Supporting information

Accessing Perfluoroaryl Sulfonimidamides and Sulfoximines via Photogenerated Perfluoroaryl Nitrenes: Synthesis and Application as a Chiral Auxiliary

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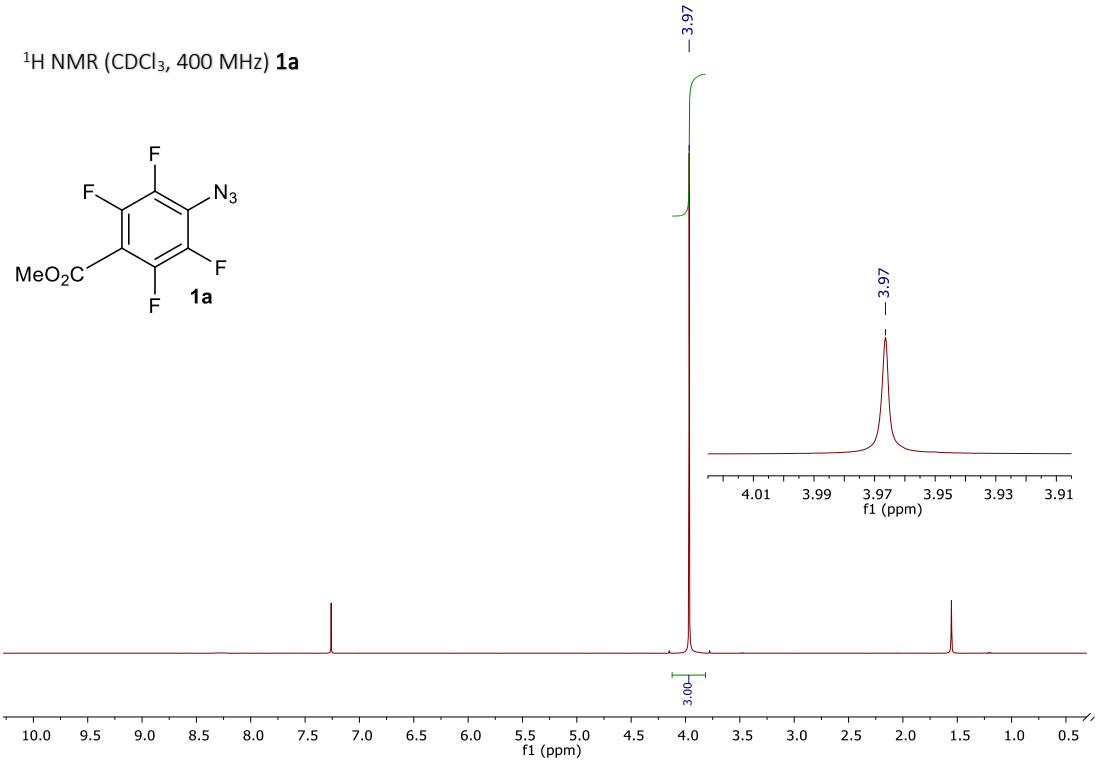
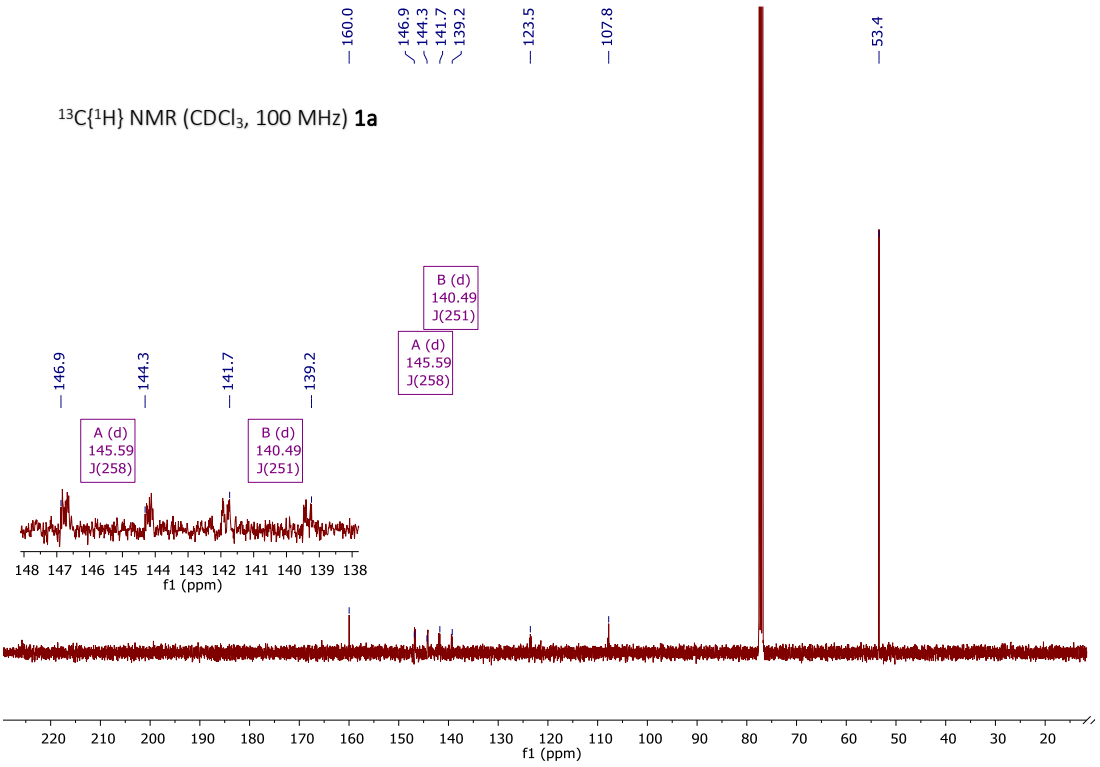
NMR Spectra synthesized starting material

Compound **1a**

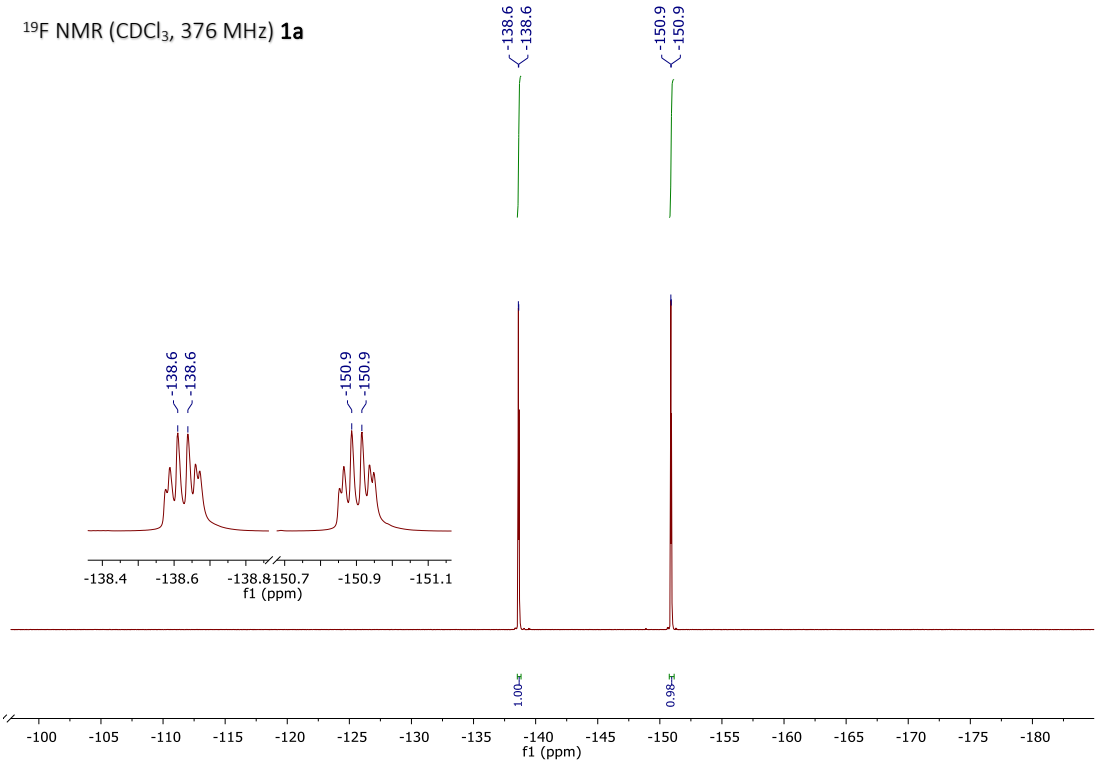
^{1}H NMR ($CDCl_3$, 400 MHz) **1a**



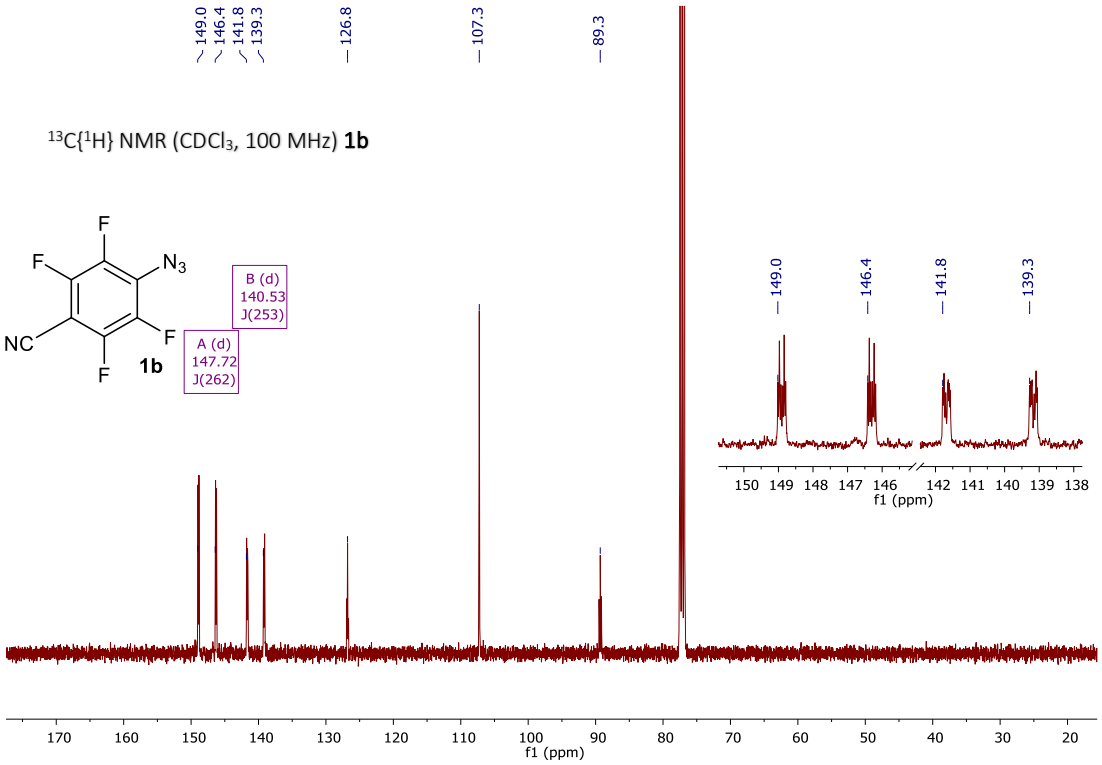
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) **1a**



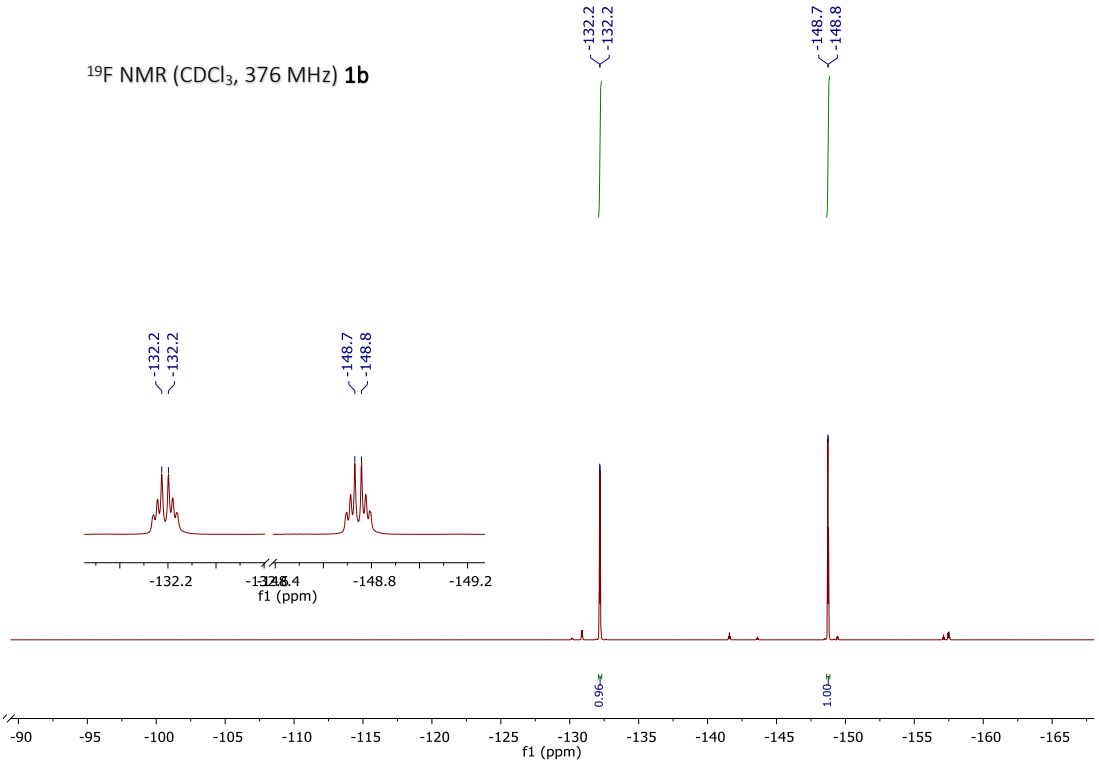
^{19}F NMR ($CDCl_3$, 376 MHz) **1a**



Compound **1b**

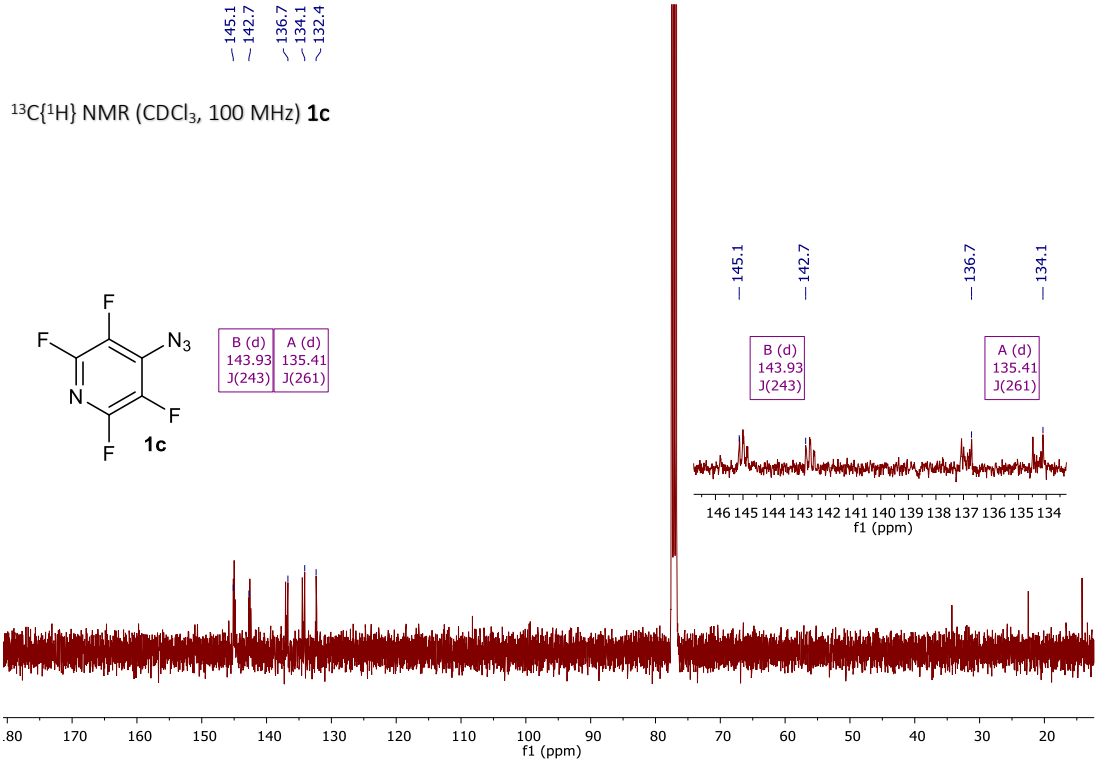


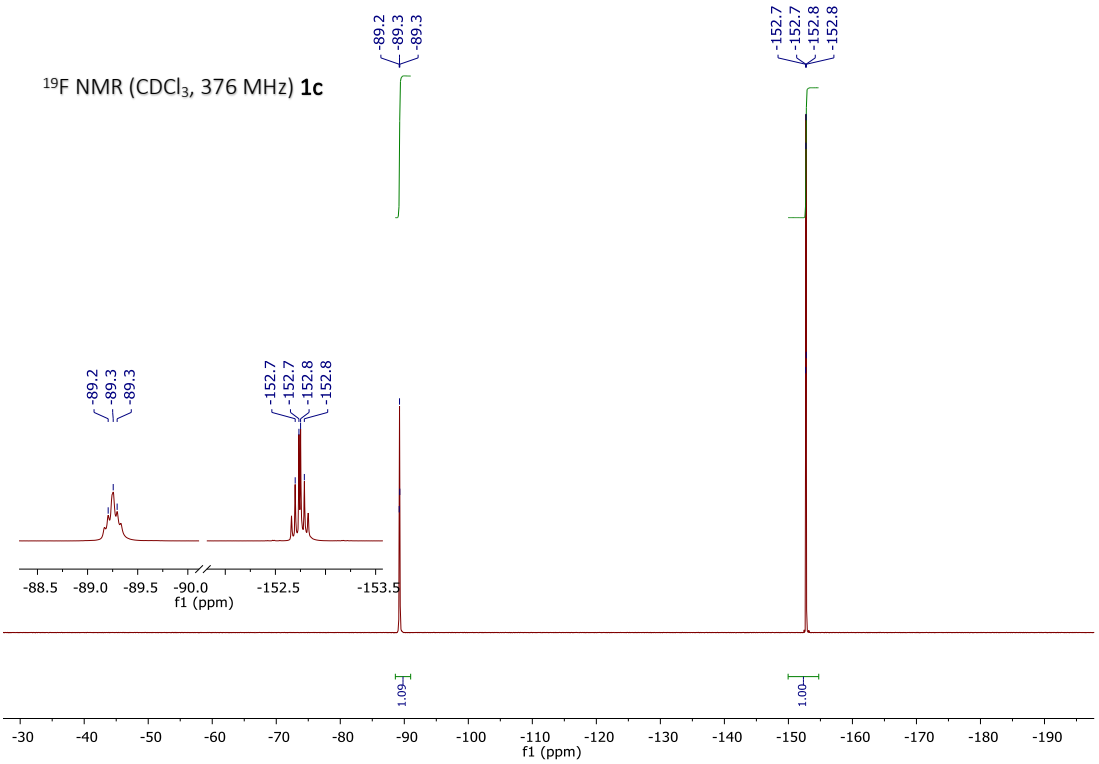
^{19}F NMR ($CDCl_3$, 376 MHz) **1b**



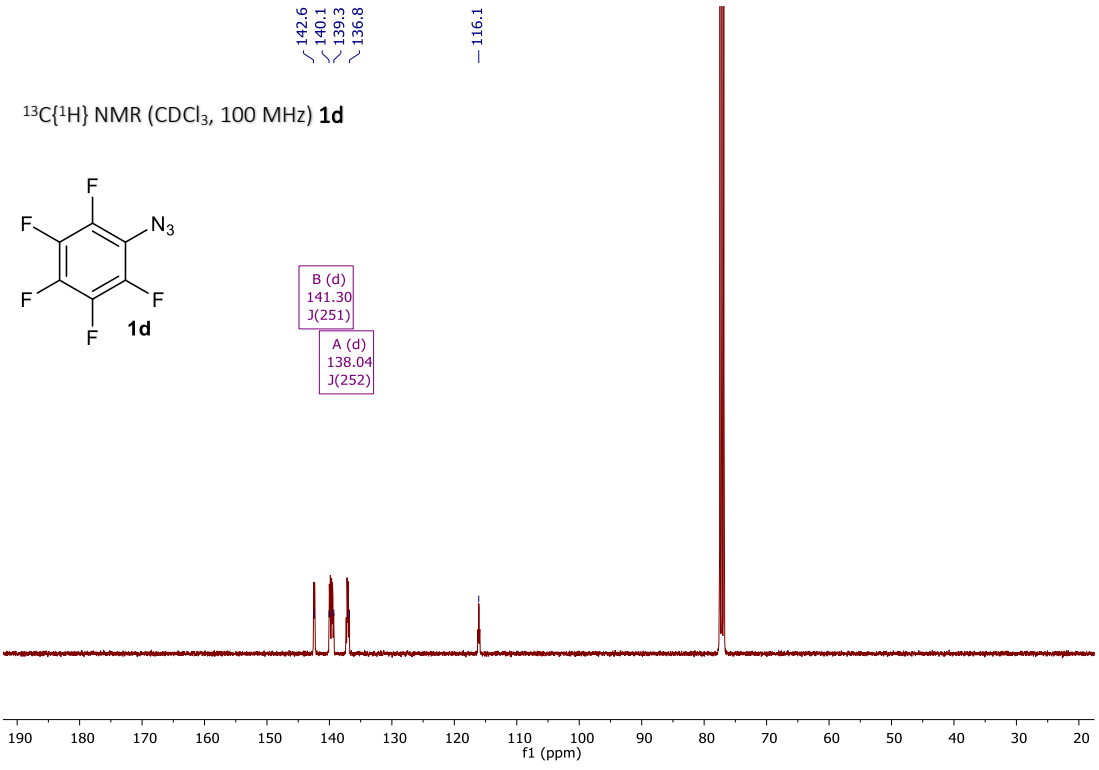
Compound **1c**

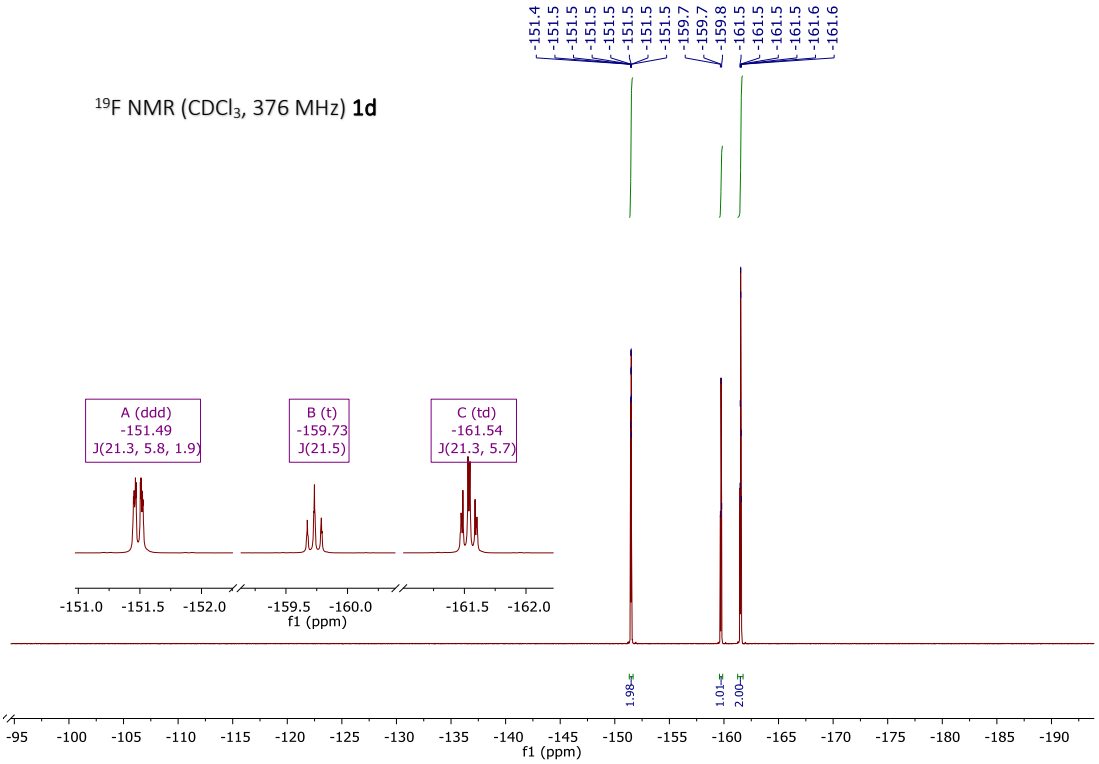
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) **1c**



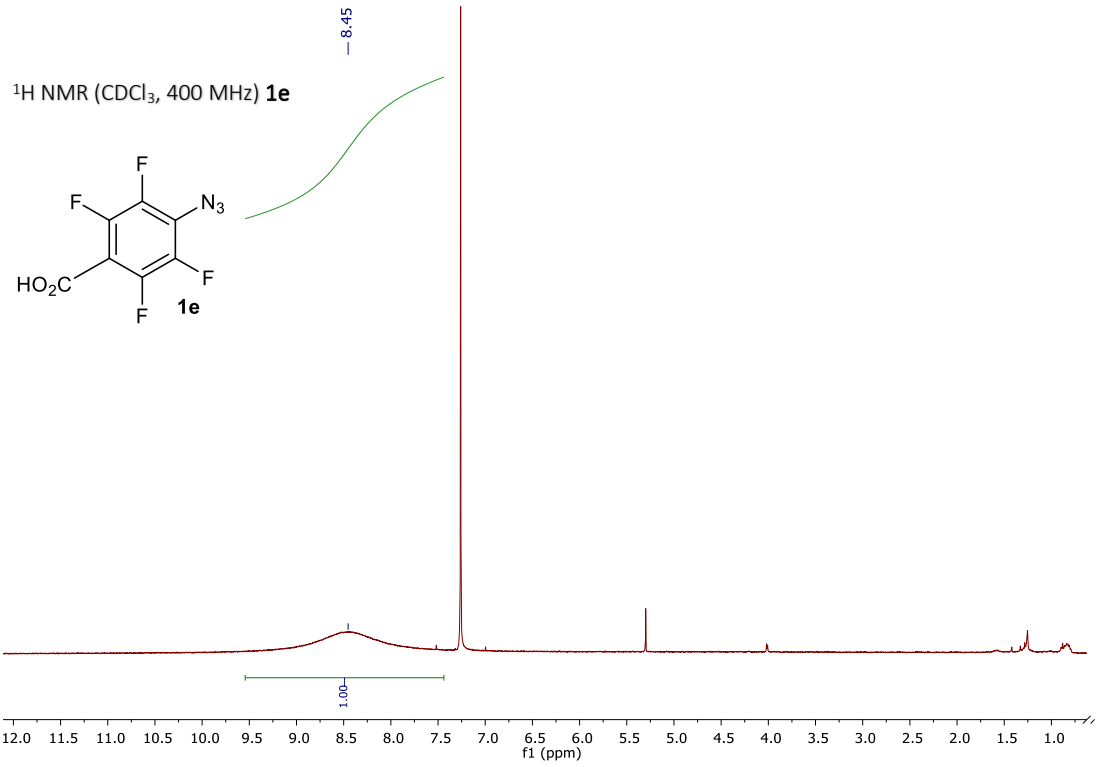

^{19}F NMR ($CDCl_3$, 376 MHz) **1c**
-89.2
-89.3
-89.3
-152.7
-152.7
-152.8
-152.8
1.09
1.00
f1 (ppm)

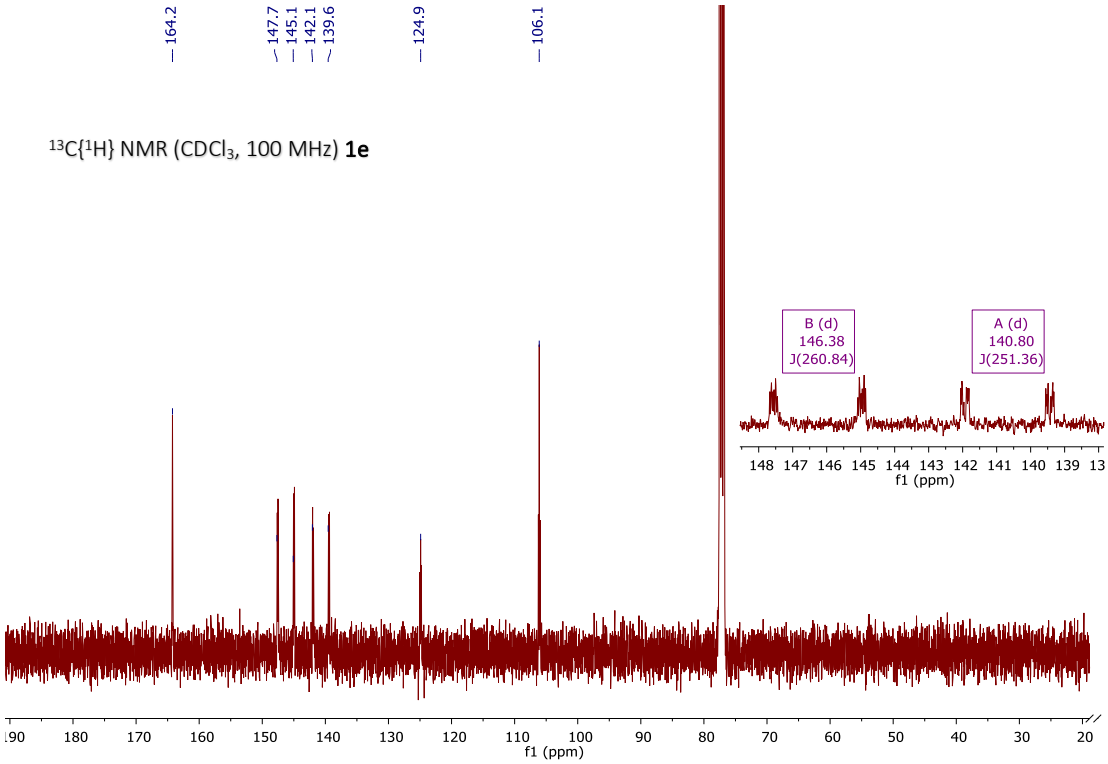
Compound **1d**


^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) **1d**
142.6
140.1
139.3
136.8
116.1
B (d)
141.30
J(251)
A (d)
138.04
J(252)
F
F
N_3
F
F
1d
f1 (ppm)

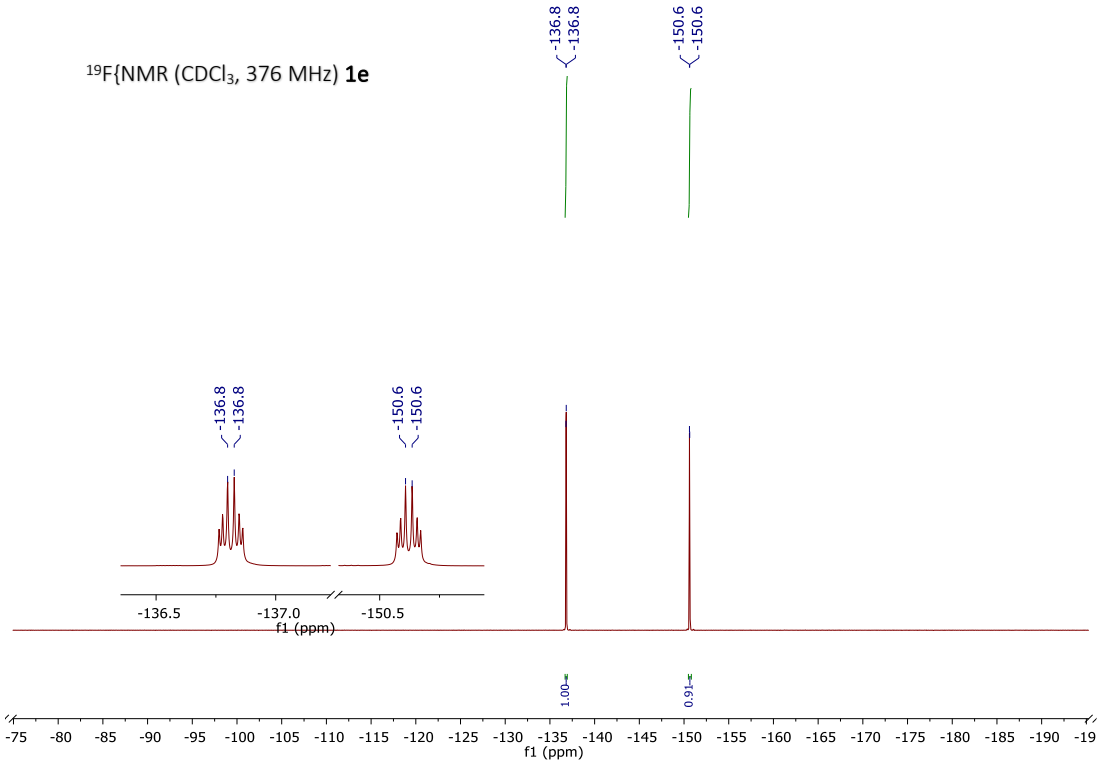

19F NMR (CDCl3, 376 MHz) 1d
-151.4
-151.5
-151.5
-151.5
-151.5
-151.5
-151.5
-151.5
-159.7
-159.7
-159.8
-161.5
-161.5
-161.5
-161.5
-161.6
-161.6
A (ddd)
-151.49
J(21.3, 5.8, 1.9)
B (t)
-159.73
J(21.5)
C (td)
-161.54
J(21.3, 5.7)
-151.0 -151.5 -152.0 -159.5 -160.0 -161.5 -162.0
f1 (ppm)
1.98
1.01
2.00
-95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180 -185 -190
f1 (ppm)

Compound **1e**


1H NMR (CDCl3, 400 MHz) 1e
8.45
F
F
N3
HO2C
F
F
1e
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) **1e**

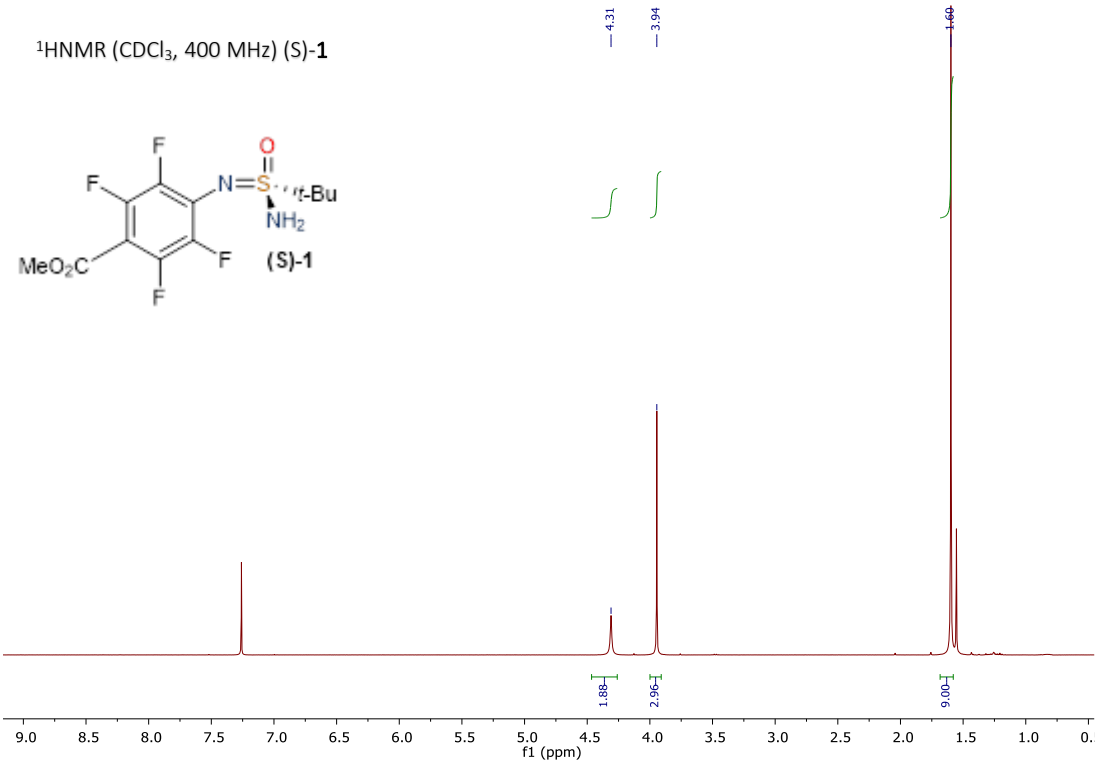


$^{19}F\{NMR$ ($CDCl_3$, 376 MHz) **1e**

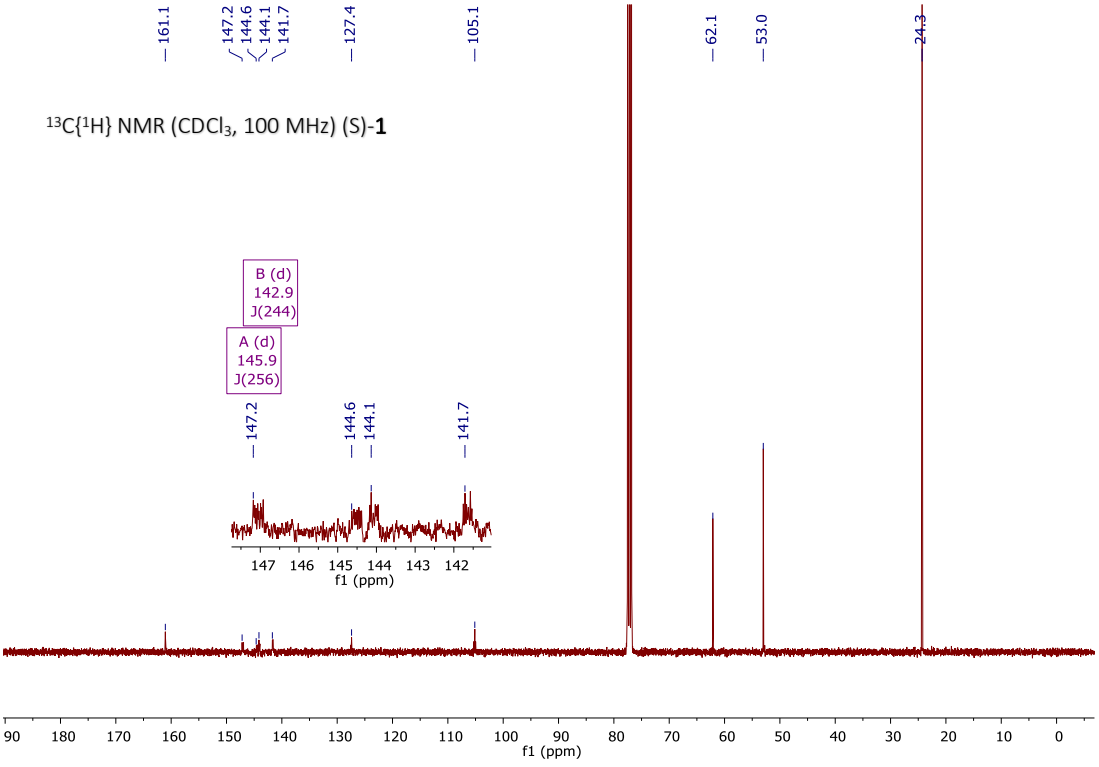
1. NMR Spectra isolated products

Compound (*S*)-**1**

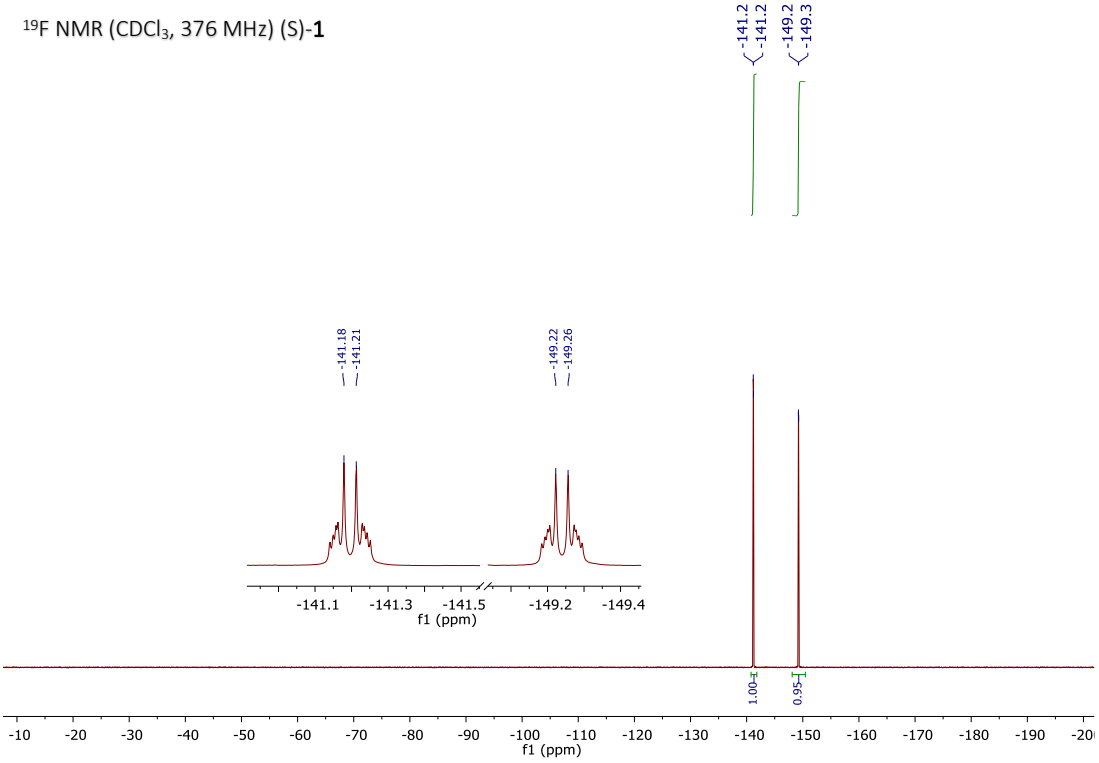
^{1}HNMR ($CDCl_3$, 400 MHz) (S)-**1**



^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) (S)-**1**



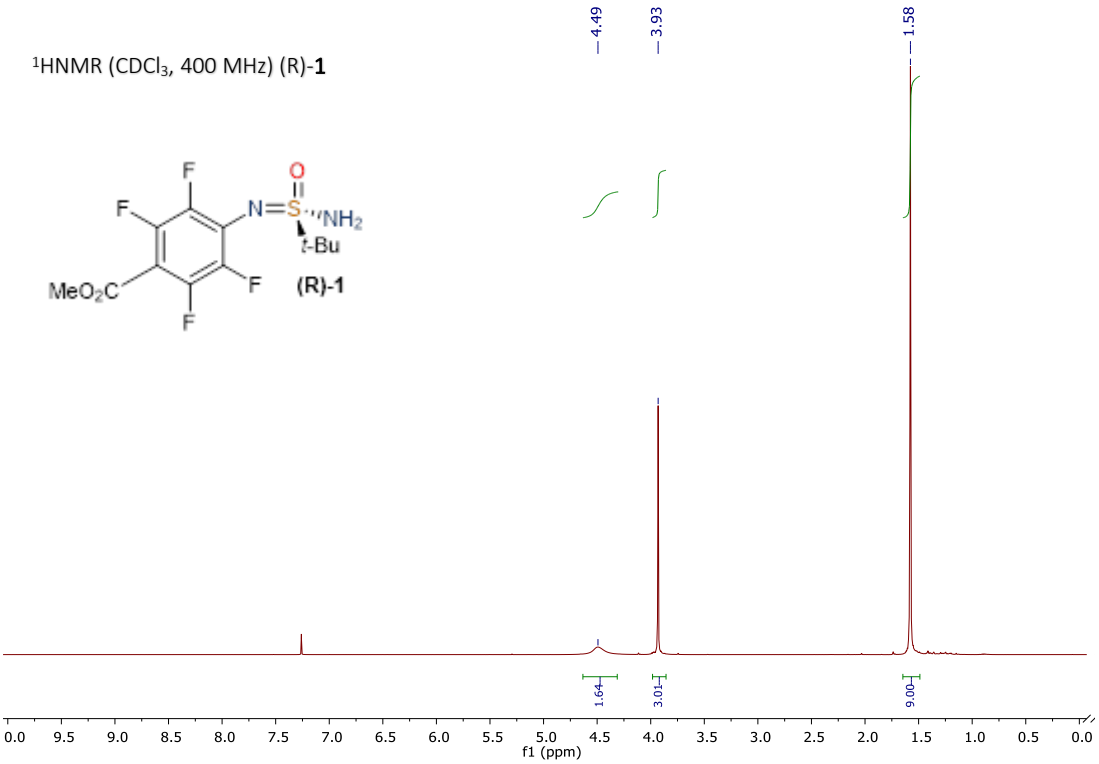
^{19}F NMR ($CDCl_3$, 376 MHz) (S)-**1**

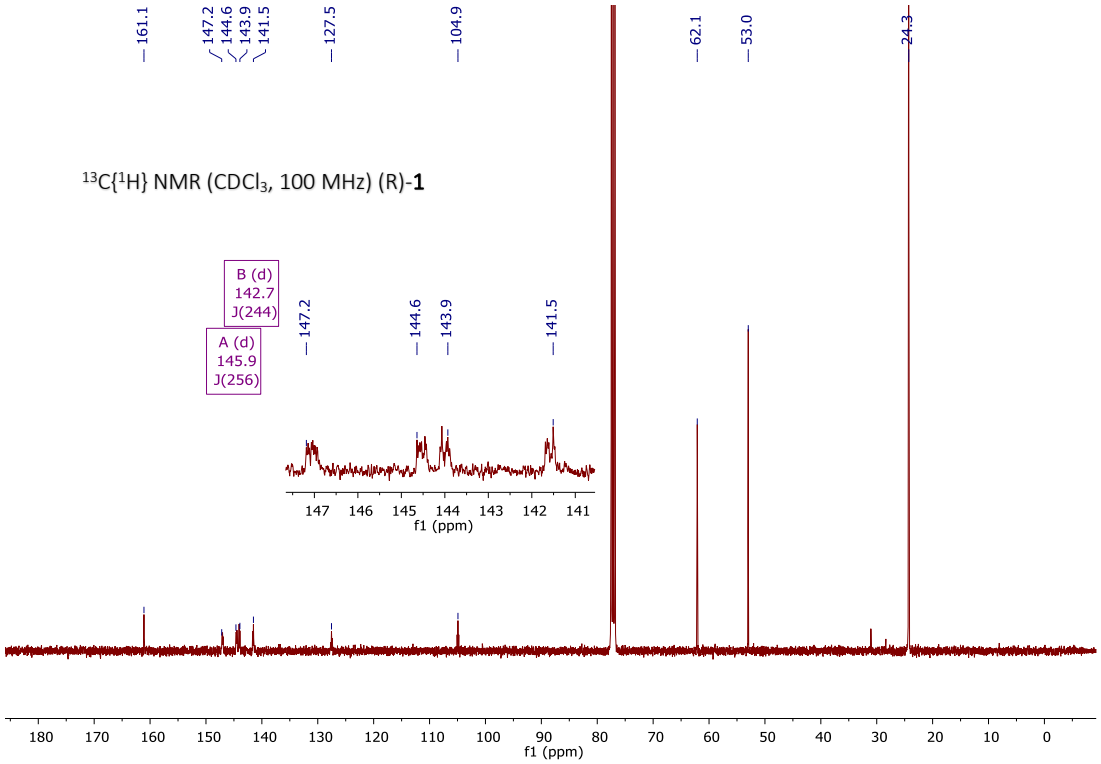


Compound (*R*)-**1**

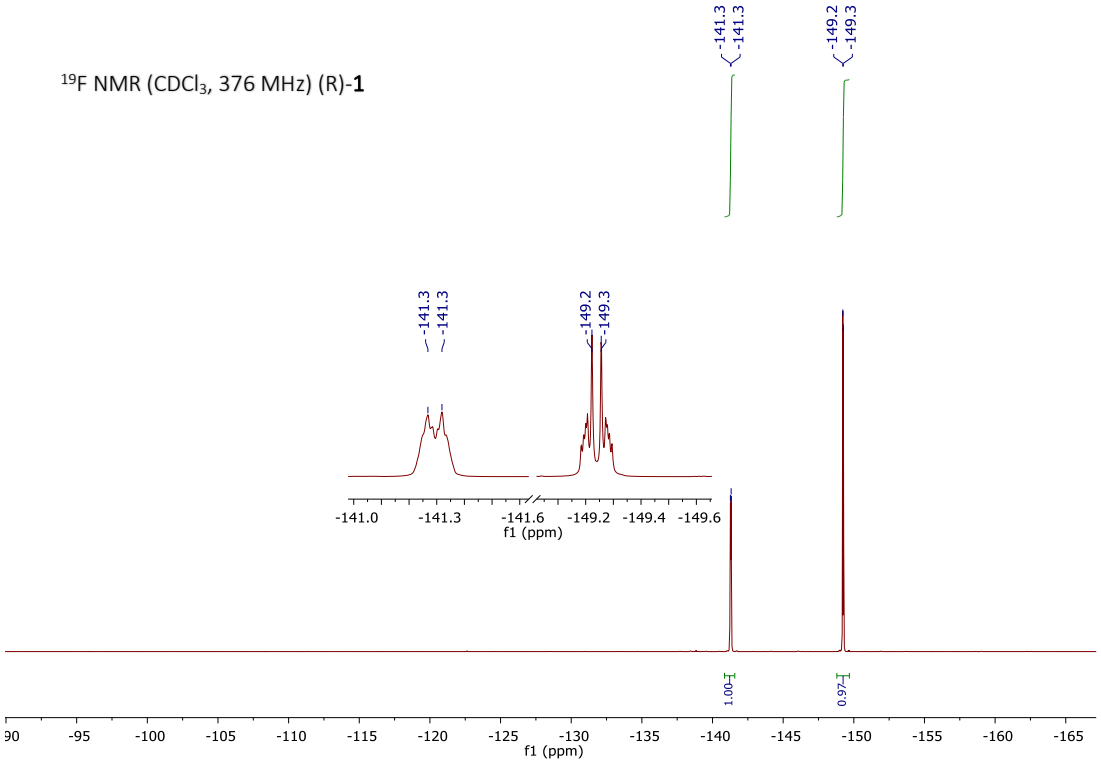
^{1}HNMR ($CDCl_3$, 400 MHz) (R)-**1**

(R)-1





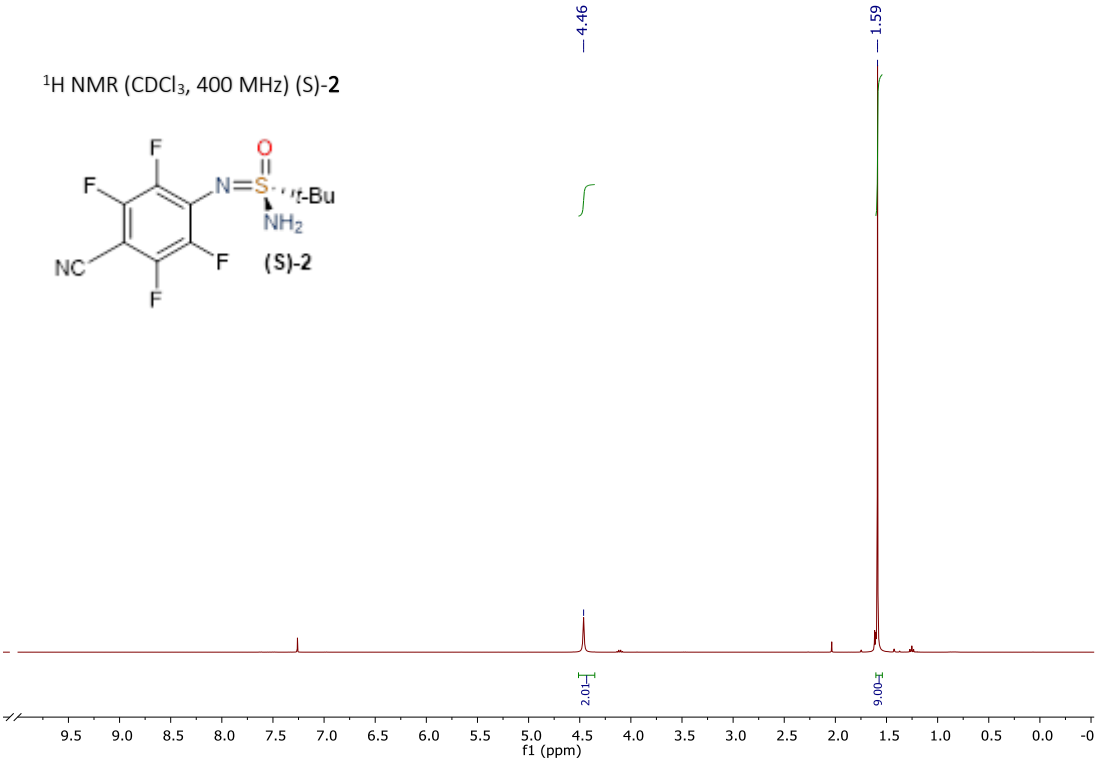
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz) (R)-**1**



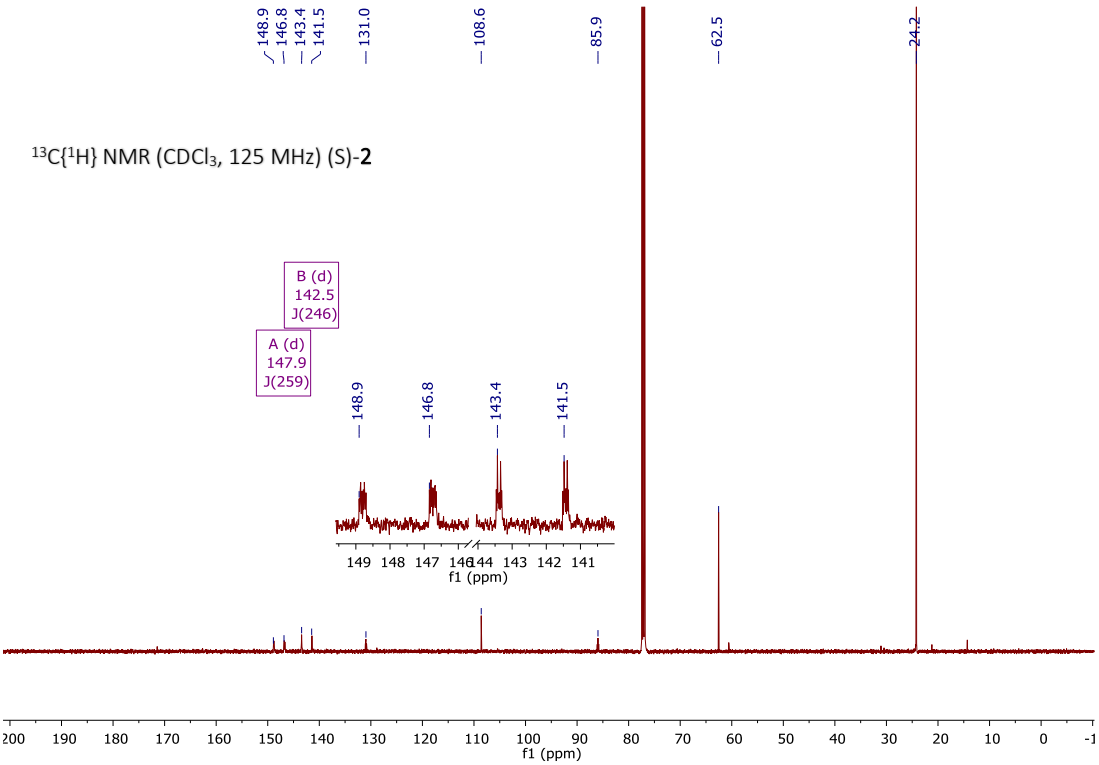
^{19}F NMR ($CDCl_3$, 376 MHz) (R)-**1**

Compound (*S*)-**2**

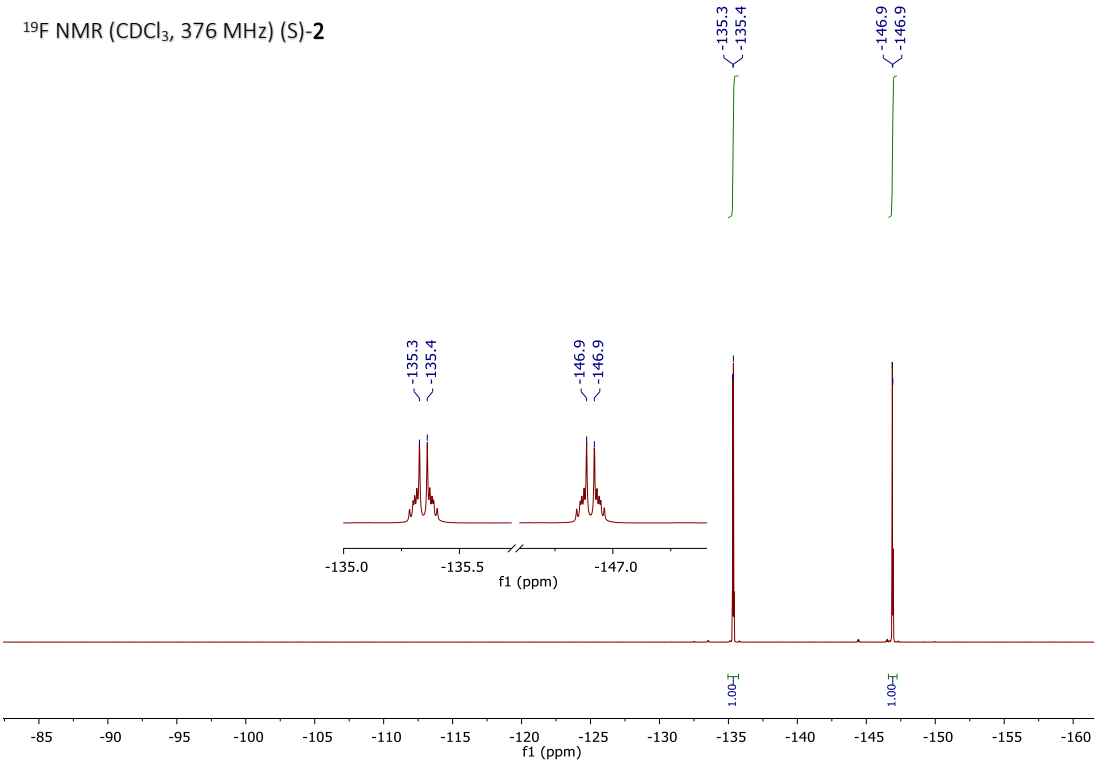
^{1}H NMR ($CDCl_3$, 400 MHz) (S)-**2**



^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz) (S)-**2**

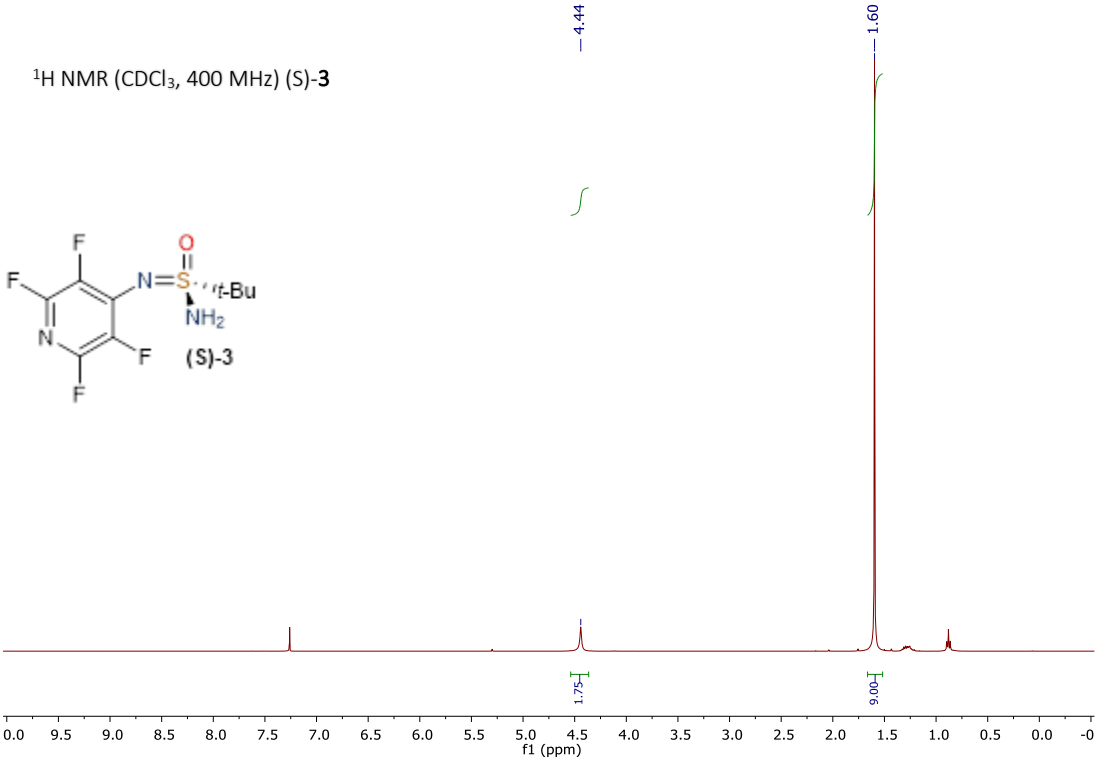


^{19}F NMR ($CDCl_3$, 376 MHz) (S)-**2**

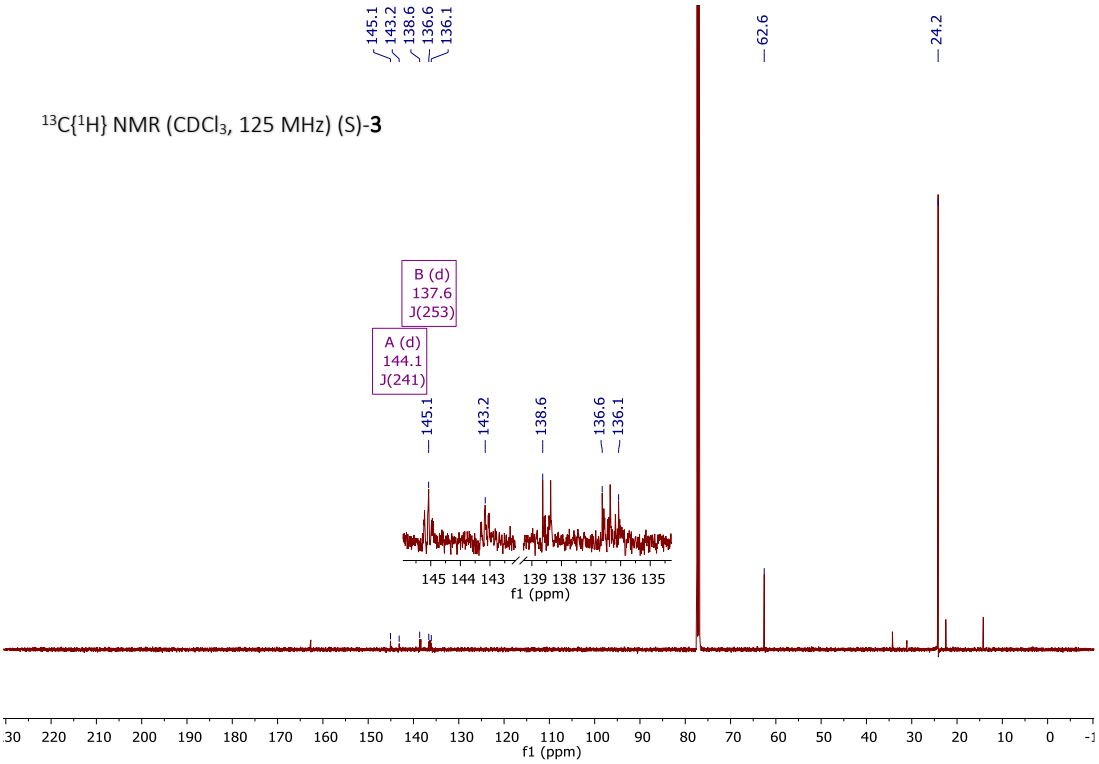


Compound (*S*)-**3**

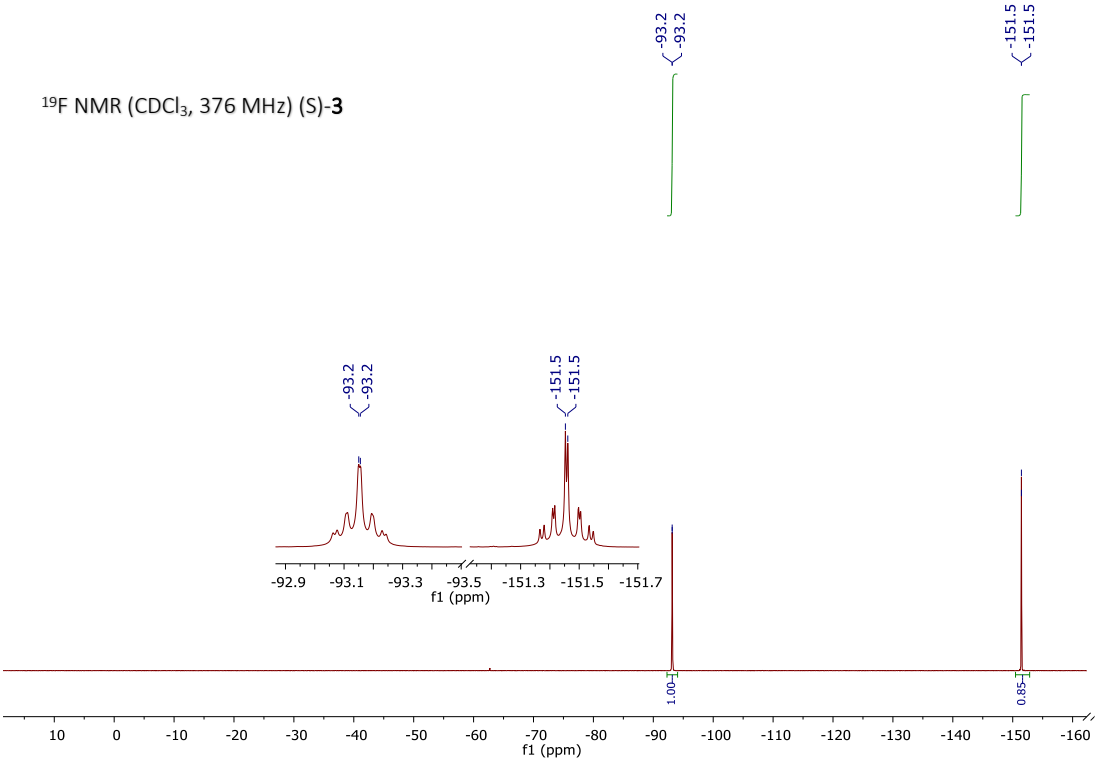
^{1}H NMR ($CDCl_3$, 400 MHz) (S)-**3**



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) (S)-**3**

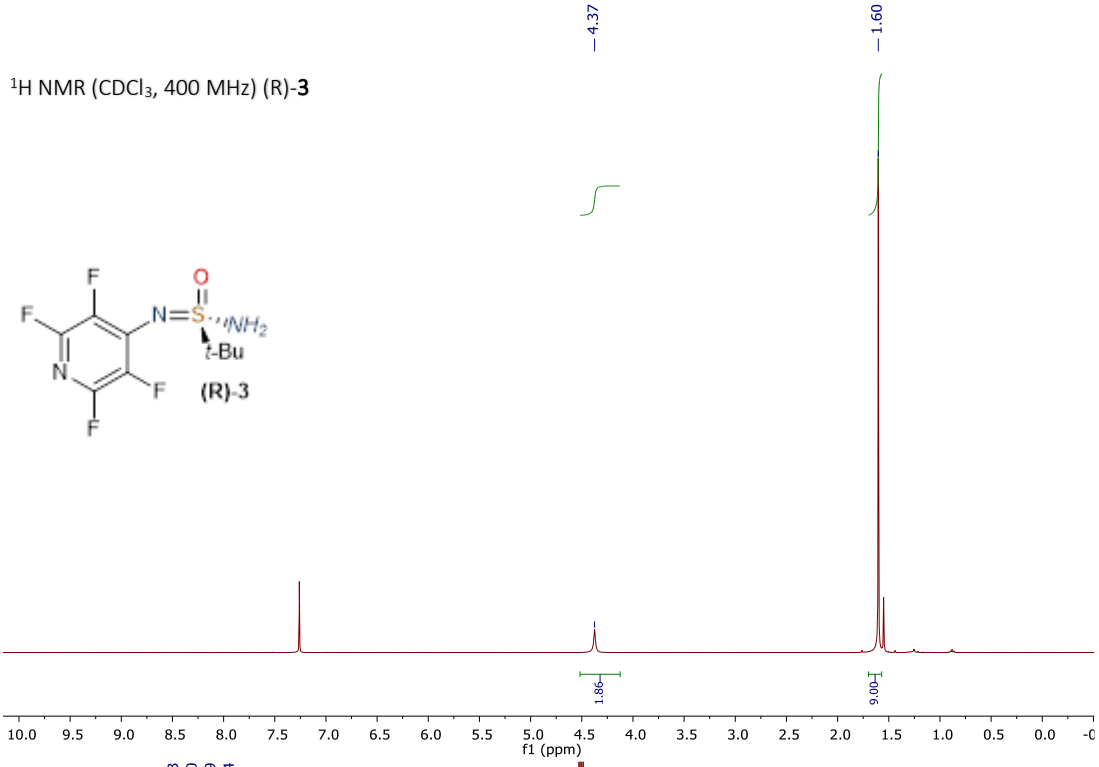


^{19}F NMR ($CDCl_3$, 376 MHz) (S)-**3**

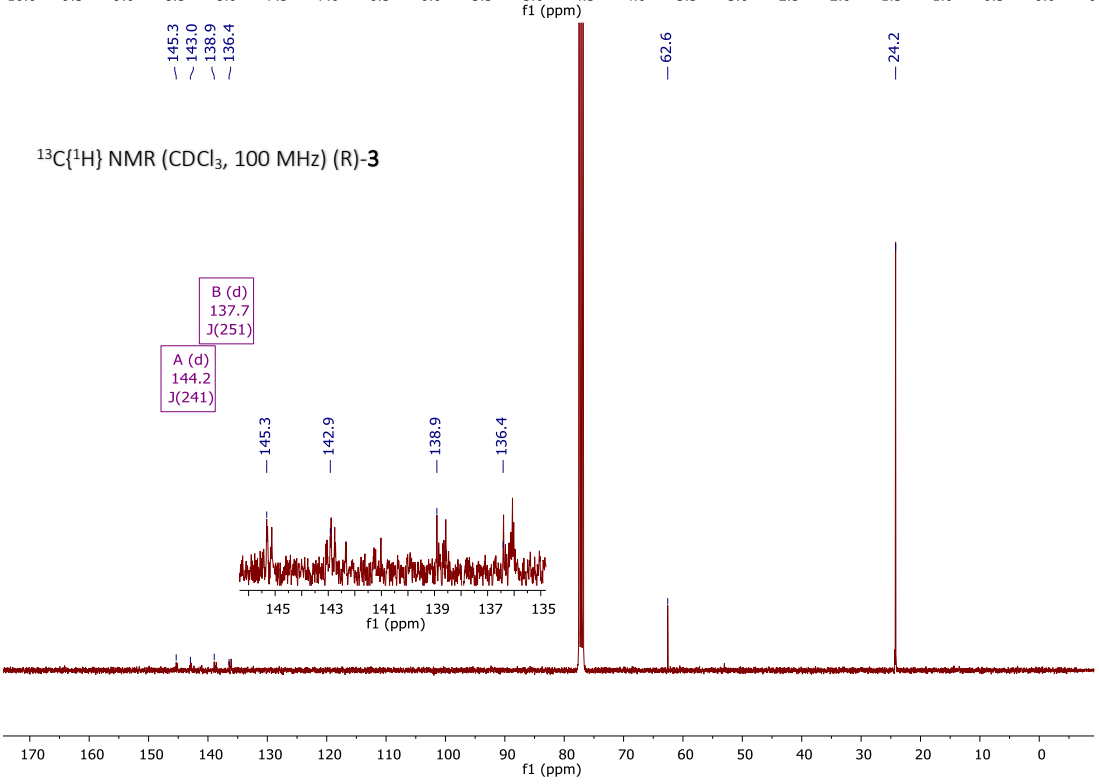


Compound (*R*)-***3***

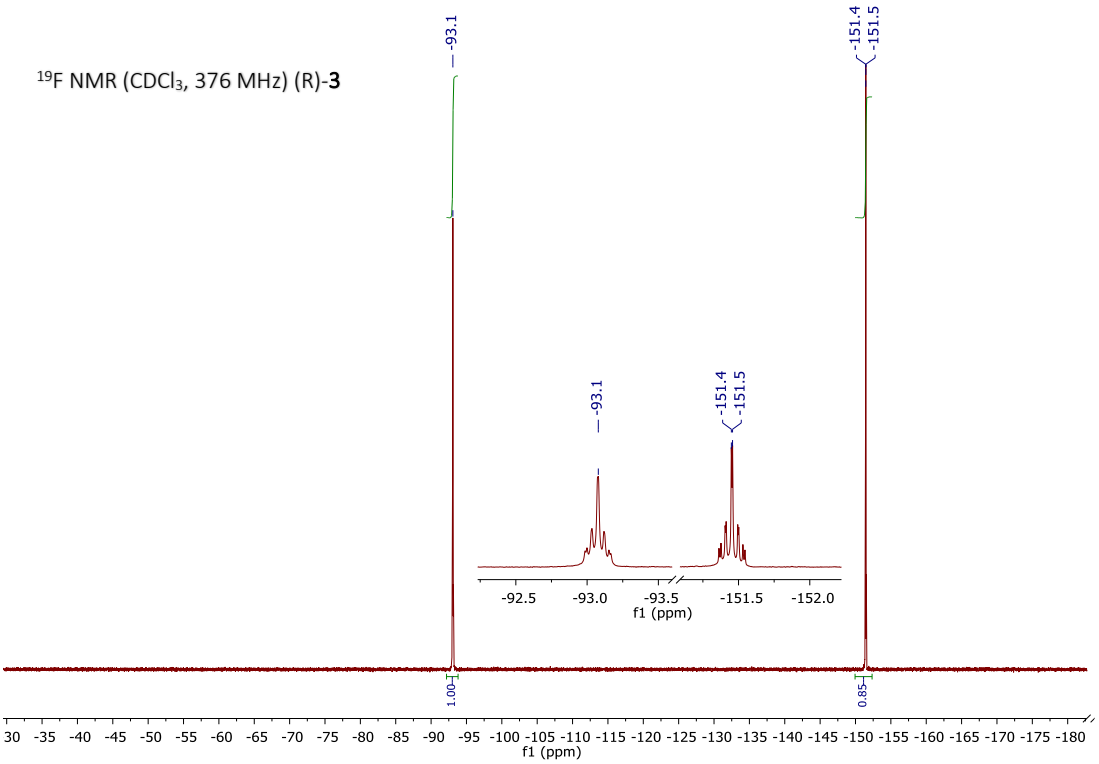
^{1}H NMR ($CDCl_3$, 400 MHz) (R)-**3**



^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) (R)-**3**



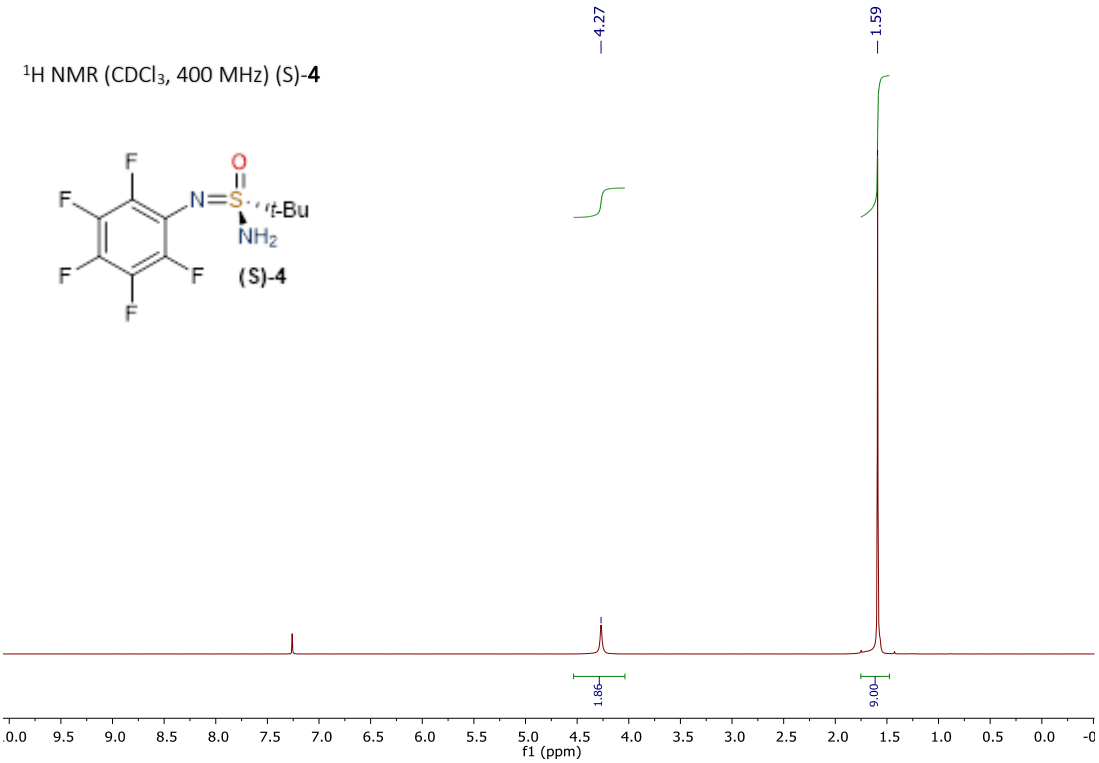
^{19}F NMR ($CDCl_3$, 376 MHz) (R)-**3**



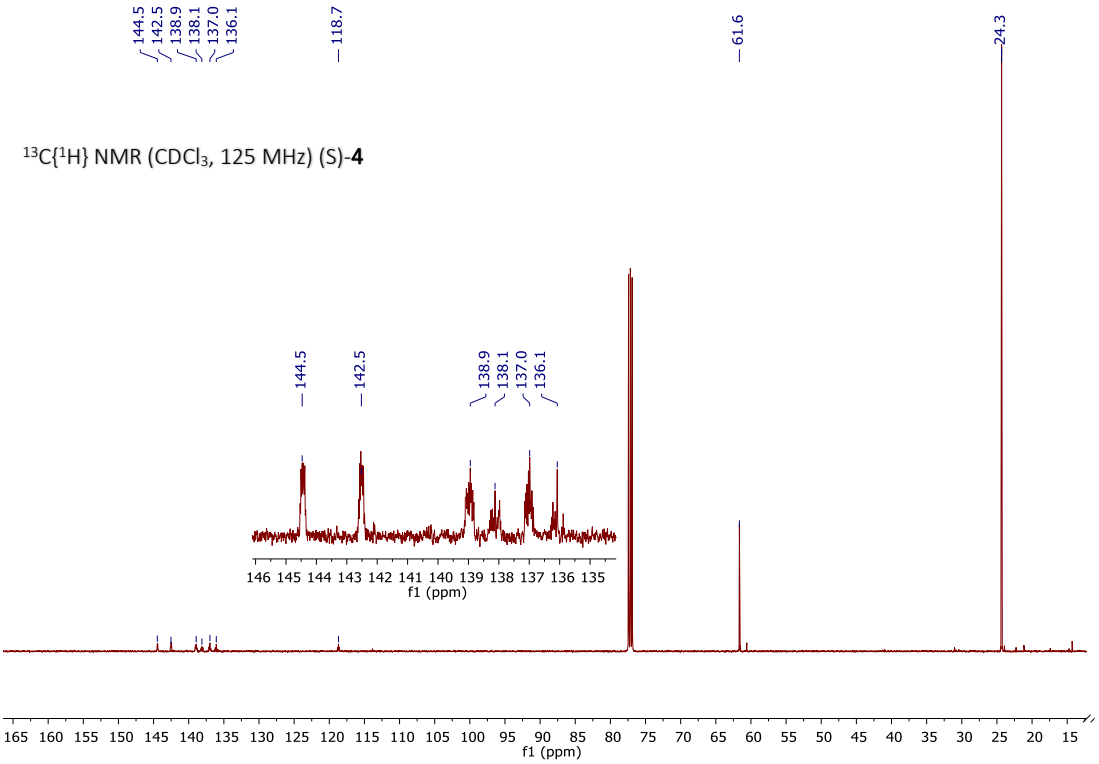
Compound (*S*)-**4**

^{1}H NMR ($CDCl_3$, 400 MHz) (S)-**4**

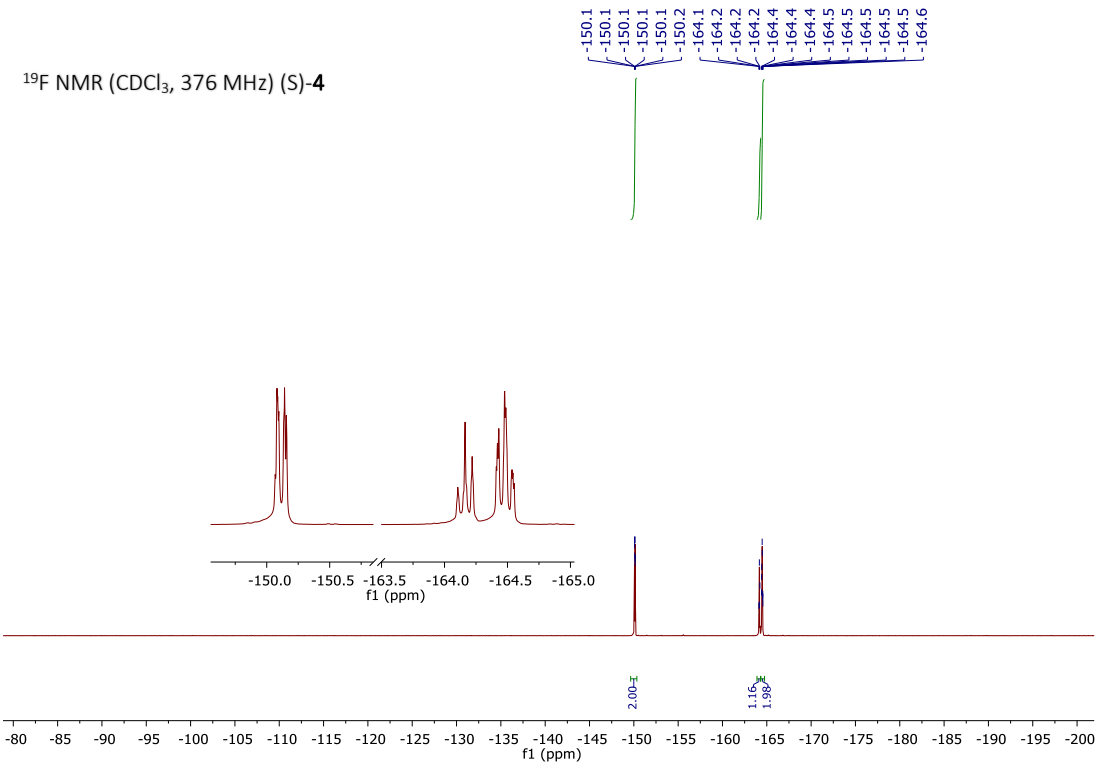
(S)-4



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) (S)-**4**



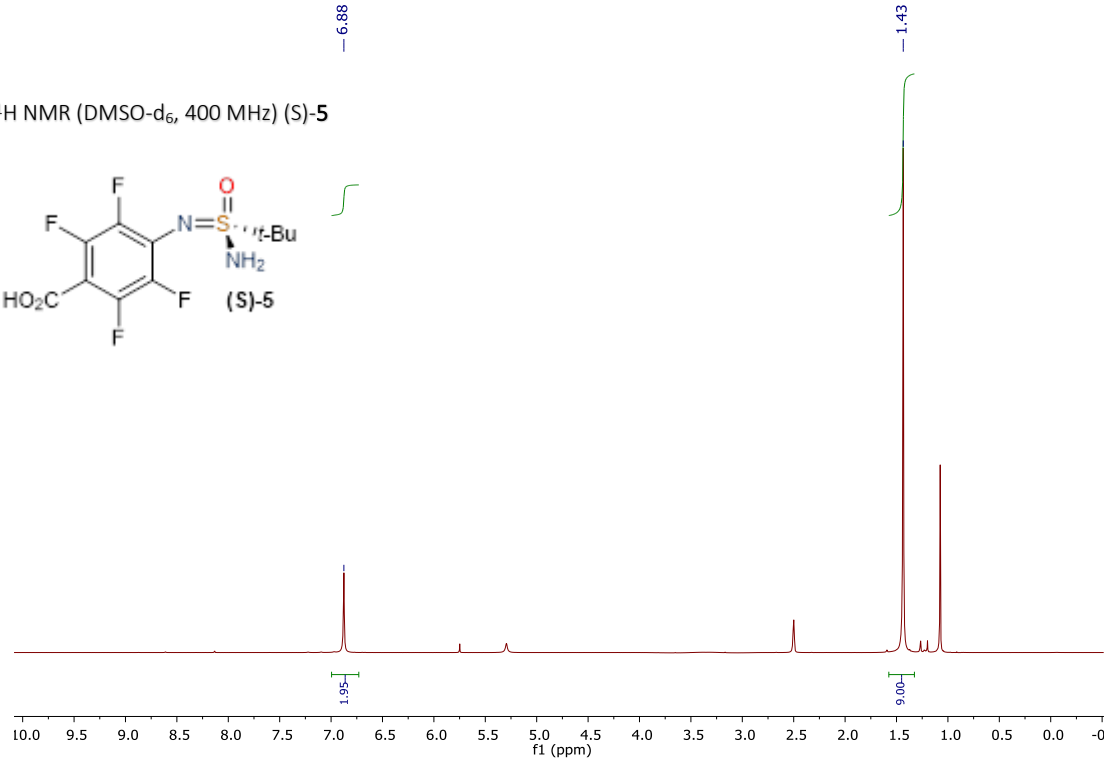
^{19}F NMR ($CDCl_3$, 376 MHz) (S)-**4**



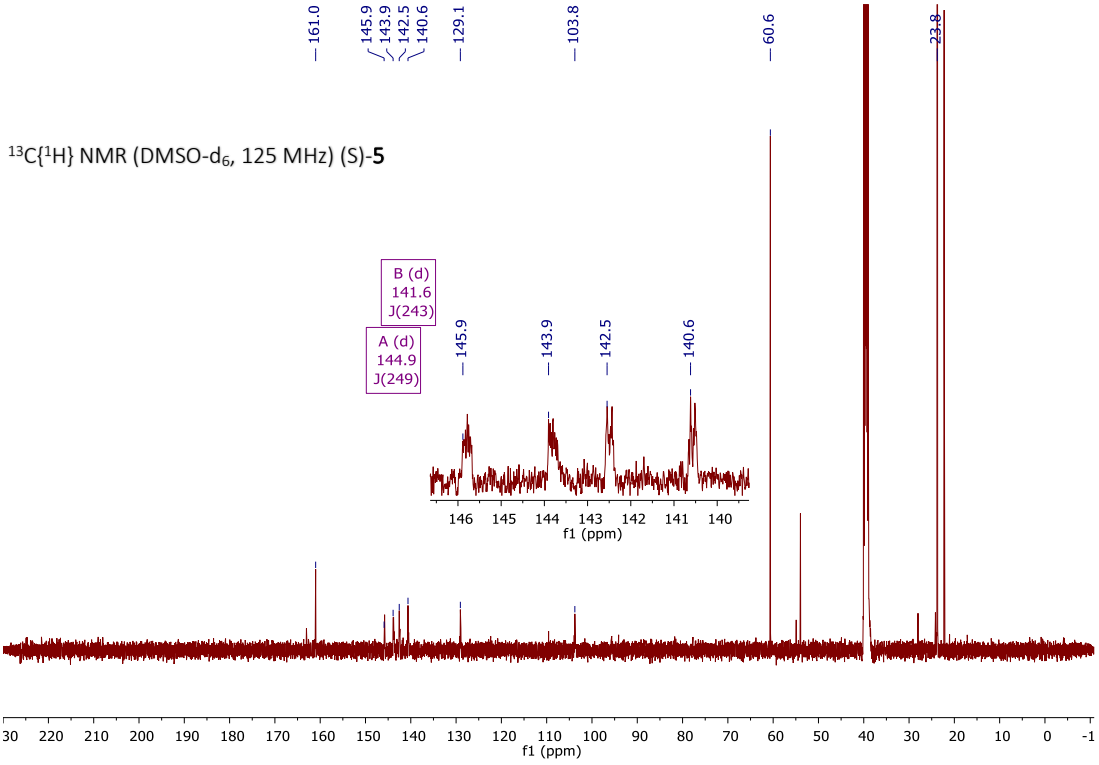
Compound (*S*)-**5**

^{1}H NMR (DMSO-d$_6$, 400 MHz) (S)-**5**

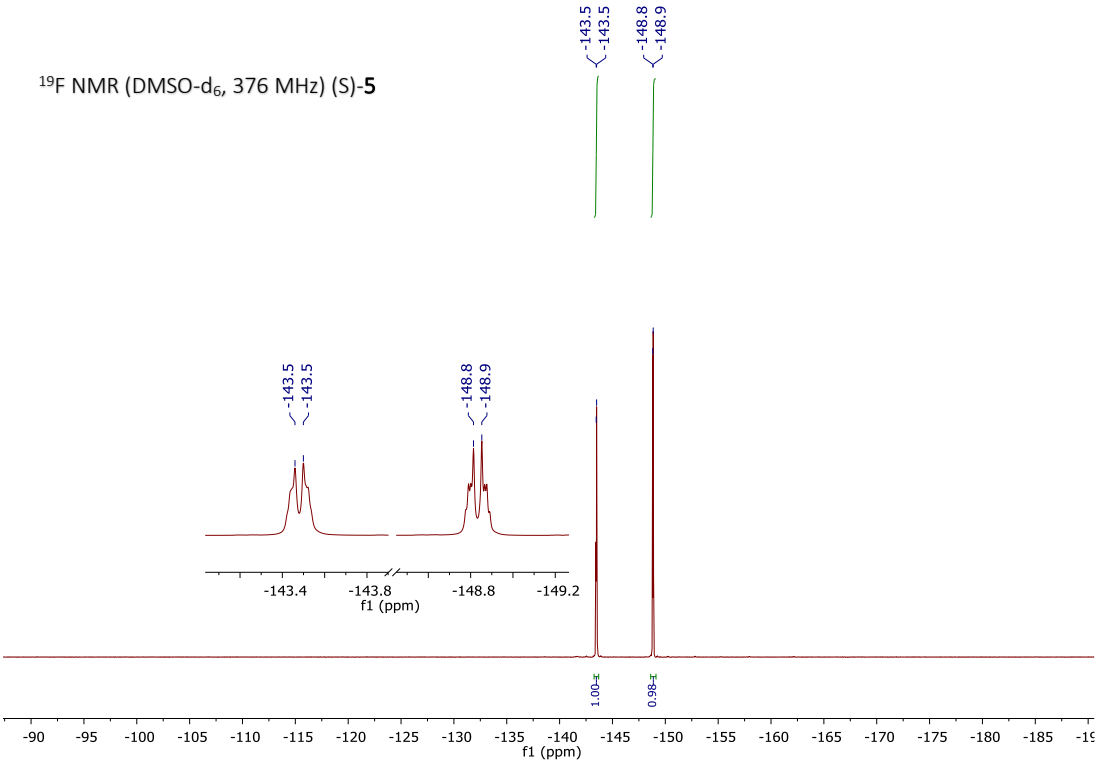
(S)-5



^{13}C{^{1}H} NMR (DMSO-d$_6$, 125 MHz) (S)-**5**



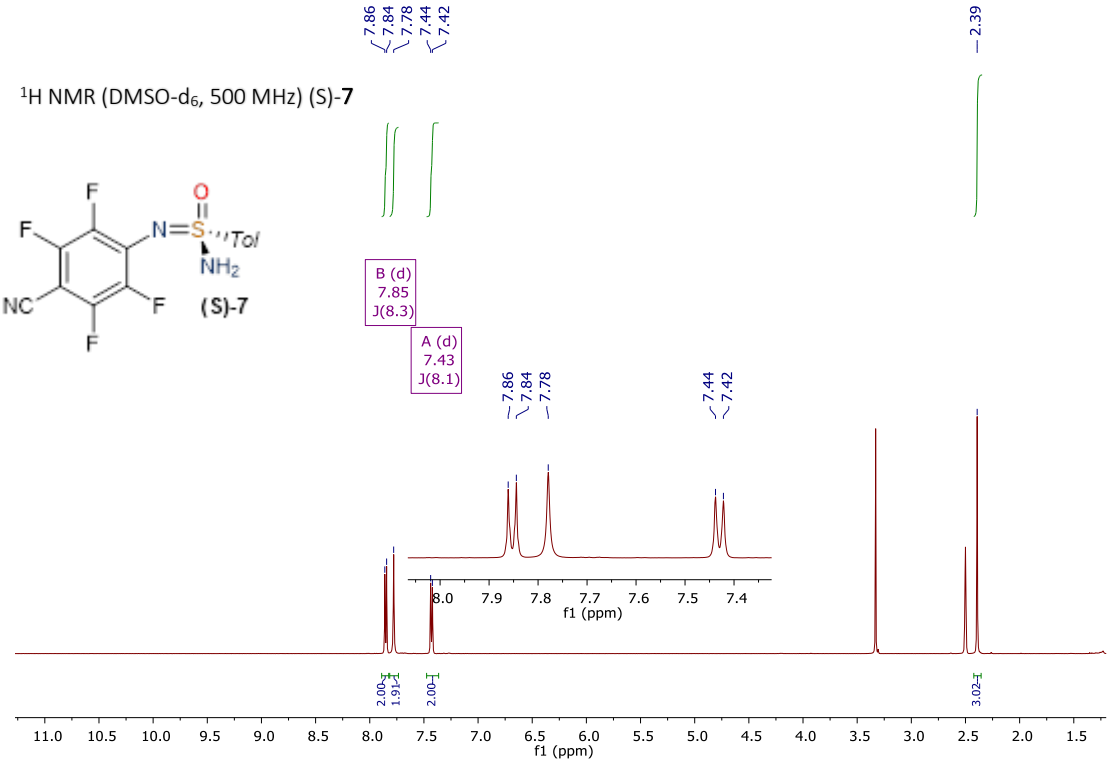
^{19}F NMR (DMSO-d_6, 376 MHz) (S)-**5**



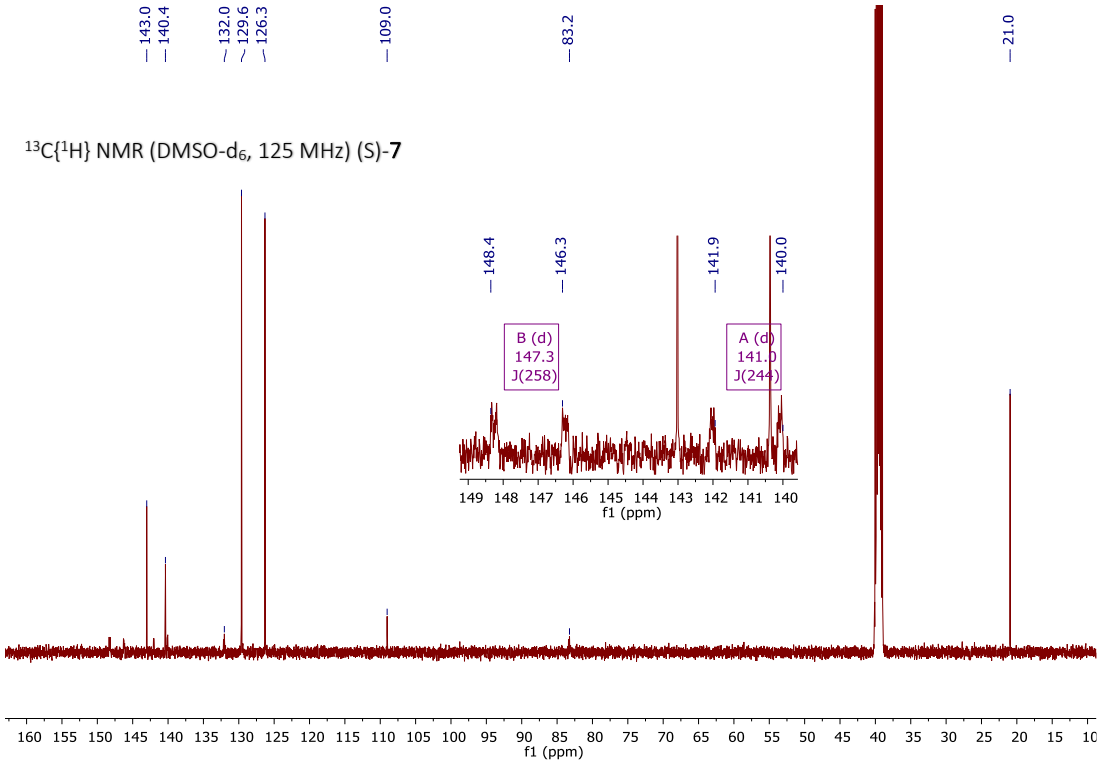
Compound (*S*)-**7**

^{1}H NMR (DMSO-d_6, 500 MHz) (S)-**7**

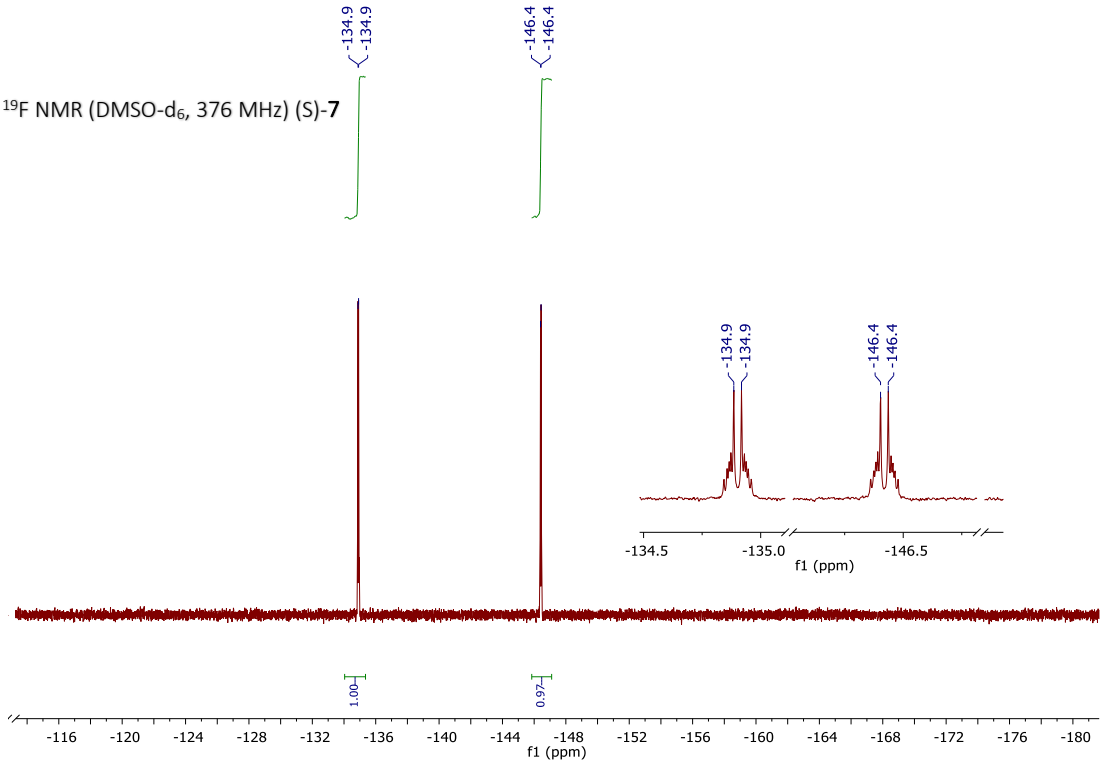
(S)-7



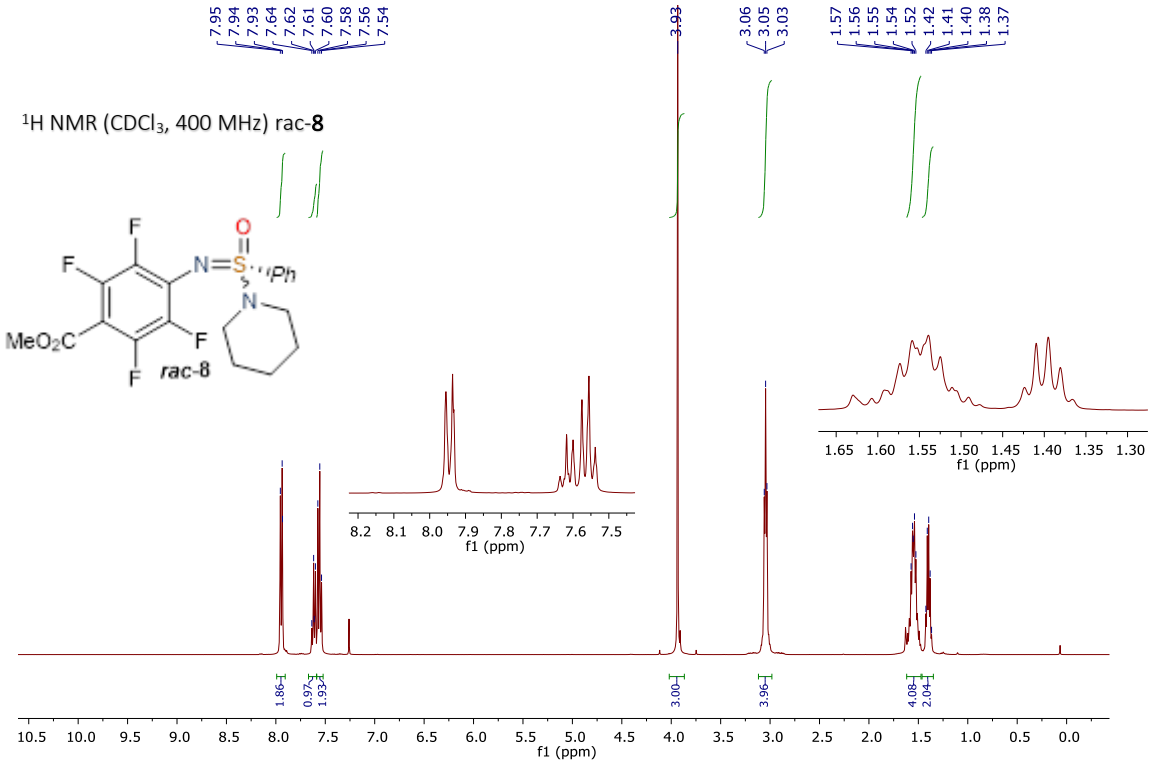
$^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 125 MHz) (S)-**7**

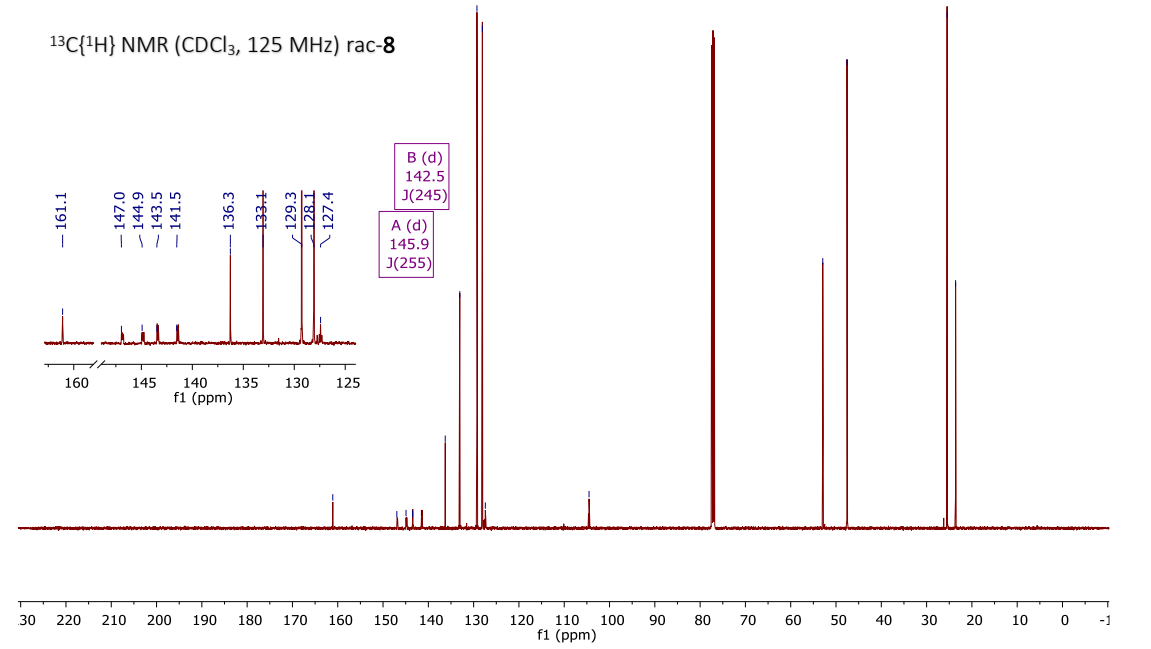


^{19}F NMR (DMSO-d_6, 376 MHz) (S)-**7**

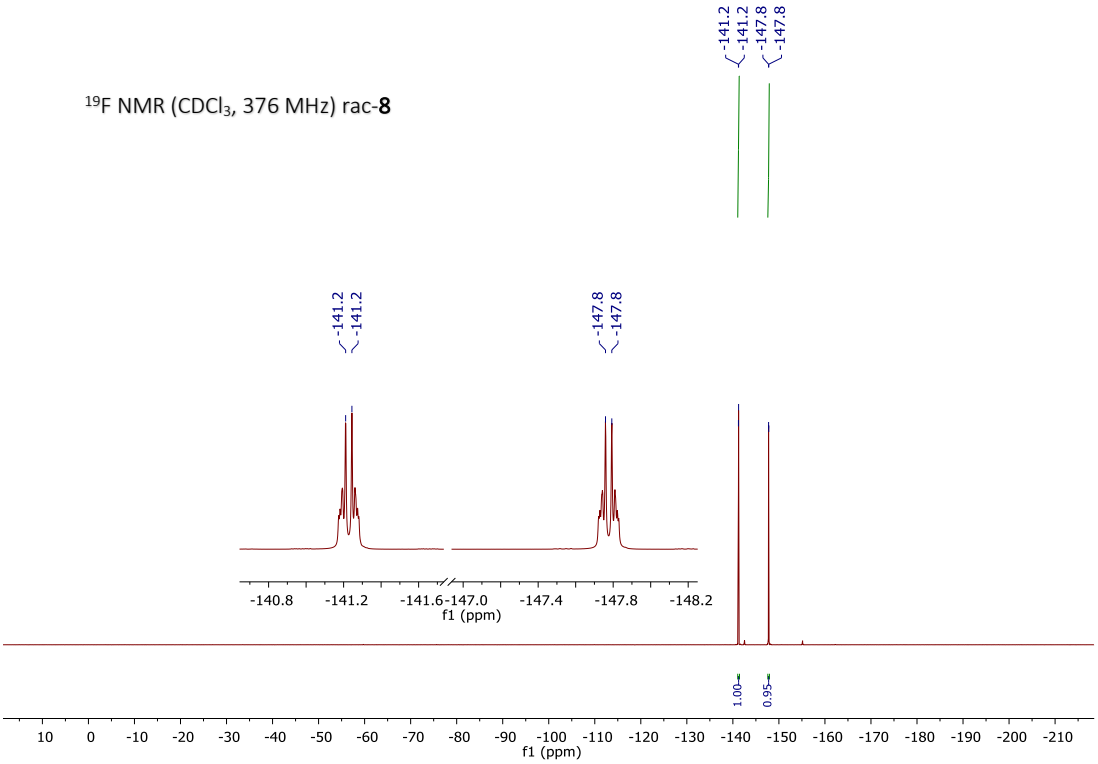


Compound *Rac*-**8**



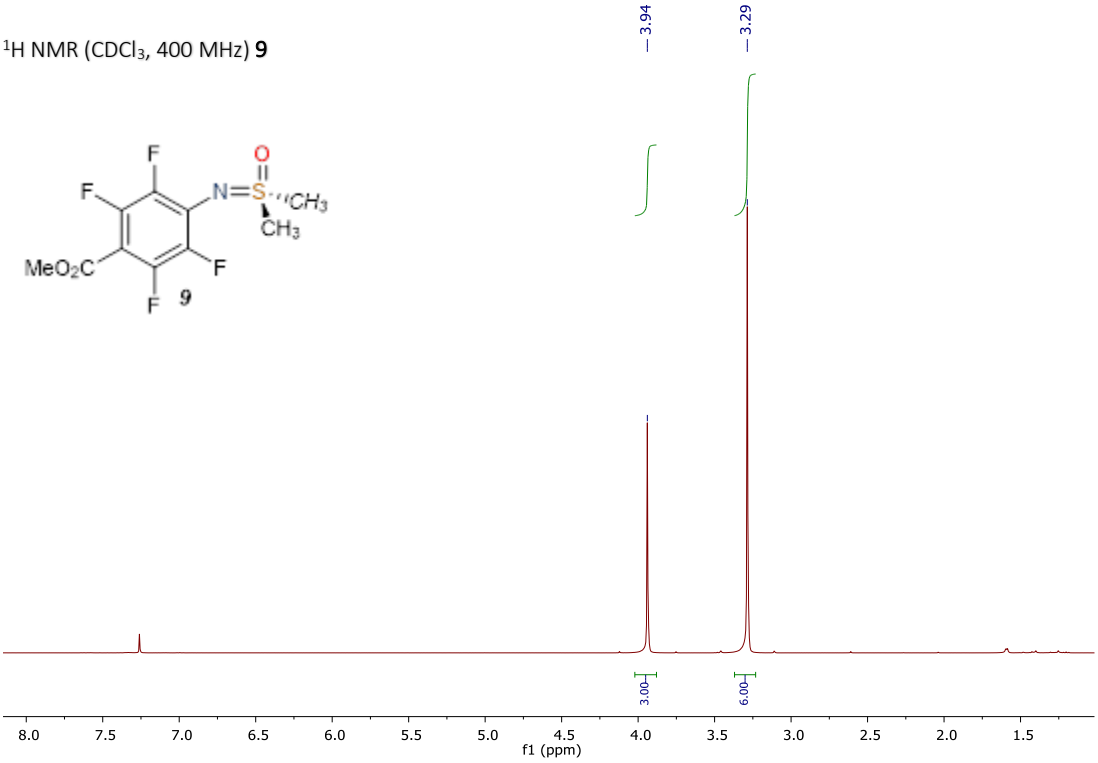


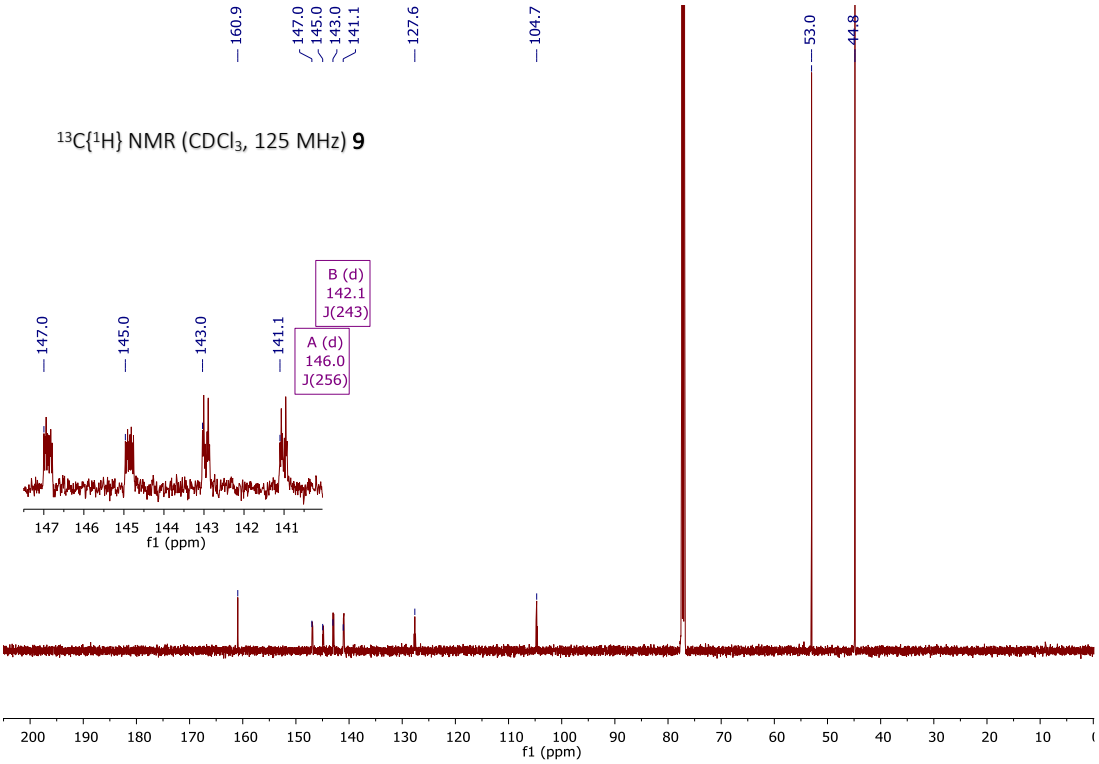
^{19}F NMR ($CDCl_3$, 376 MHz) rac-**8**

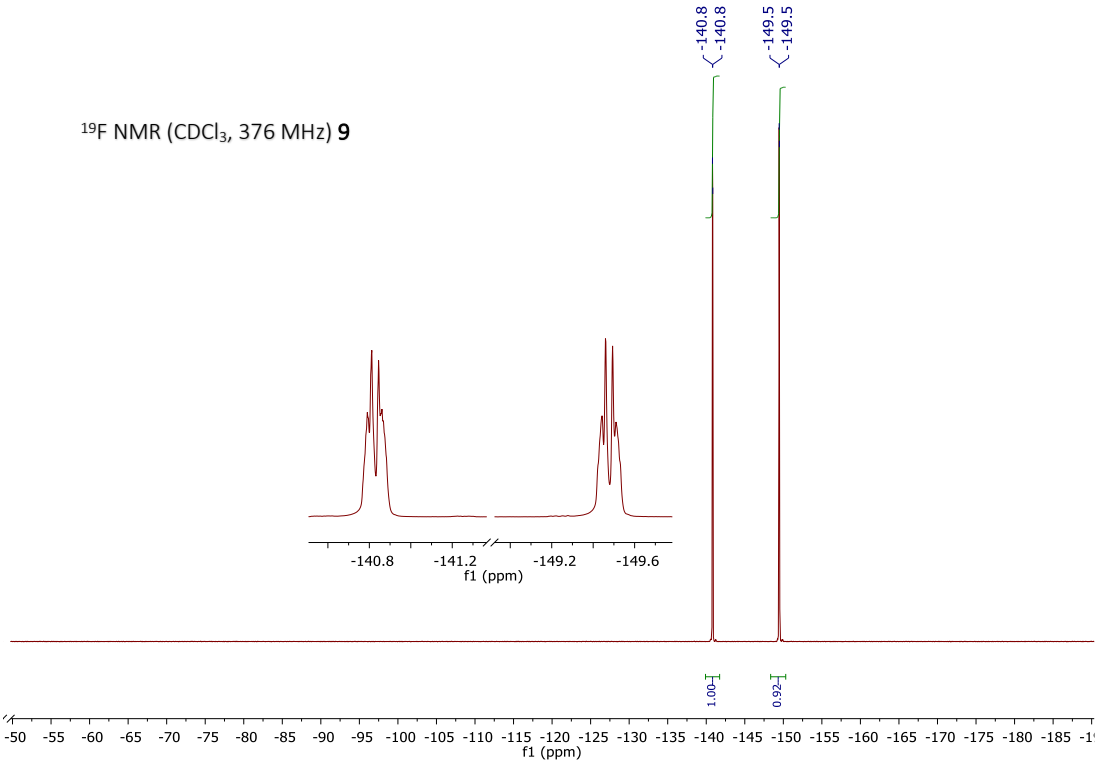


Compound **9**

^{1}H NMR ($CDCl_3$, 400 MHz) **9**

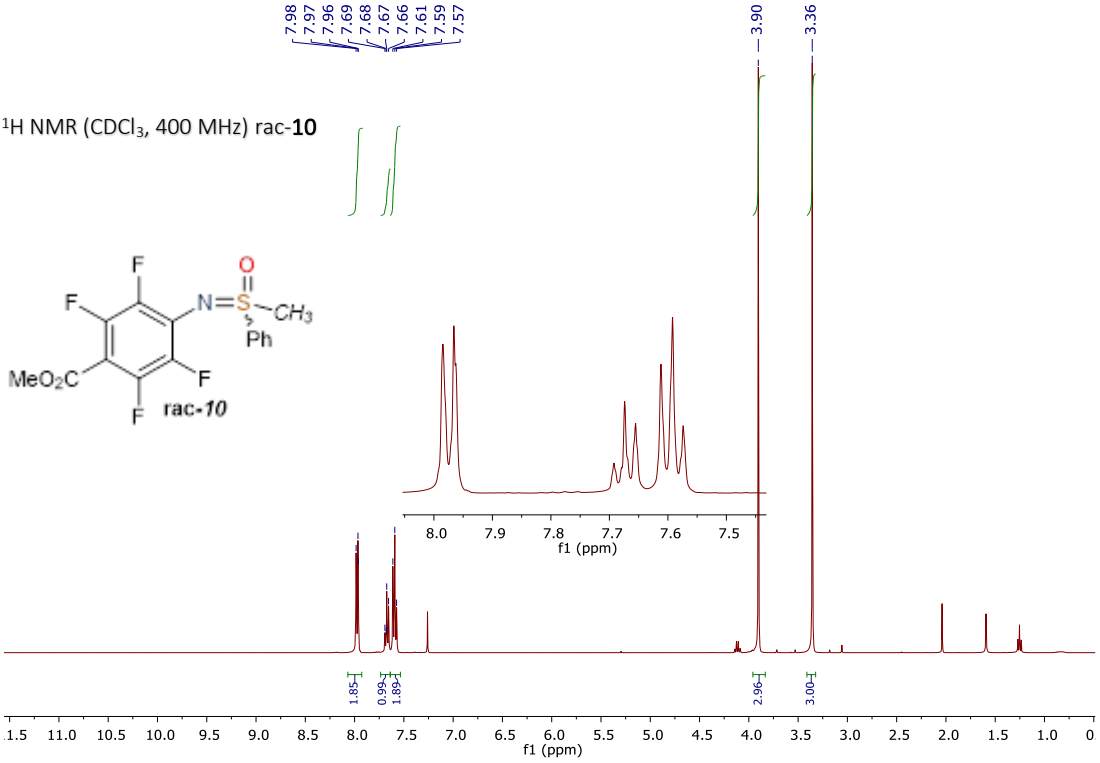



160.9
147.0
145.0
143.0
141.1
127.6
104.7
53.0
44.8
13C{1H} NMR (CDCl3, 125 MHz) 9
B (d)
142.1
J(243)
A (d)
146.0
J(256)
147.0
145.0
143.0
141.1
147 146 145 144 143 142 141
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

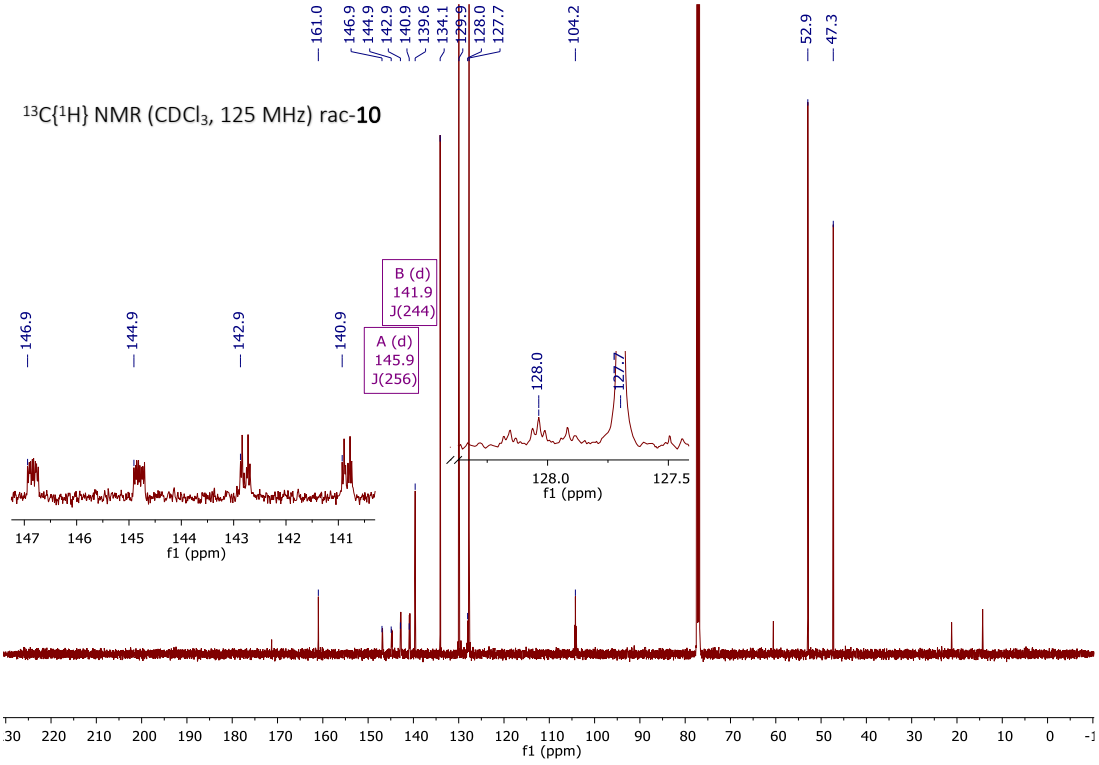

-140.8
-140.8
-149.5
-149.5
19F NMR (CDCl3, 376 MHz) 9
-140.8 -141.2 -149.2 -149.6
f1 (ppm)
1.00
0.92
-50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180 -185
f1 (ppm)

Compound *rac*-**10**

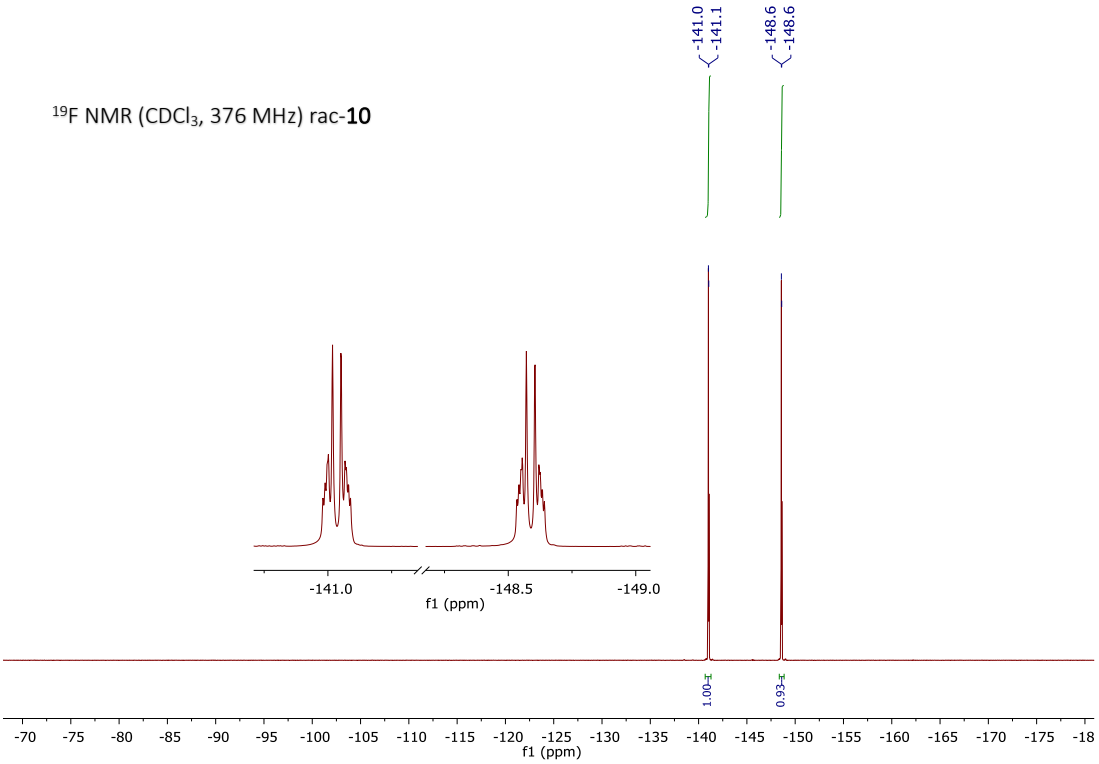
^{1}H NMR ($CDCl_3$, 400 MHz) rac-**10**



^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz) rac-**10**

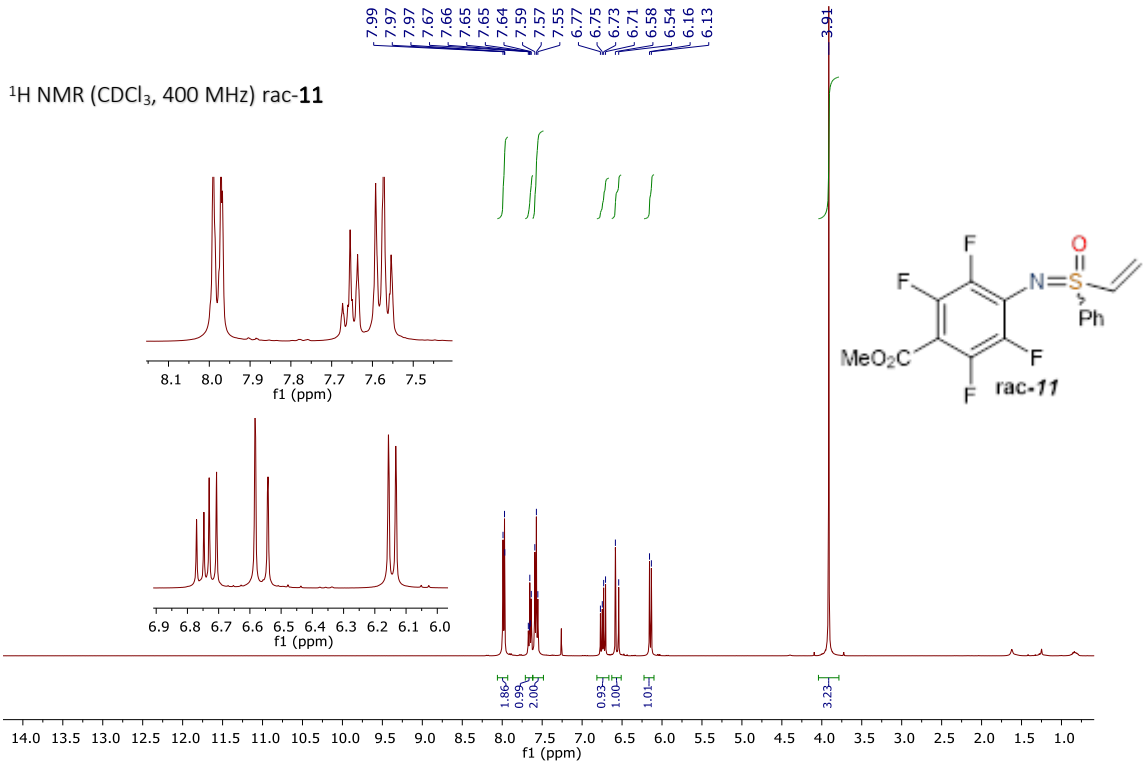


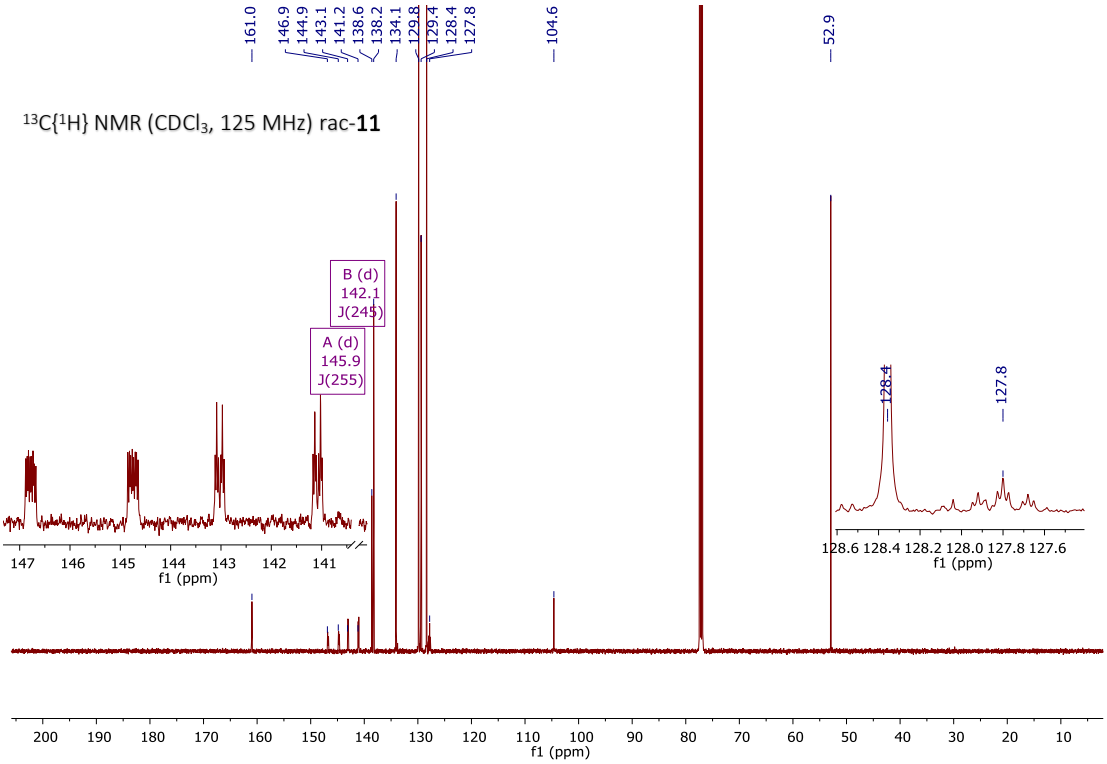
^{19}F NMR ($CDCl_3$, 376 MHz) rac-**10**

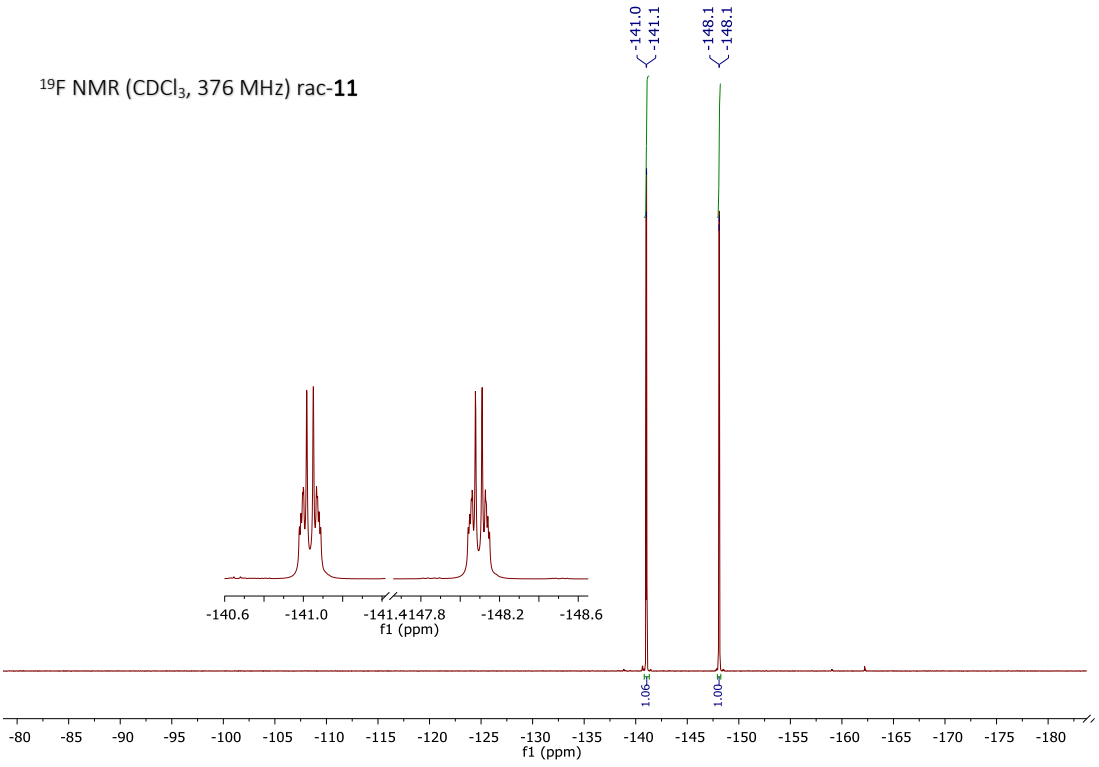


Compound *rac*-**11**

^{1}H NMR ($CDCl_3$, 400 MHz) rac-**11**

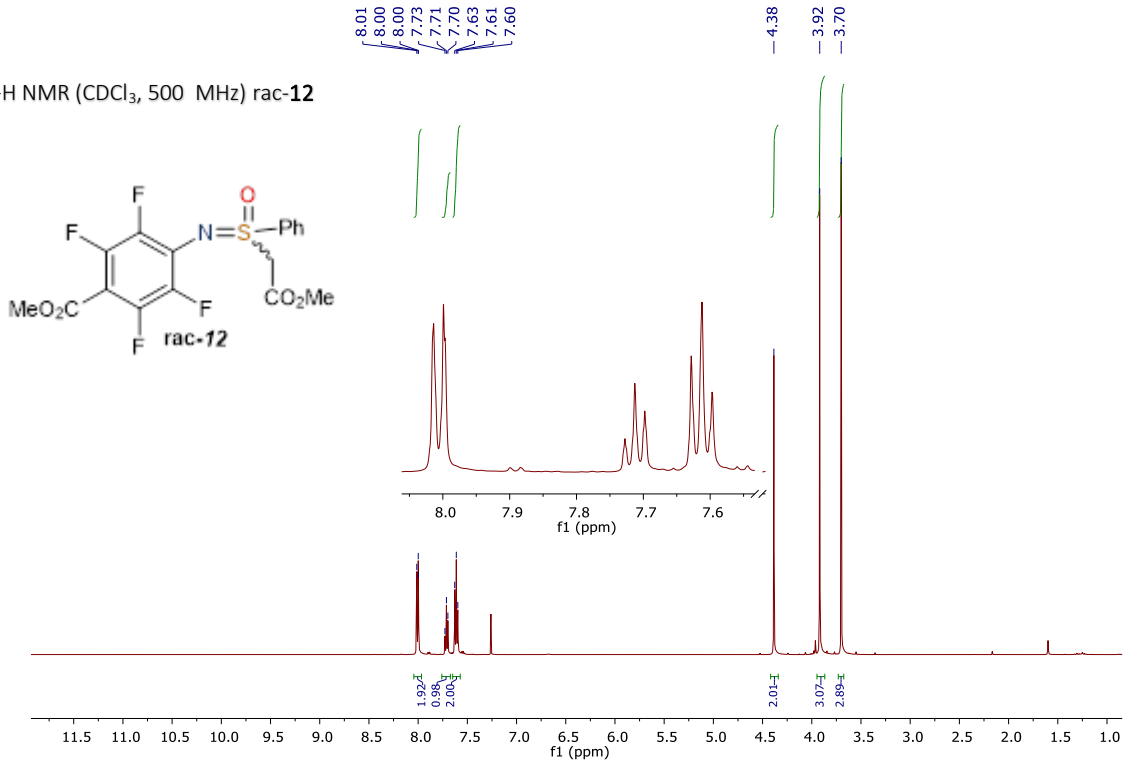


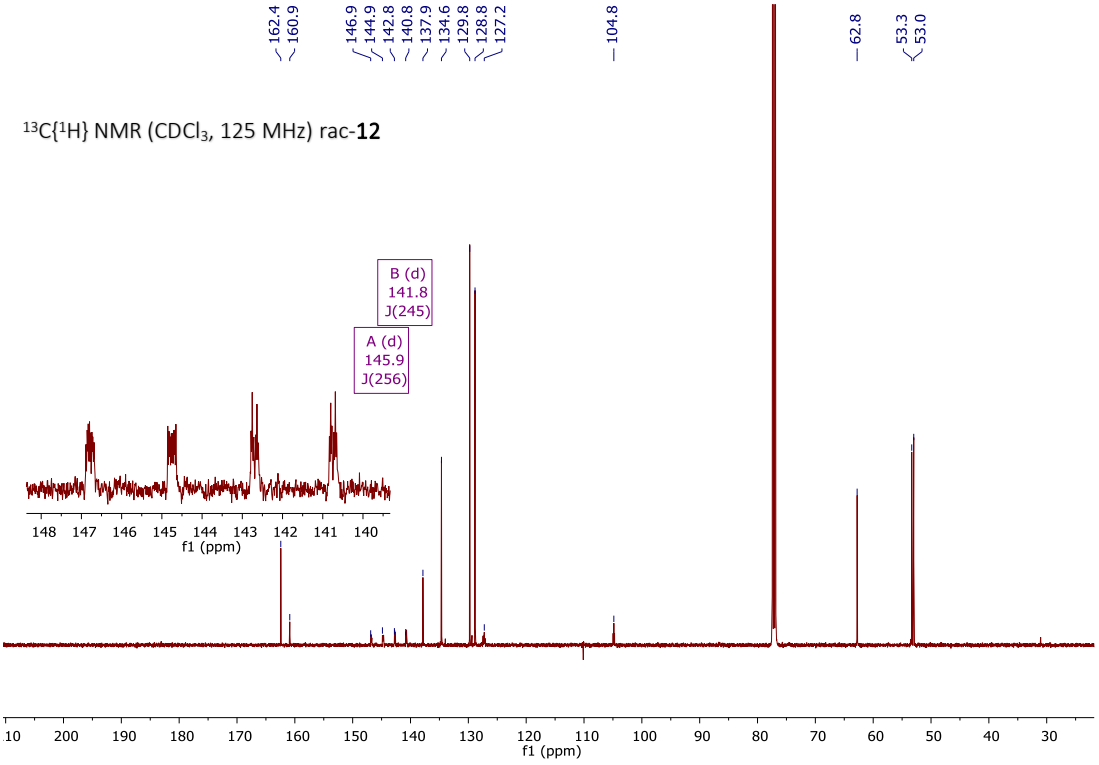

161.0
146.9
144.9
143.1
141.2
138.6
138.2
134.1
129.8
129.4
128.4
127.8
104.6
52.9
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) rac-**11**
B (d)
142.1
J(245)
A (d)
145.9
J(255)
128.4
127.8
f1 (ppm)


-141.0
-141.1
-148.1
-148.1
^{19}F NMR ($CDCl_3$, 376 MHz) rac-**11**
1.06
1.00
f1 (ppm)

Compound *rac*-**12**

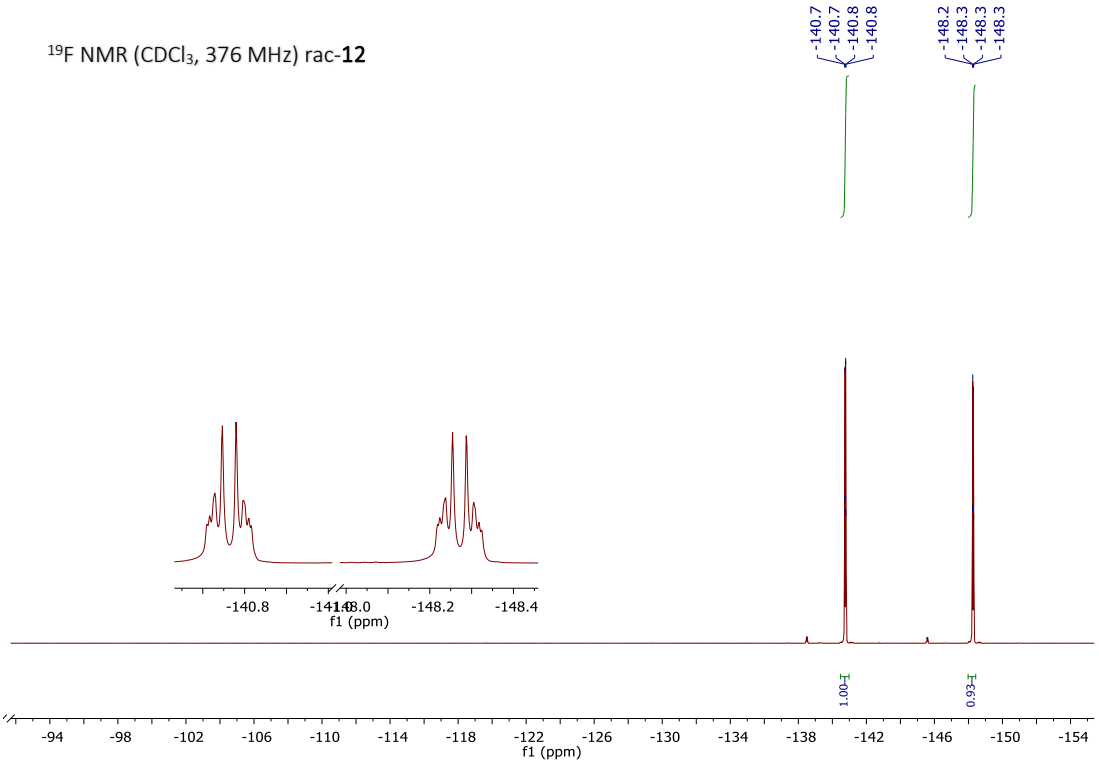
^{1}H NMR ($CDCl_3$, 500 MHz) rac-**12**





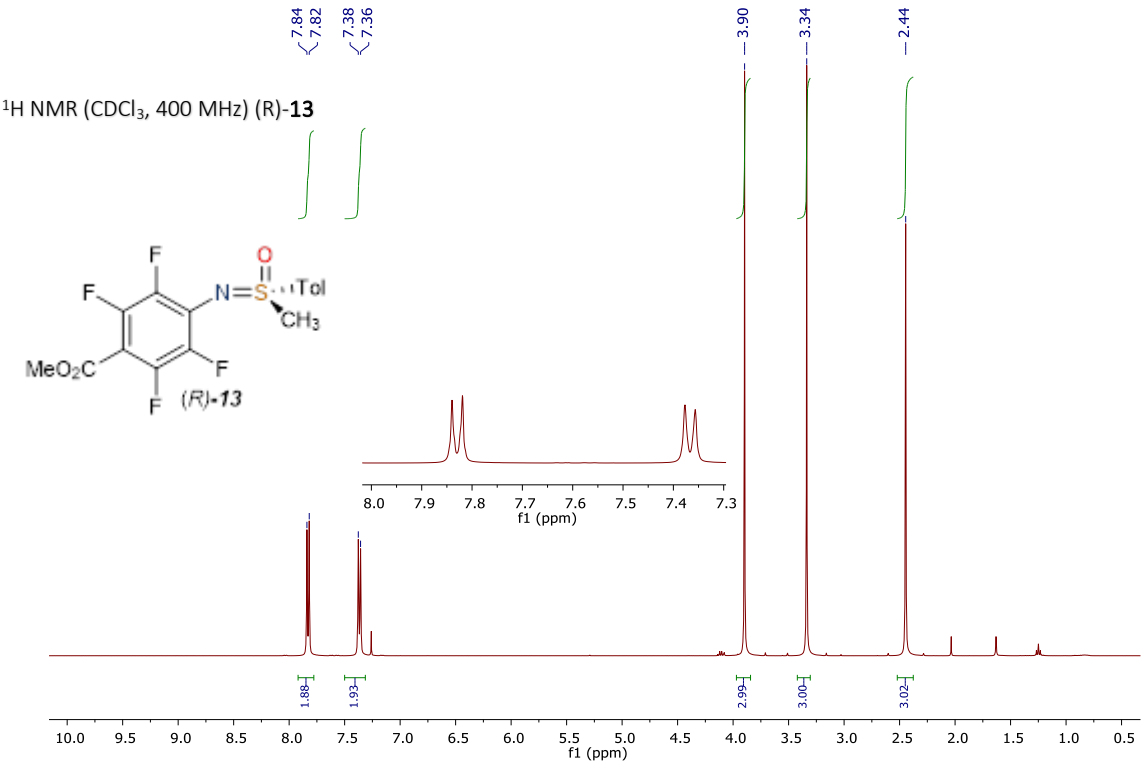
^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz) rac-**12**

^{19}F NMR ($CDCl_3$, 376 MHz) rac-**12**

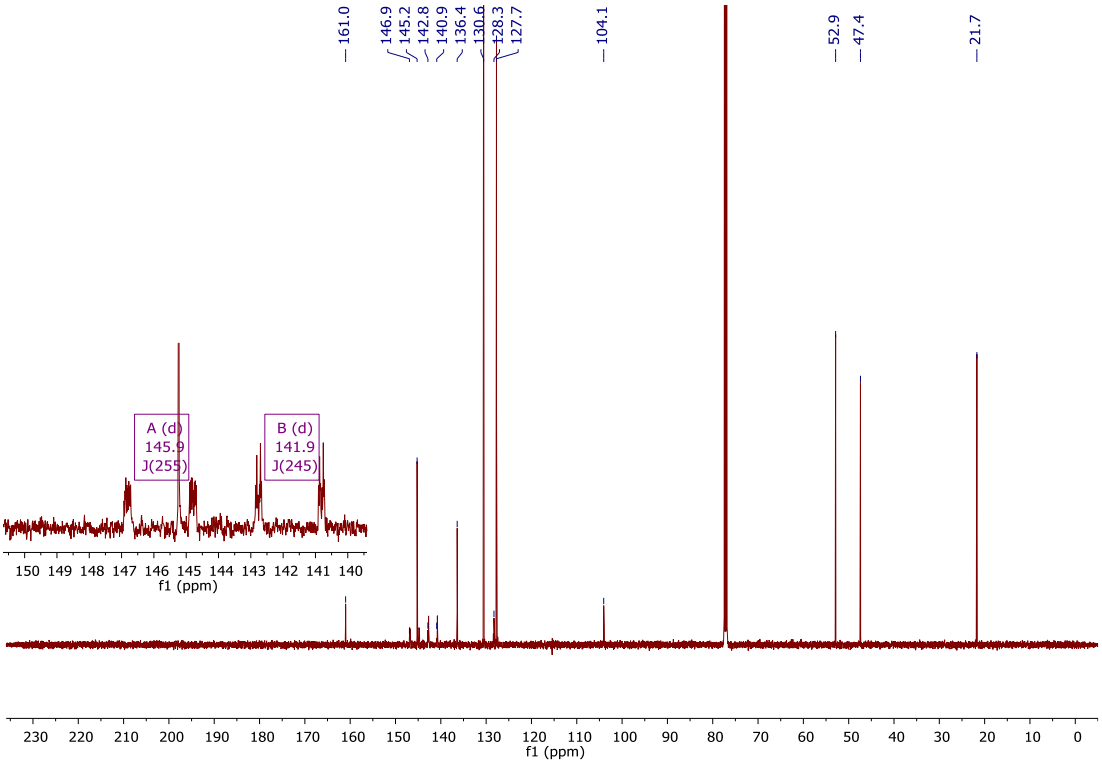


Compound (*R*)-**13**

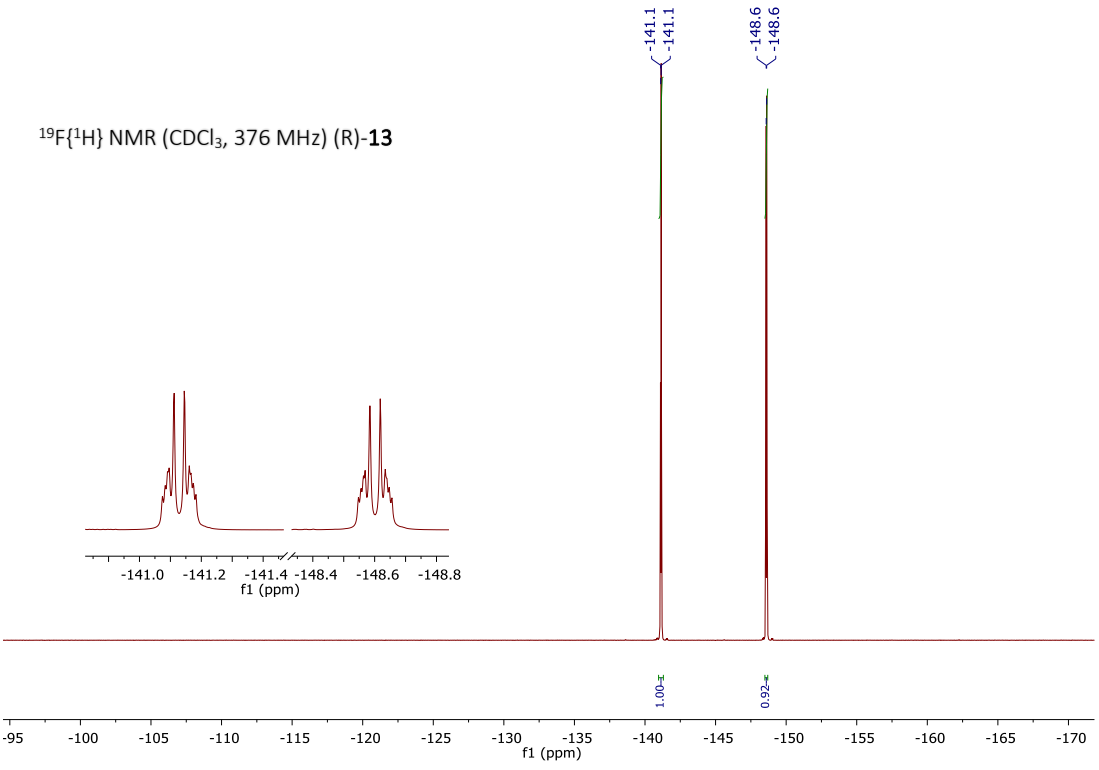
^{1}H NMR ($CDCl_3$, 400 MHz) (R)-**13**



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) (R)-**13**

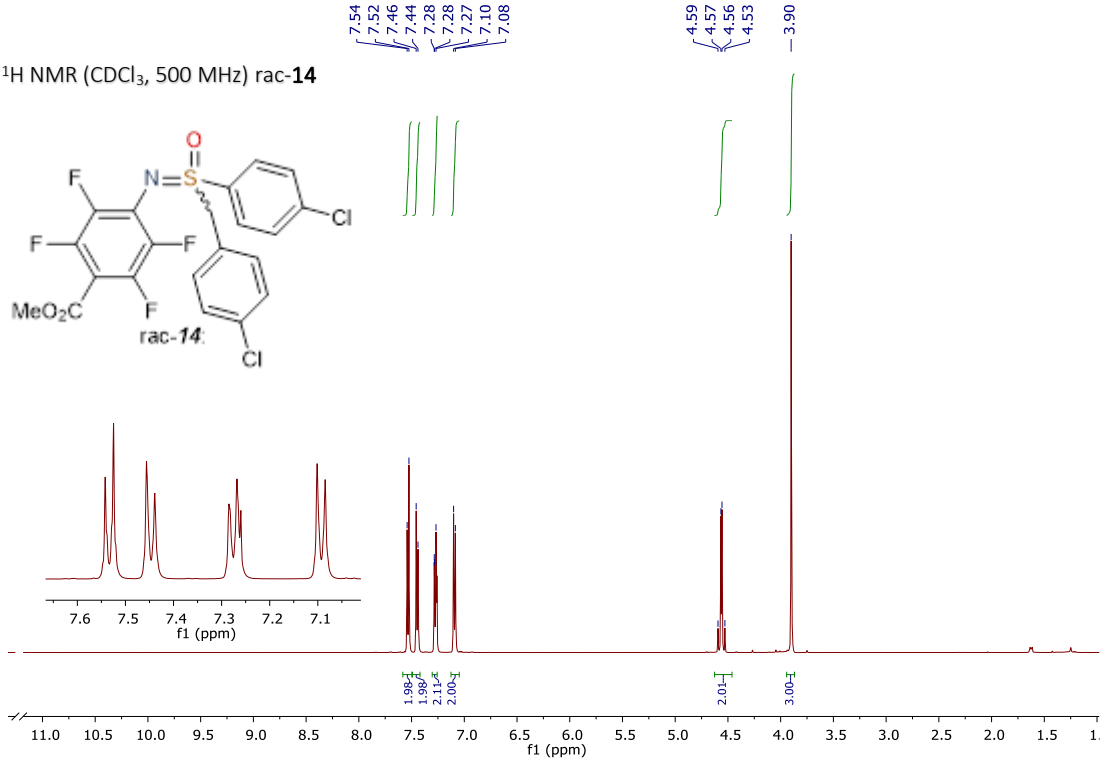


$^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 376 MHz) (R)-**13**

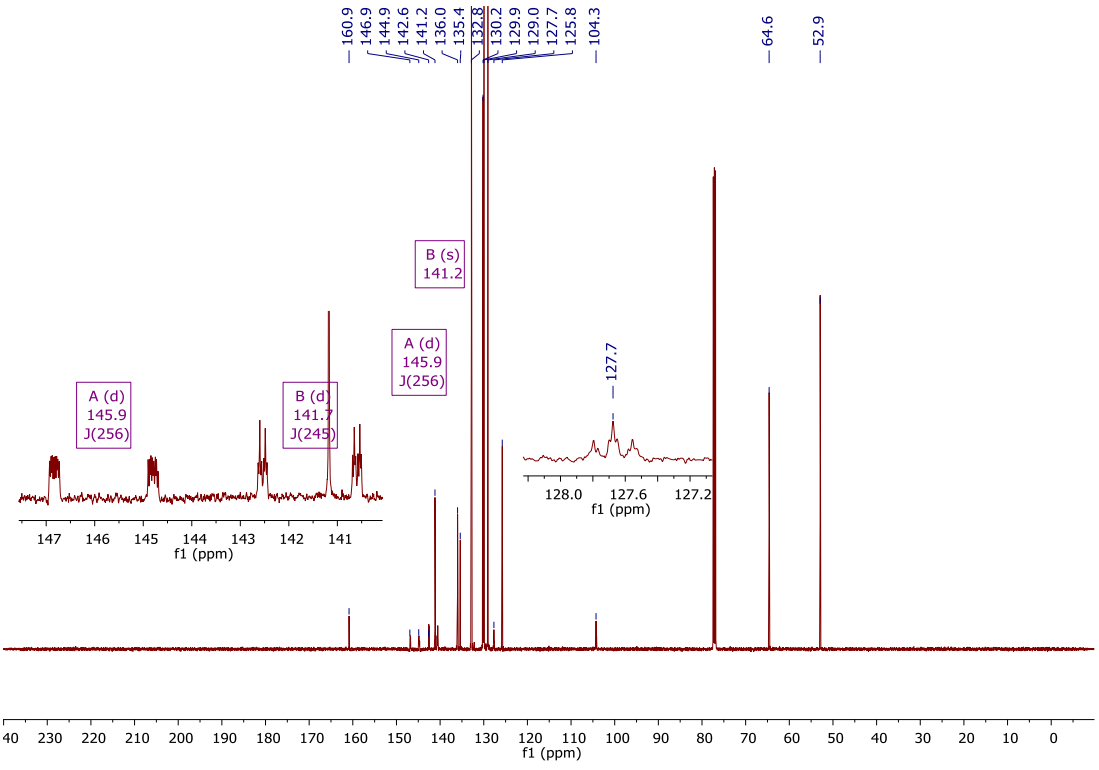


Compound *rac*-**14**

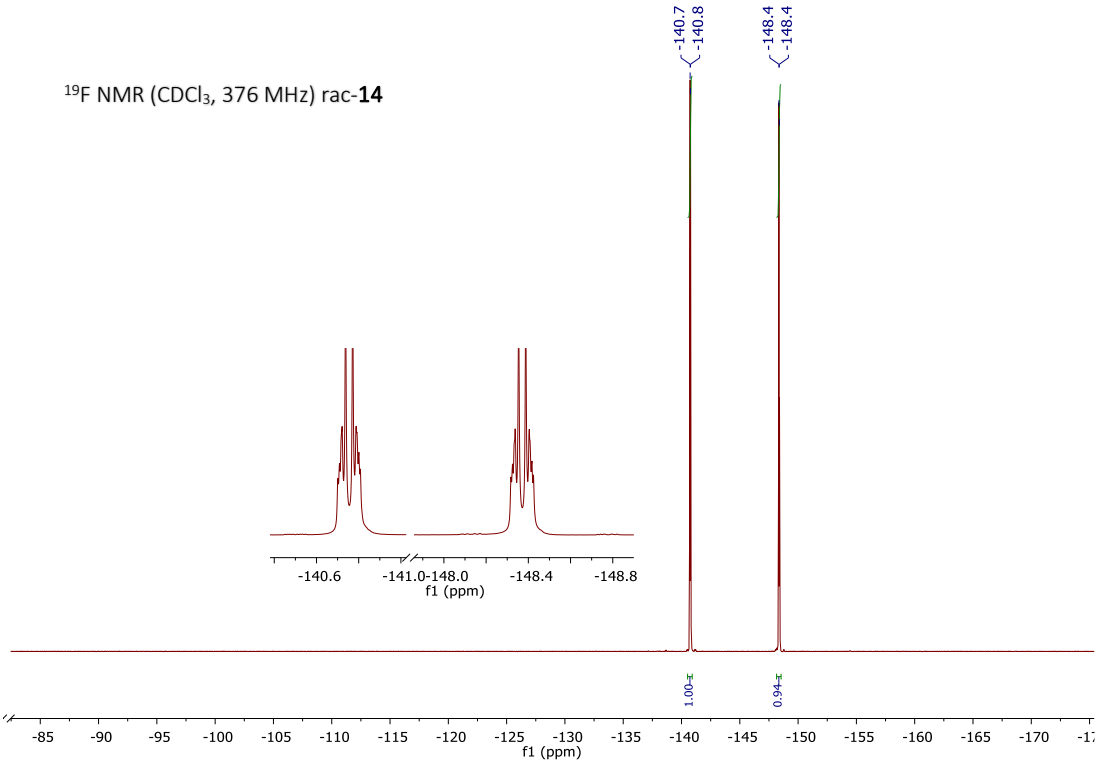
^{1}H NMR ($CDCl_3$, 500 MHz) rac-**14**



^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz) rac-**14**

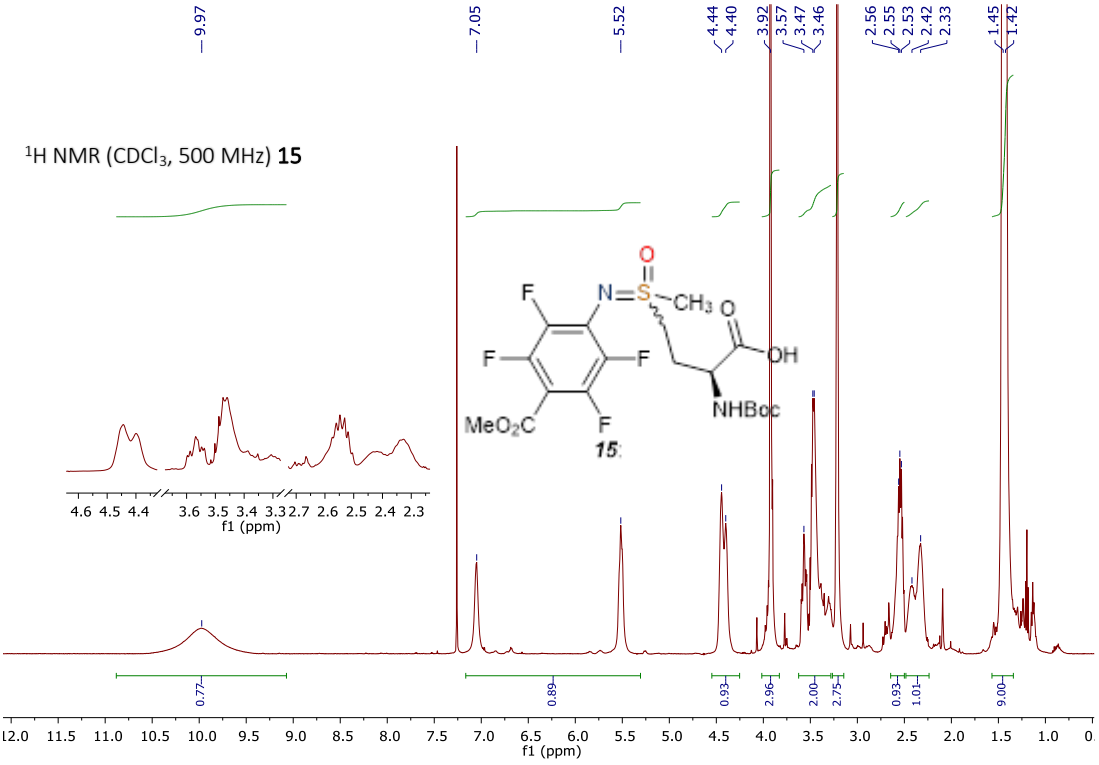


^{19}F NMR ($CDCl_3$, 376 MHz) rac-**14**

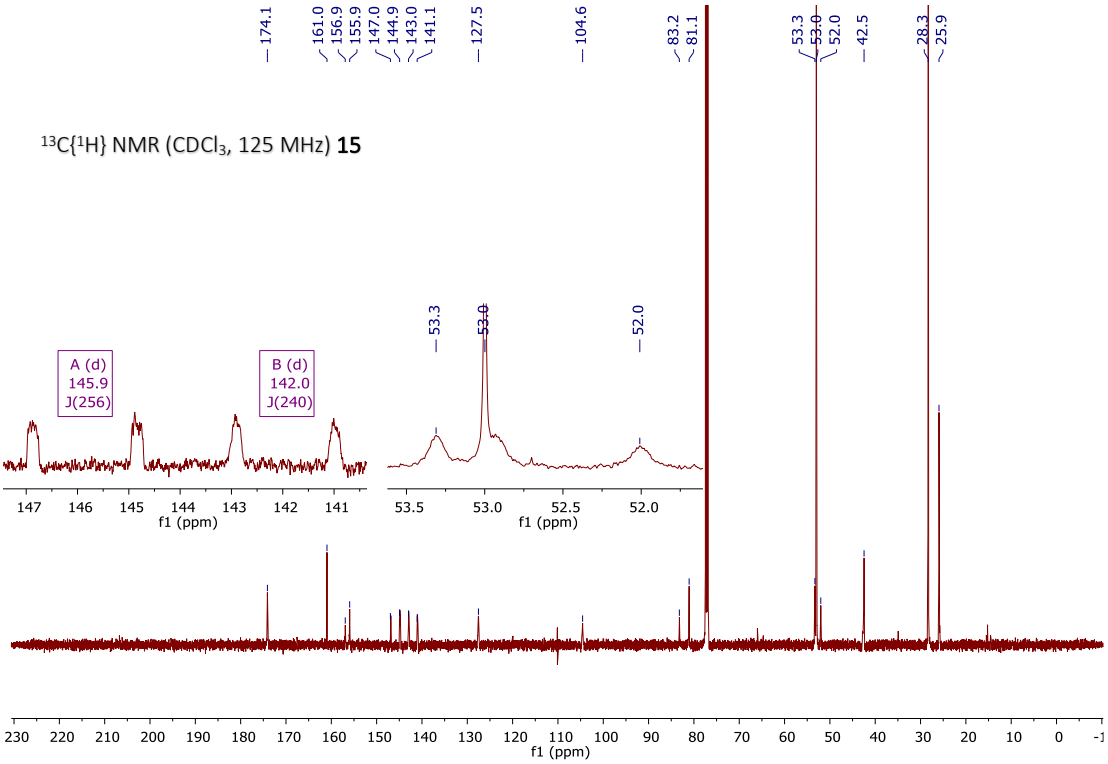


Compound **15**

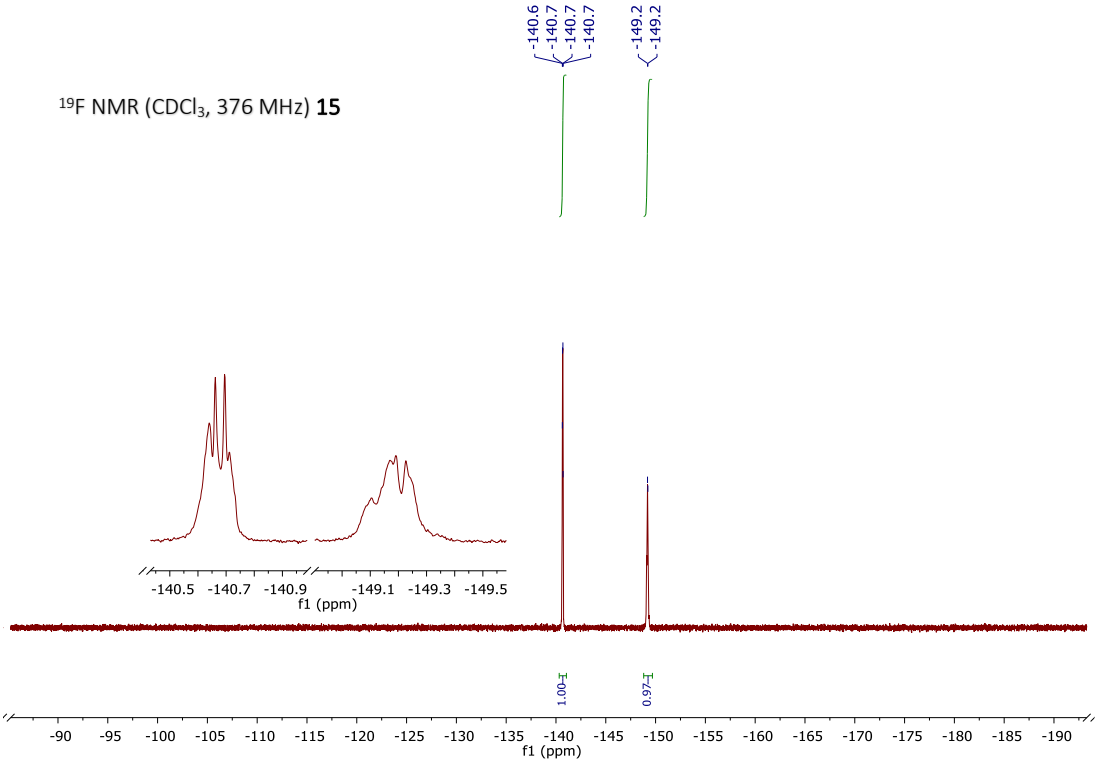
^{1}H NMR ($CDCl_3$, 500 MHz) **15**



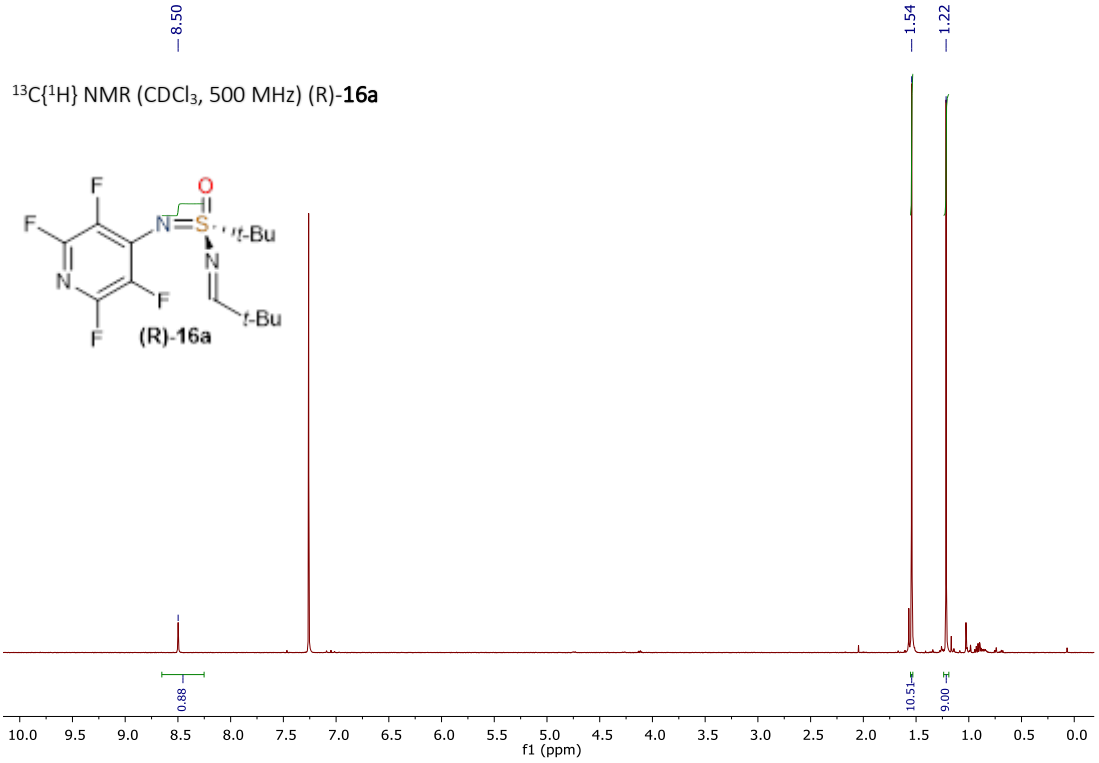
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) **15**



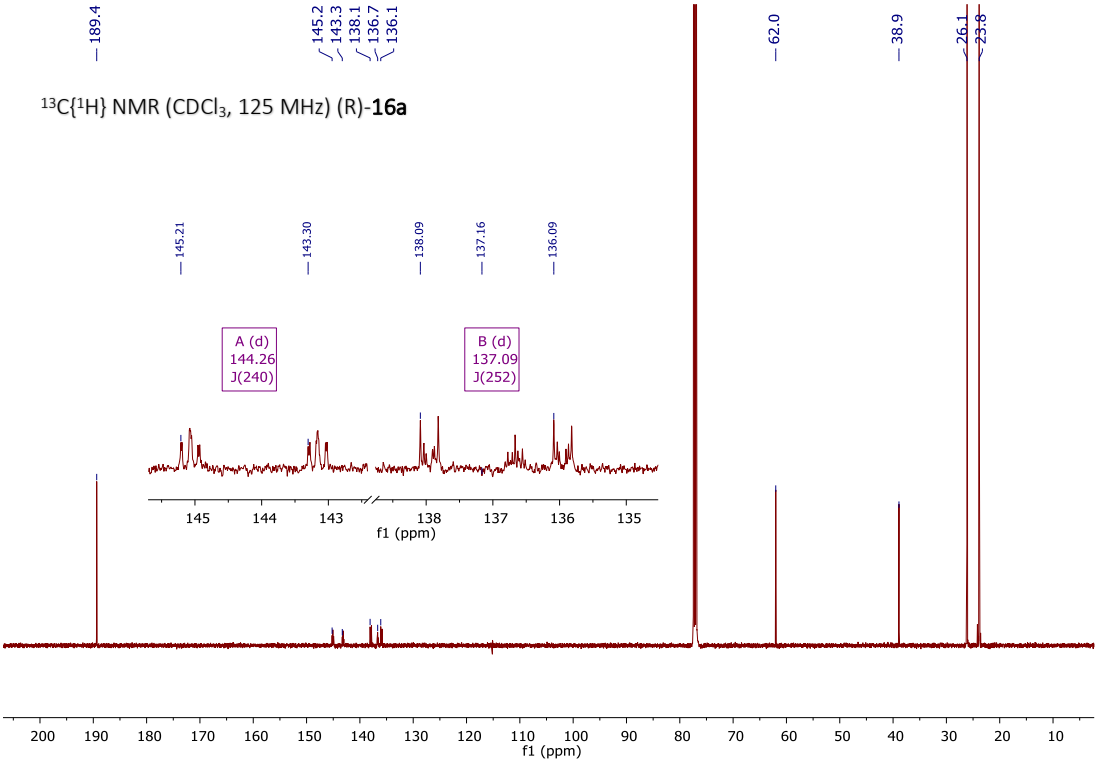
^{19}F NMR ($CDCl_3$, 376 MHz) **15**



Compound (*R*)-**16a**

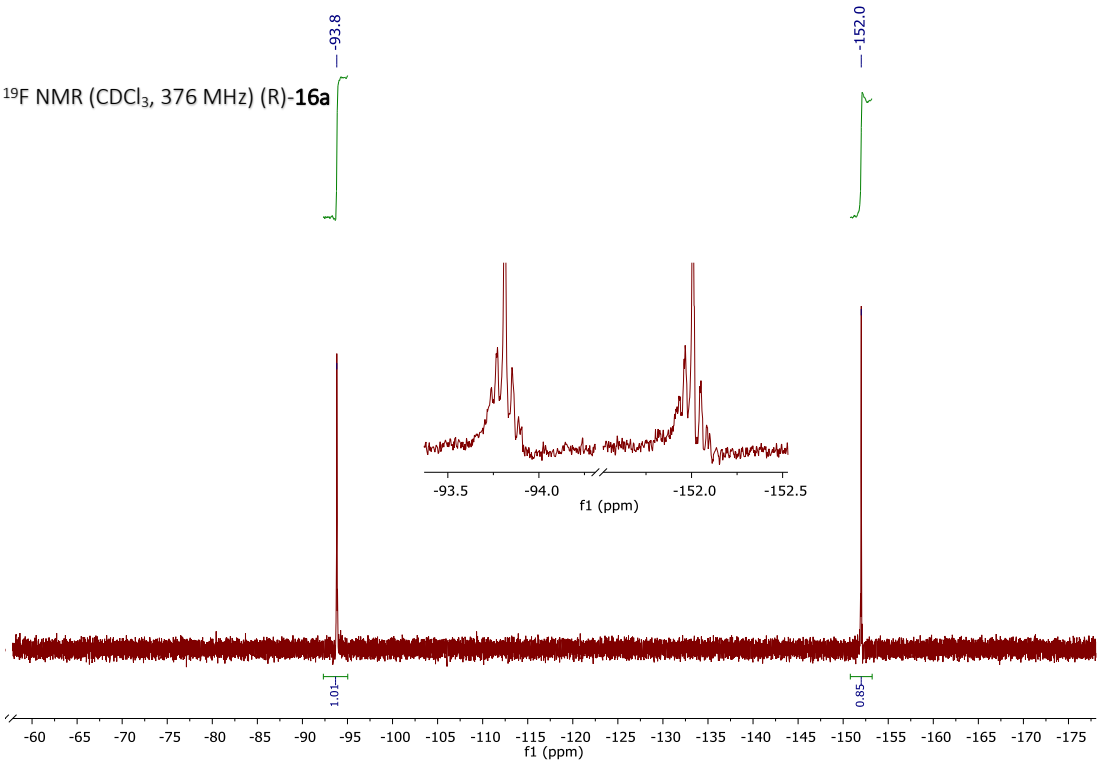


$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 500 MHz) (R)-**16a**



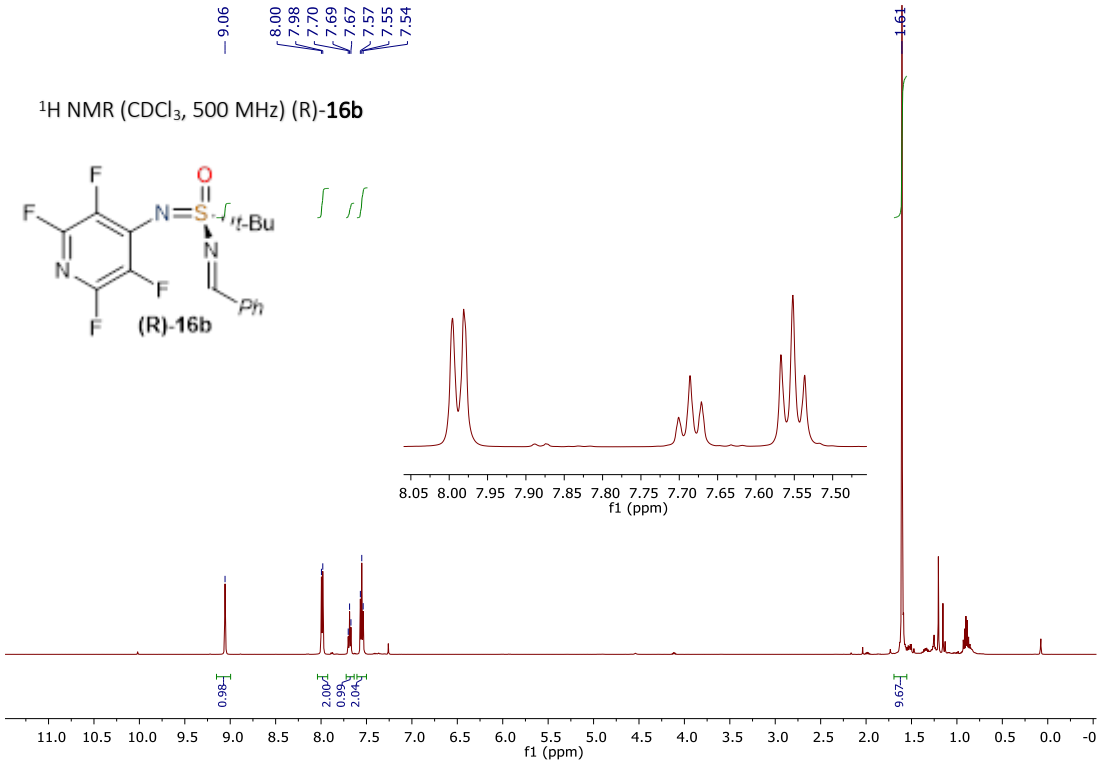
$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) (R)-**16a**

^{19}F NMR ($CDCl_3$, 376 MHz) (R)-**16a**

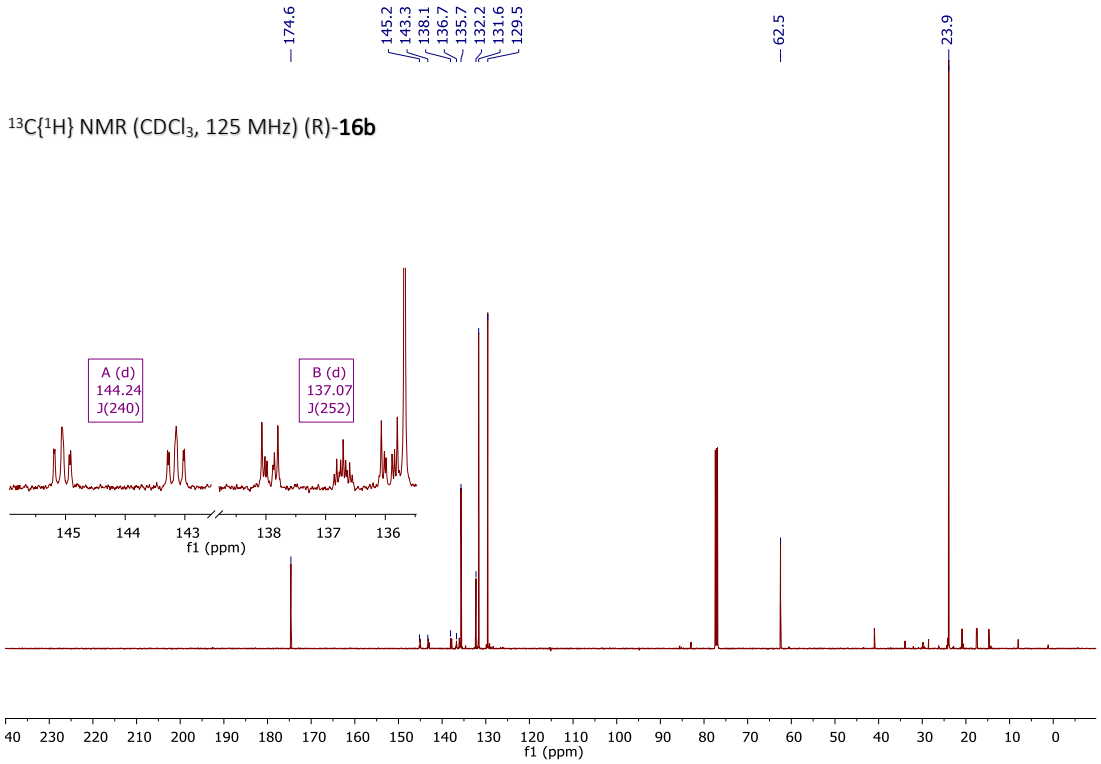


Compound (*R*)-**16b**

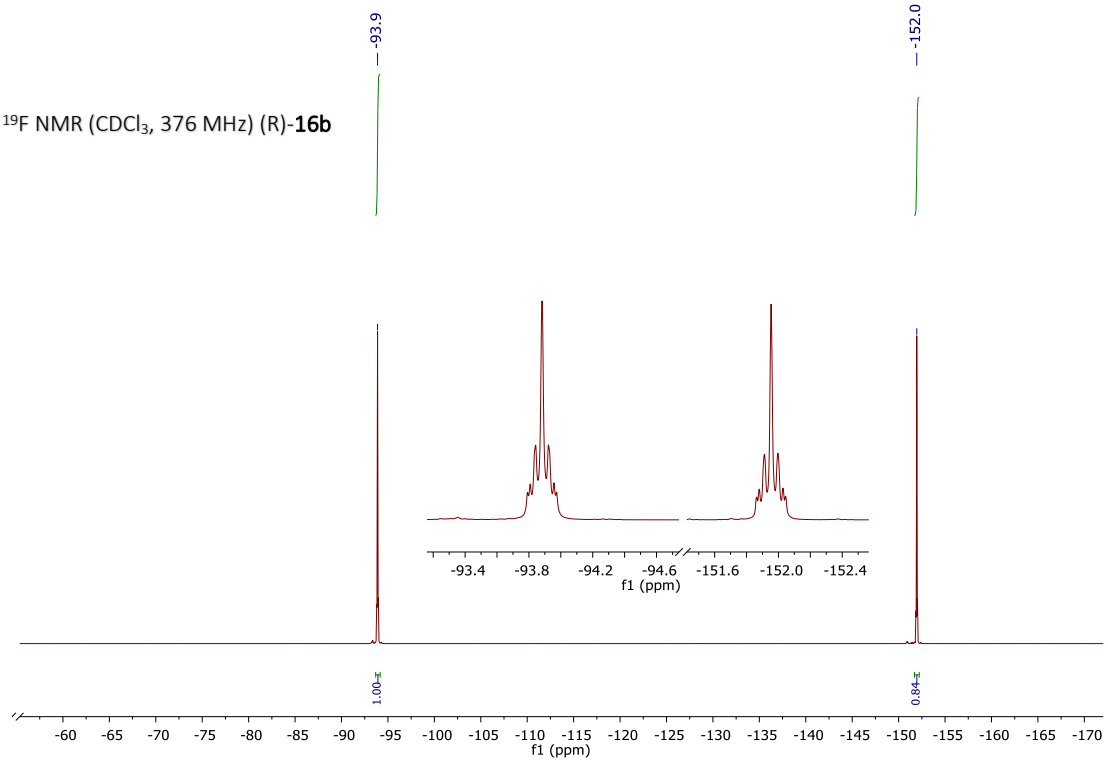
^{1}H NMR ($CDCl_3$, 500 MHz) (R)-**16b**



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) (R)-**16b**

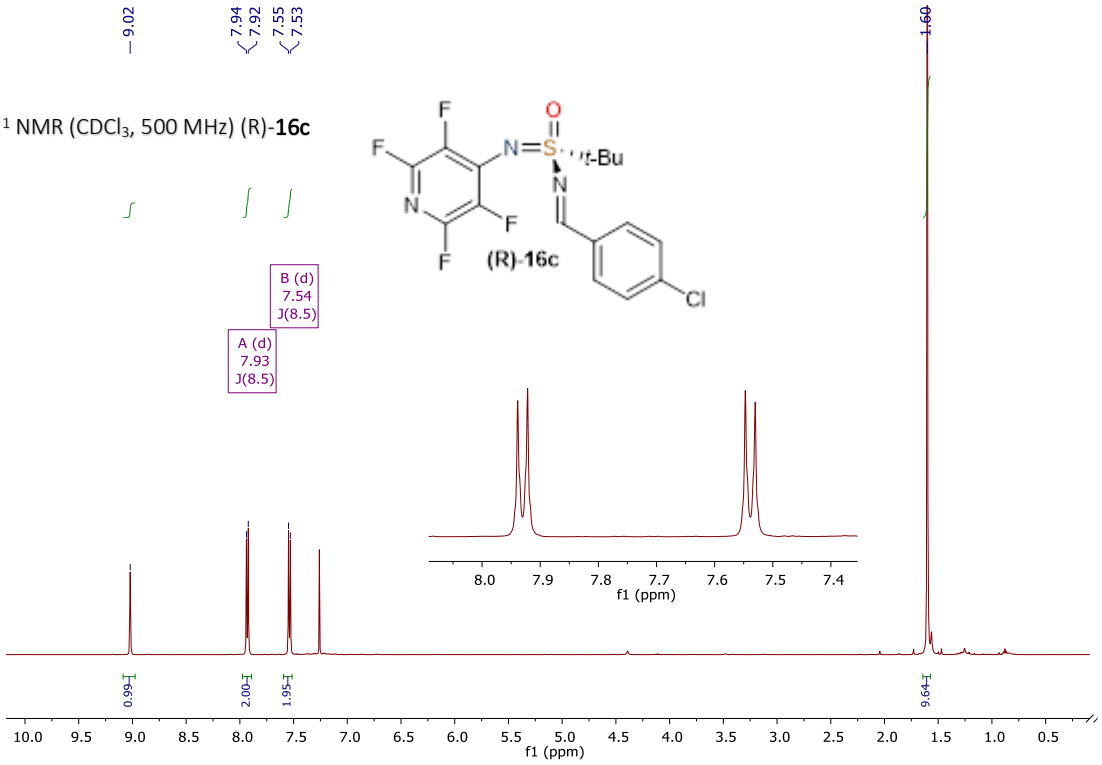


^{19}F NMR ($CDCl_3$, 376 MHz) (R)-**16b**

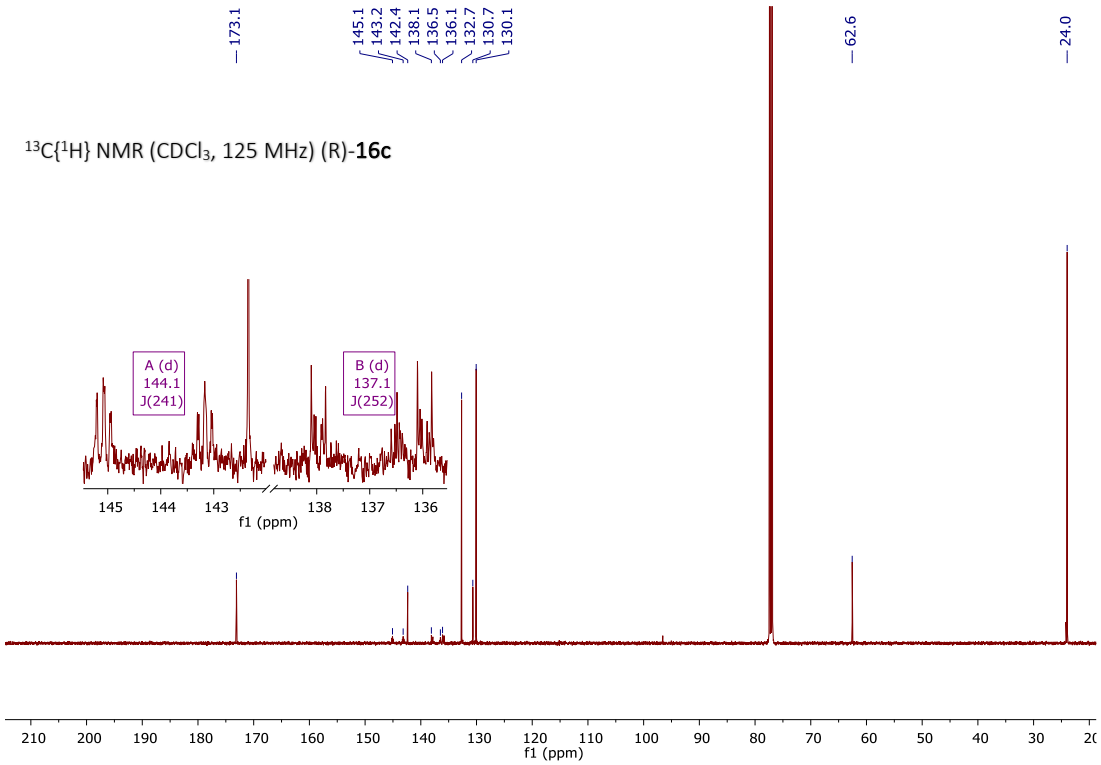


Compound (*R*)-**16c**

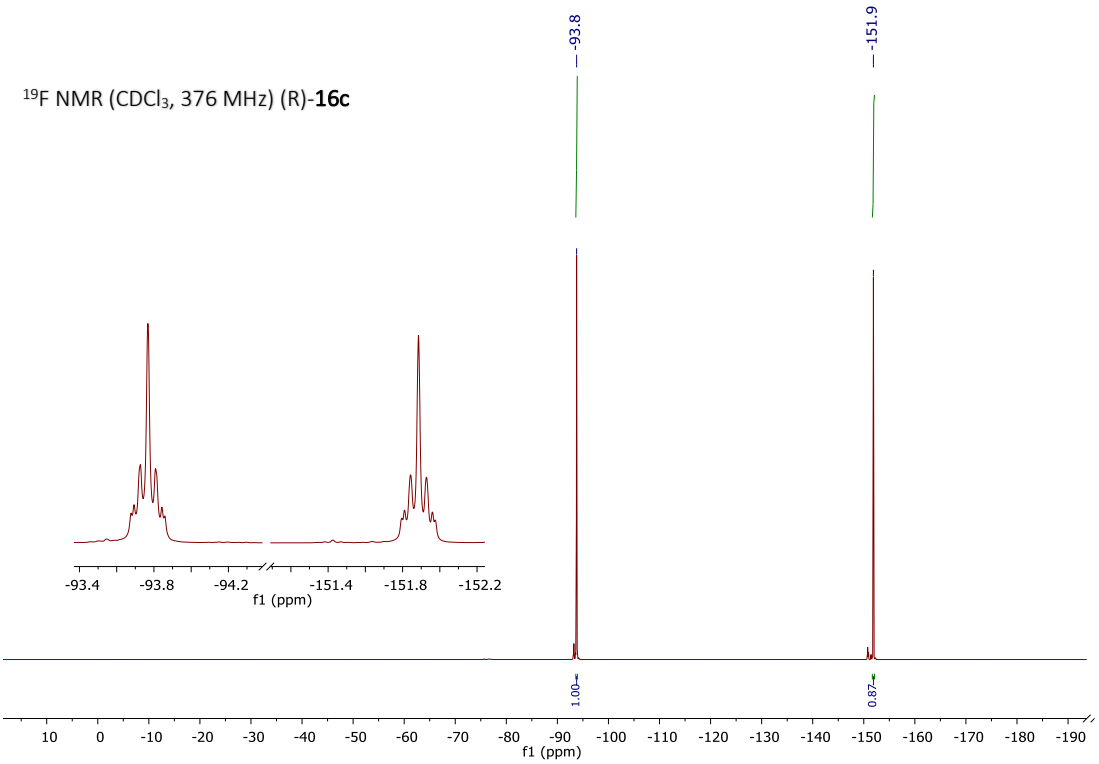
^{1} NMR ($CDCl_3$, 500 MHz) (R)-**16c**



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) (R)-**16c**

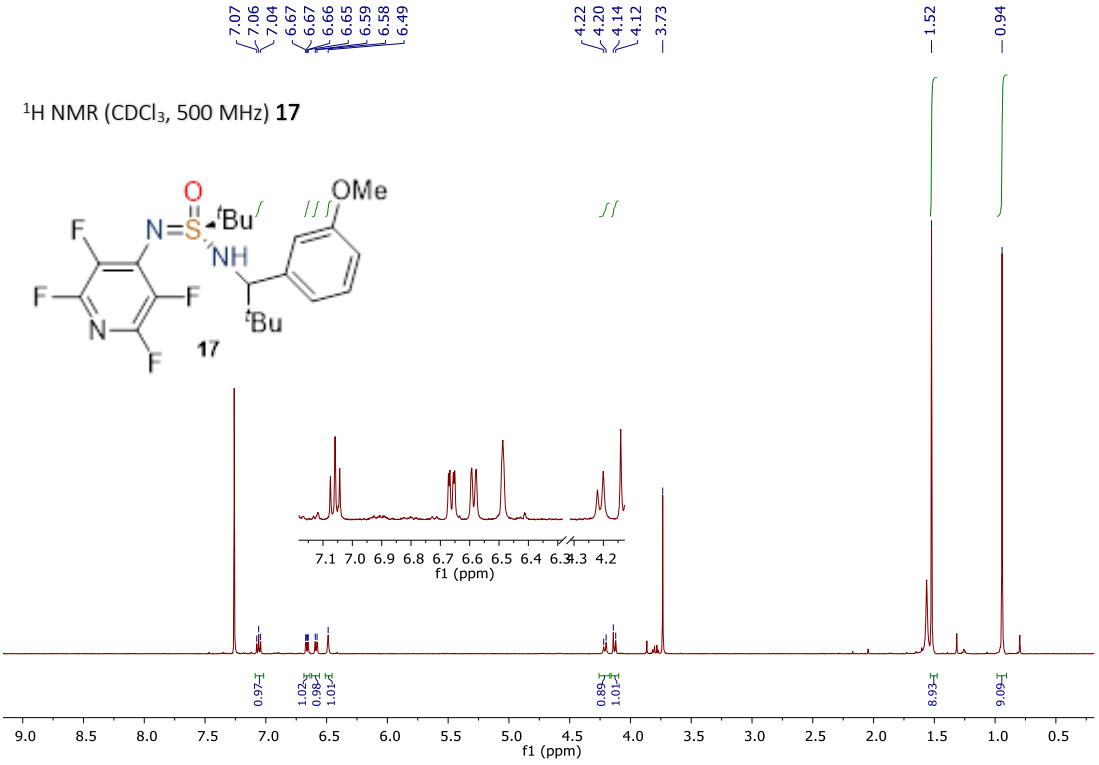


^{19}F NMR ($CDCl_3$, 376 MHz) (R)-**16c**

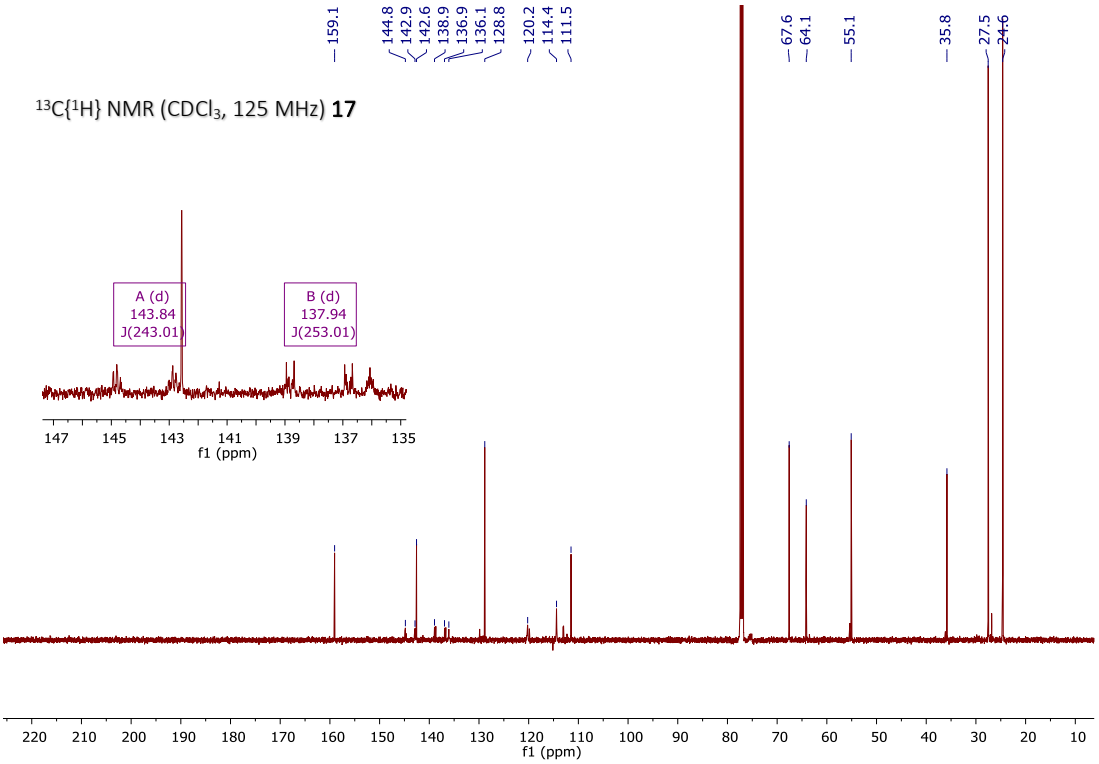


Compound **17**

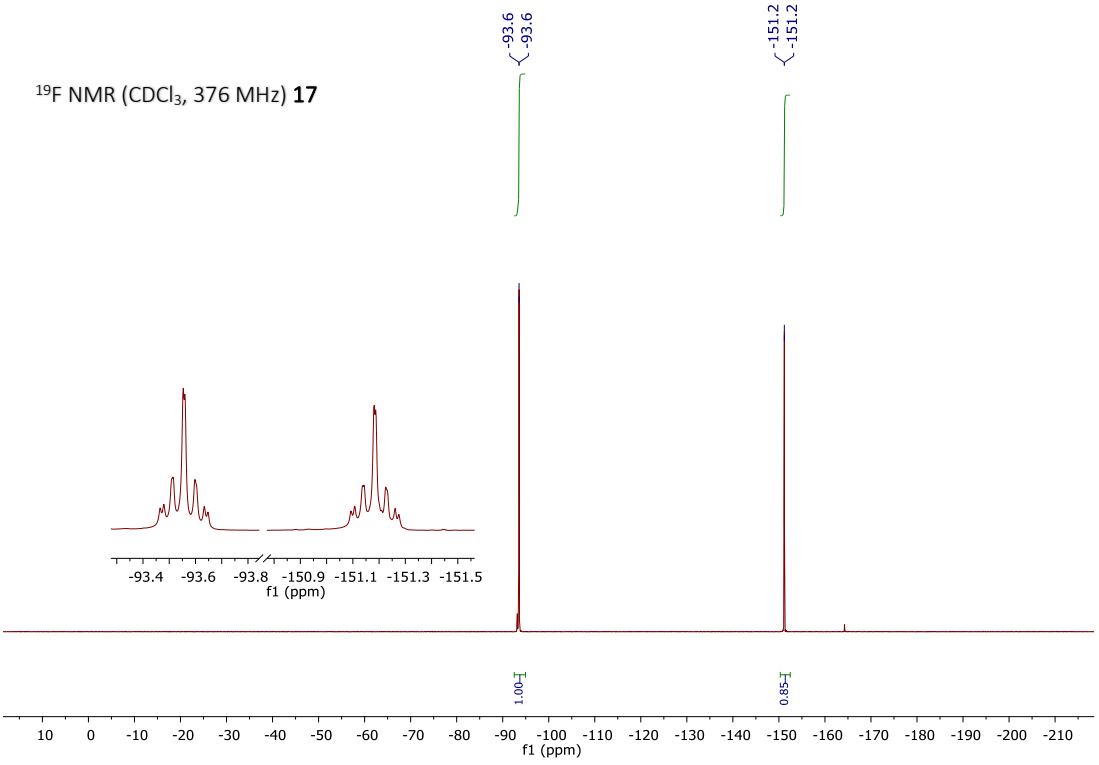
^{1}H NMR ($CDCl_3$, 500 MHz) **17**



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz) **17**

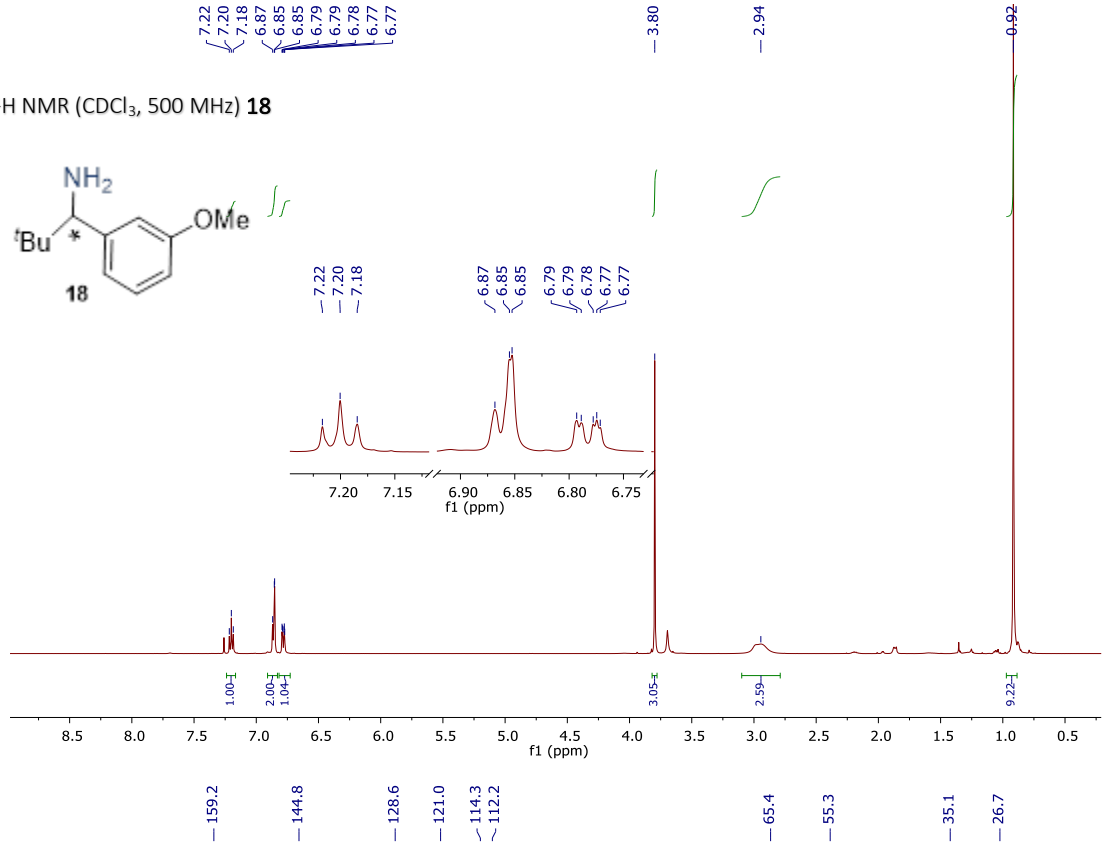


^{19}F NMR ($CDCl_3$, 376 MHz) **17**

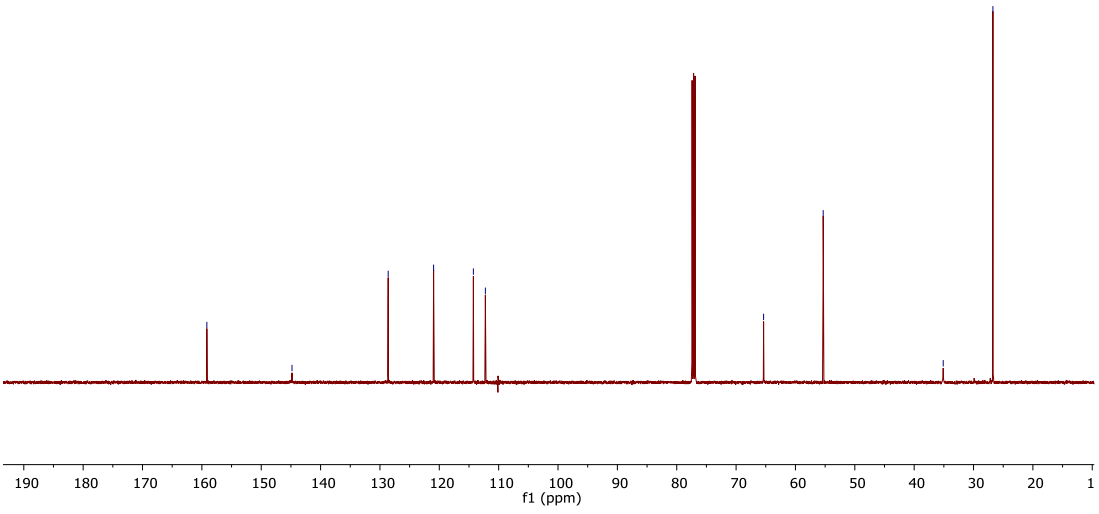


Compound **18**

^{1}H NMR ($CDCl_3$, 500 MHz) **18**

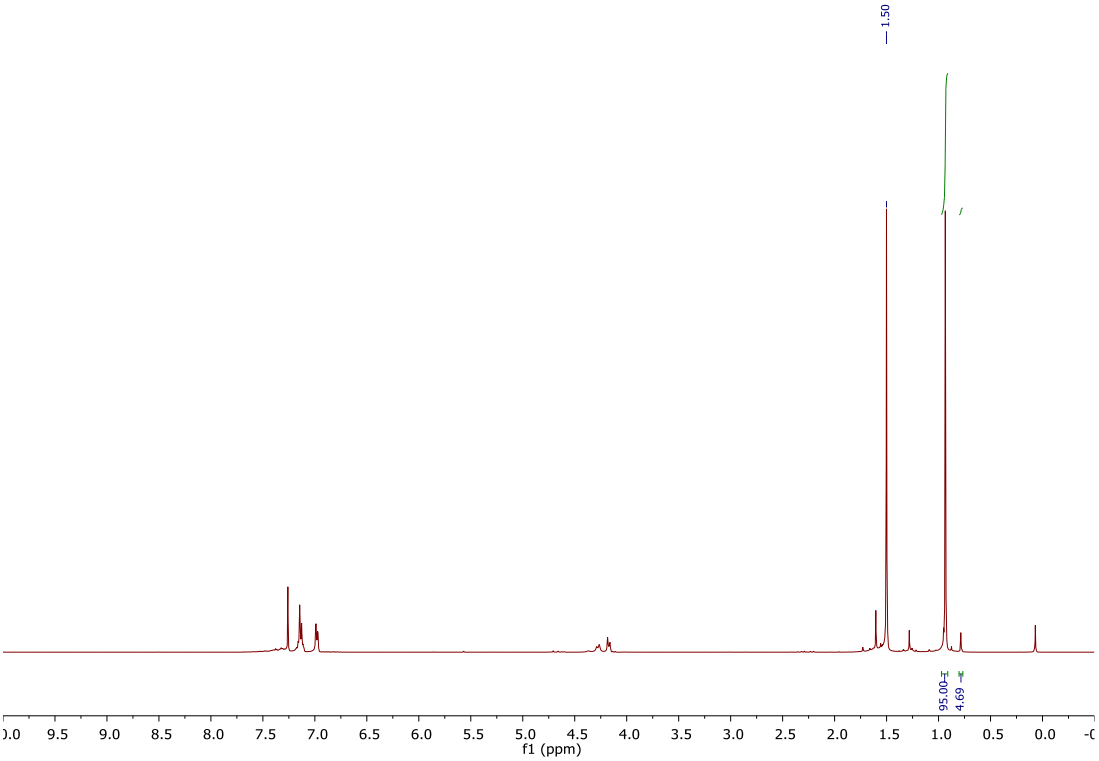


^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz) **18**

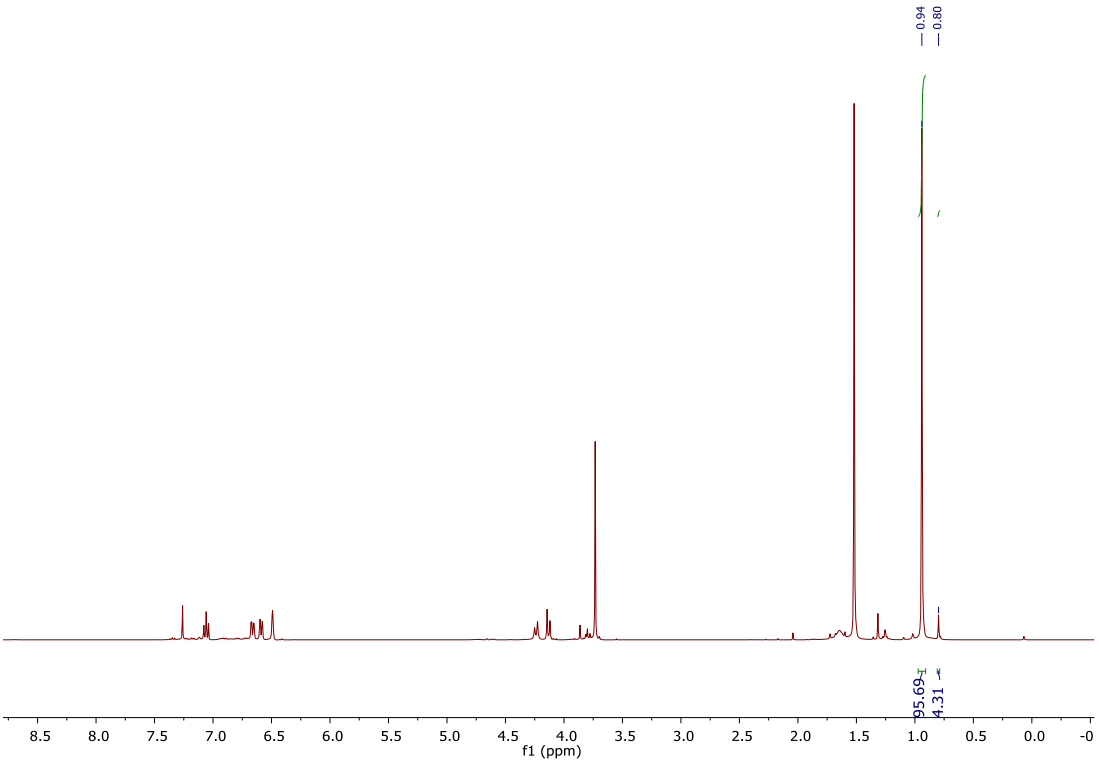


2. NMR spectra and HPLC chromatograms for the Grignard additions screening

^{1}H NMR (Table 4, entry 1)



^{1}H NMR (Table 4, entry 2)



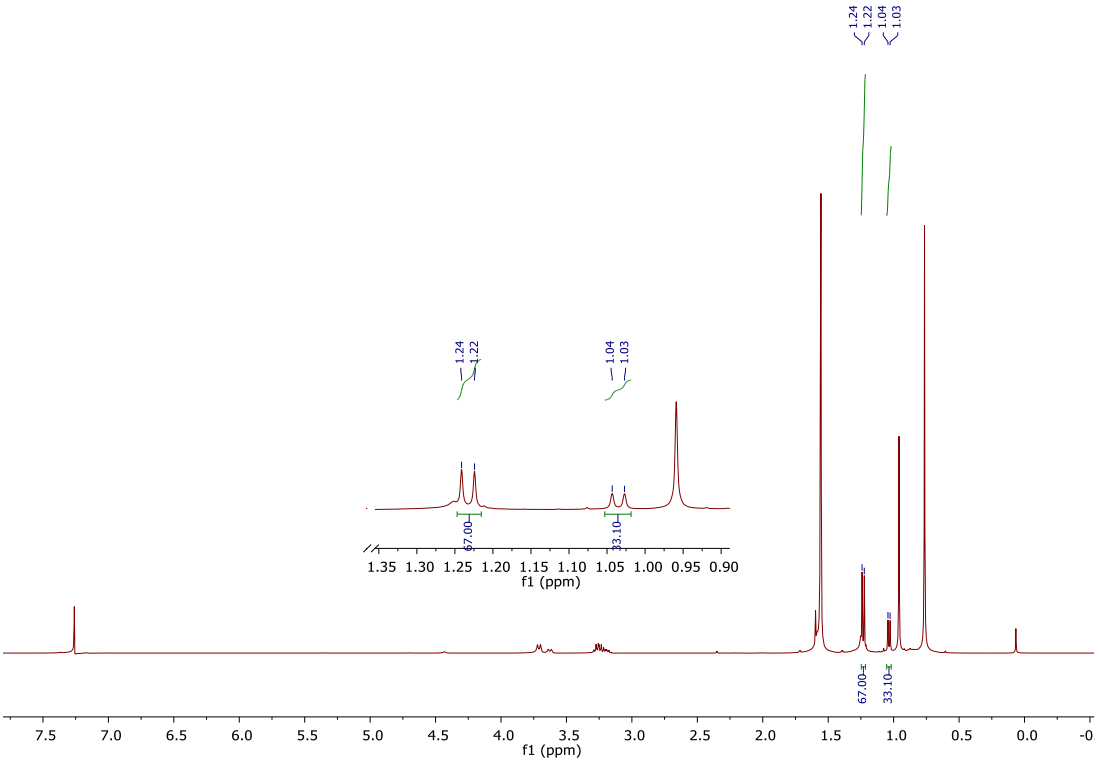
HPLC chromatogram (Table 4, entry 3)

Ret time[a]	Area	Height	Peak start	Peak end	% Area
8.3	1252887	58187	7.875	9.542	6.8
16.9	17063923	323836	16.158	20.858	93.2

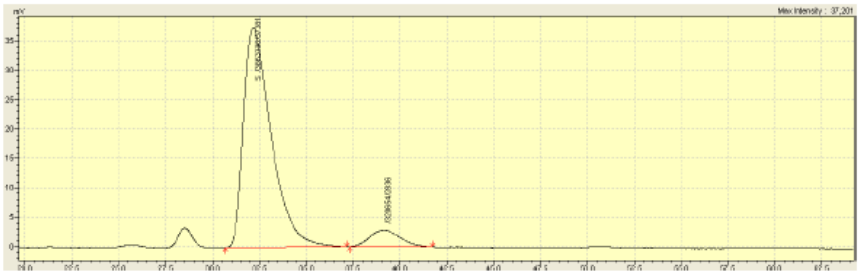
[a]0.5% *i*-PrOH

HPLC (Kromasil 5-CelluCoat RP, 0.46 cm × 25 cm, n-hexane/*iso*-propanol = 99.5/0.5, flow rate = 1.0 mL/min, λ = 220 nm) tR = 8.3 min (minor), 16.9 min (major).

^{1}H NMR (Table 4, entry 4)



HPLC chromatogram (Table 4, entry 6)

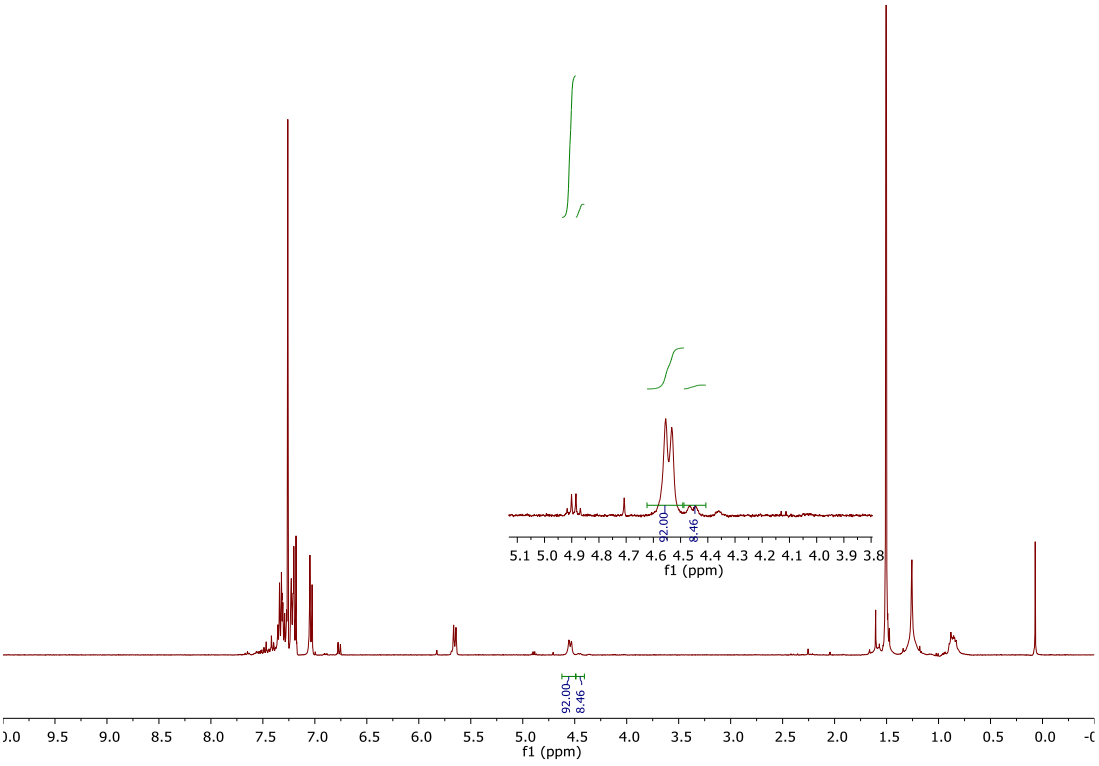


Ret time[a]	Area	Height	Peak start	Peak end	% Area
32.2	3863336	37381	30.692	37.15	92.3
39.1	320654	2836	37.292	41.733	7.7

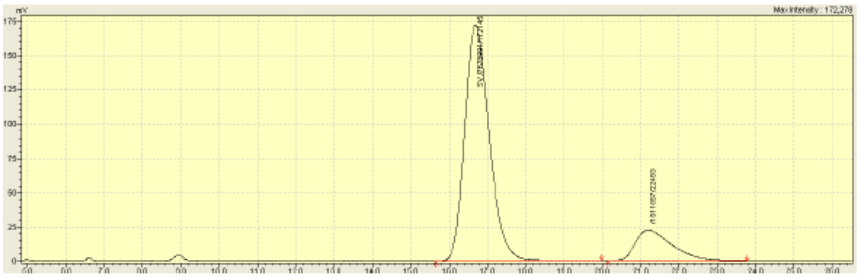
[a]0.2% *i*-PrOH

HPLC (Kromasil 5-CelluCoat RP, 0.46 cm × 25 cm, n-hexane/*iso*-propanol = 98.8/0.2, flow rate = 1.0 mL/min, λ = 220 nm) tR = 32.2 min (major), 39.1 min (minor).

^{1}H NMR (Table 4, entry 7)



HPLC chromatogram Table 4, entry 8

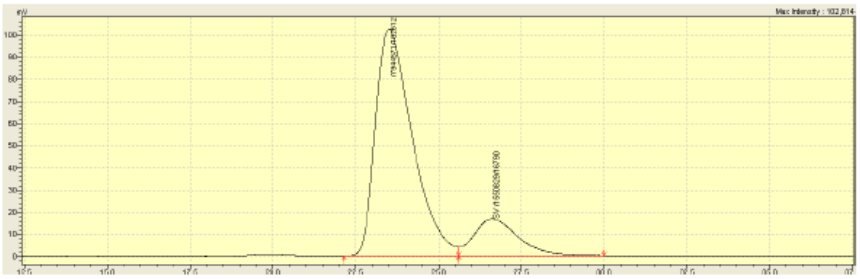


Ret time[a]	Area	Height	Peak start	Peak end	% Area
16.7	7678991	172145	15.667	19.975	81.0
21.2	1511857	22493	20.142	23.783	15.9

[a]2% *i*-PrOH

HPLC (Kromasil 5-CelluCoat RP, 0.46 cm × 25 cm, n-hexane/*iso*-propanol = 98/2, flow rate = 1.0 mL/min, λ = 220 nm) tR = 16.7 min (major), 21.2 min (minor).

HPLC chromatogram (Table 4, entry 9)

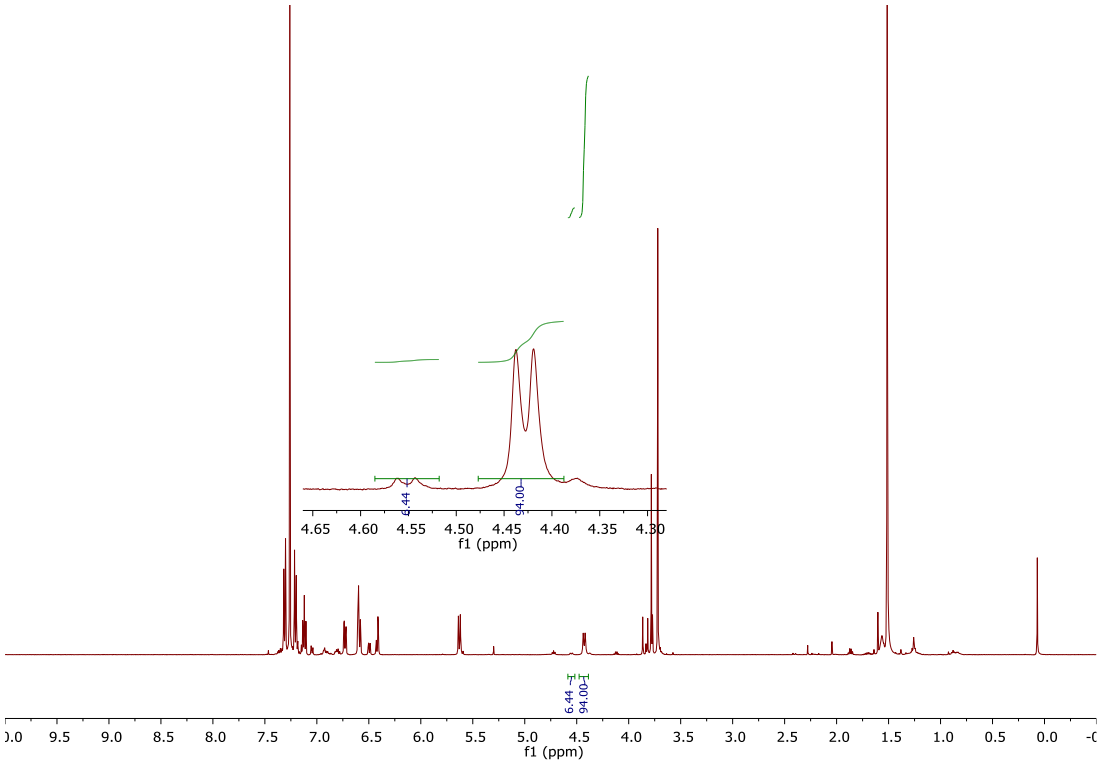


Ret time[a]	Area	Height	Peak start	Peak end	% Area
23.5	7944571	102612	22.15	25.608	83.7
26.6	1550829	16790	25.608	30	16.3

[a]0.5% *i*-PrOH

HPLC (Kromasil 5-CelluCoat RP, 0.46 cm × 25 cm, n-hexane/*iso*-propanol = 99.5/0.5, flow rate = 1.0 mL/min, λ = 220 nm) tR = 23.5 min (major), 26.6 min (minor).

^{1}H NMR (Table 4, entry 10)



3. HRMS spectra

Compound (*S*)-**1**

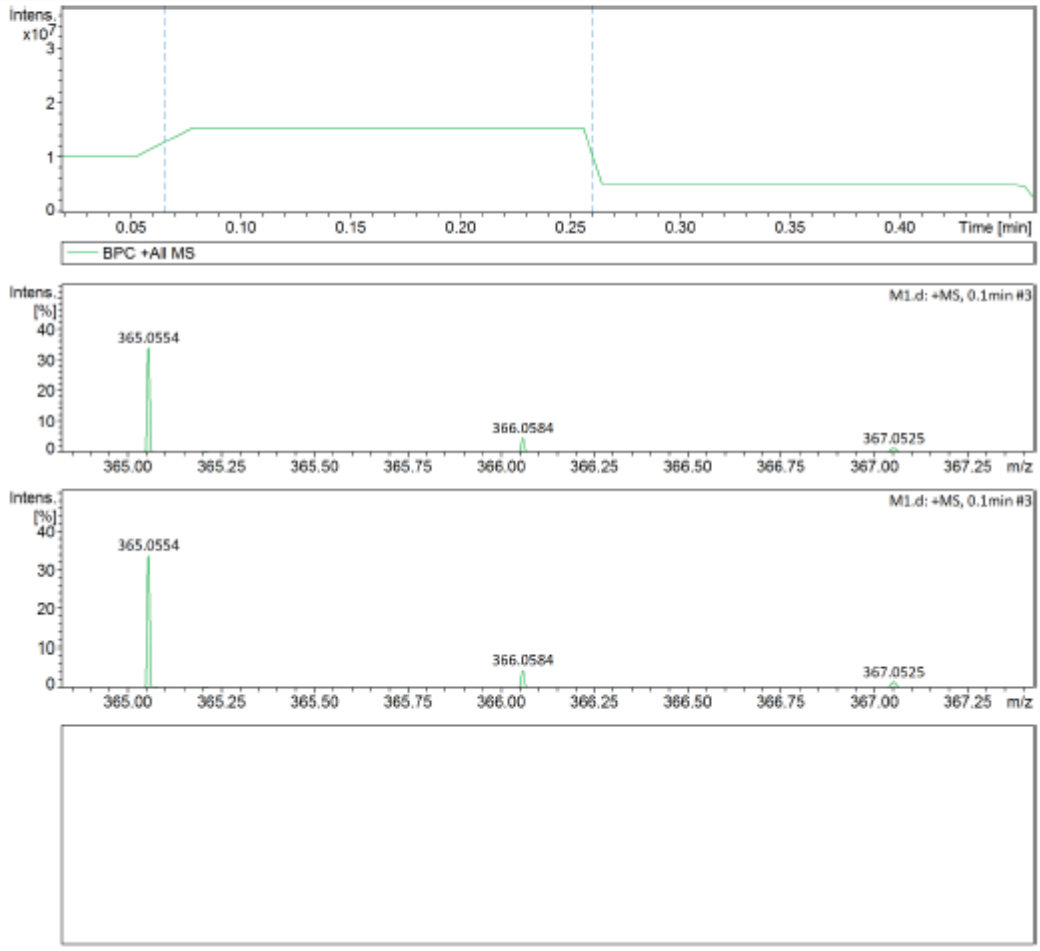
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M1.d	Acquisition Date	8/22/2021 12:47:18 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



M1.d

Bruker Compass DataAnalysis 4.4 printed: 8/22/2021 5:58:37 PM by: demo Page 1 of 1

Compound (*R*)-**1**

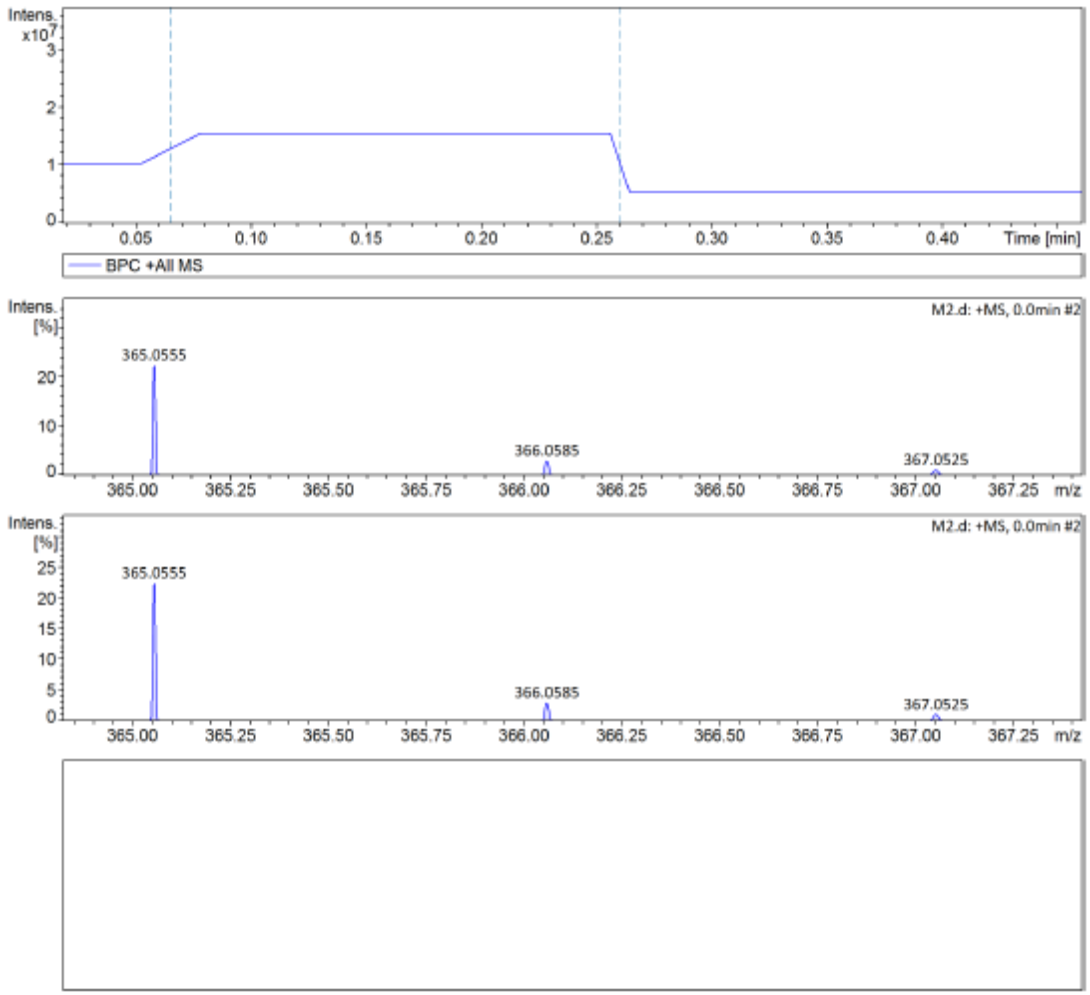
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M2.d	Acquisition Date	8/22/2021 1:06:27 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



M2.d

Bruker Compass DataAnalysis 4.4 printed: 8/22/2021 6:00:11 PM by: demo Page 1 of 1

Compound (*S*)-**2**

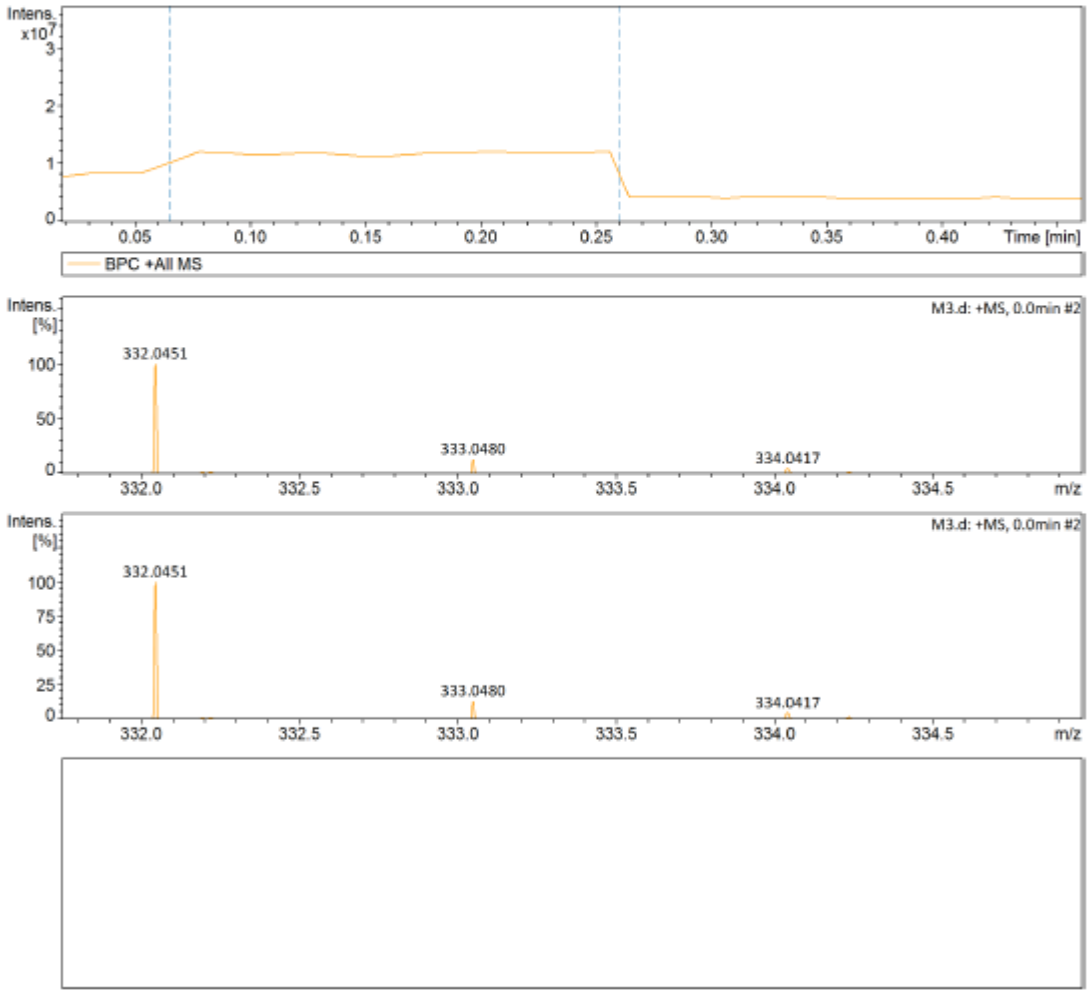
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M3.d	Acquisition Date	8/22/2021 1:08:57 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



Compound (*S*)-**3**

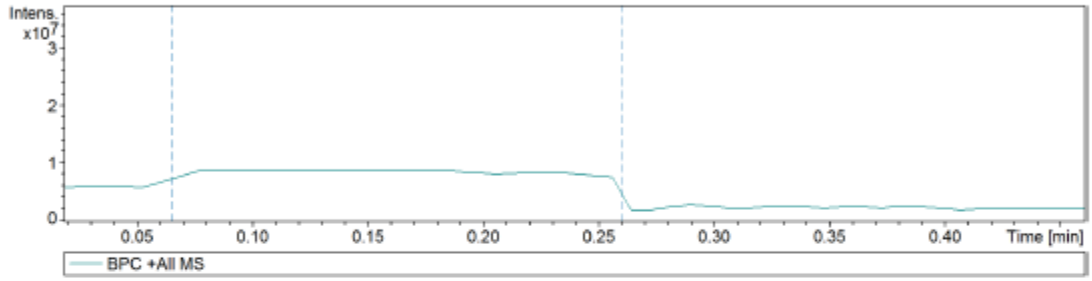
Display Report

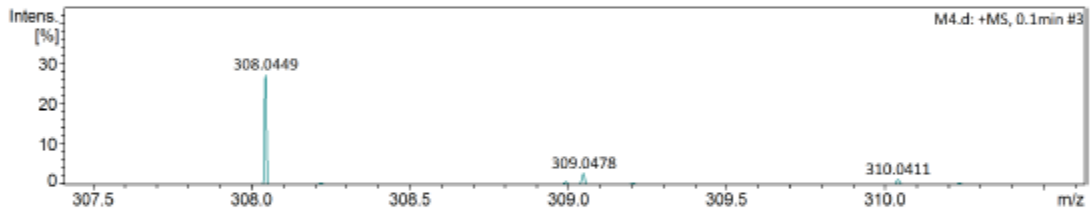
Analysis Info

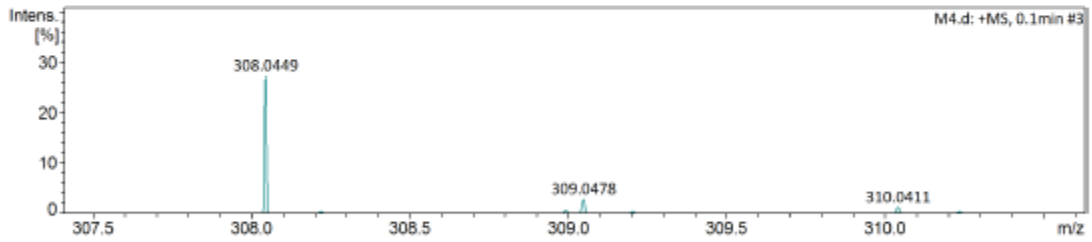
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M4.d	Acquisition Date	8/22/2021 12:00:36 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M4.d

Bruker Compass DataAnalysis 4.4 printed: 8/22/2021 6:03:04 PM by: demo Page 1 of 1

Compound (*R*)-**3**

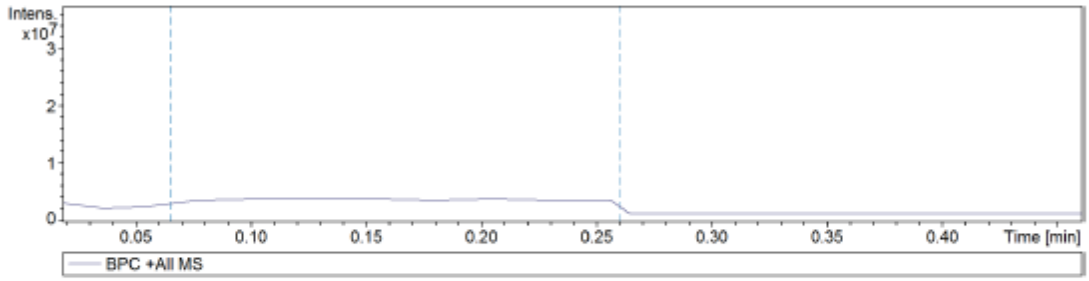
Display Report

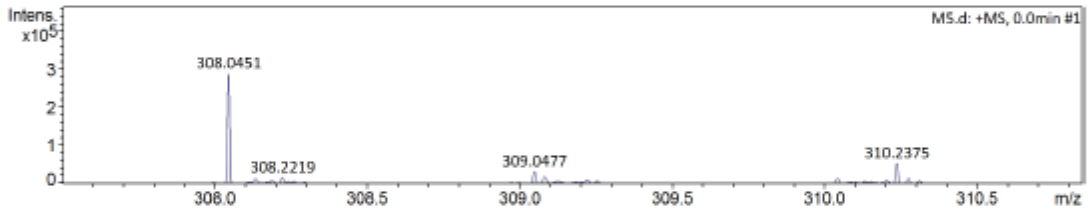
Analysis Info

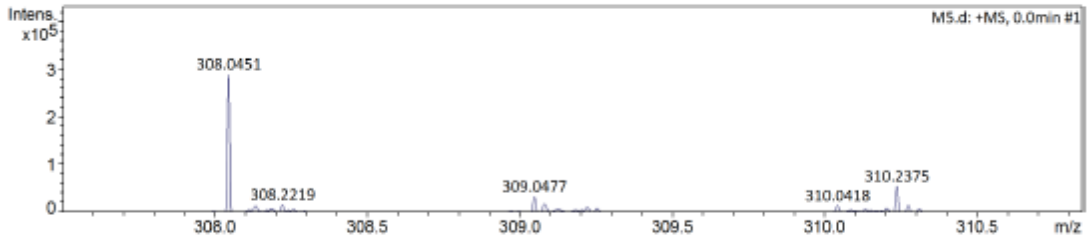
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M5.d	Acquisition Date	8/22/2021 12:41:50 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M5.d

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Compound (*S*)-**4**

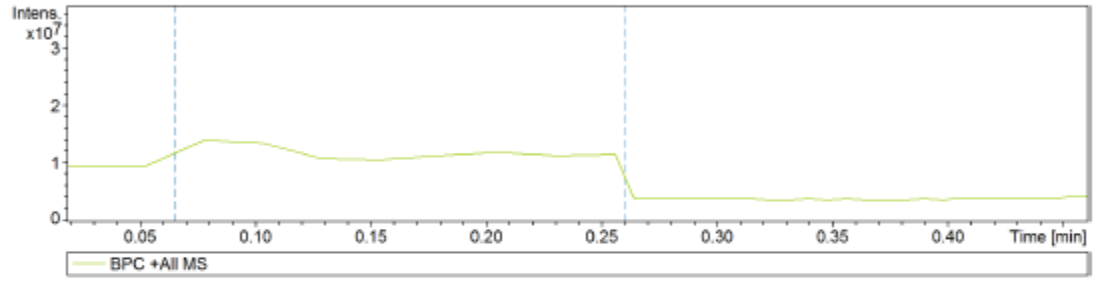
Display Report

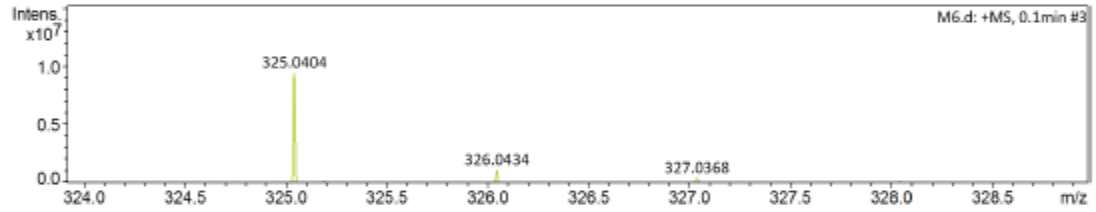
Analysis Info

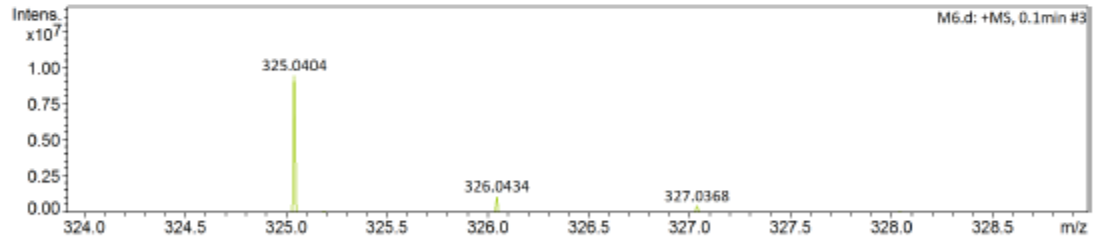
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M6.d	Acquisition Date	8/22/2021 12:34:27 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M6.d

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Compound (*S*)-**5**

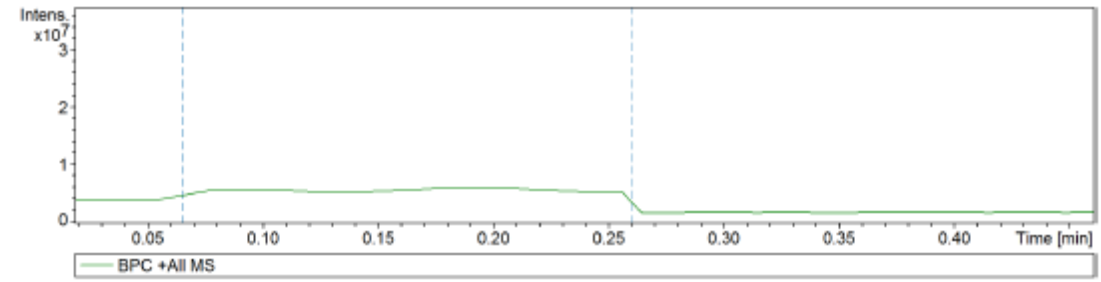
Display Report

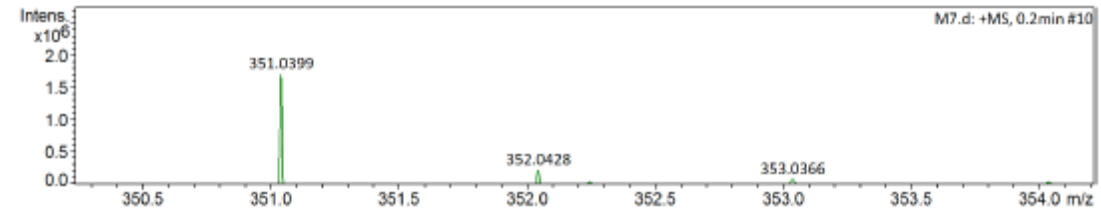
Analysis Info

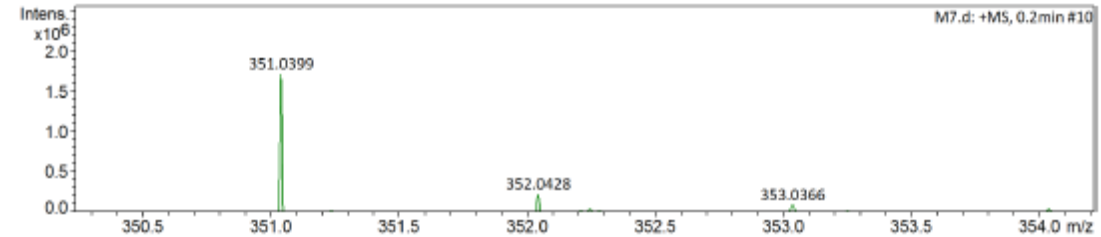
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M7.d	Acquisition Date	8/22/2021 12:11:18 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M7.d

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Compound (*S*)-**7**

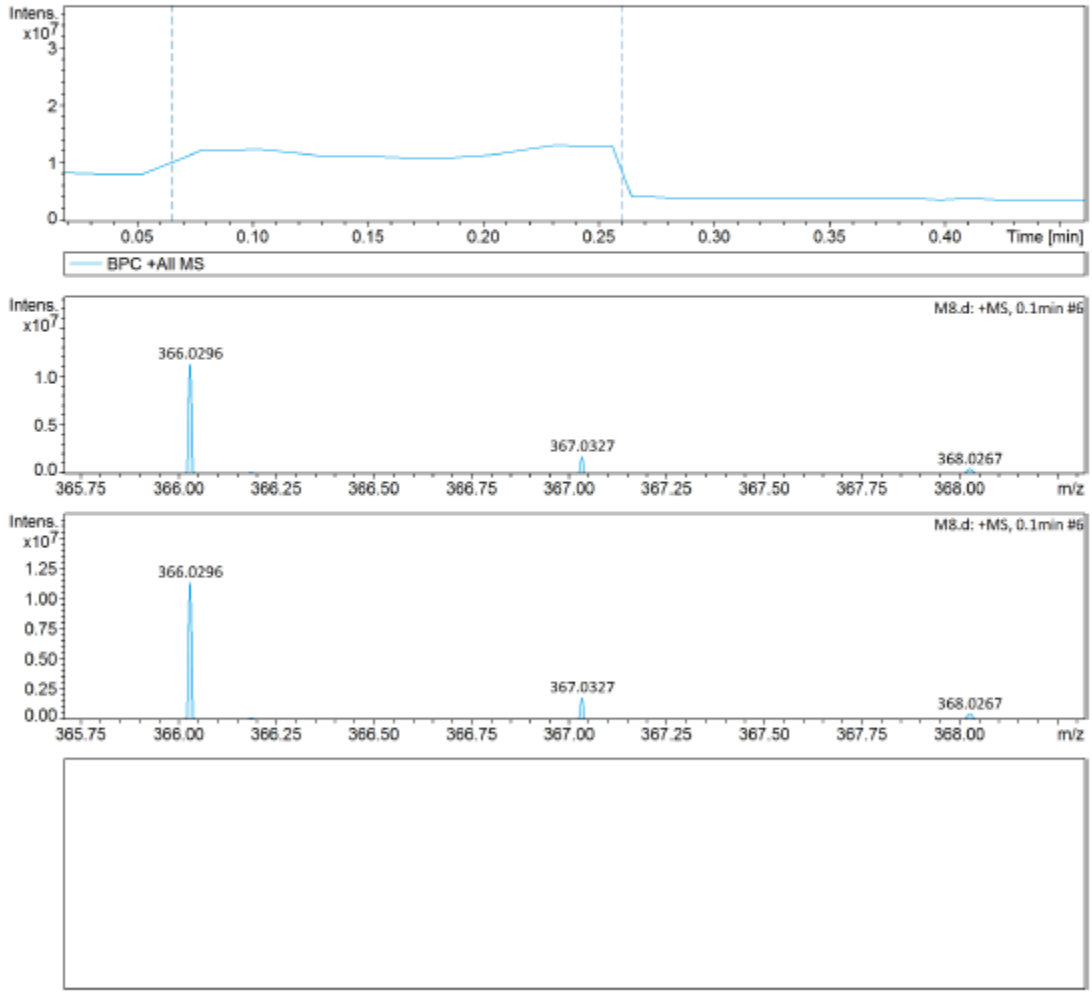
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M8.d	Acquisition Date	8/22/2021 12:31:53 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



M8.d

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Compound Rac-**8**

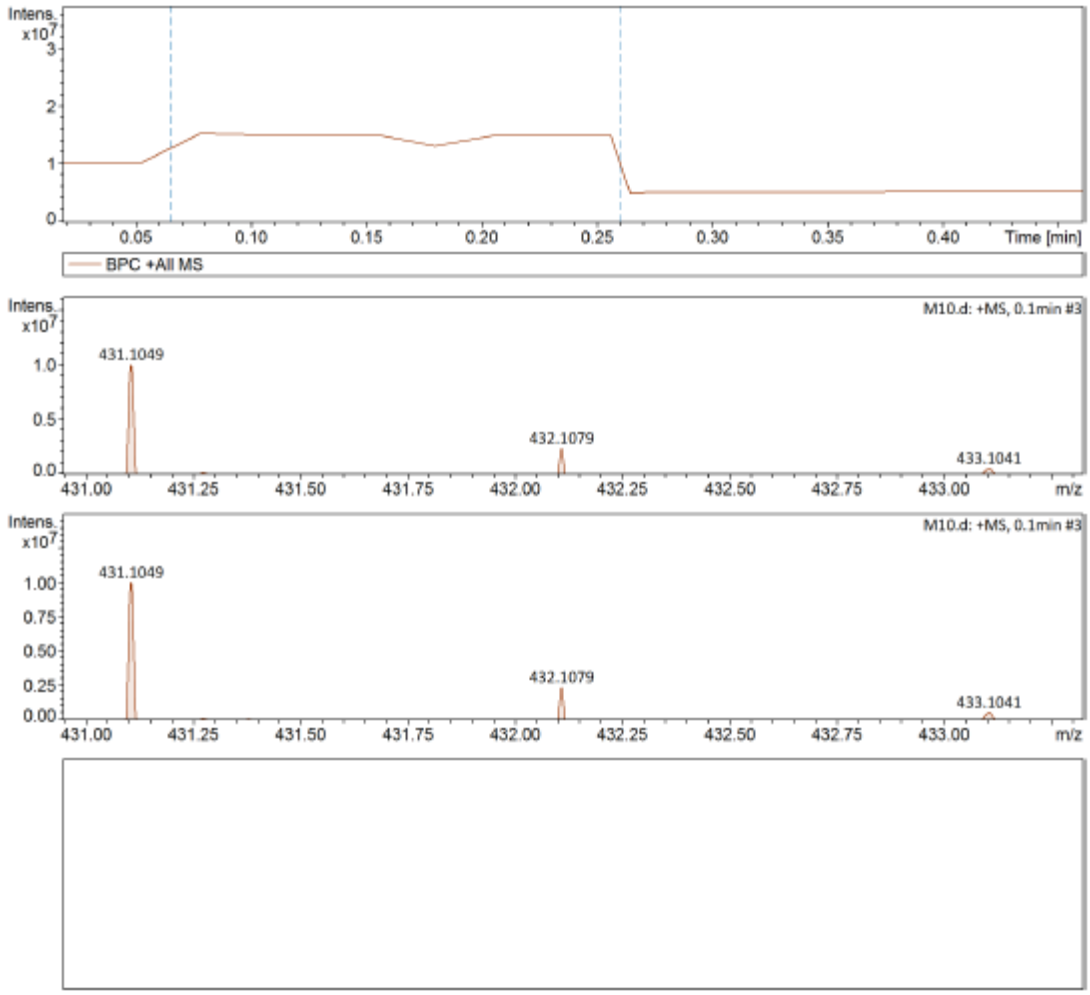
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M10.d	Acquisition Date	8/22/2021 12:08:39 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



Compound **9**

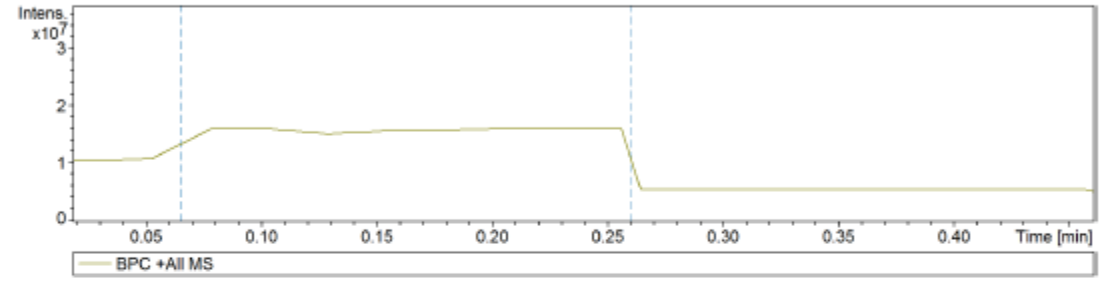
Display Report

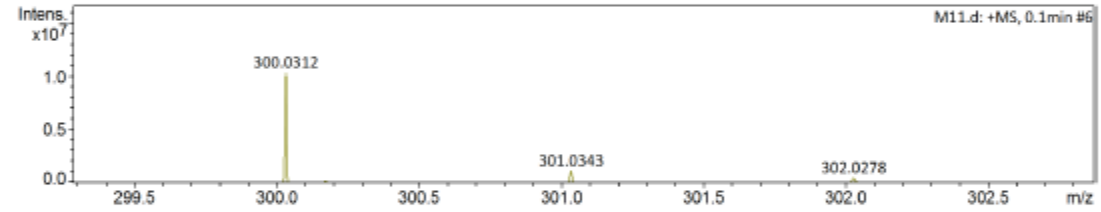
Analysis Info

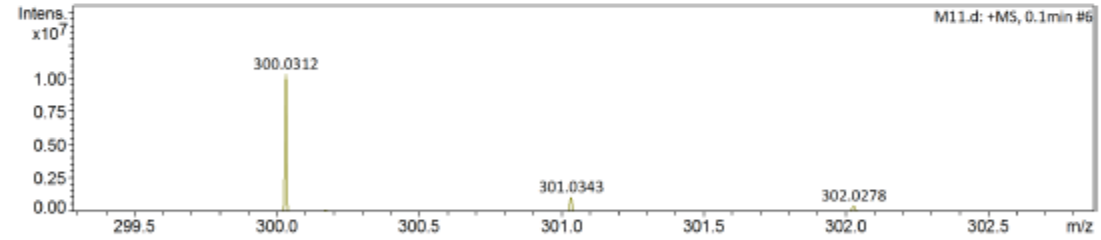
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M11.d	Acquisition Date	8/22/2021 12:54:55 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M11.d

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Compound Rac-**10**

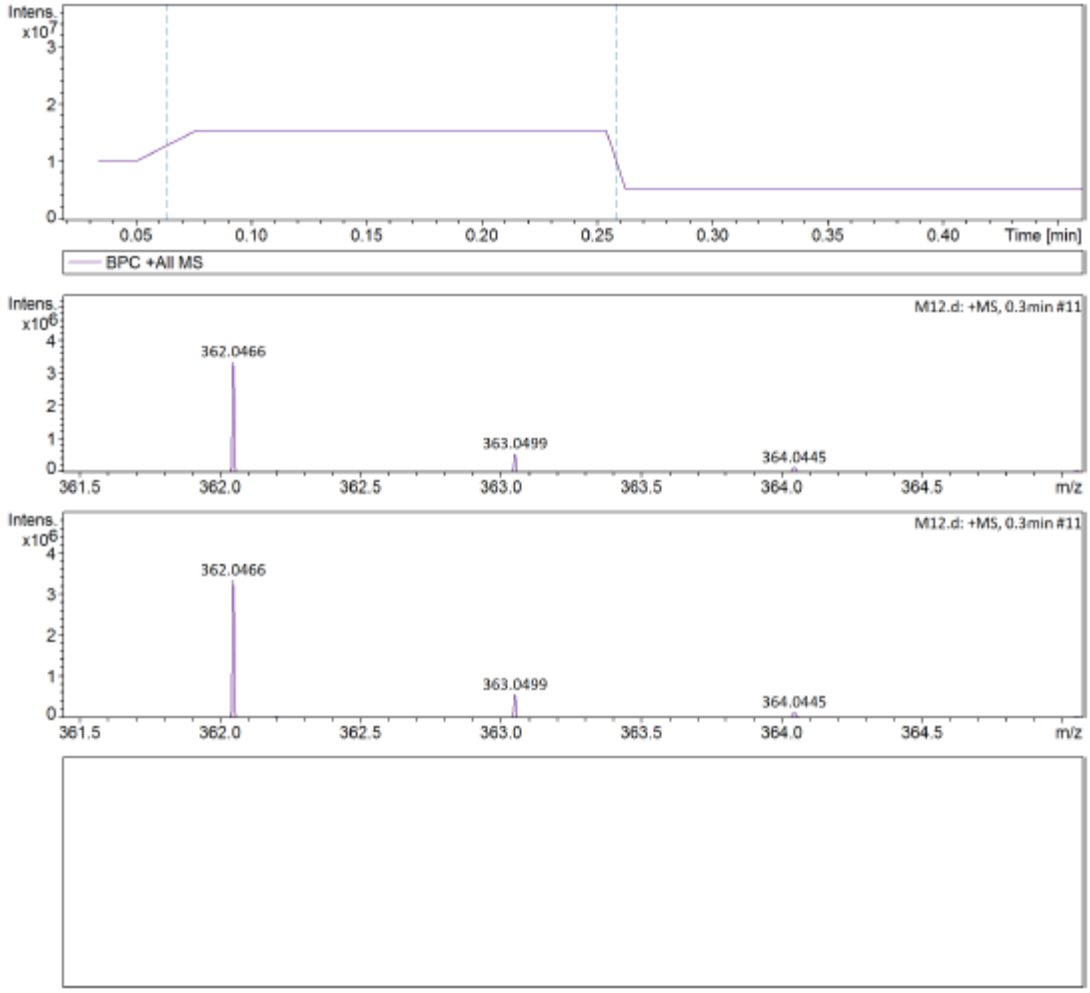
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M12.d	Acquisition Date	8/22/2021 12:03:09 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



Rac-**11**

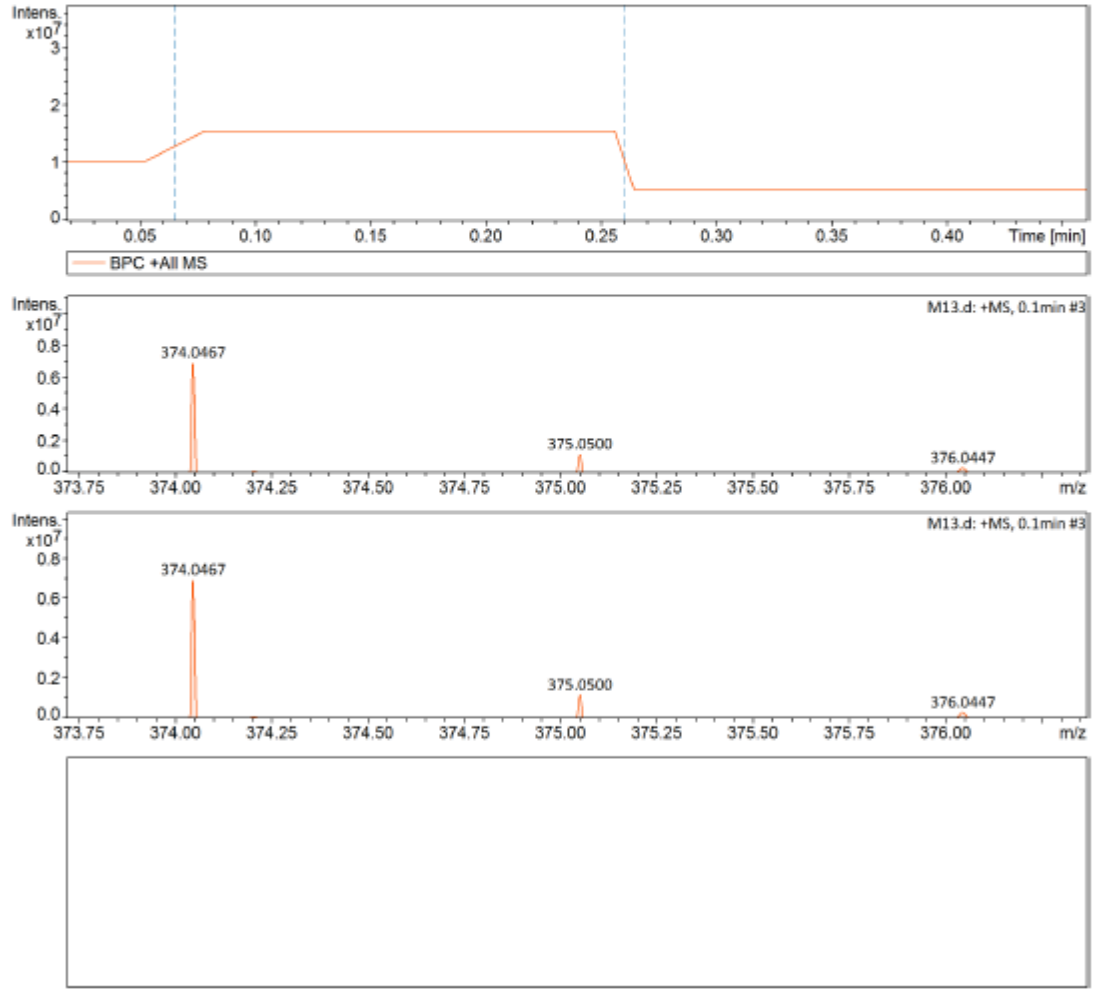
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M13.d	Acquisition Date	8/22/2021 12:37:33 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



Compound Rac-**12**

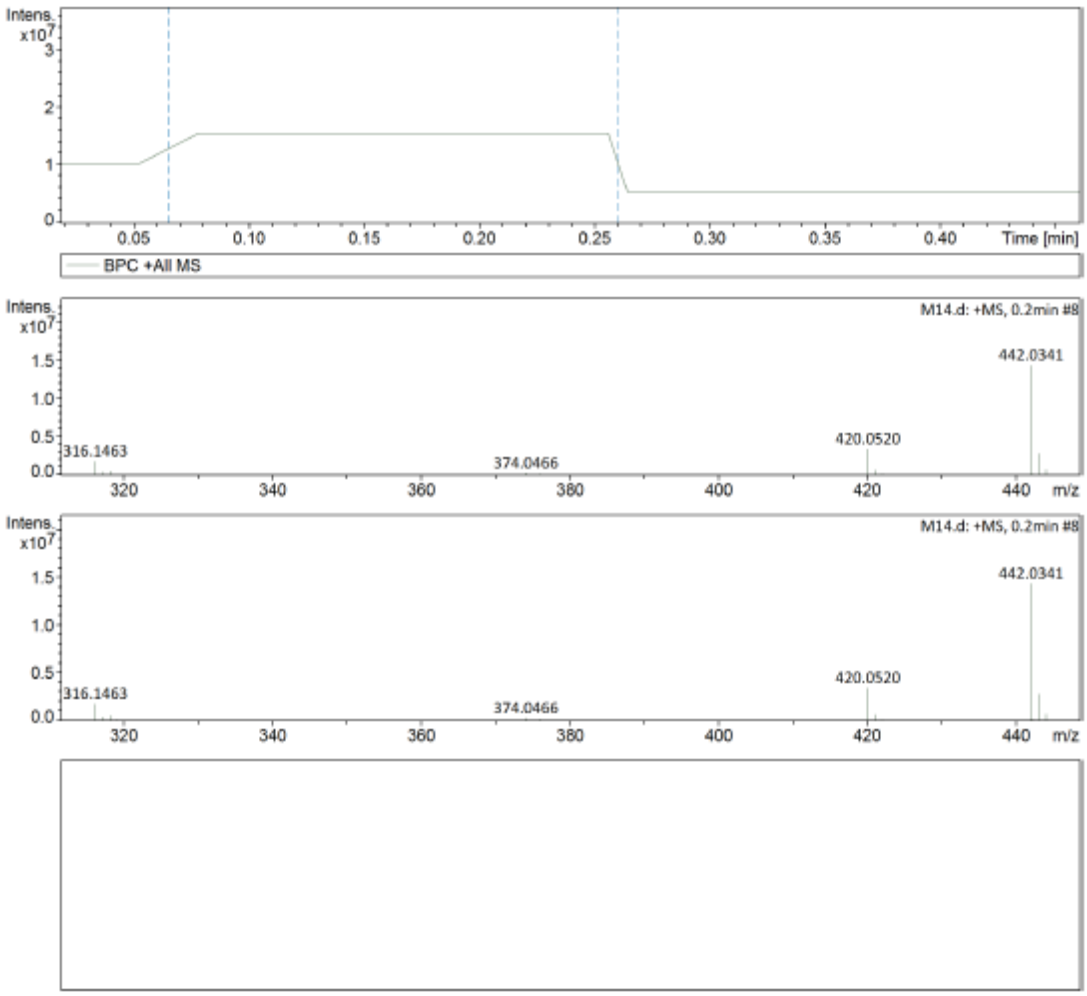
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M14.d	Acquisition Date	8/22/2021 1:03:44 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



Compound (*R*)-**13**

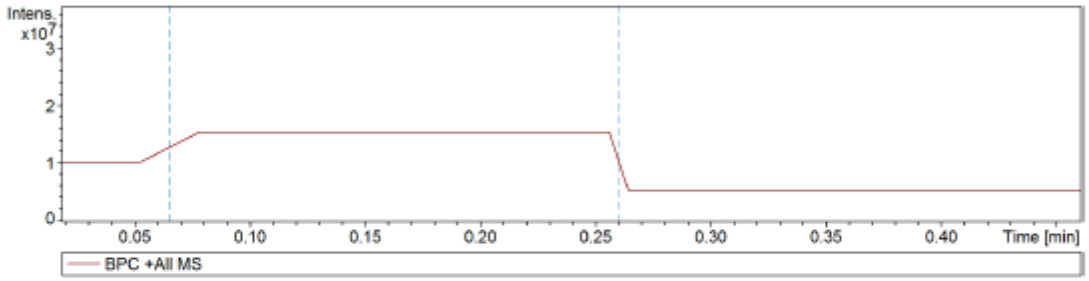
Display Report

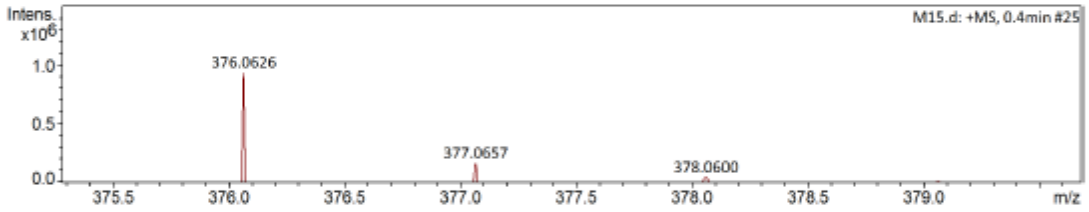
Analysis Info

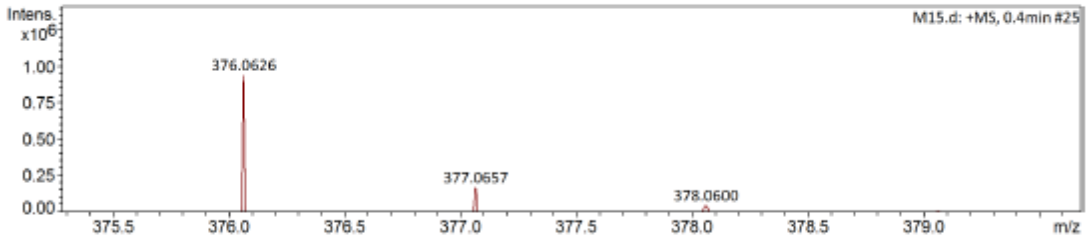
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M15.d	Acquisition Date	8/22/2021 12:57:23 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M15.d

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Compound rac-**14**

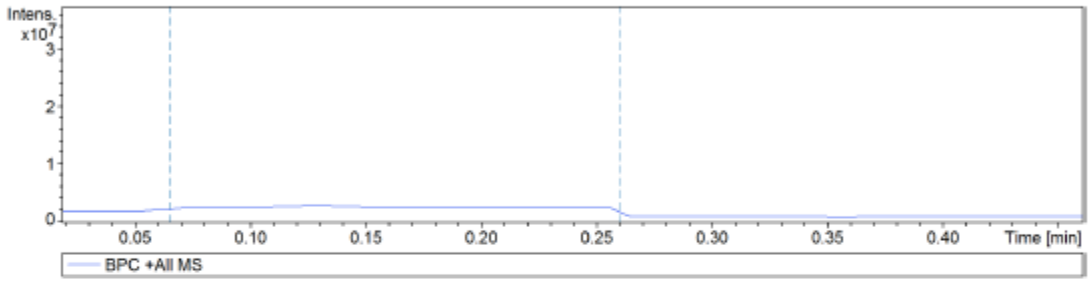
Display Report

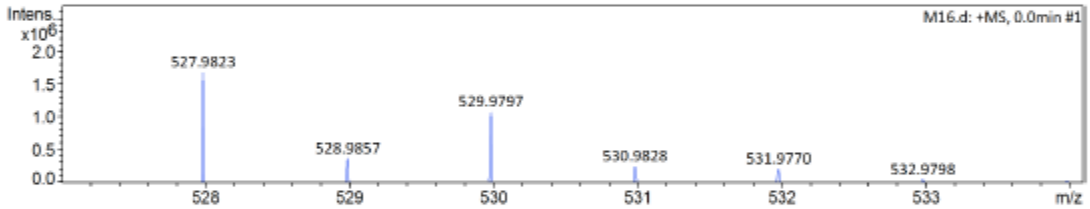
Analysis Info

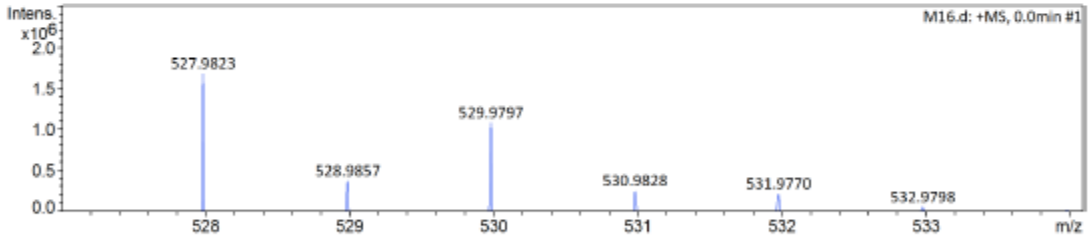
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M16.d	Acquisition Date	8/22/2021 12:13:59 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M16.d

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Compound **15**

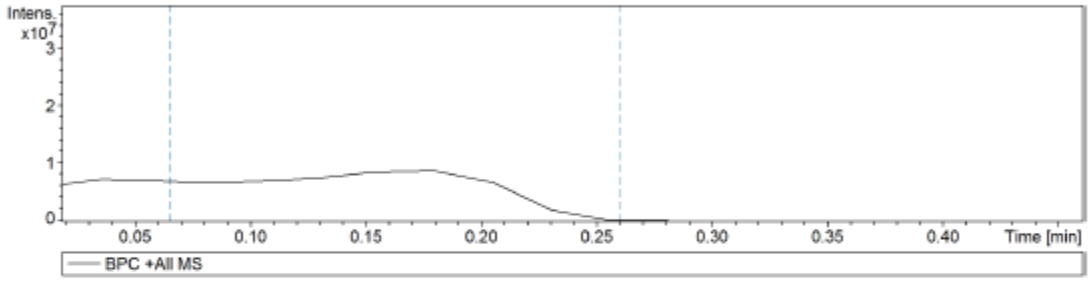
Display Report

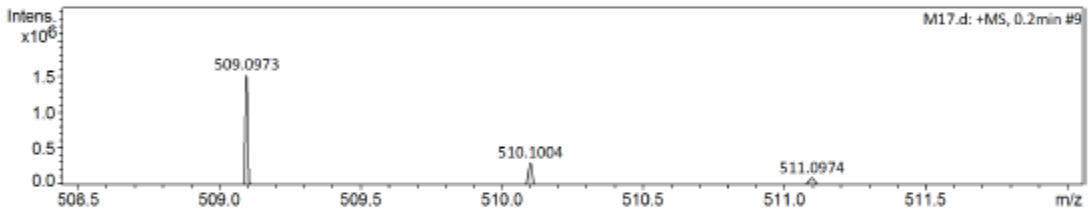
Analysis Info

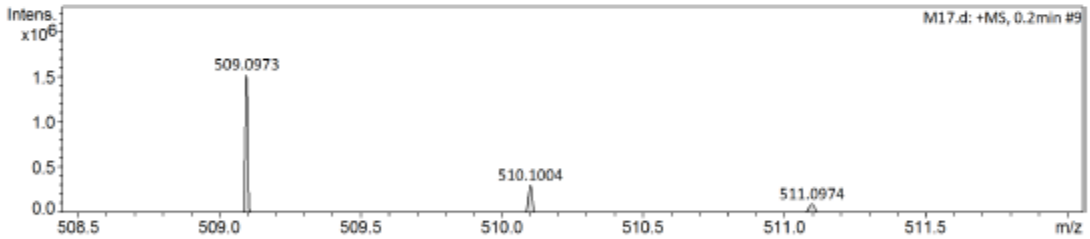
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M17.d	Acquisition Date	8/22/2021 1:11:36 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M17.d

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Compound (*R*)-**16a**

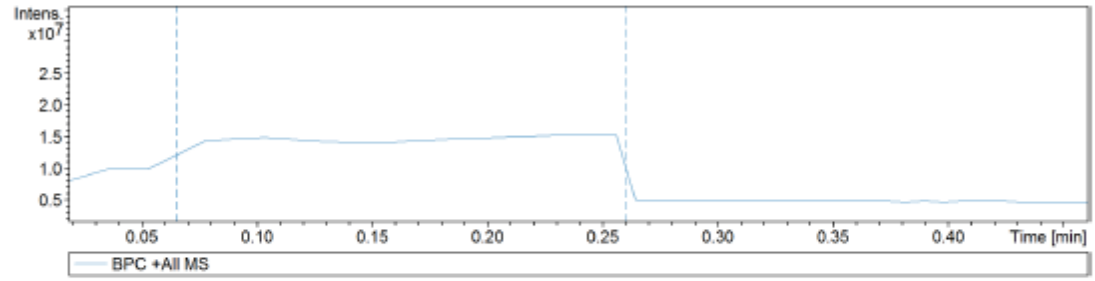
Display Report

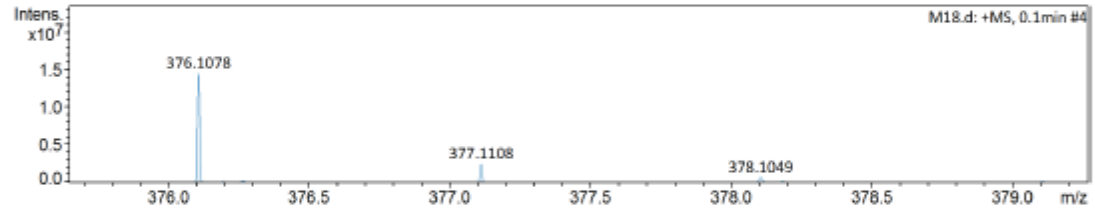
Analysis Info

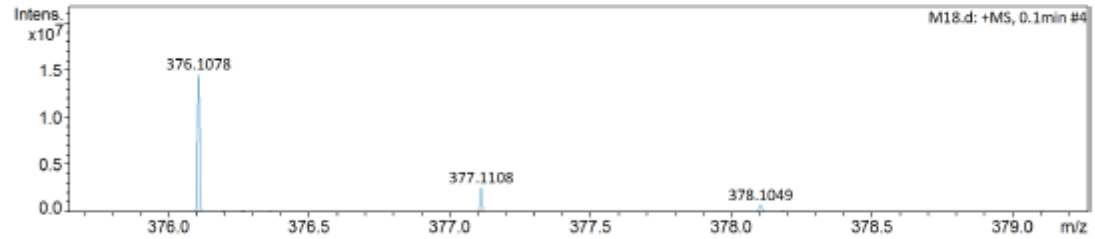
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M18.d	Acquisition Date	8/22/2021 1:13:21 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







Compound (*R*)-**16b**

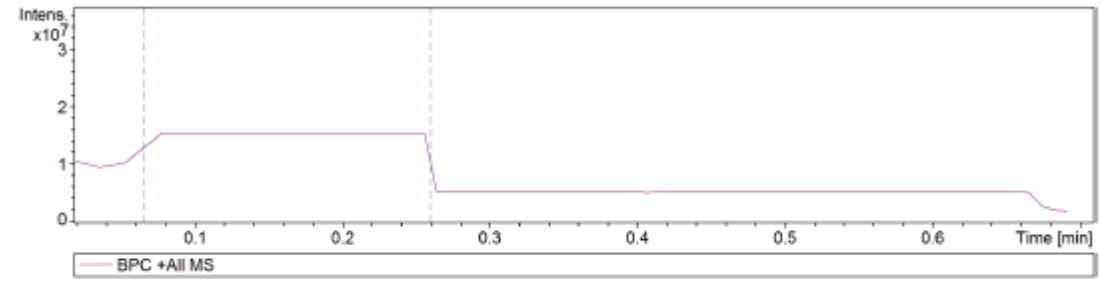
Display Report

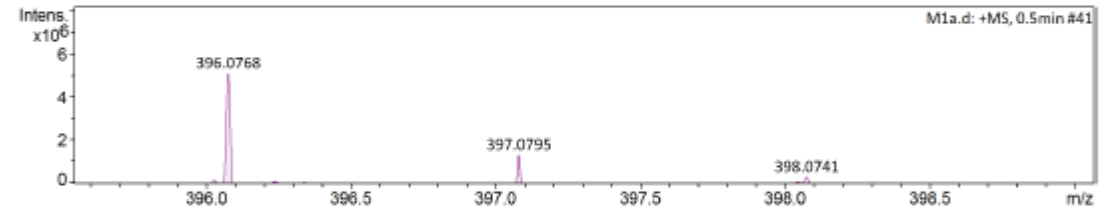
Analysis Info

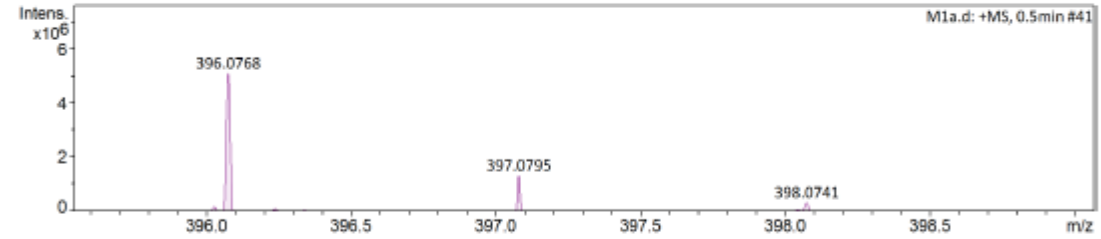
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M1a.d	Acquisition Date	8/22/2021 1:15:54 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M1a.d

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Compound (*R*)-**16c**

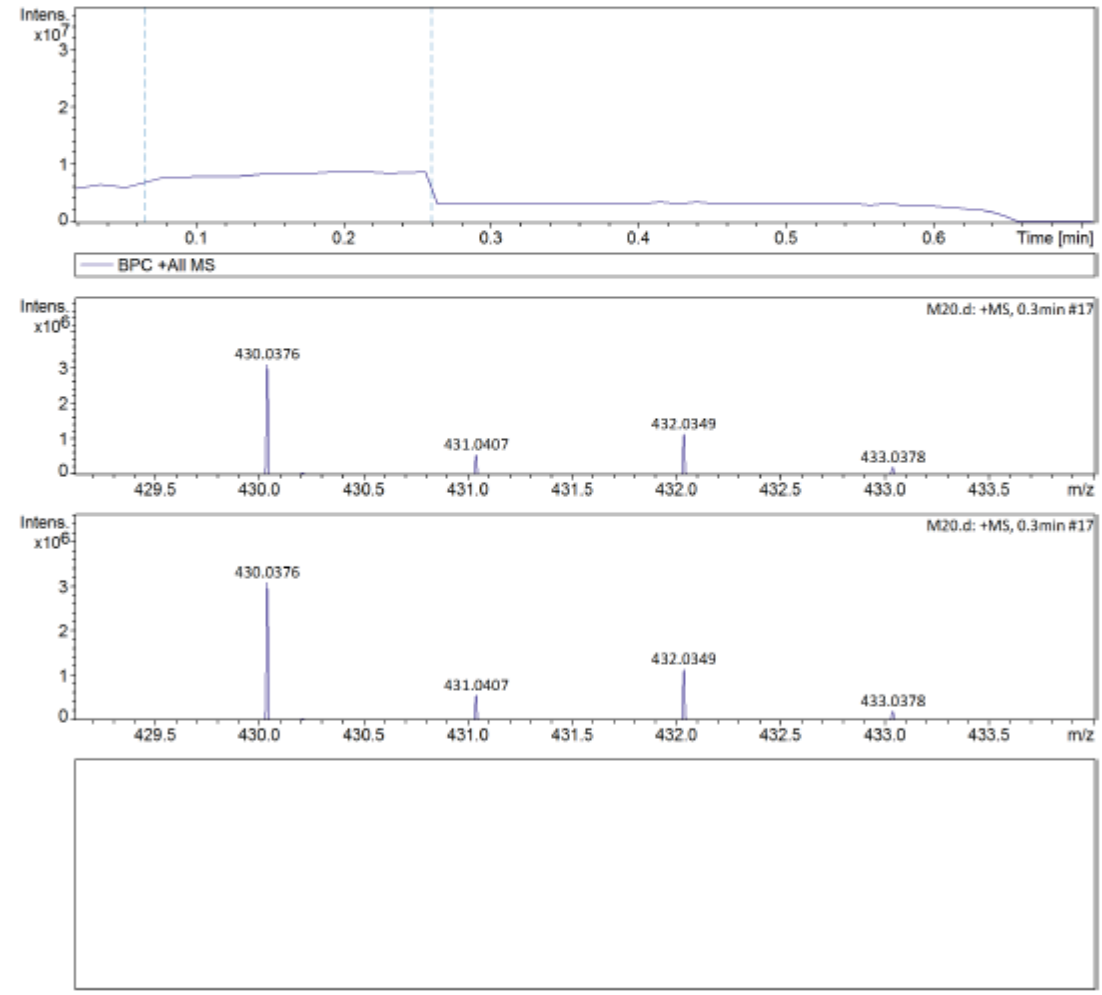
Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M20.d	Acquisition Date	8/22/2021 12:44:11 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C



Compound **17**

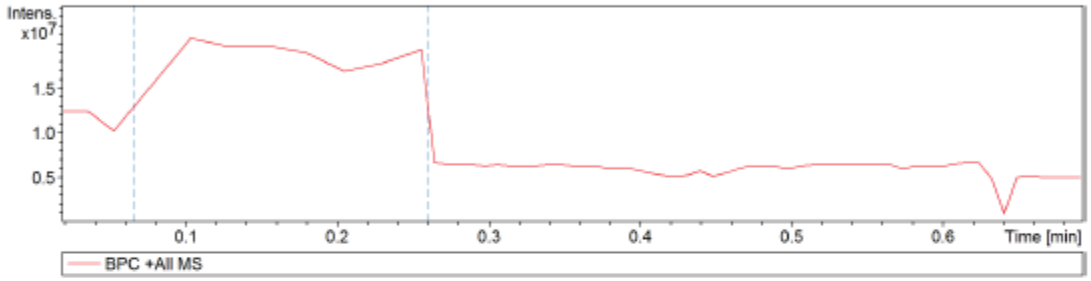
Display Report

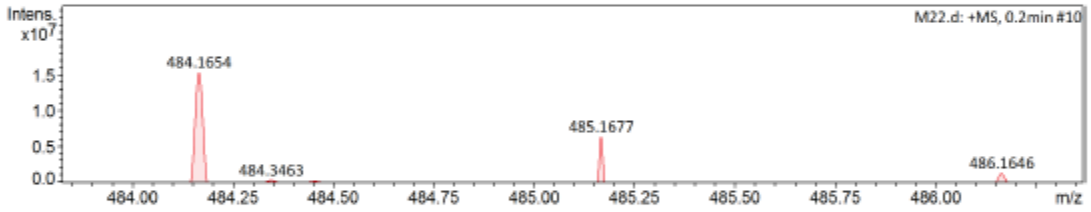
Analysis Info

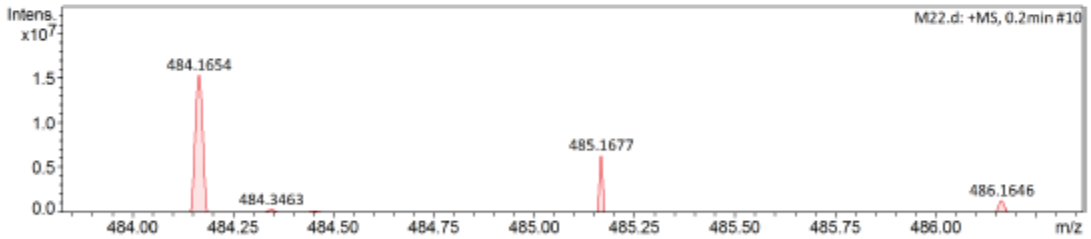
Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M22.d	Acquisition Date	8/22/2021 12:29:10 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825265.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C







M22.d

Bruker Compass DataAnalysis 4.4 printed: 8/22/2021 6:40:12 PM by: demo Page 1 of 1

Compound **18**

Display Report

Analysis Info

Analysis Name	D:\Data\RawData\Azamat\KTH\Batch_2_final\M21.d	Acquisition Date	8/22/2021 12:59:57 PM
Method	MS_fullscan_positive.m	Operator	Demo User
Sample Name	NaFormate	Instrument	impact II 1825285.10235
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	250 °C
Scan Begin	150 m/z	Set End Plate Offset	-400 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	4000 nA	Set APCI Heater	200 °C