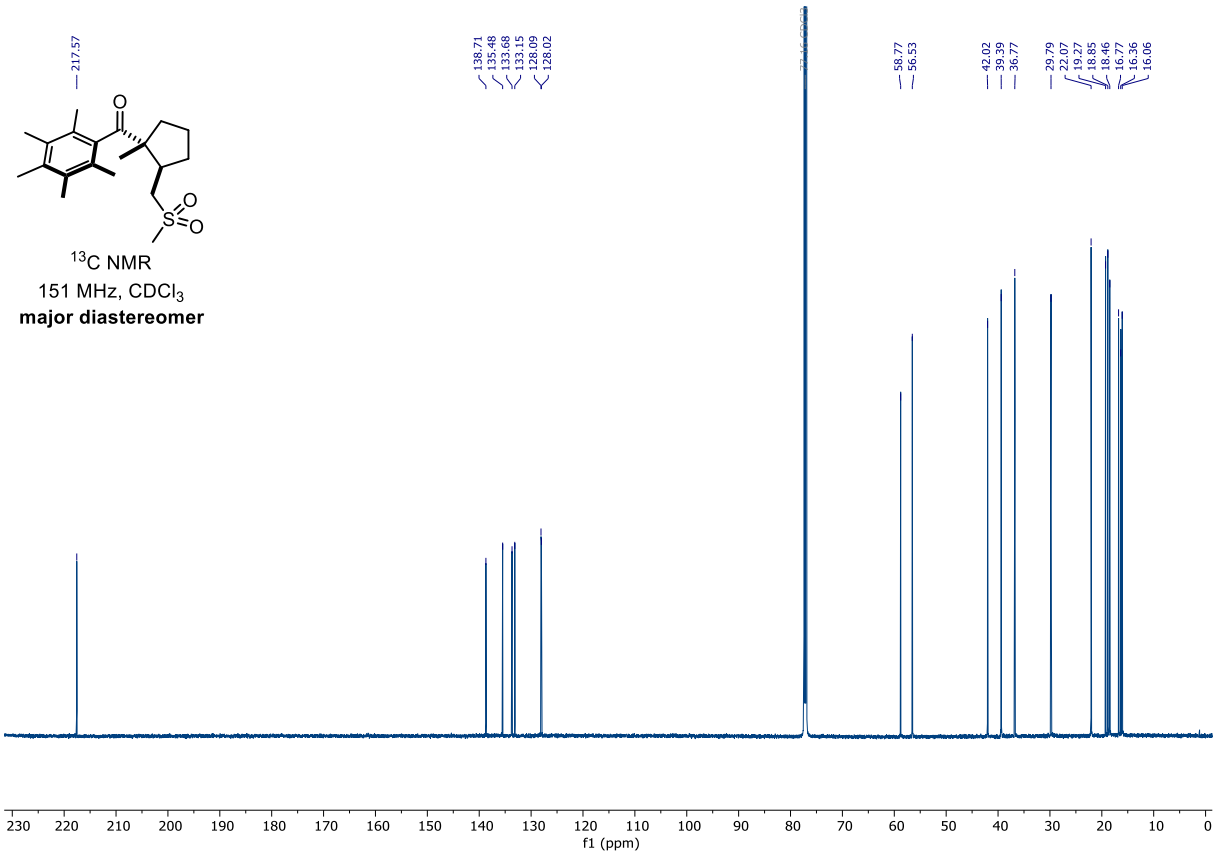
151 MHz, $CDCl_3$

mixture of diastereomers

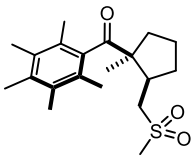
[94:6] d.r.

***trans*-3g ((1*RS*, 2*RS*)-1-Methyl-2-((methylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

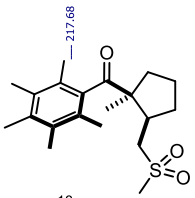




***cis*-3g ((1*SR*, 2*RS*) -1-Methyl-2-((methylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

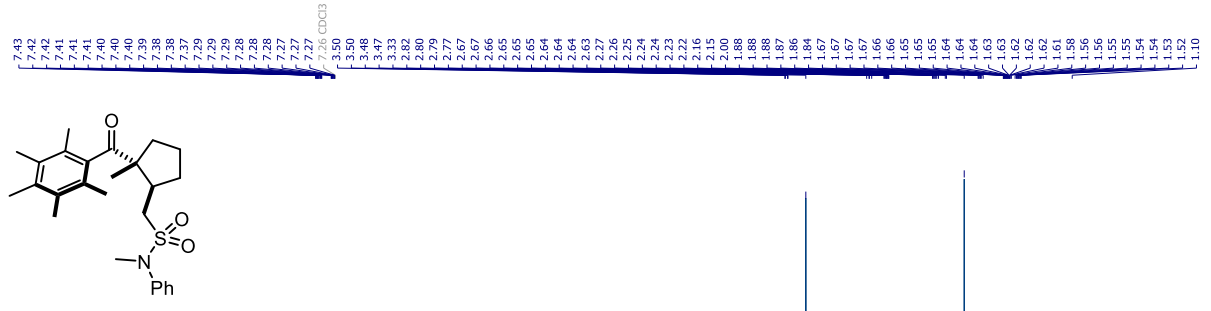


^{1}H NMR
600 MHz, $CDCl_3$
minor diastereomer

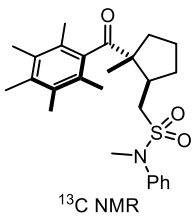


^{13}C NMR
151 MHz, $CDCl_3$
minor diastereomer

***trans*-3h *N*-Methyl-1-((1*RS*, 2*RS*)-2-methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)-*N*-phenylmethanesulfonamide**

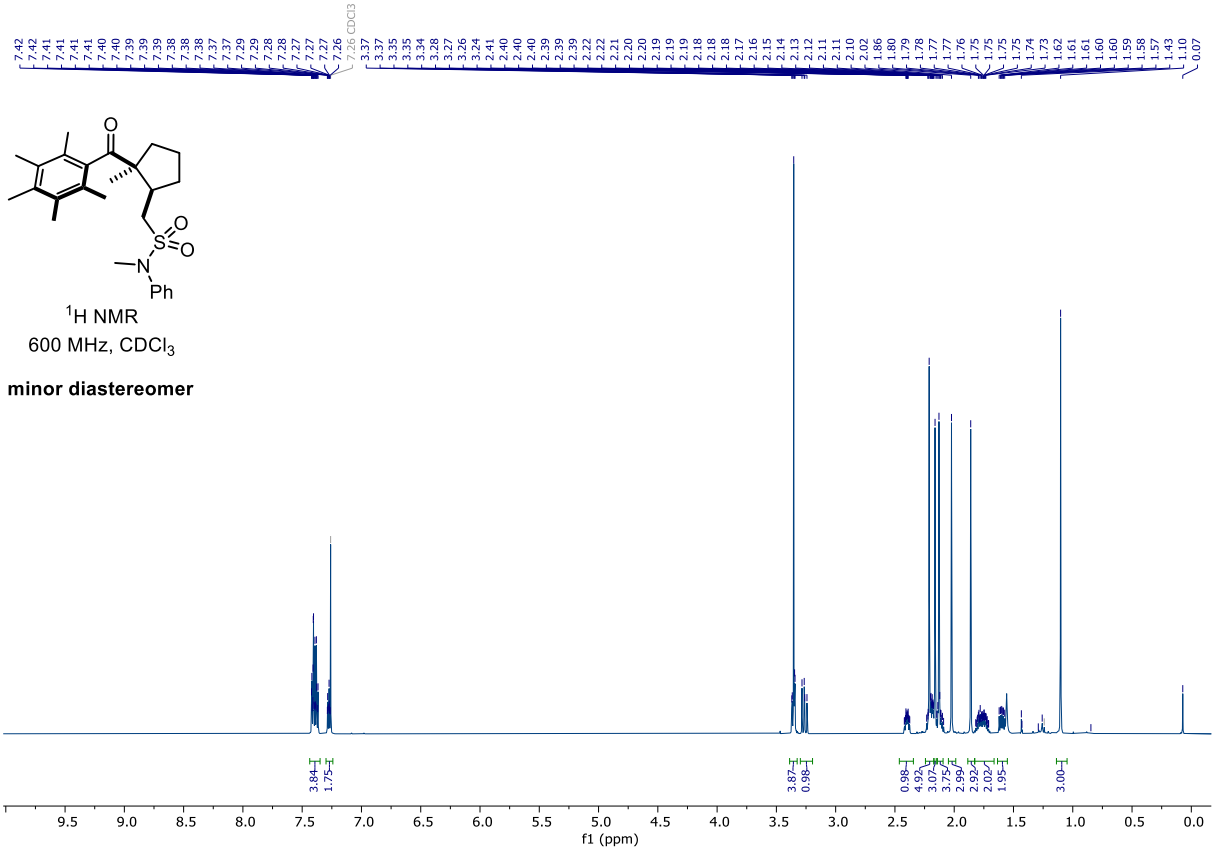


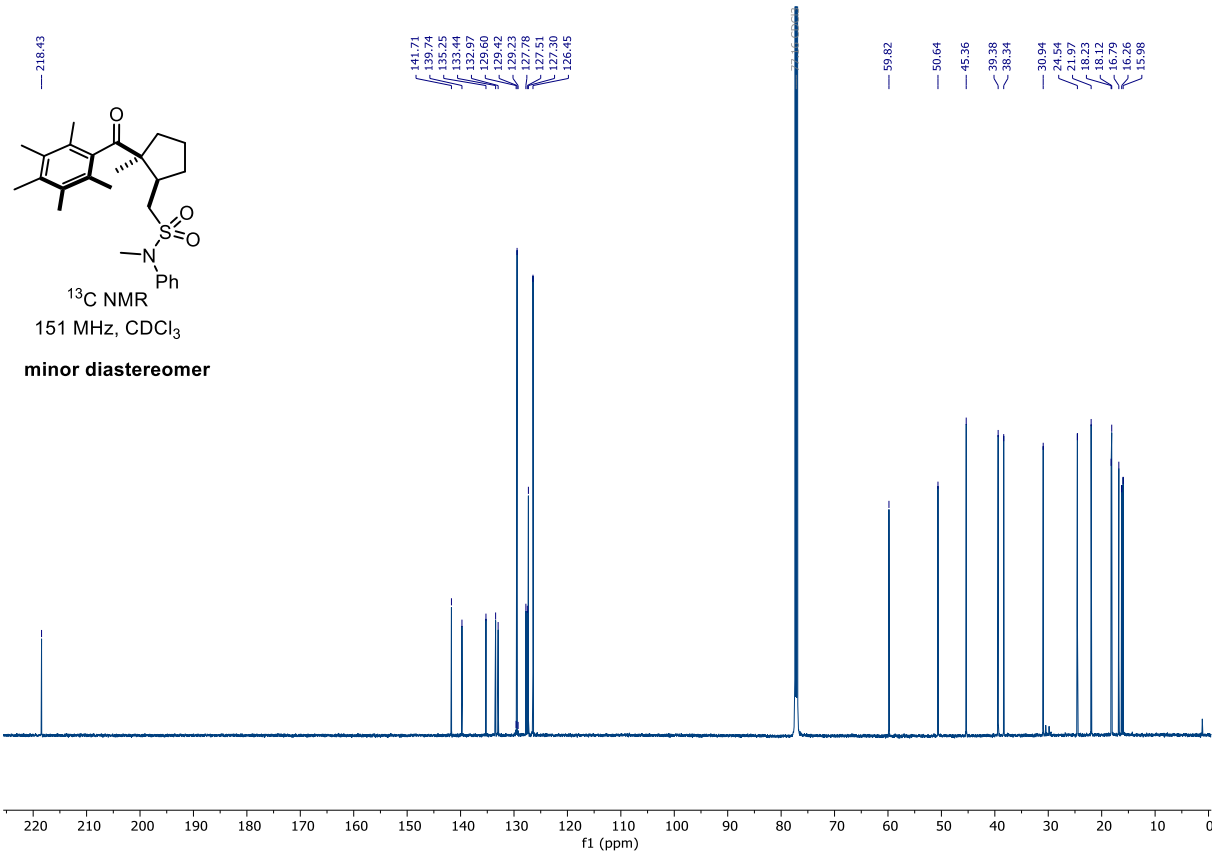
^{1}H NMR
600 MHz, $CDCl_3$
major diastereomer



^{13}C NMR
151 MHz, $CDCl_3$
major diastereomer

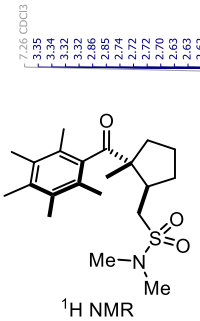
***cis*-3h *N*-Methyl-1-(2-(1*SR*, 2*RS*)methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)-*N*-phenylmethanesulfonamide**





***trans*-3i *N*,*N*-Dimethyl-1-((1*RS*, 2*RS*)-**

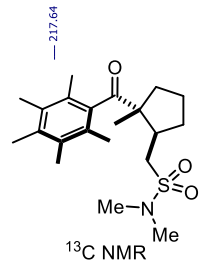
2-methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)methanesulfonamide



^{1}H NMR

600 MHz, $CDCl_3$

major diastereomer



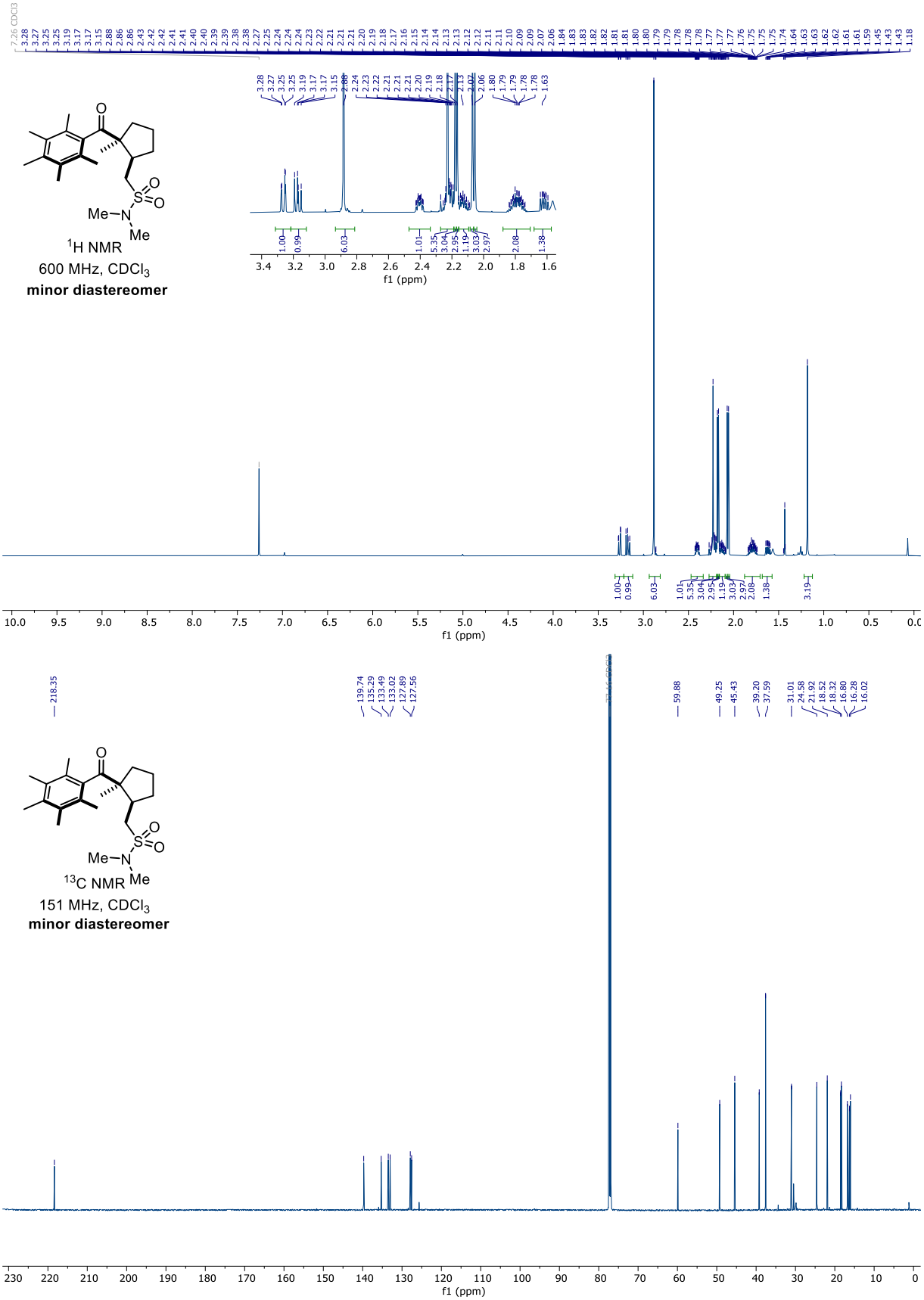
^{13}C NMR

151 MHz, $CDCl_3$

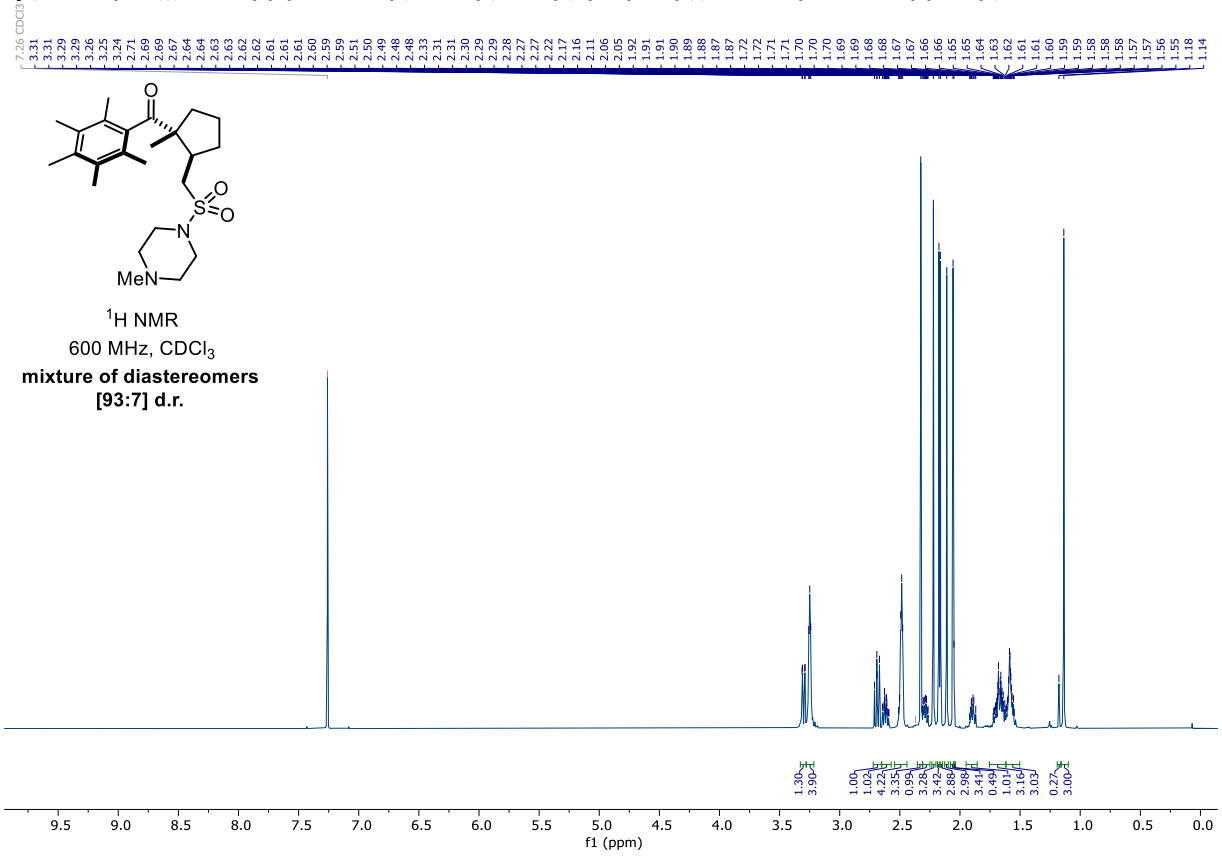
major diastereomer

***cis*-3i *N*,*N*-Dimethyl-1-((1*SR*, 2*RS*)-**

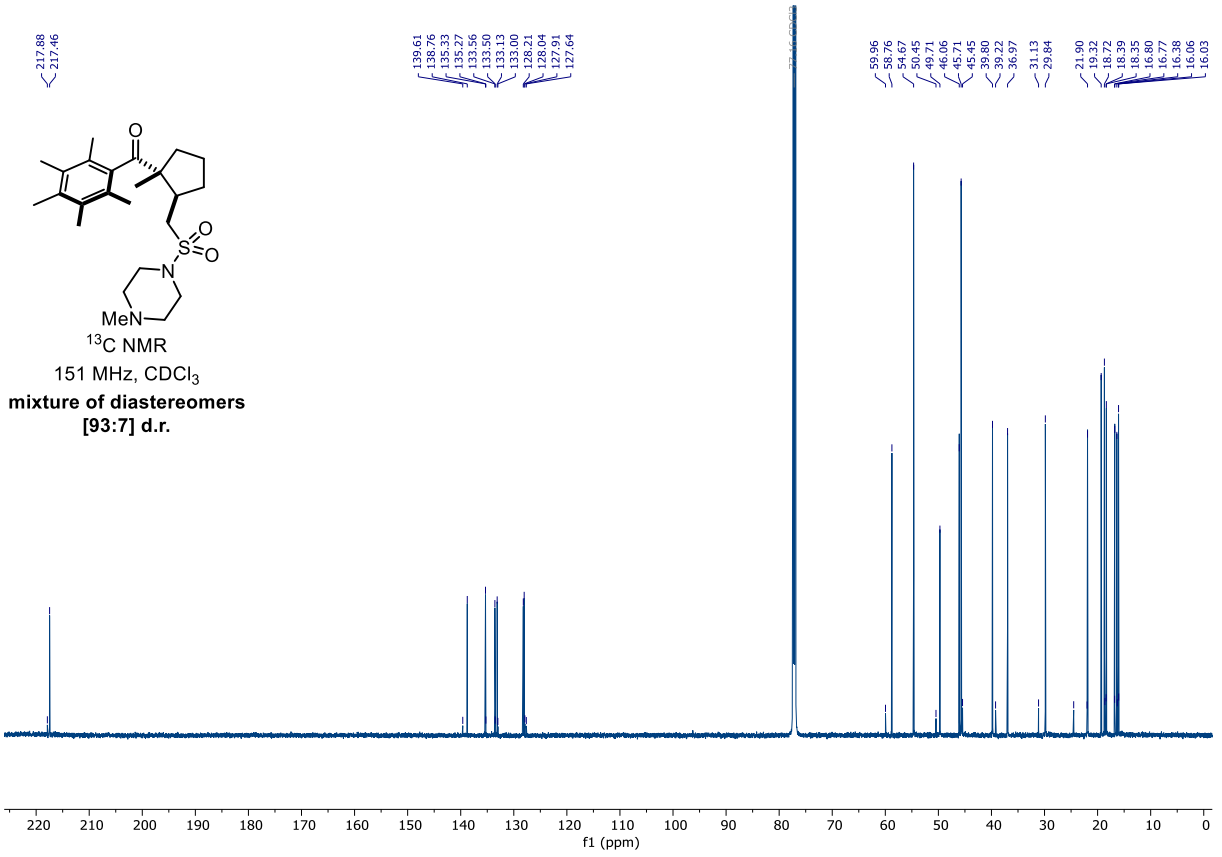
2-methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)methanesulfonamide



3j (1-Methyl-2-(((4-methylpiperazin-1-yl)sulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone

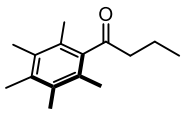


^{1}H NMR
600 MHz, $CDCl_3$
mixture of diastereomers
[93:7] d.r.

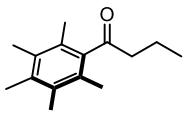


^{13}C NMR
151 MHz, $CDCl_3$
mixture of diastereomers
[93:7] d.r.

S10 1-(2,3,4,5,6-Pentamethylphenyl)butan-1-one

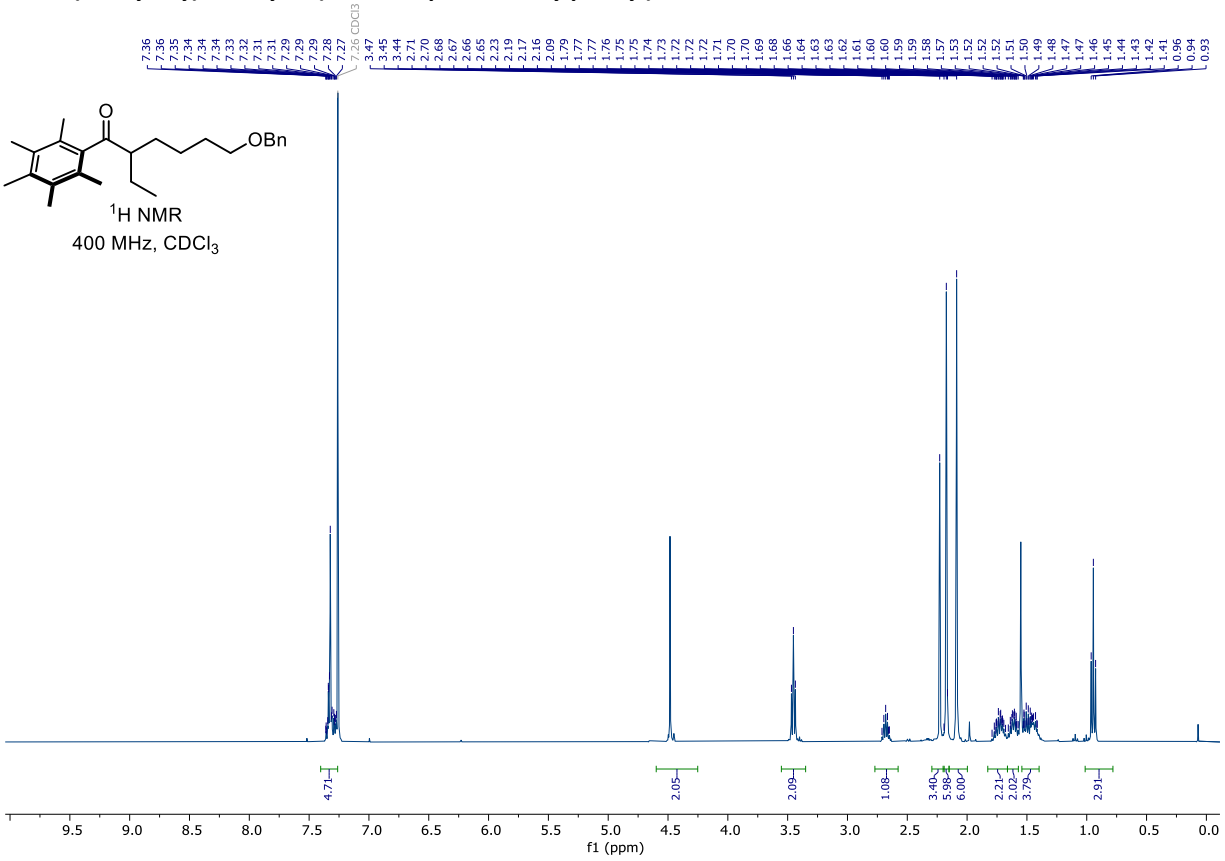


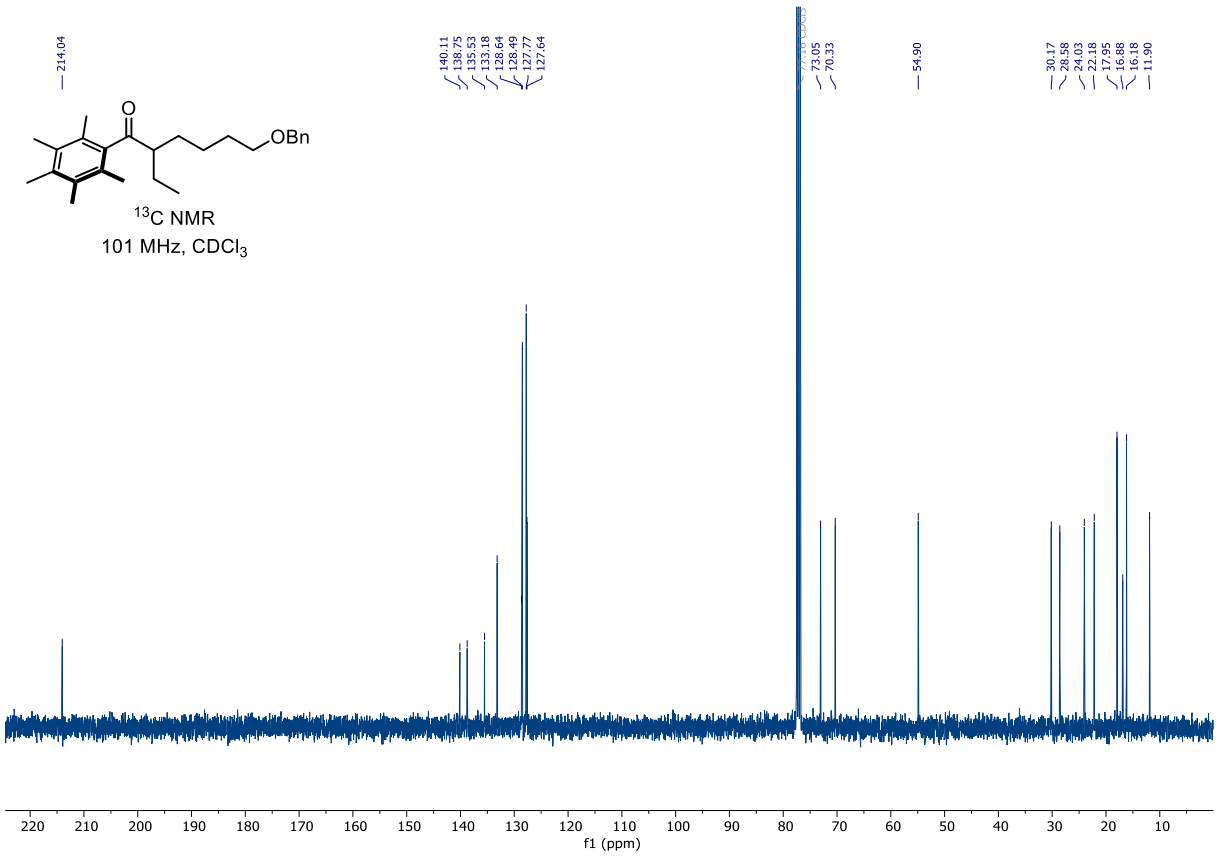
^{1}H NMR
400 MHz, $CDCl_3$



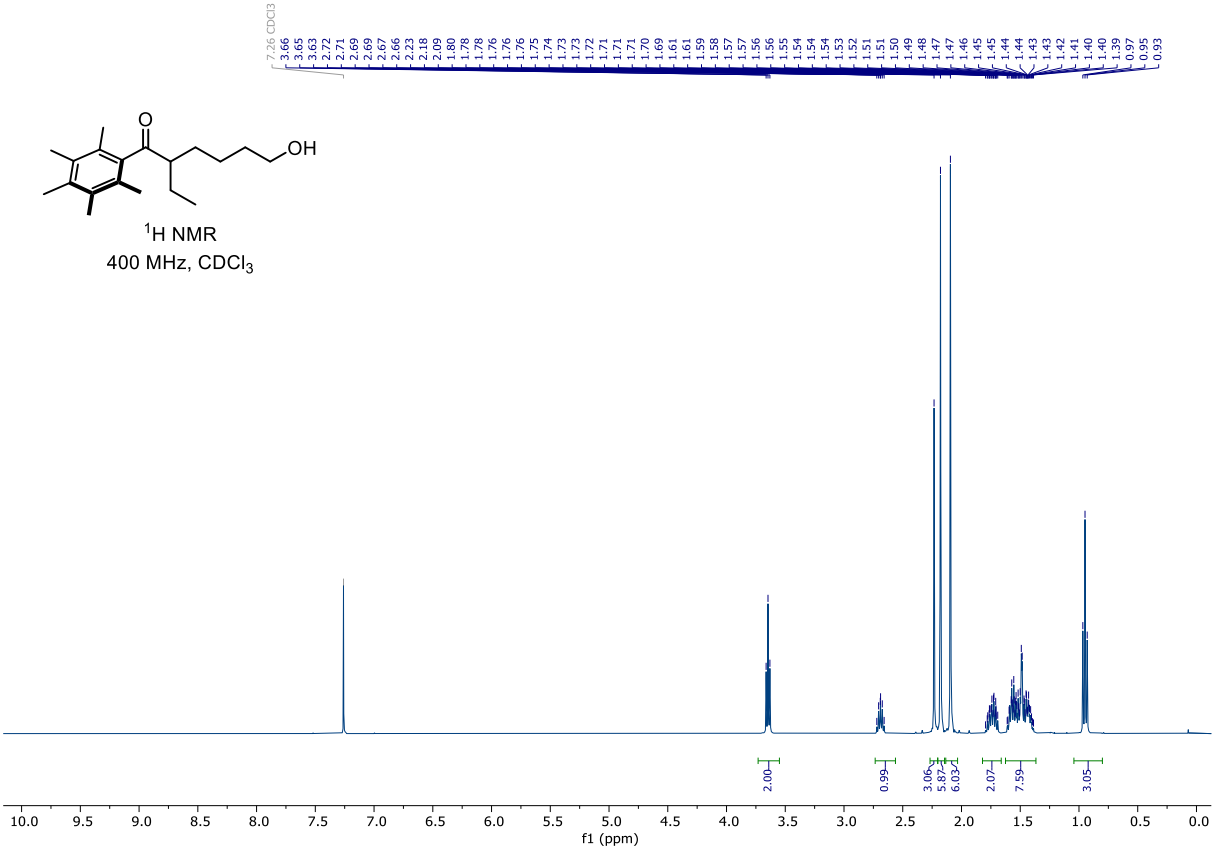
^{13}C NMR
101 MHz, $CDCl_3$

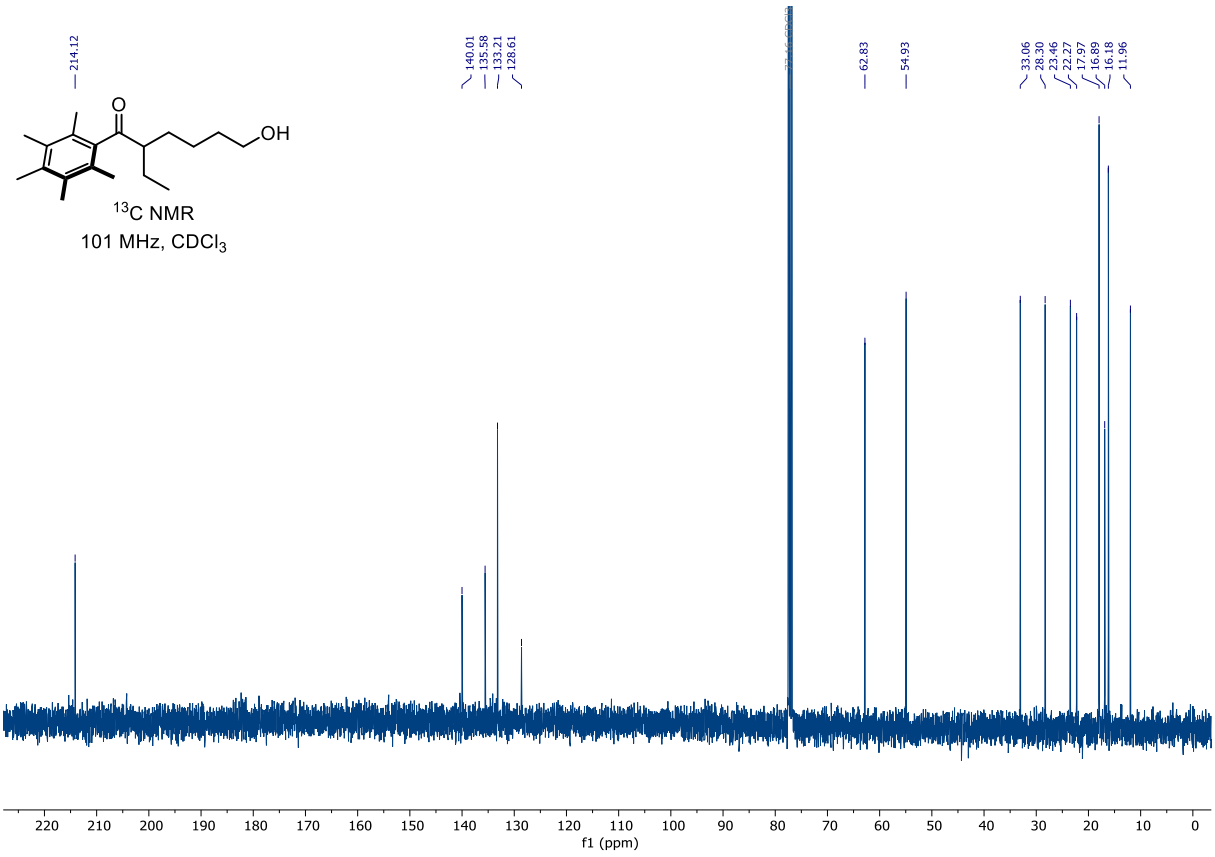
S11 6-(Benzyloxy)-2-ethyl-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one



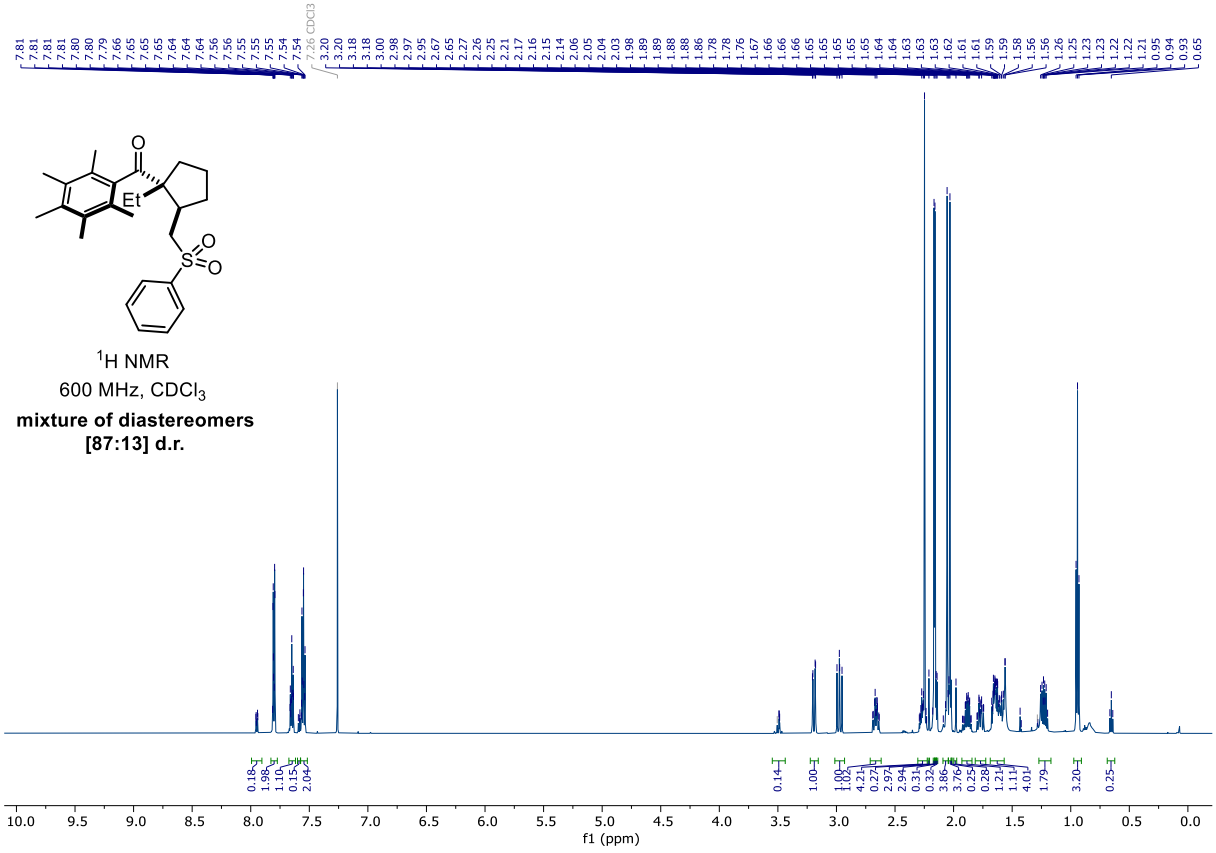


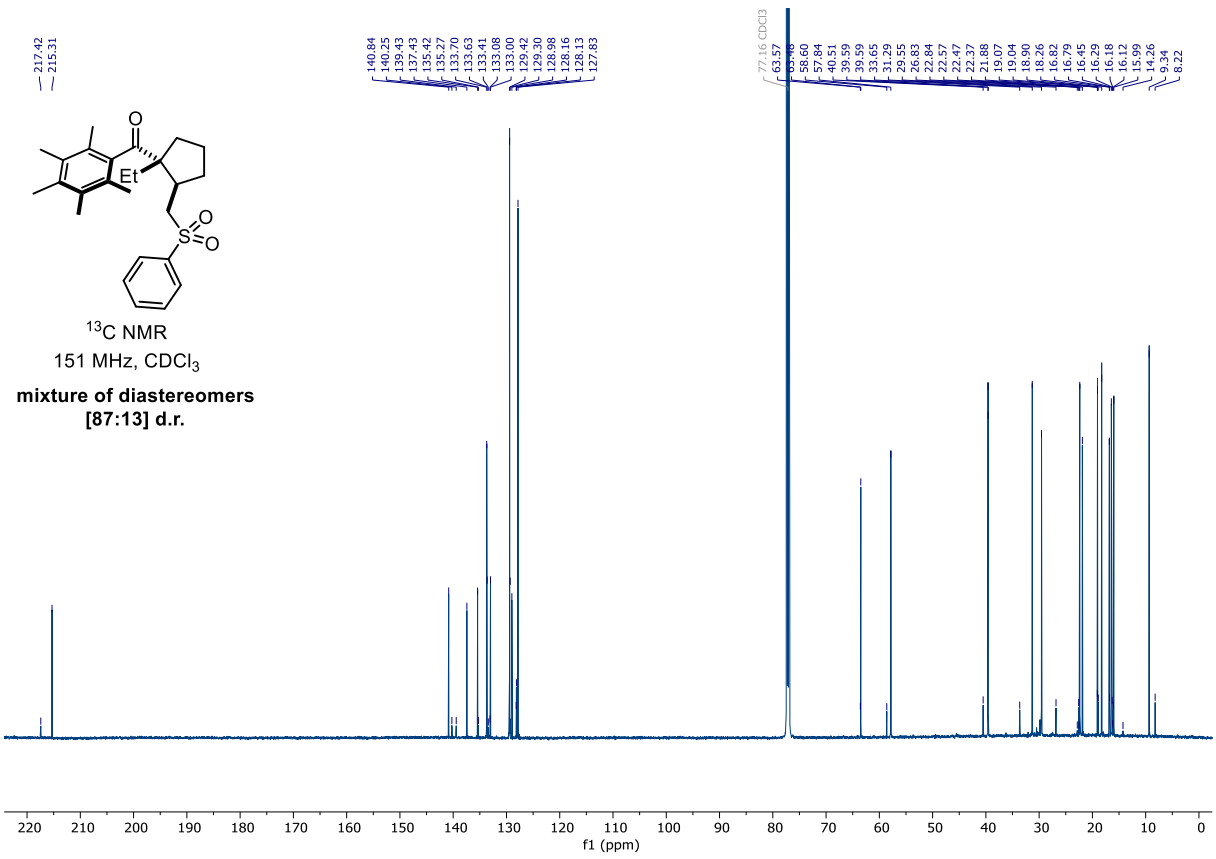
1k 2-Ethyl-6-hydroxy-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one



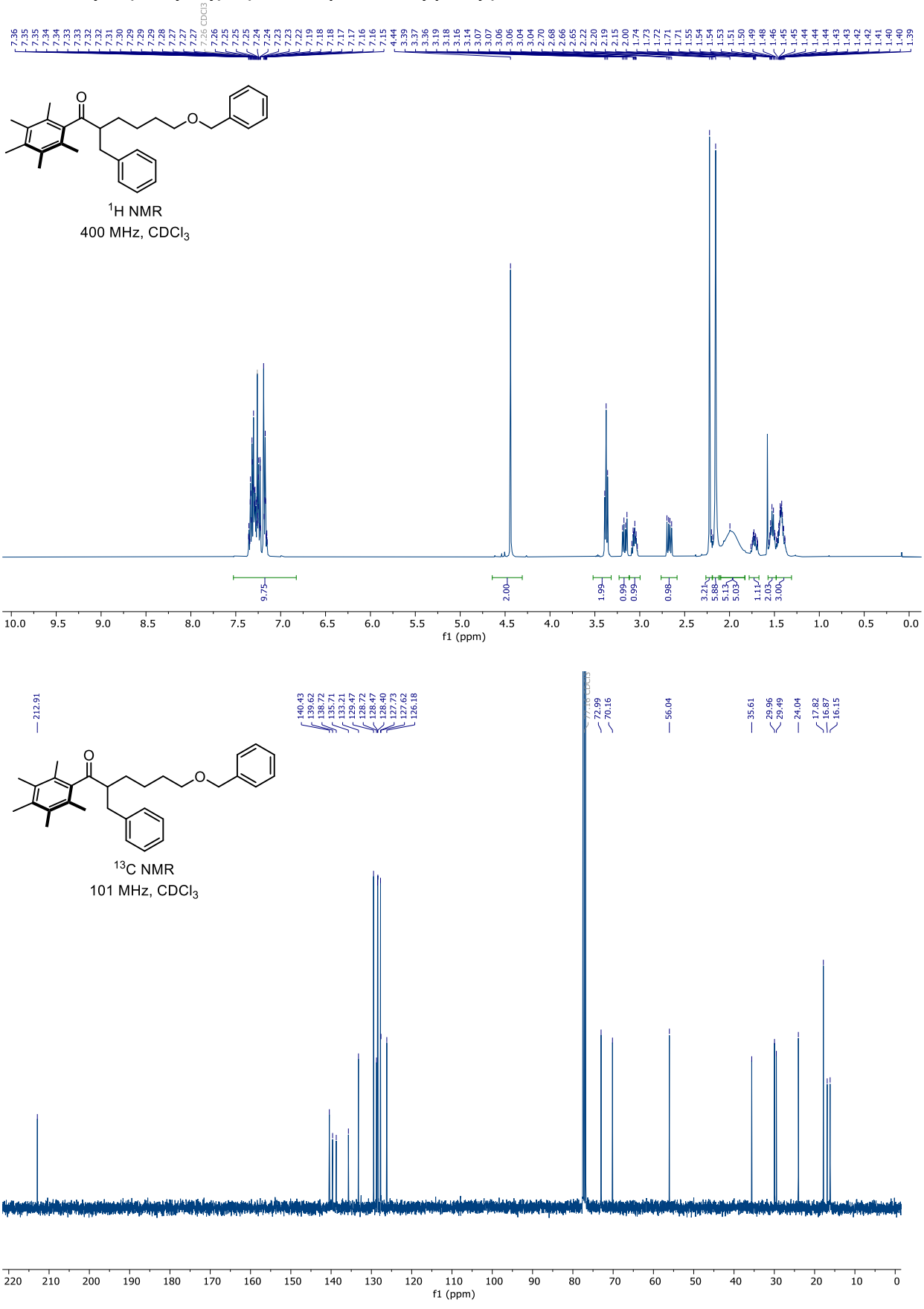


3k (1-Ethyl-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone

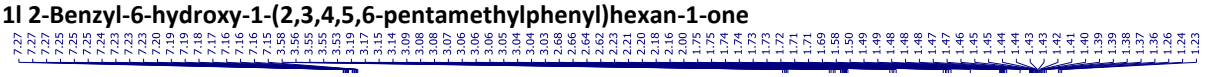


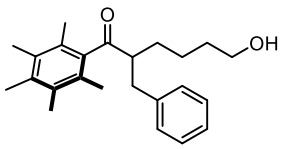


S13 2-Benzyl-6-(benzyloxy)-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one

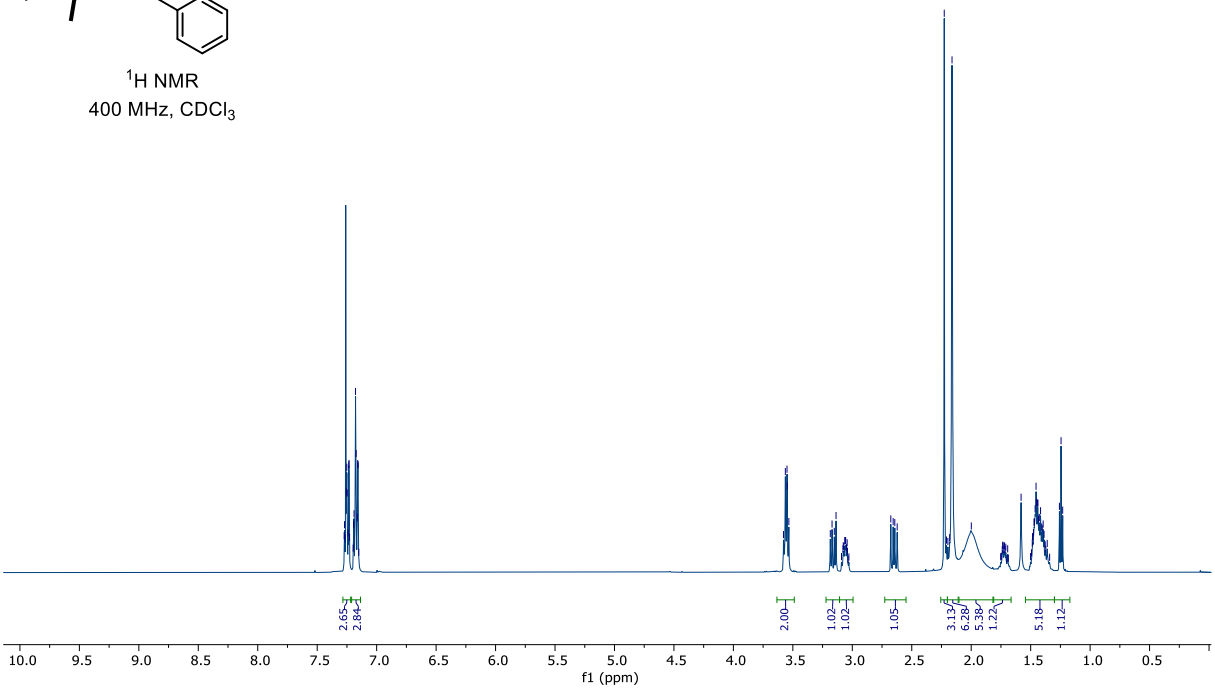


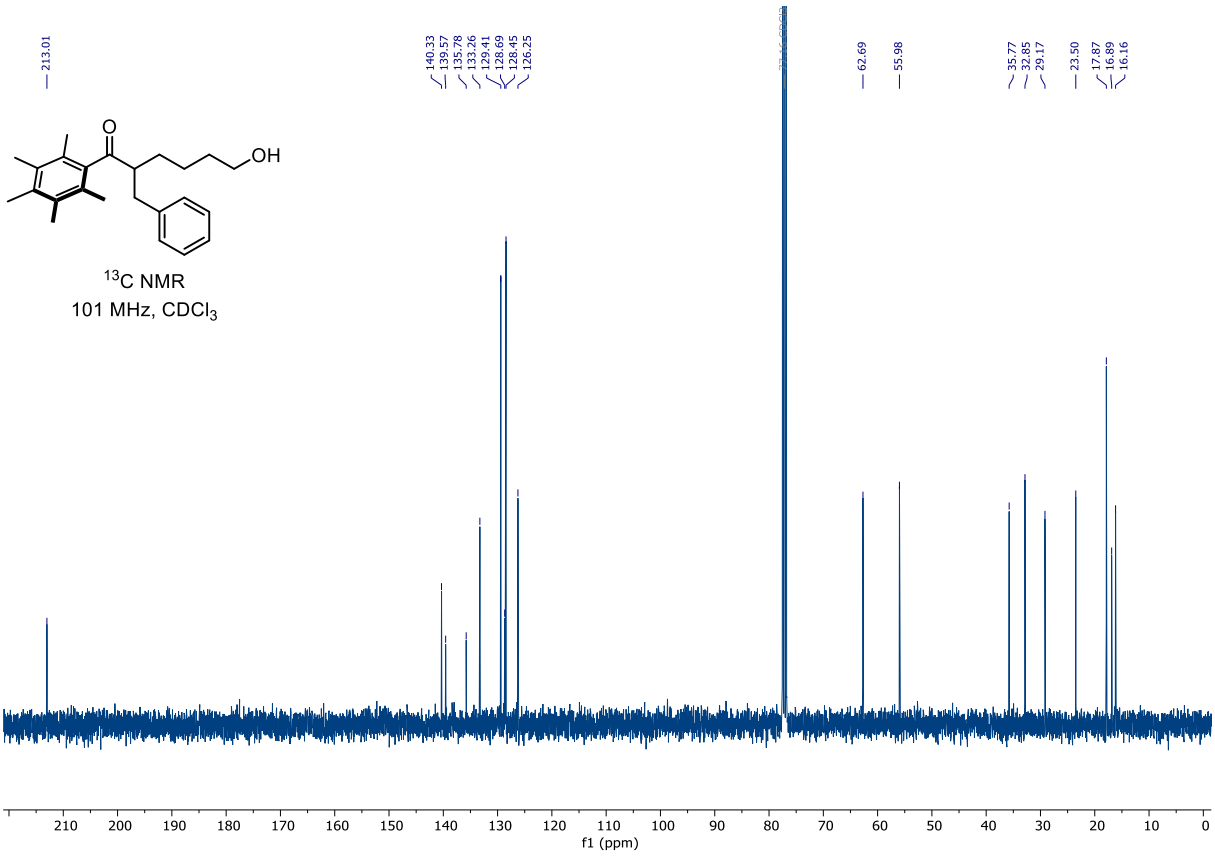
1l 2-Benzyl-6-hydroxy-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one





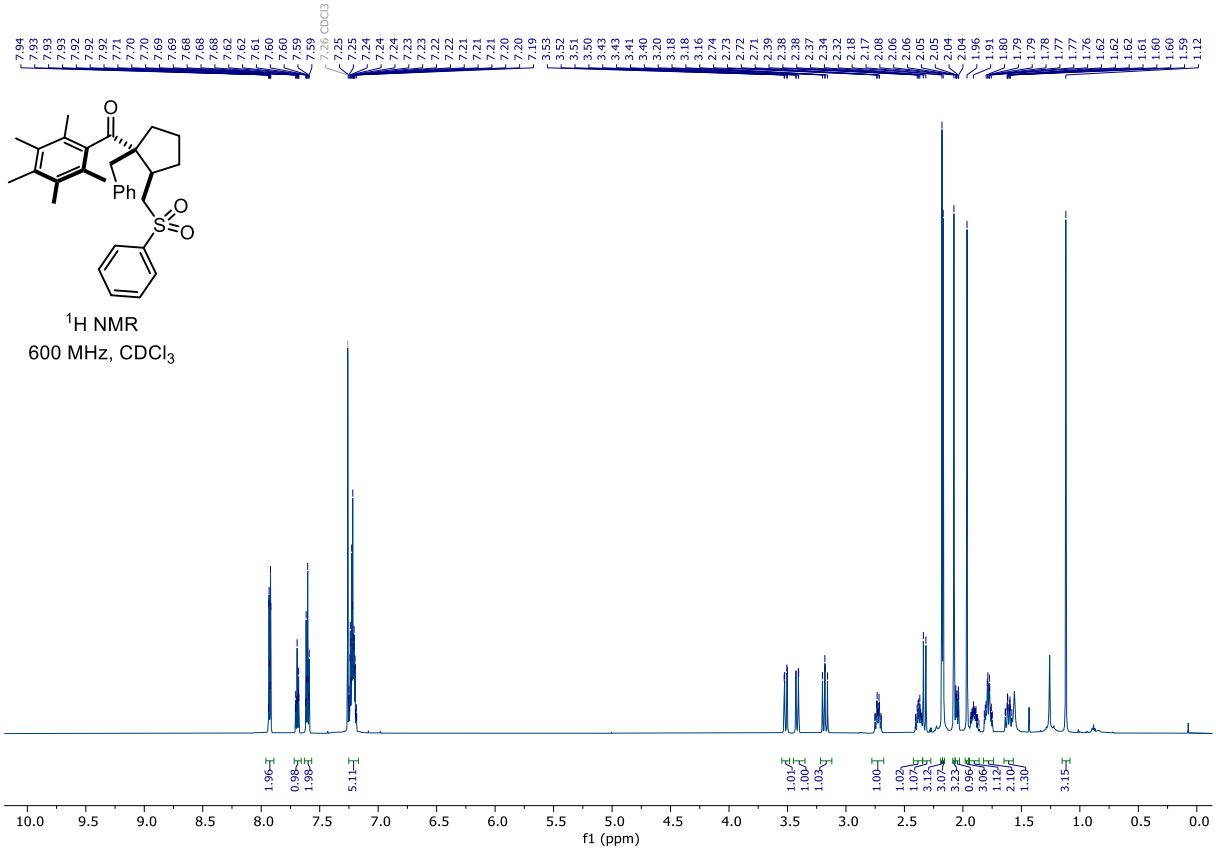
^{1}H NMR
400 MHz, $CDCl_3$

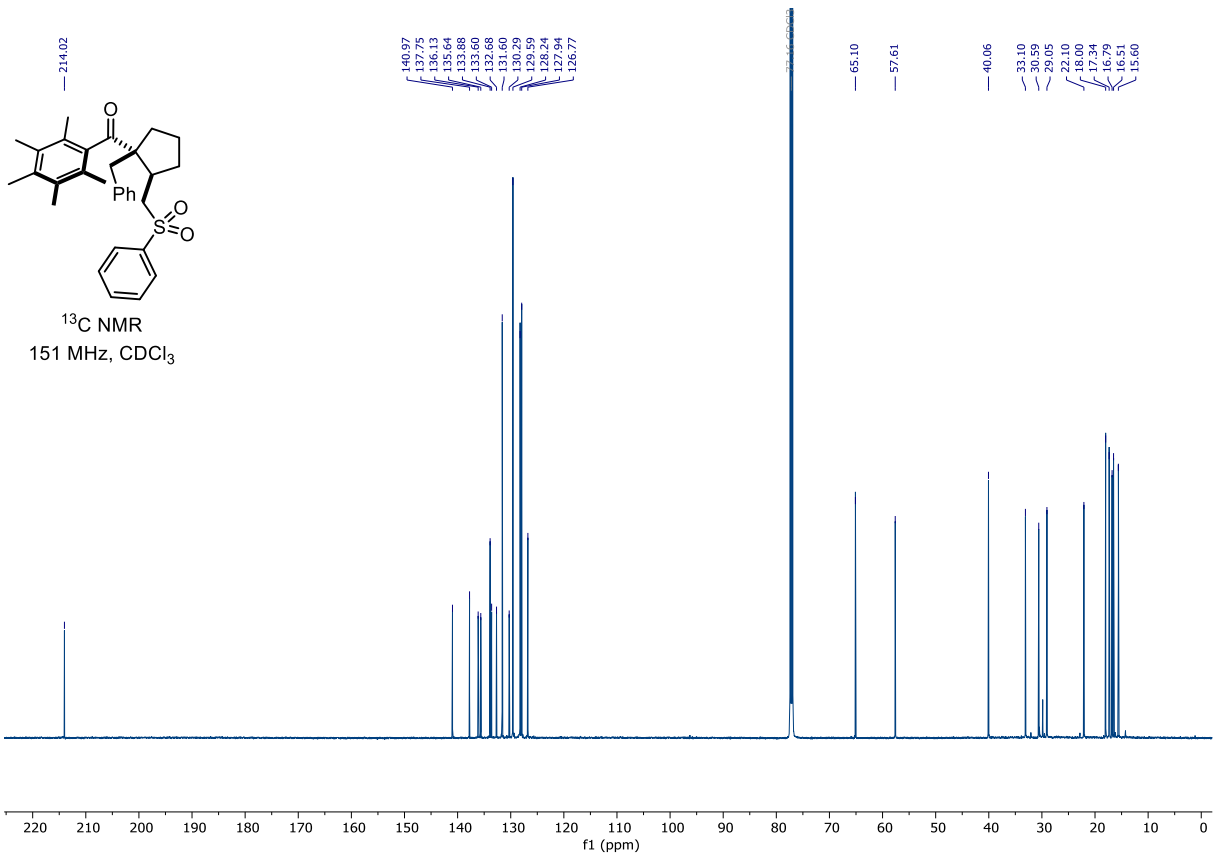




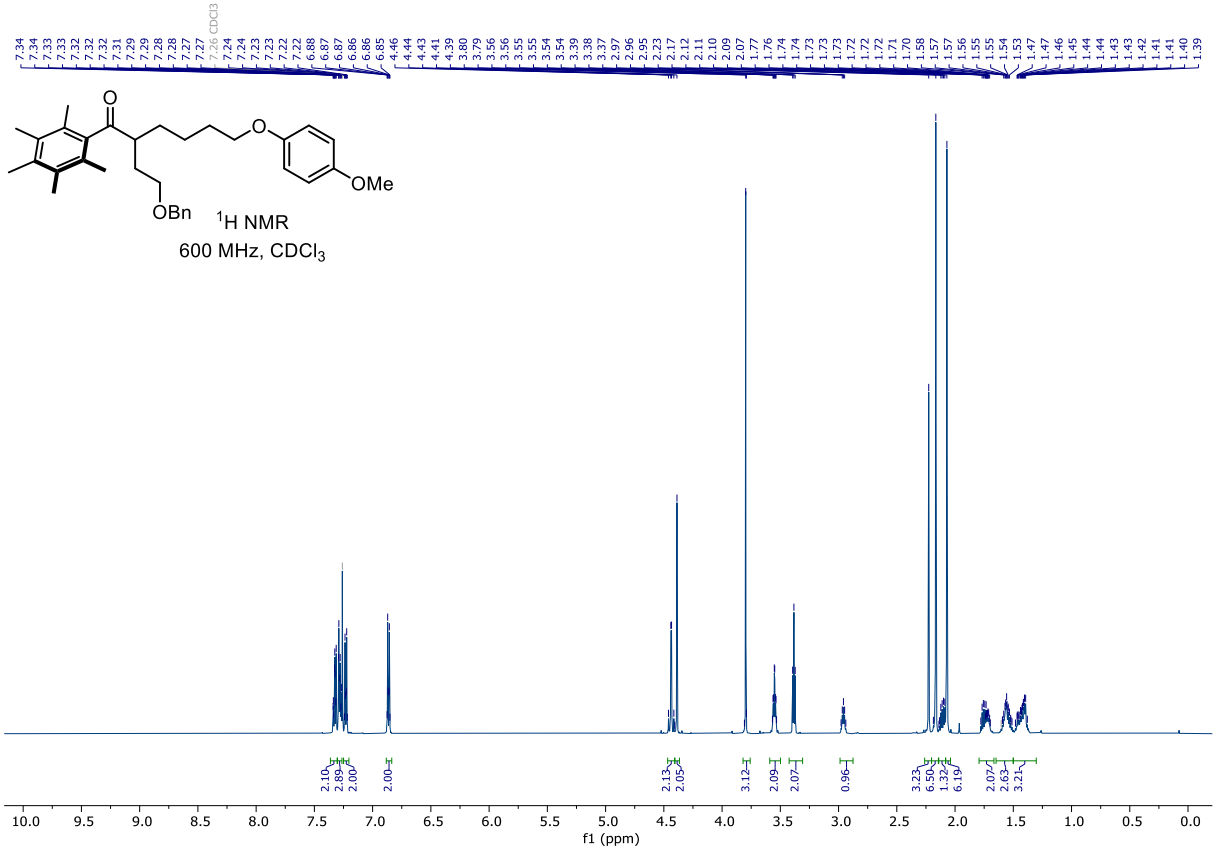
^{13}C NMR
101 MHz, $CDCl_3$

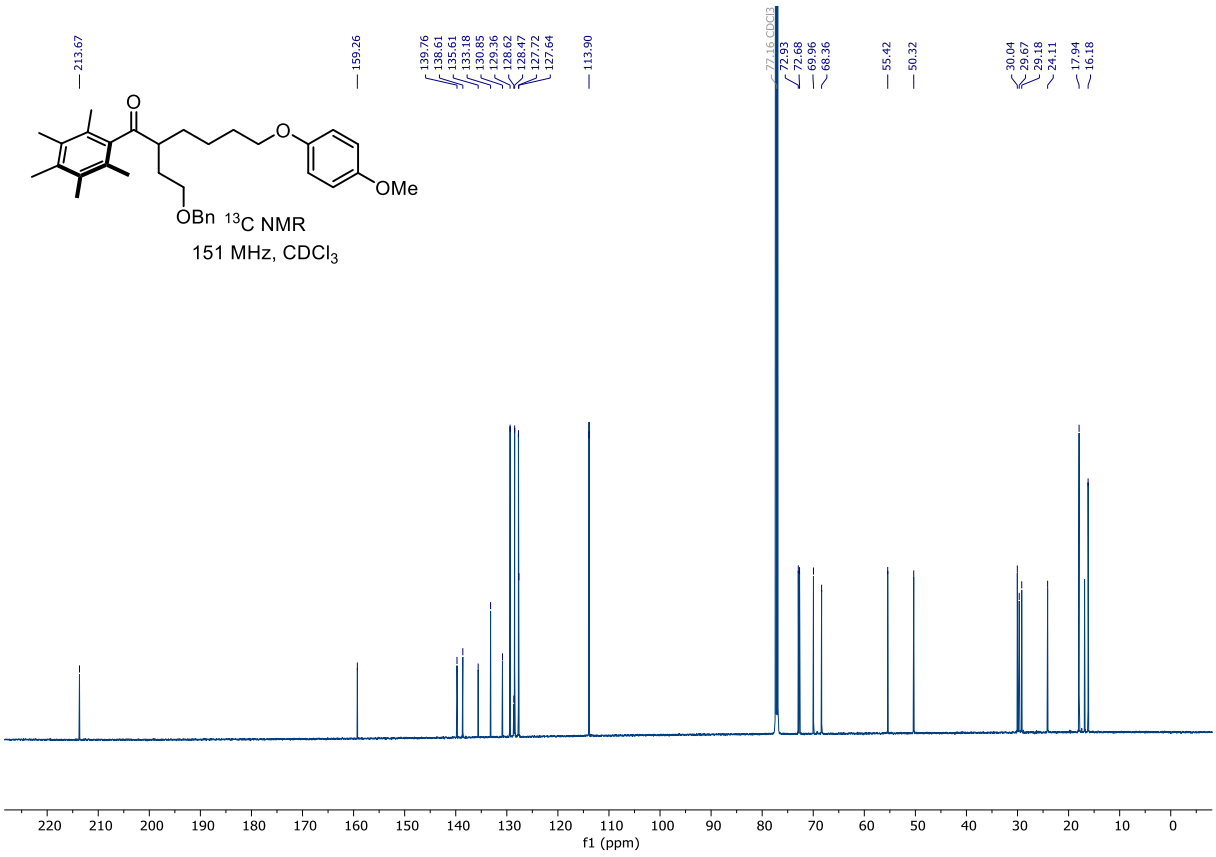
3l ((1*S*,2*R*))-1-Benzyl-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone



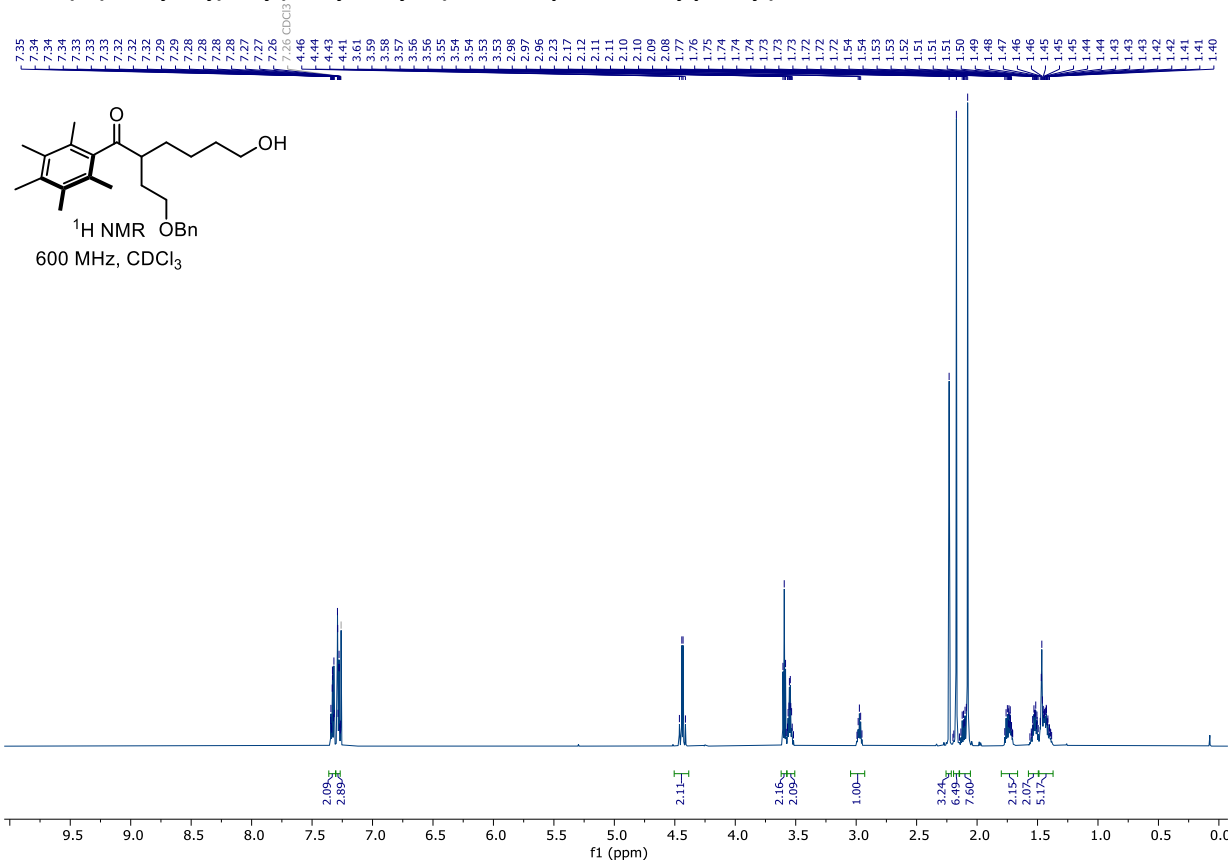


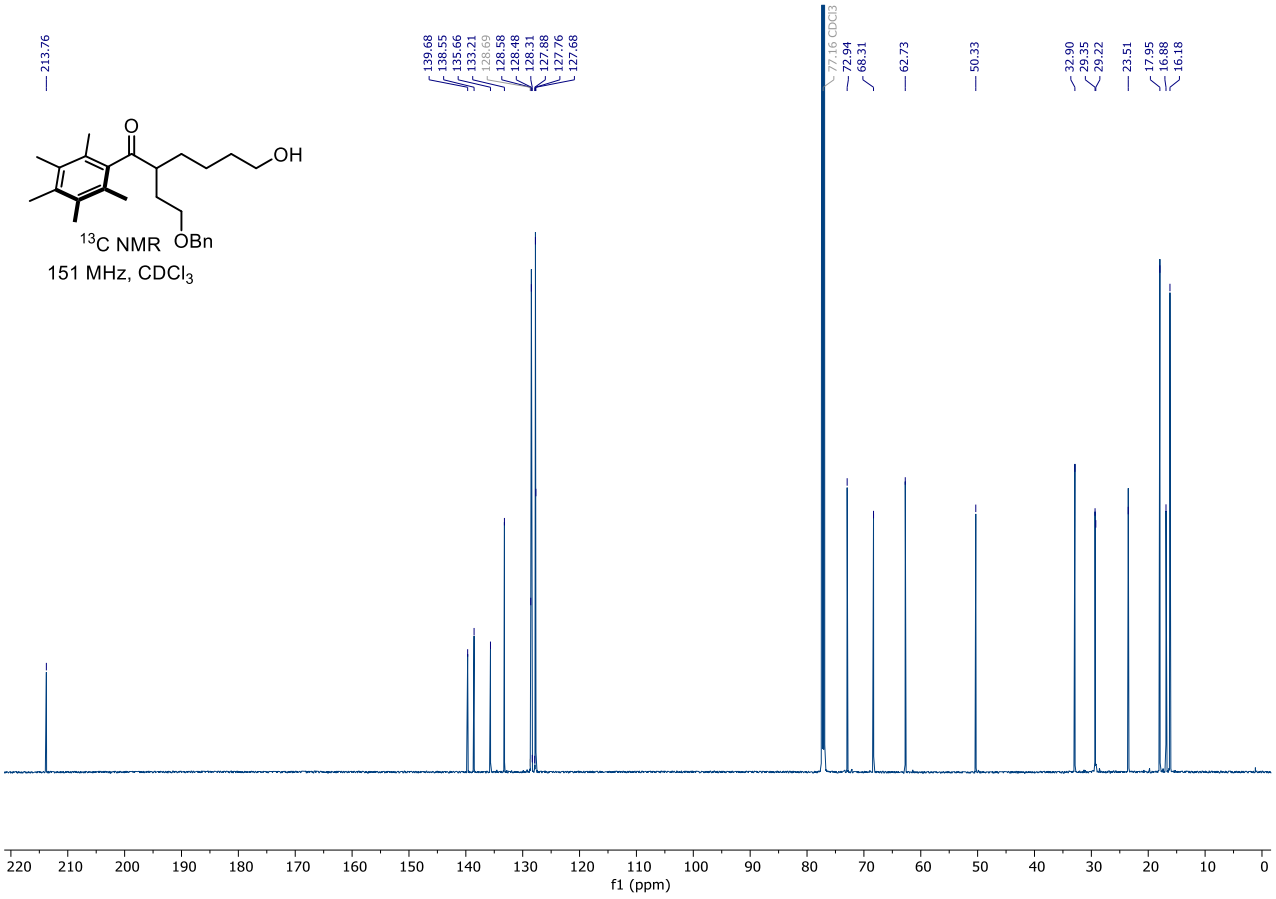
S18 2-(2-(Benzyloxy)ethyl)-6-((4-methoxybenzyl)oxy)-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one



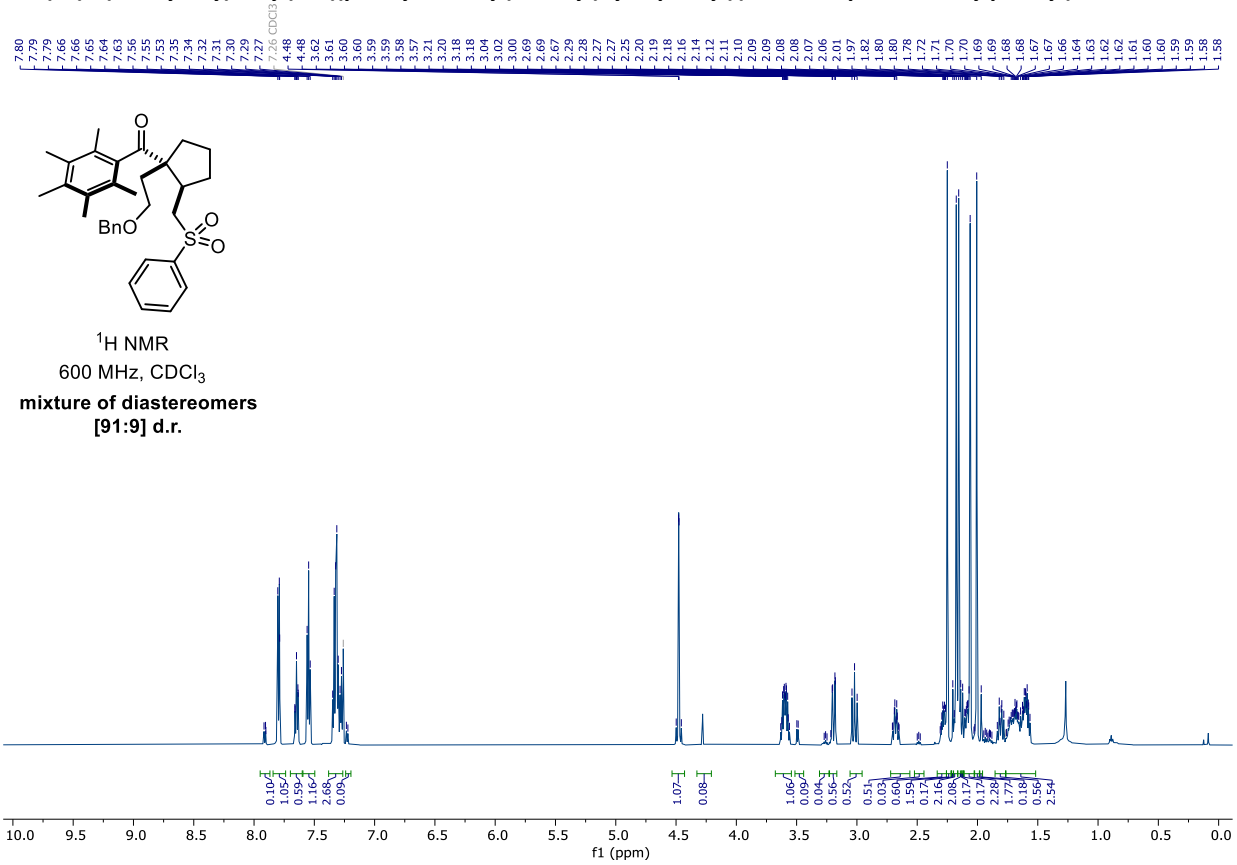


1m 2-(2-(Benzyloxy)ethyl)-6-hydroxy-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one

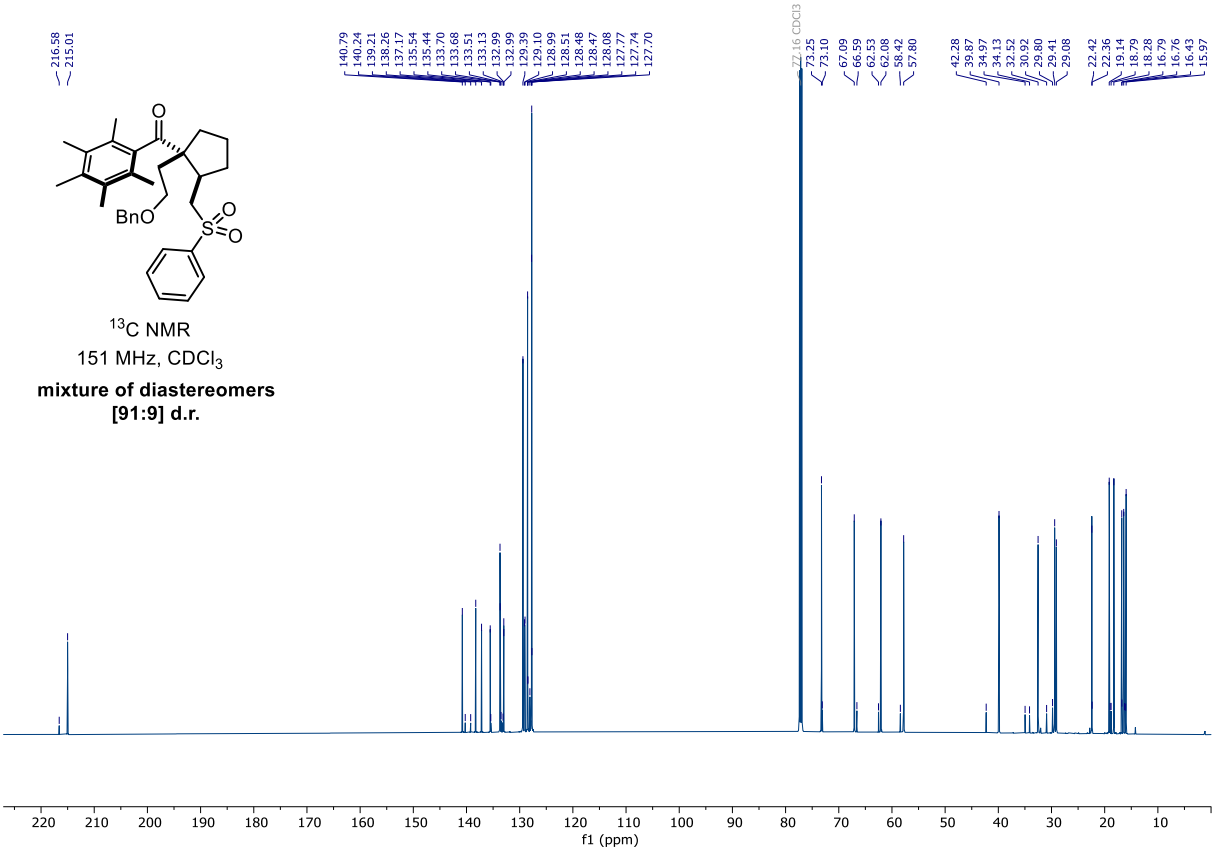




3m (1-(2-(Benzyloxy)ethyl)-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone

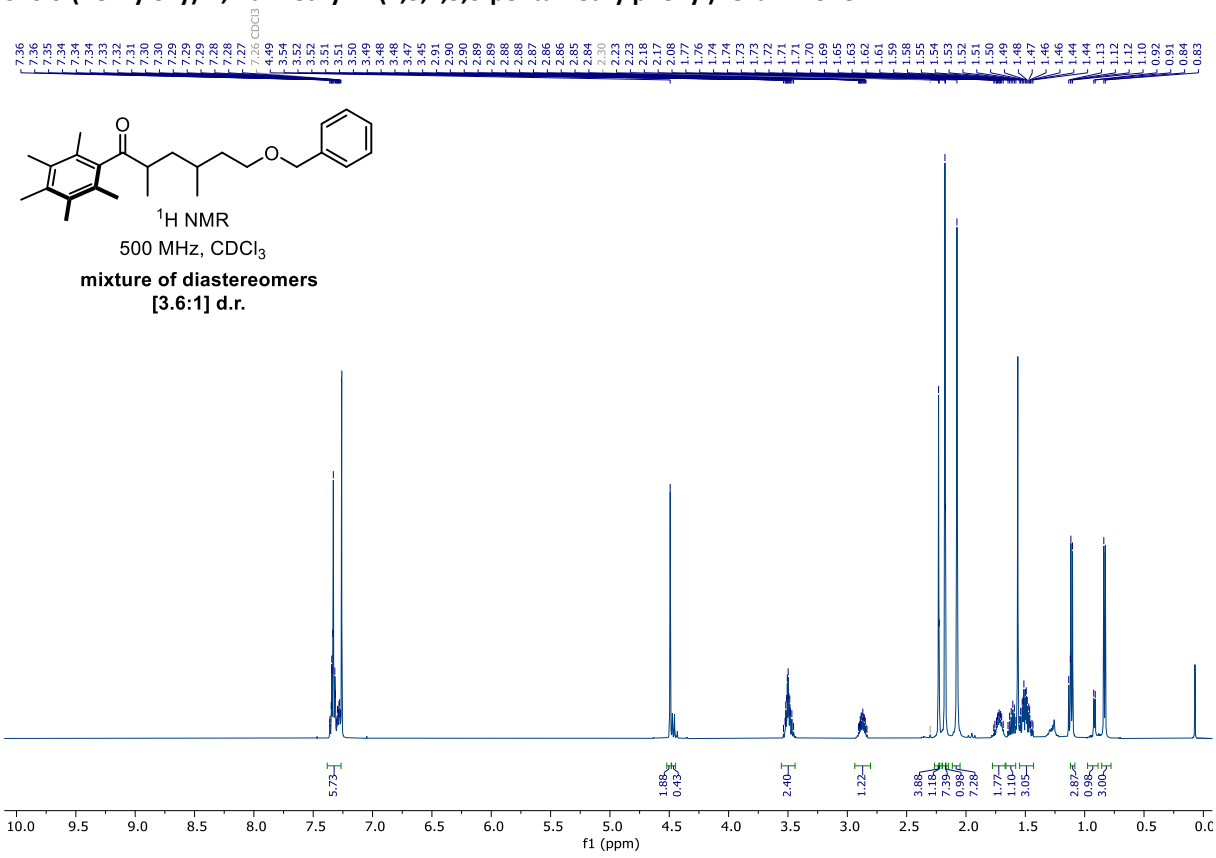


^{1}H NMR
600 MHz, $CDCl_3$
mixture of diastereomers
[91:9] d.r.

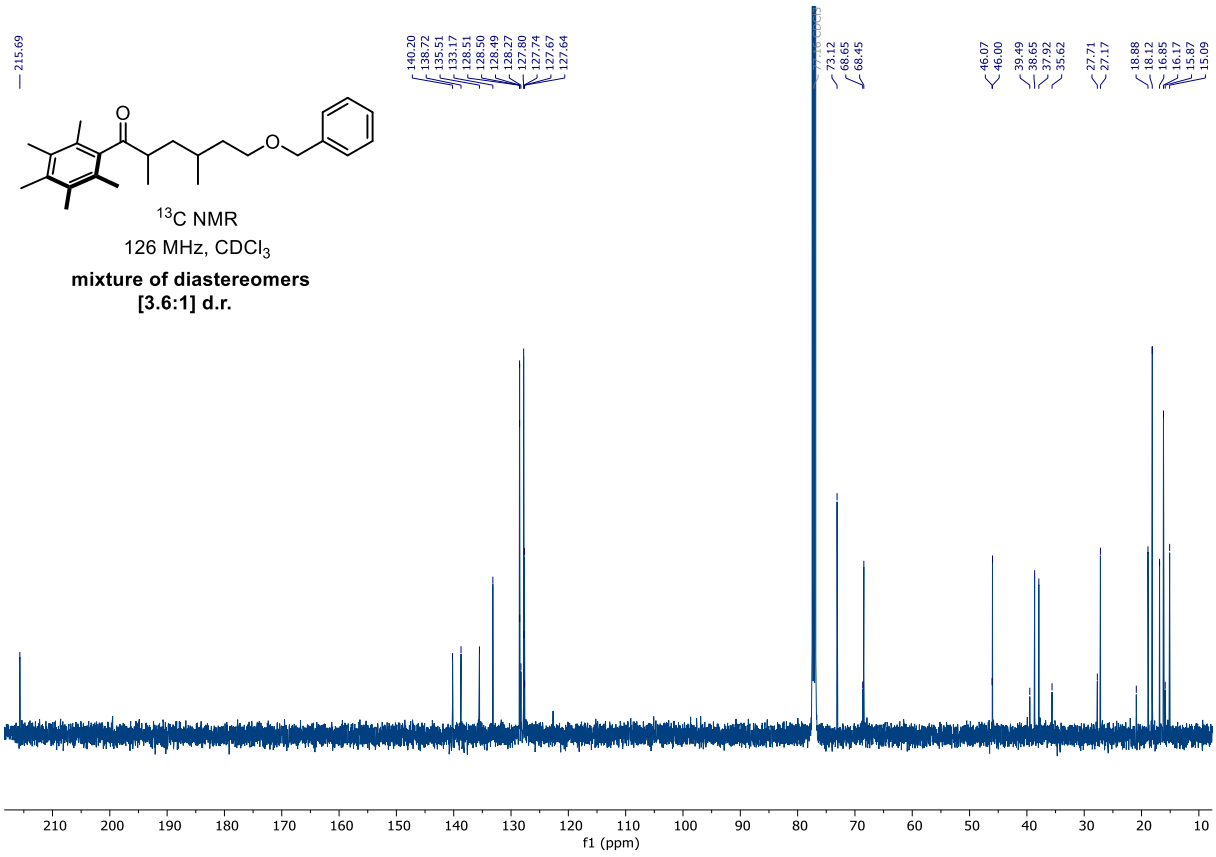


^{13}C NMR
151 MHz, $CDCl_3$
mixture of diastereomers
[91:9] d.r.

S20 6-(Benzyloxy)-2,4-dimethyl-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one

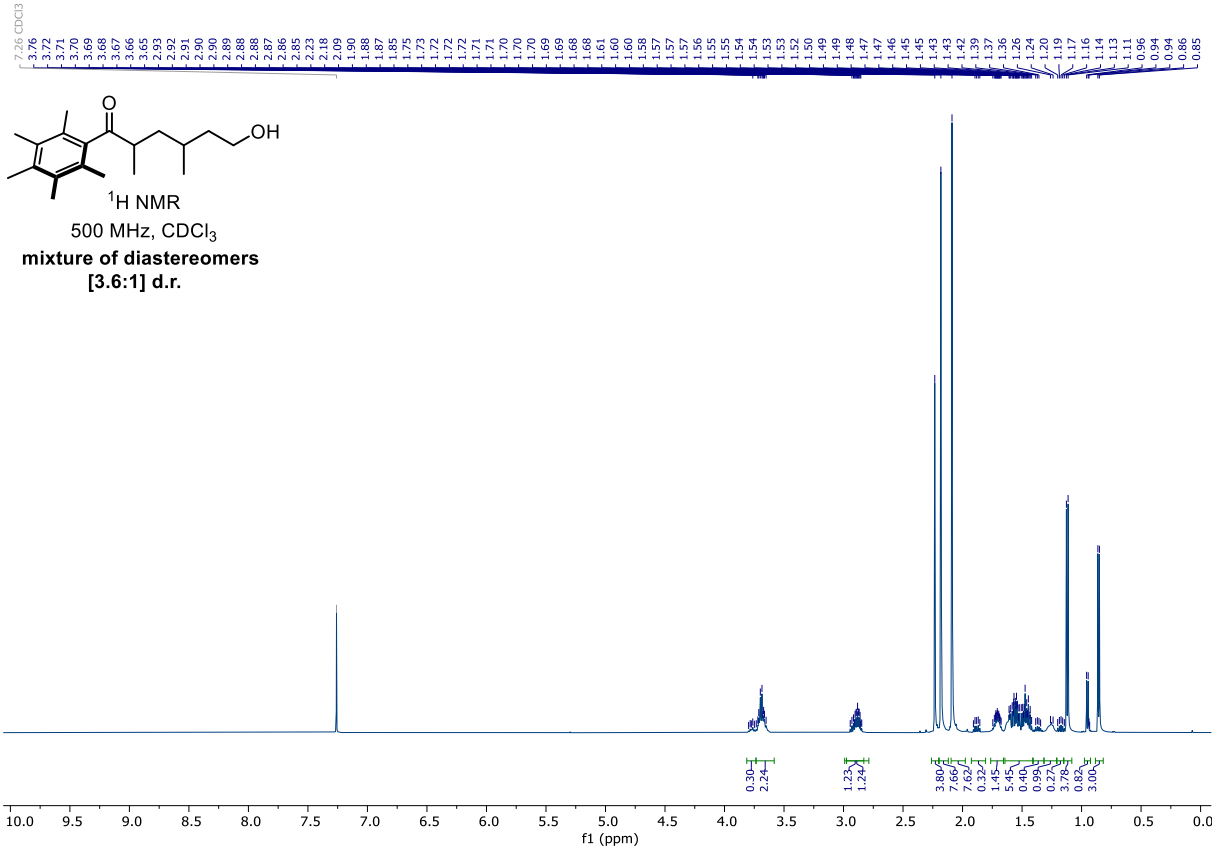


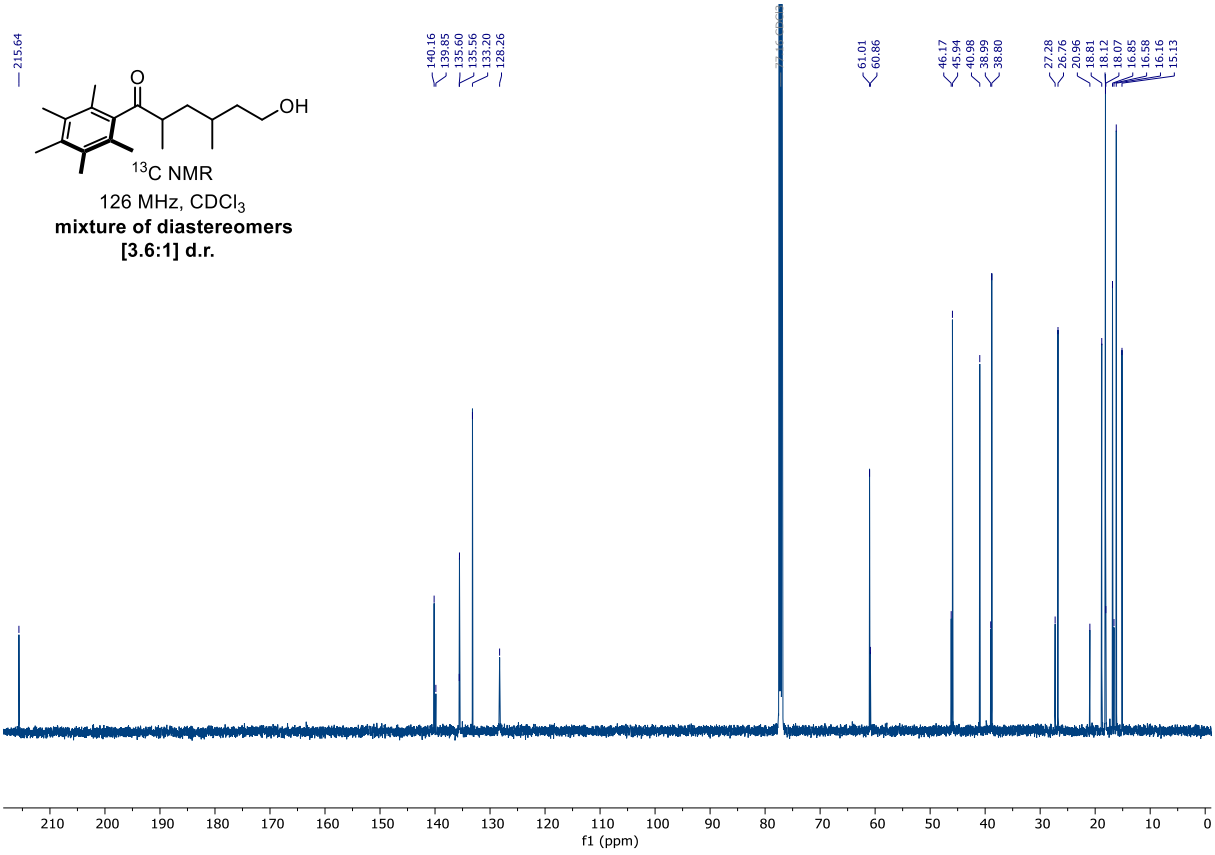
^{1}H NMR
500 MHz, $CDCl_3$
mixture of diastereomers
[3.6:1] d.r.



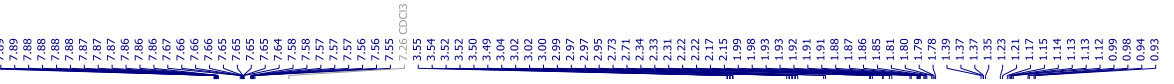
^{13}C NMR
126 MHz, $CDCl_3$
mixture of diastereomers
[3.6:1] d.r.

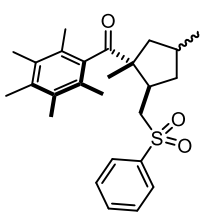
1n 6-Hydroxy-2,4-dimethyl-1-(2,3,4,5,6-pentamethylphenyl)hexan-1-one

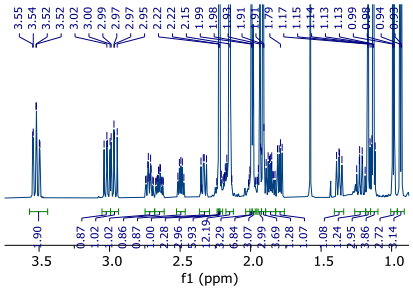




***trans*- 3n (((1*R*,2*R*,4*SR*) & (1*S*,2*S*,4*RS*))-1,4-Dimethyl-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

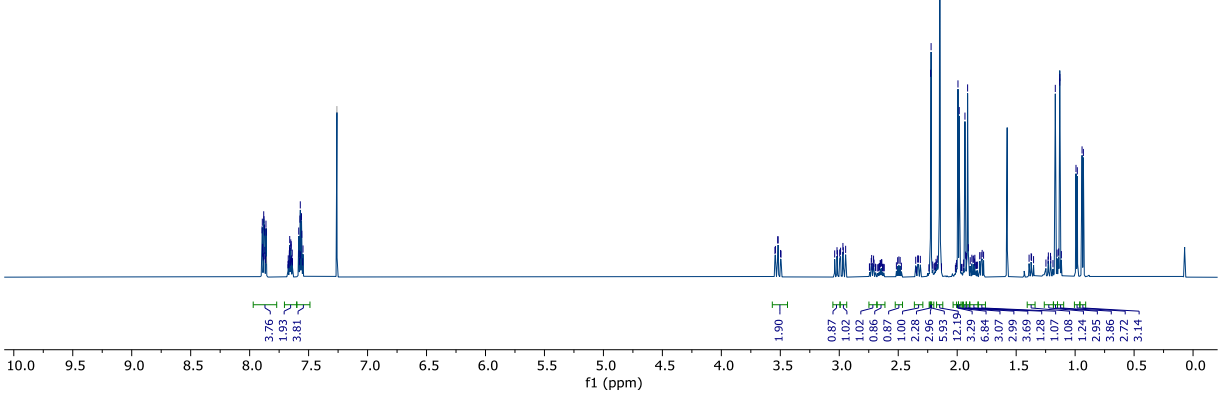


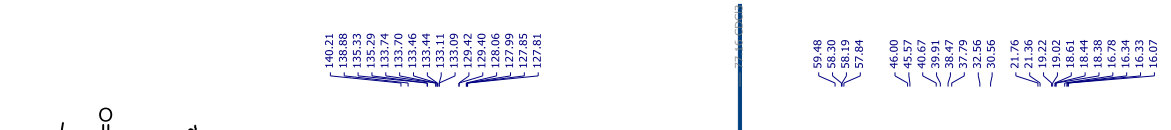




^{1}H NMR
600 MHz, $CDCl_3$

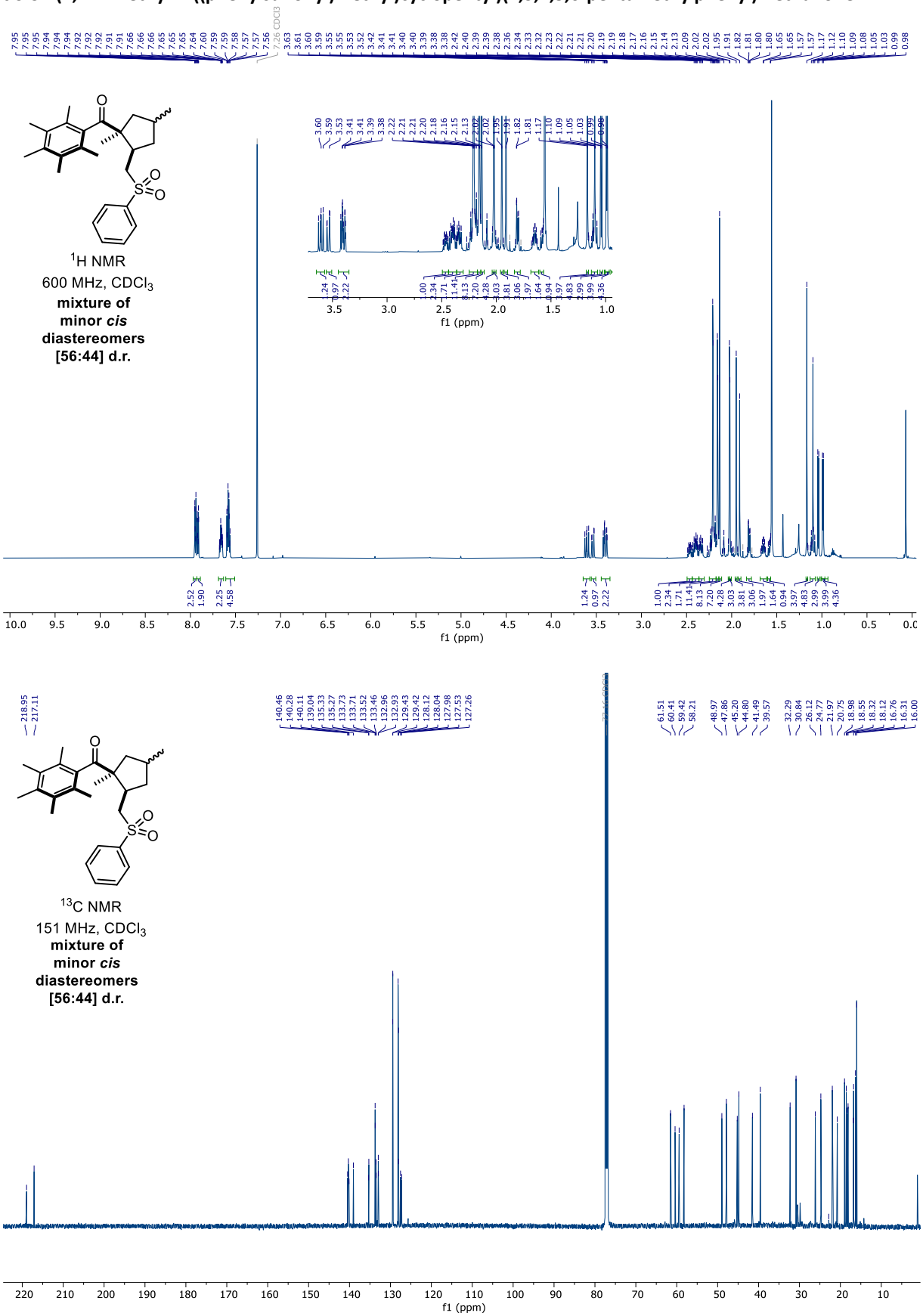
mixture of major *trans* diastereomers [53:47] d.r.



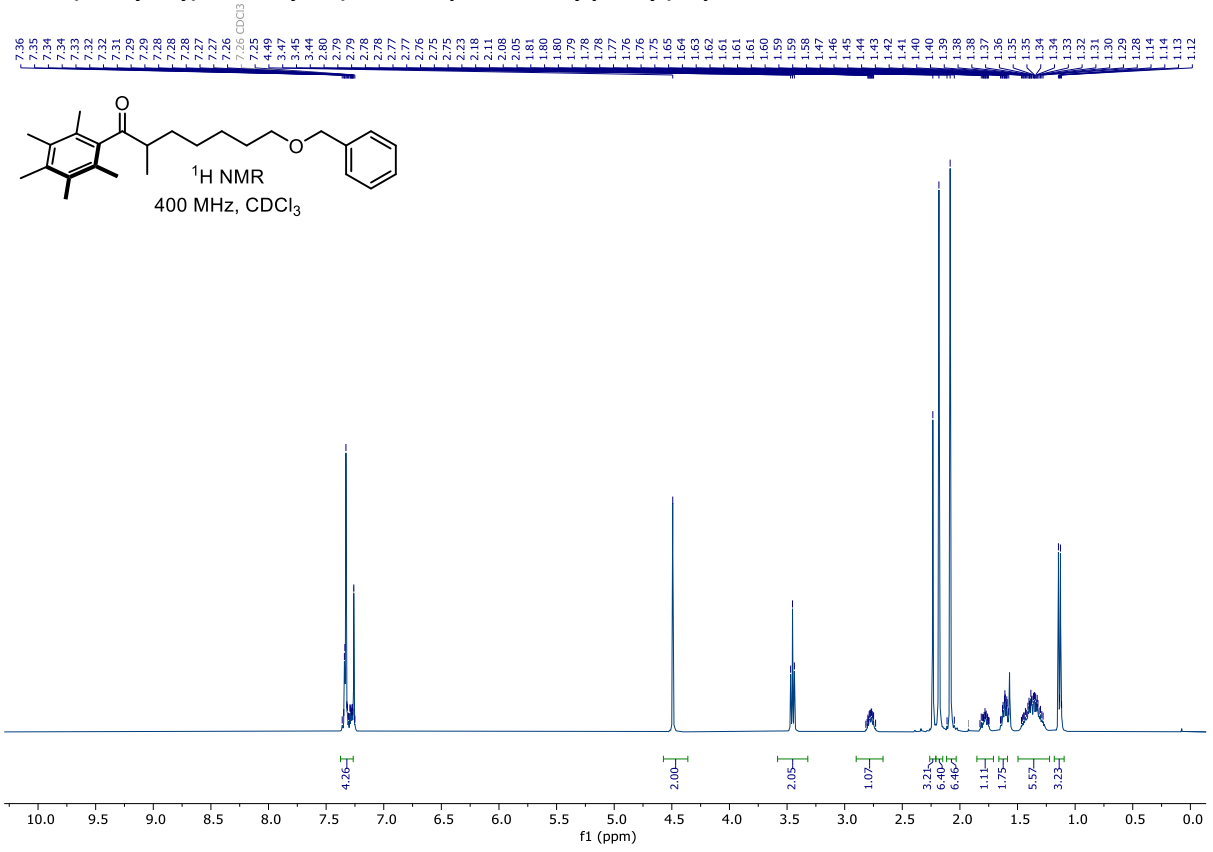


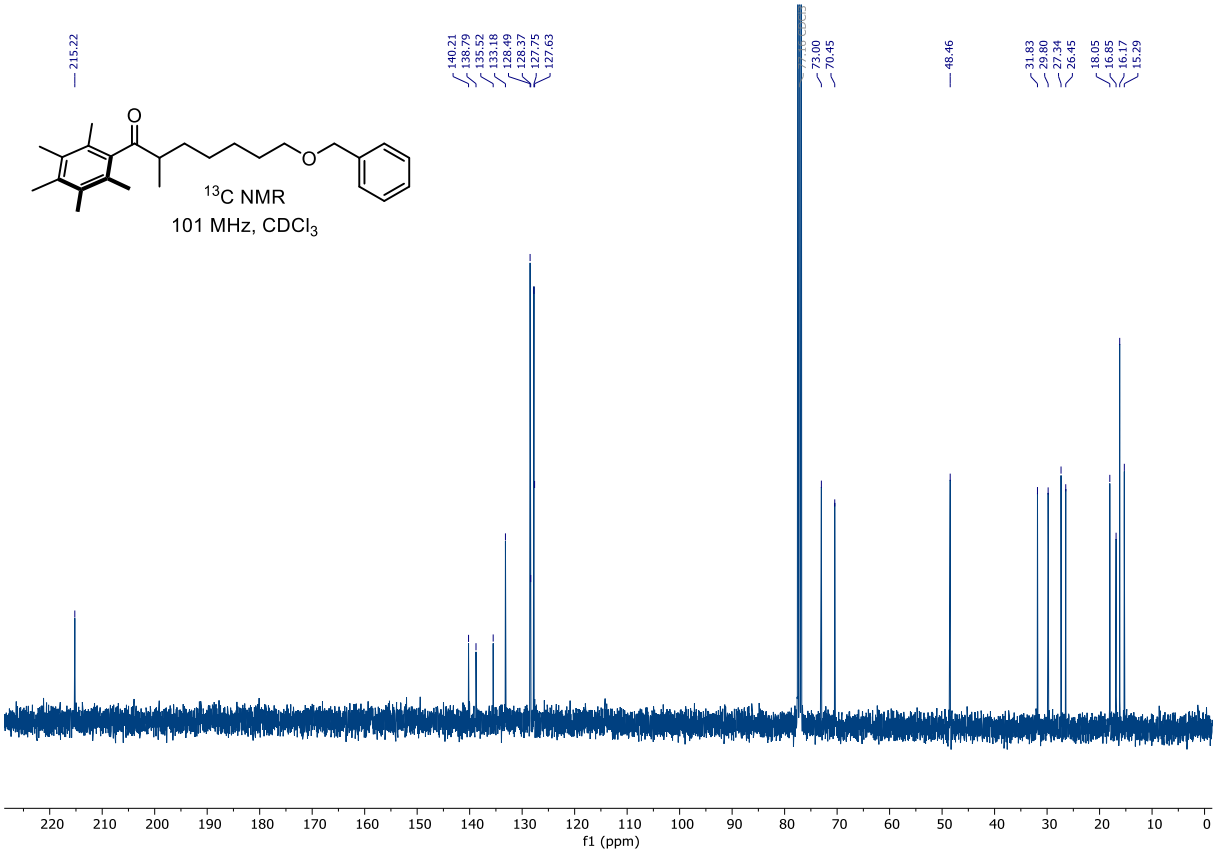


***cis*-3n (1,4-Dimethyl-2-((phenylsulfonyl)methyl)cyclopentyl)(2,3,4,5,6-pentamethylphenyl)methanone**

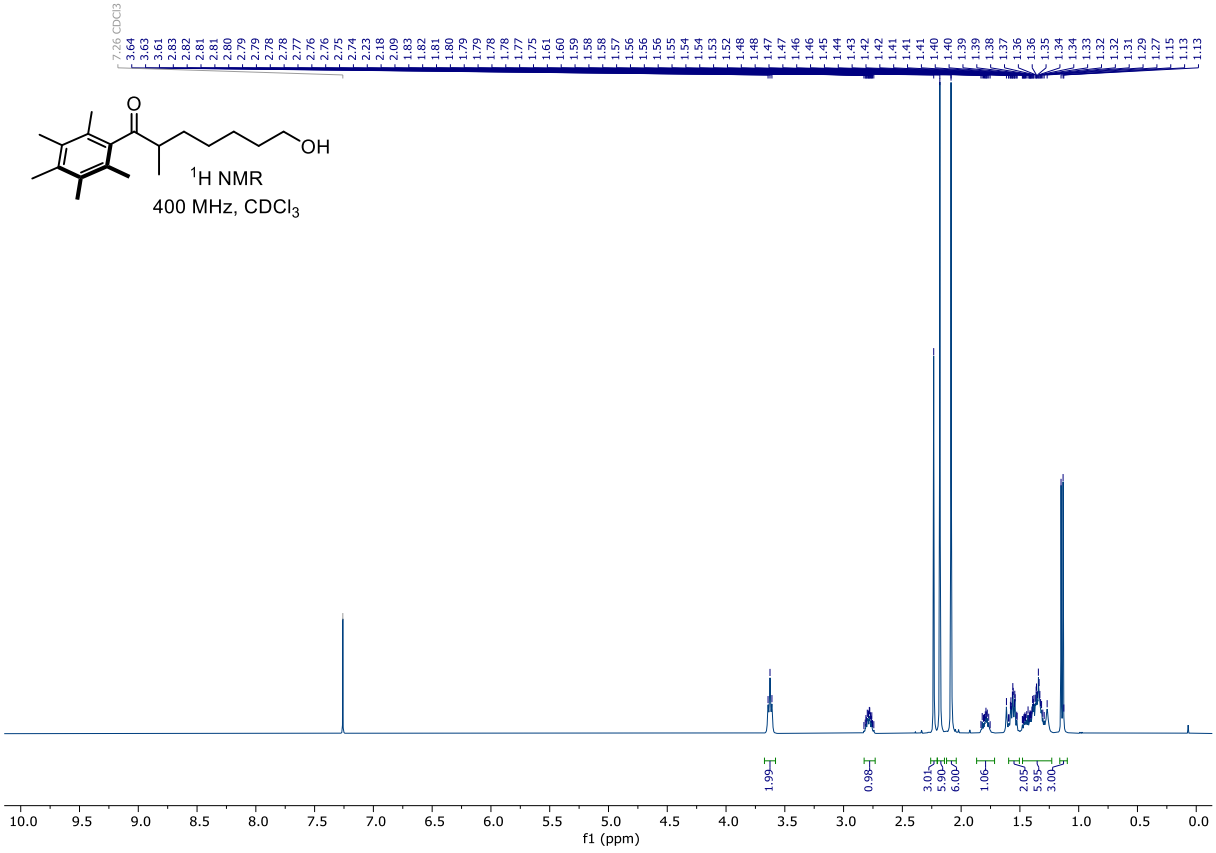


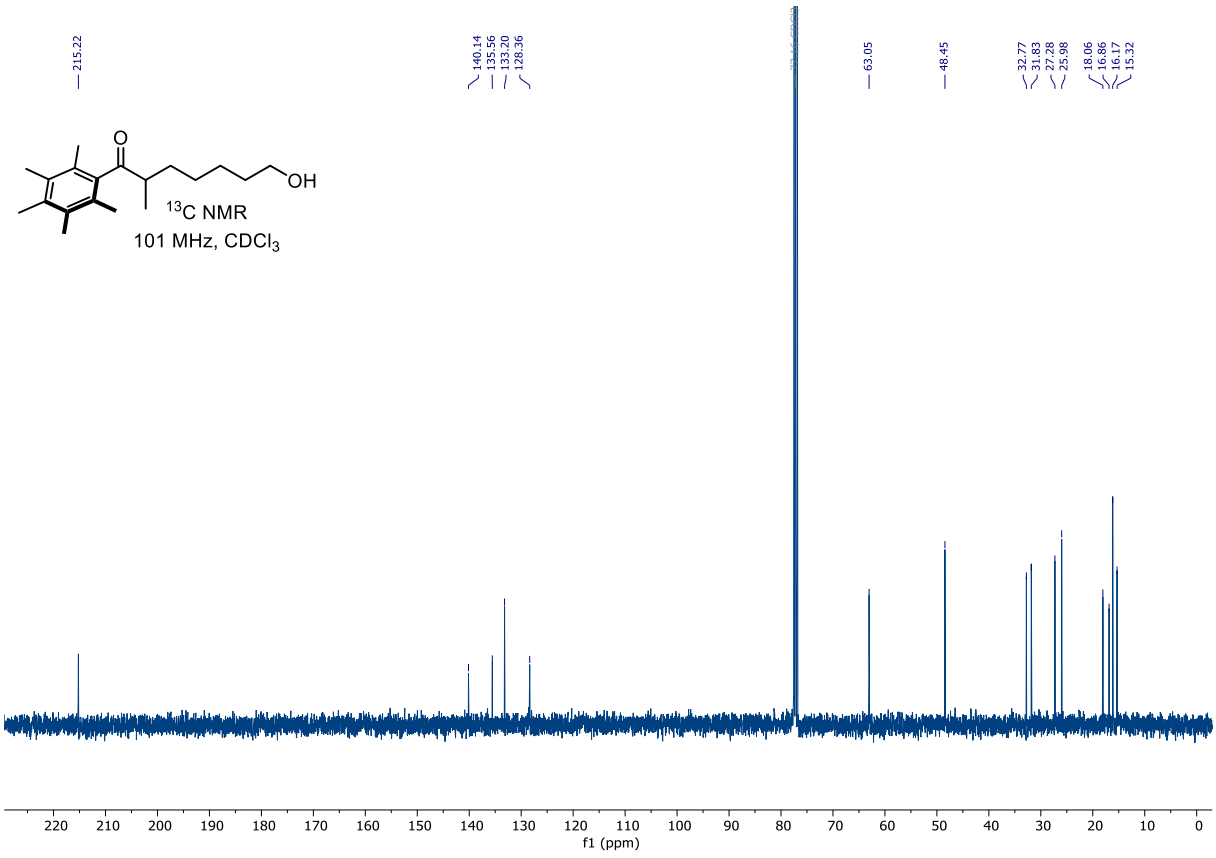
S22 7-(Benzyloxy)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)heptan-1-one



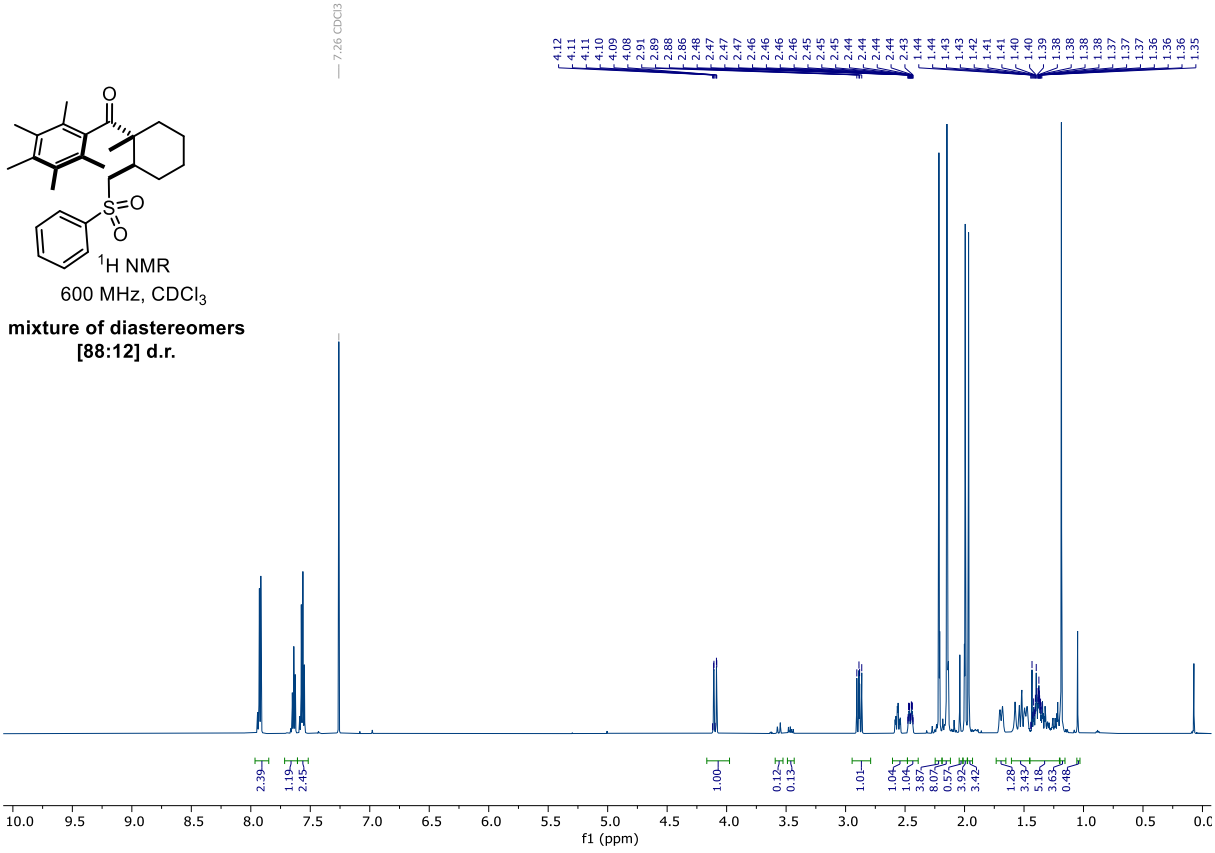


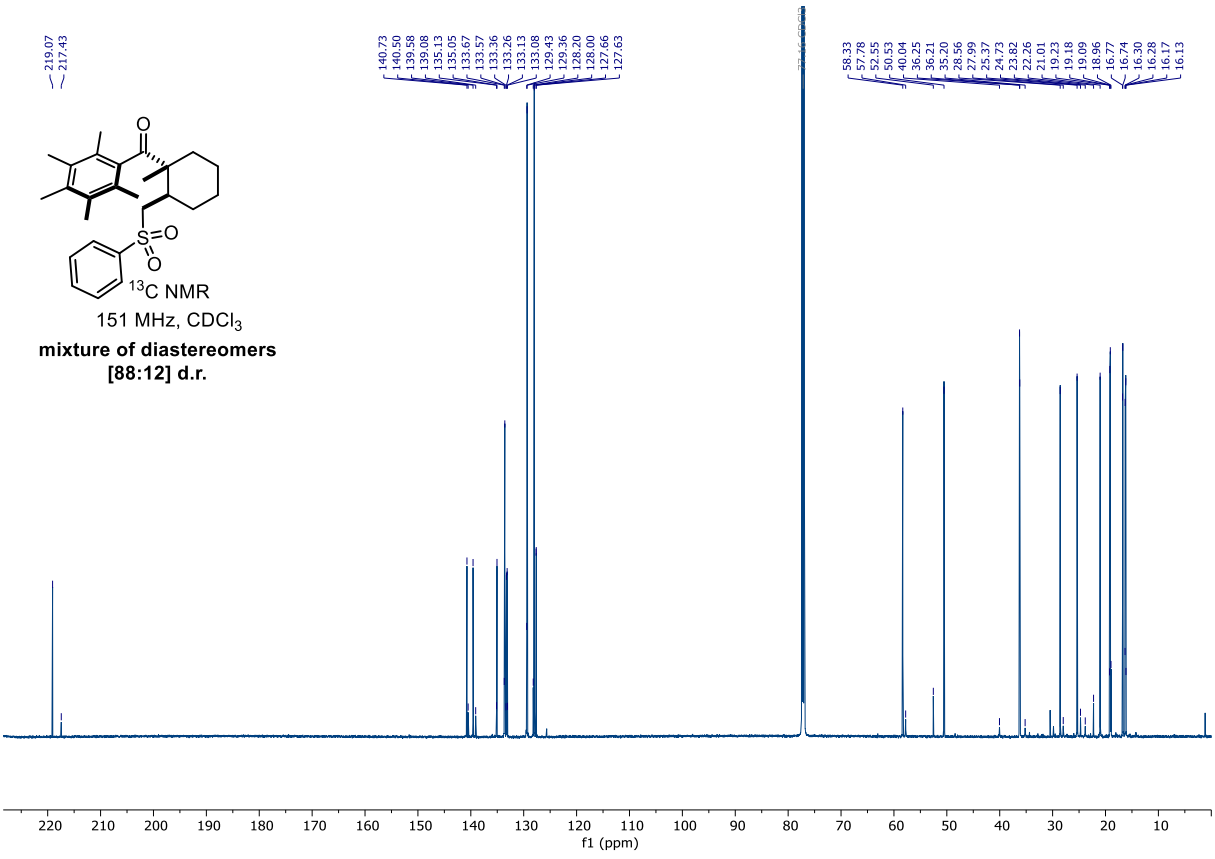
1o 7-Hydroxy-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)heptan-1-one



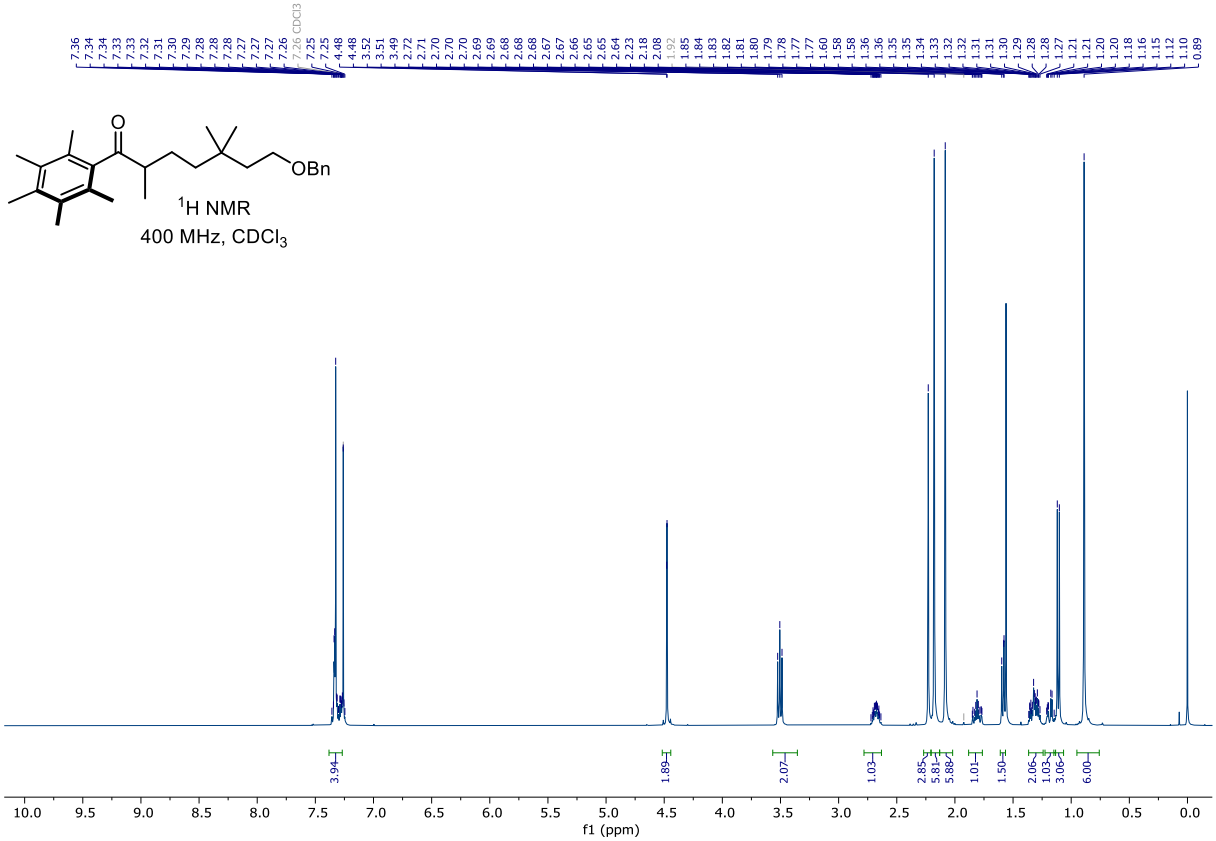


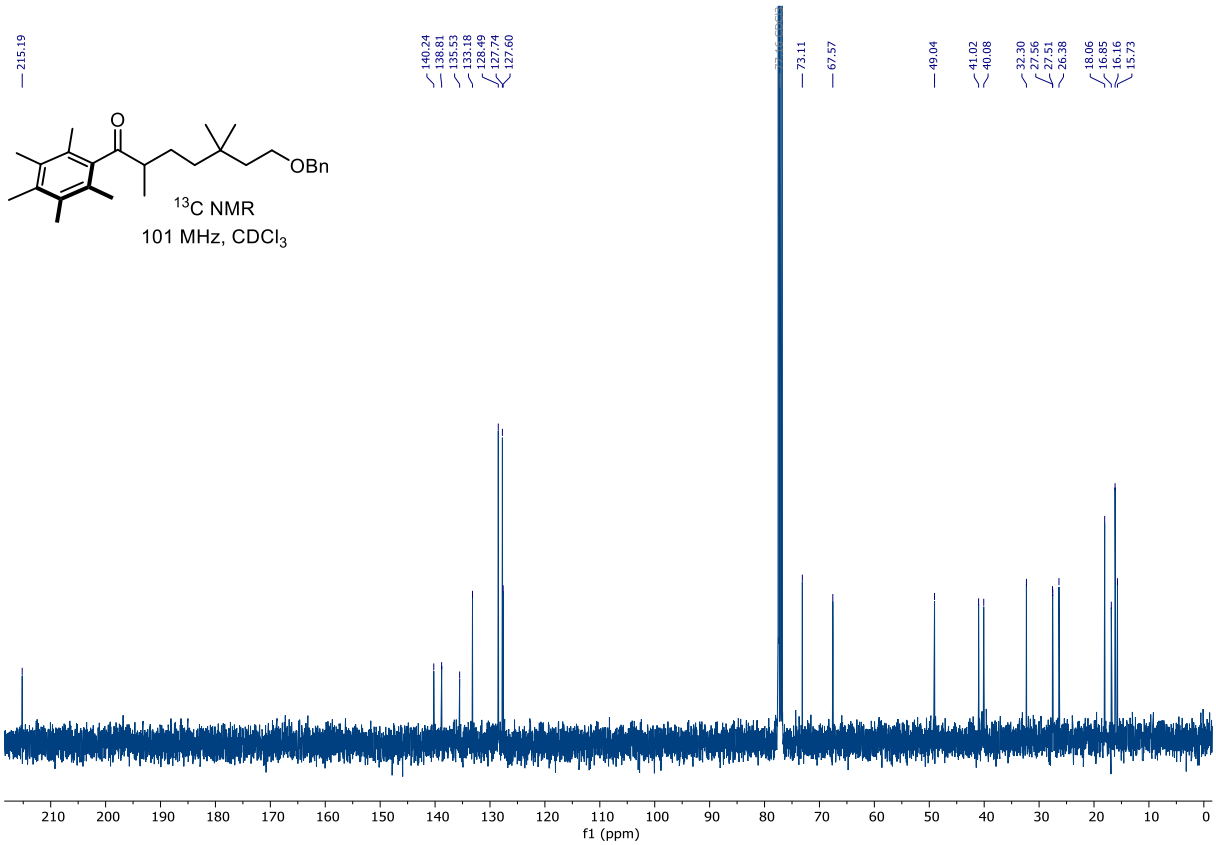
3o (1-Methyl-2-((phenylsulfonyl)methyl)cyclohexyl)(2,3,4,5,6-pentamethylphenyl)methanone



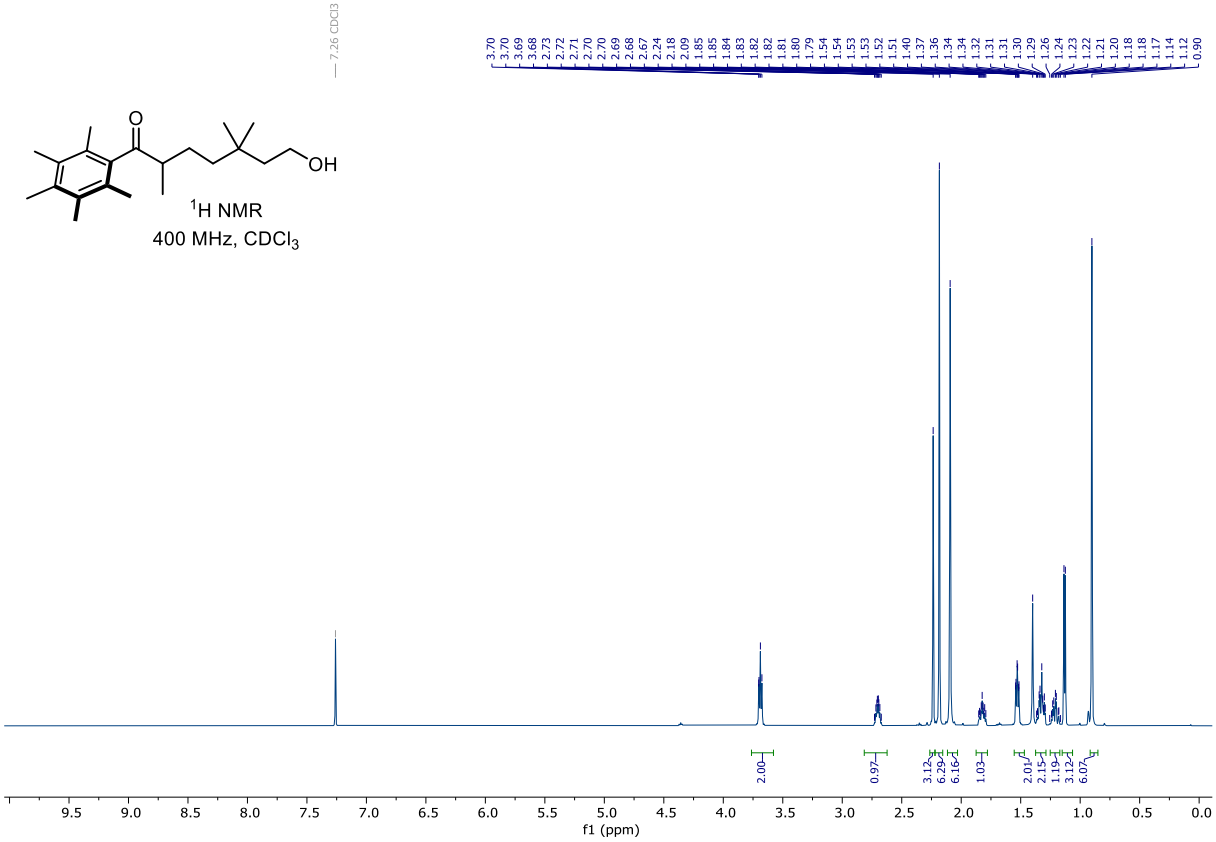


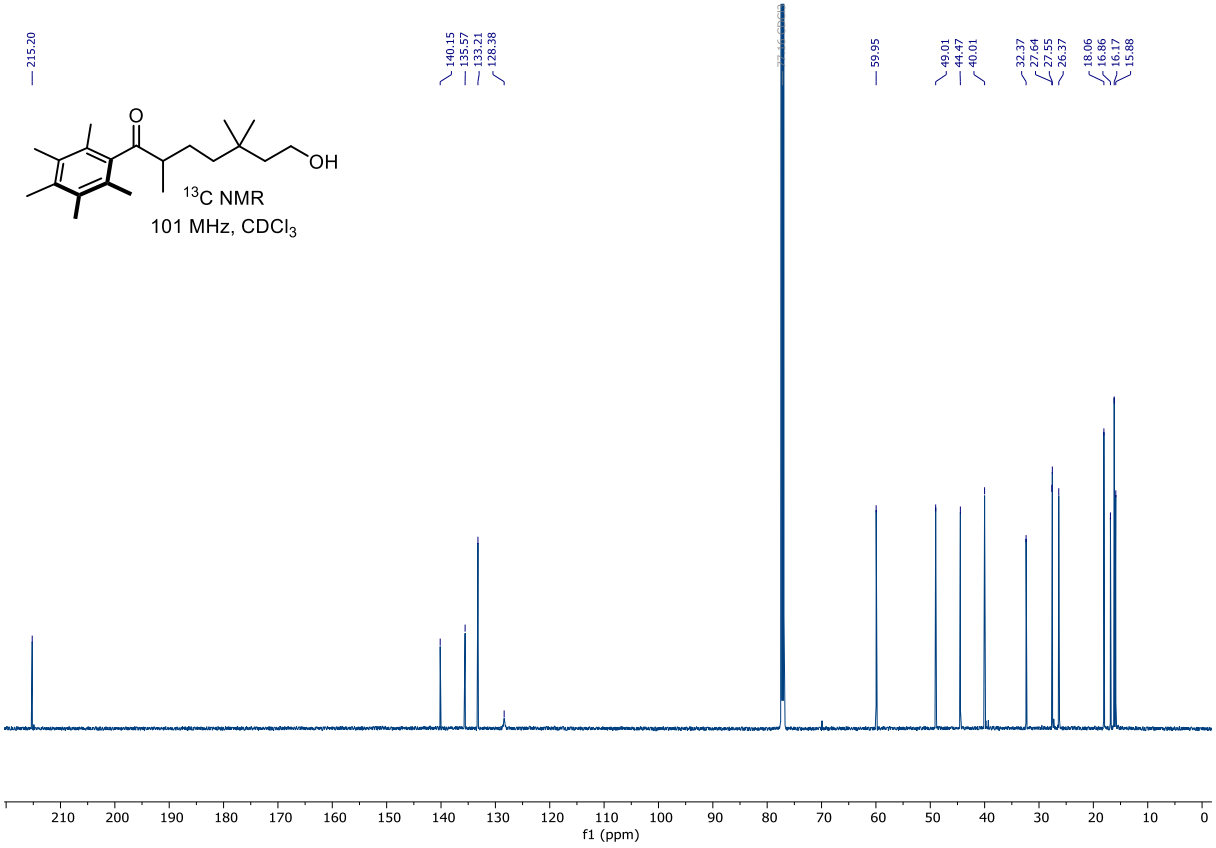
S25 7-(Benzyloxy)-2,5,5-trimethyl-1-(2,3,4,5,6-pentamethylphenyl)heptan-1-one



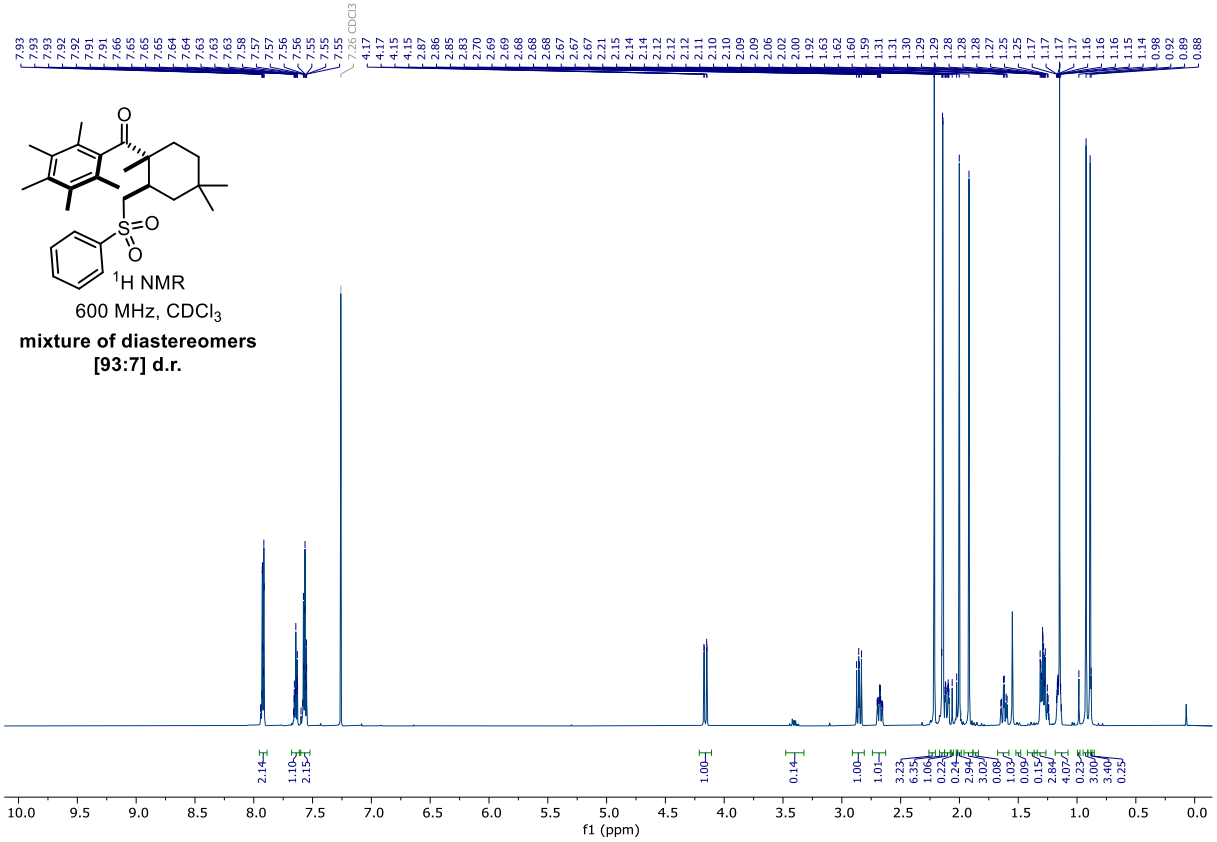


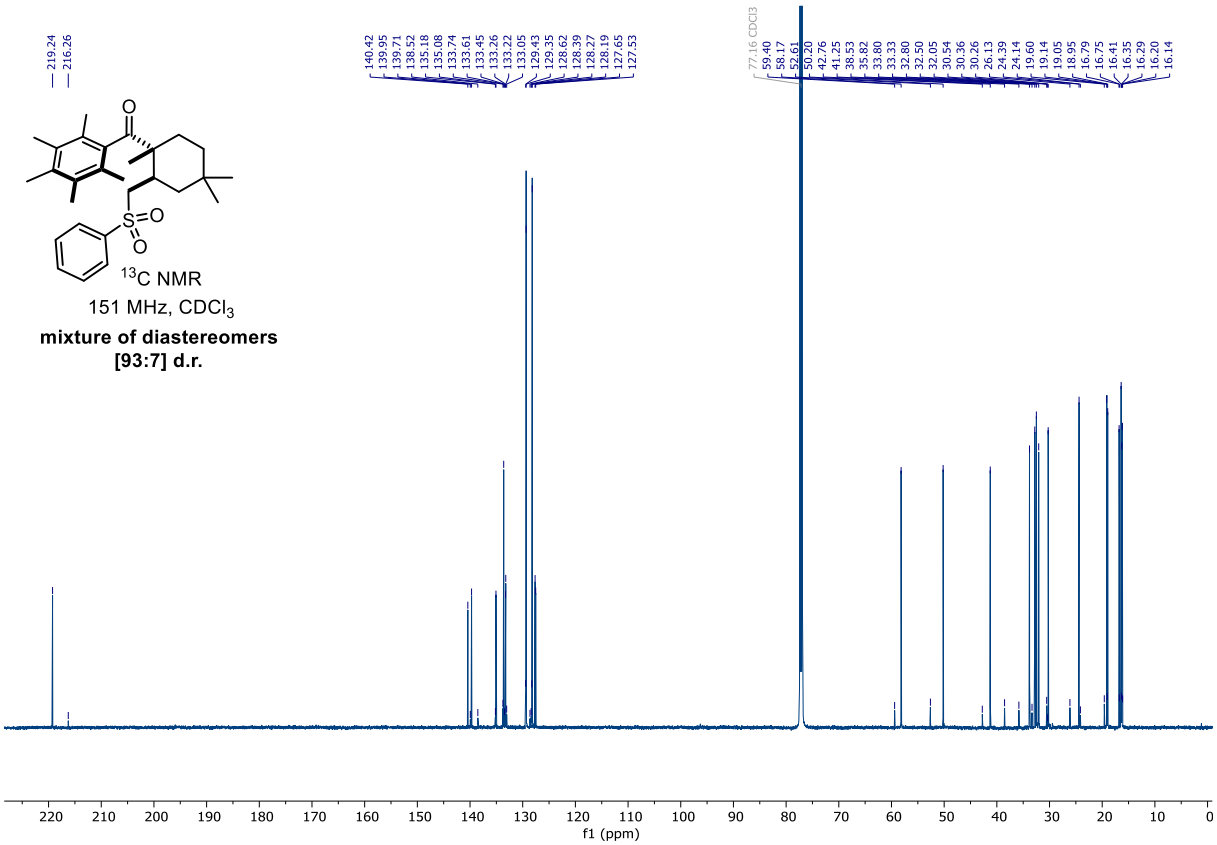
1p 7-Hydroxy-2,5,5-trimethyl-1-(2,3,4,5,6-pentamethylphenyl)heptan-1-one



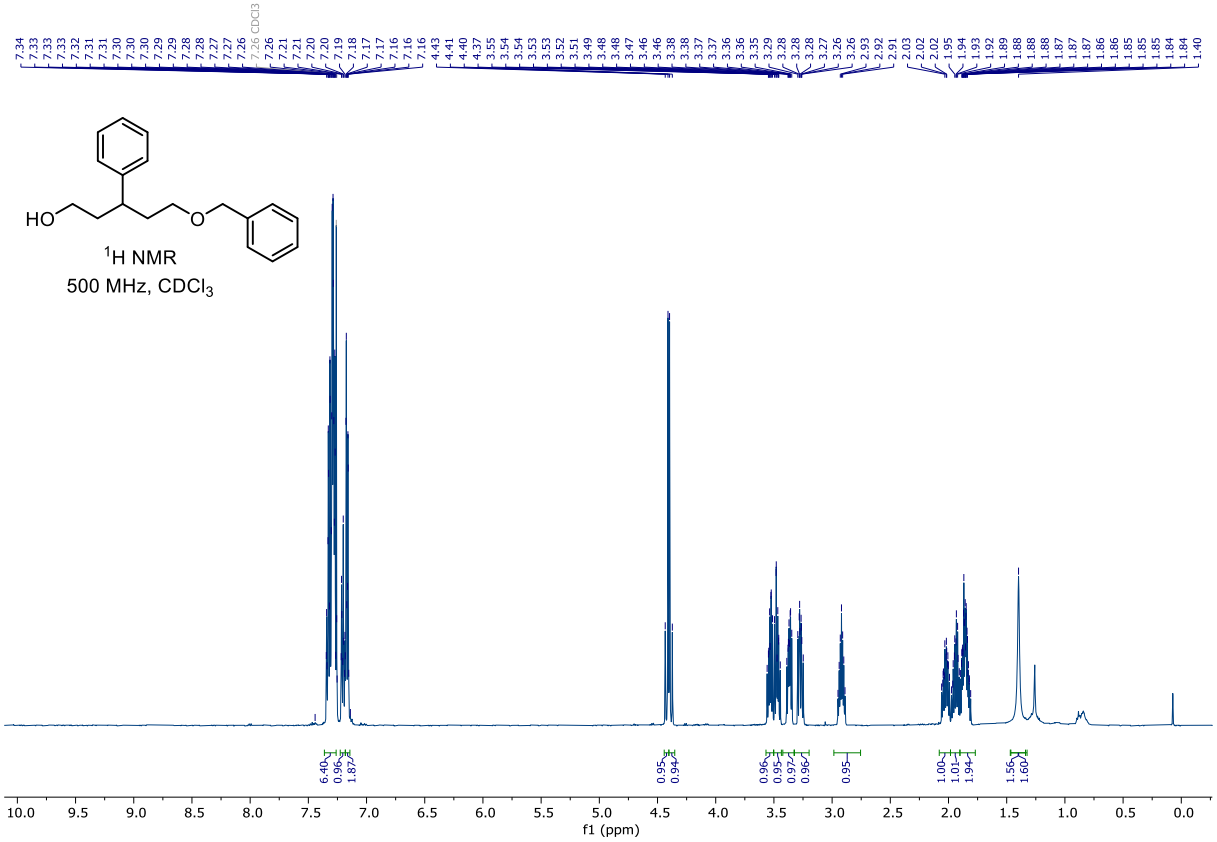


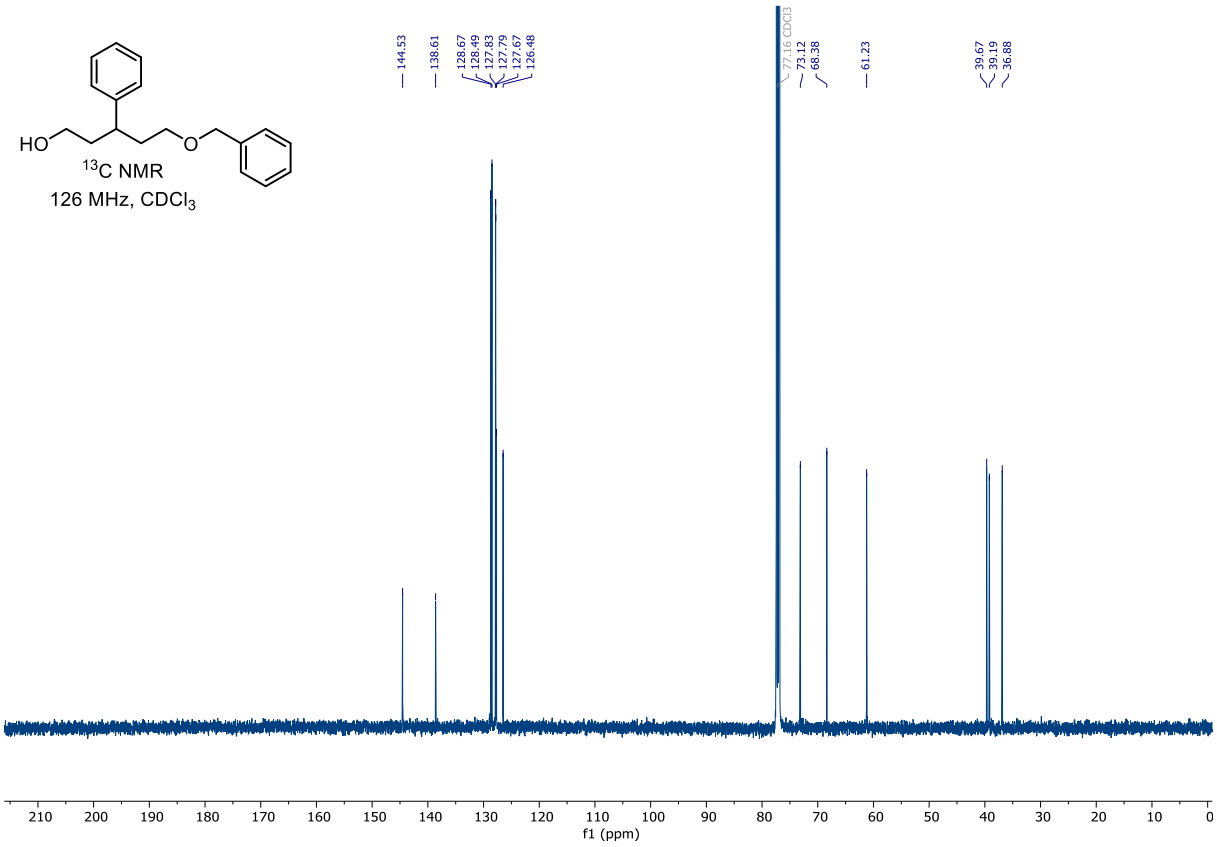
3p (2,3,4,5,6-Pentamethylphenyl)(1,4,4-trimethyl-2-((phenylsulfonyl)methyl)cyclohexyl)methanone



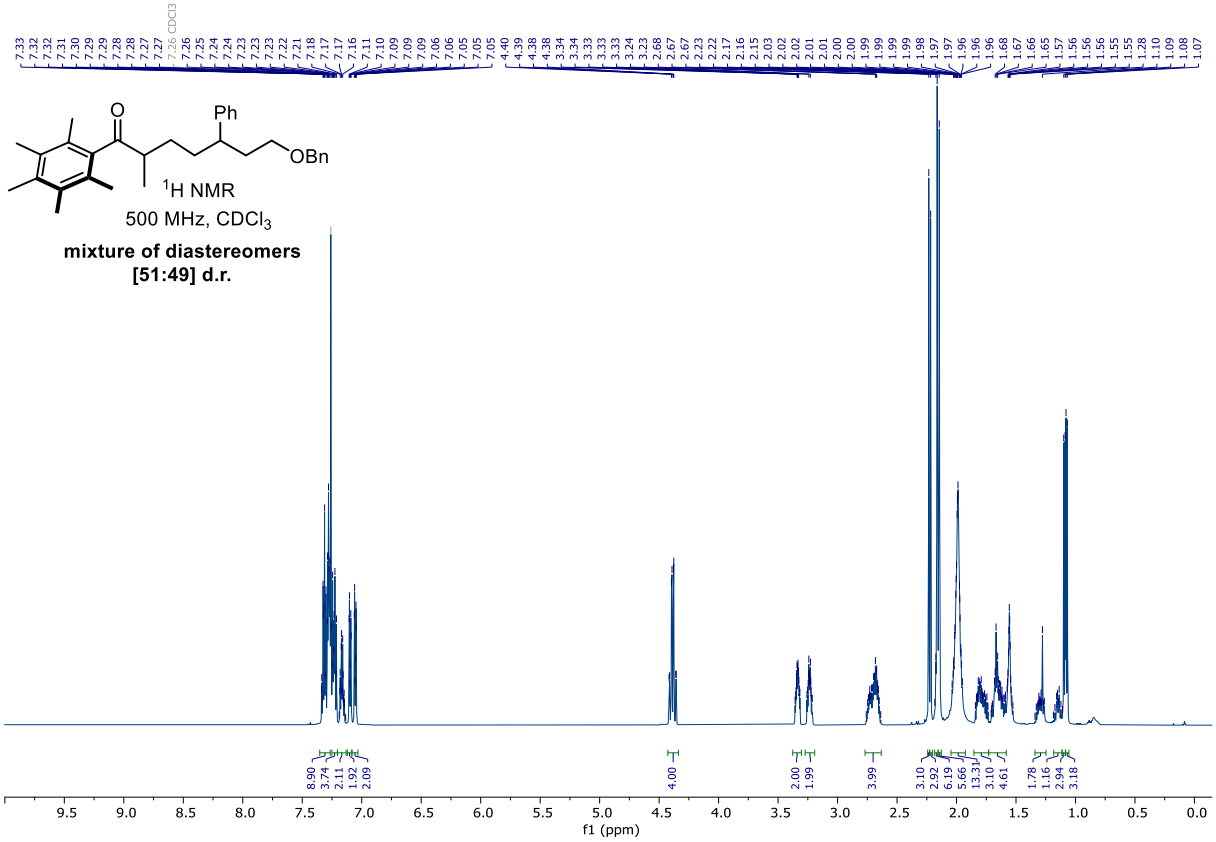


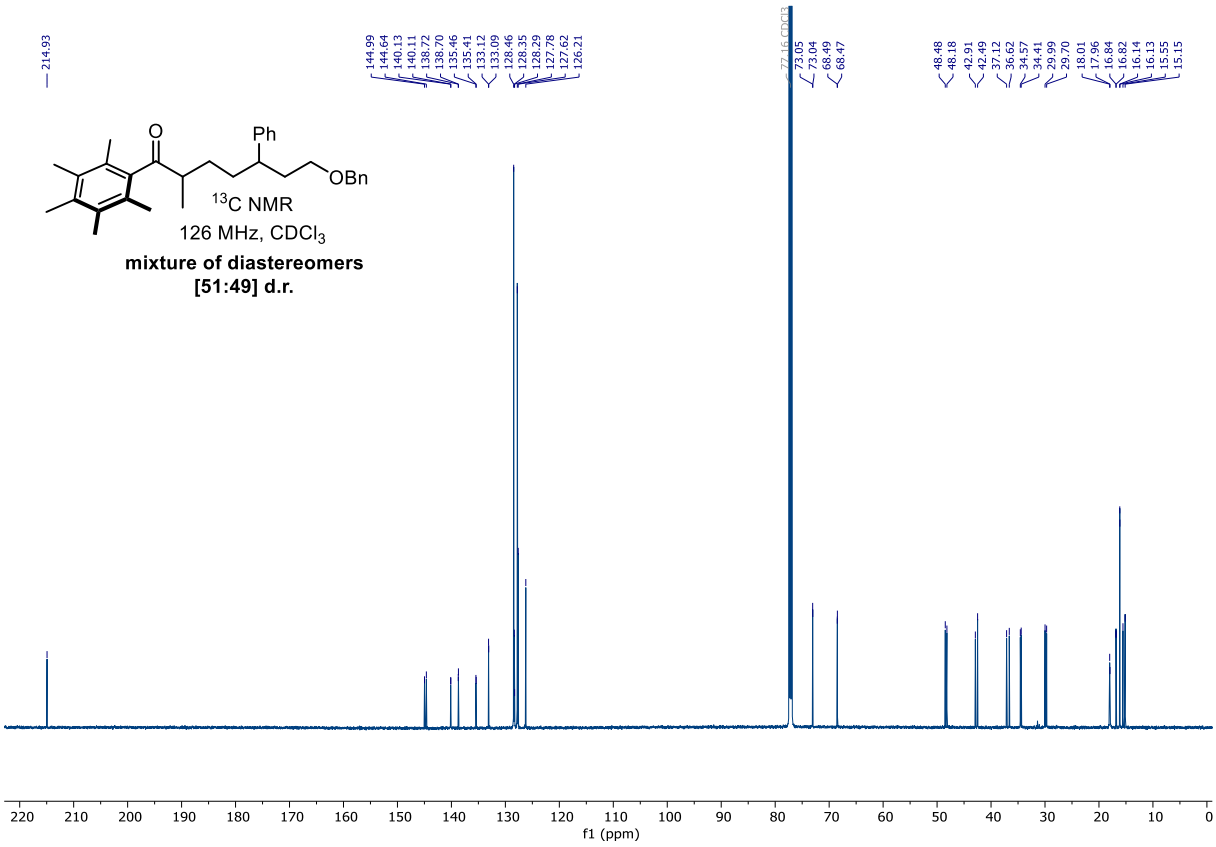
S27 5-(Benzyloxy)-3-phenylpentan-1-ol



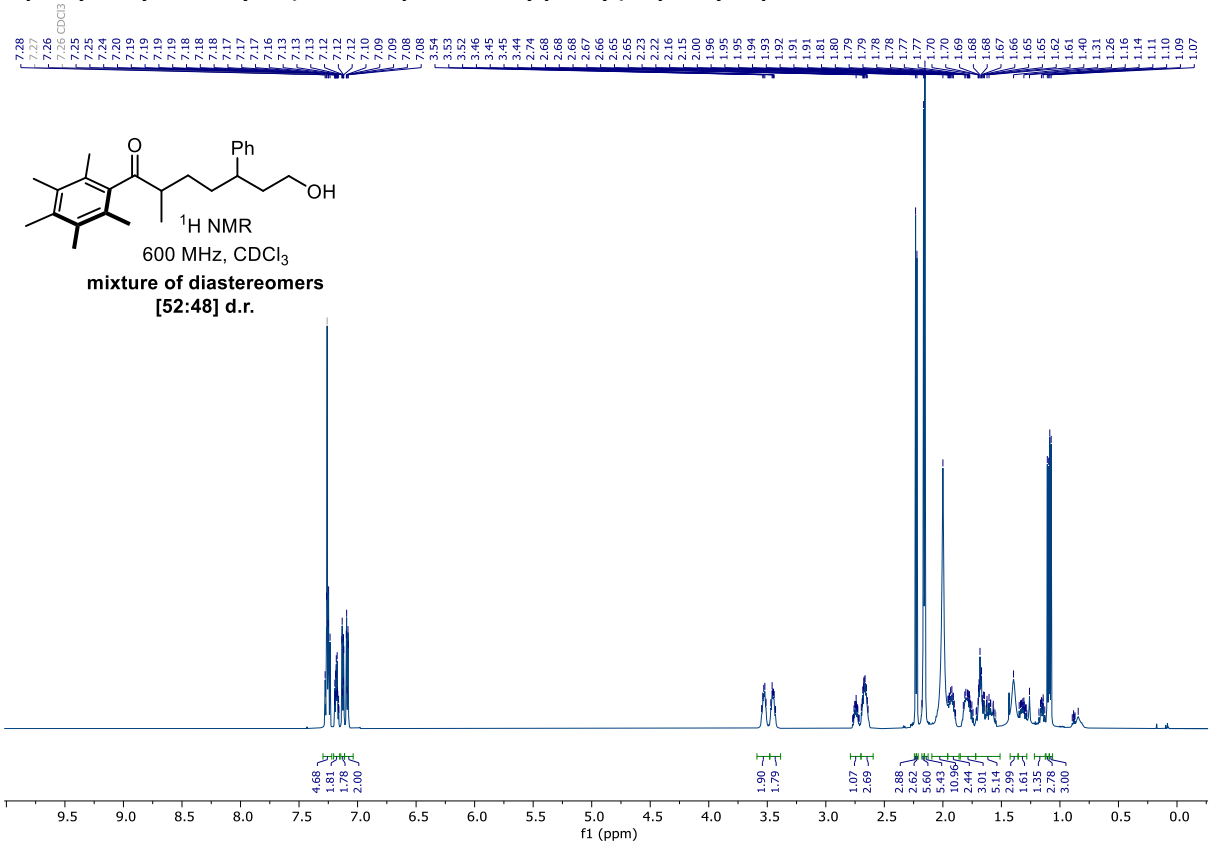


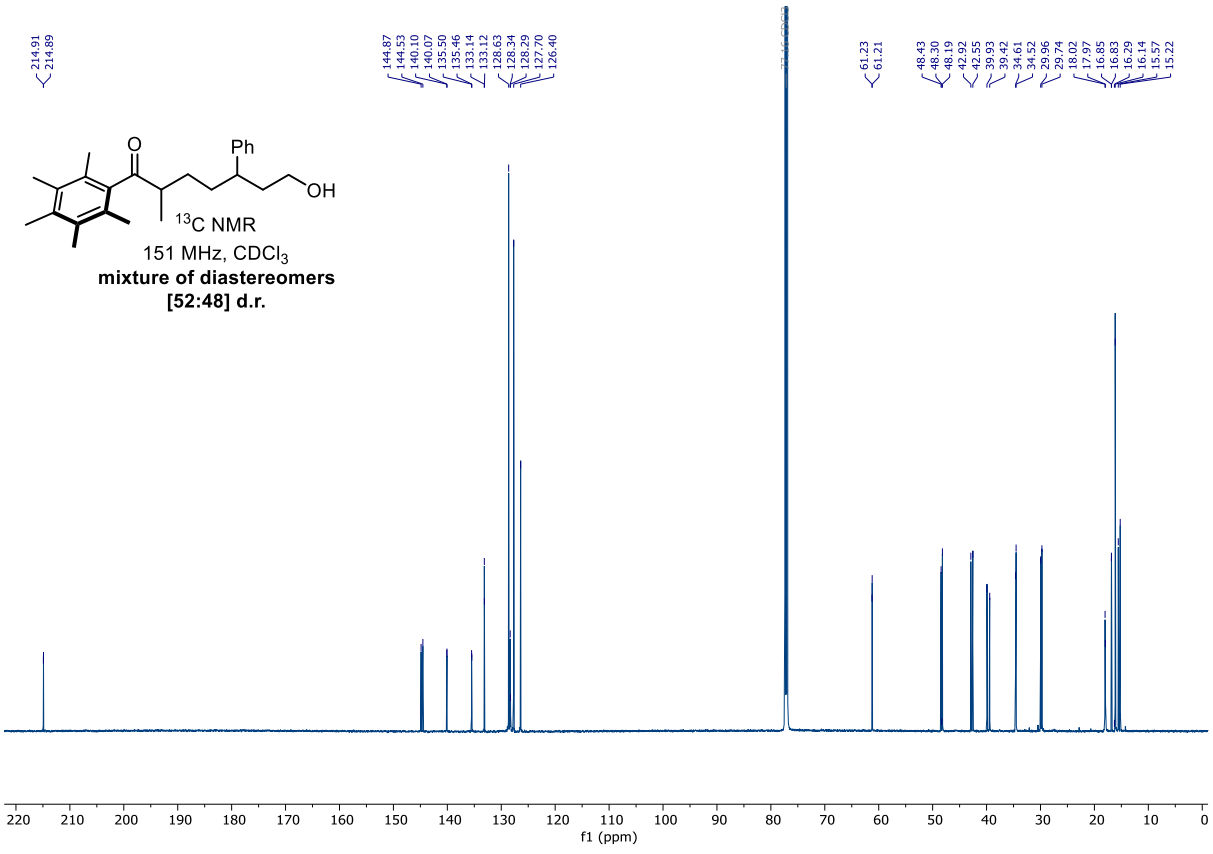
S28 7-(Benzyloxy)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)-5-phenylheptan-1-one





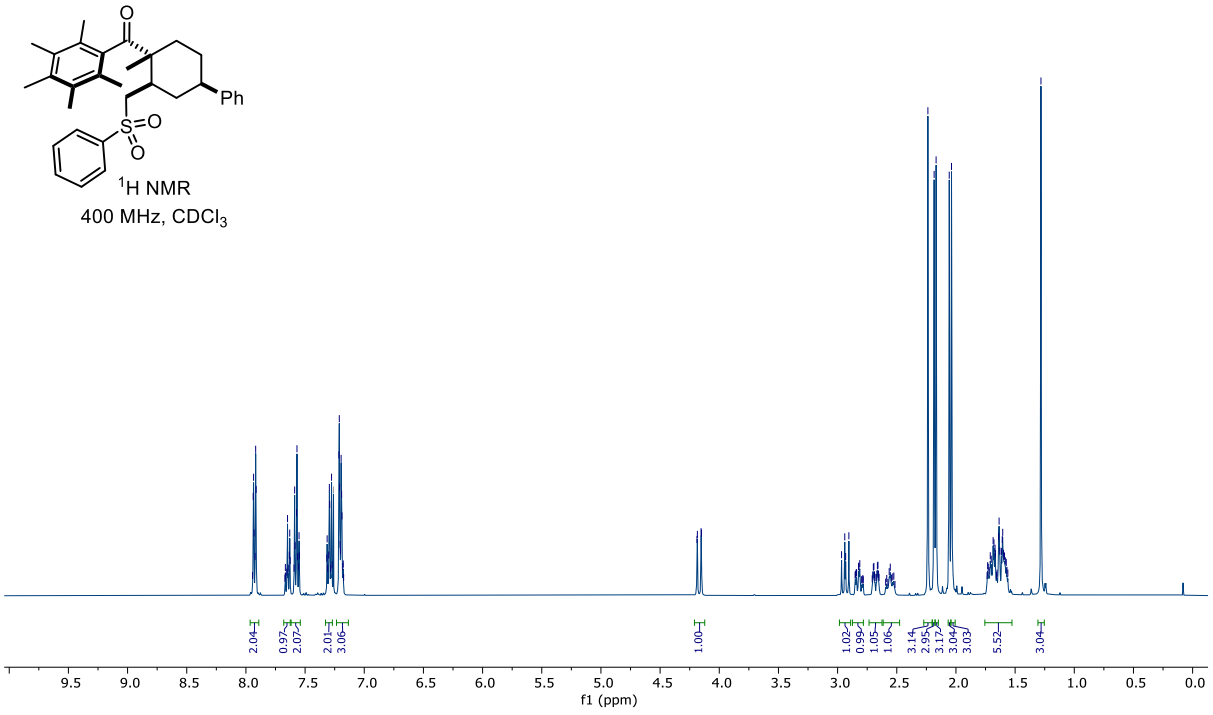
1q 7-Hydroxy-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)-5-phenylheptan-1-one

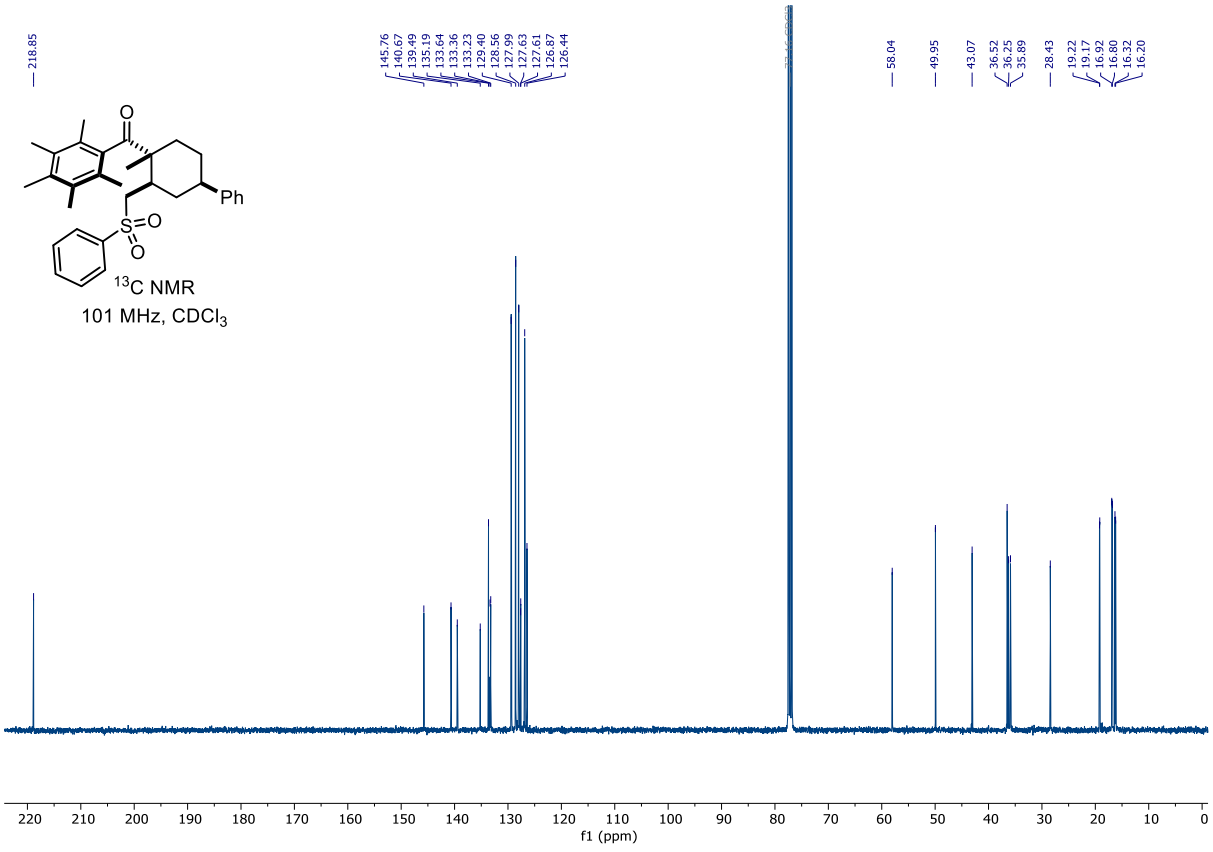




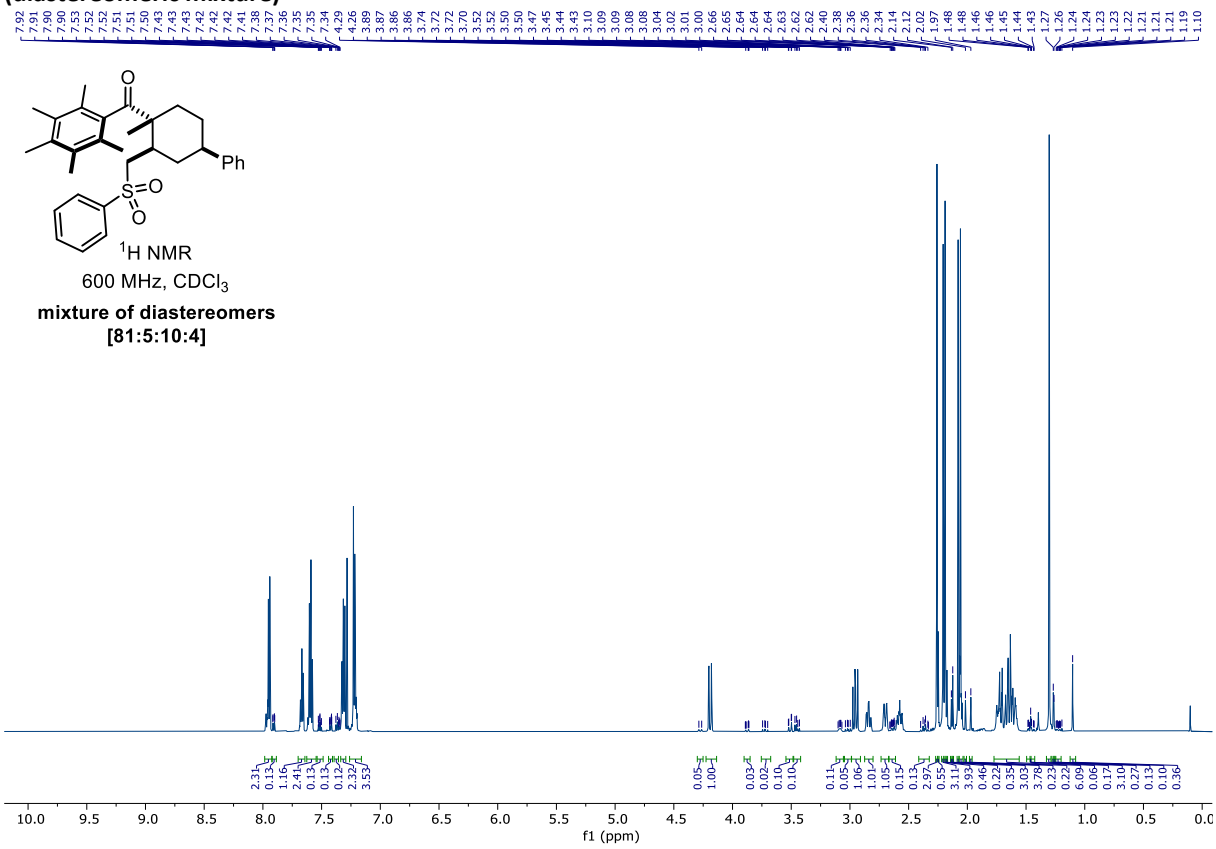
3q ((1*RS*,2*RS*,4*RS*) -1-Methyl-4-phenyl-2-((phenylsulfonyl)methyl)cyclohexyl)(2,3,4,5,6-pentamethylphenyl)methanone

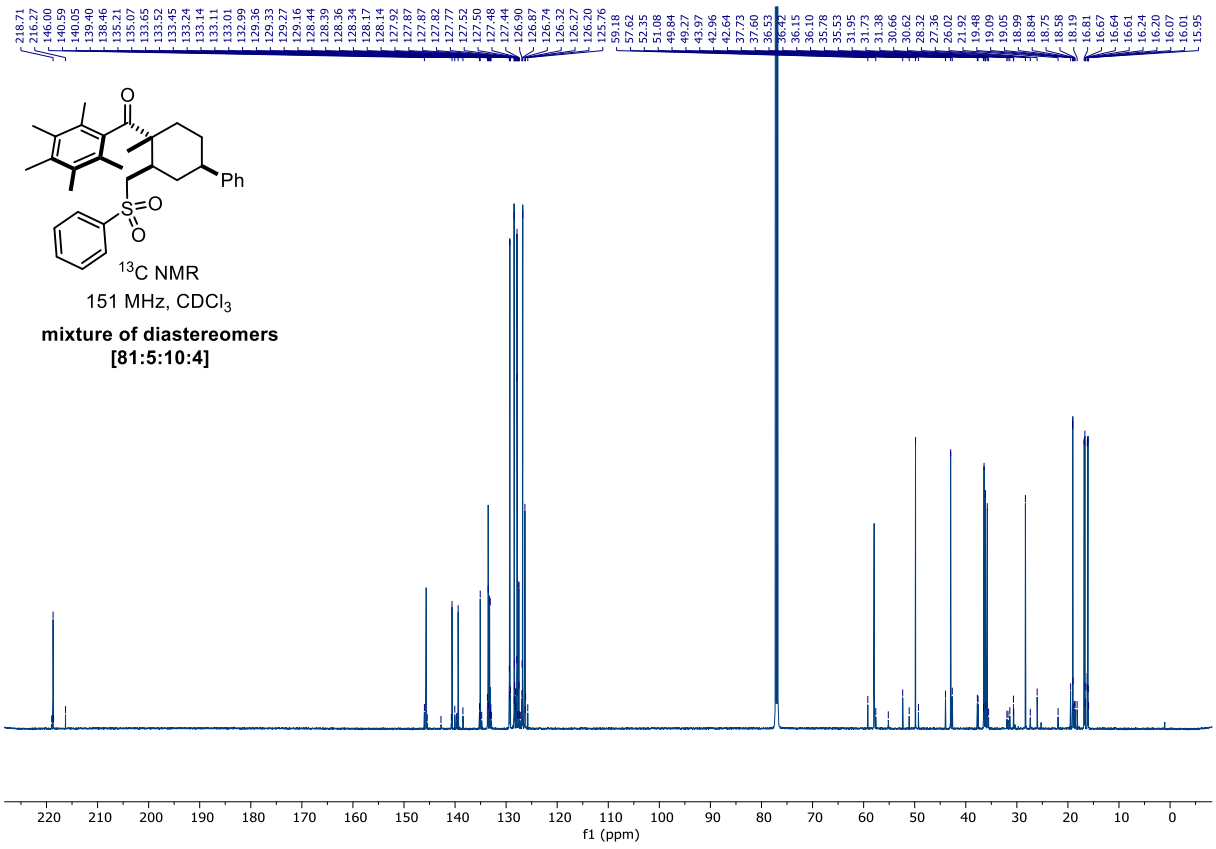




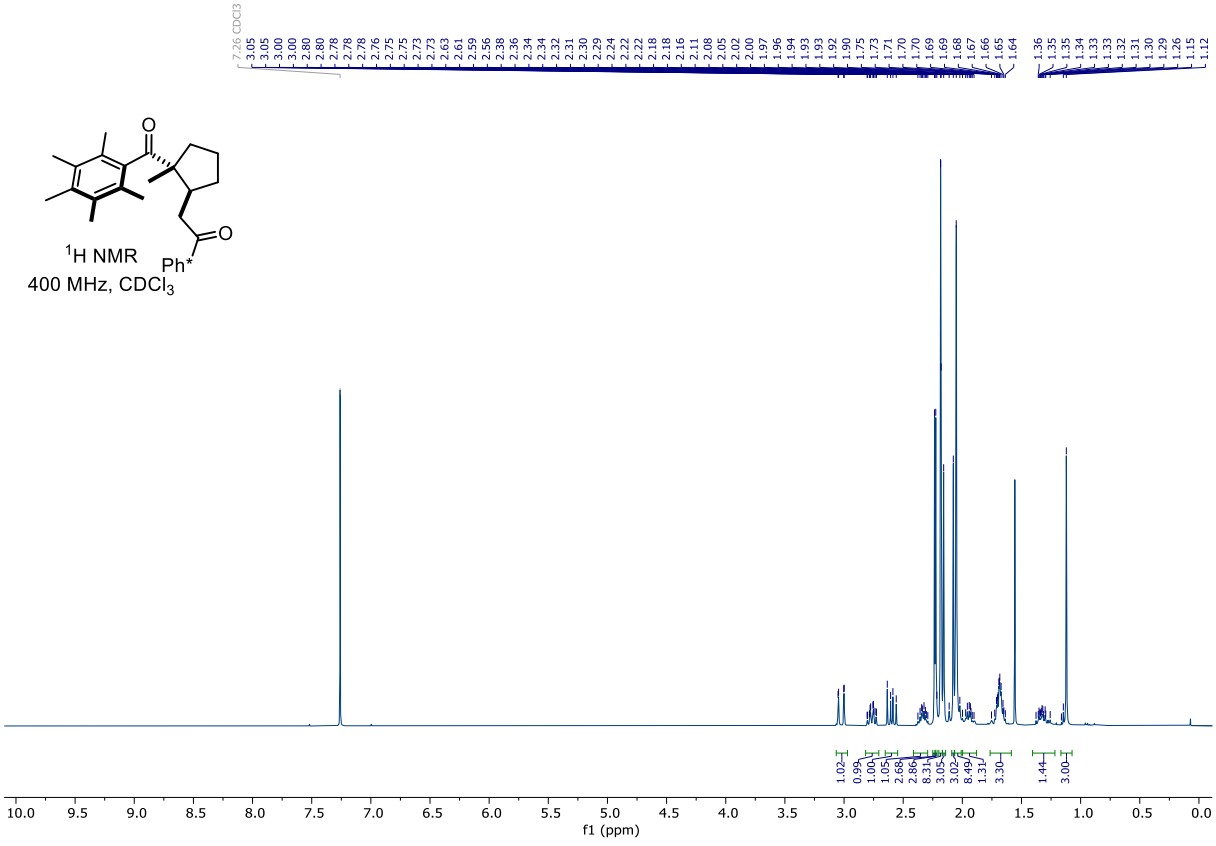


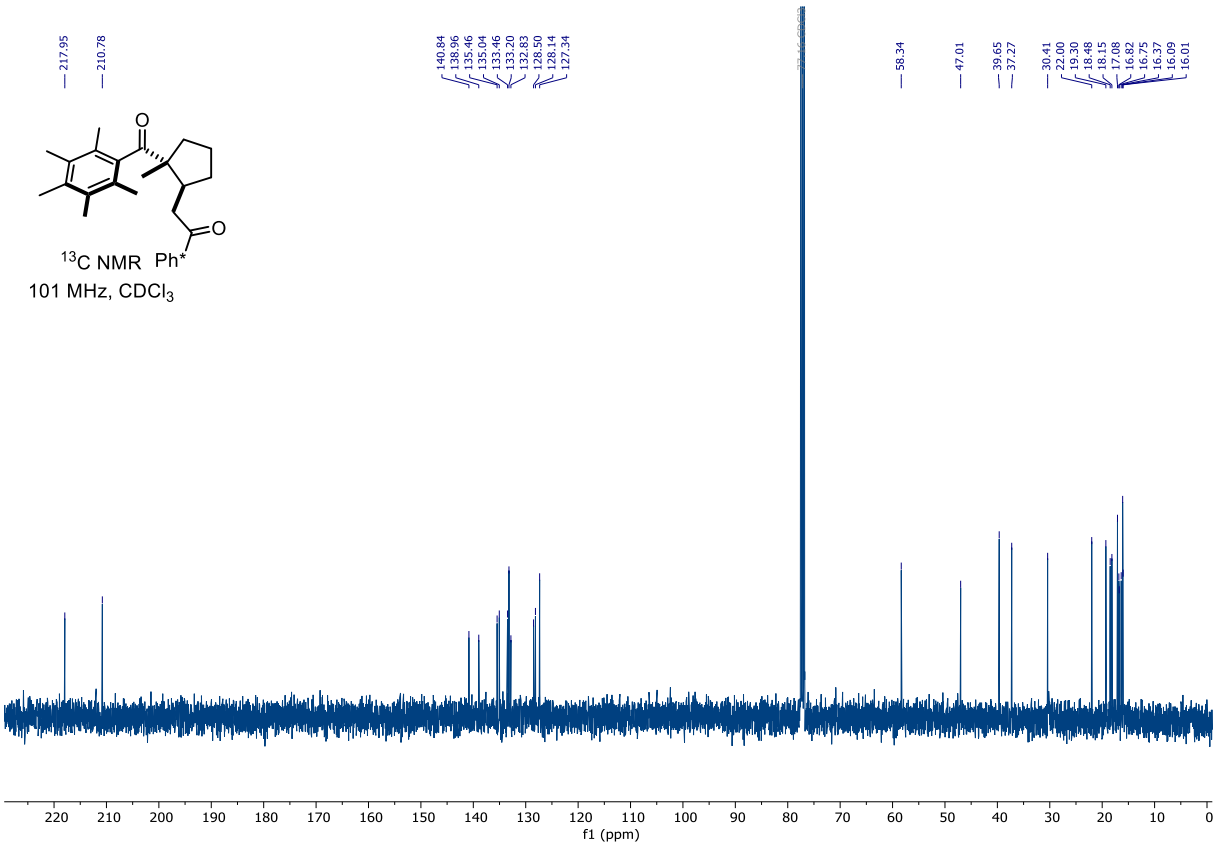
3q (1-Methyl-4-phenyl-2-((phenylsulfonyl)methyl)cyclohexyl)(2,3,4,5,6-pentamethylphenyl)methanone (diastereomeric mixture)



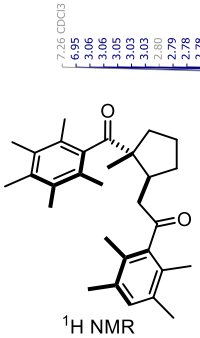


3r 2-((1*SR*,2*RS*)-2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)-1-(2,3,4,5,6-pentamethylphenyl)ethan-1-one





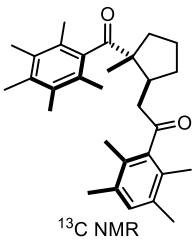
3s 2-(2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)-1-(2,3,5,6-tetramethylphenyl)ethan-1-one



^{1}H NMR

600 MHz, $CDCl_3$

mixture of diastereomers
[95:5] d.r.

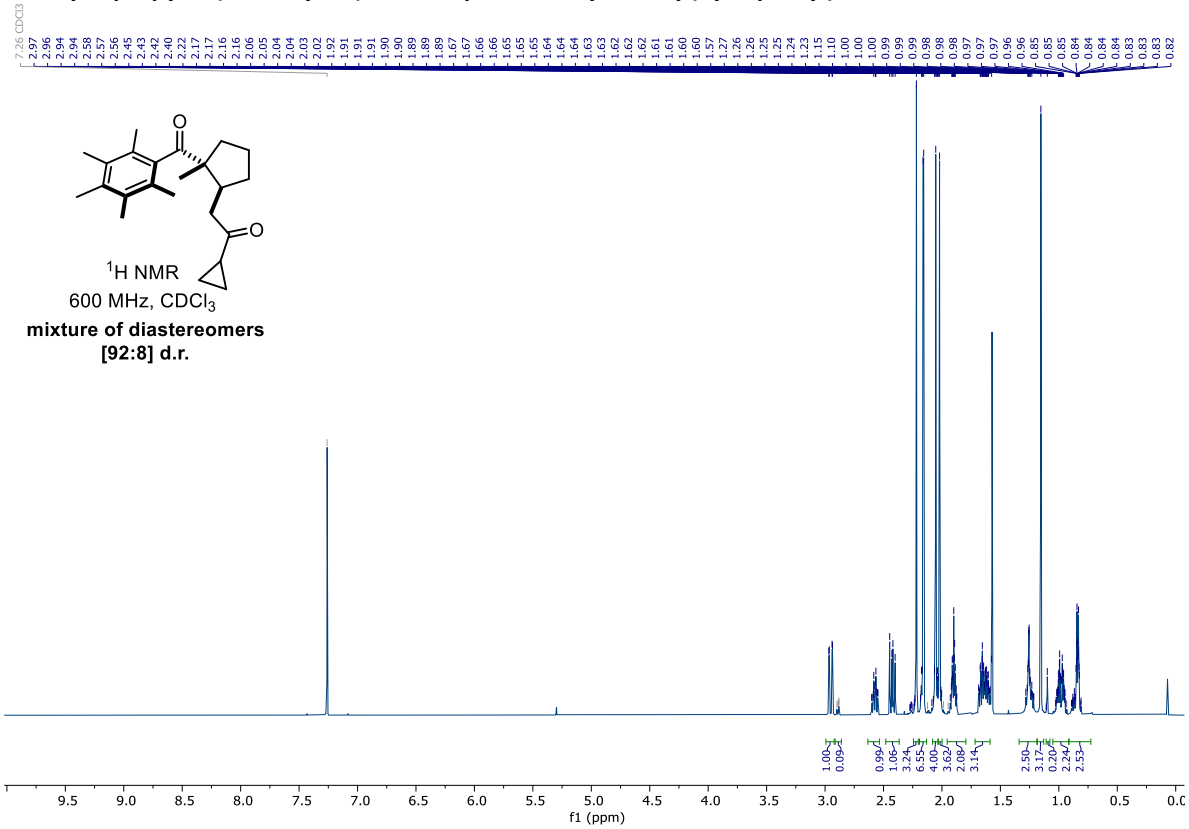


^{13}C NMR

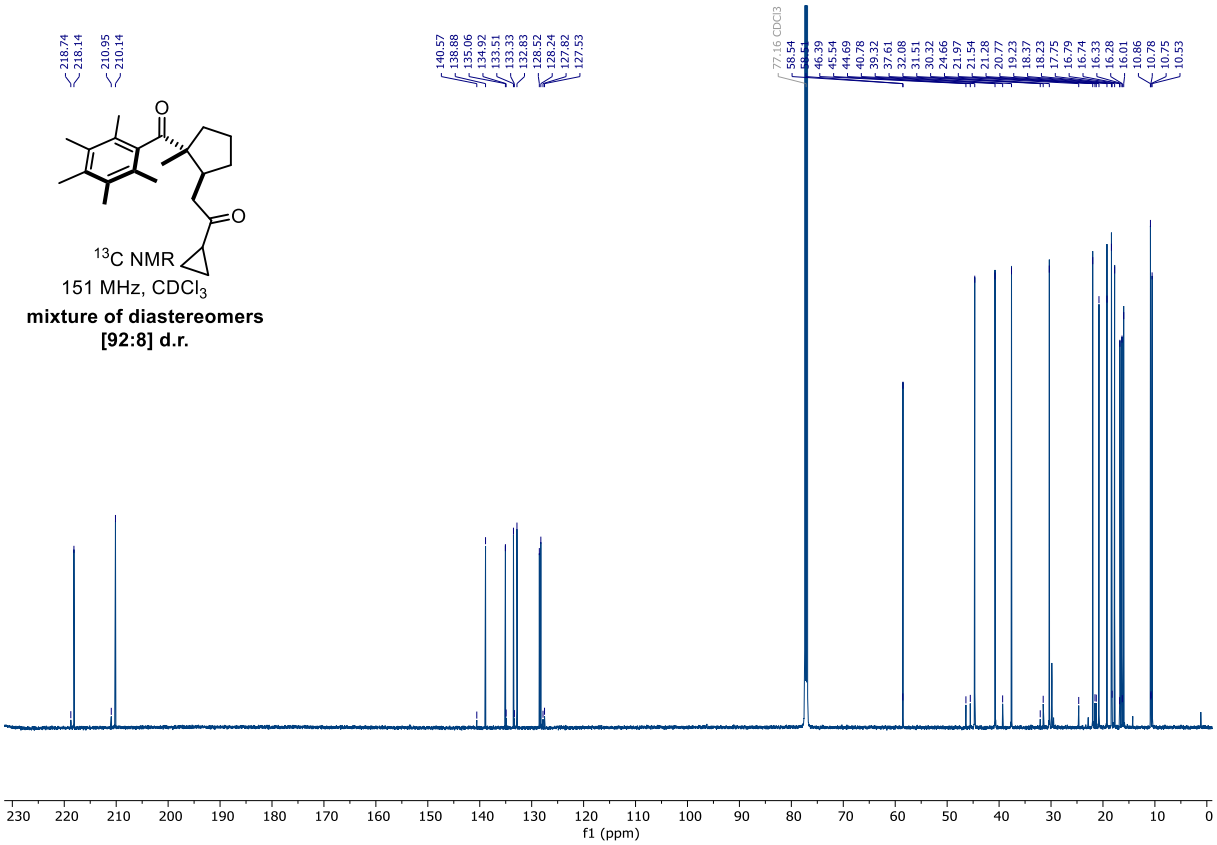
151 MHz, $CDCl_3$

mixture of diastereomers
[95:5] d.r.

3t 1-Cyclopropyl-2-(2-methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)ethan-1-one

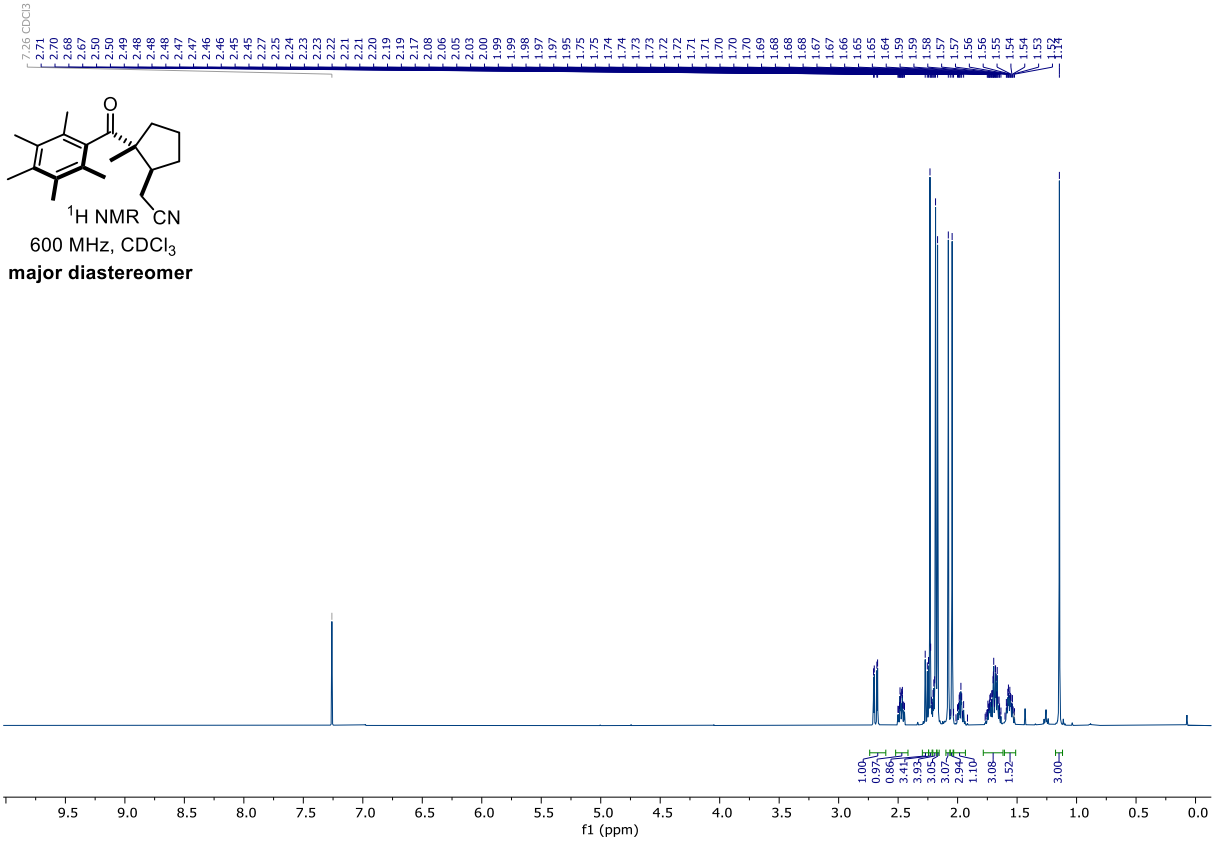


^{1}H NMR
600 MHz, $CDCl_3$
mixture of diastereomers
[92:8] d.r.



^{13}C NMR
151 MHz, $CDCl_3$
mixture of diastereomers
[92:8] d.r.

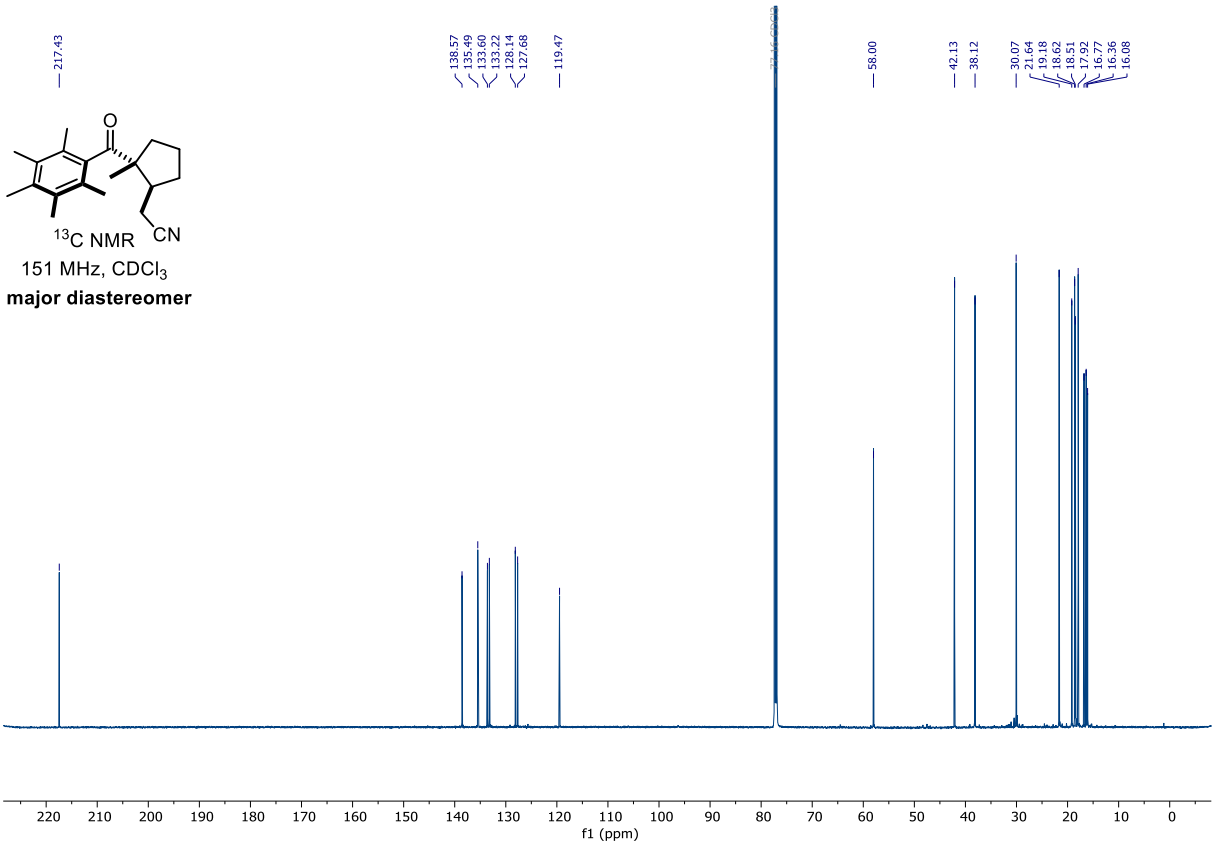
***trans*-3u 2-((1*SR*, 2RS)-2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)acetonitrile**



^{1}H NMR

600 MHz, $CDCl_3$

major diastereomer

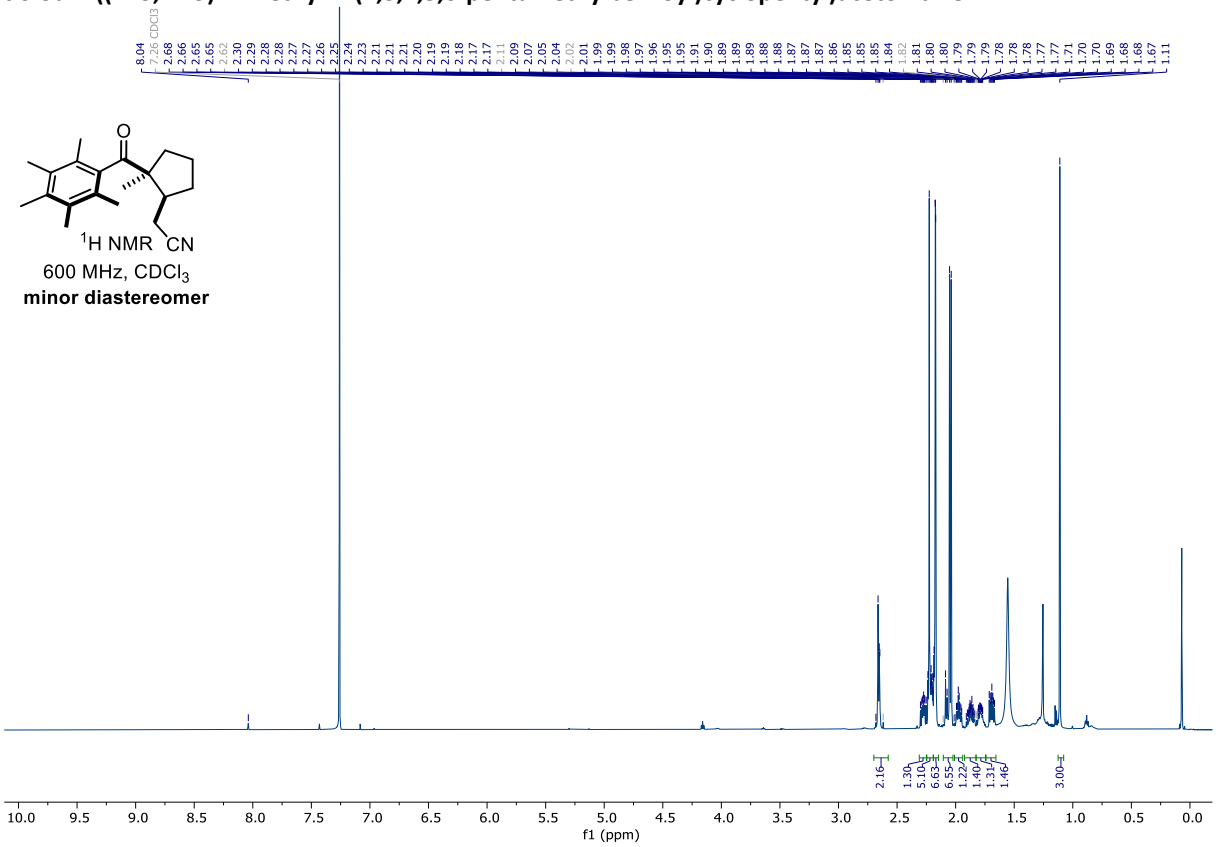


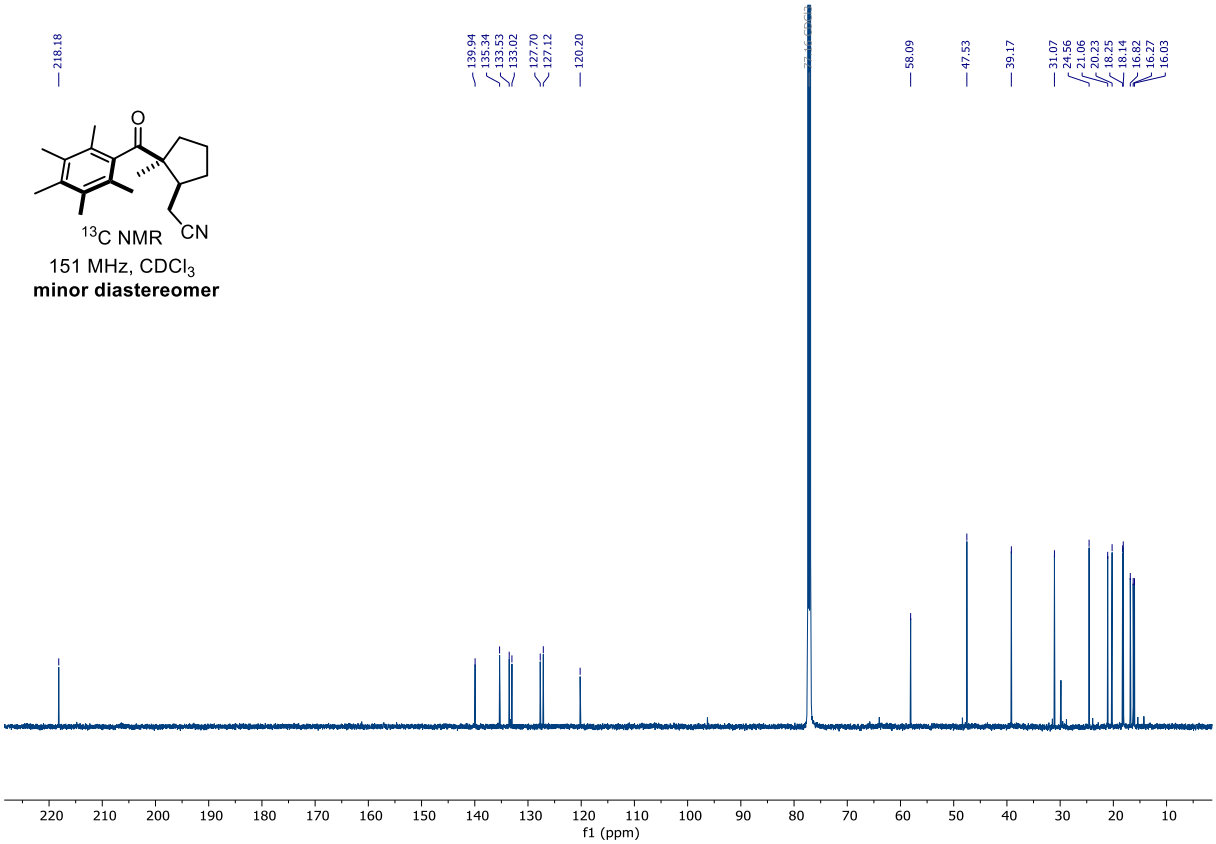
^{13}C NMR

151 MHz, $CDCl_3$

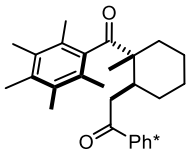
major diastereomer

***cis*-3u 2-((1*RS*, 2*RS*)-2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclopentyl)acetonitrile**





3v 2-(2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)cyclohexyl)-1-(2,3,4,5,6-pentamethylphenyl)ethan-1-one

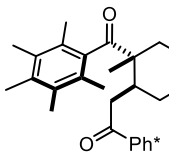


^{1}H NMR

600 MHz, $CDCl_3$

mixture of diastereomers

[86:14] d.r.



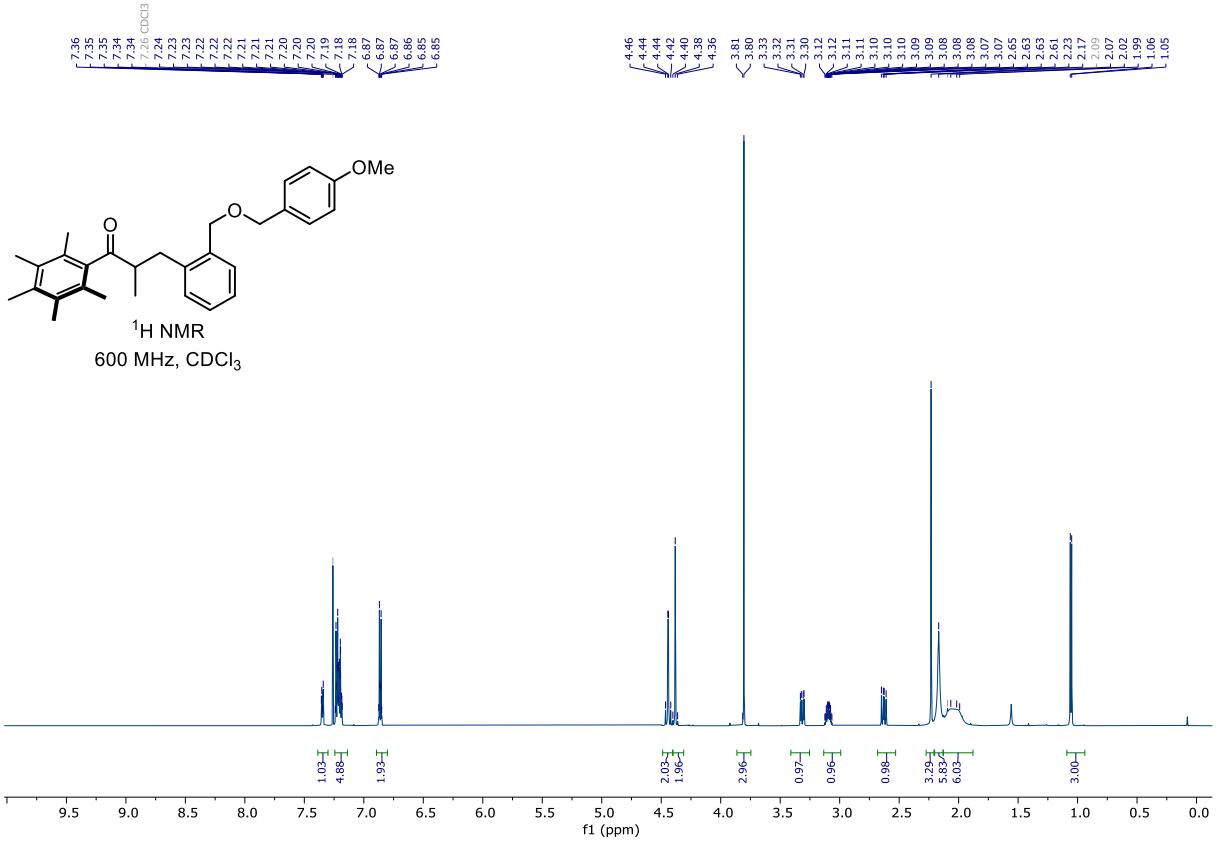
^{13}C NMR

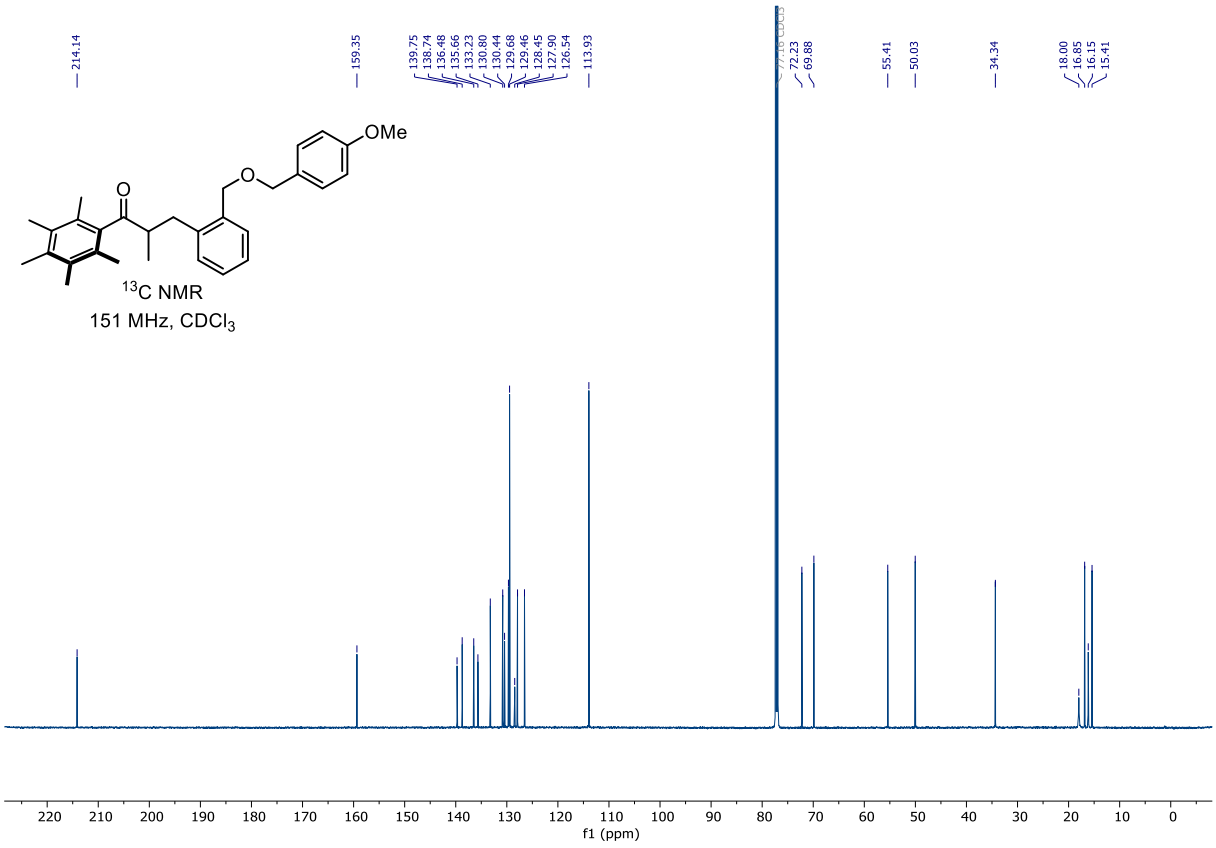
151 MHz, $CDCl_3$

mixture of diastereomers

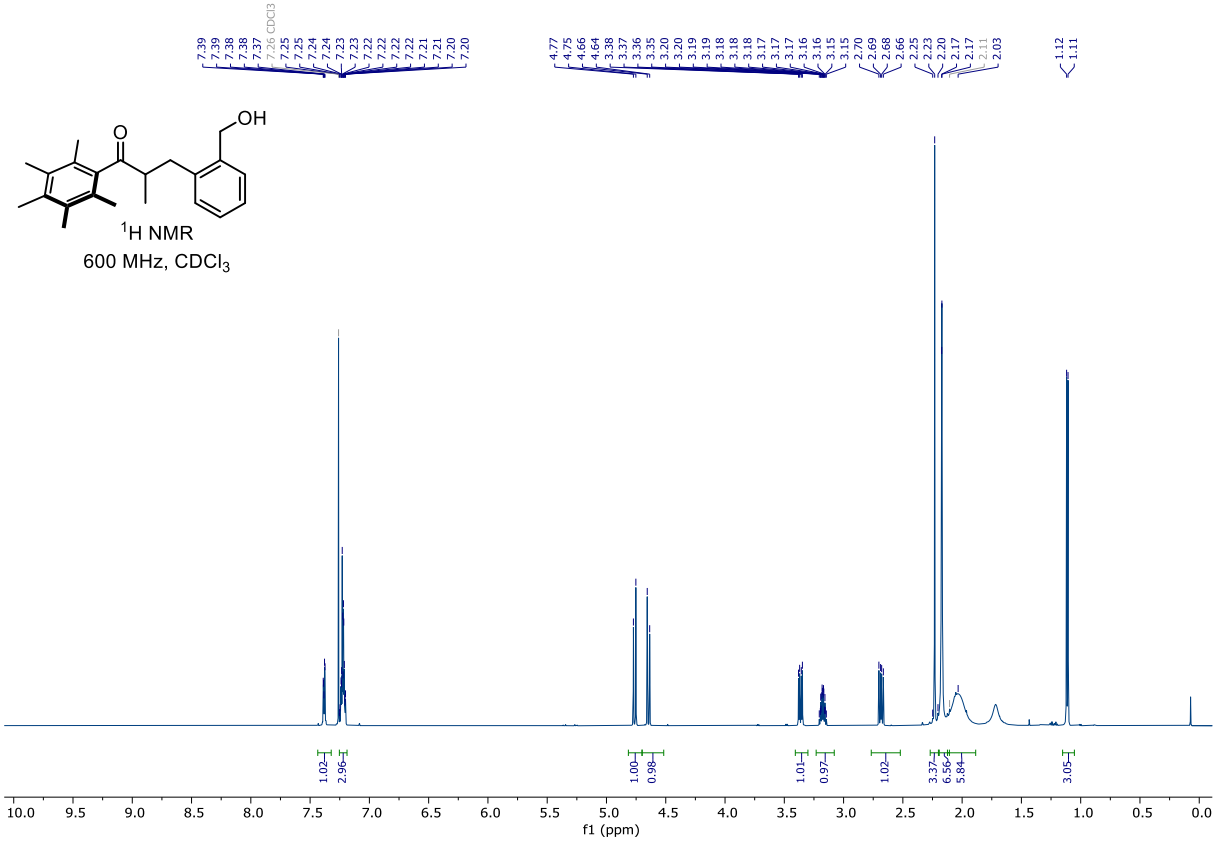
[86:14] d.r.

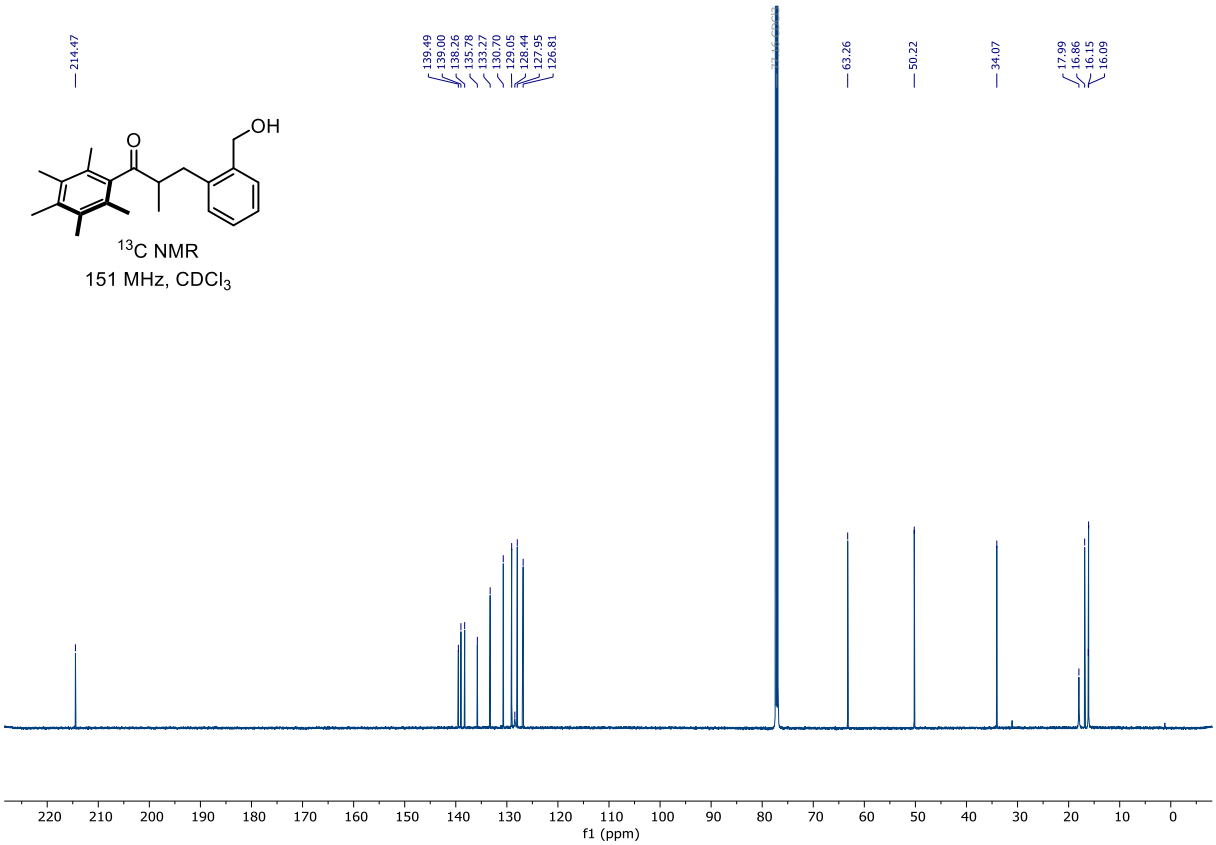
S33 3-(2-(((4-Methoxybenzyl)oxy)methyl)phenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



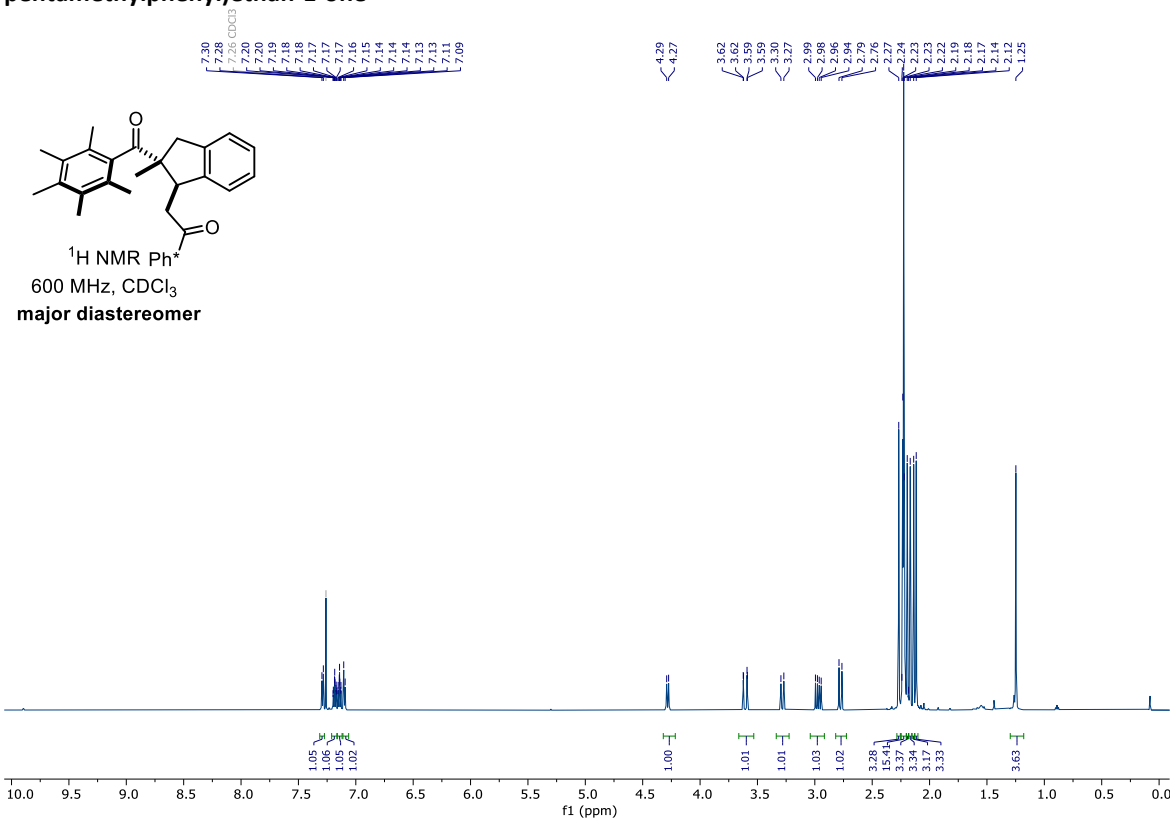


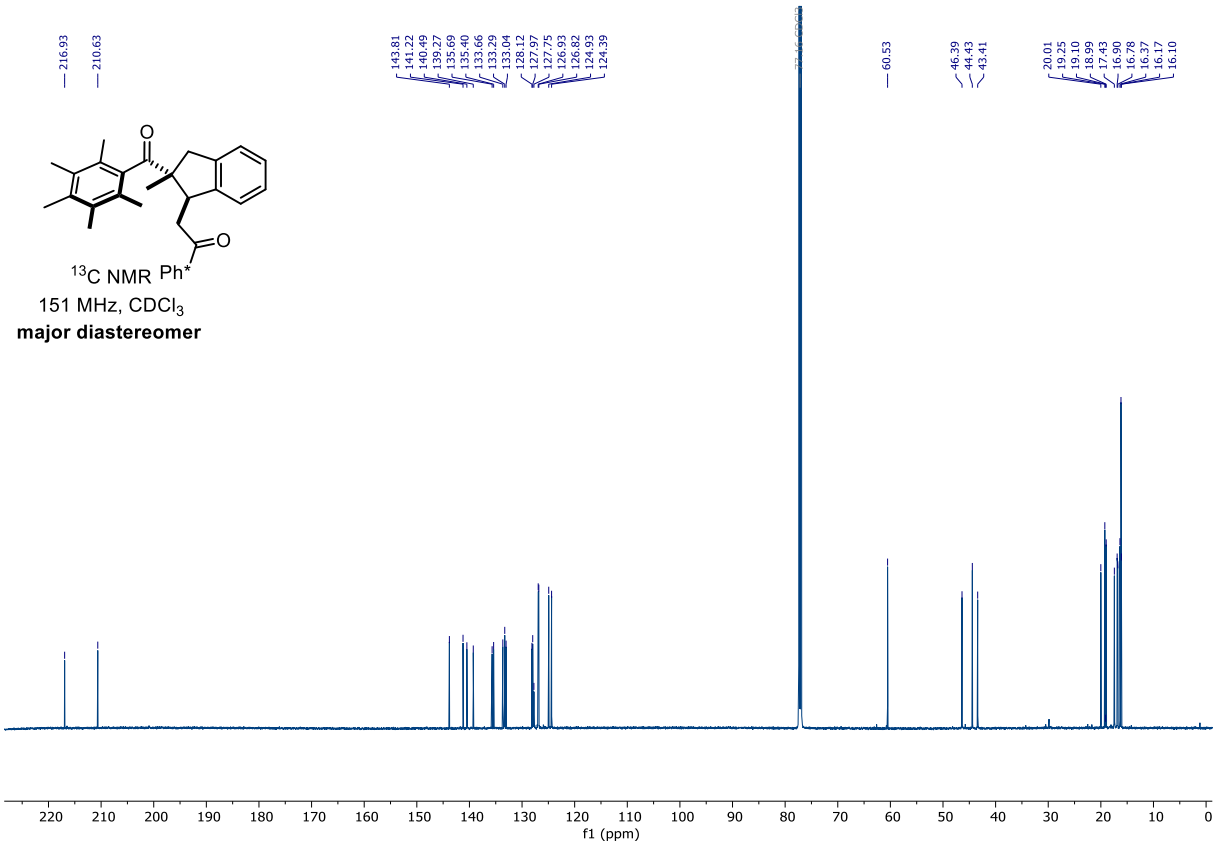
11a 3-(2-(Hydroxymethyl)phenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



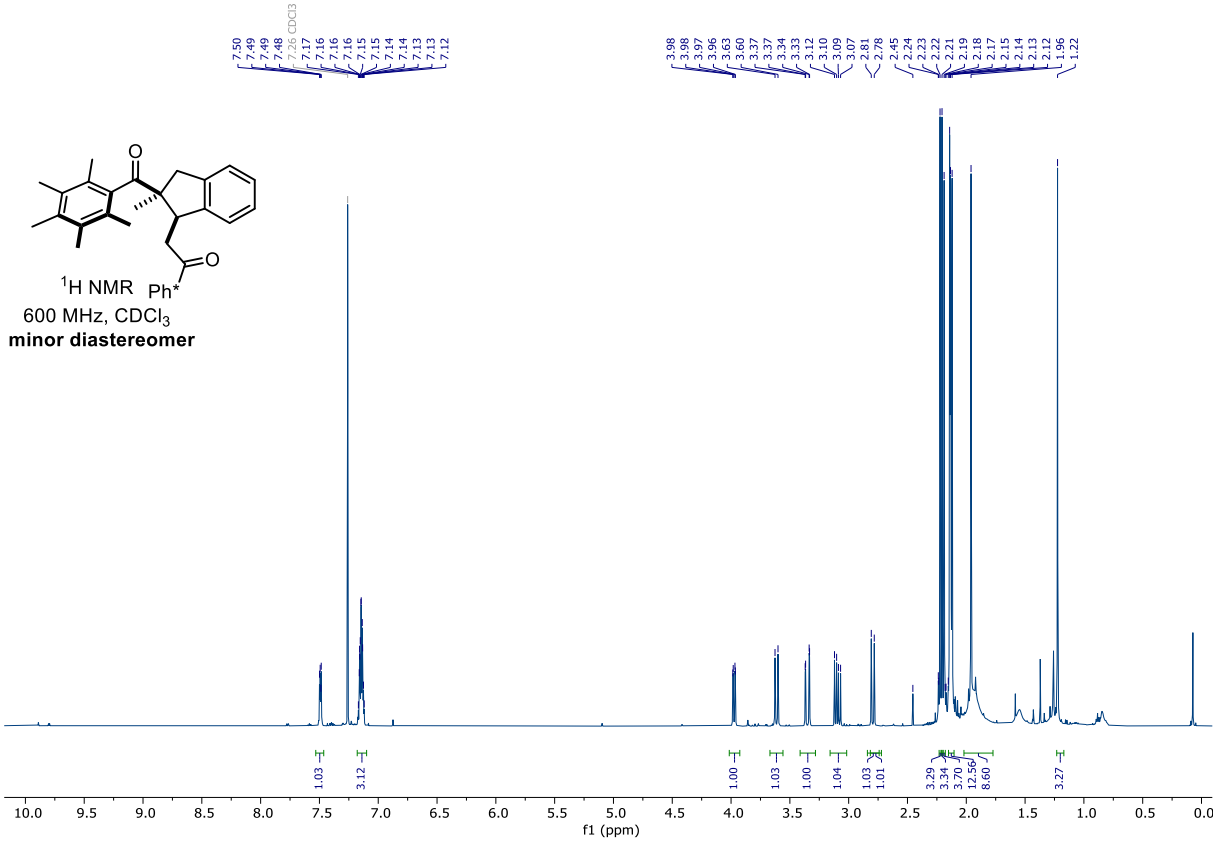


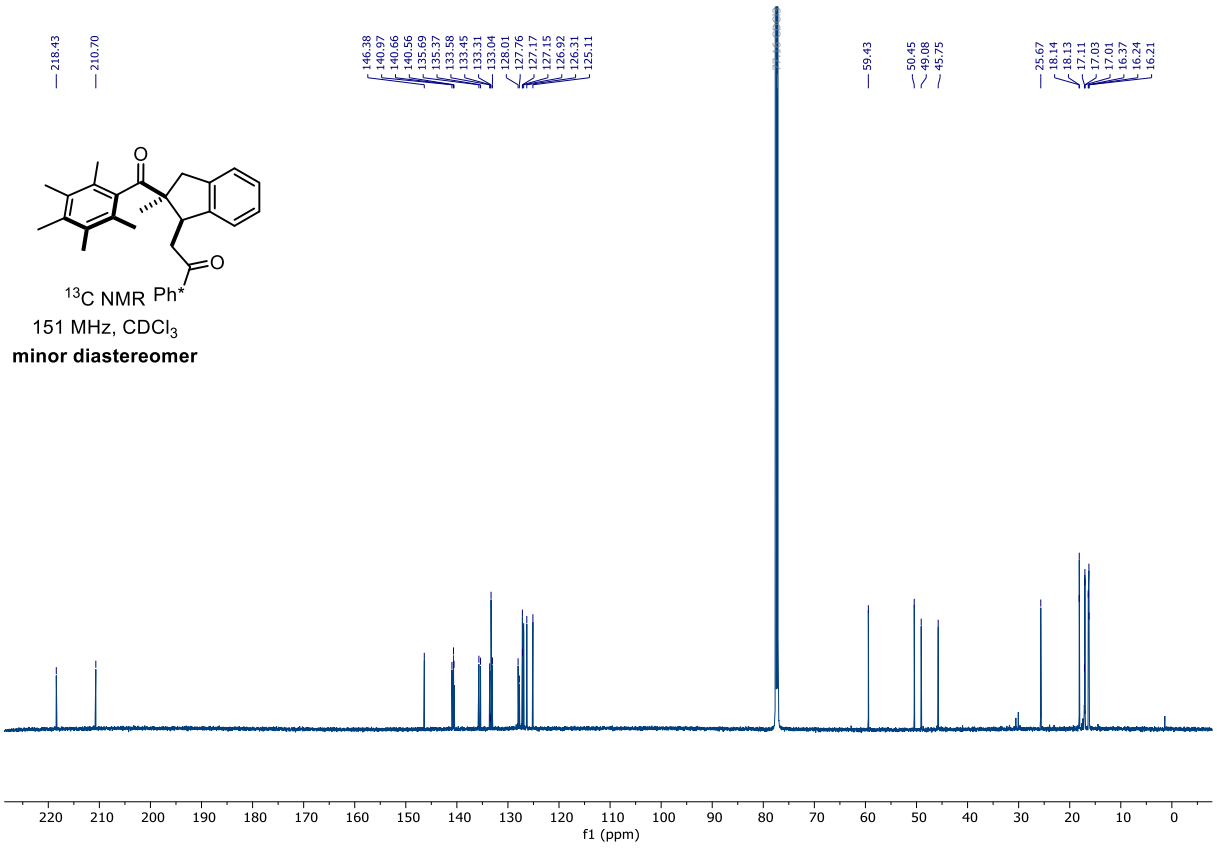
***trans*-3w 2-((1*RS,* 2*RS*)-2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)-2,3-dihydro-1*H*-inden-1-yl)-1-(2,3,4,5,6-pentamethylphenyl)ethan-1-one**



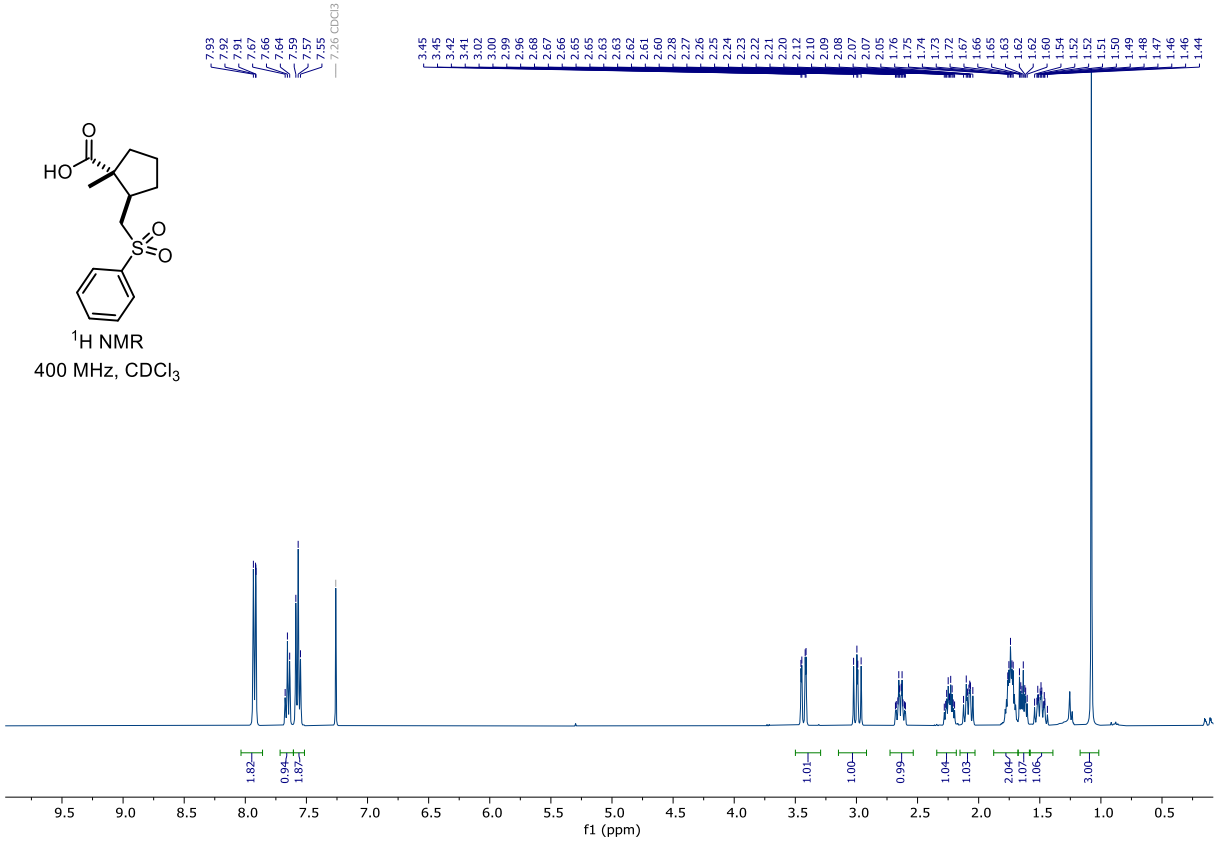


***cis*-3w 2-((1*SR*, 2*RS*)-2-Methyl-2-(2,3,4,5,6-pentamethylbenzoyl)-2,3-dihydro-1*H*-inden-1-yl)-1-(2,3,4,5,6-pentamethylphenyl)ethan-1-one**

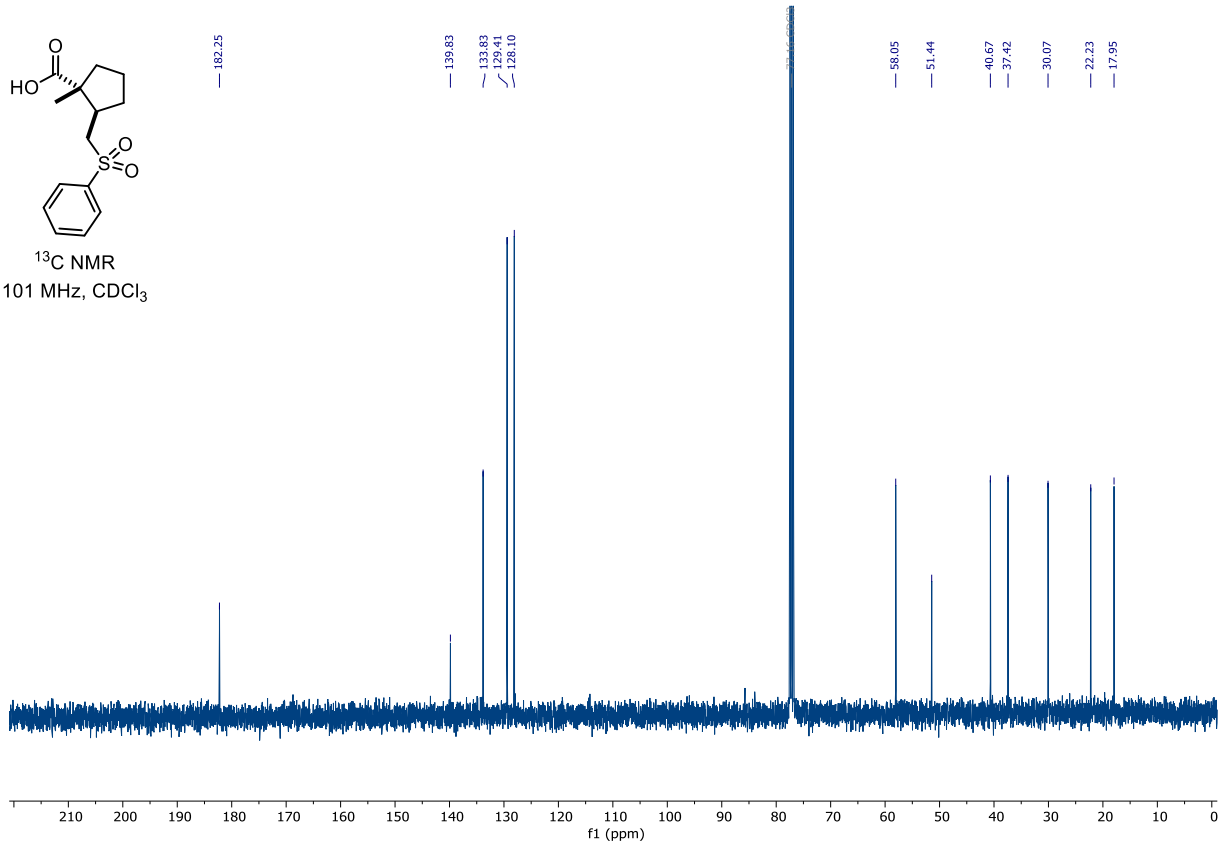




5 (1*SR*,2*SR*)-1-Methyl-2-((phenylsulfonyl)methyl)cyclopentane-1-carboxyli acid

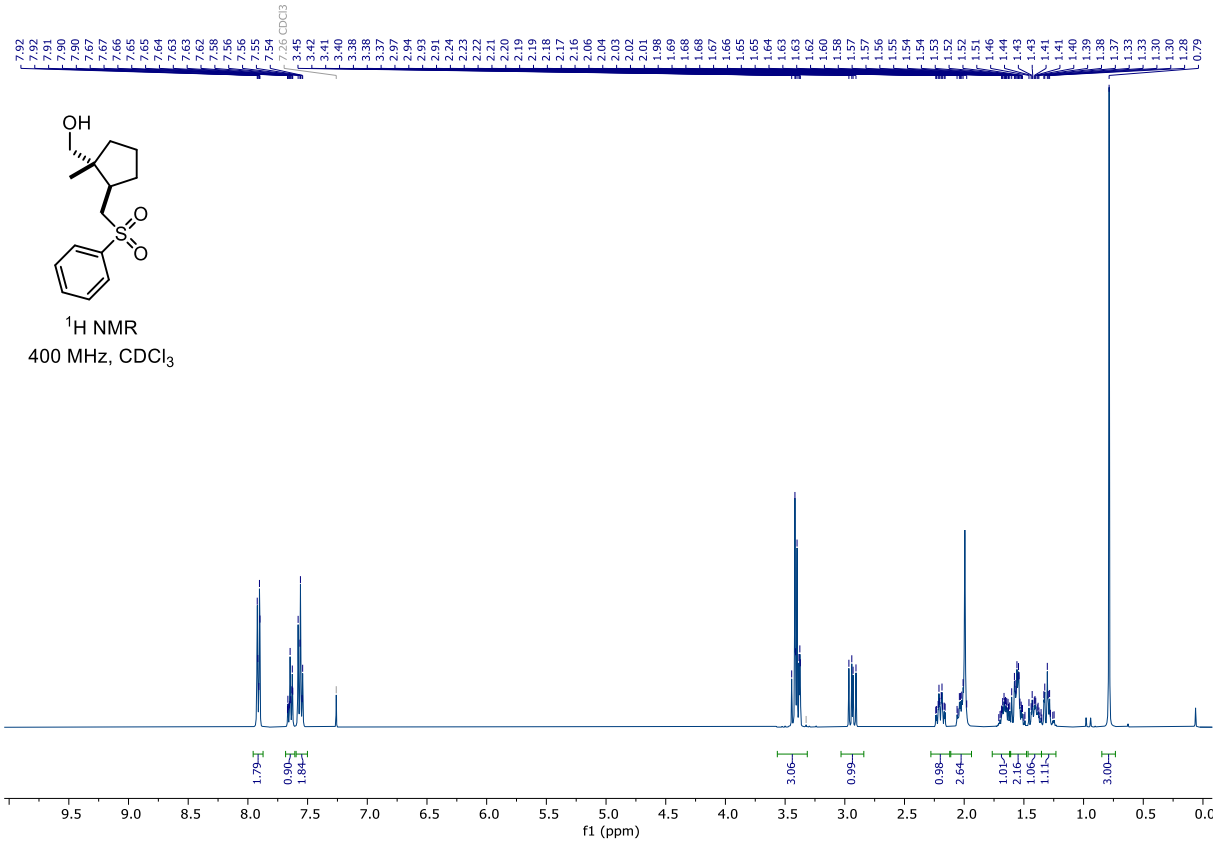


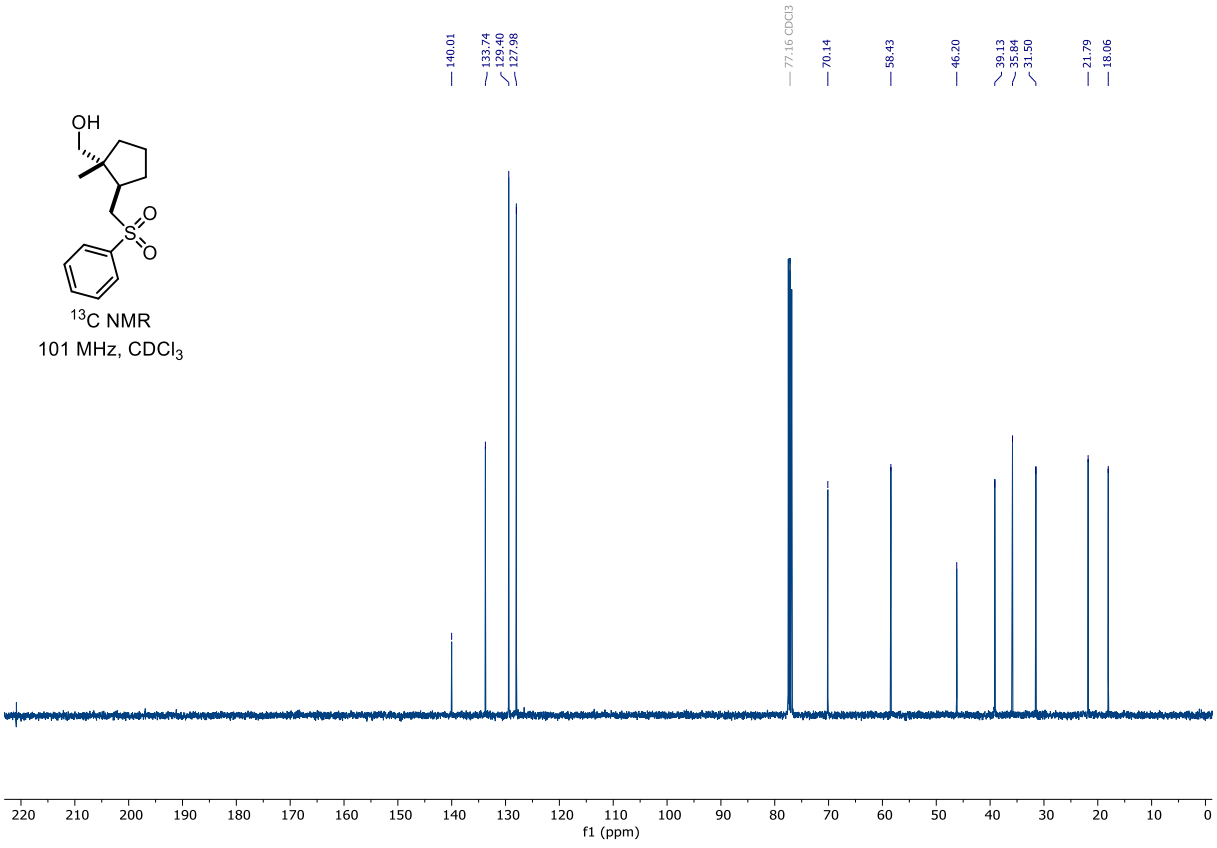
^{1}H NMR
400 MHz, $CDCl_3$



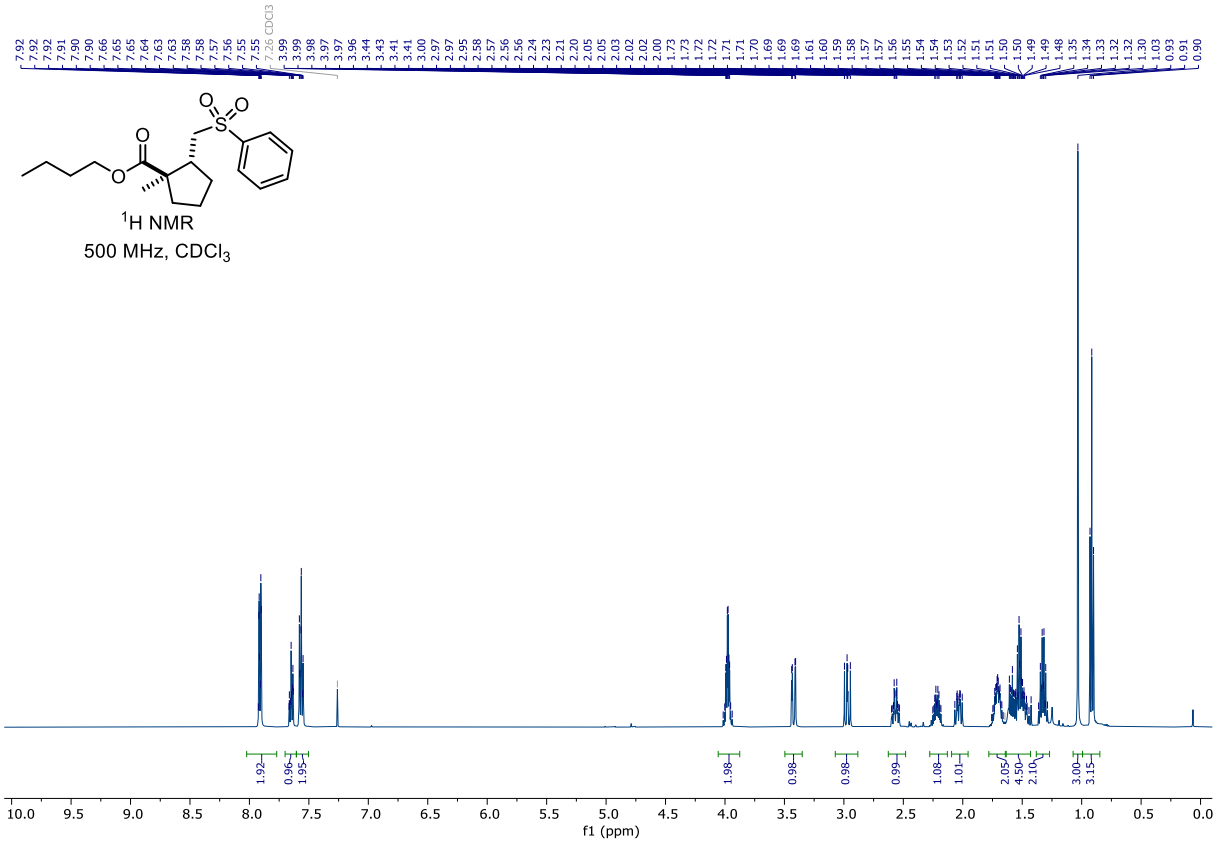
^{13}C NMR
101 MHz, $CDCl_3$

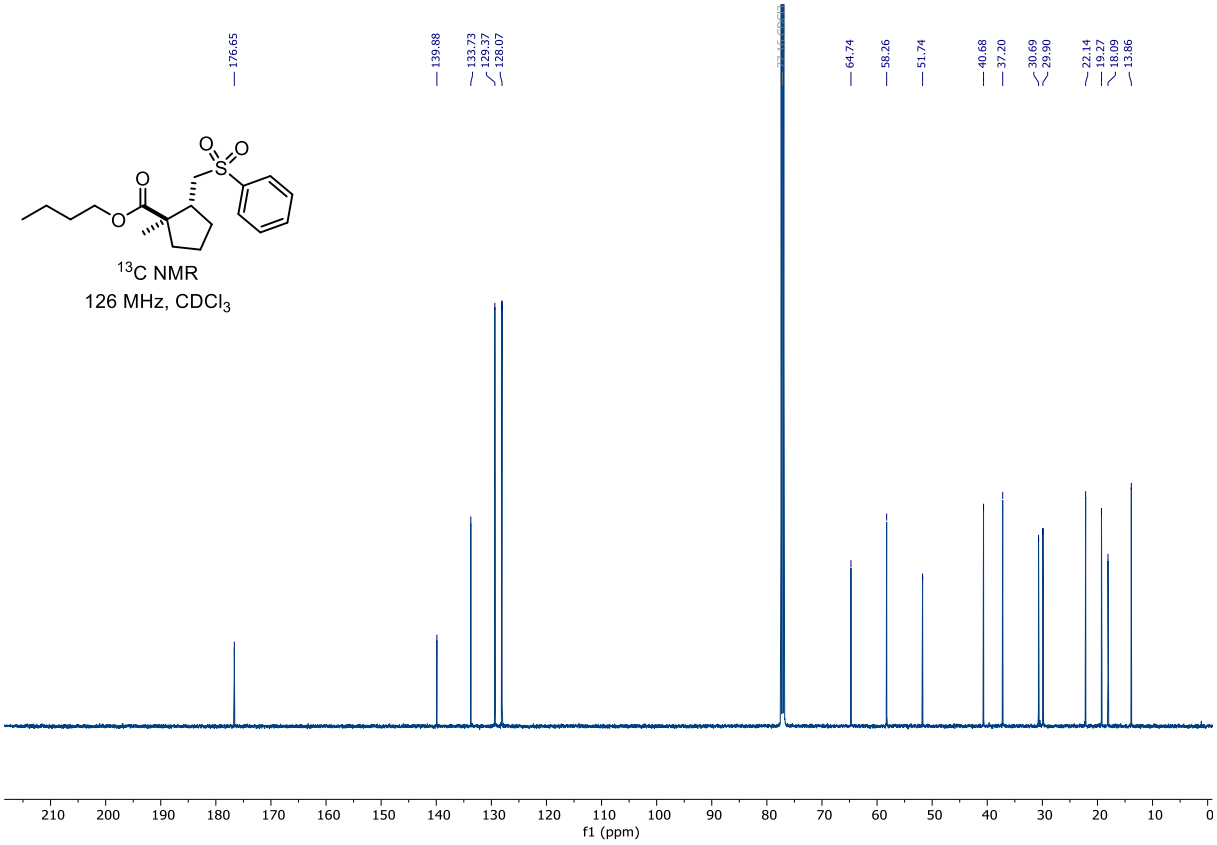
6 ((1*RS*,2*RS*)-1-Methyl-2-((phenylsulfonyl)methyl)cyclopentyl)methanol



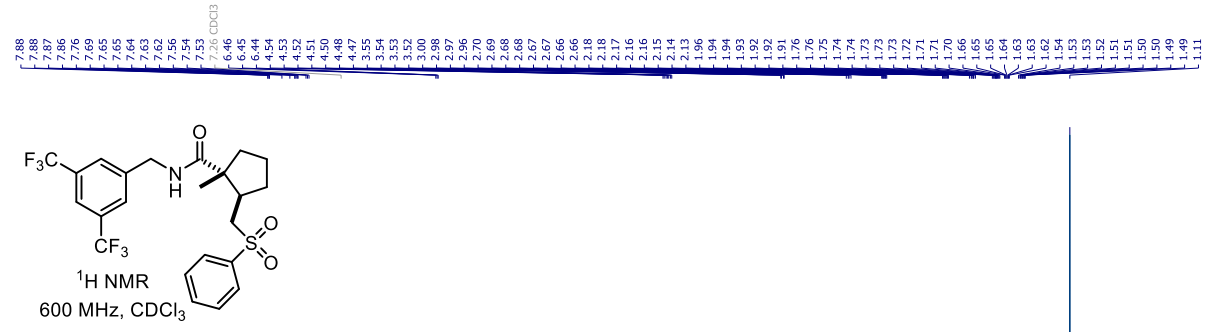


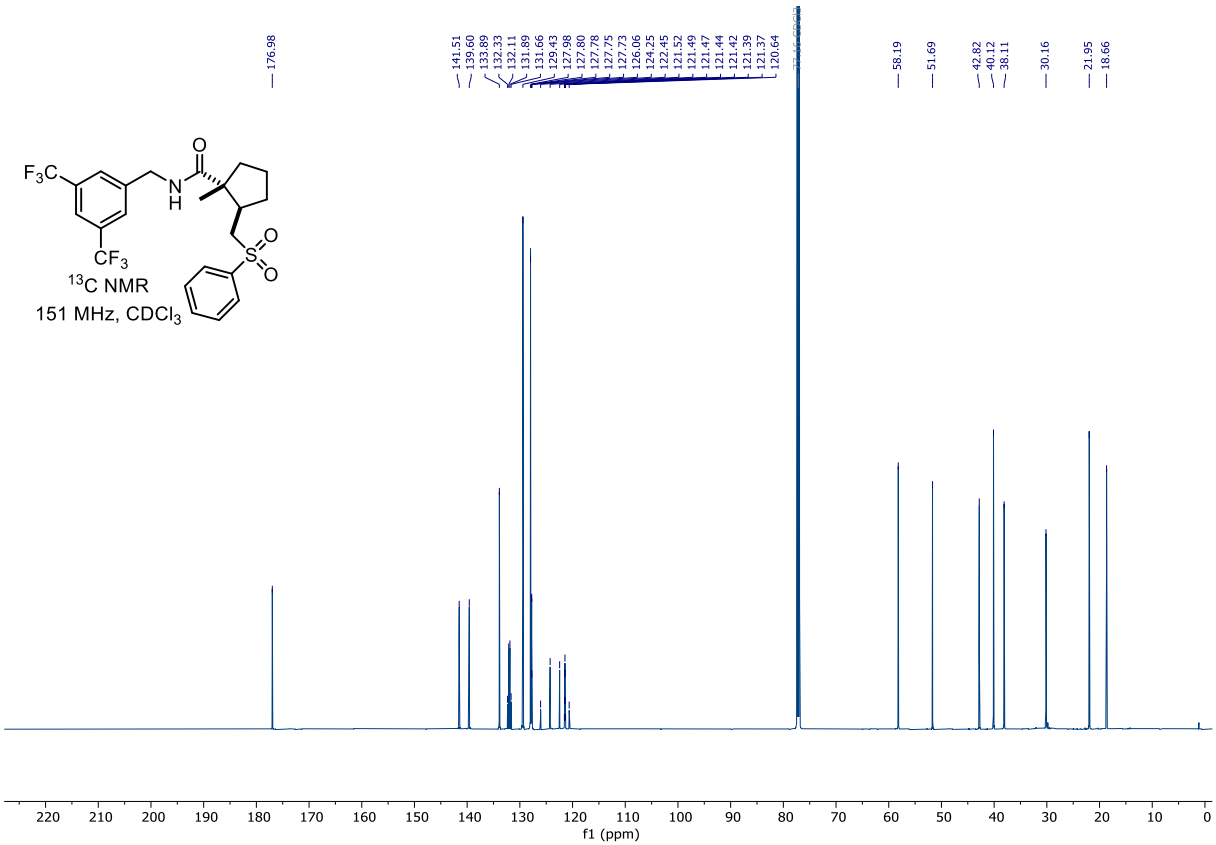
7 Butyl (1*RS*,2*RS*)-1-methyl-2-((phenylsulfonyl)methyl)cyclopentane-1-carboxylate

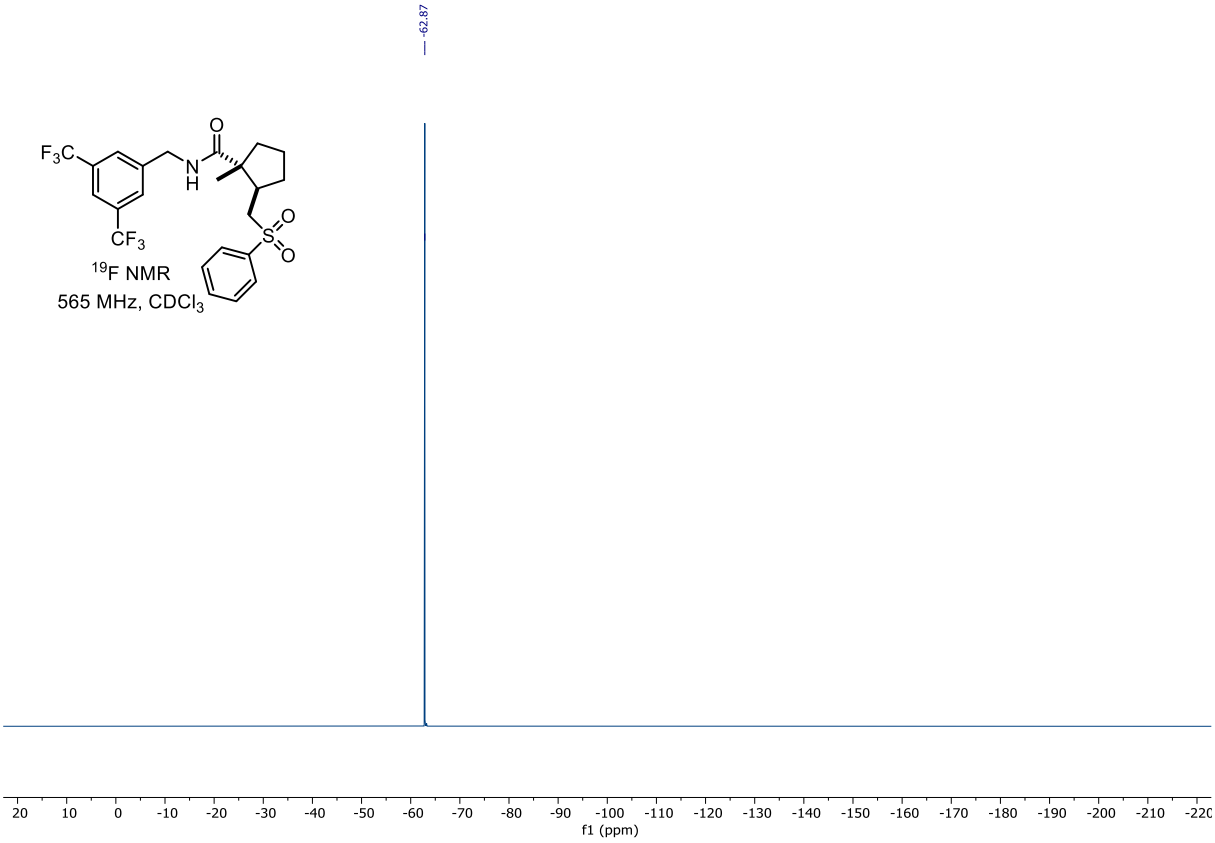




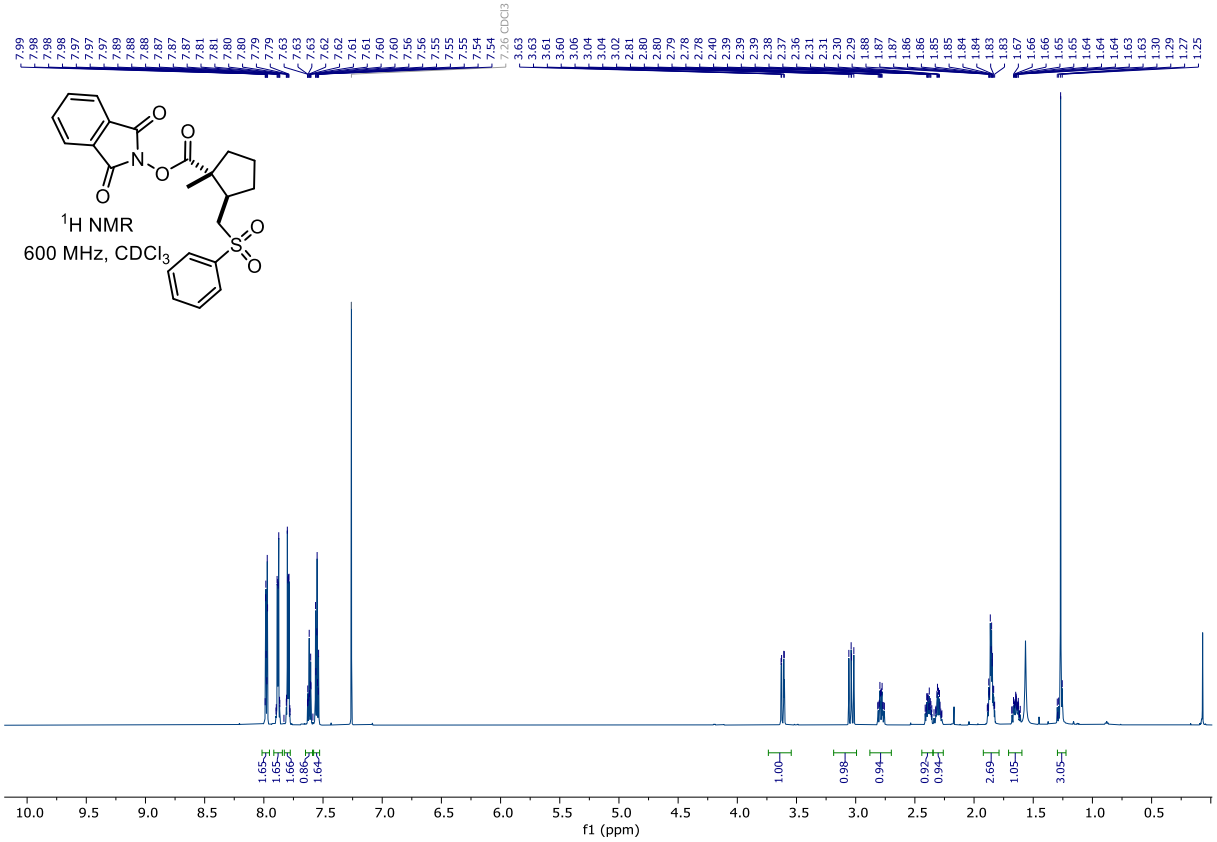
8 (1*RS*,2*RS*)-*N*-(3,5-Bis(trifluoromethyl)benzyl)-1-methyl-2-((phenylsulfonyl)methyl)cyclopentane-1-carboxamide

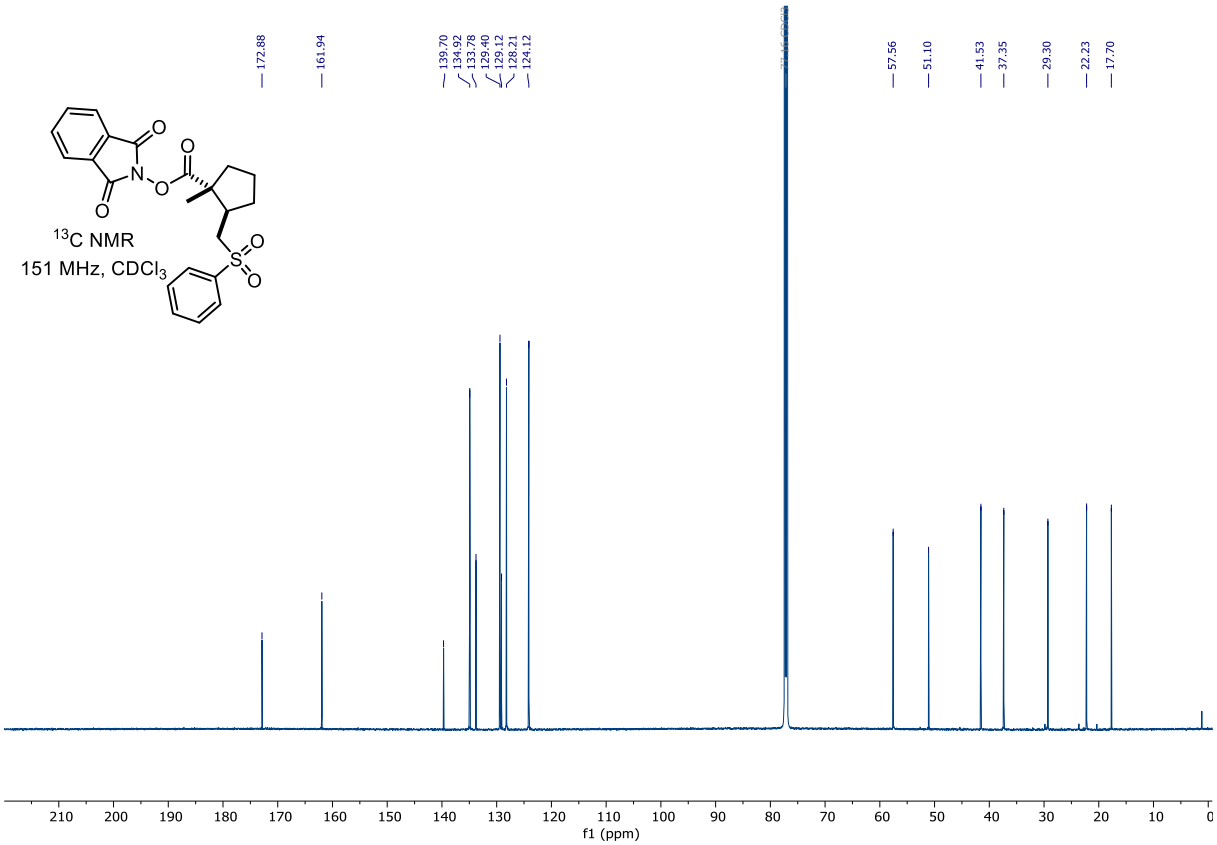




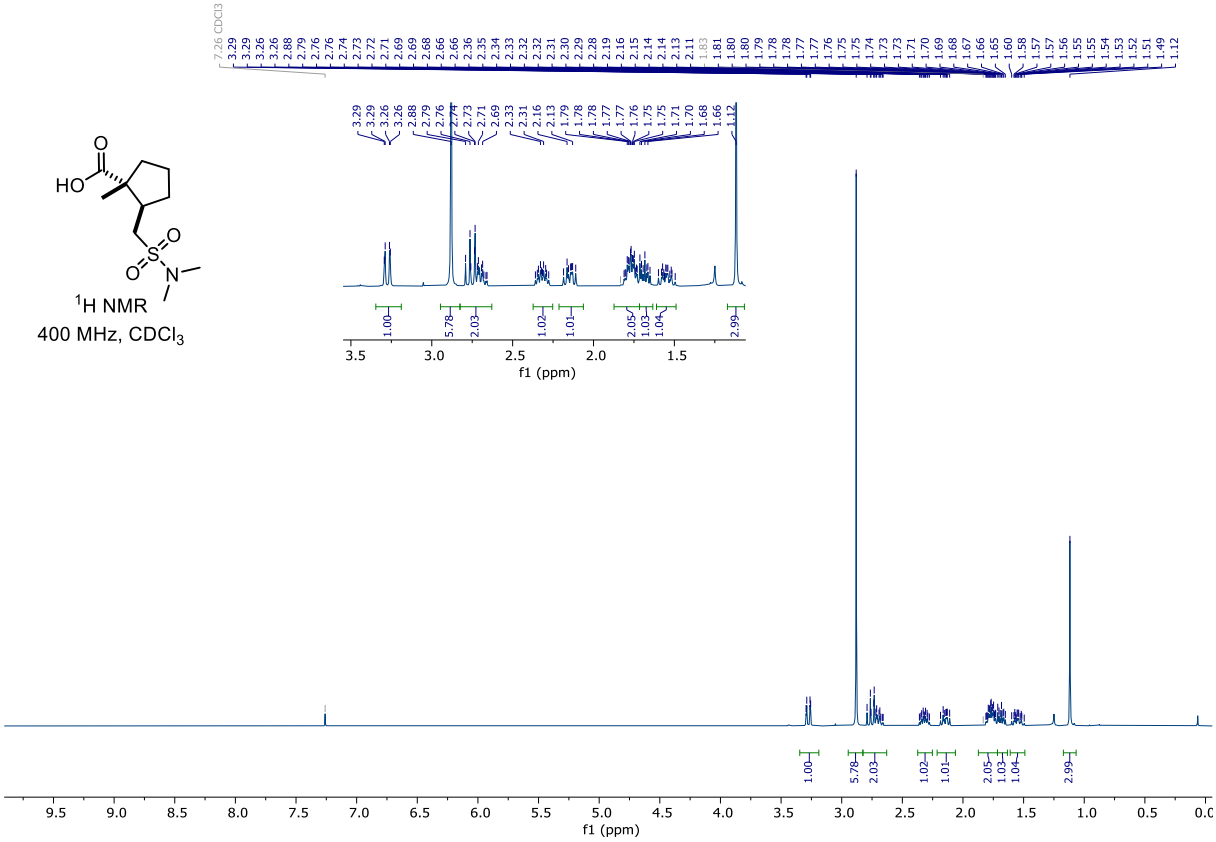

-62.87
F3C
CF3
O
N
H
O
S
O
19F NMR
565 MHz, CDCl3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

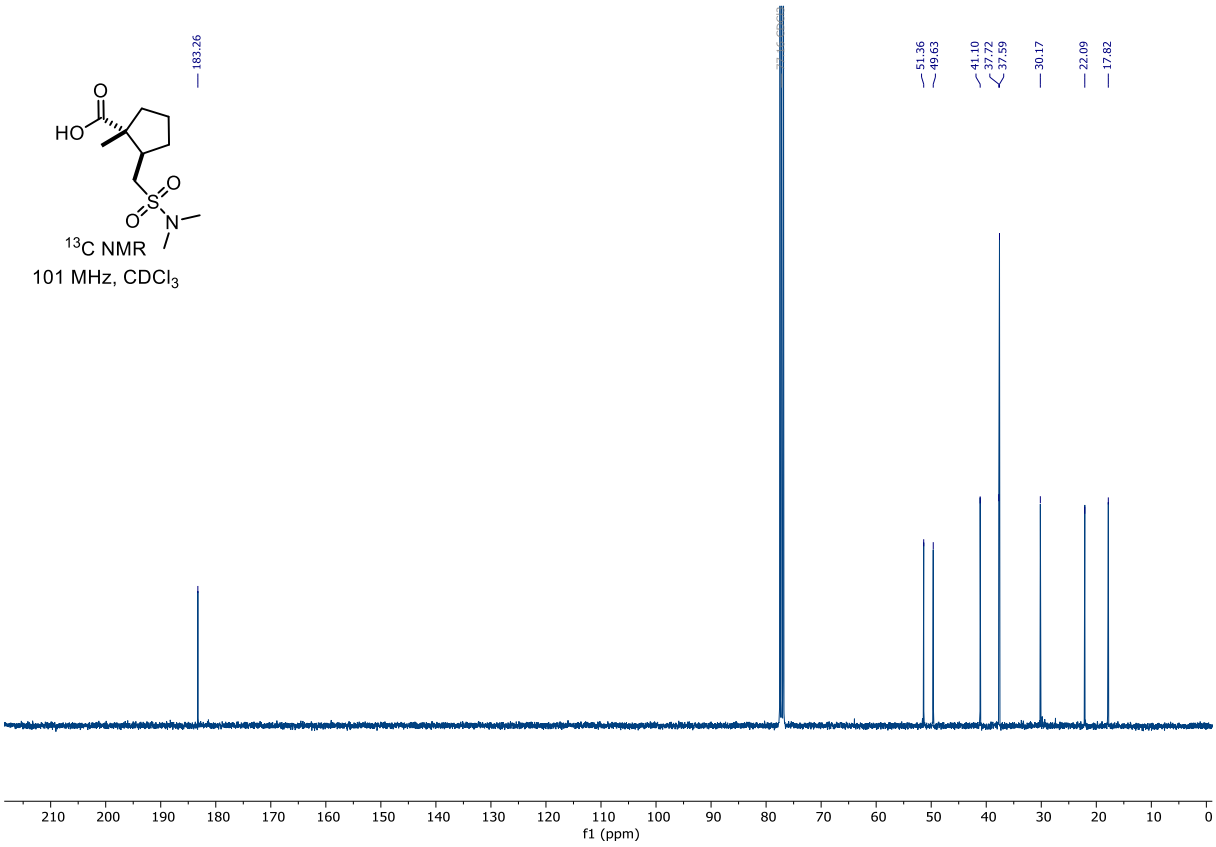
9 1,3-Dioxoisoindolin-2-yl (1*RS*,2*RS*)-1-methyl-2-((phenylsulfonyl)methyl)cyclopentane-1-carboxylate



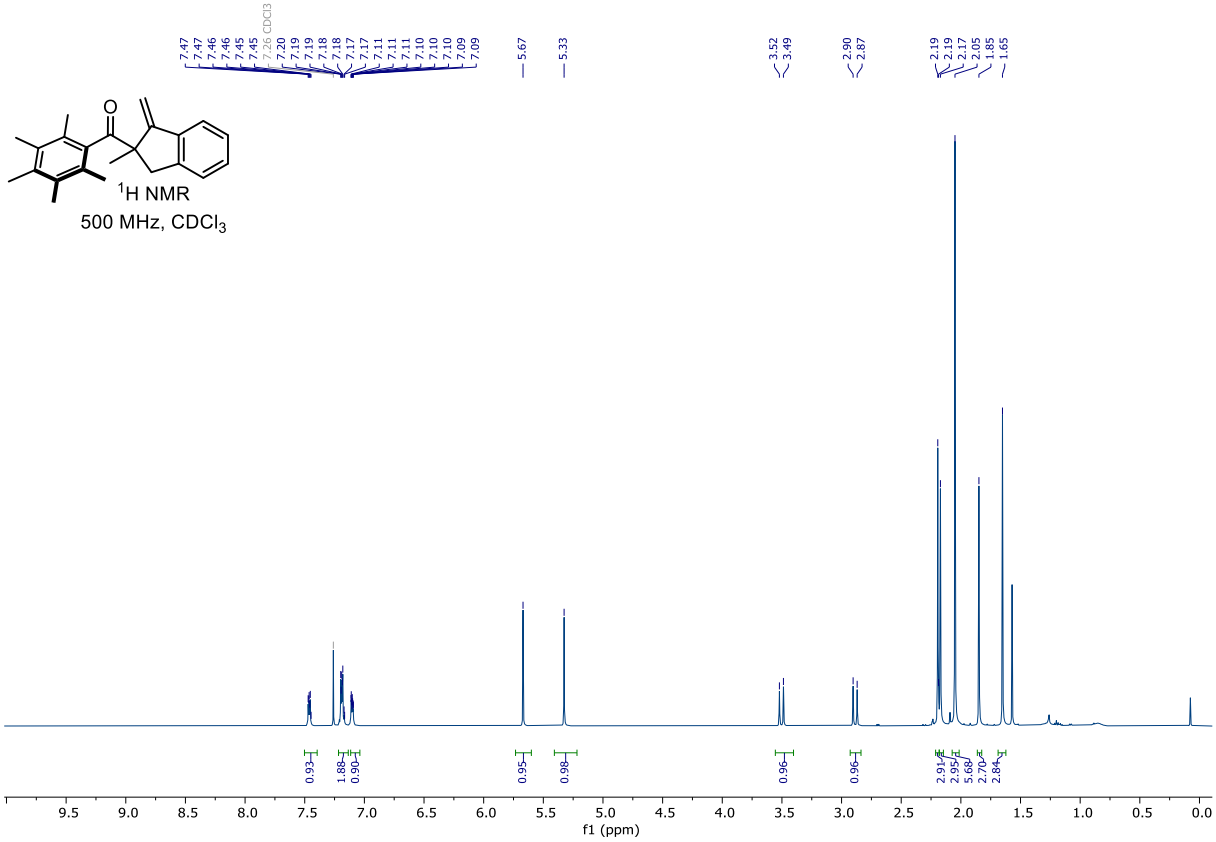


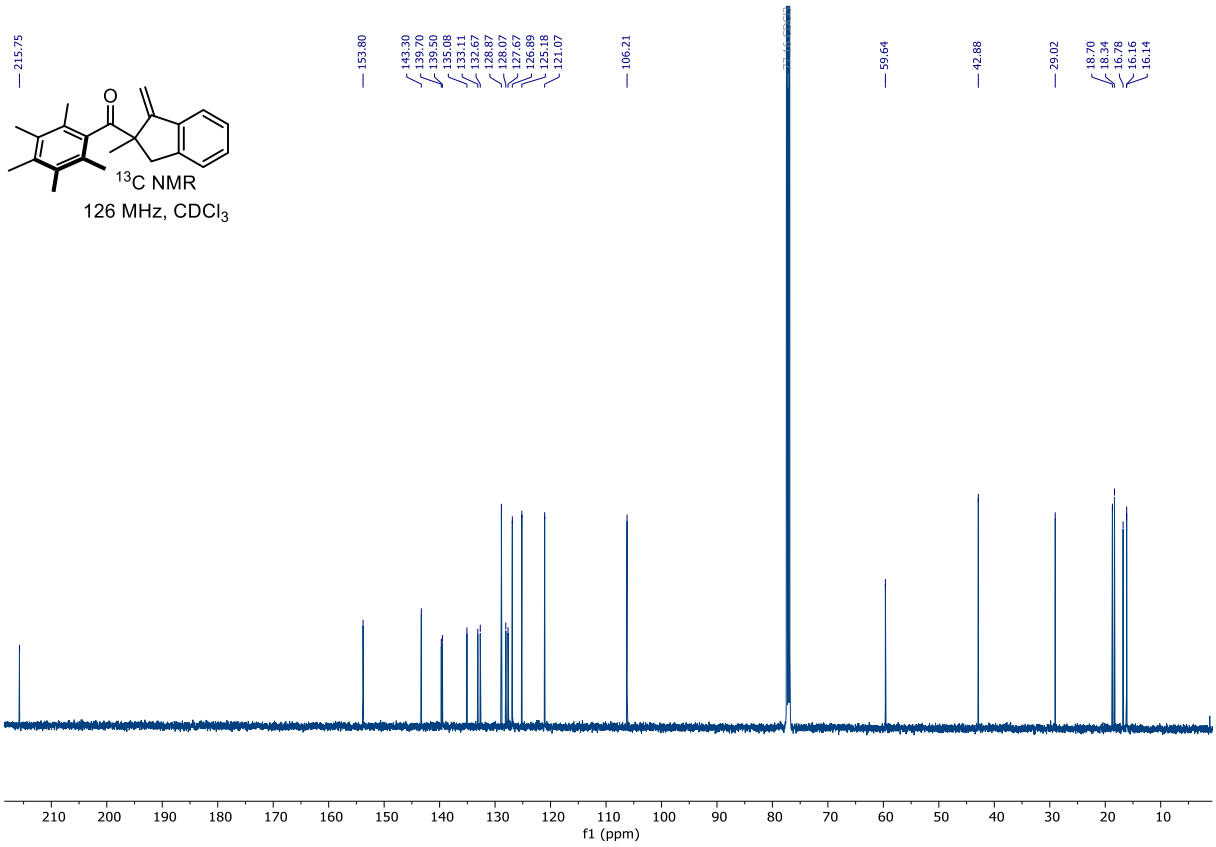
10 (1*RS*,2*RS*)-2-((*N*,*N*-Dimethylsulfamoyl)methyl)-1-methylcyclopentane-1-carboxylic acid



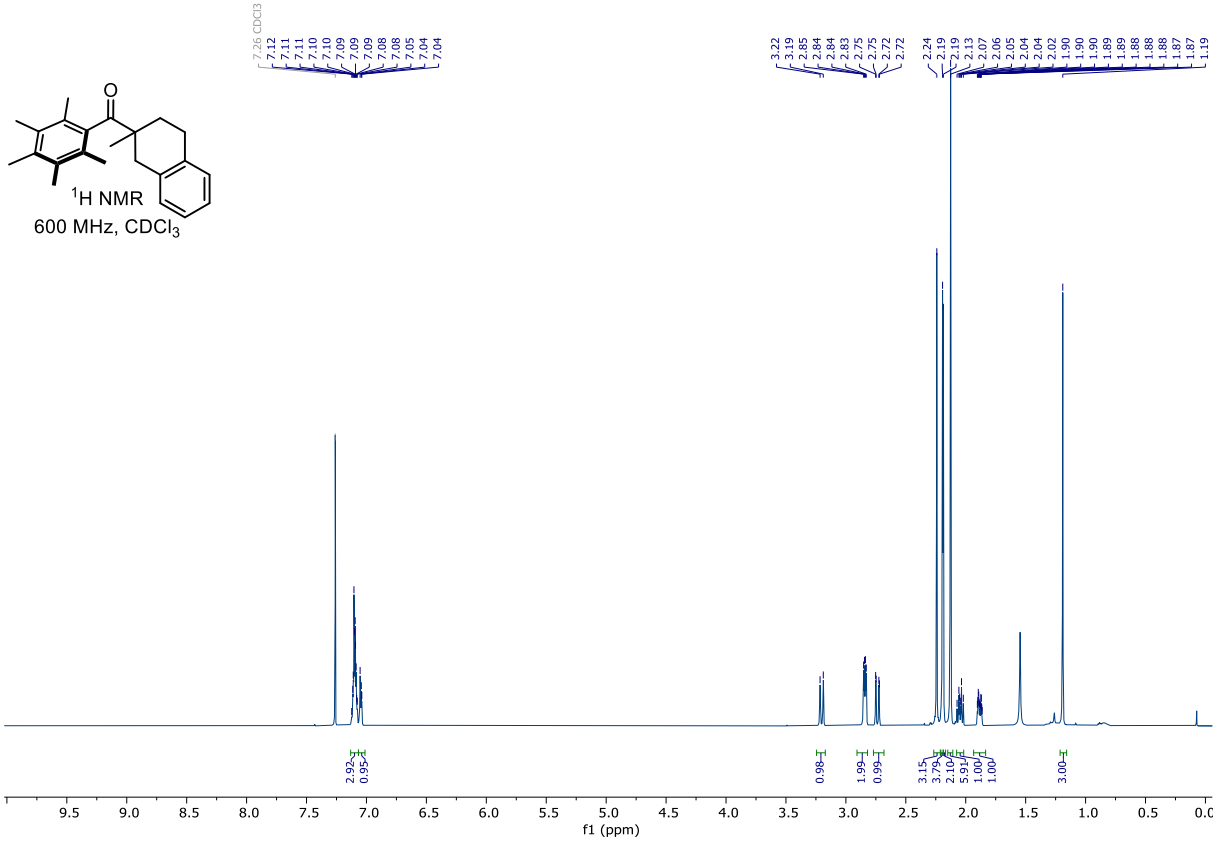


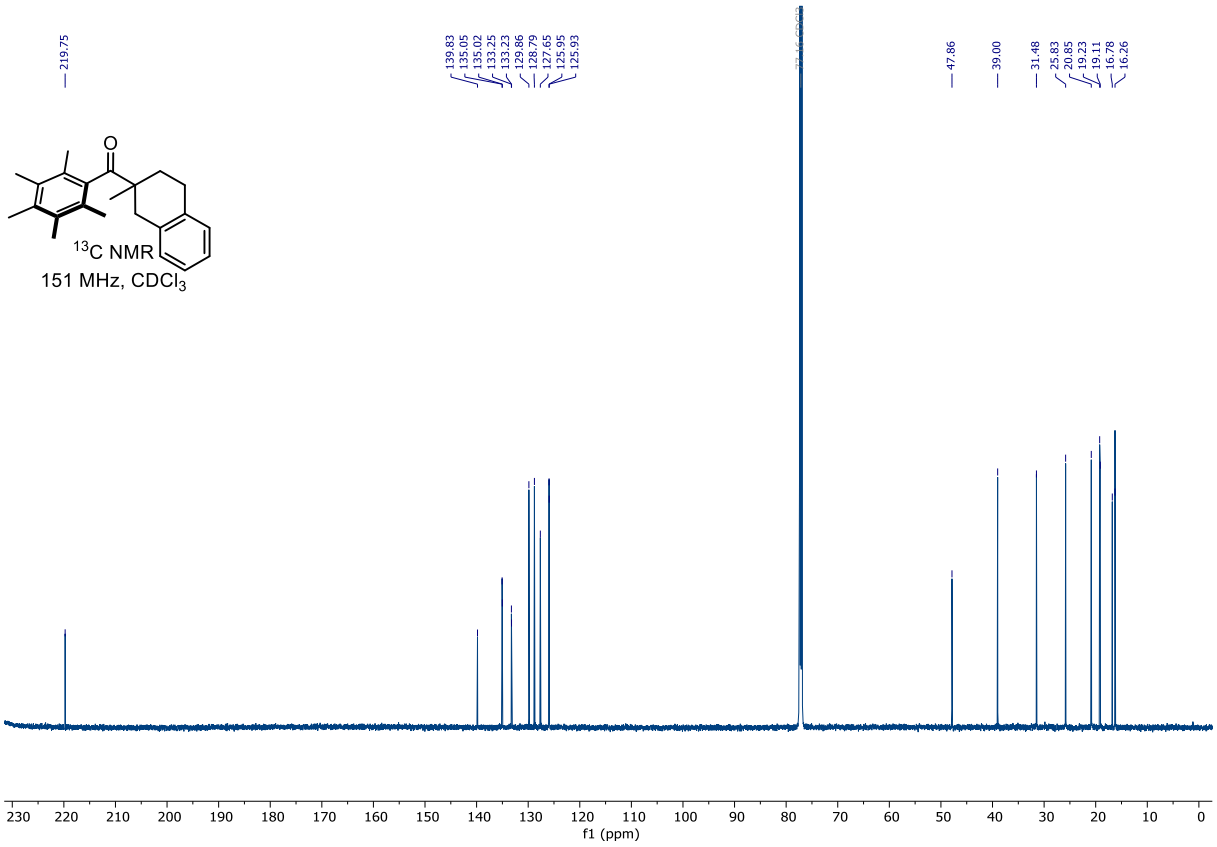
12a (2-Methyl-1-methylene-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



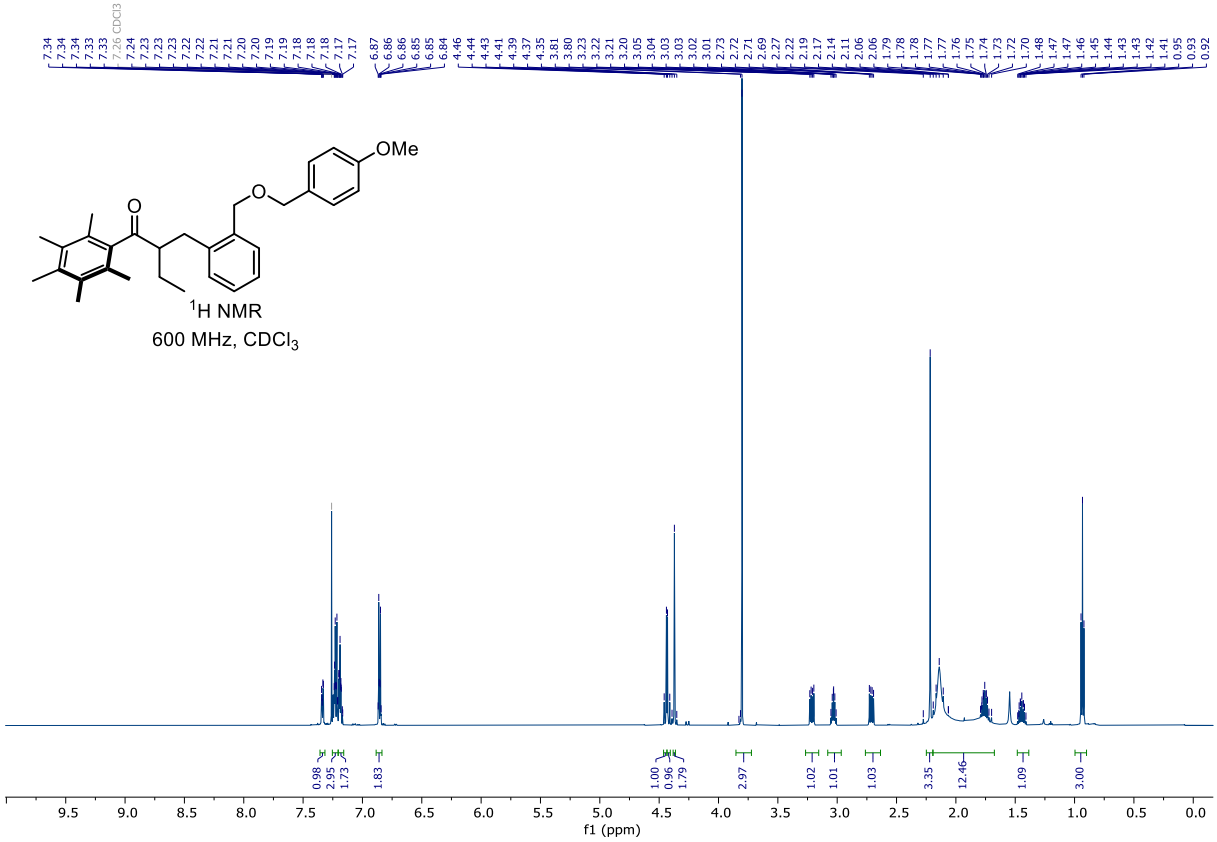


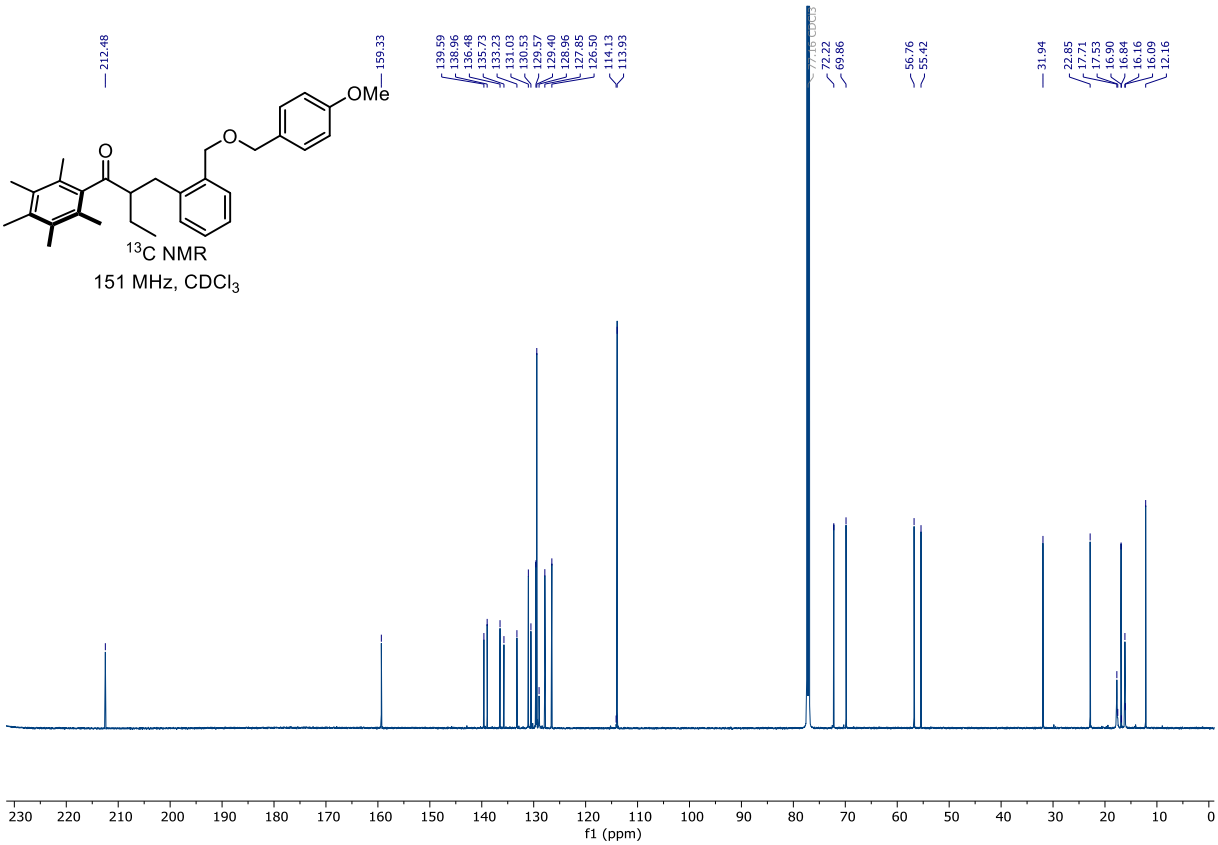
13a (2-Methyl-1,2,3,4-tetrahydronaphthalen-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



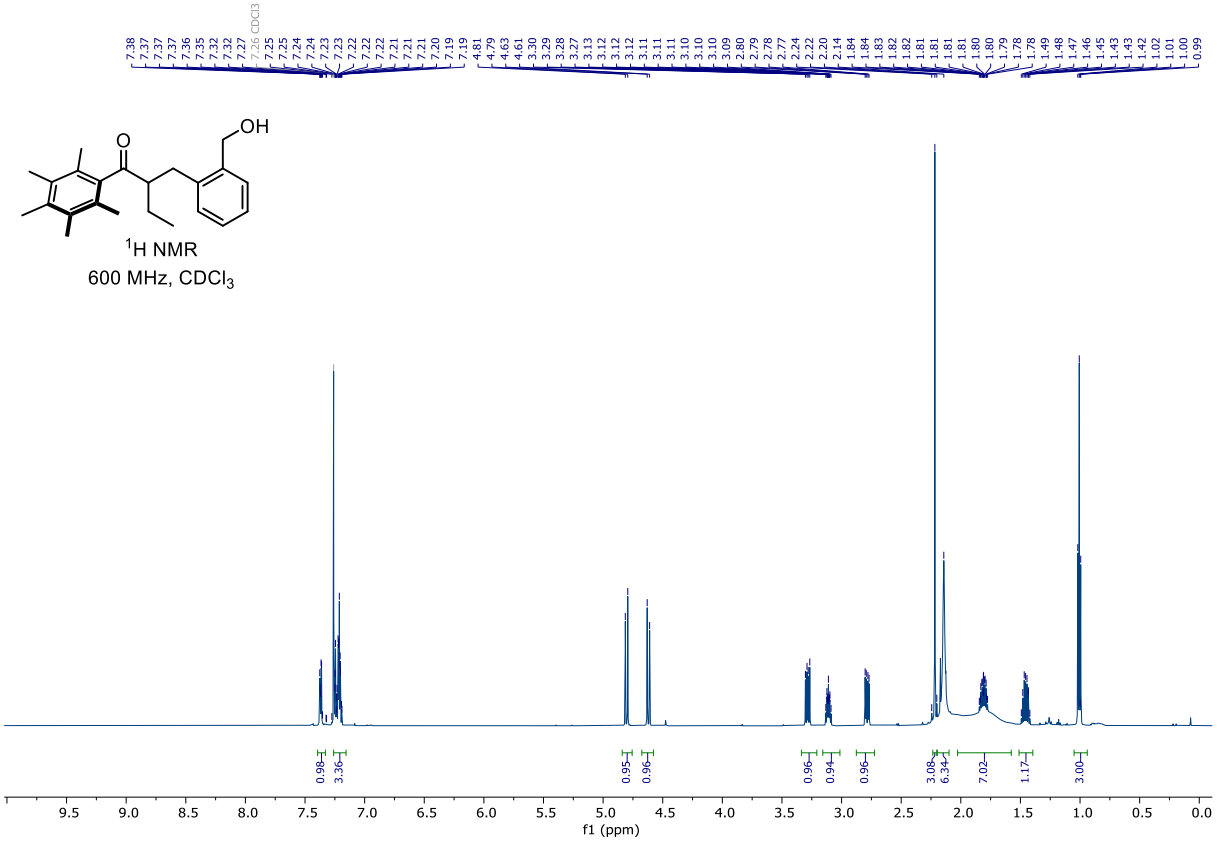


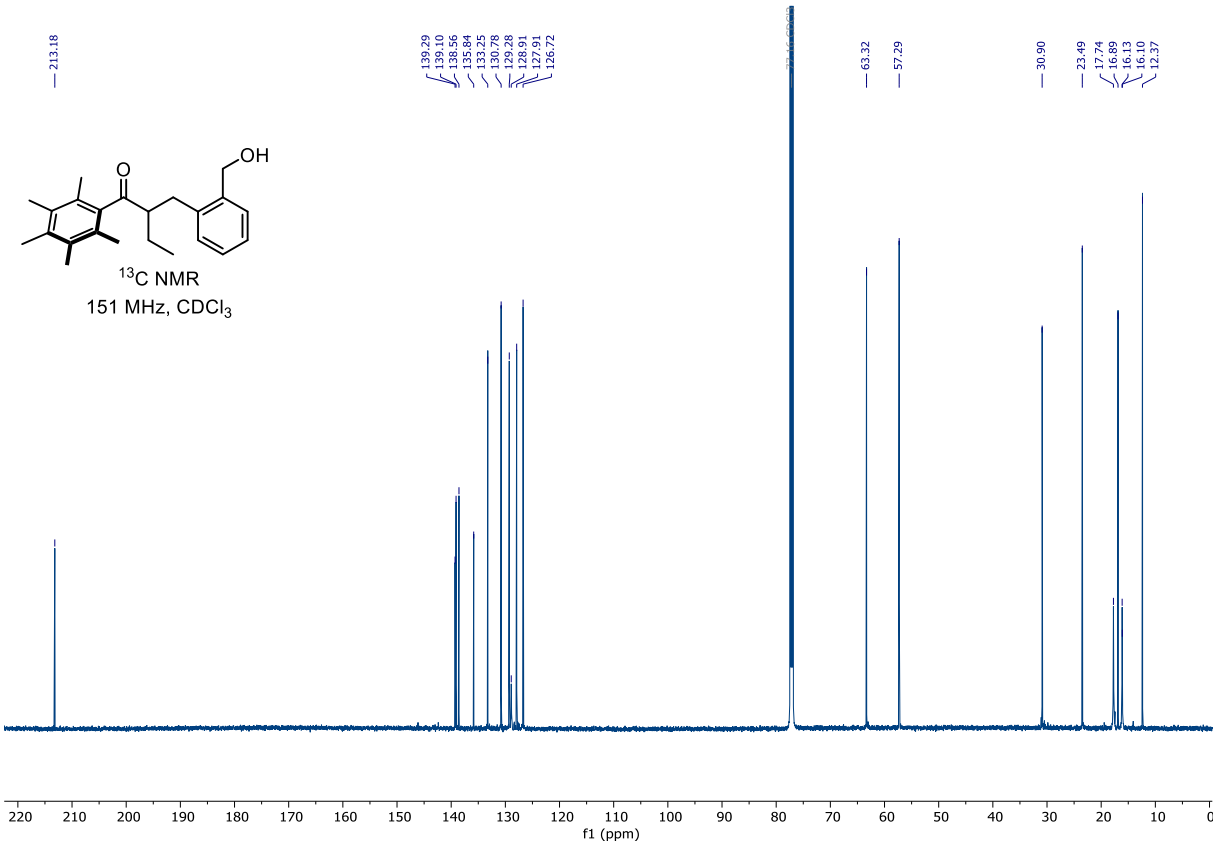
S34 2-(2-(((4-Methoxybenzyl)oxy)methyl)benzyl)-1-(2,3,4,5,6-pentamethylphenyl)butan-1-one



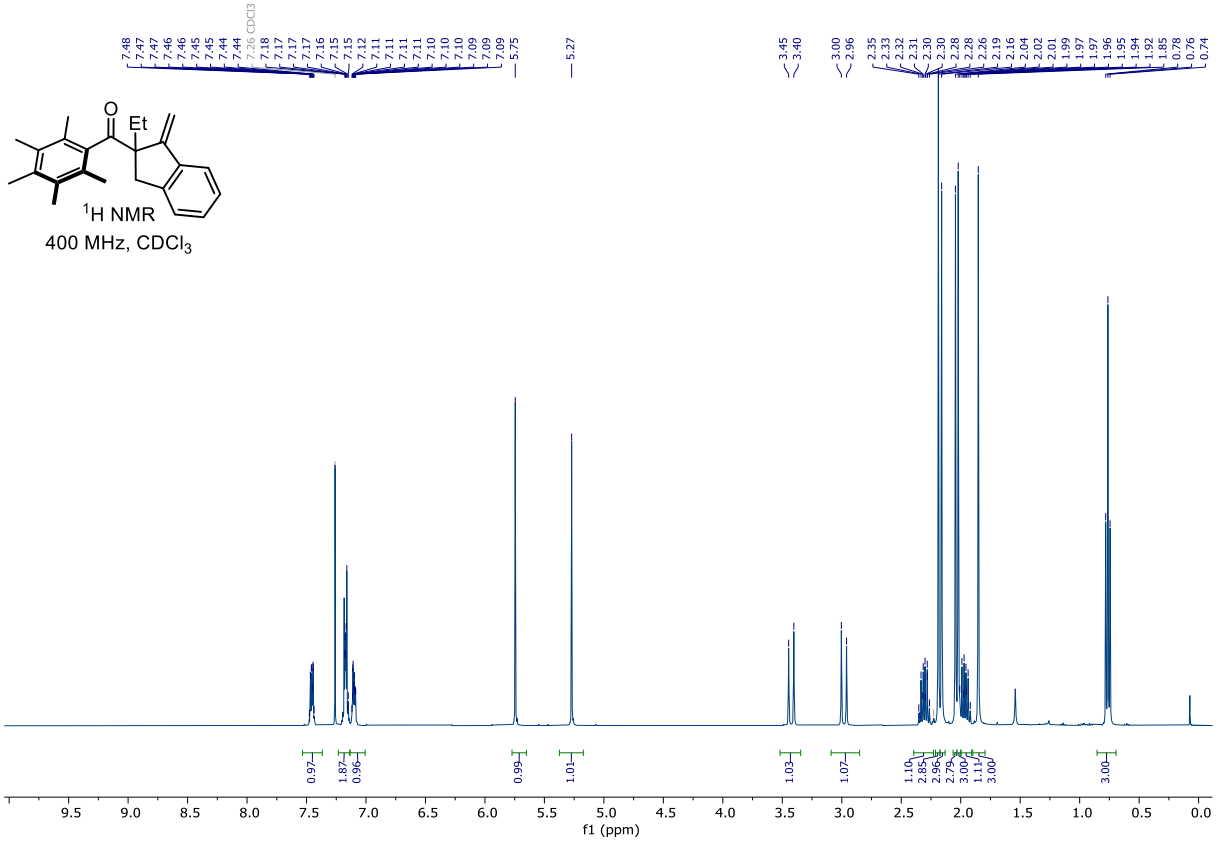


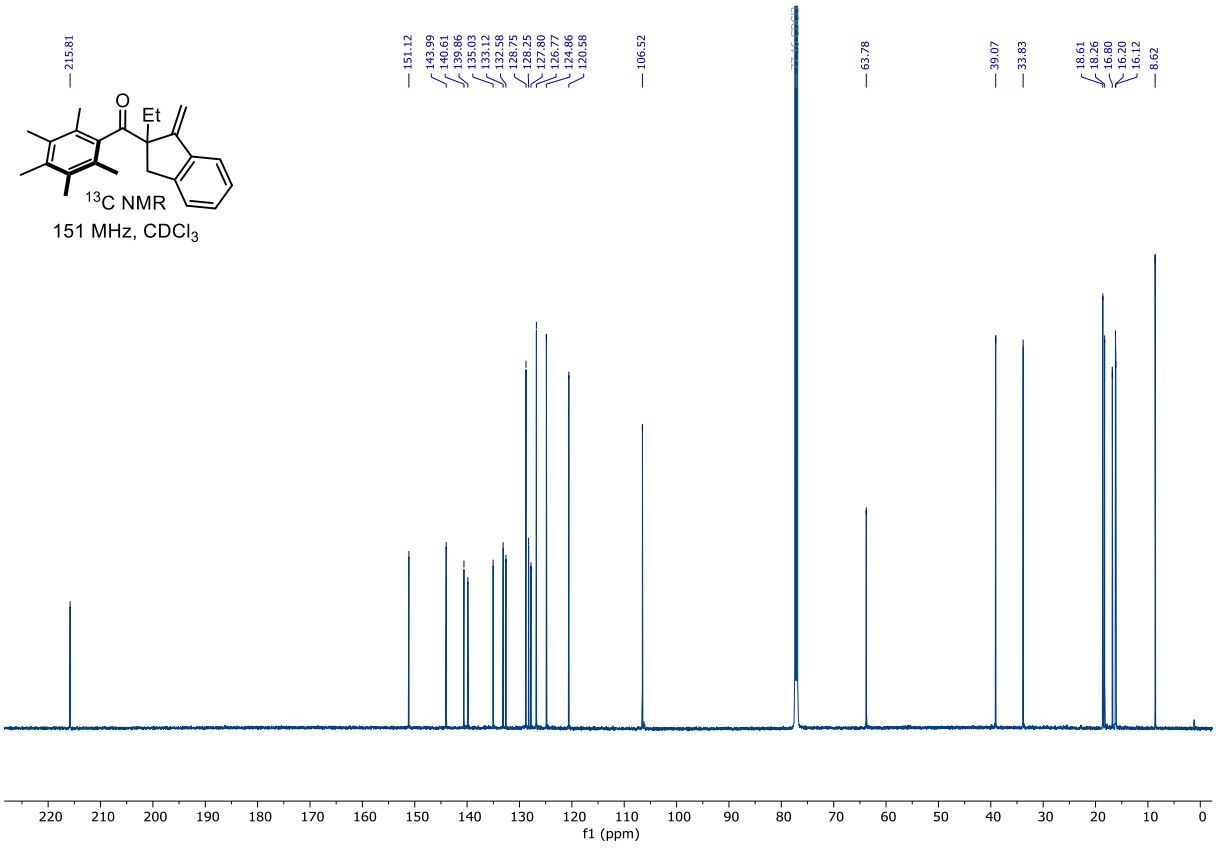
11b 2-(2-(Hydroxymethyl)benzyl)-1-(2,3,4,5,6-pentamethylphenyl)butan-1-one



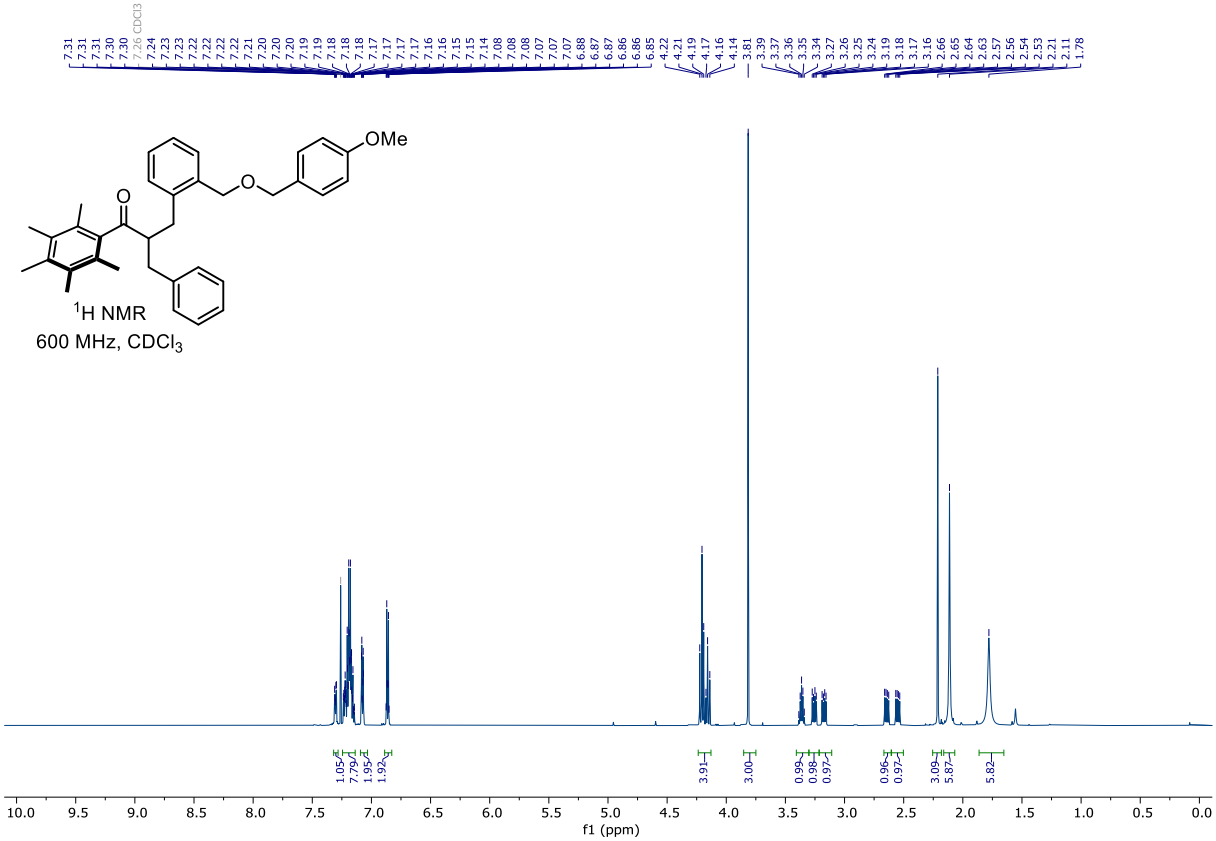


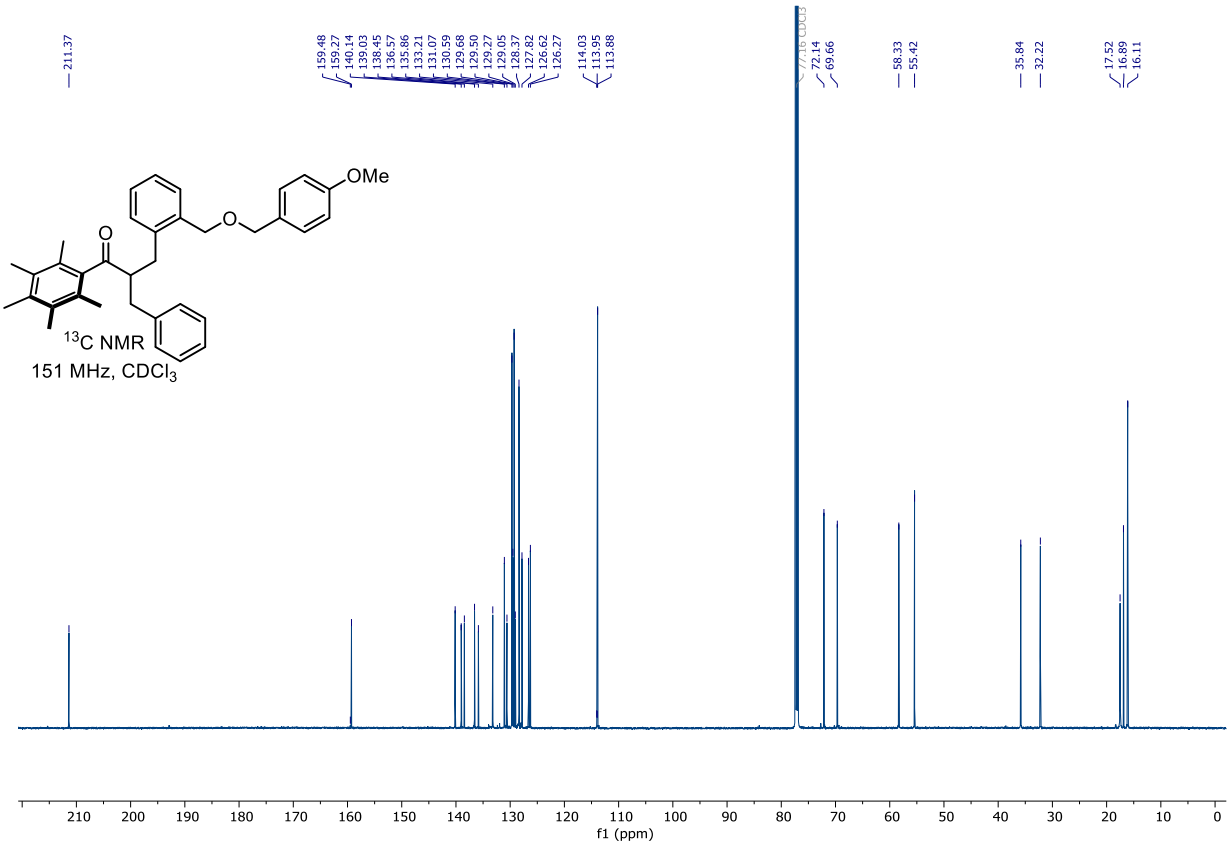
12b (2-Ethyl-1-methylene-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



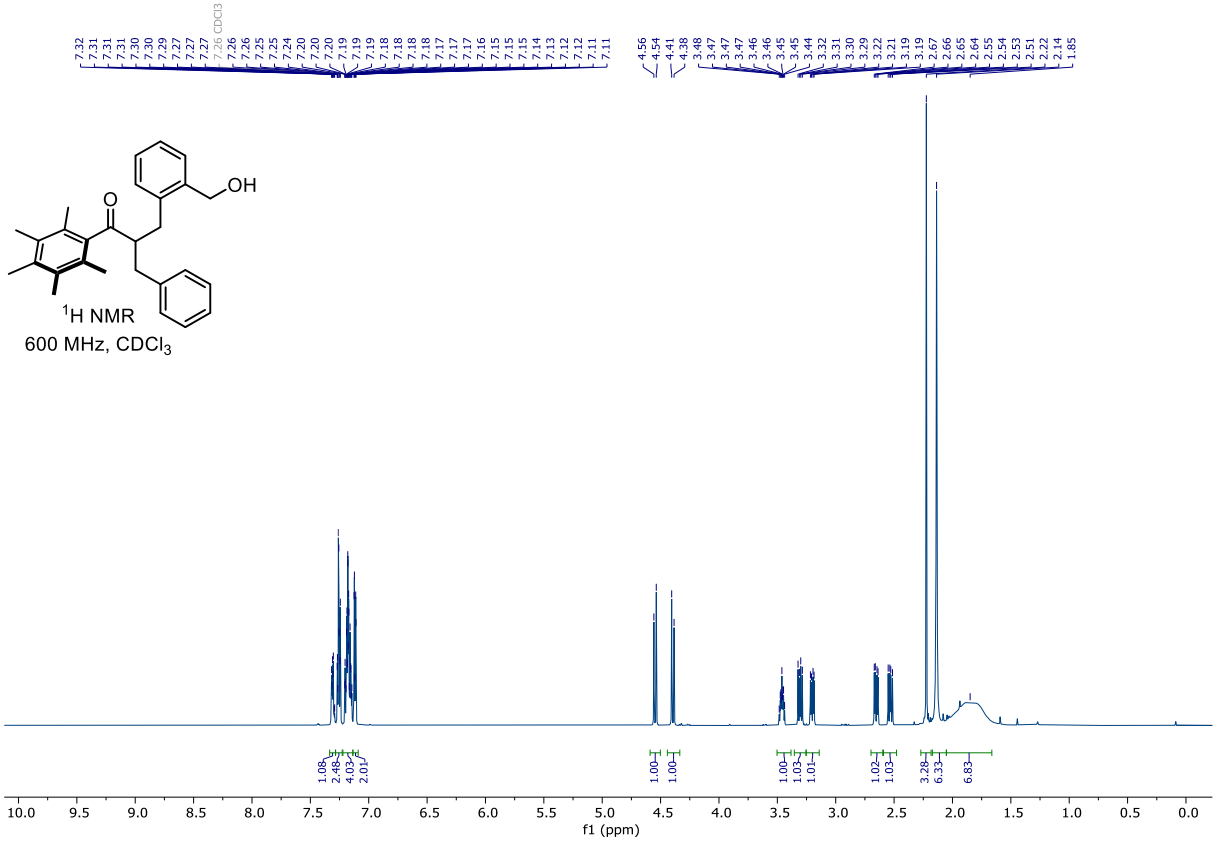


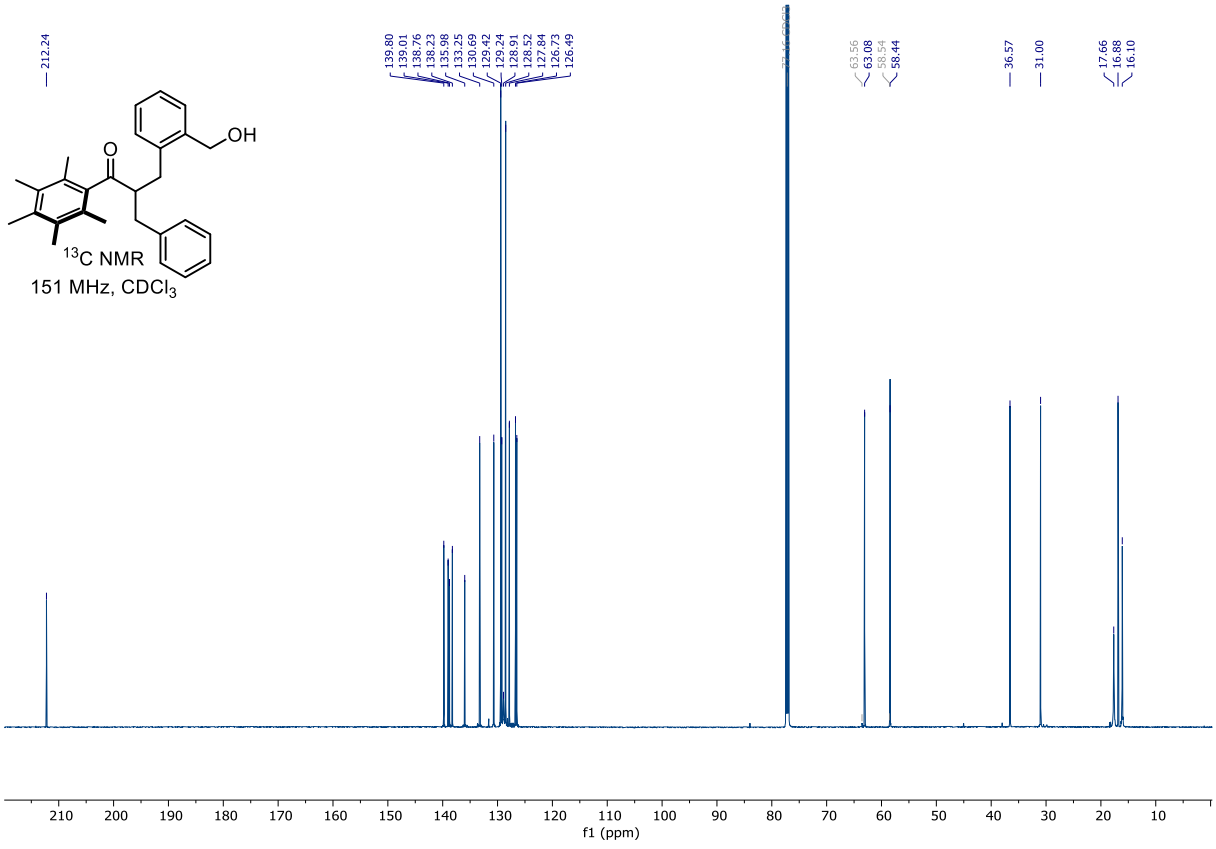
S35 2-Benzyl-3-(2-(((4-methoxybenzyl)oxy)methyl)phenyl)-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



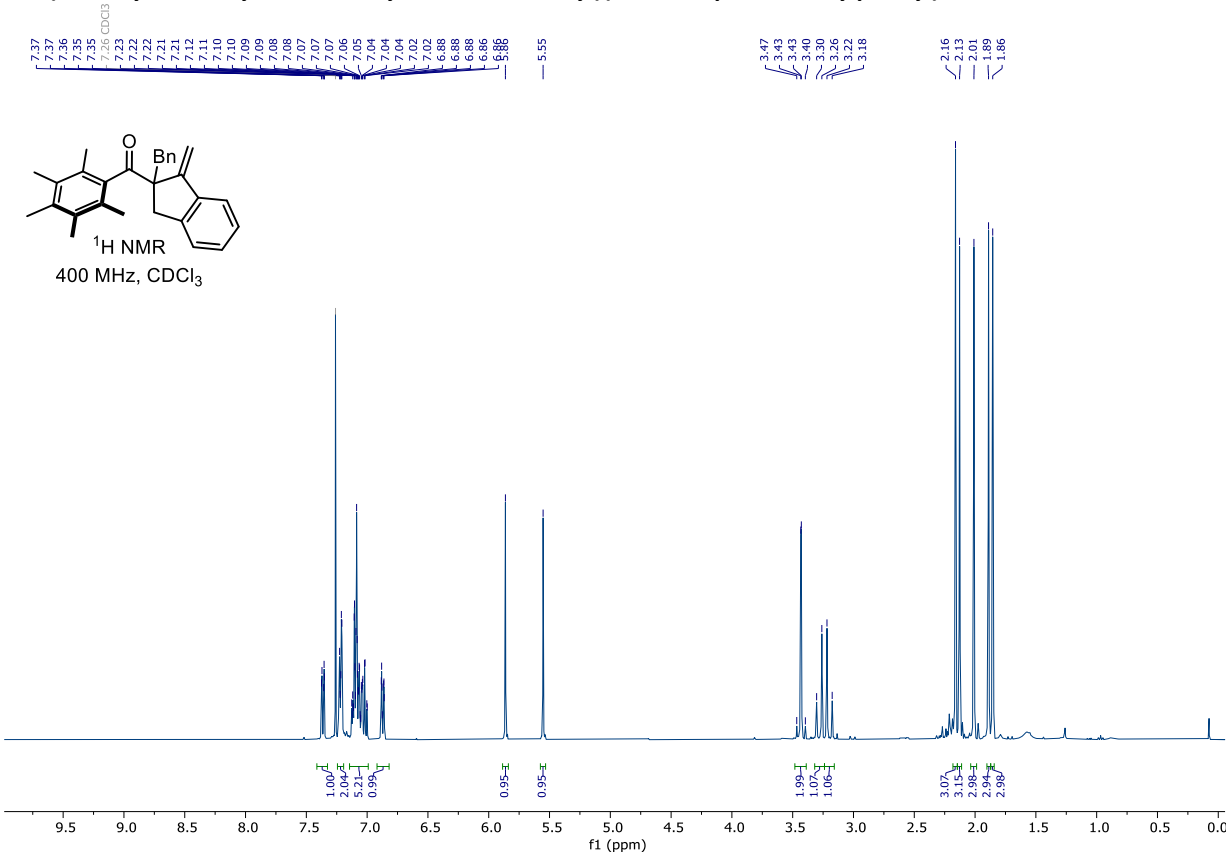


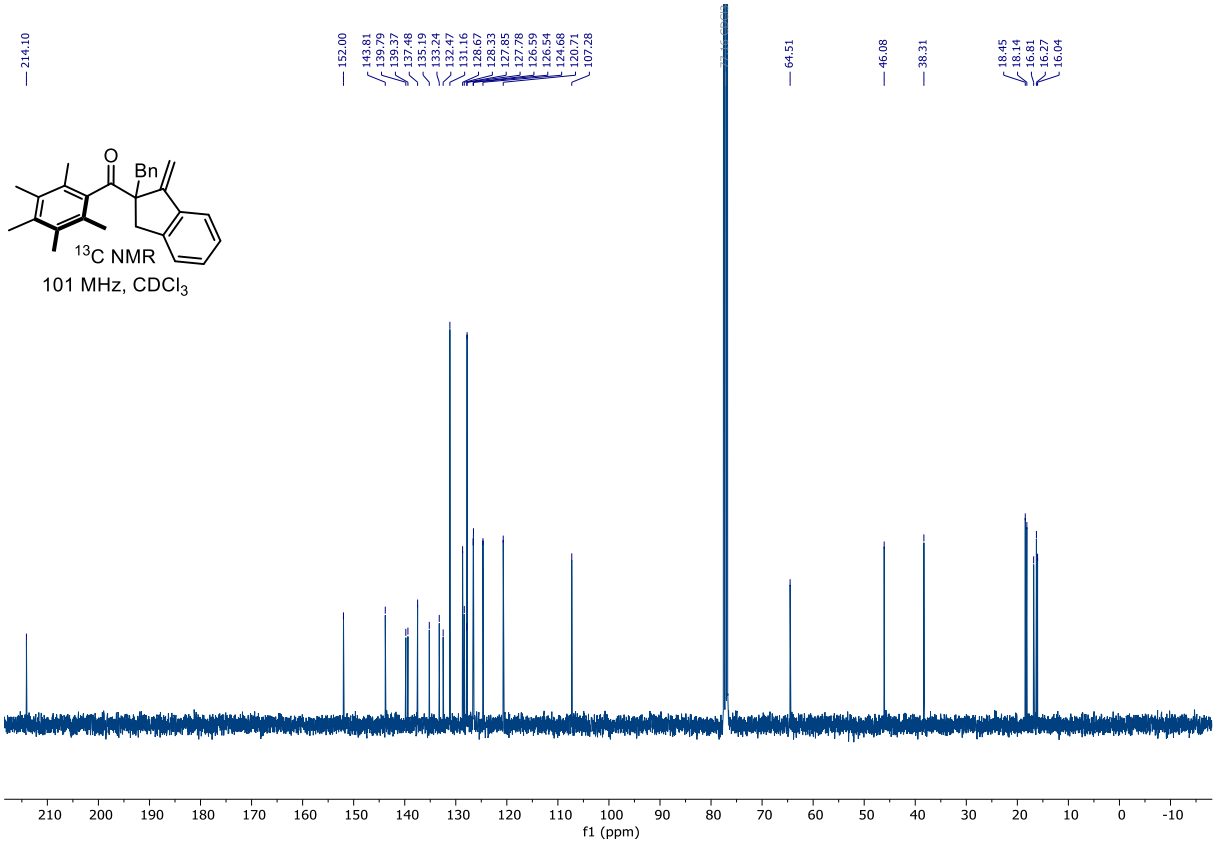
11c 2-Benzyl-3-(2-(hydroxymethyl)phenyl)-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



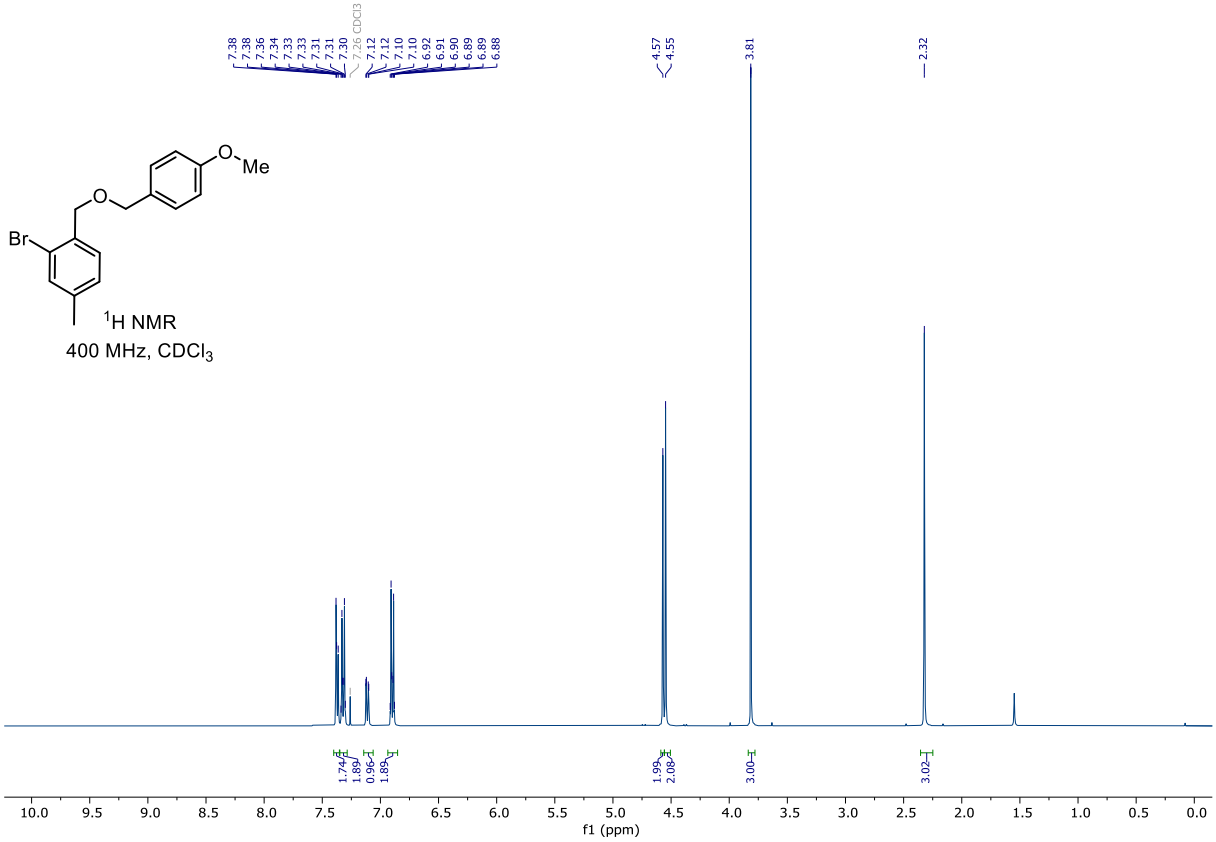


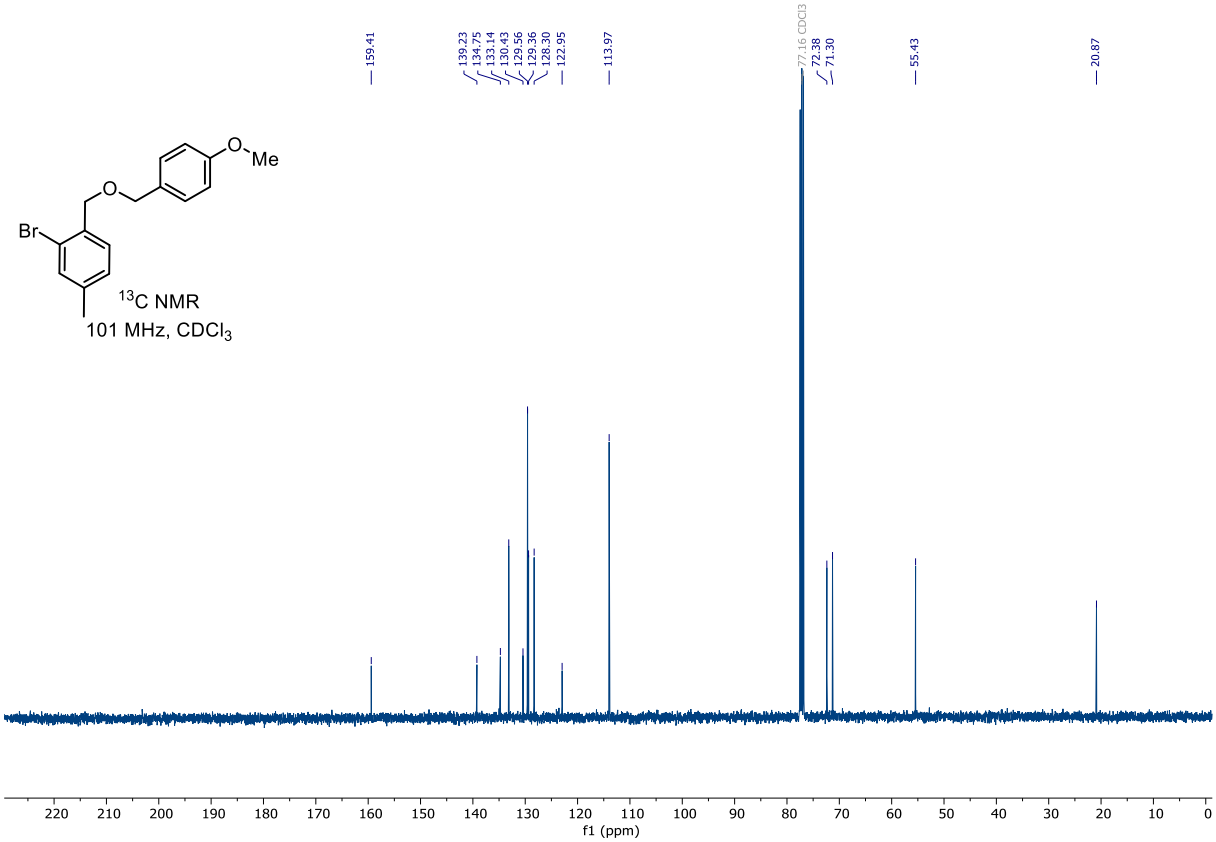
12c (2-Benzyl-1-methylene-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



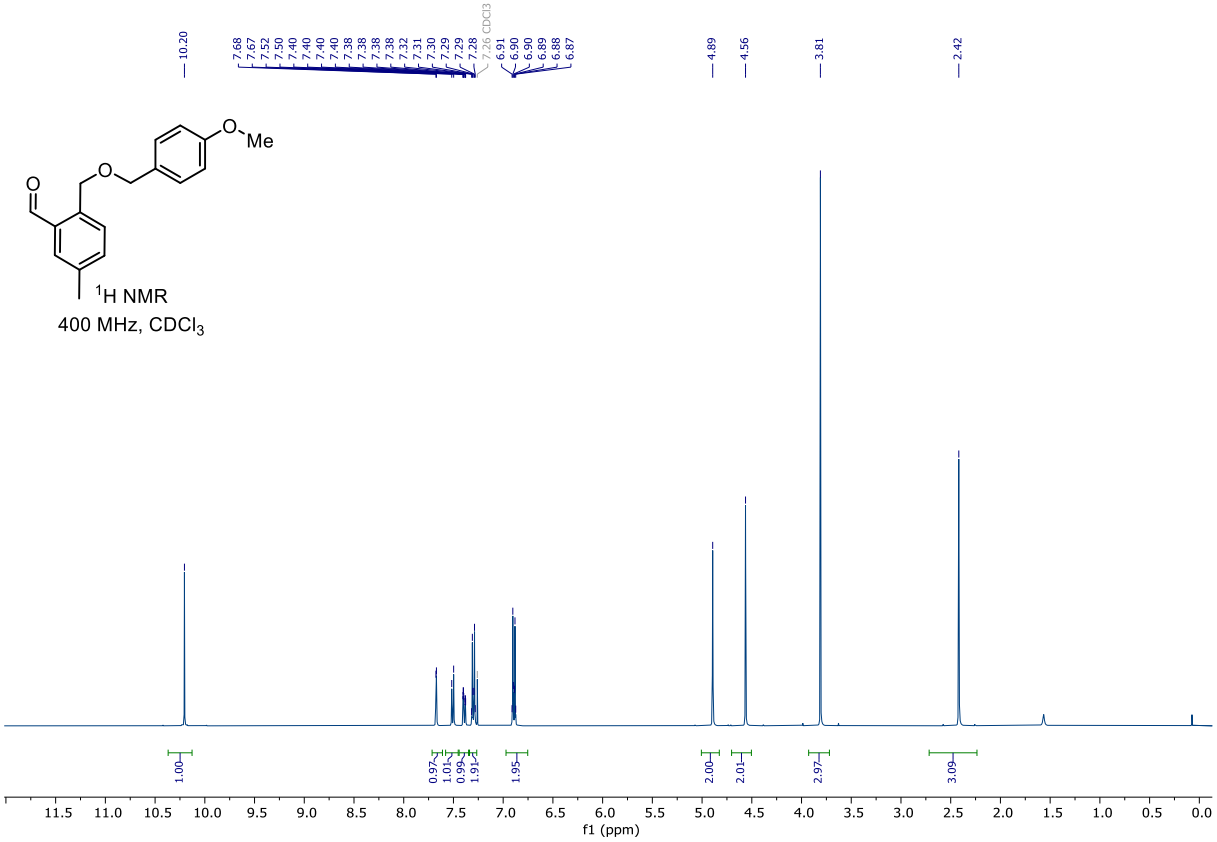


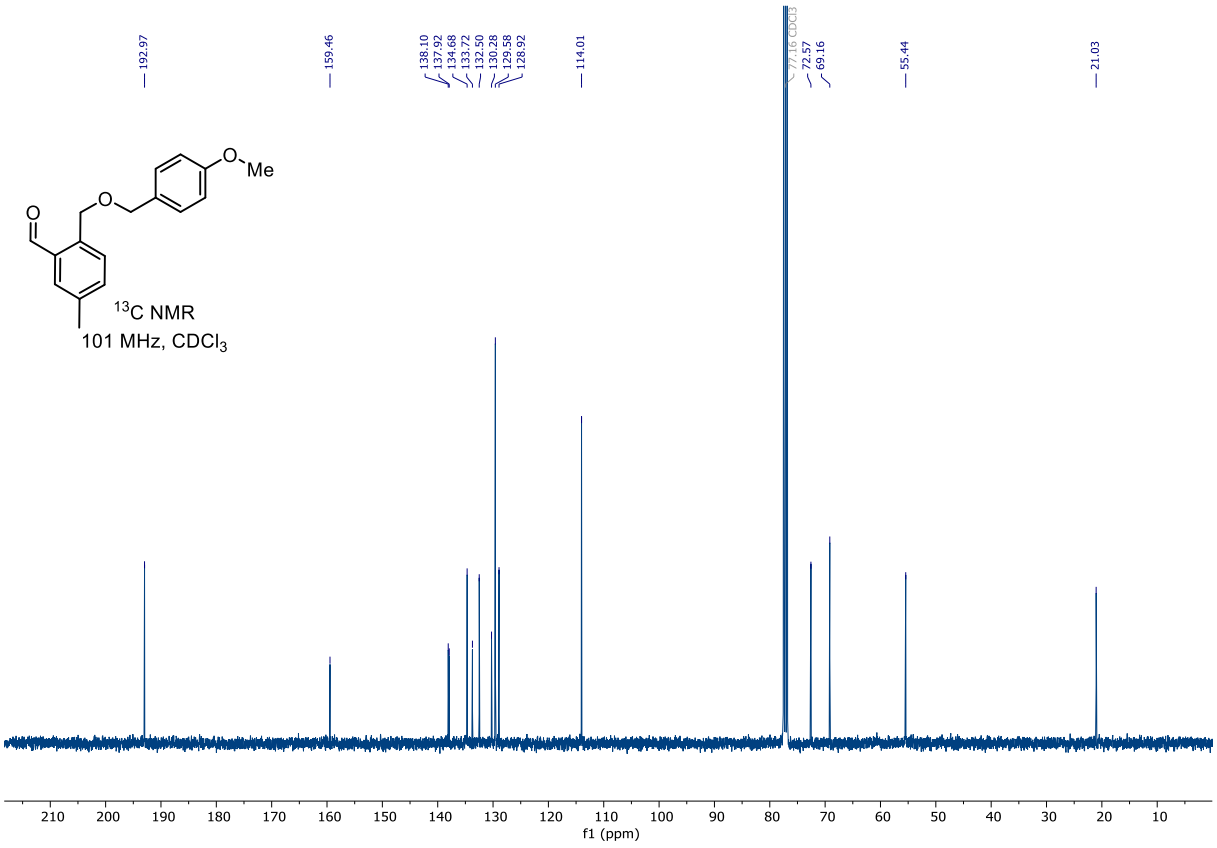
S37 2-Bromo-1-(((4-methoxybenzyl)oxy)methyl)-4-methylbenzene



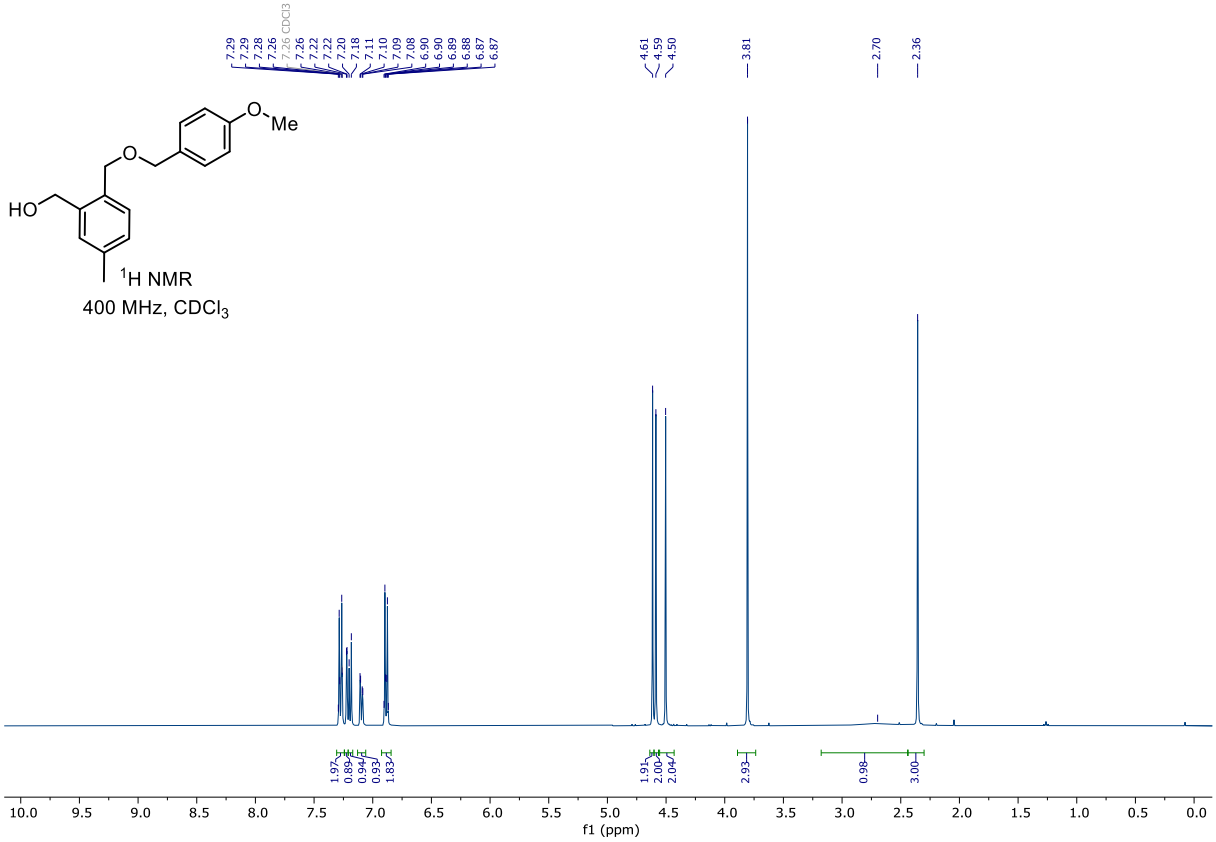


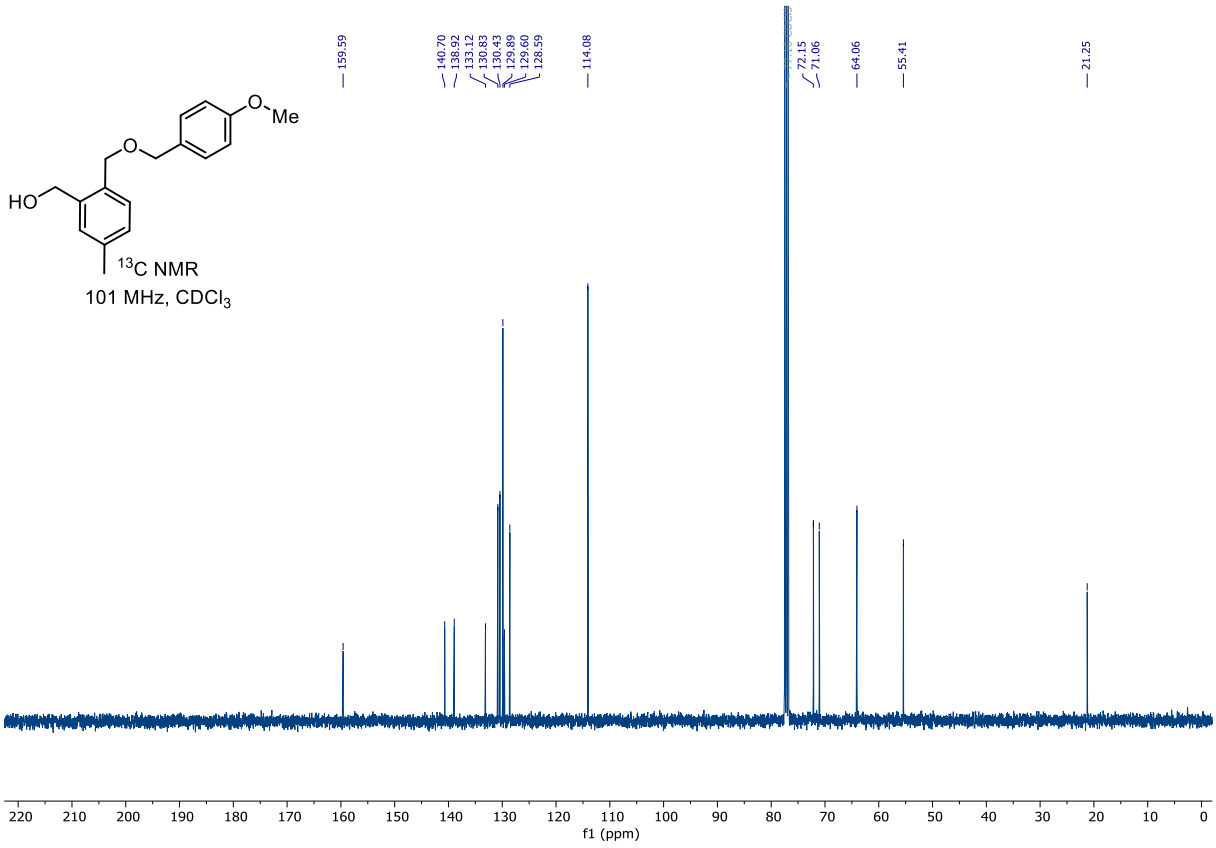
S38 2-(((4-Methoxybenzyl)oxy)methyl)-5-methylbenzaldehyde



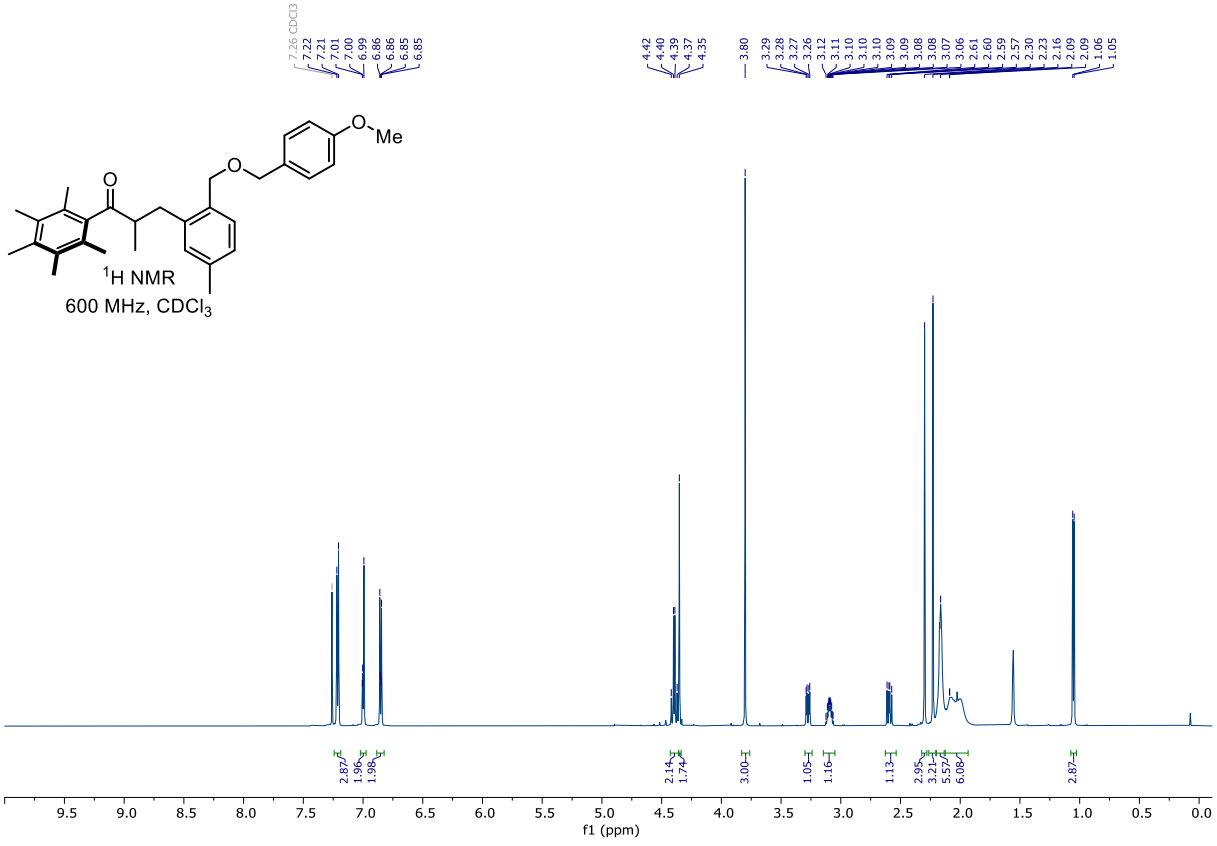


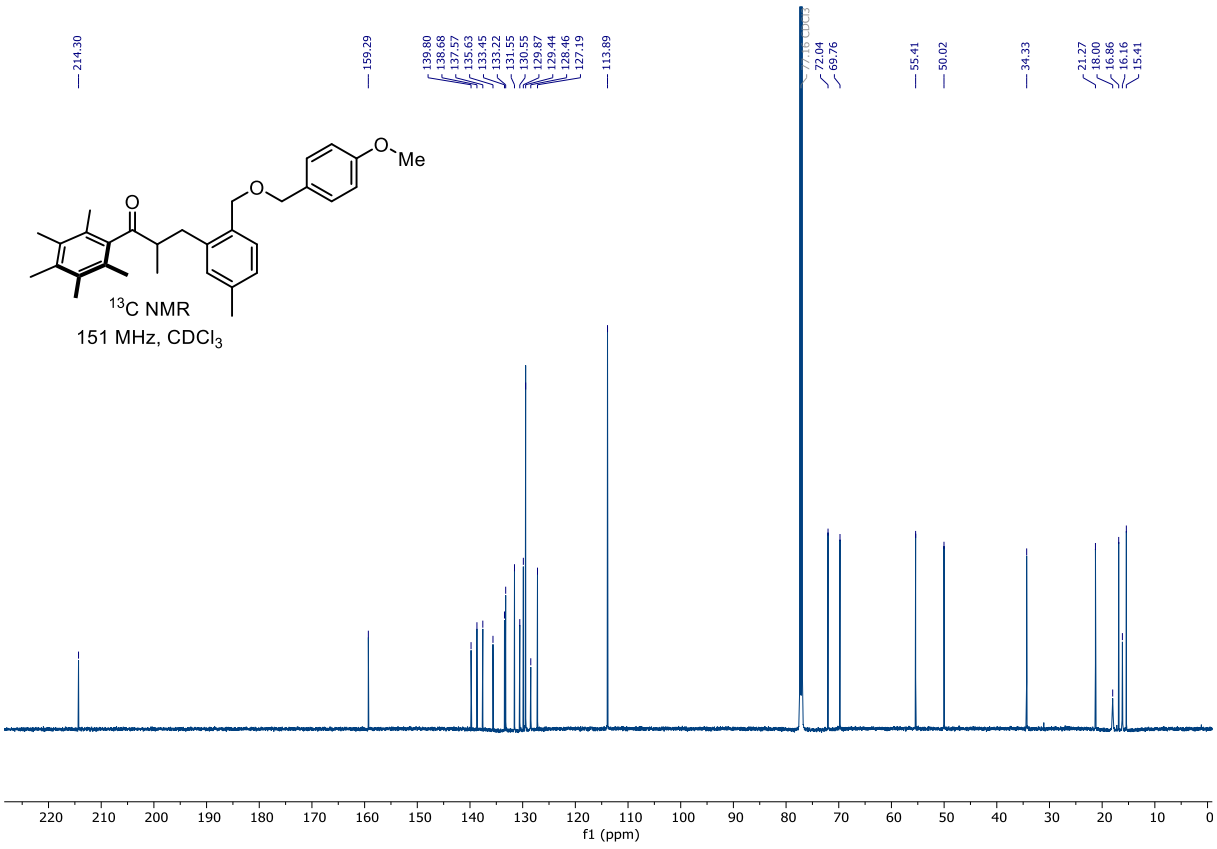
S39 (2-(((4-Methoxybenzyl)oxy)methyl)-5-methylphenyl)methanol



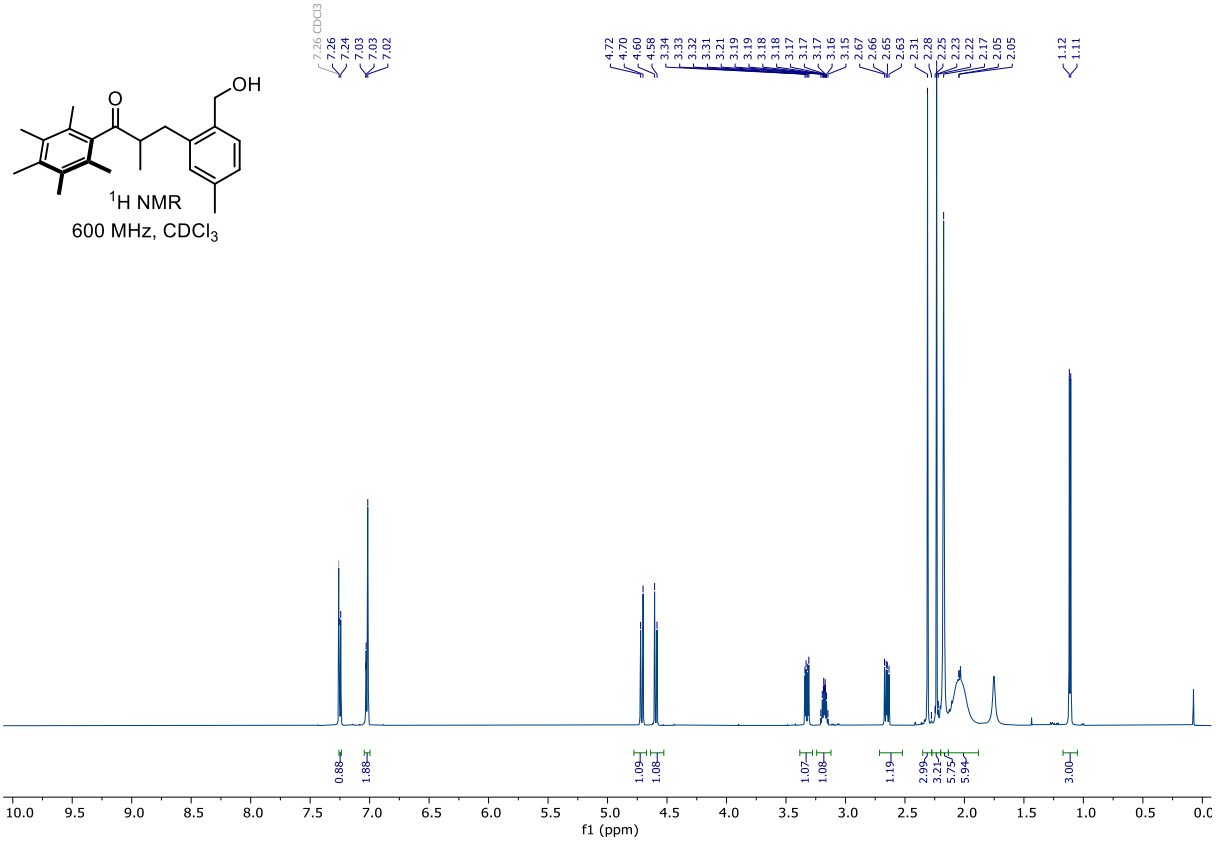


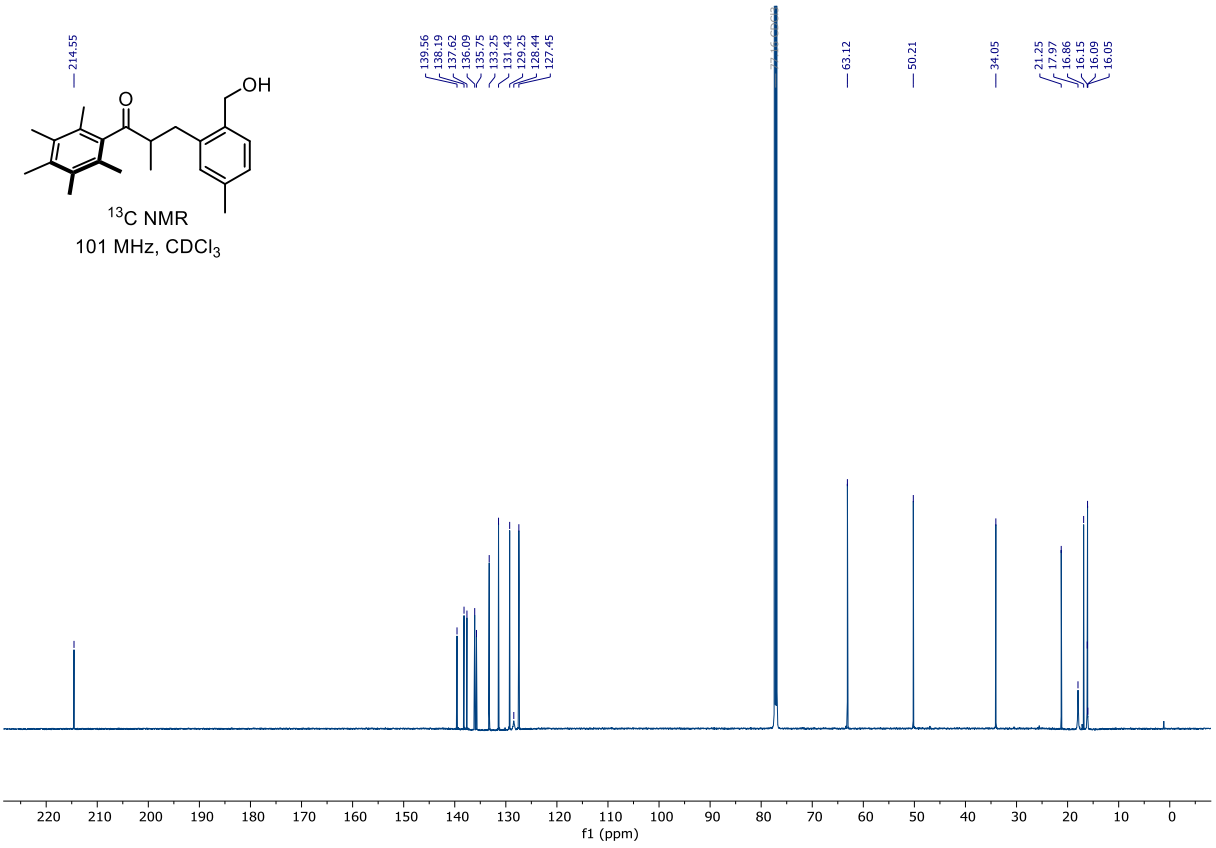
S40 **3-(2-(((4-Methoxybenzyl)oxy)methyl)-5-methylphenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one**



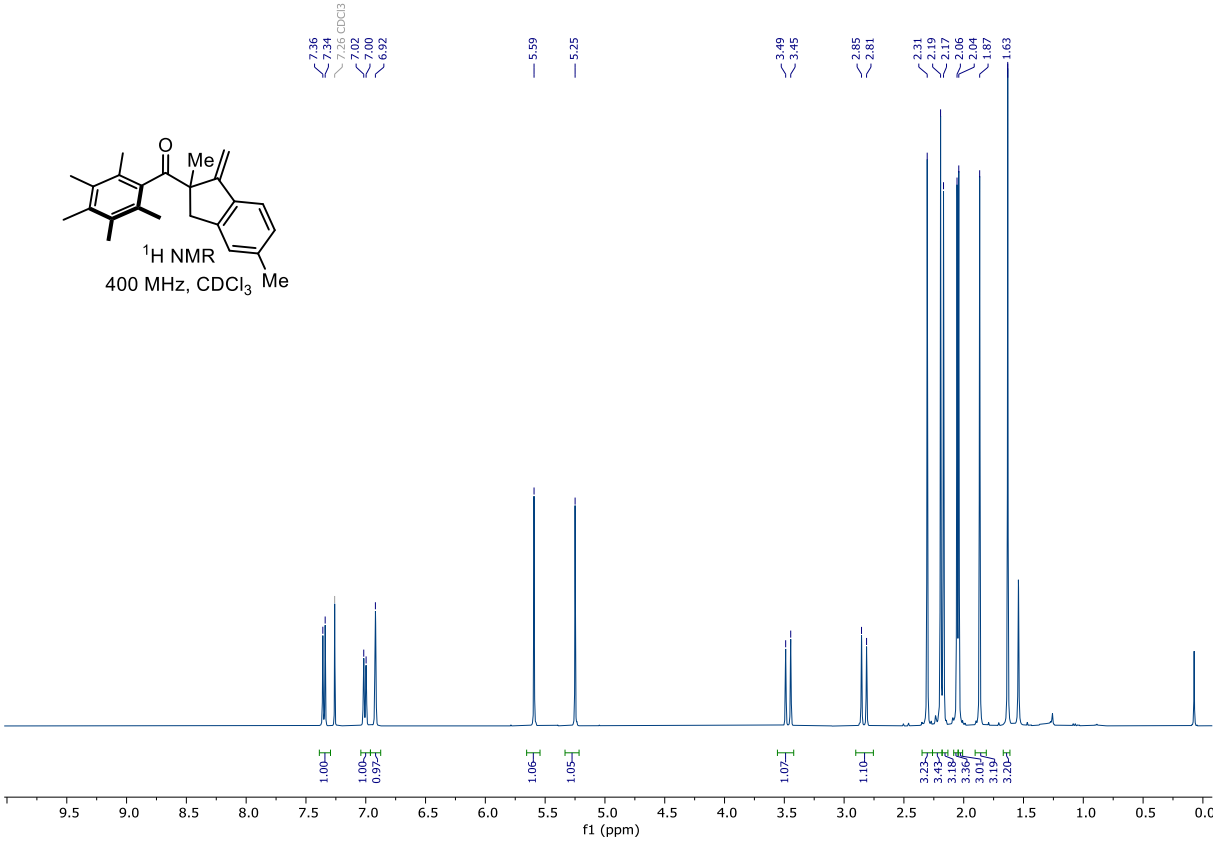


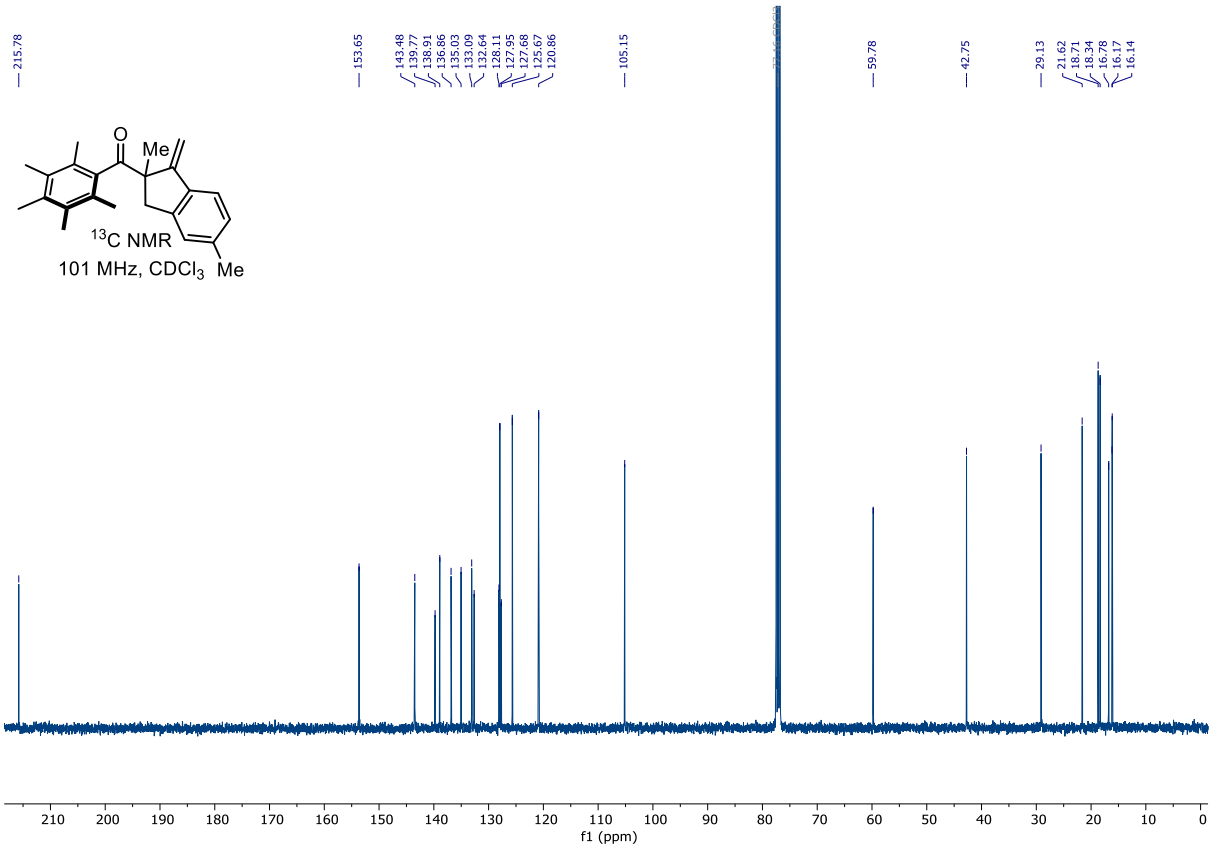
11d 3-(2-(Hydroxymethyl)-5-methylphenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



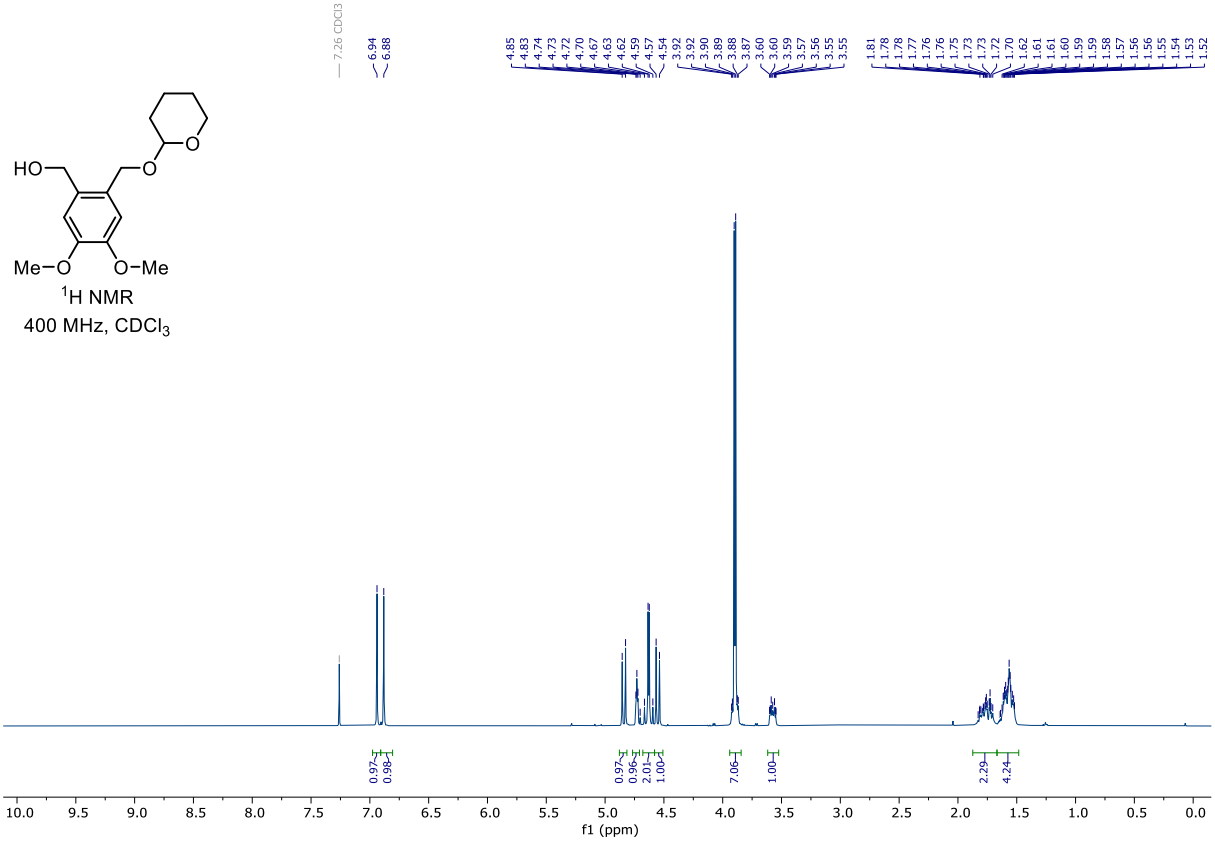


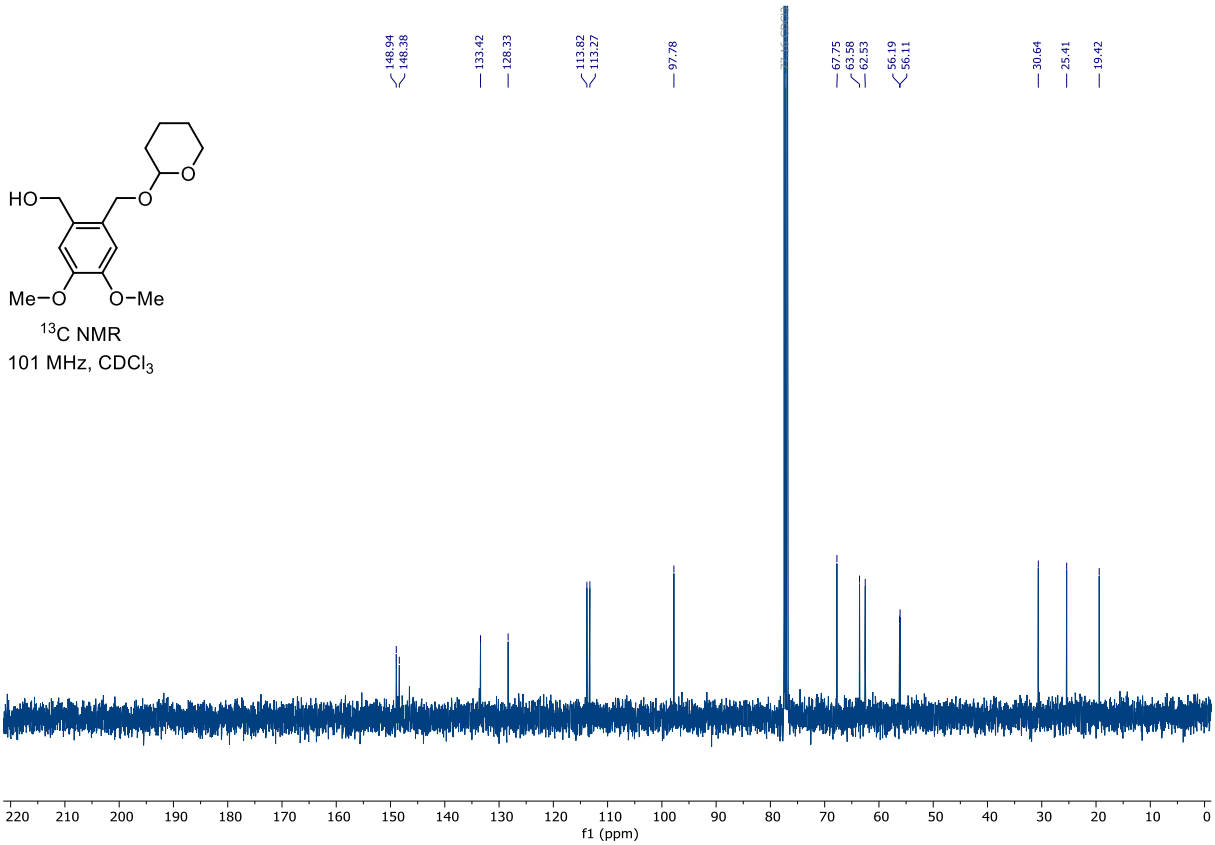
12d (2,5-Dimethyl-1-methylene-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



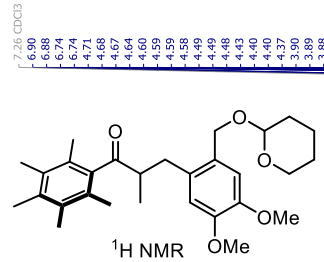


S42 (4,5-Dimethoxy-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)methanol

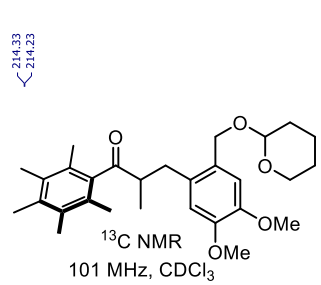




S43 3-(4,5-Dimethoxy-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one

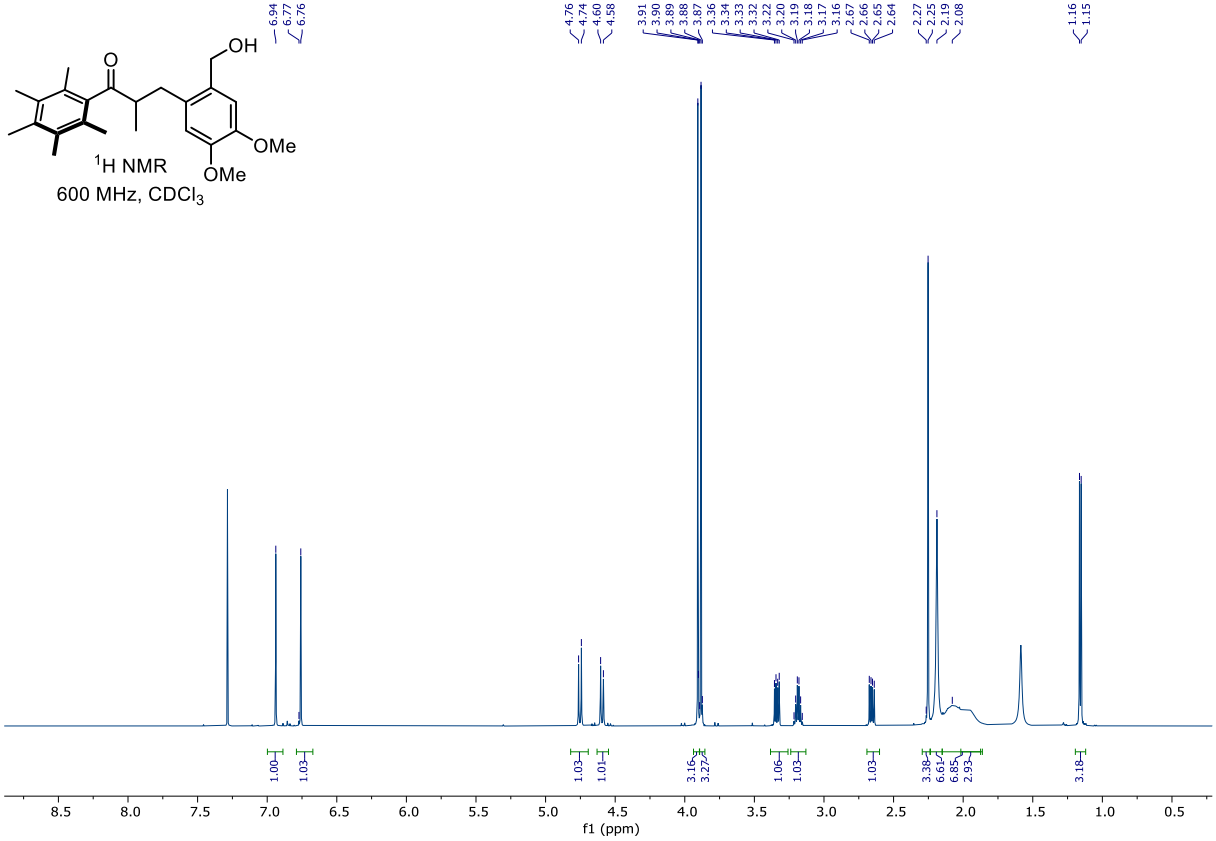


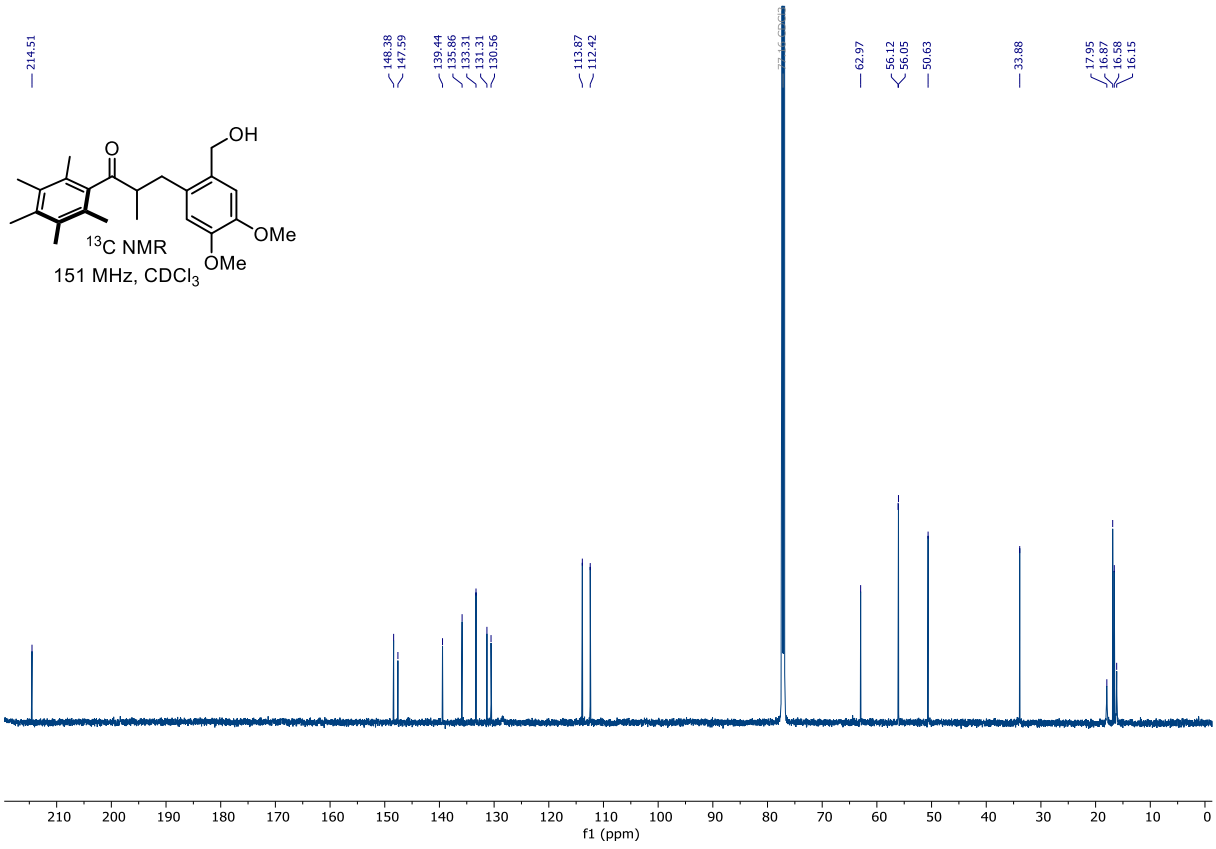
^{1}H NMR
400 MHz, $CDCl_3$
mixture of diastereomers
[49:51] d.r.



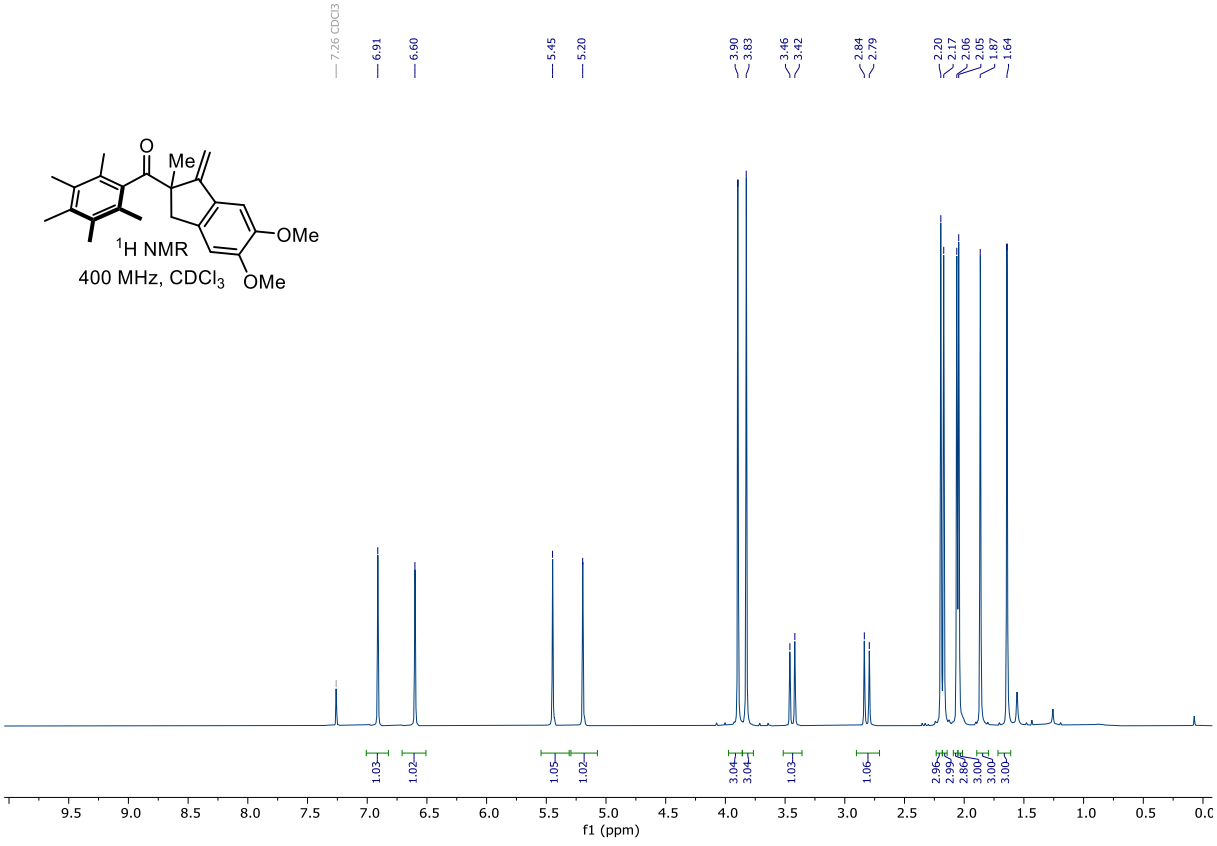
^{13}C NMR
101 MHz, $CDCl_3$
mixture of diastereomers
[51:49] d.r.

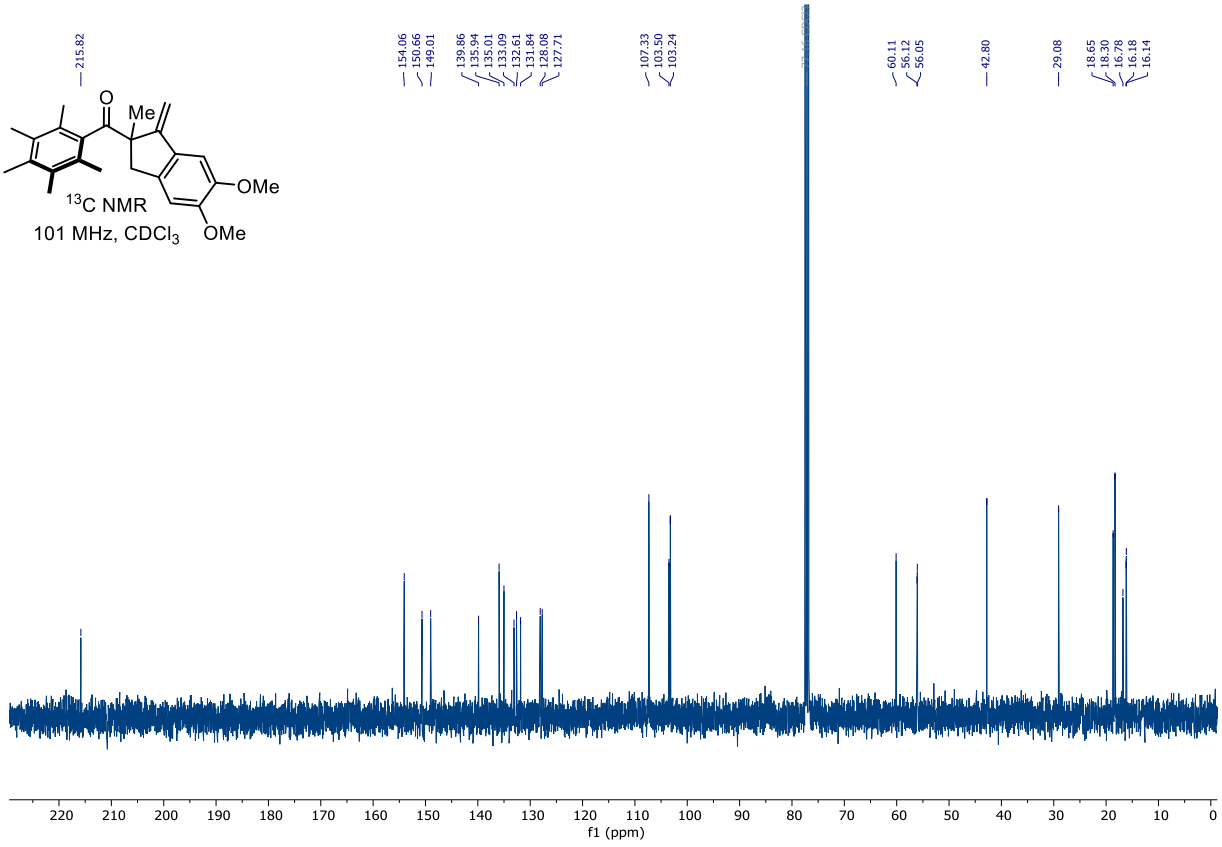
11e 3-(2-(Hydroxymethyl)-4,5-dimethoxyphenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



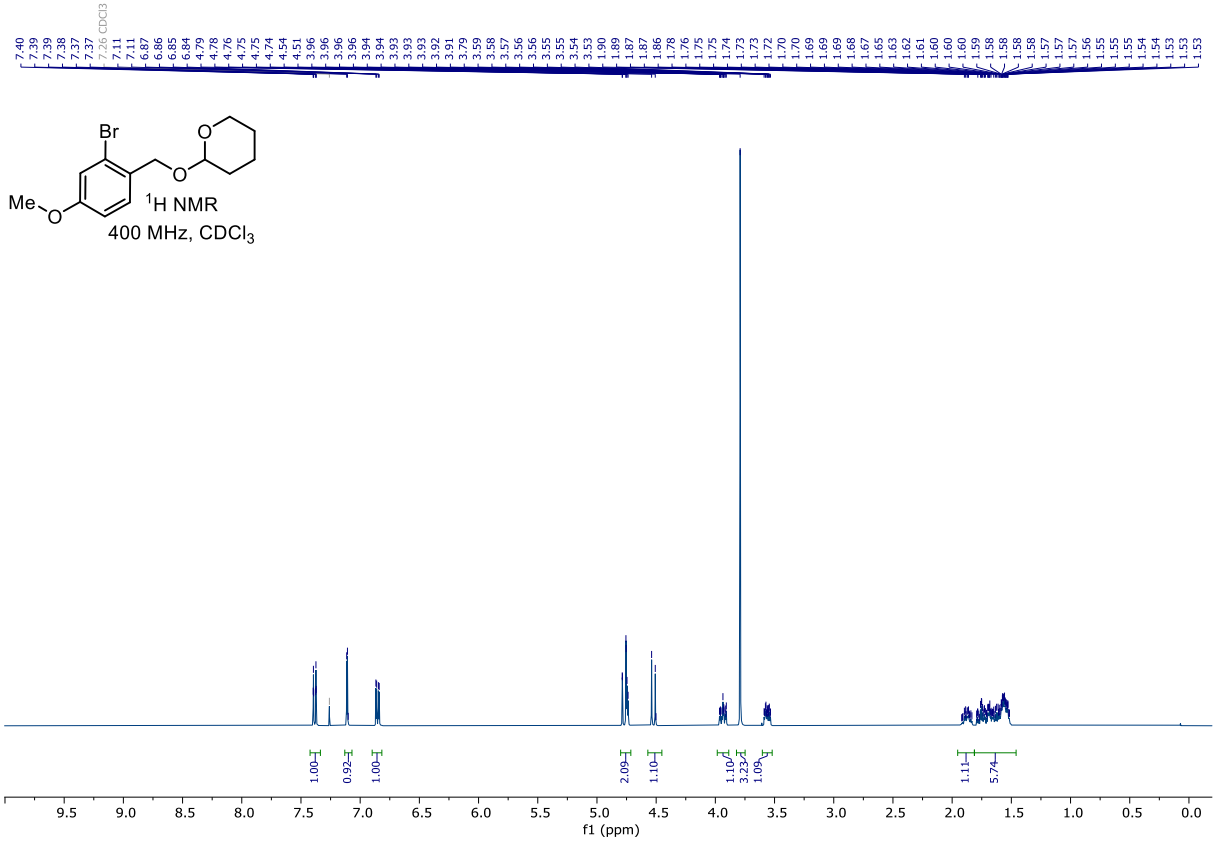


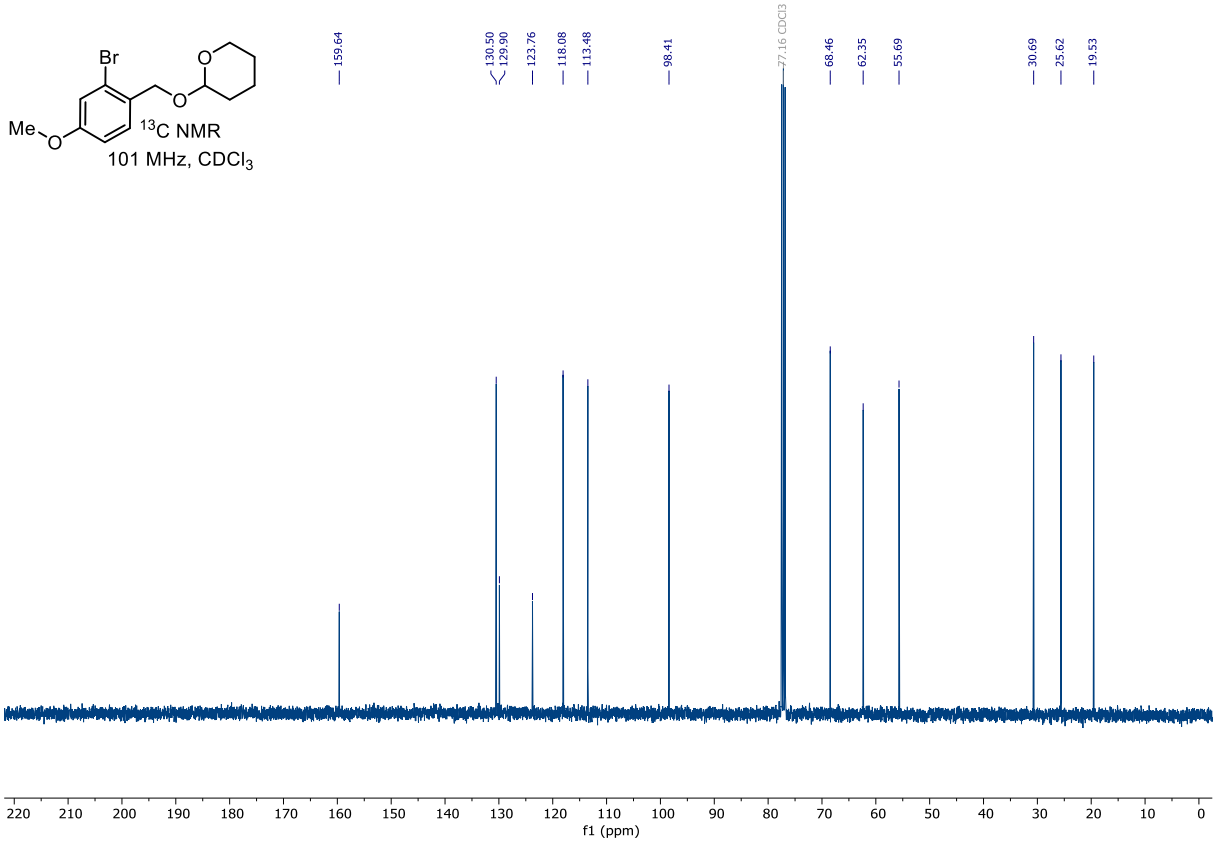
12e (5,6-Dimethoxy-2-methyl-1-methylene-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



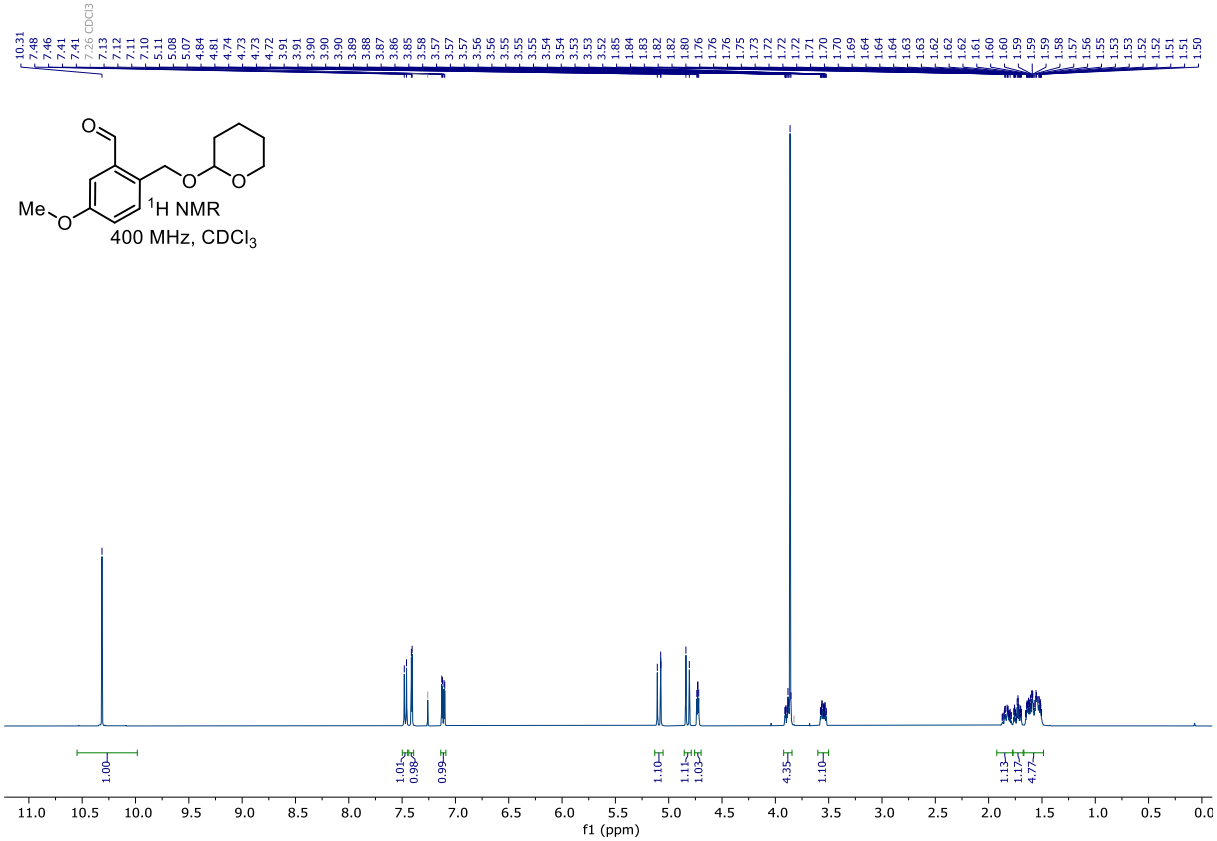


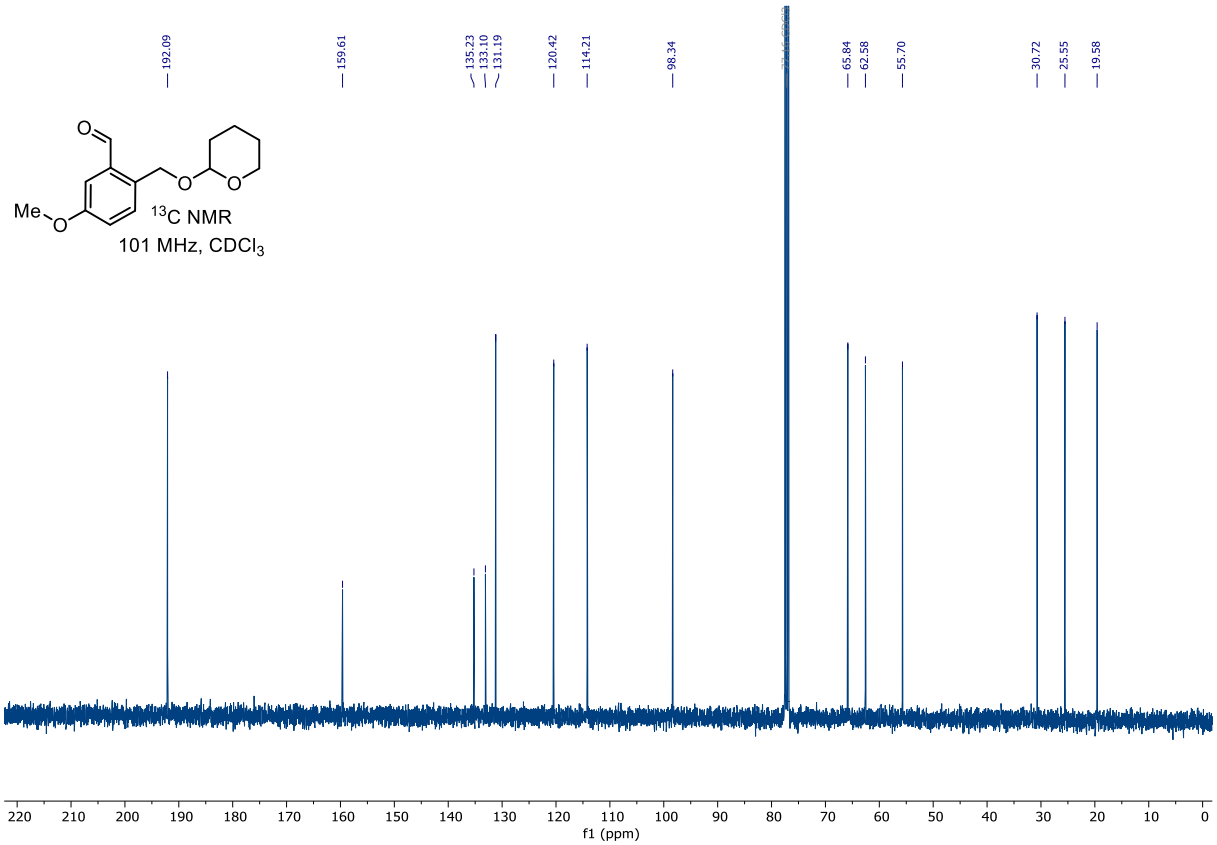
S45 2-((2-Bromo-4-methoxybenzyl)oxy)tetrahydro-2*H*-pyran



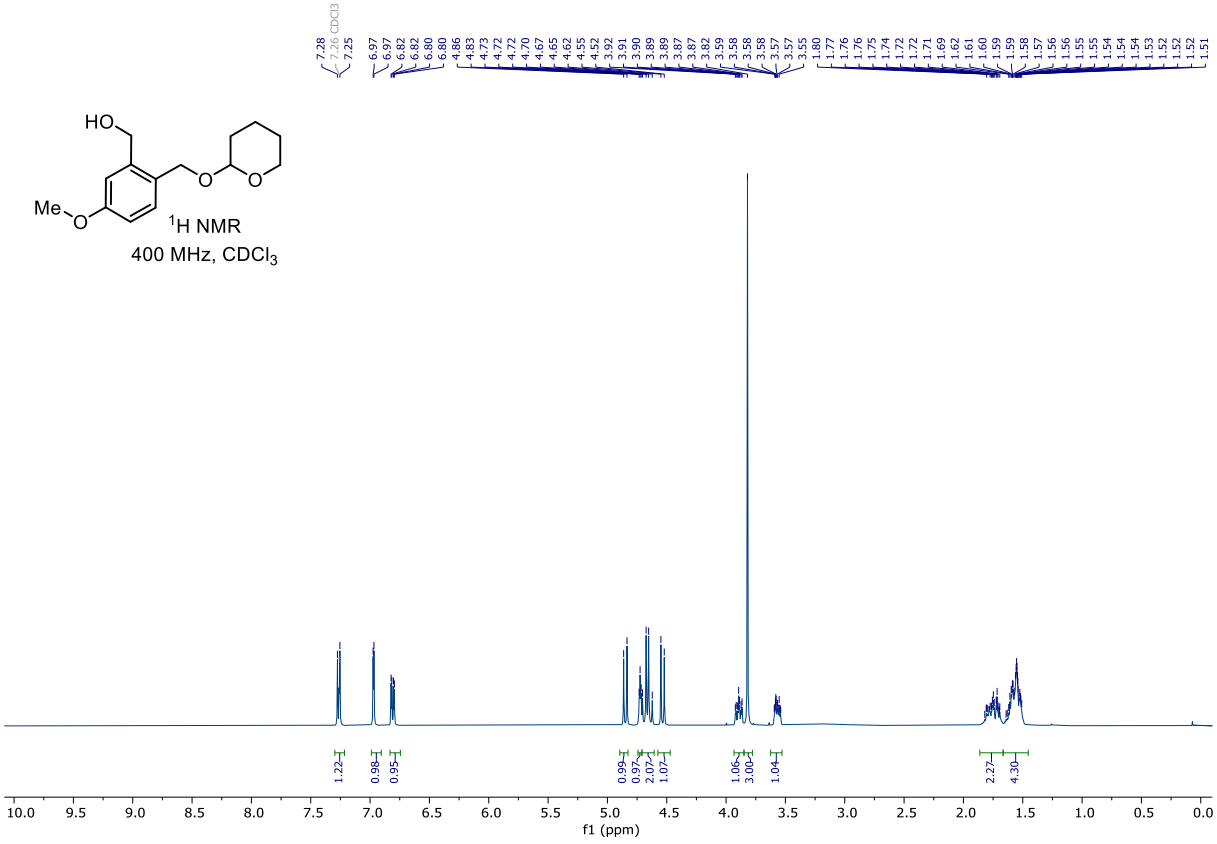


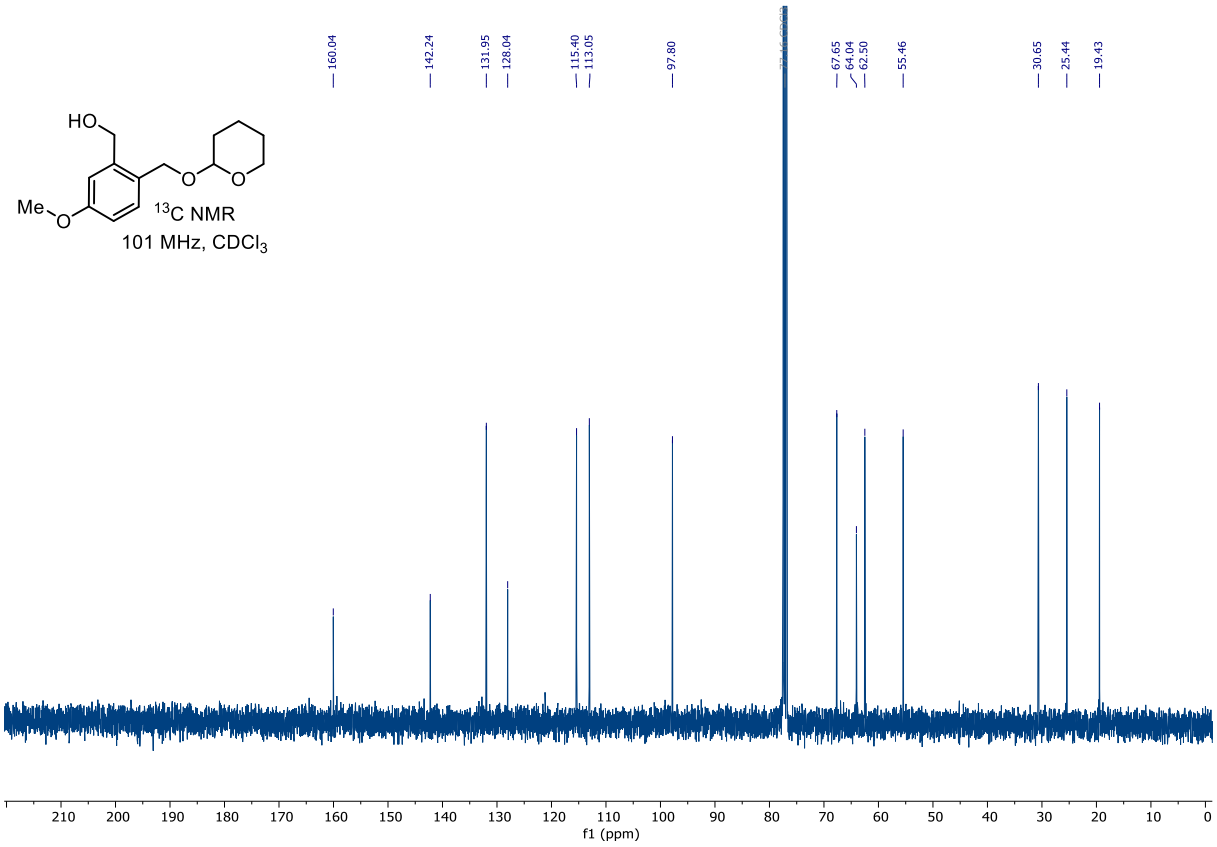
S46 5-Methoxy-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)benzaldehyde





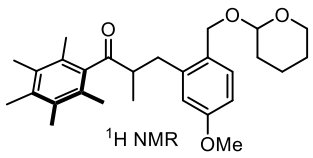
S47 (5-Methoxy-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)methanol



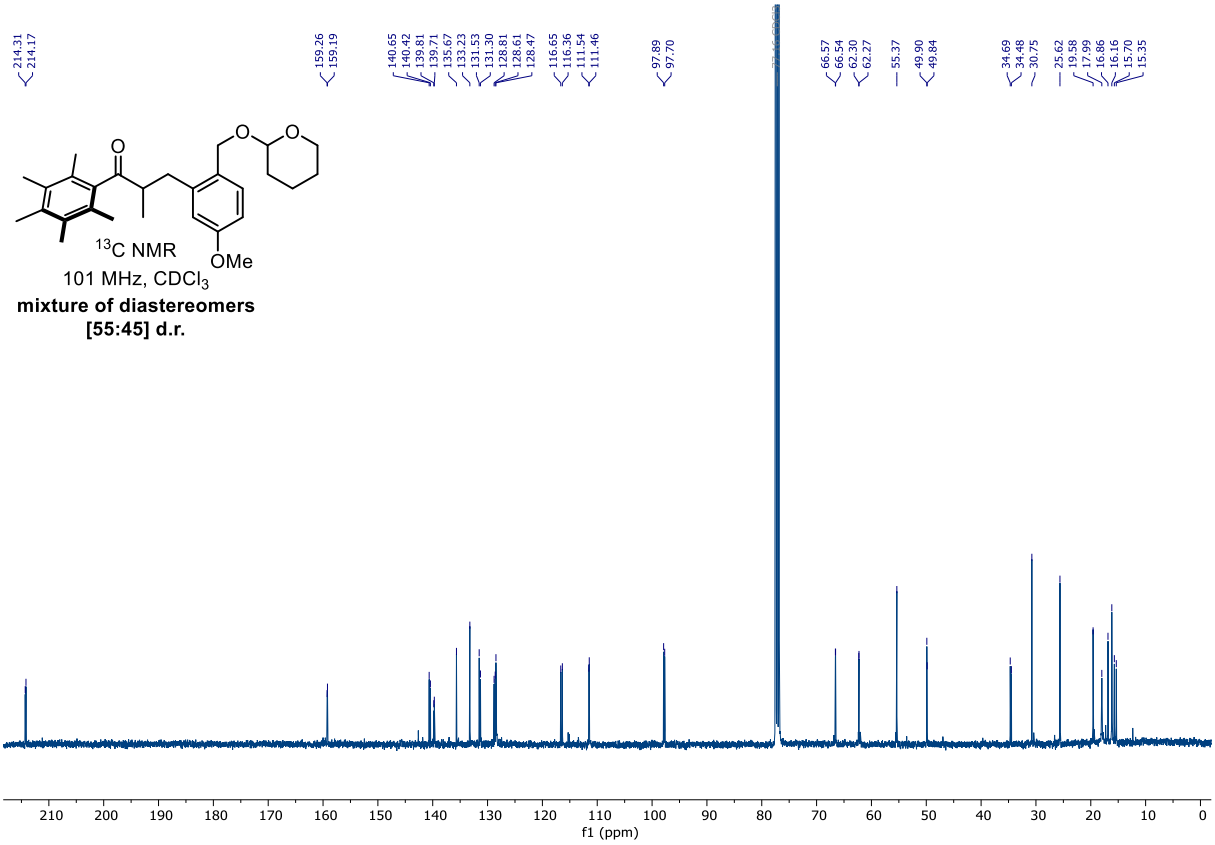


S48 3-(5-Methoxy-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



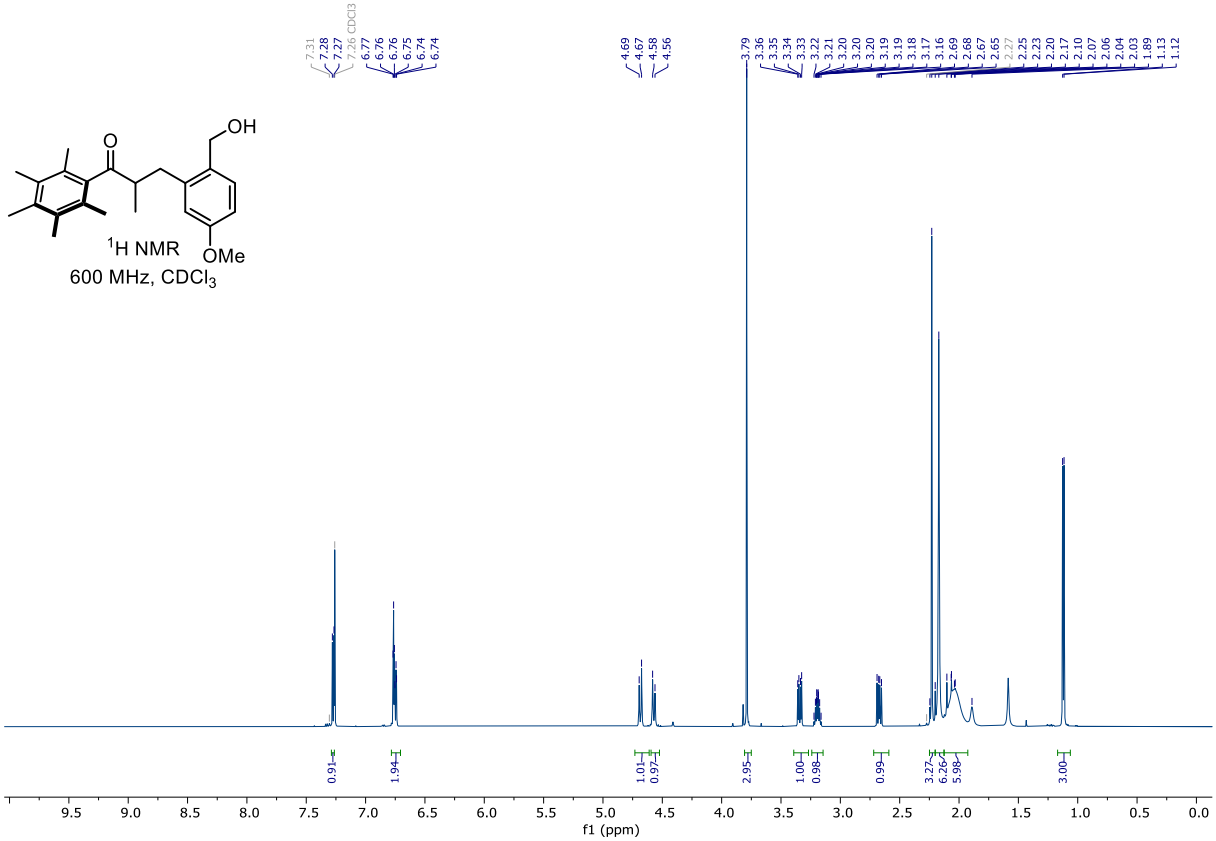


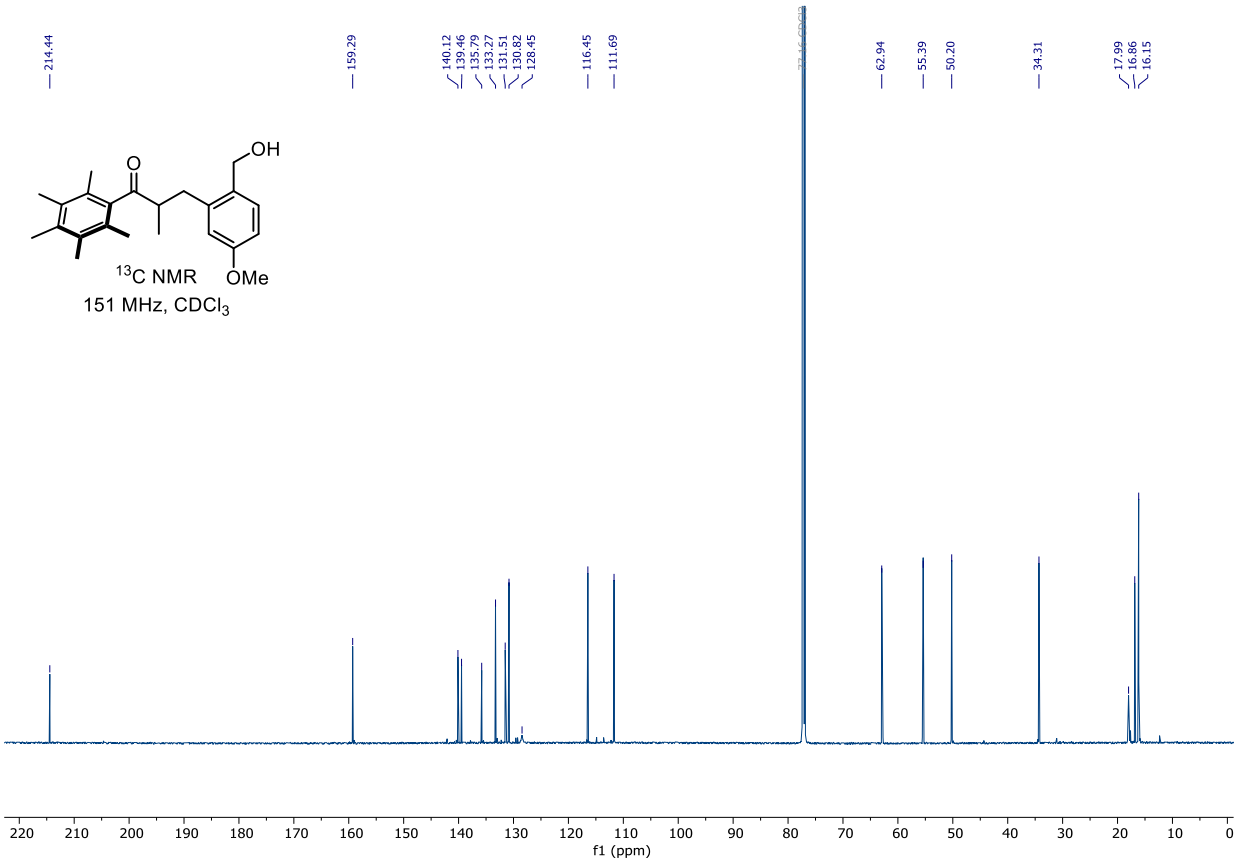
^{1}H NMR
400 MHz, $CDCl_3$
mixture of diastereomers [55:45] d.r.



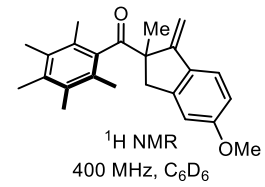
^{13}C NMR
101 MHz, $CDCl_3$
mixture of diastereomers [55:45] d.r.

11f 3-(2-(Hydroxymethyl)-5-methoxyphenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one

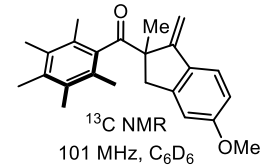




12f (5-Methoxy-2-methyl-1-methylene-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone

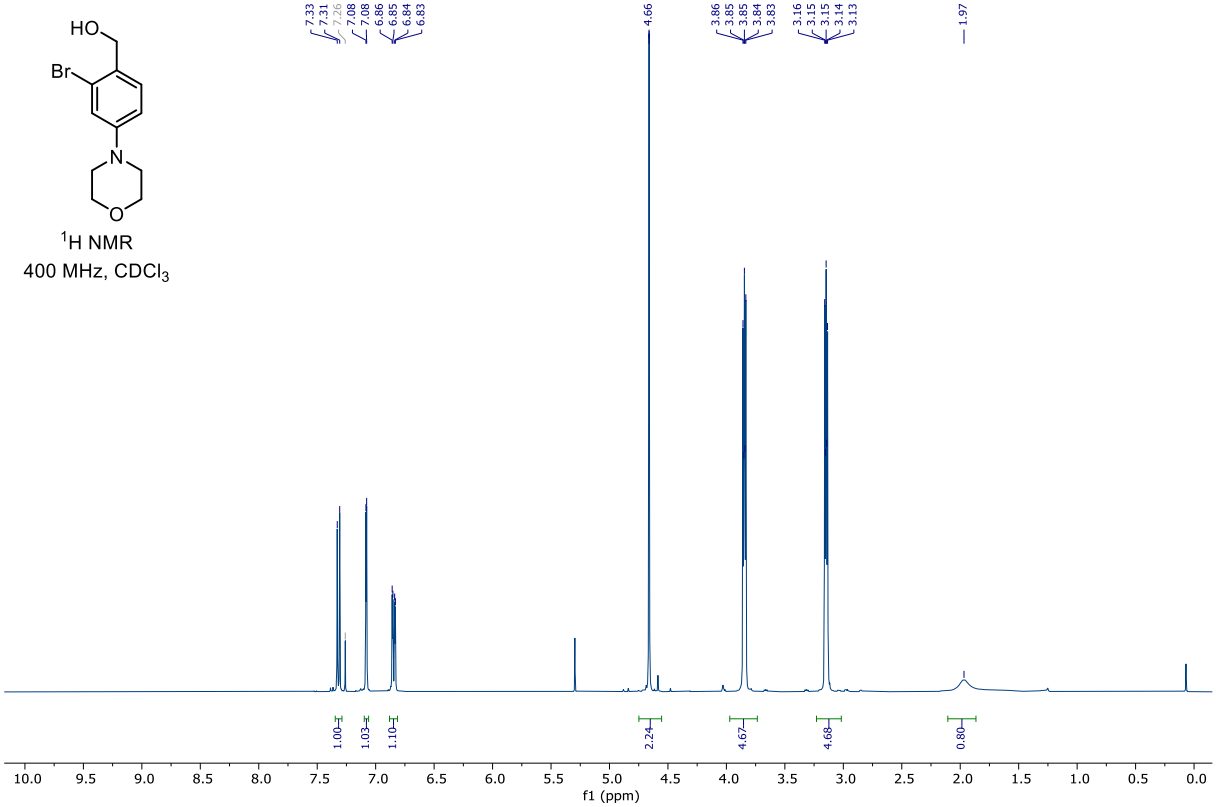


^{1}H NMR
400 MHz, C_6D_6

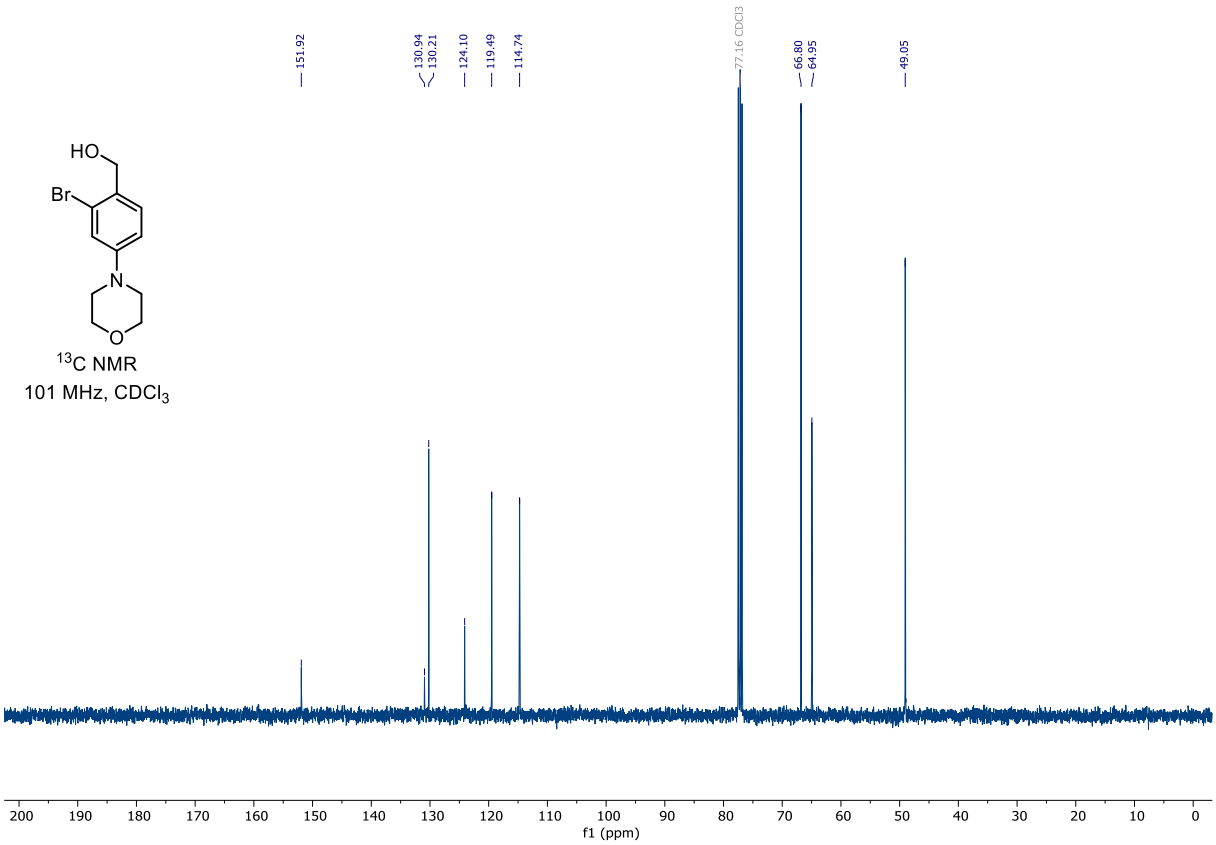


^{13}C NMR
101 MHz, C_6D_6

S50 (2-Bromo-4-morpholinophenyl)methanol

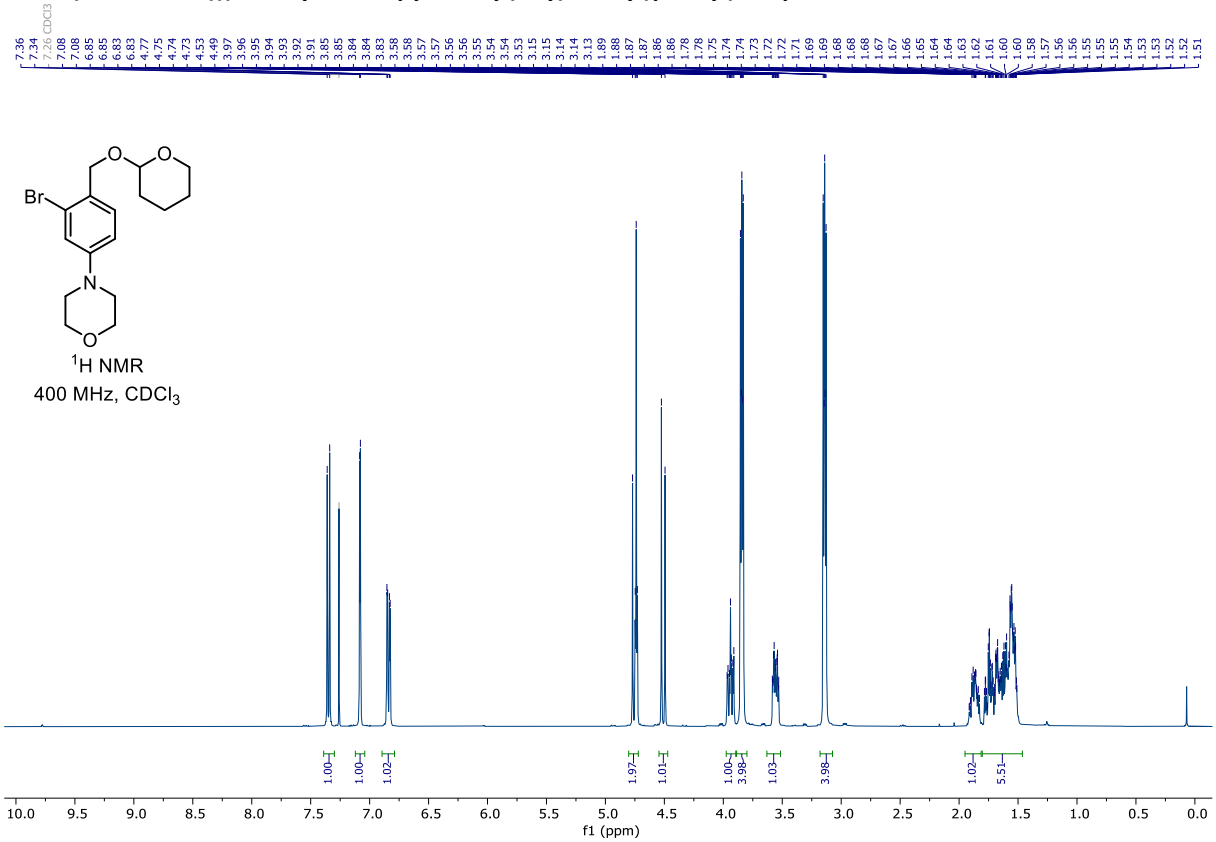


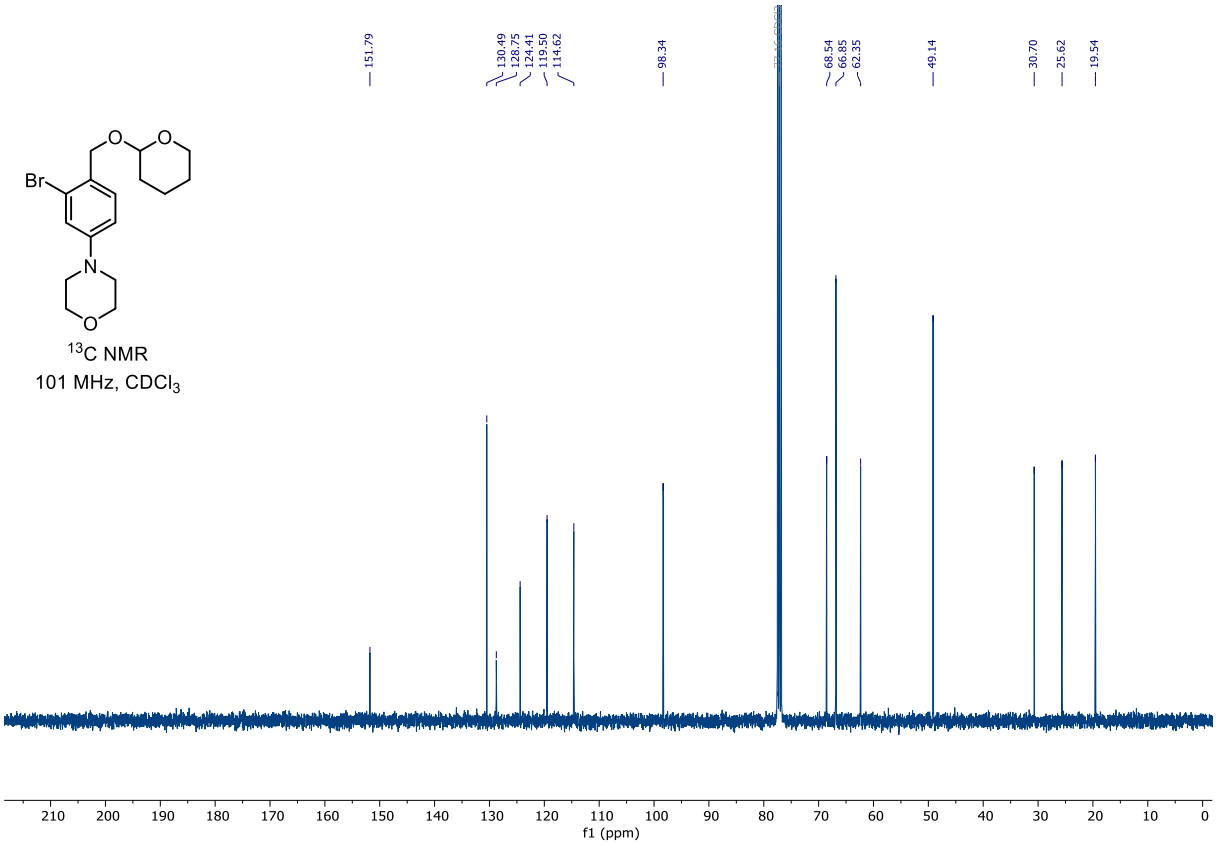
^{1}H NMR
400 MHz, $CDCl_3$



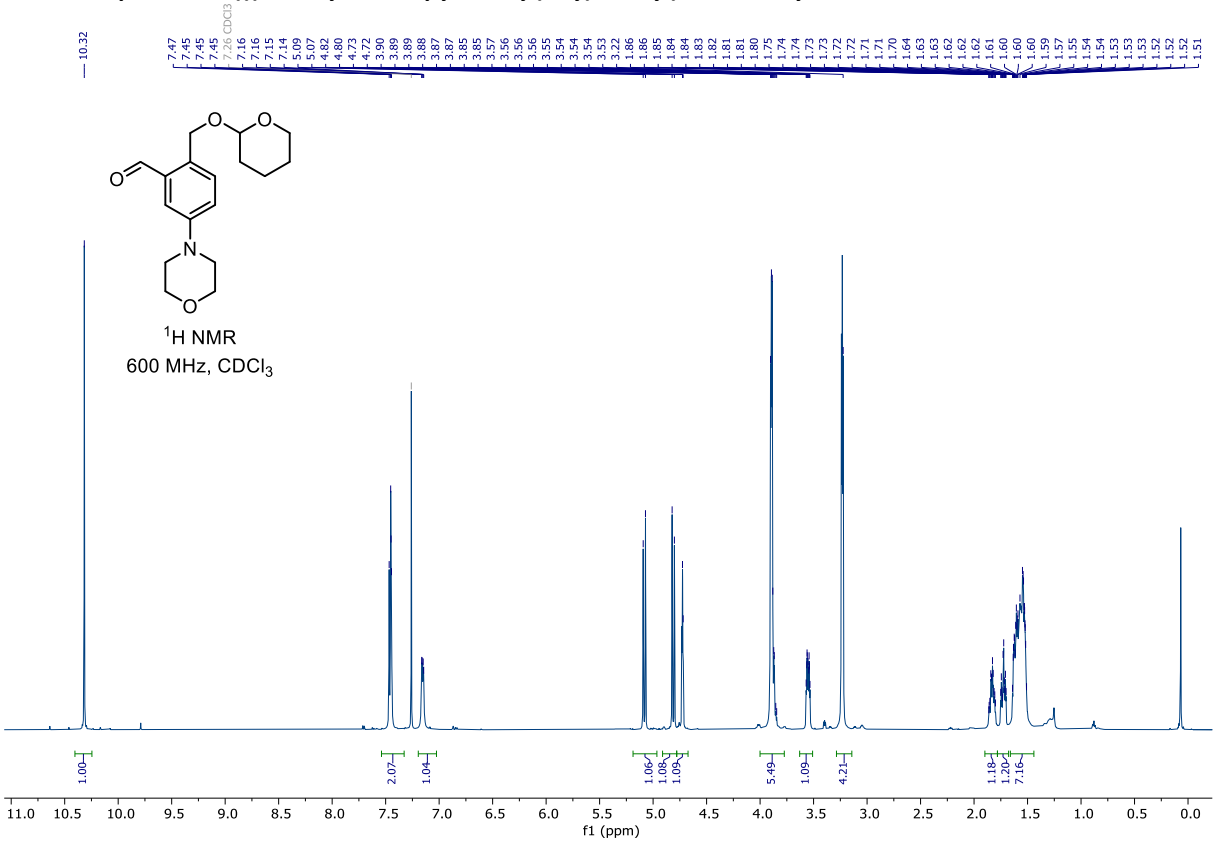
^{13}C NMR
101 MHz, $CDCl_3$

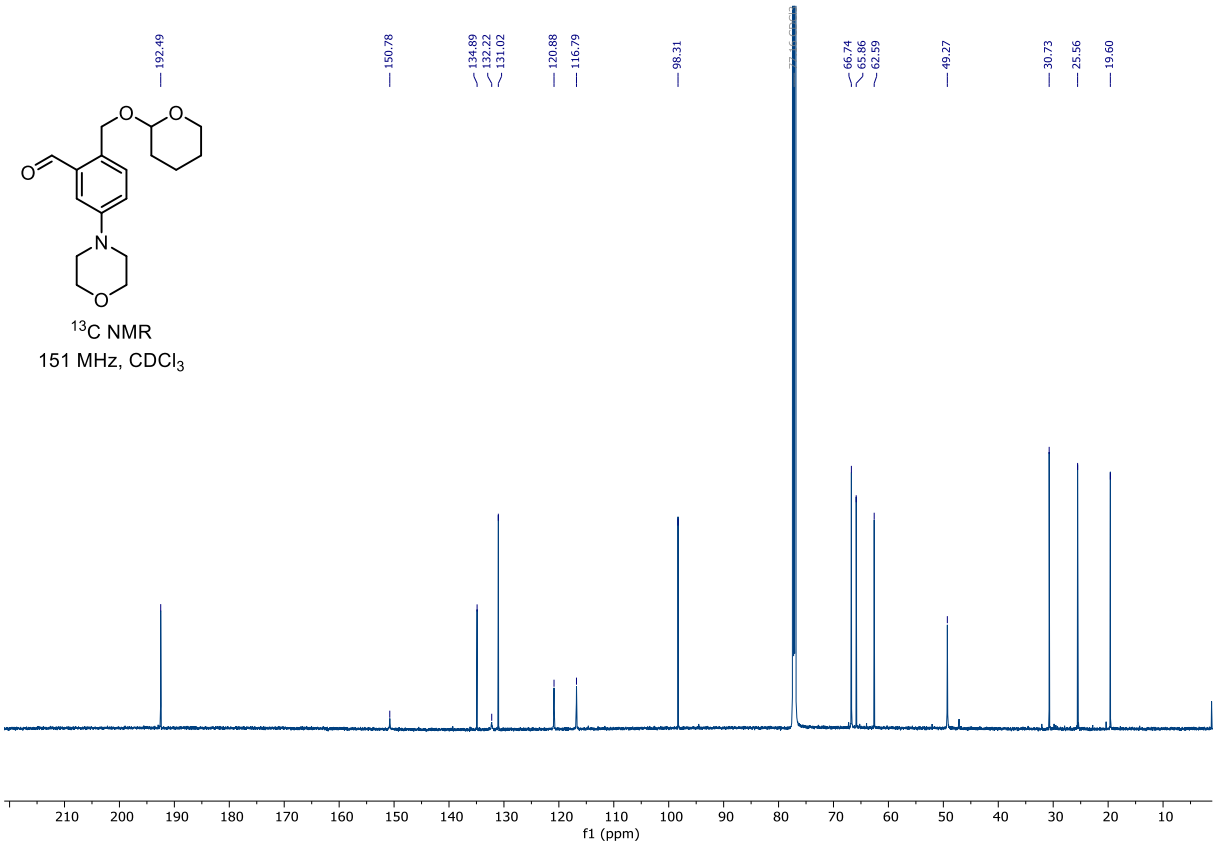
S51 4-(3-Bromo-4-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)morpholine





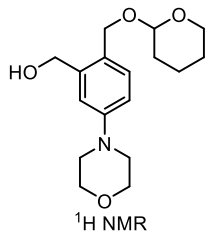
S52 5-Morpholino-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)benzaldehyde



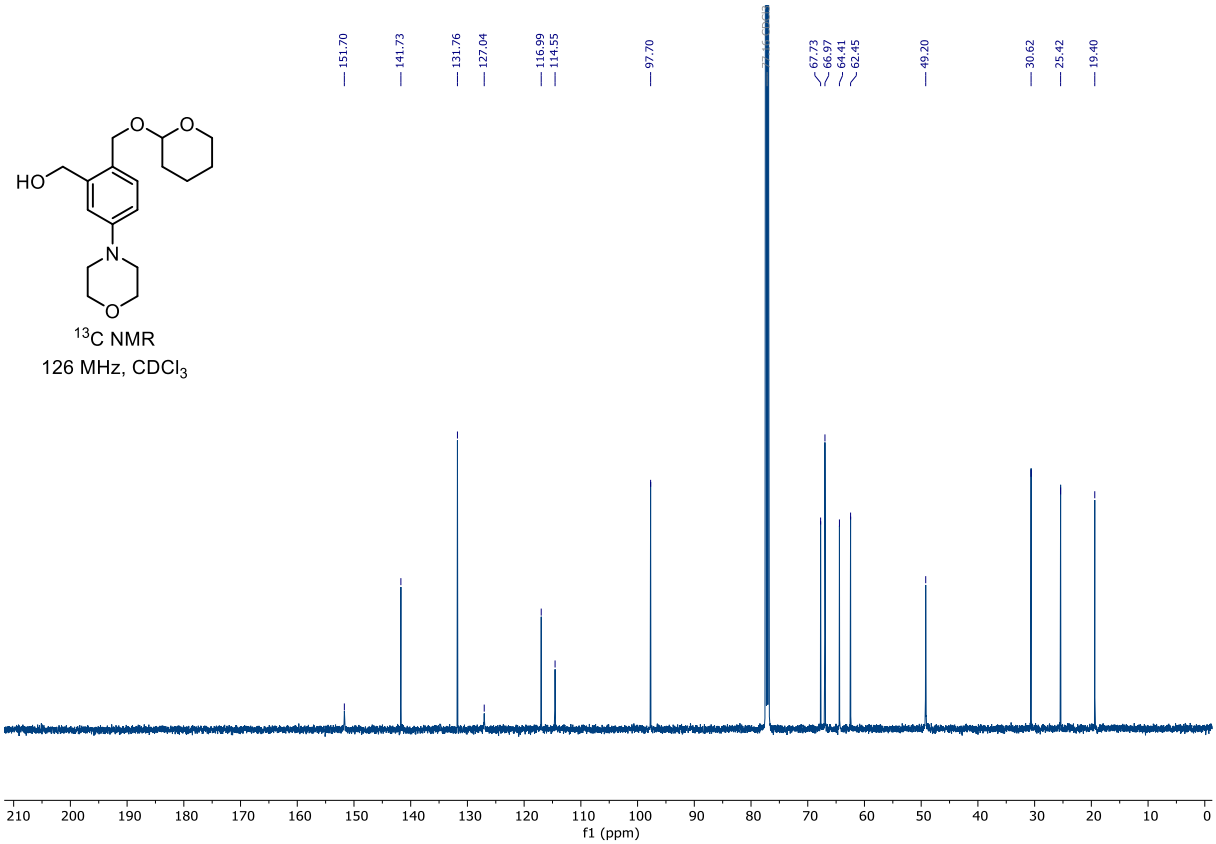


S53 (5-Morpholino-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)methanol



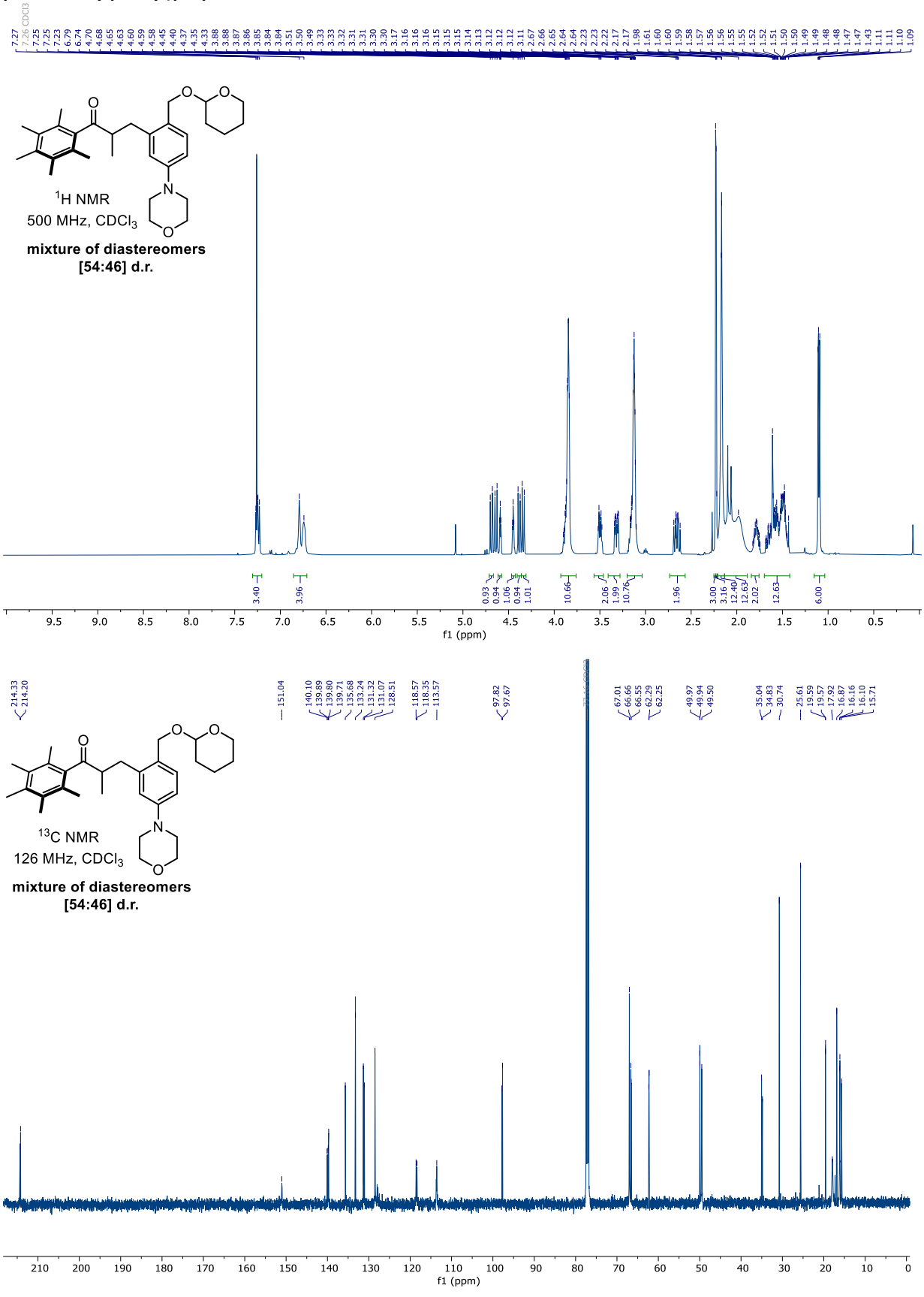


^{1}H NMR
500 MHz, $CDCl_3$

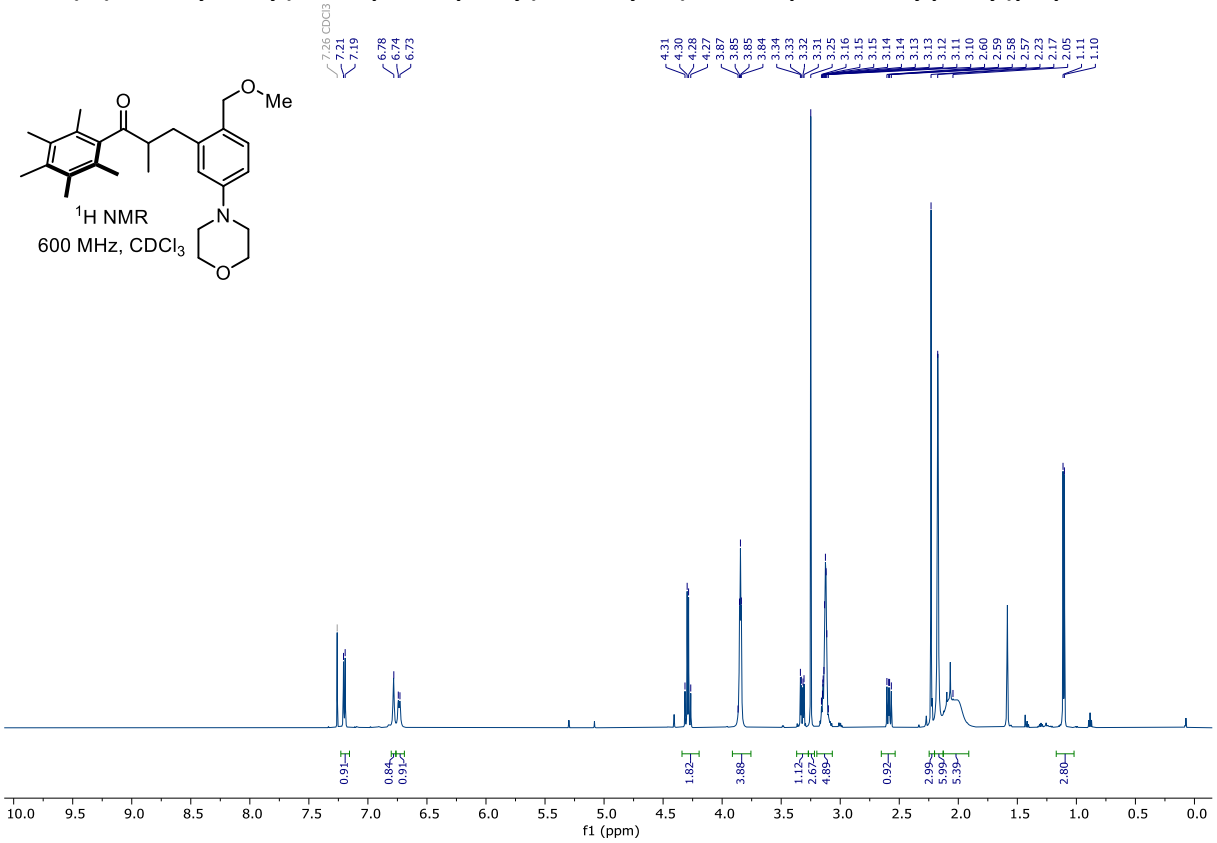


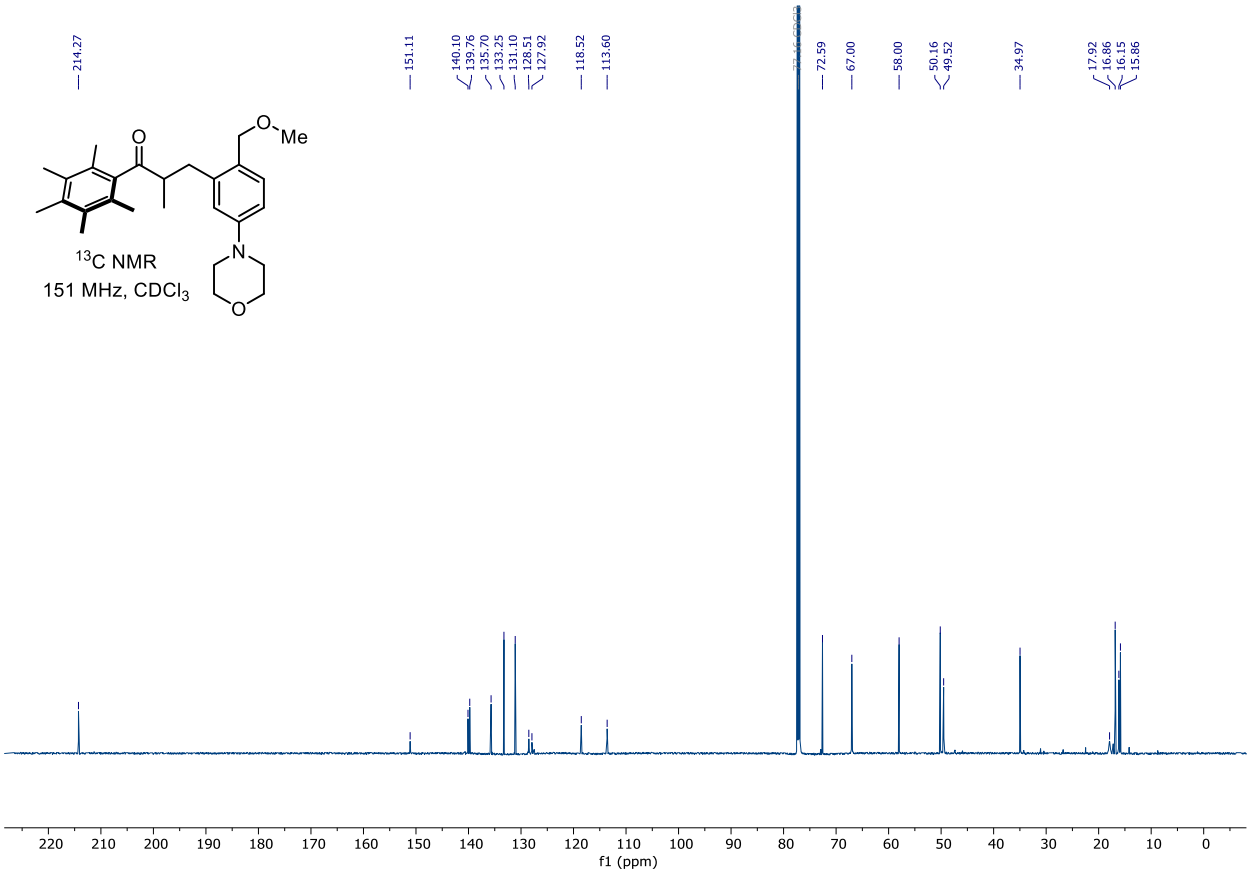
^{13}C NMR
126 MHz, $CDCl_3$

S54 **2-Methyl-3-(5-morpholino-2-(((tetrahydro-2*H*-pyran-2-yl)oxy)methyl)phenyl)-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one**

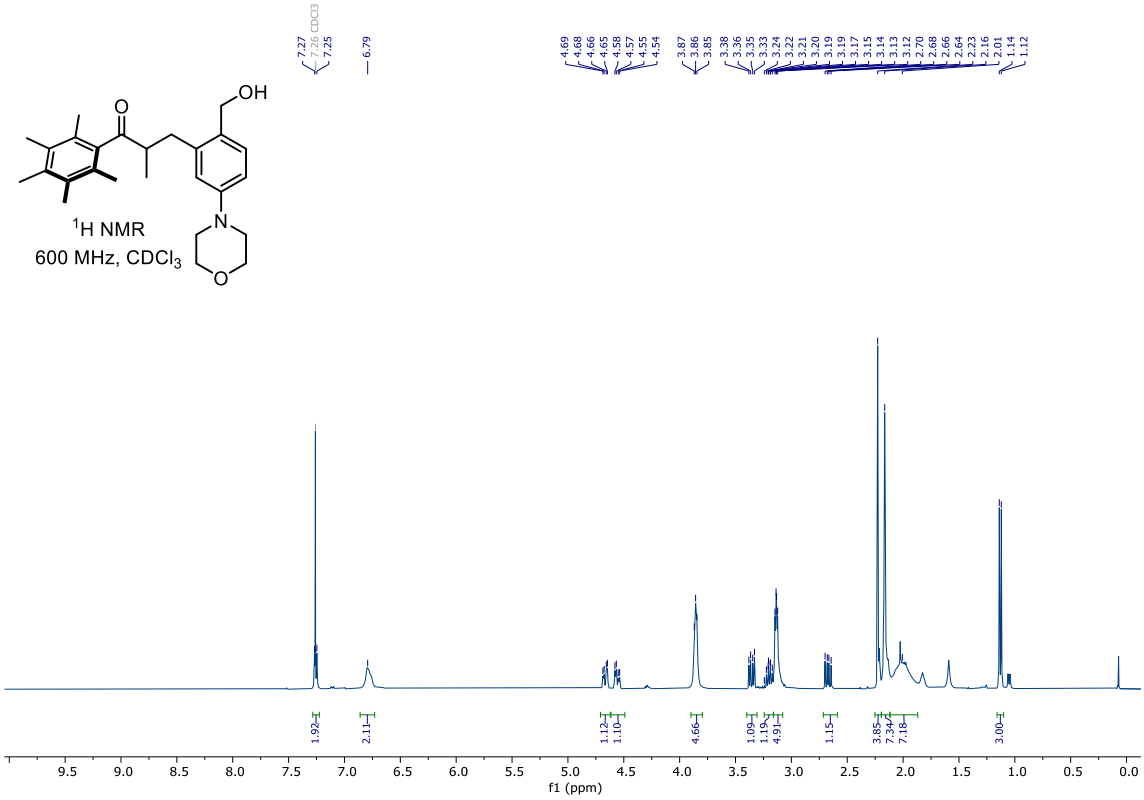


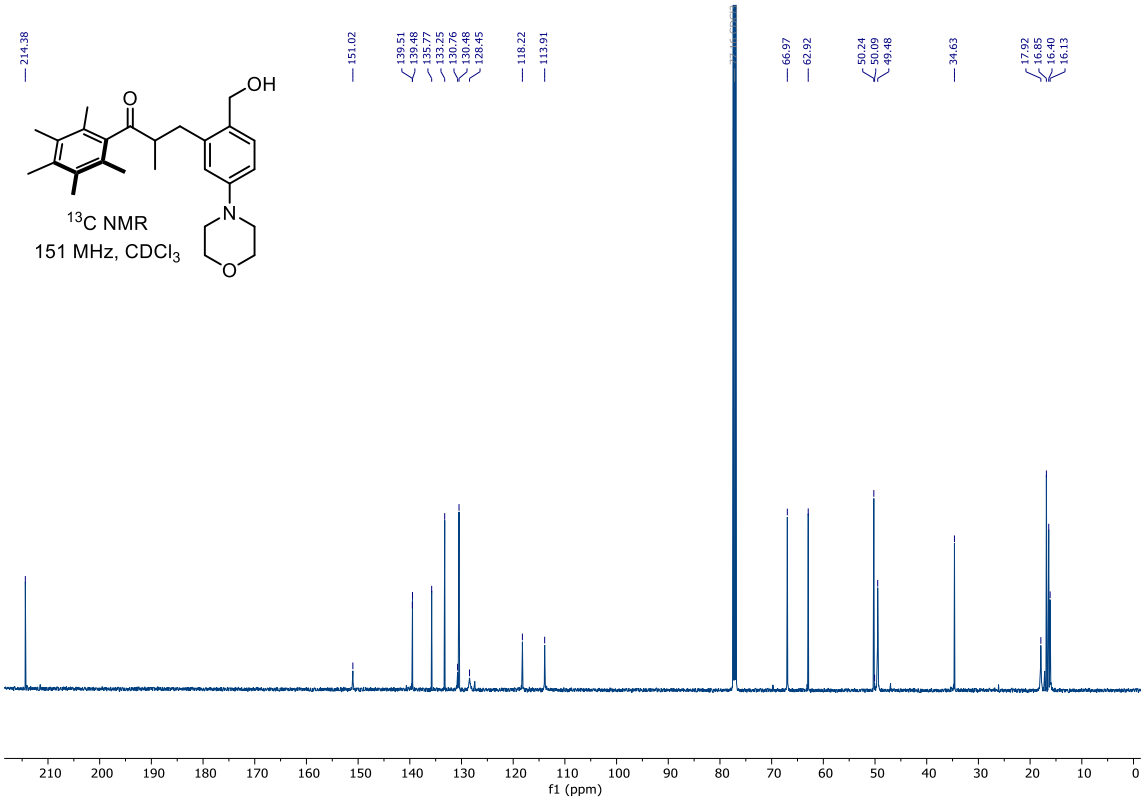
S55 3-(2-(Methoxymethyl)-5-morpholinophenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



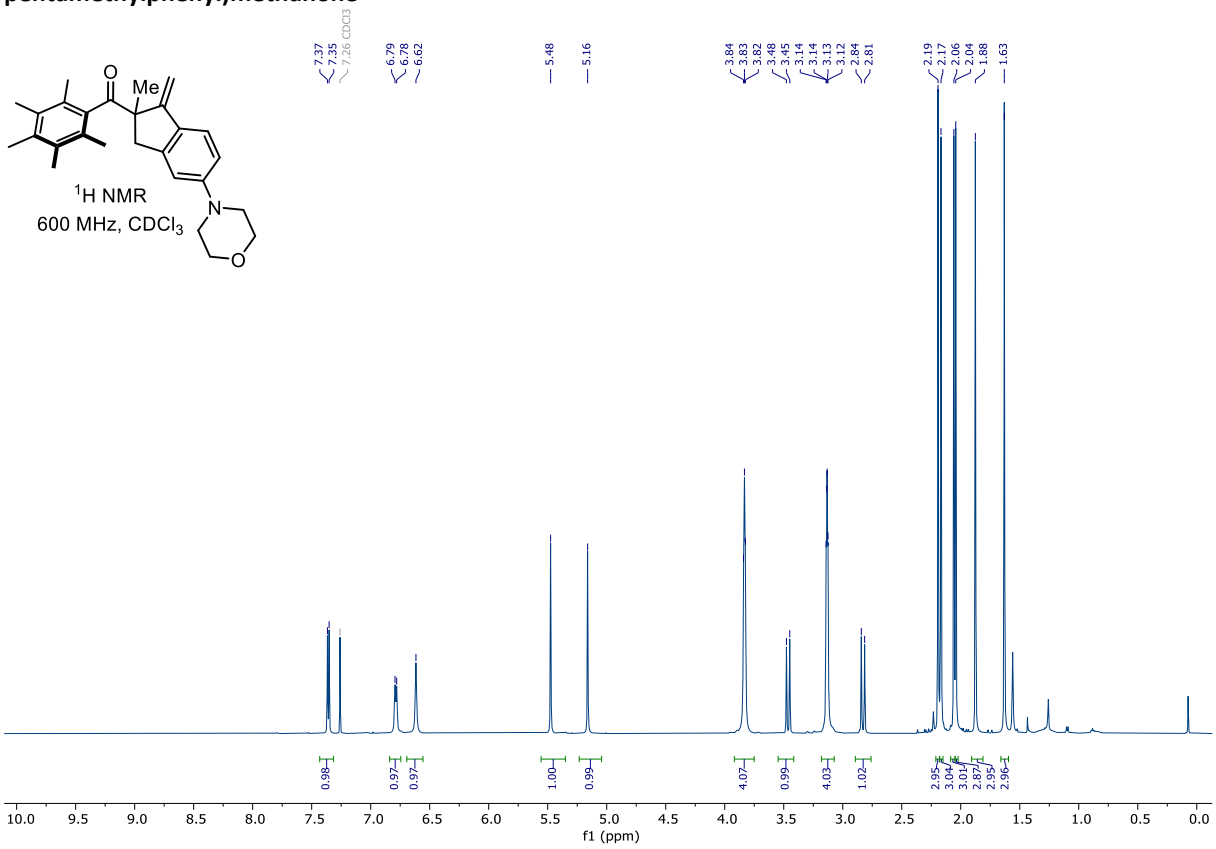


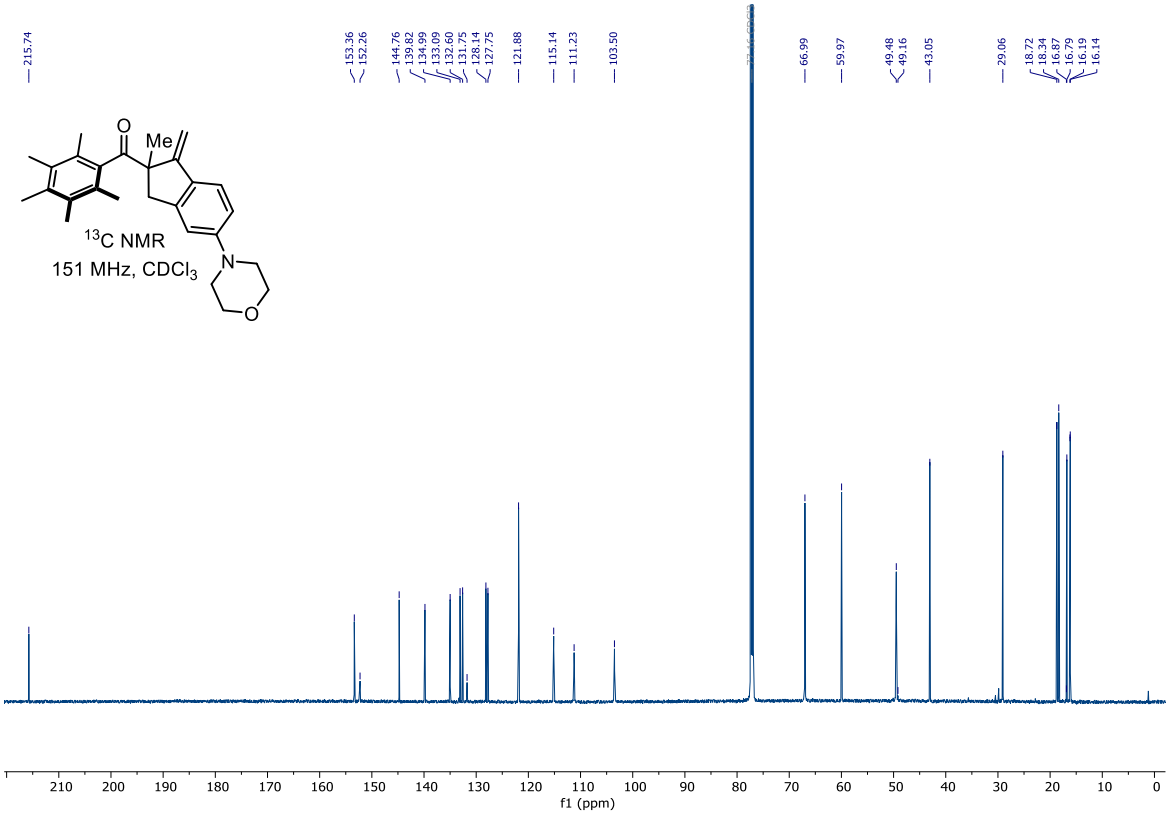
11g 3-(2-(Hydroxymethyl)-5-morpholinophenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one



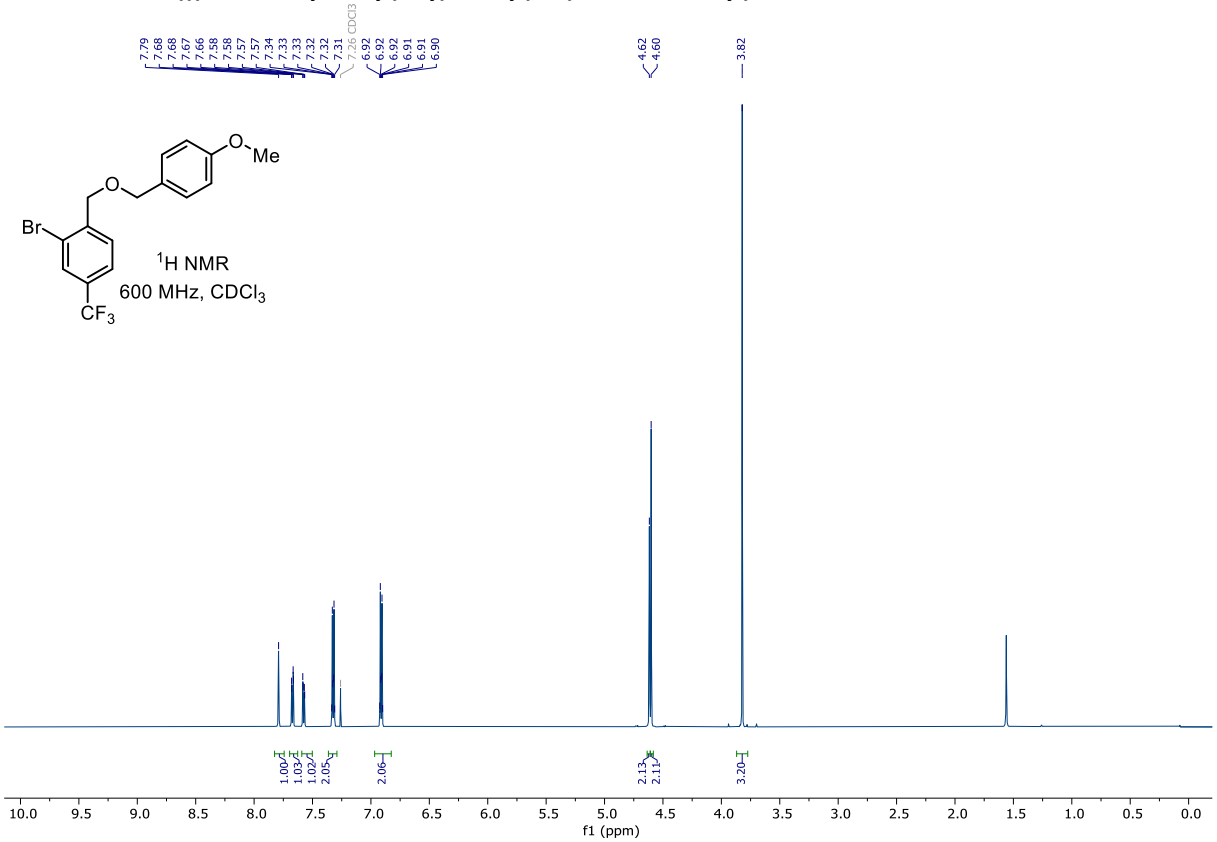


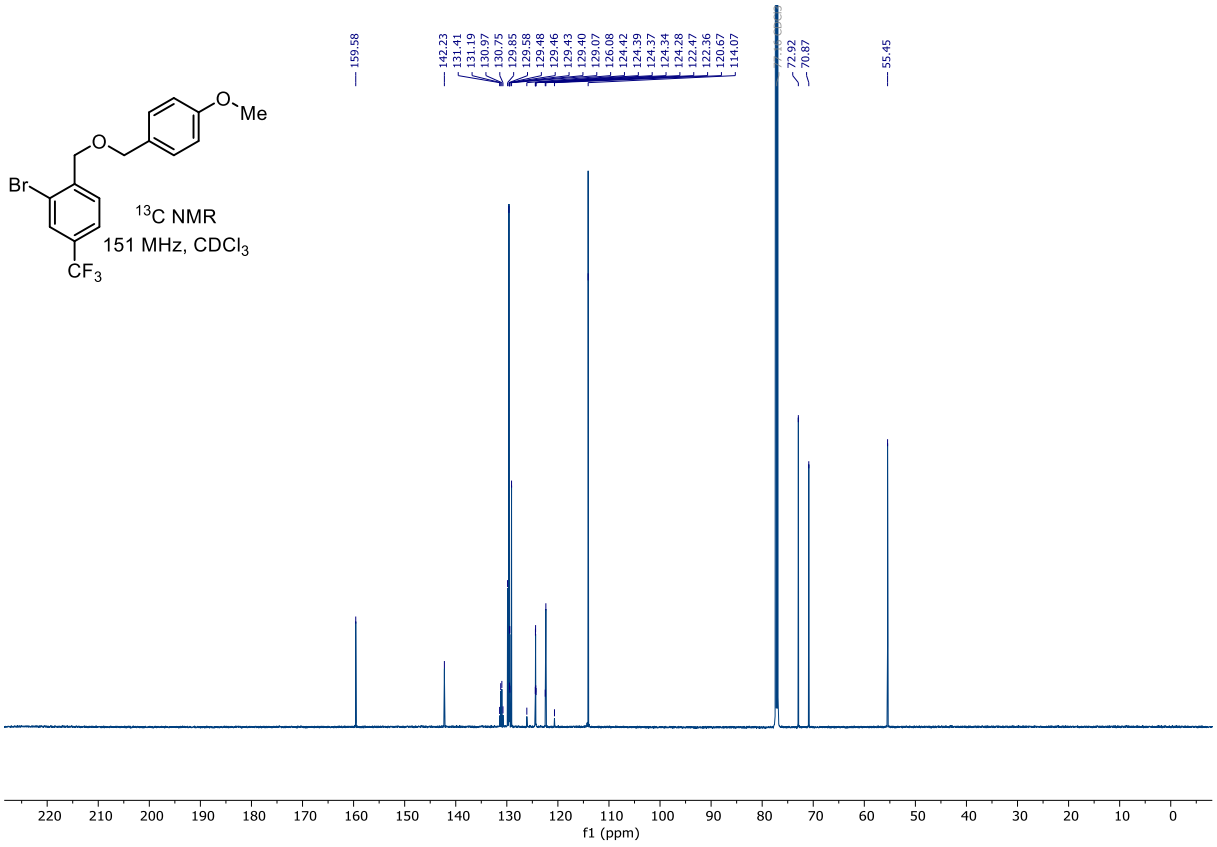
12g **(2-Methyl-1-methylene-5-morpholino-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone**

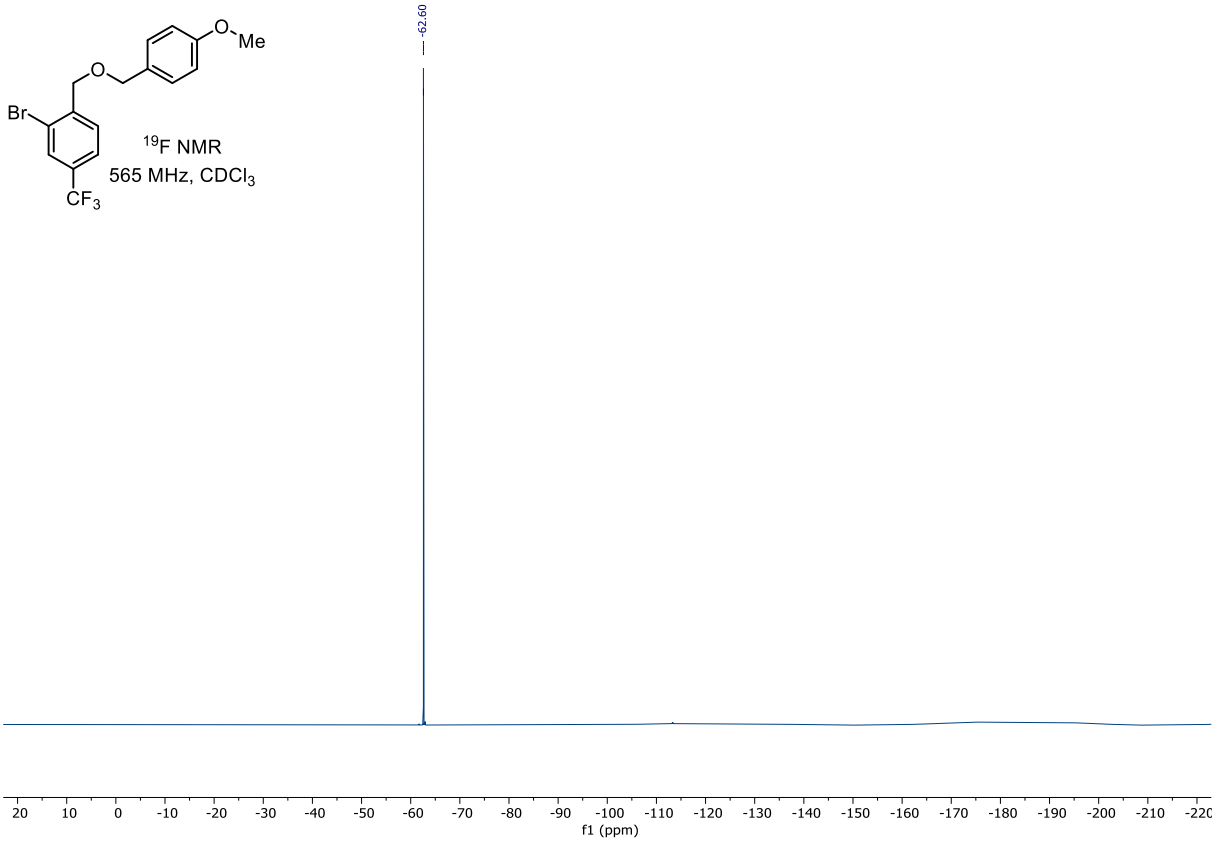




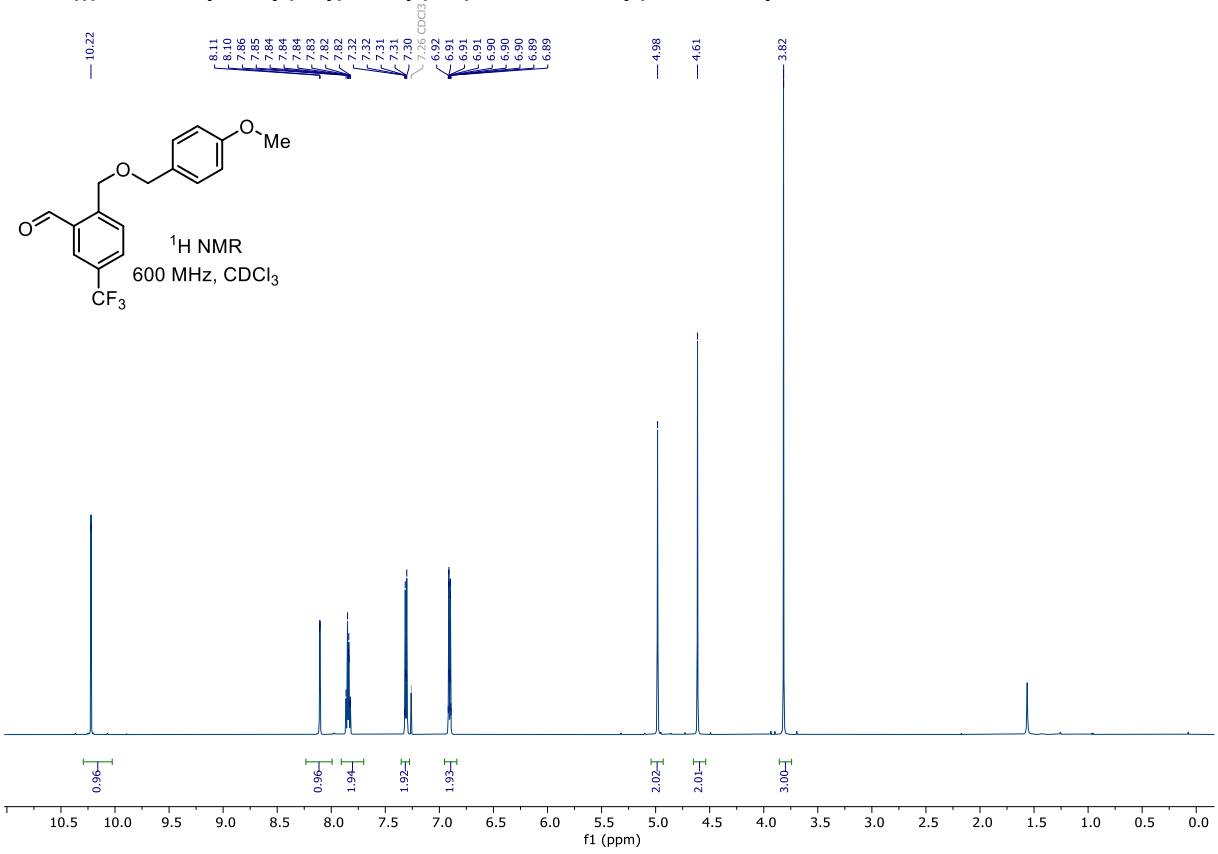
S56 2-Bromo-1-(((4-methoxybenzyl)oxy)methyl)-4-(trifluoromethyl)benzene

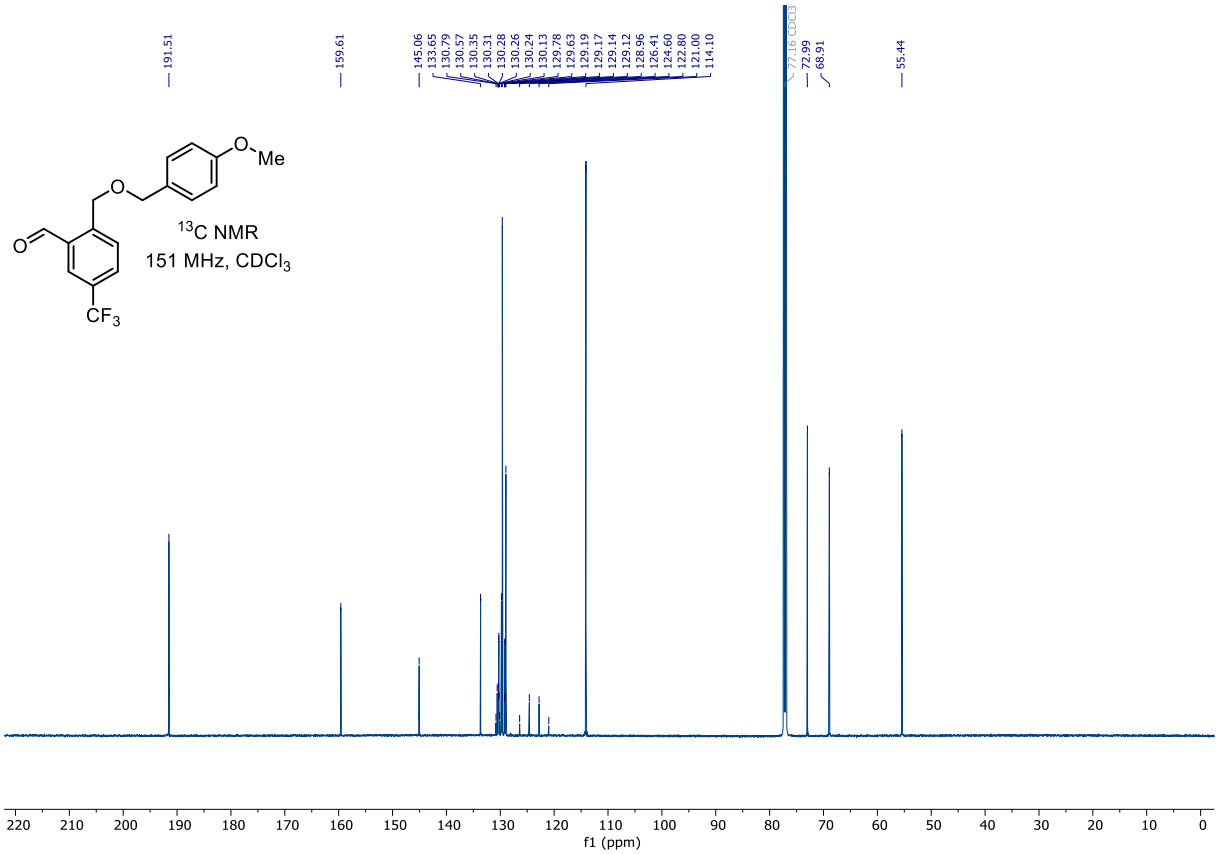


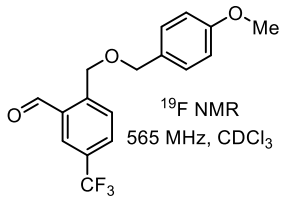



Me
O
O
Br
CF3
19F NMR
565 MHz, CDCl3
-62.60
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

S57 2-(((4-Methoxybenzyl)oxy)methyl)-5-(trifluoromethyl)benzaldehyde



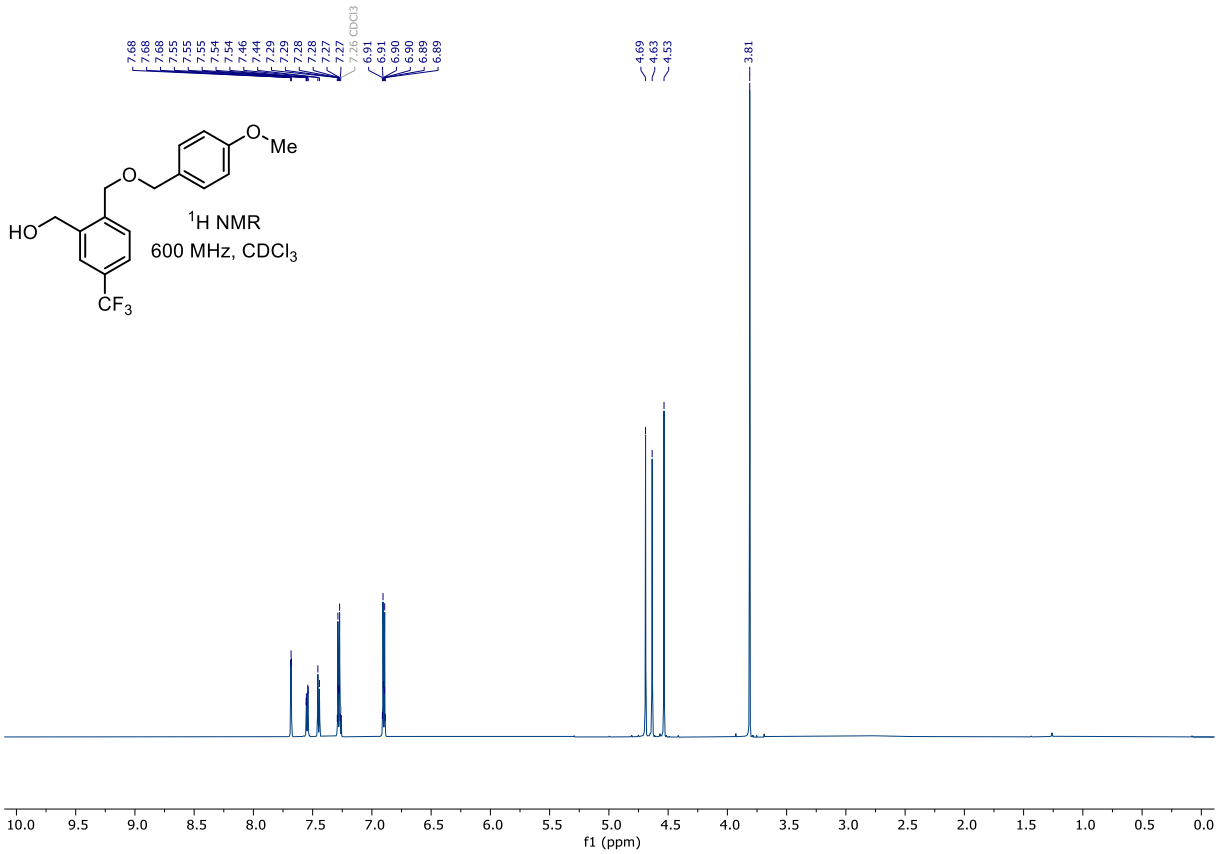


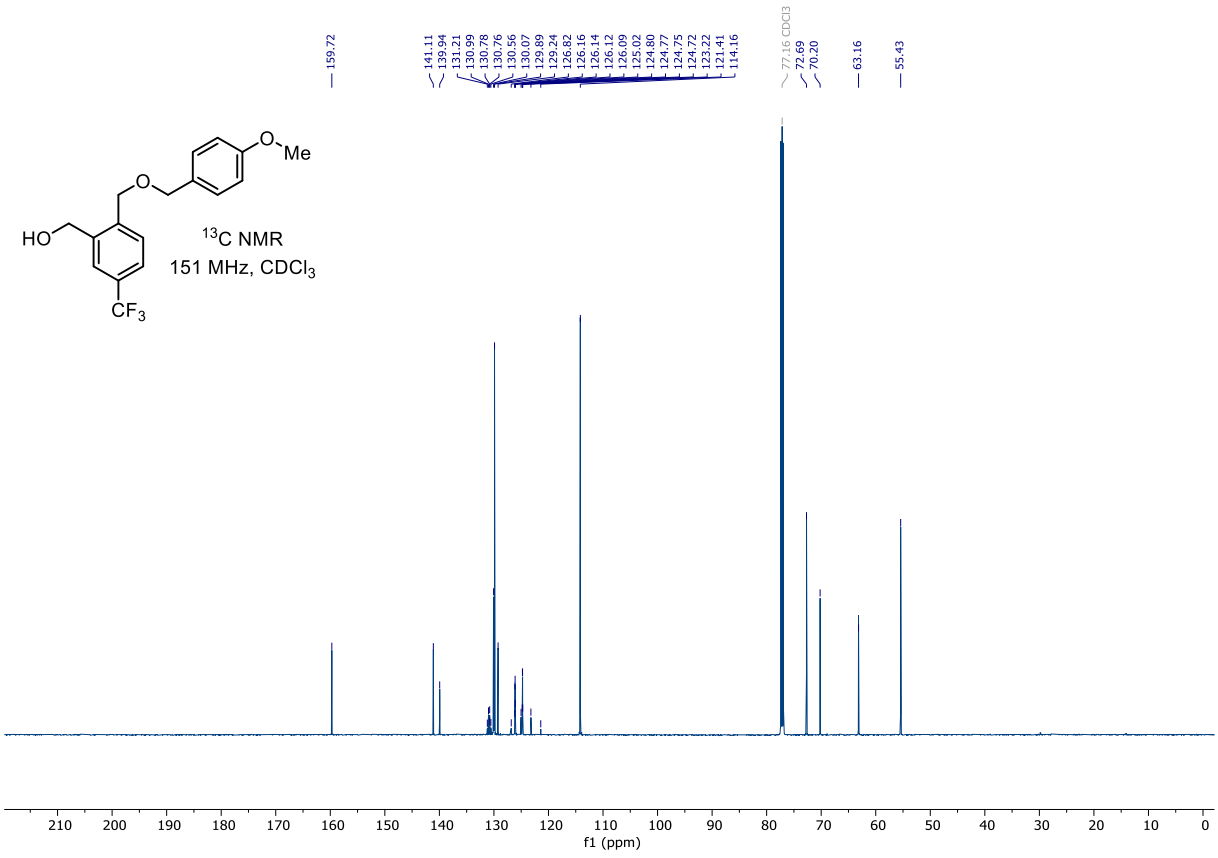


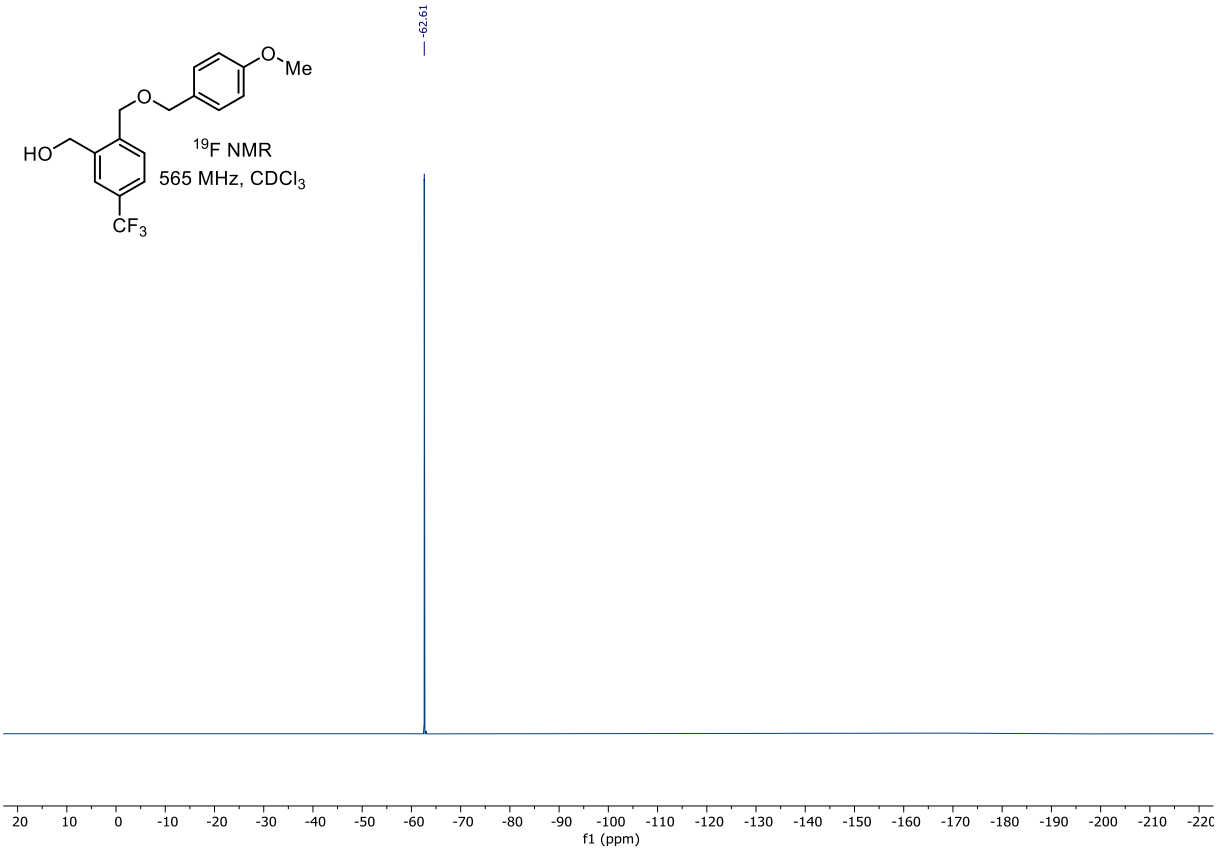
^{19}F NMR

565 MHz, $CDCl_3$

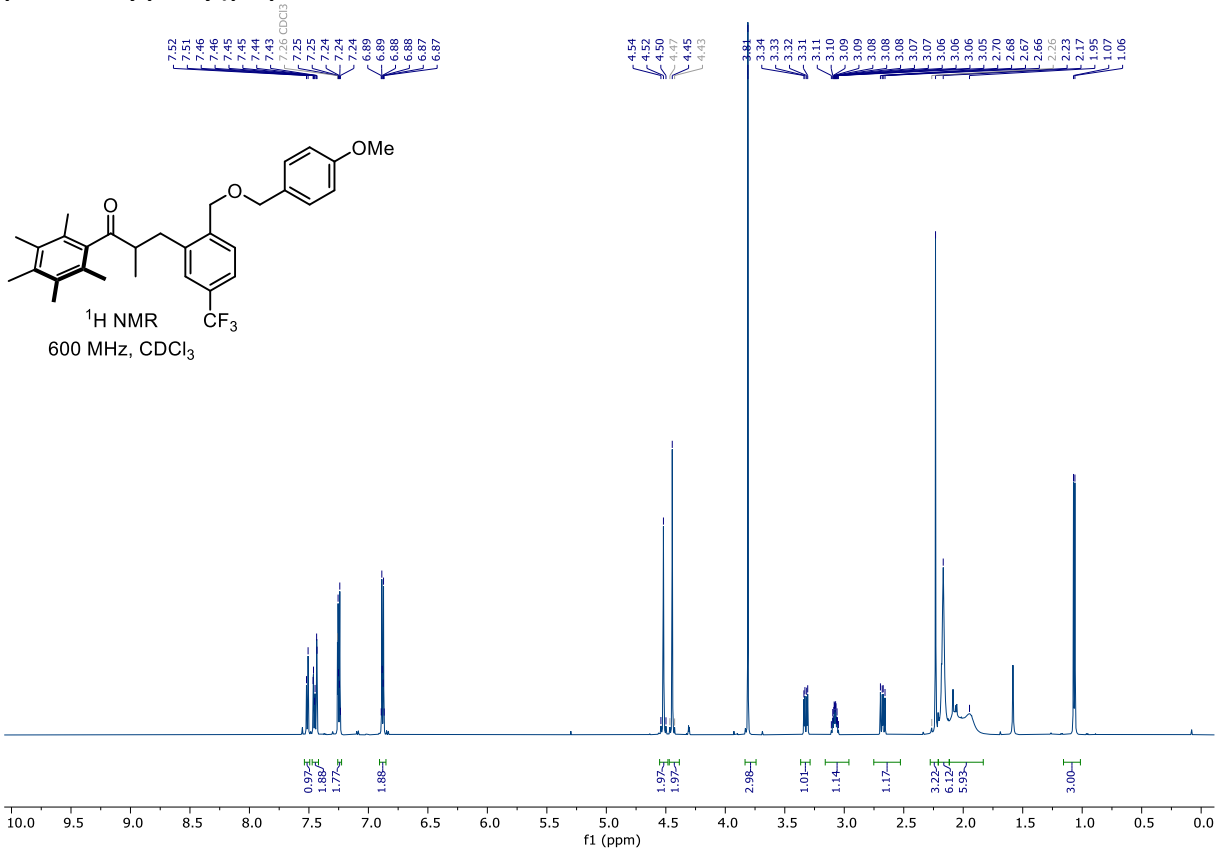
S58 (2-(((4-Methoxybenzyl)oxy)methyl)-5-(trifluoromethyl)phenyl)methanol

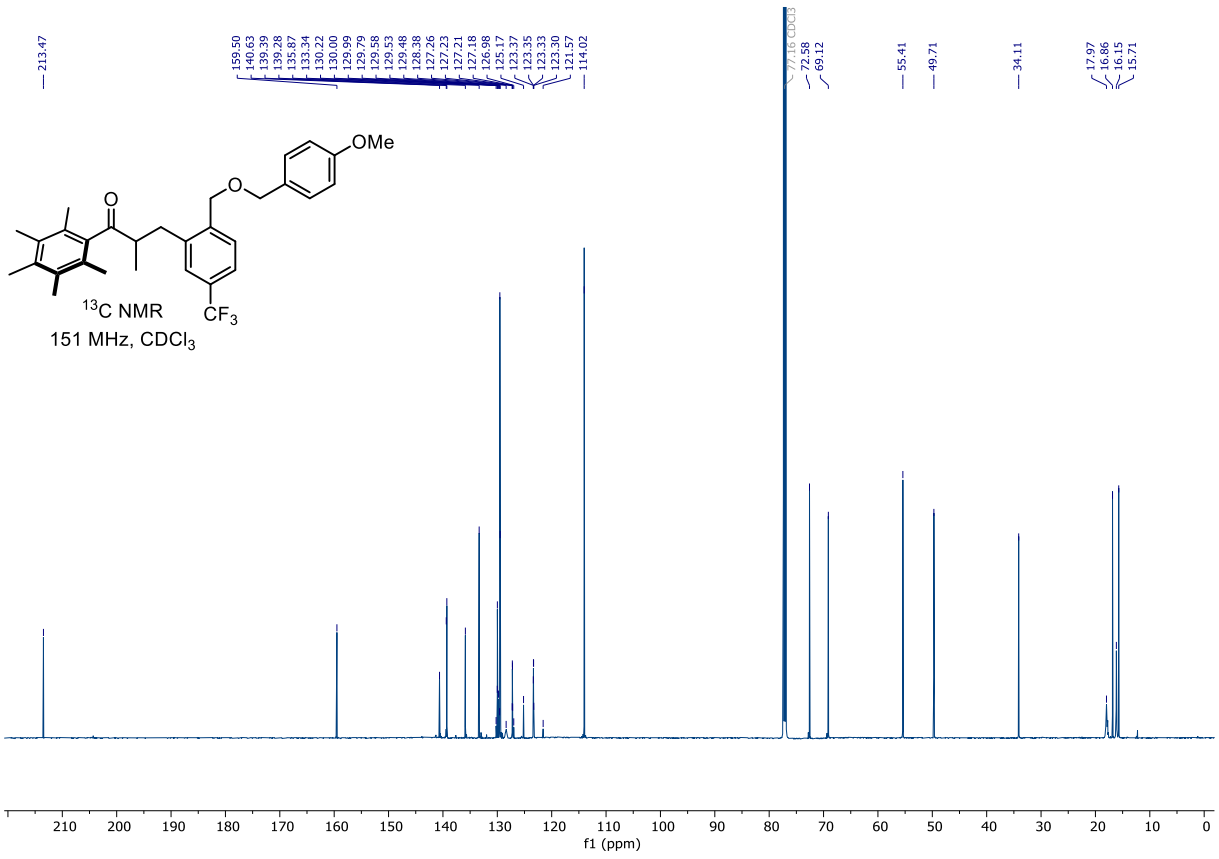


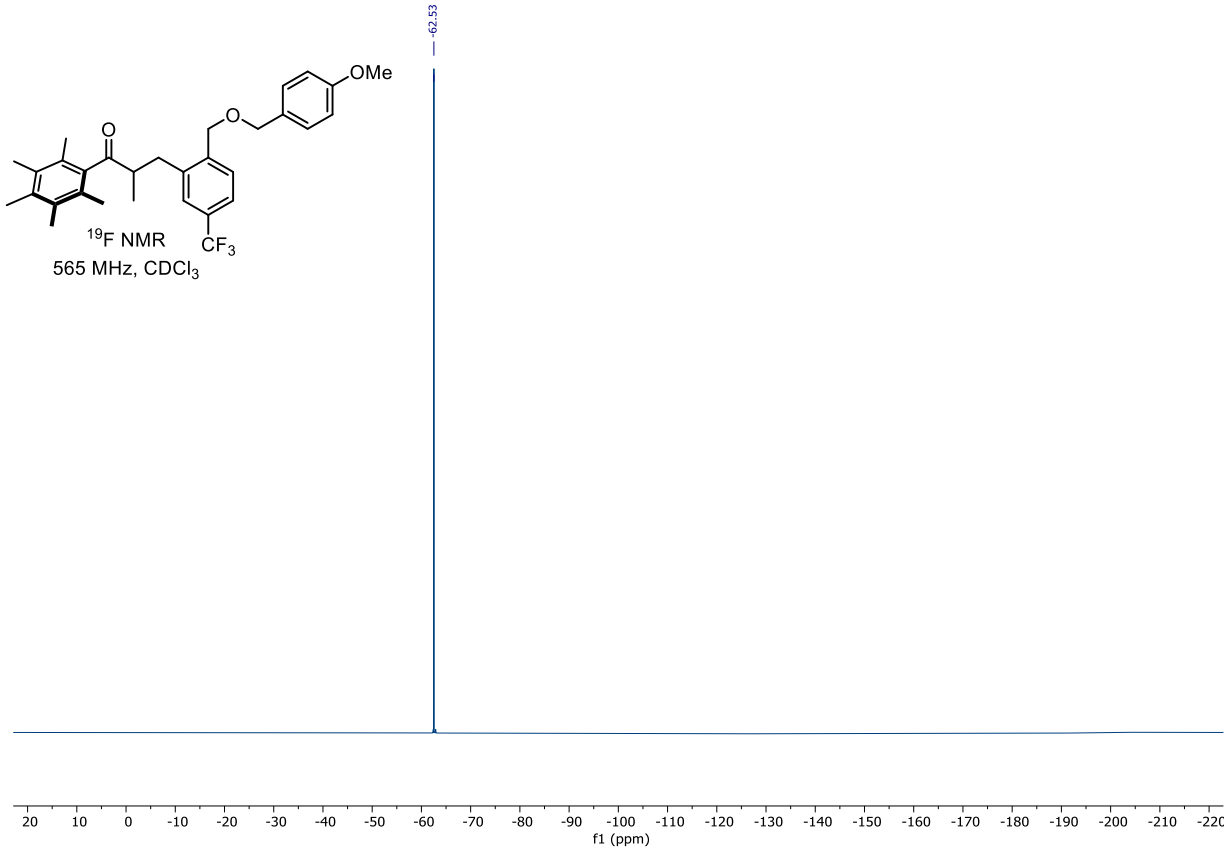



-62.61
O
Me
O
HO
CF3
19F NMR
565 MHz, CDCl3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

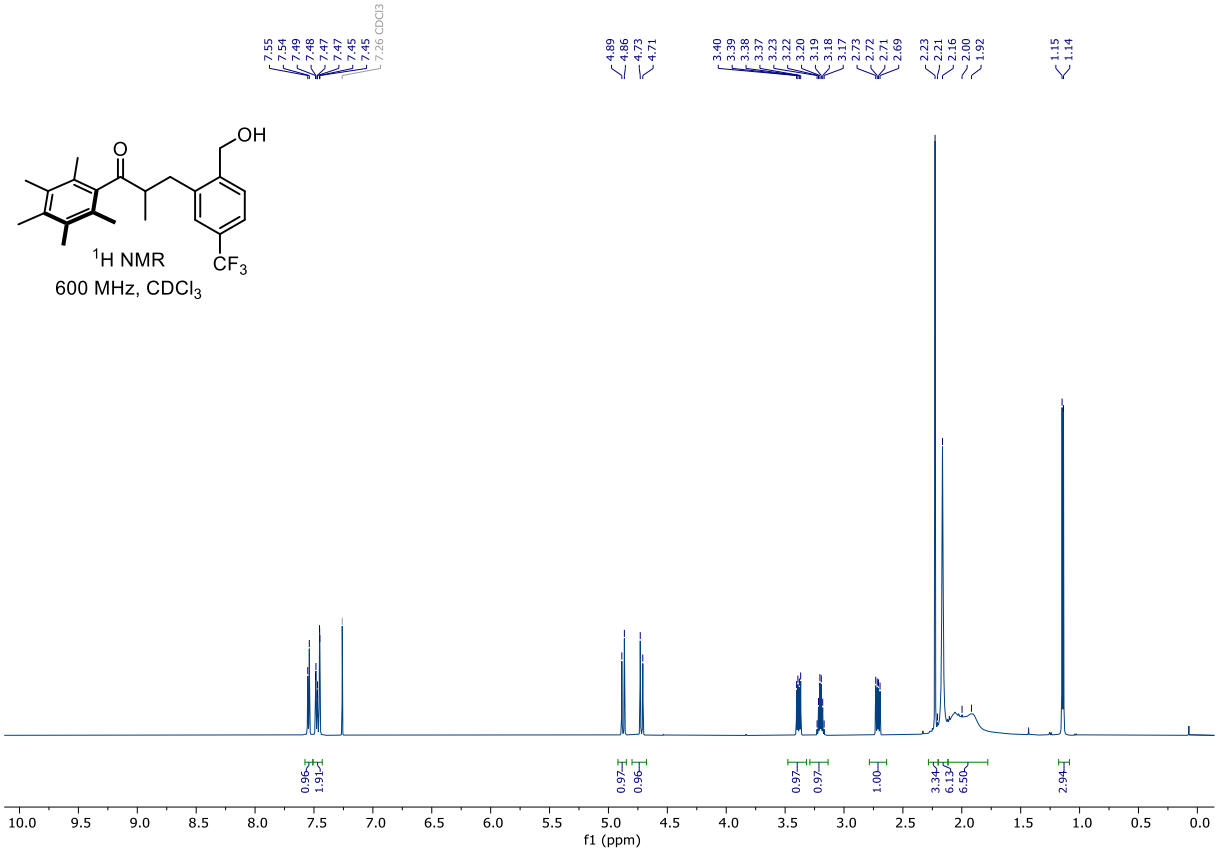
S59 **3-(2-(((4-Methoxybenzyl)oxy)methyl)-5-(trifluoromethyl)phenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one**

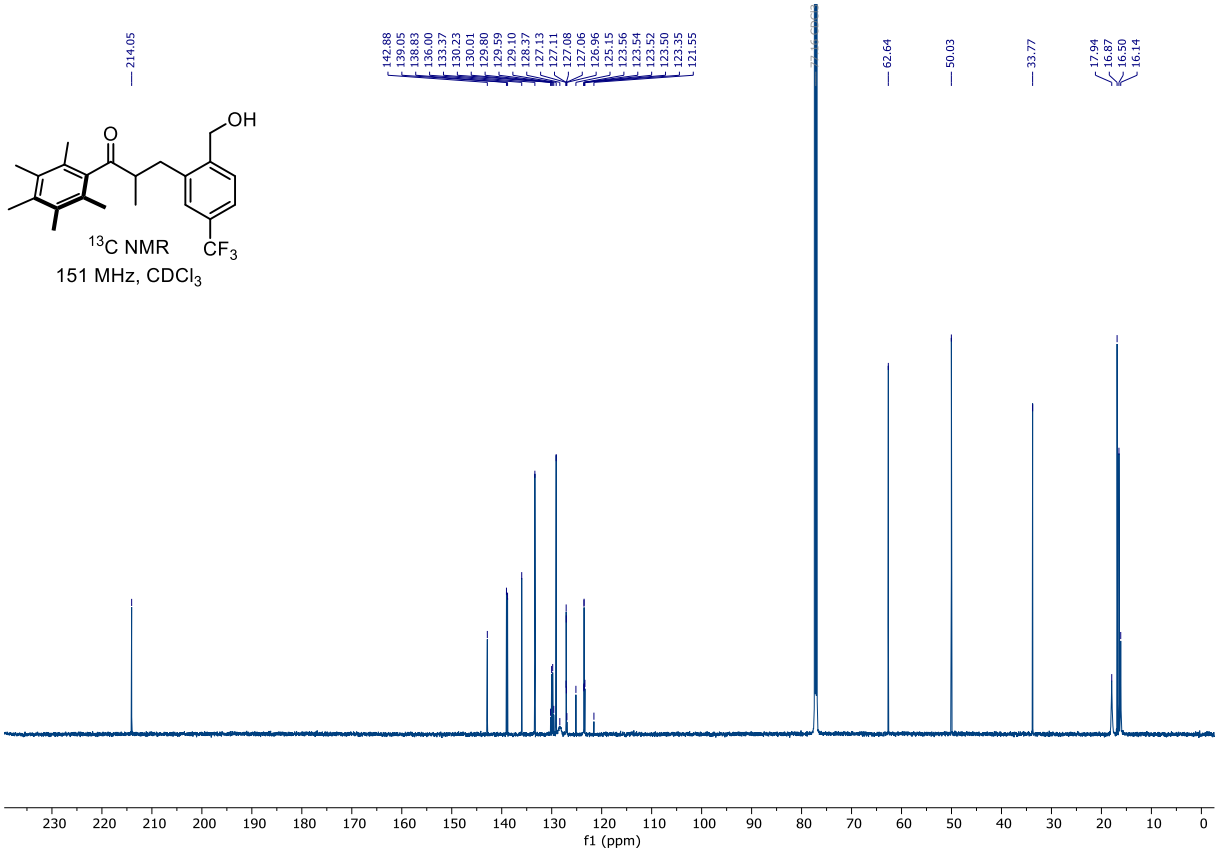


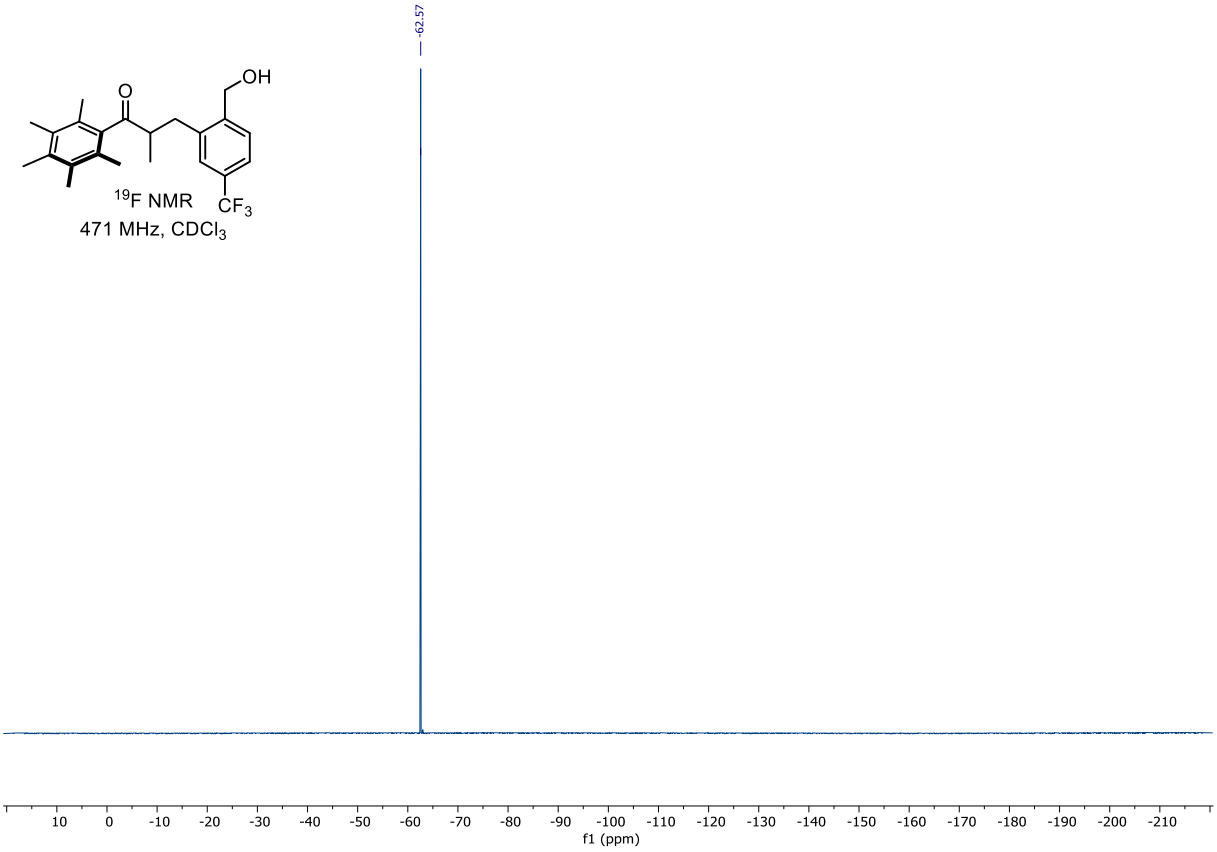



-62.53
OMe
O
O
CF3
19F NMR
565 MHz, CDCl3
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

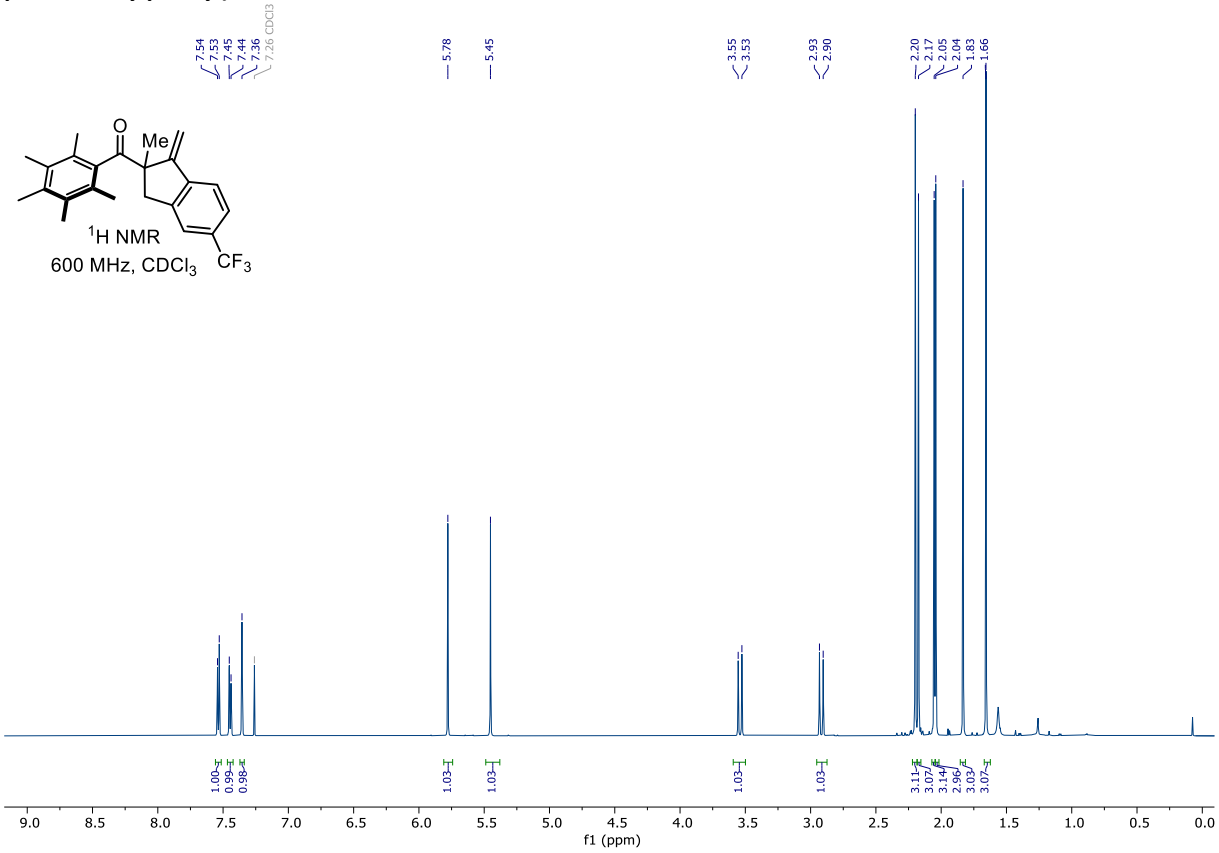
11h 3-(2-(Hydroxymethyl)-5-(trifluoromethyl)phenyl)-2-methyl-1-(2,3,4,5,6-pentamethylphenyl)propan-1-one

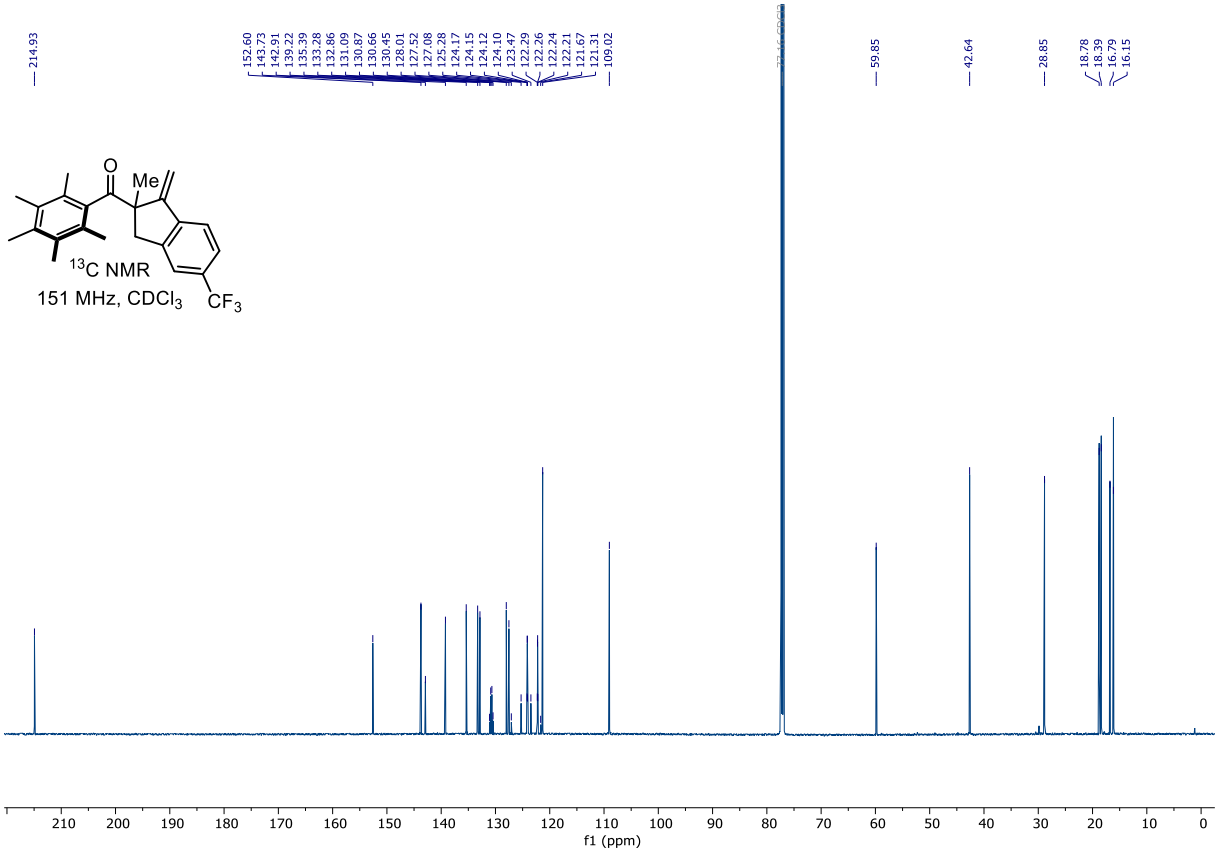


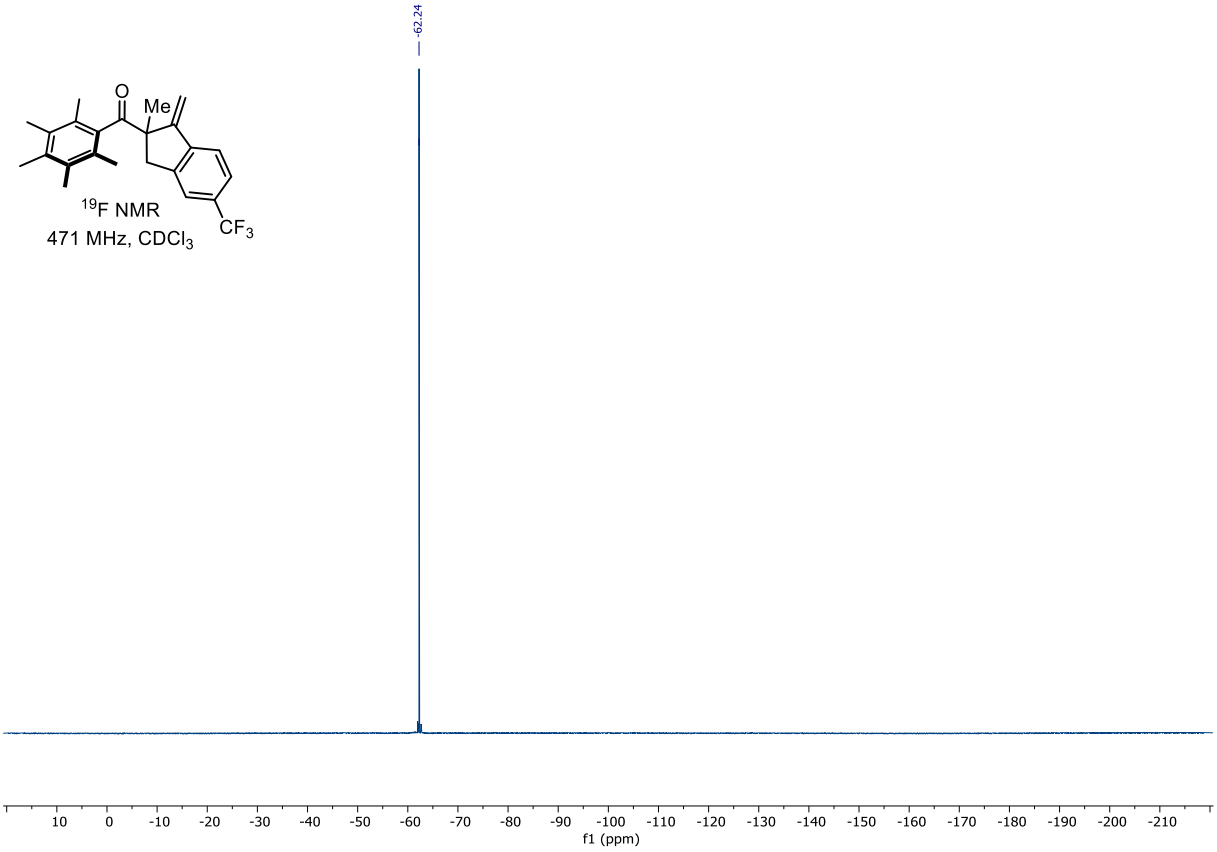



-62.57
OH
O
CF3
19F NMR
471 MHz, CDCl3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

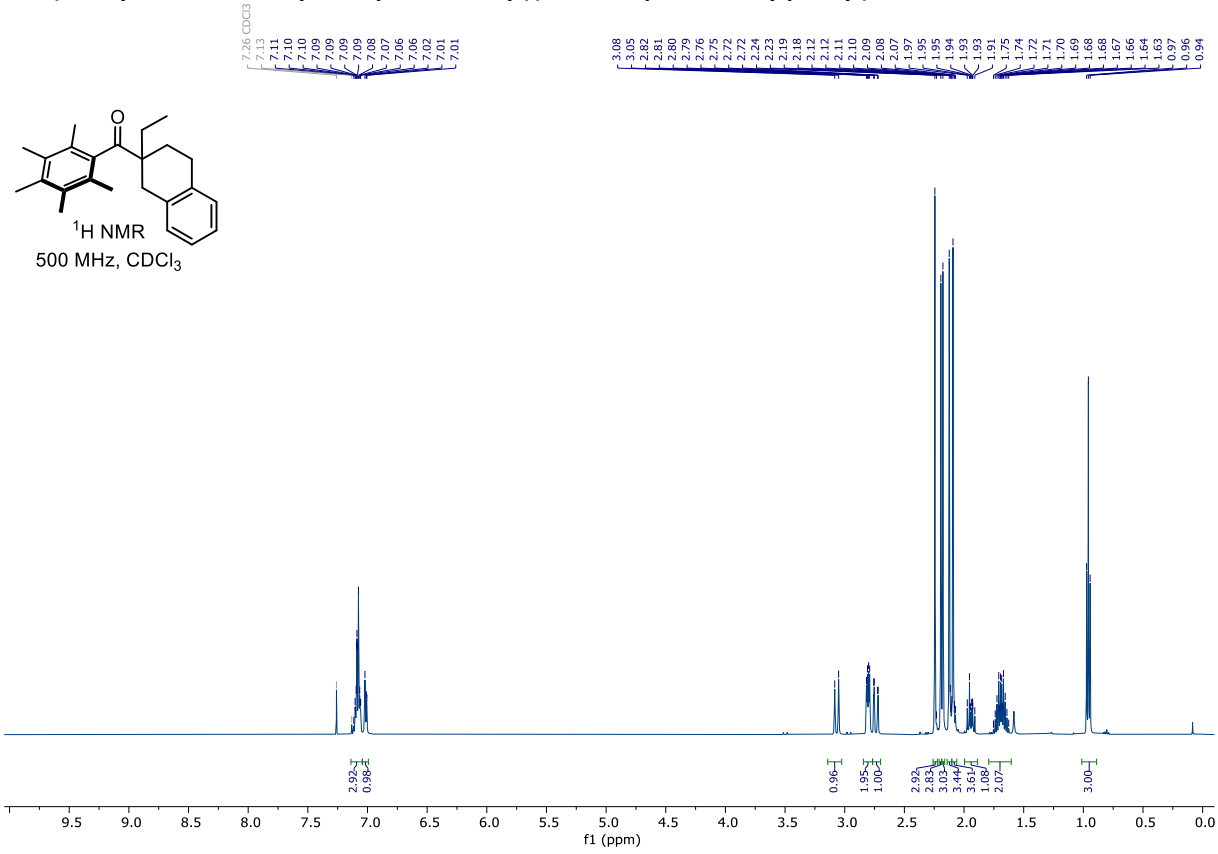
12h (2-Methyl-1-methylene-5-(trifluoromethyl)-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone

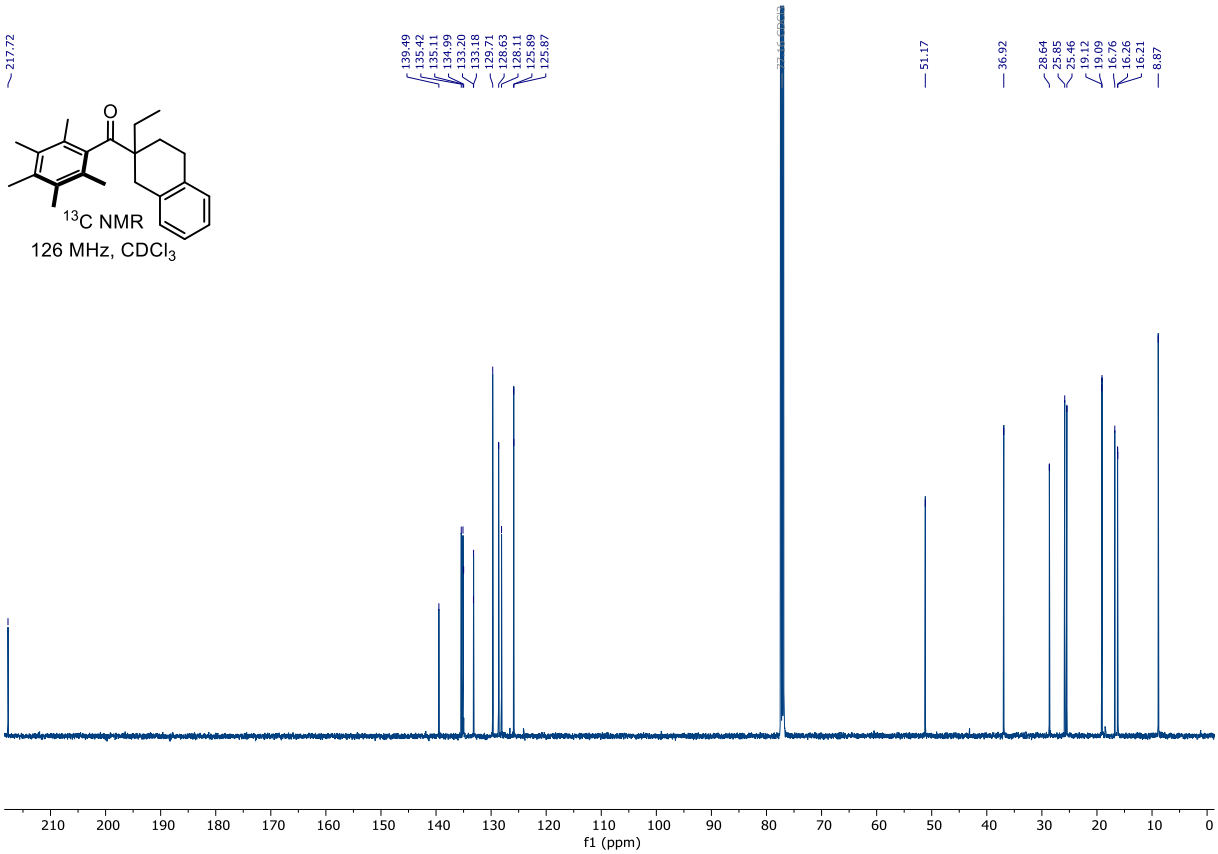




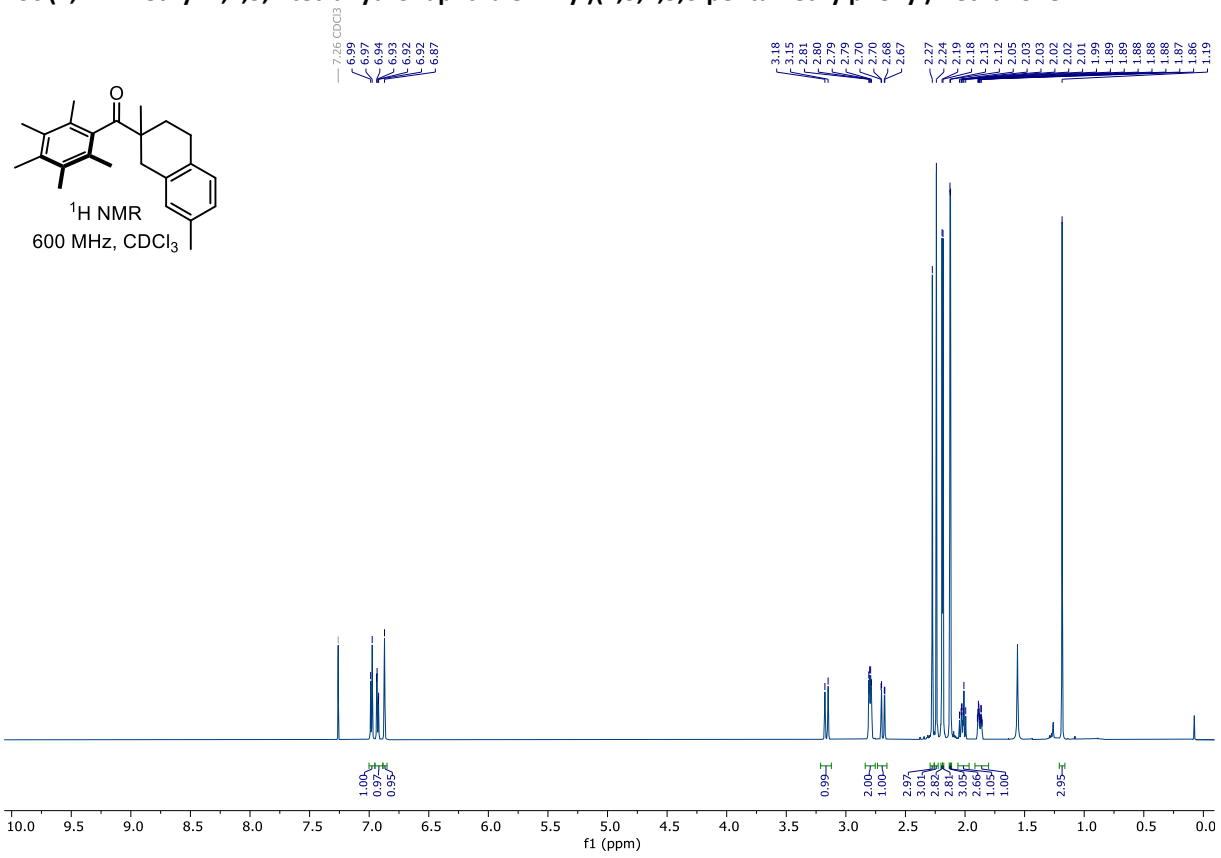

-62.24
O
Me
CF3
19F NMR
471 MHz, CDCl3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

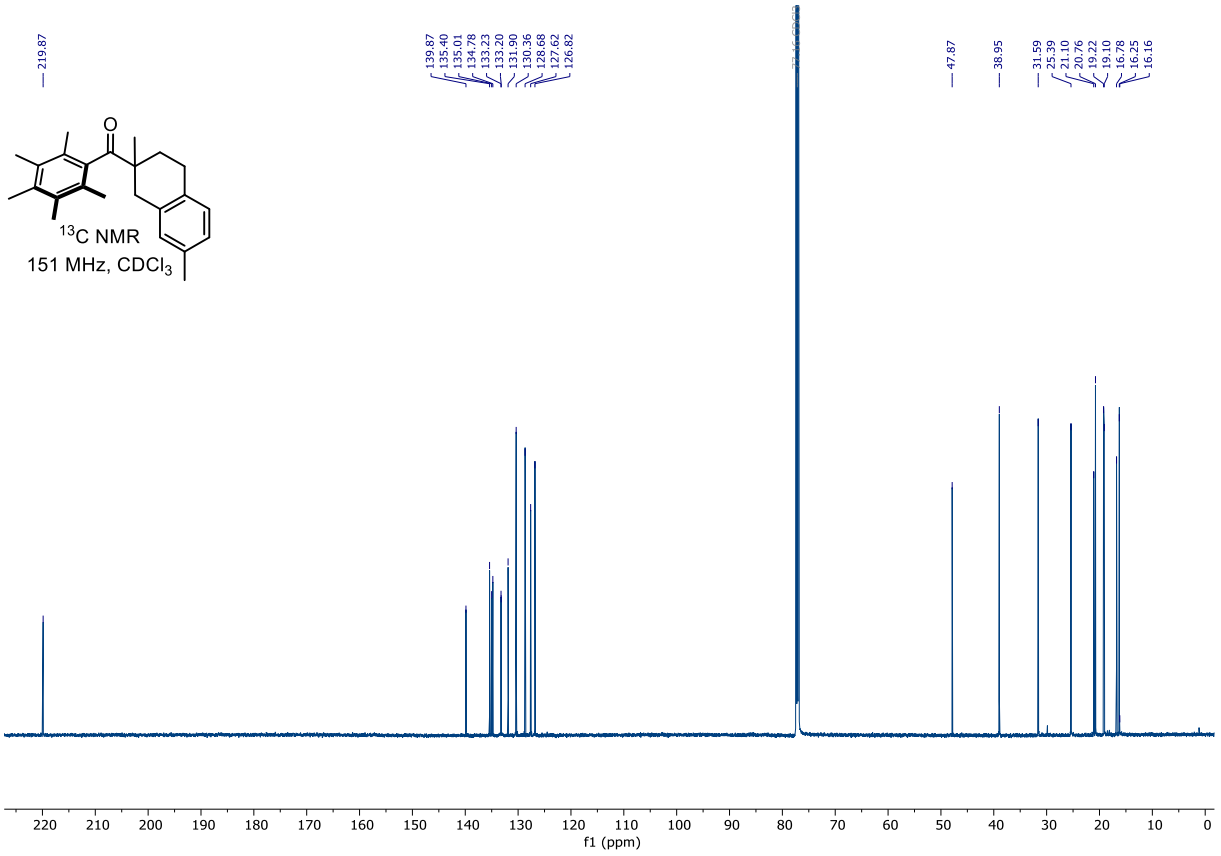
13b (2-Ethyl-1,2,3,4-tetrahydronaphthalen-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



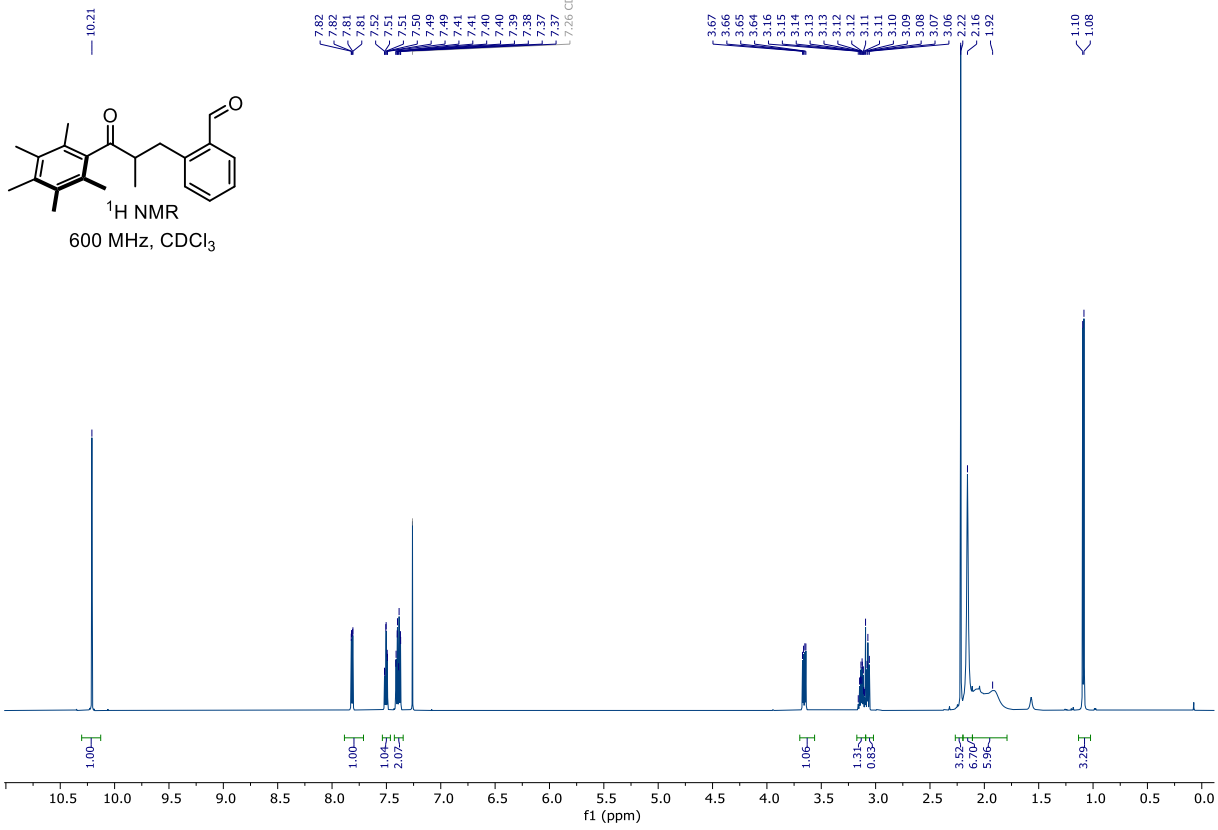


13c (2,7-Dimethyl-1,2,3,4-tetrahydronaphthalen-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone

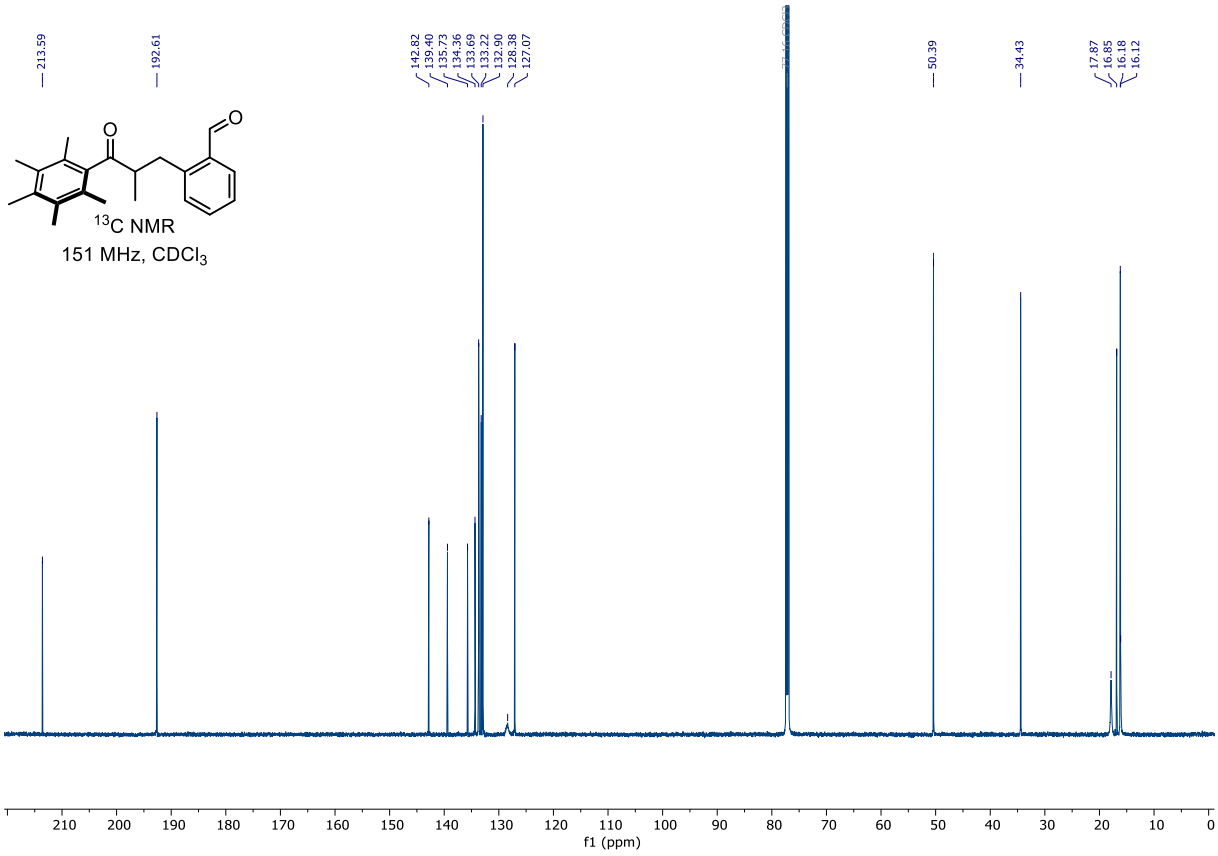




14 2-(2-Methyl-3-oxo-3-(2,3,4,5,6-pentamethylphenyl)propyl)benzaldehyde

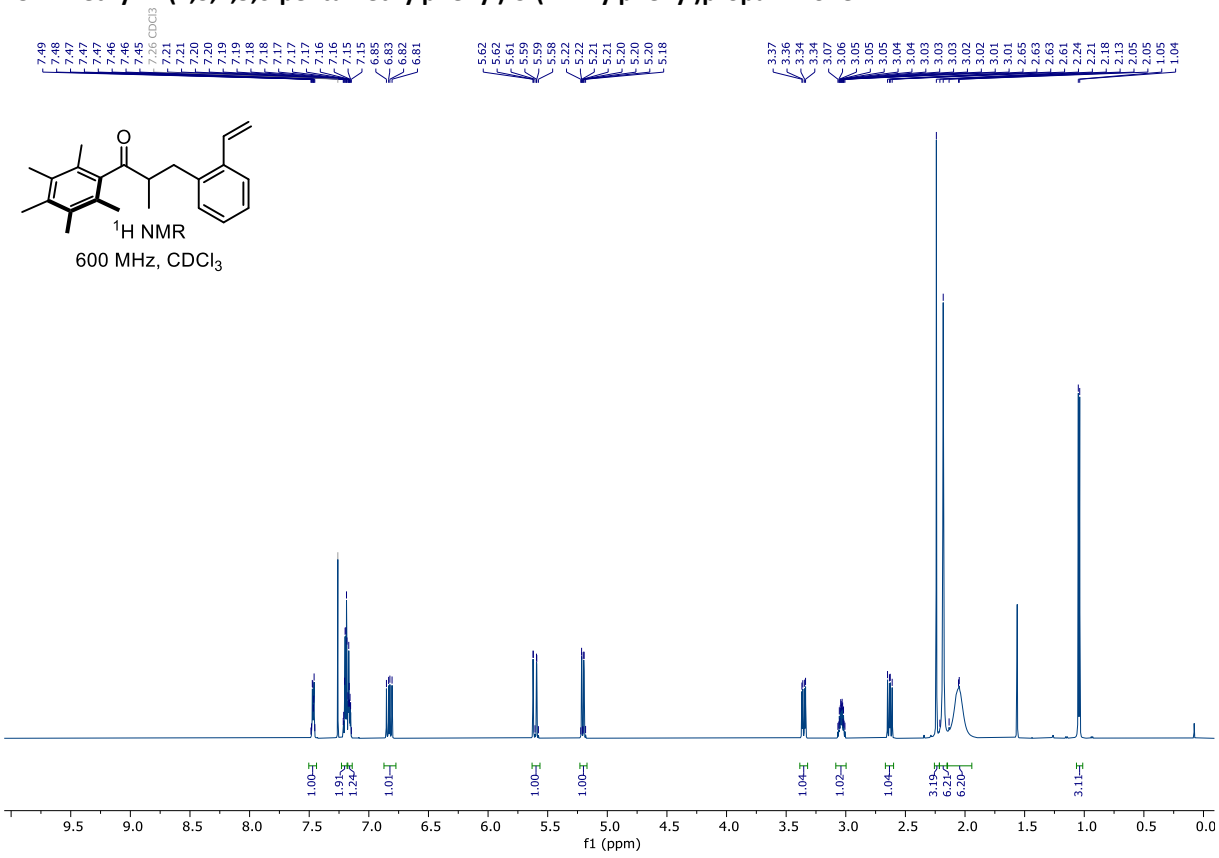


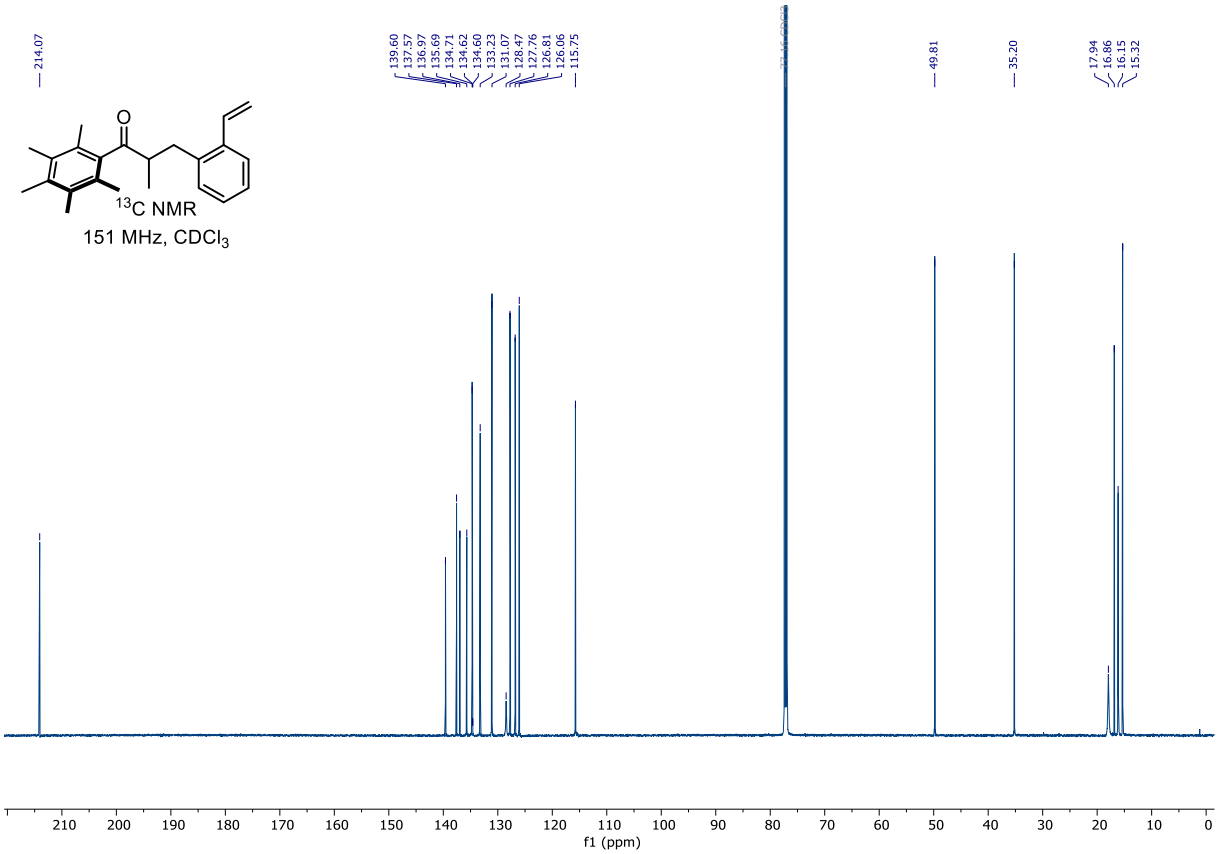
^{1}H NMR
600 MHz, $CDCl_3$



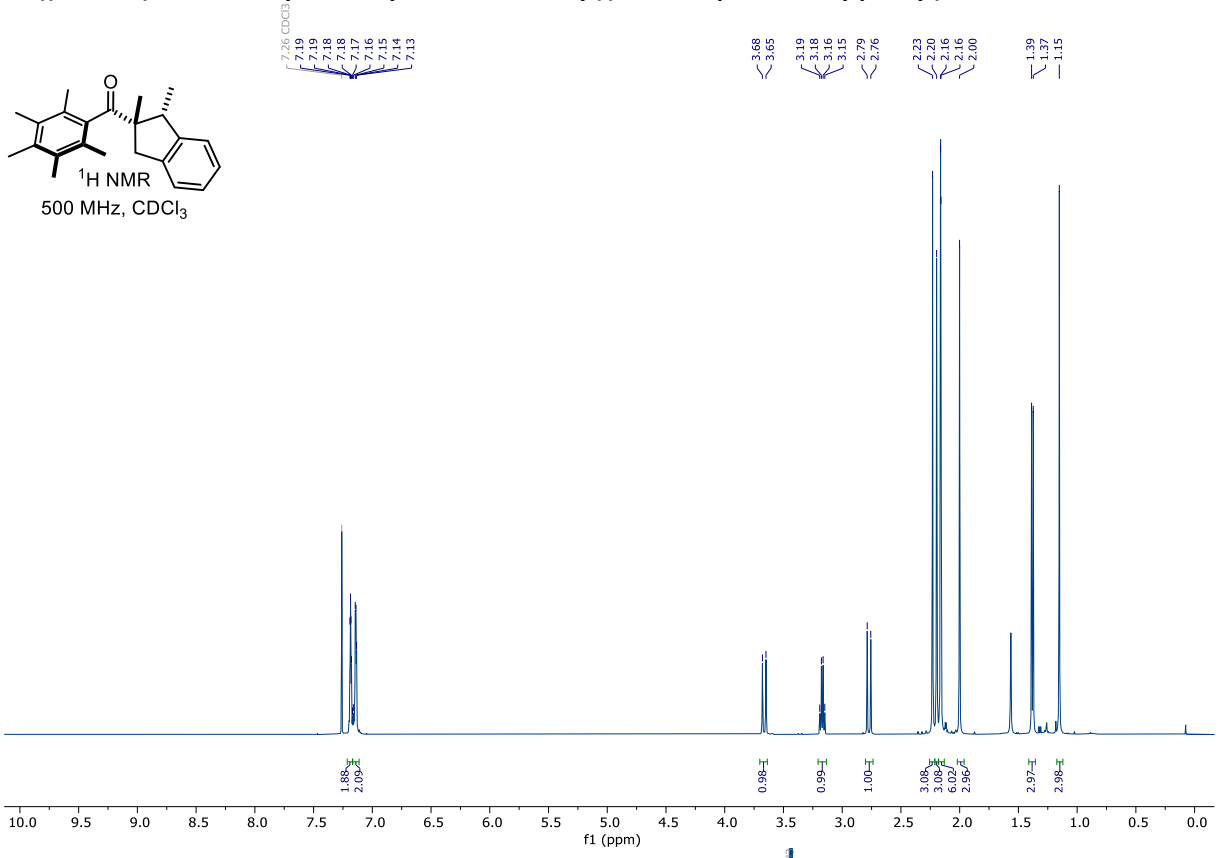
^{13}C NMR
151 MHz, $CDCl_3$

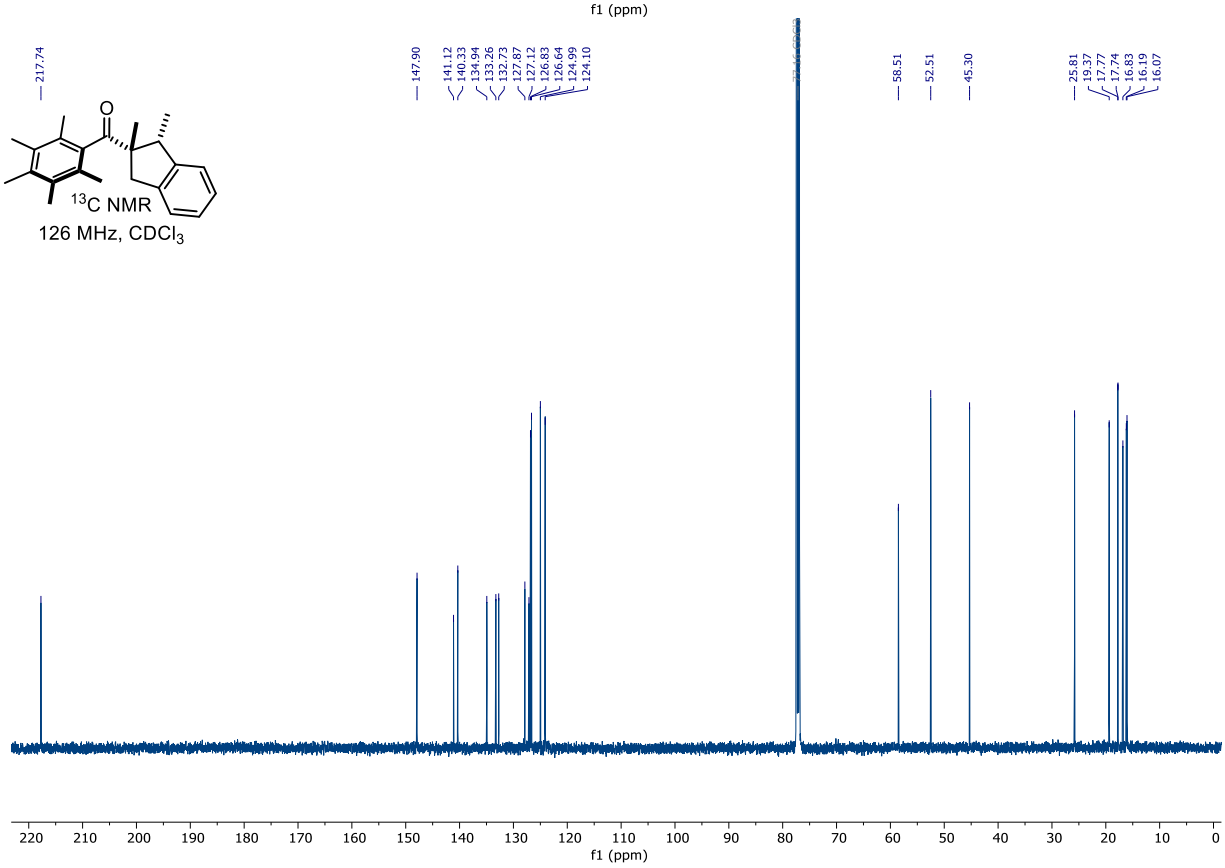
15 2-Methyl-1-(2,3,4,5,6-pentamethylphenyl)-3-(2-vinylphenyl)propan-1-one



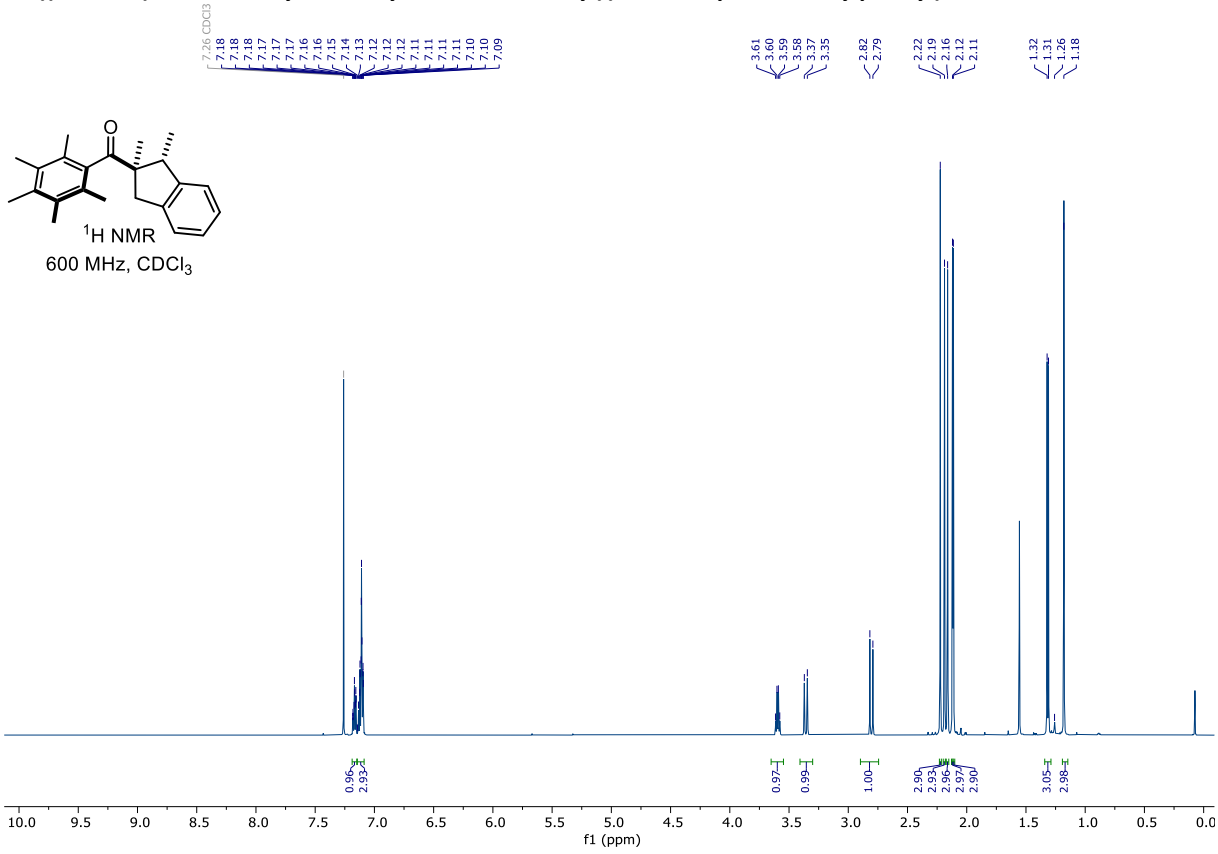


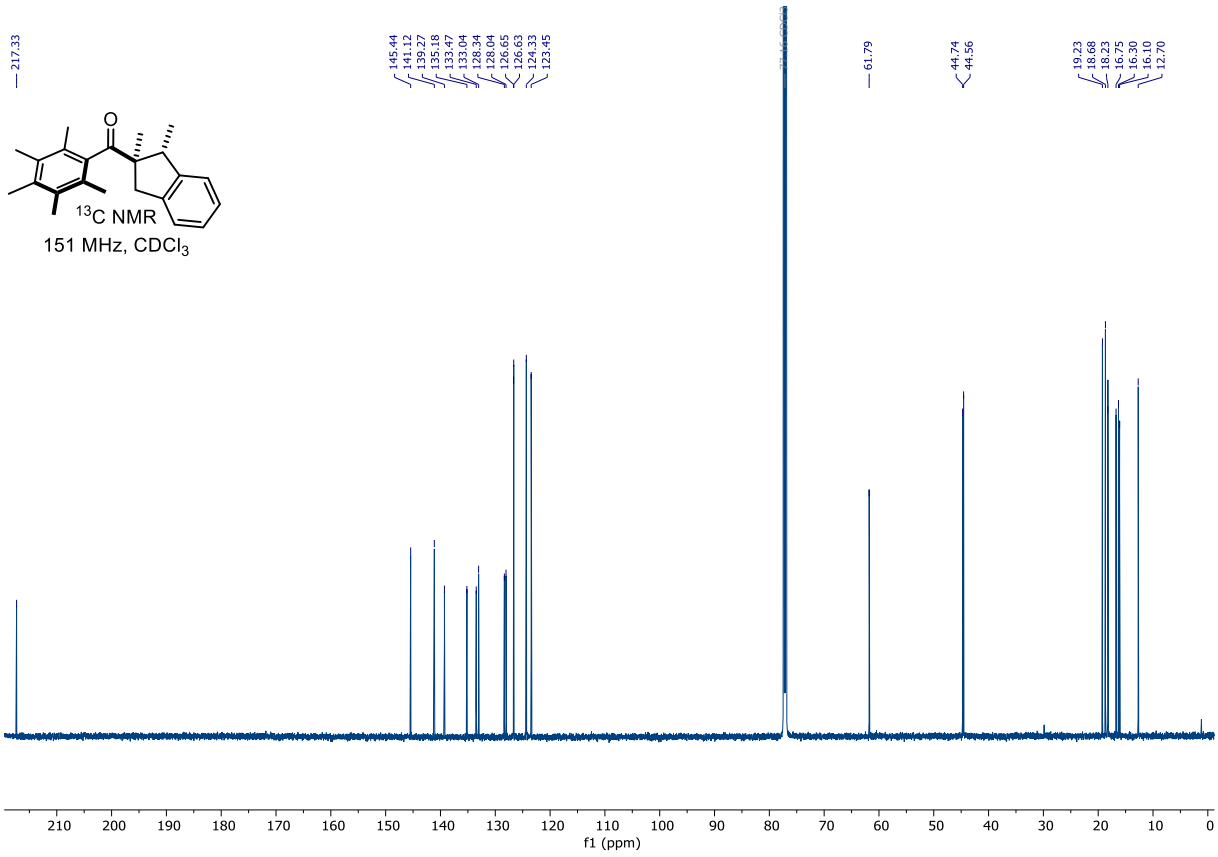
17 ((1*RS*,2*SR*)-1,2-Dimethyl-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone



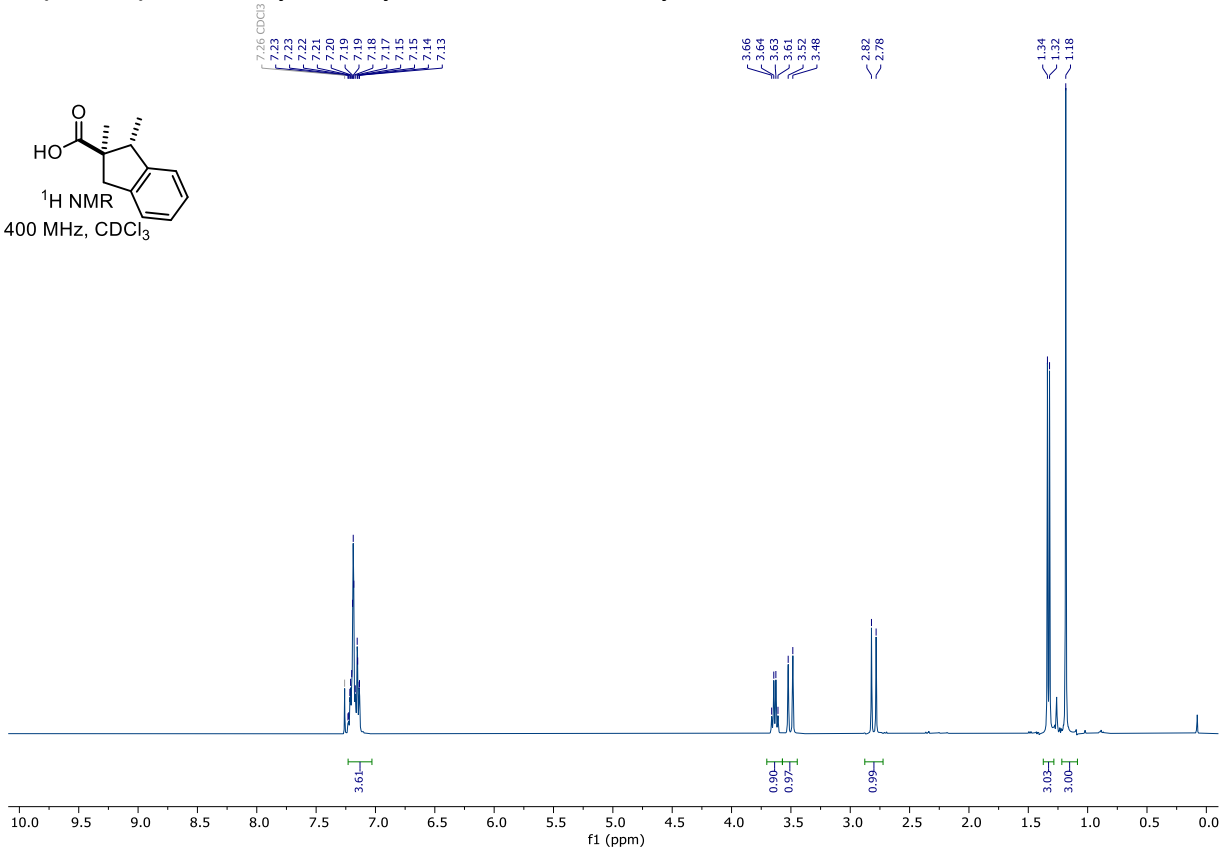


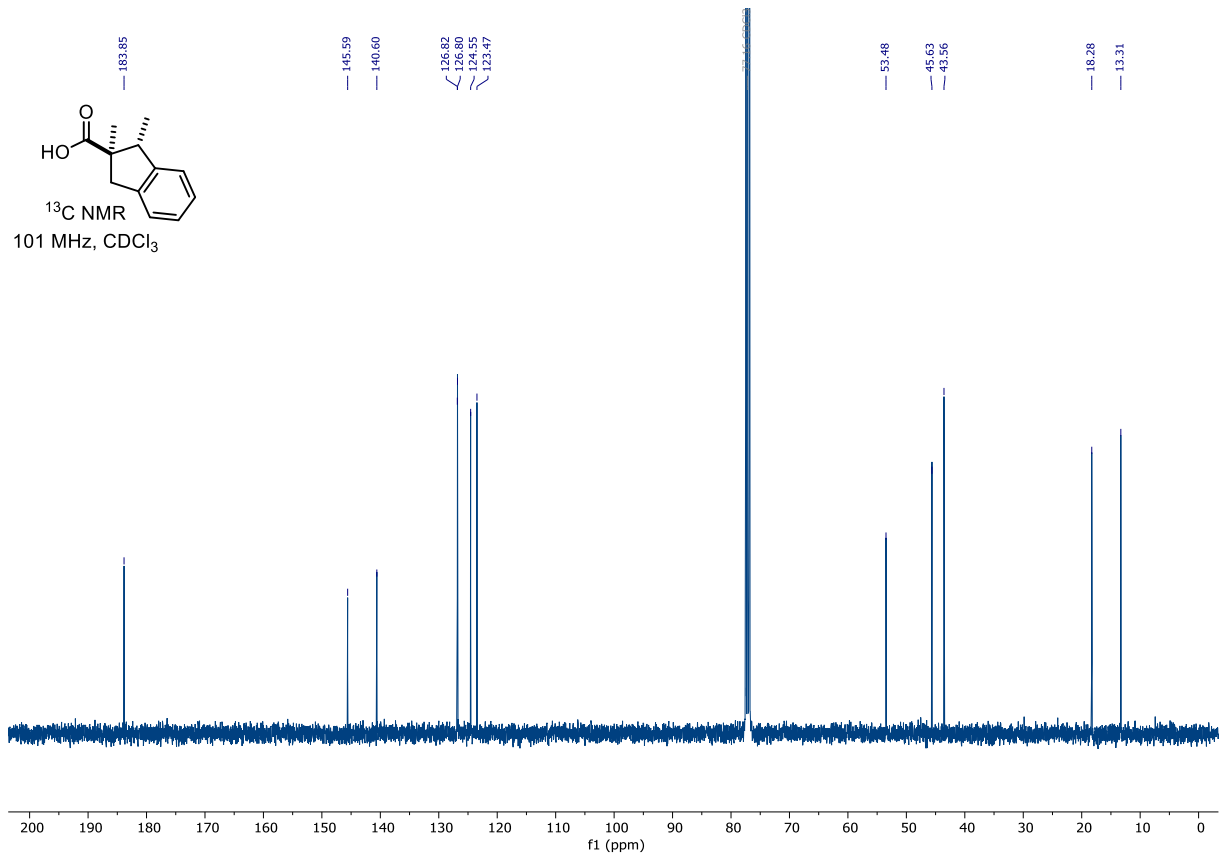
18 ((1*RS*,2*RS*)-1,2-Dimethyl-2,3-dihydro-1*H*-inden-2-yl)(2,3,4,5,6-pentamethylphenyl)methanone





19 (1*RS*,2*RS*)-1,2-dimethyl-2,3-dihydro-1*H*-indene-2-carboxylic acid





21 (1*RS*,2*SR*)-1,2-Dimethyl-*N*-(thiazol-2-yl)-2,3-dihydro-1*H*-indene-2-carboxamide

