Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Persistent azulene α-carbocations: Synthesis from aldehydes, spectroscopic and crystallographic properties

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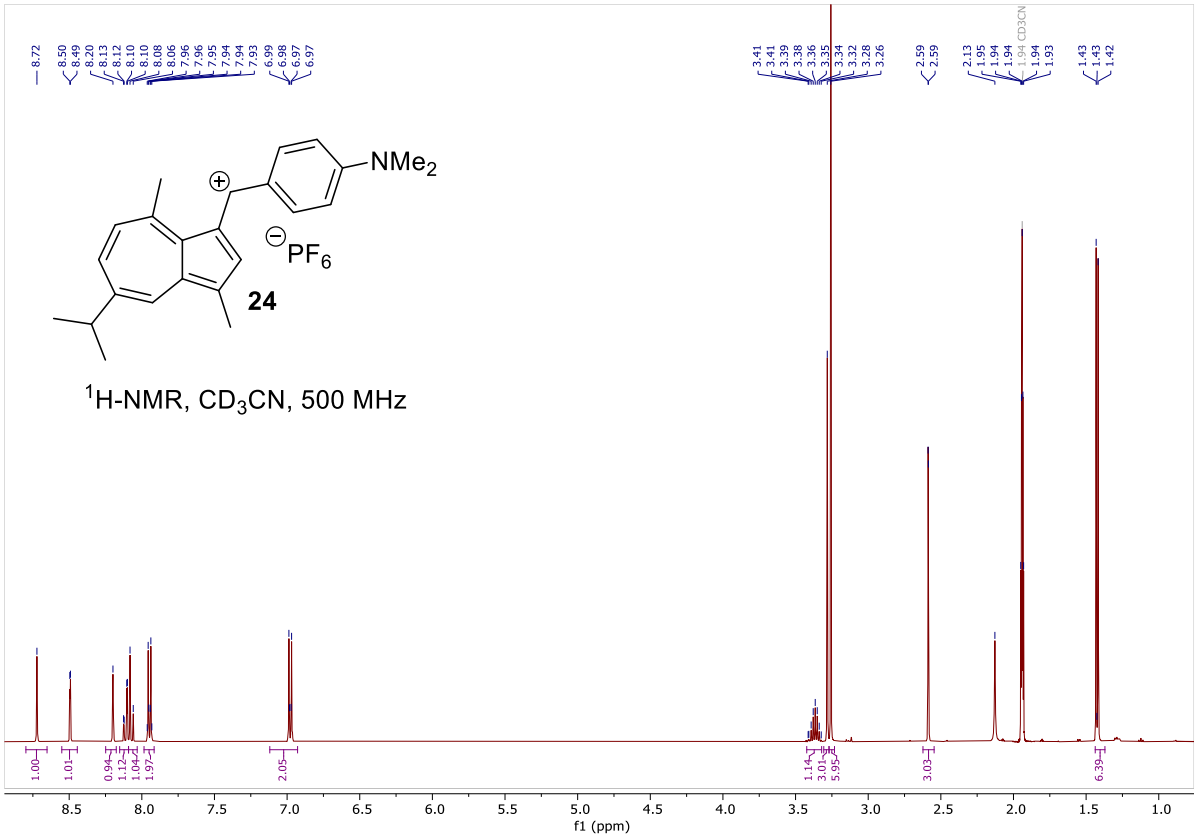
ELECTRONIC SUPPORTING INFORMATION

General Experimental Details

Synthetic chemistry and compound characterisation. Reagents were purchased from Fluorochem, Merck and Alfa-Aesar. Reactions were carried out under an atmosphere of air. Solvents were removed using Büchi rotary evaporators and with high vacuum on a Schlenk line. Capillary melting points were recorded on a Büchi 535 melting point apparatus and are uncorrected. UV-Vis experiments were performed on a Shimadzu UV-1800 UV spectrometer, for which a quartz cuvette of 1 cm path length was used. ^{1}H and ^{13}C NMR spectra were obtained using a 500 MHz Agilent ProPulse 500 or a 300 MHz Bruker NMR spectrometer, for which proton decoupling was active for ^{13}C NMR. Spectra were acquired at 298 K and were referenced to residual solvent peaks; chemical shifts are reported in parts per million (ppm) relative to residual acetonitrile (δ = 1.94 ppm, ^{1}H; 1.32 ppm, ^{13}C). Coupling constants, *J*, reported in Hz, were calculated using MestreNova 9.0 to the nearest 0.1 Hz. ^{1}H and ^{13}C{^{1}H} assignments for novel compounds are corroborated though 2D (COSY, HSQC, HMBC). Infrared (IR) spectra were recorded on a Perkin-Elmer Spectrum 100 ATR-FTIR spectrometer with only selected absorbances quoted as ν in cm^{-1}. For mass spectrometry a microTOF electrospray time-of-flight (ESI-TOF) mass spectrometer (Bruker Daltonik GmbH, Bremen, Germany) was used. Data are reported in the form of *m*/*z*. The observed mass and isotope pattern matched the corresponding theoretical values as calculated from the expected molecular formula. X-Ray crystallography was recorded on a Nonius Kappa CCD diffractometer with Mo-Kα radiation (λ=0.71074 Å). All structures were solved by direct methods and refined on all F2 data using SHELX-97 suite of programs.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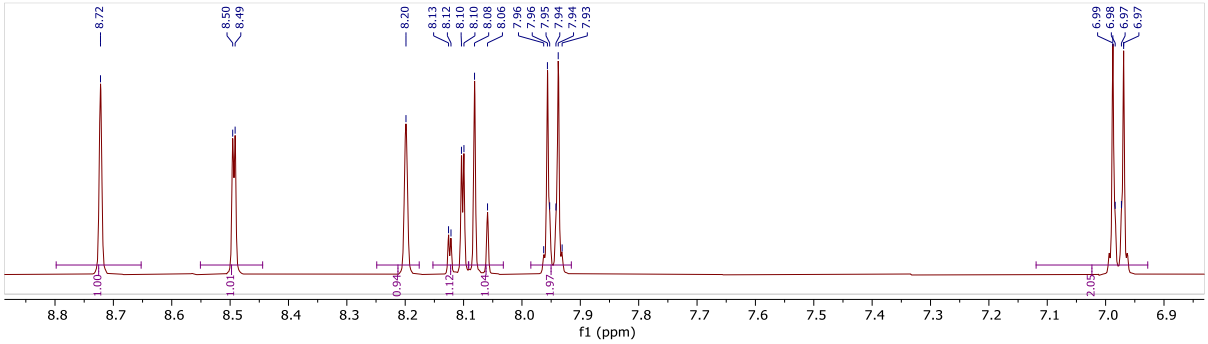
f1 (ppm)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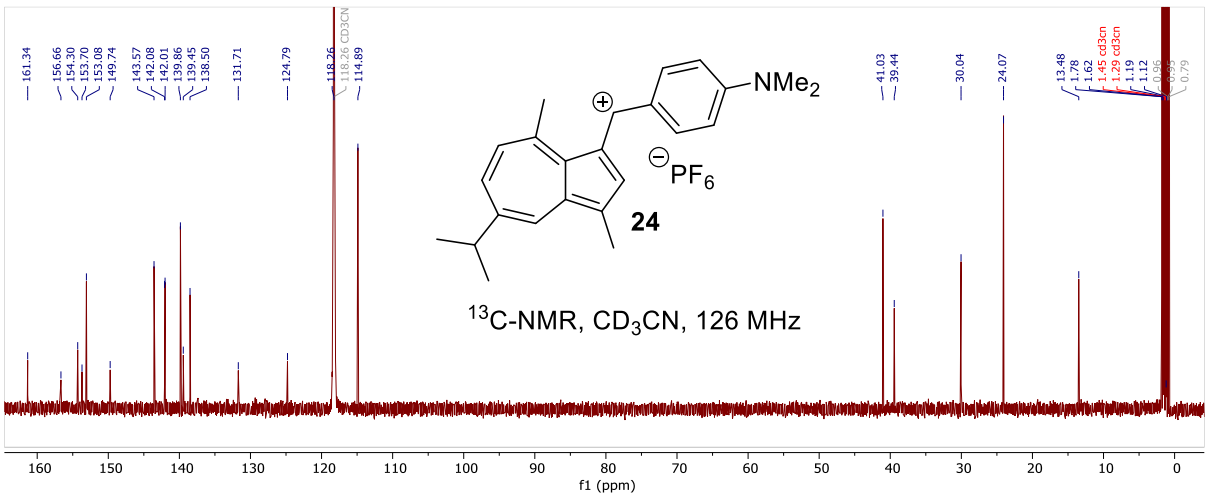
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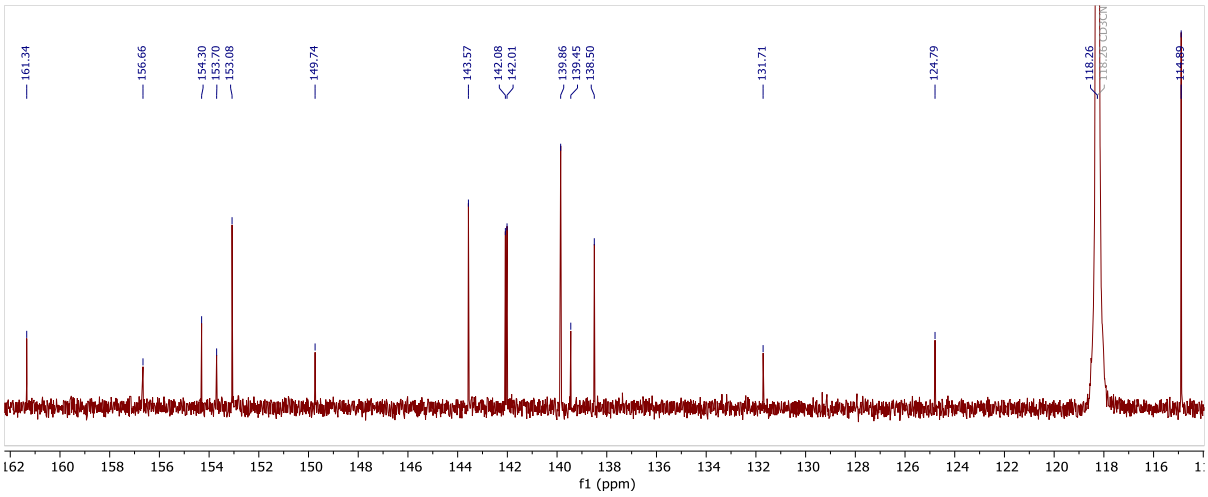
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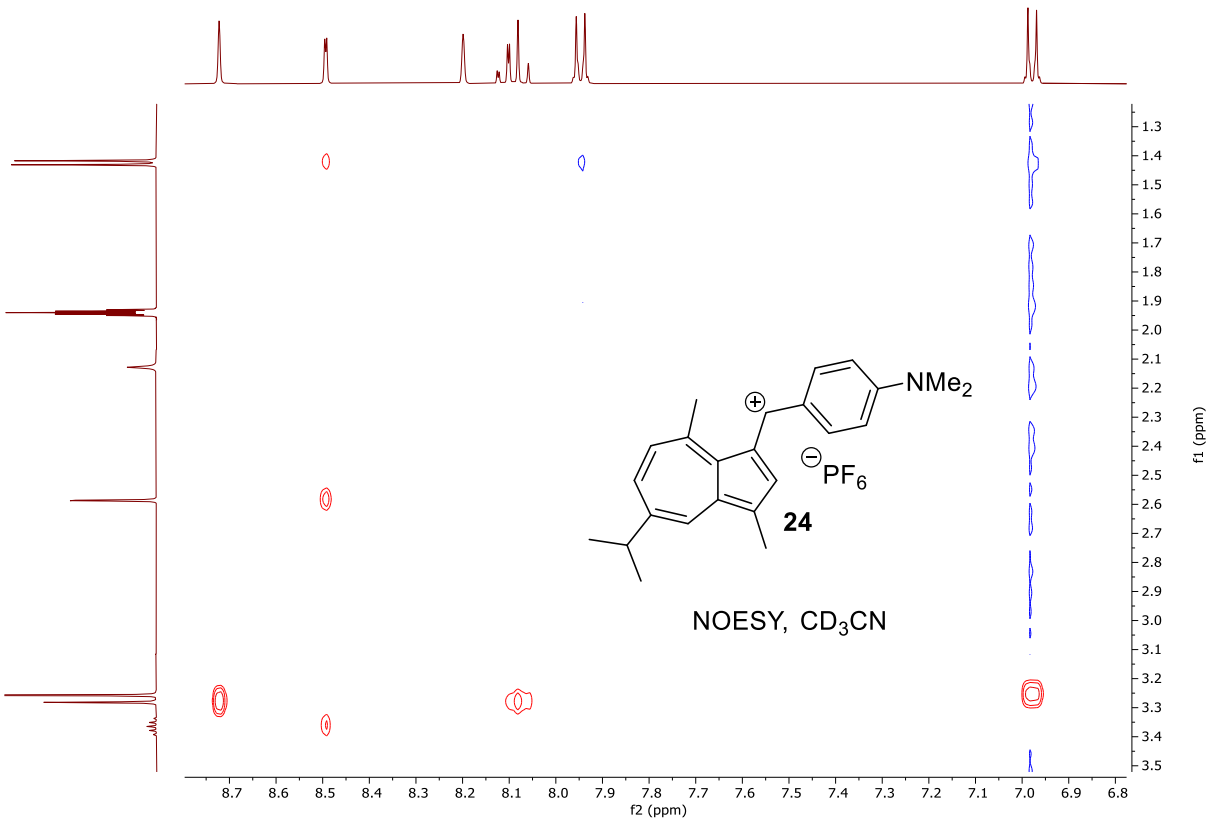
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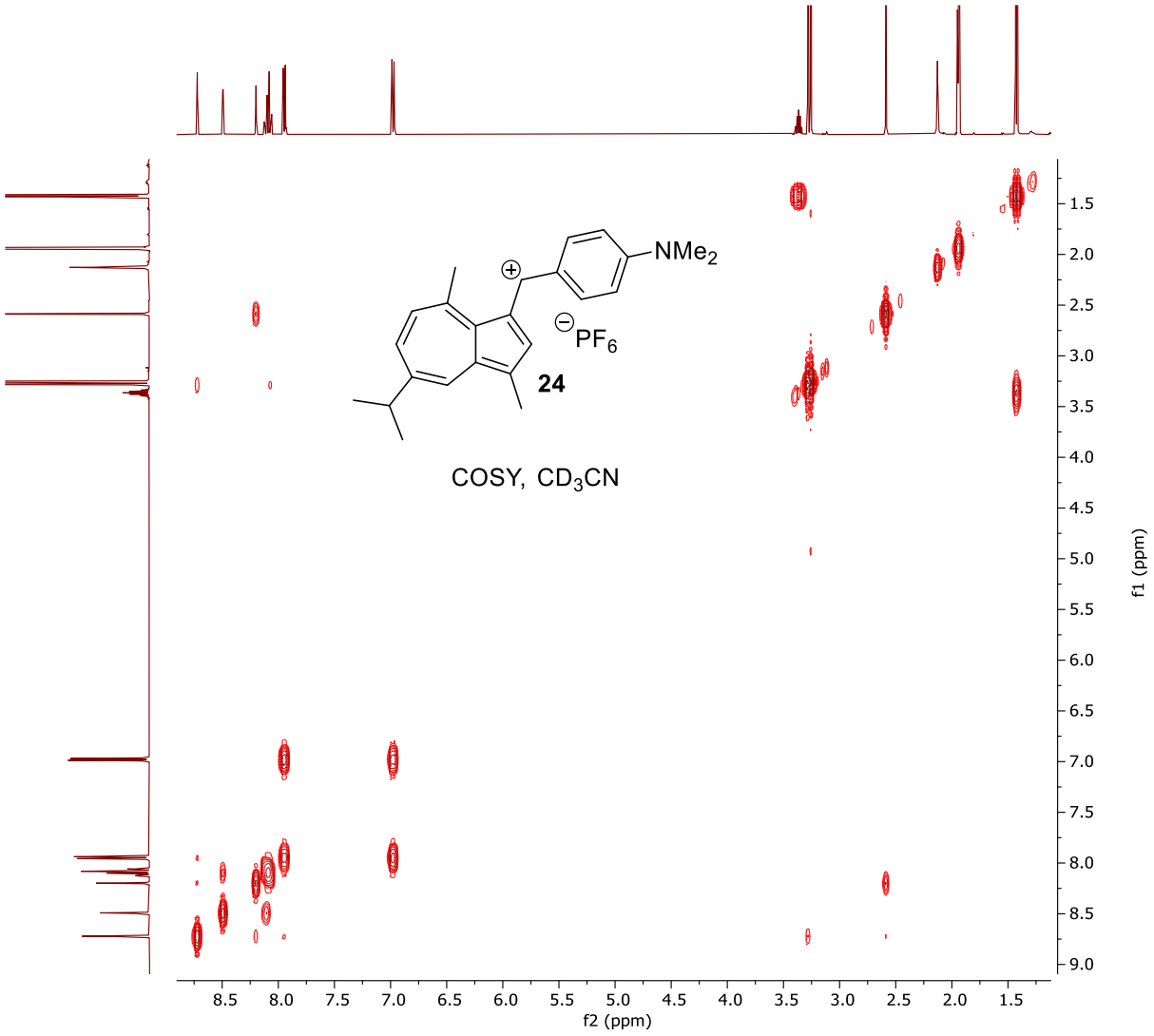
f1 (ppm)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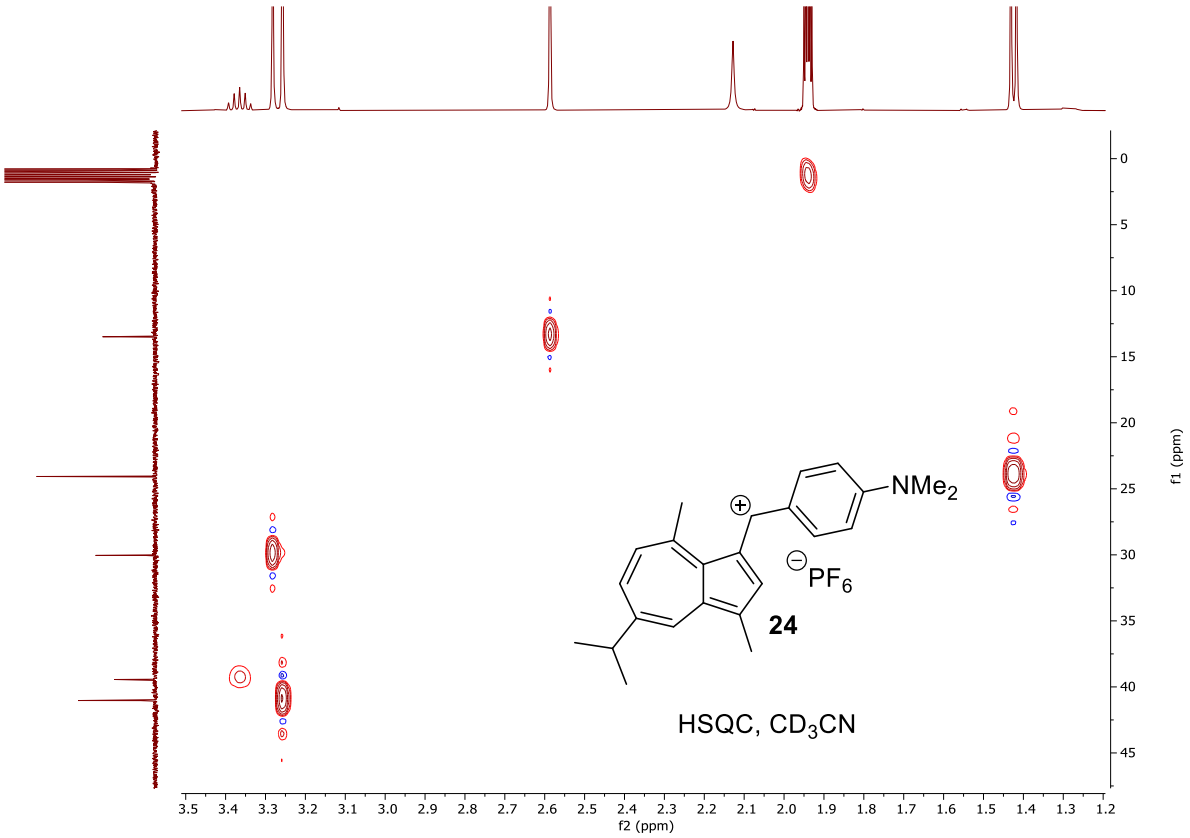
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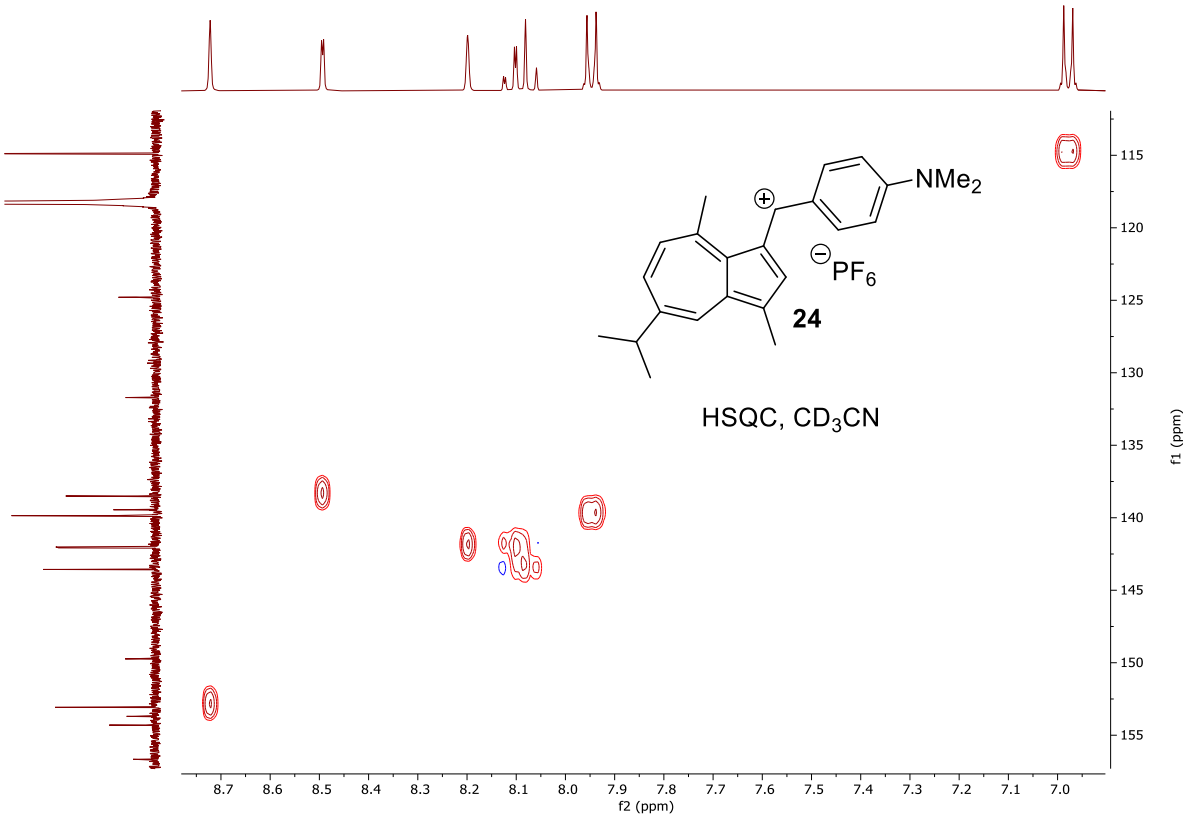
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HSQC, CD3CN
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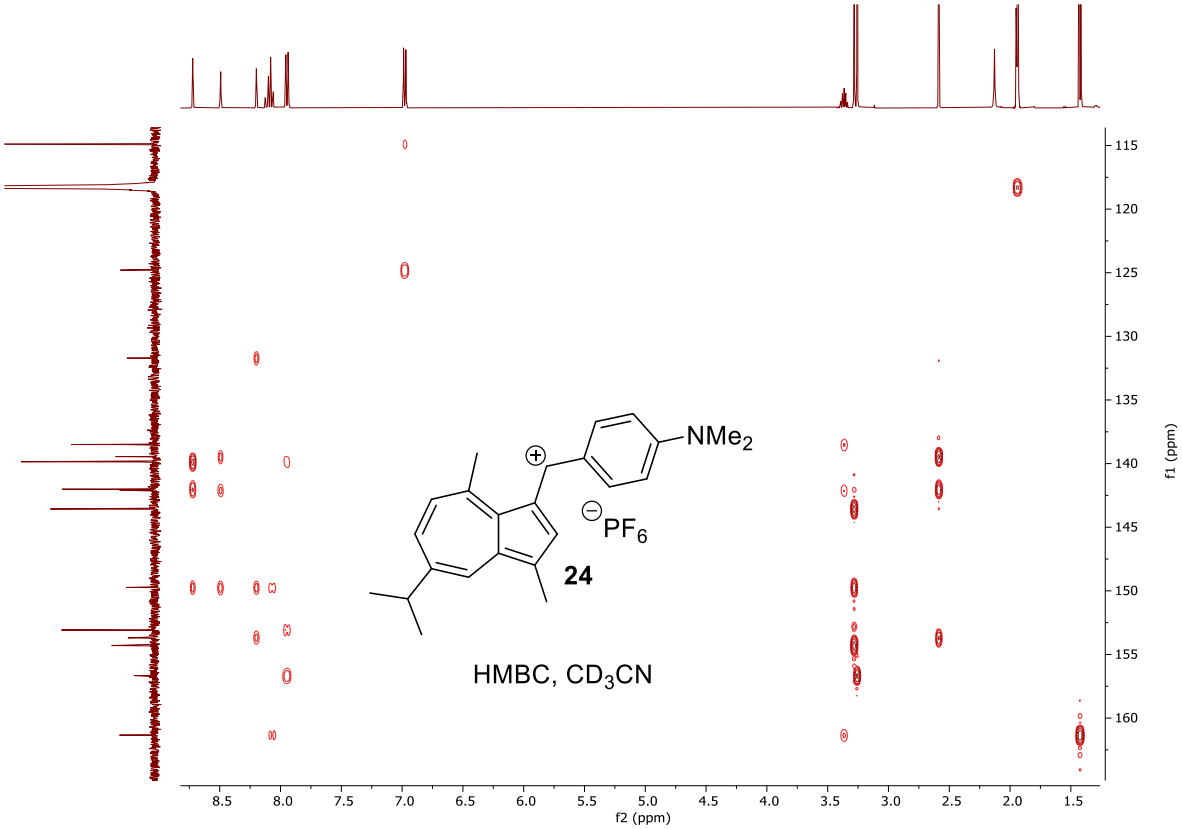
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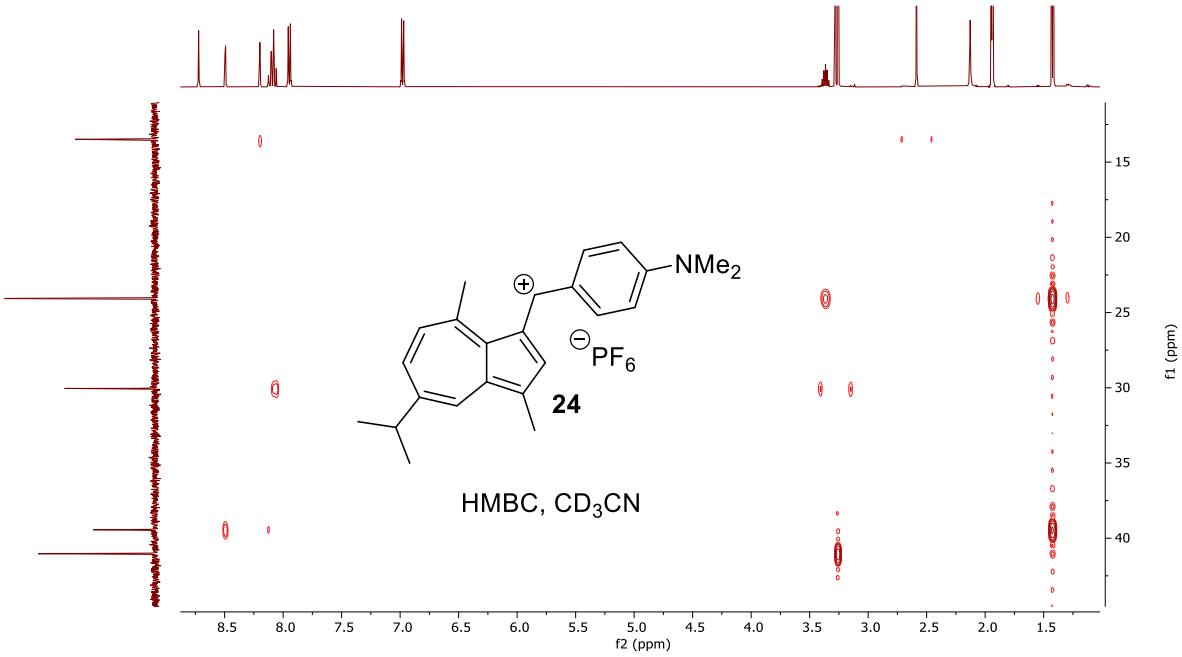
f2 (ppm)
f1 (ppm)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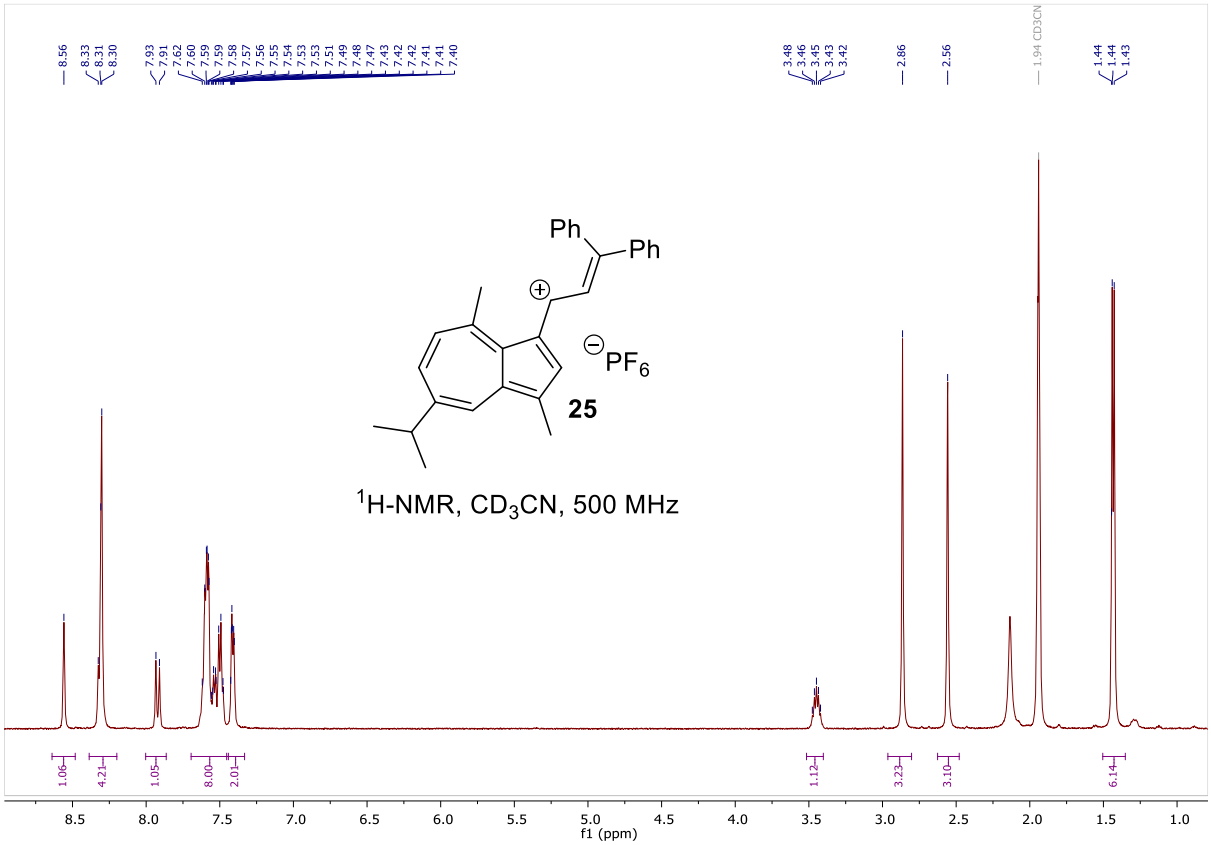
HMBC, CD3CN
f2 (ppm)
f1 (ppm)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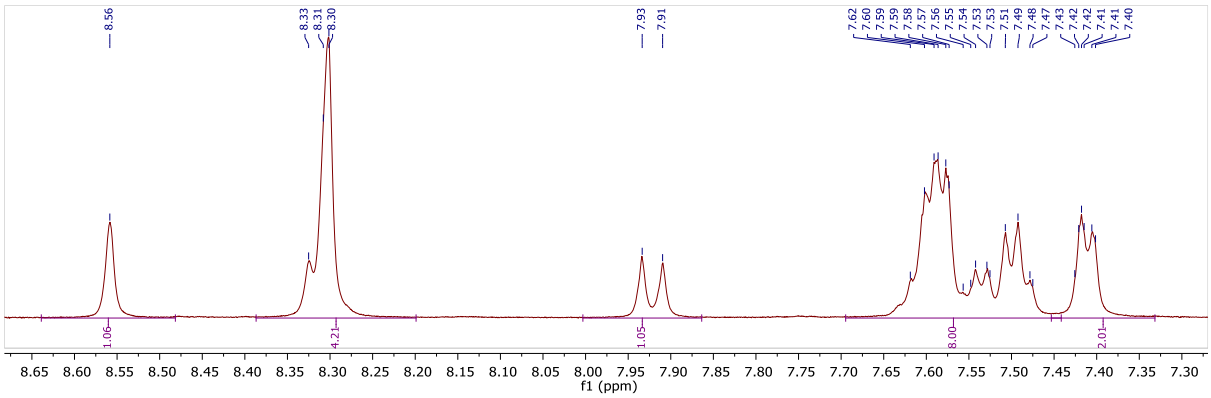
f1 (ppm)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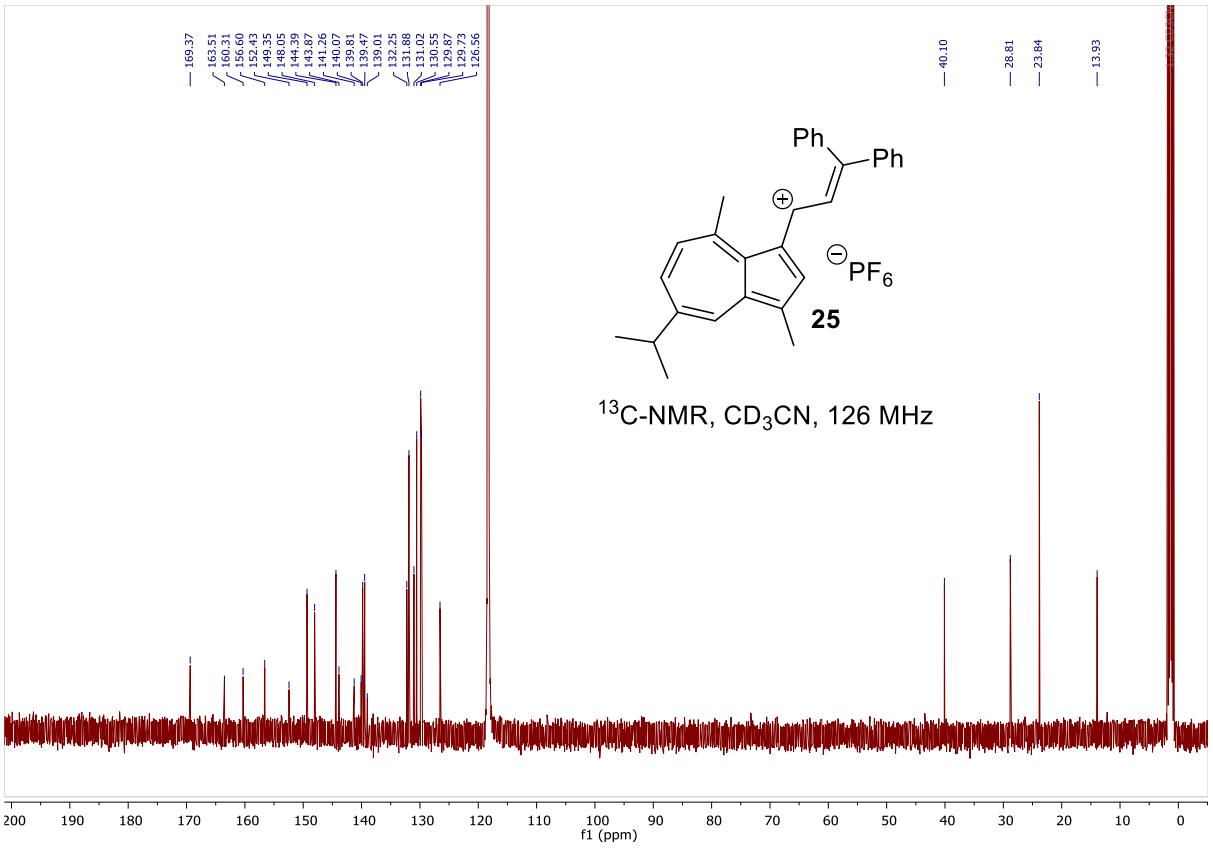
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Ph
Ph
PF6
25
13C-NMR, CD3CN, 126 MHz
200
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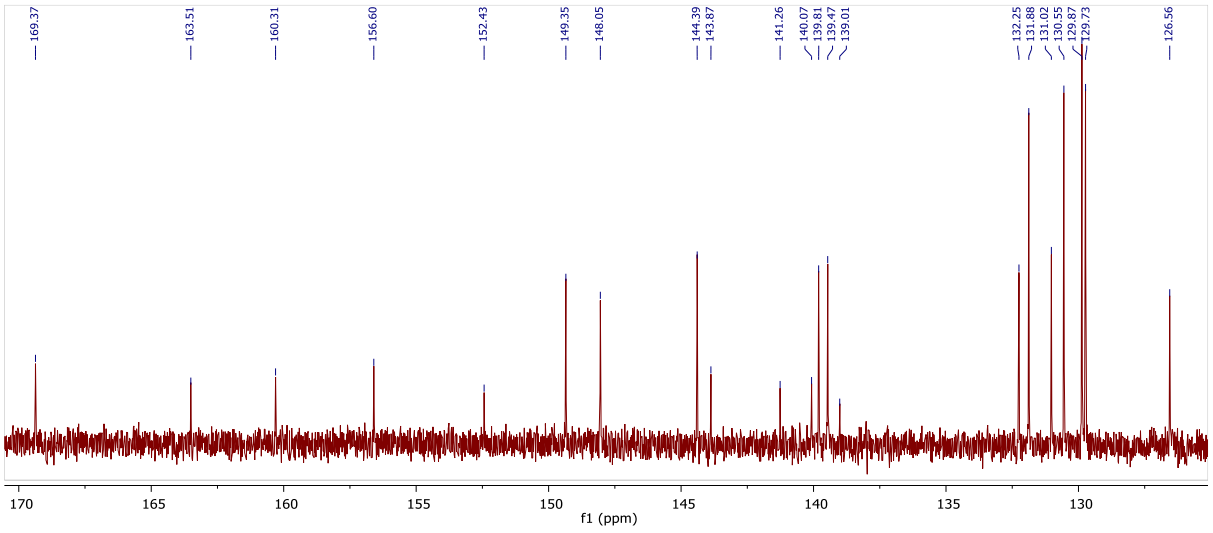
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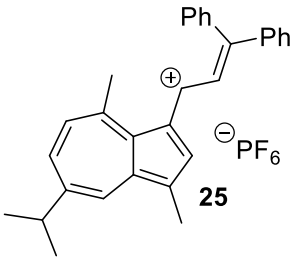
f1 (ppm)



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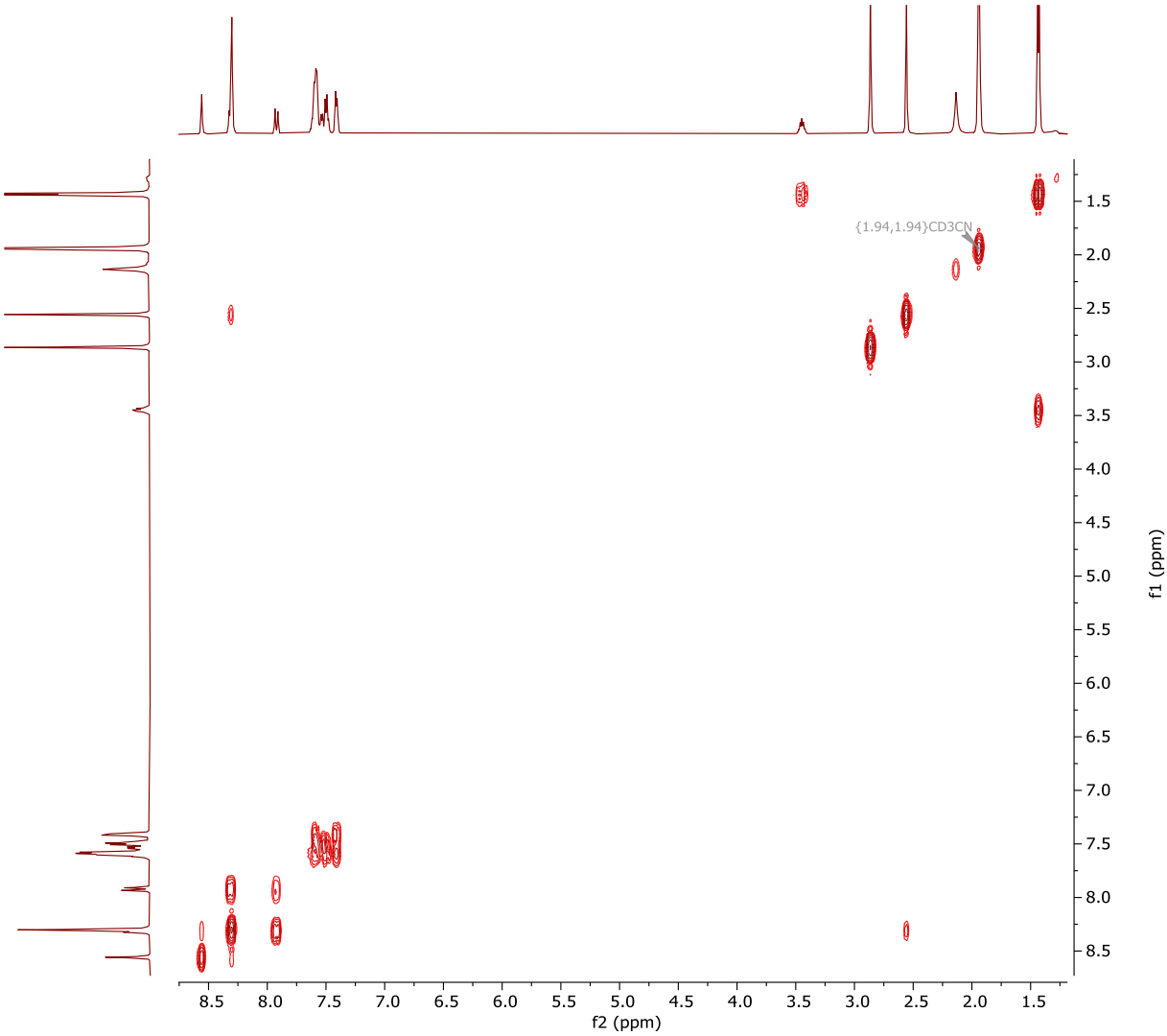
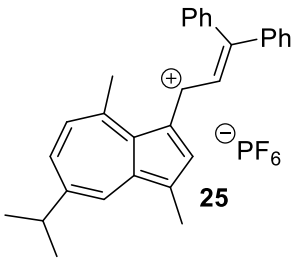
COSY, CD_3CN





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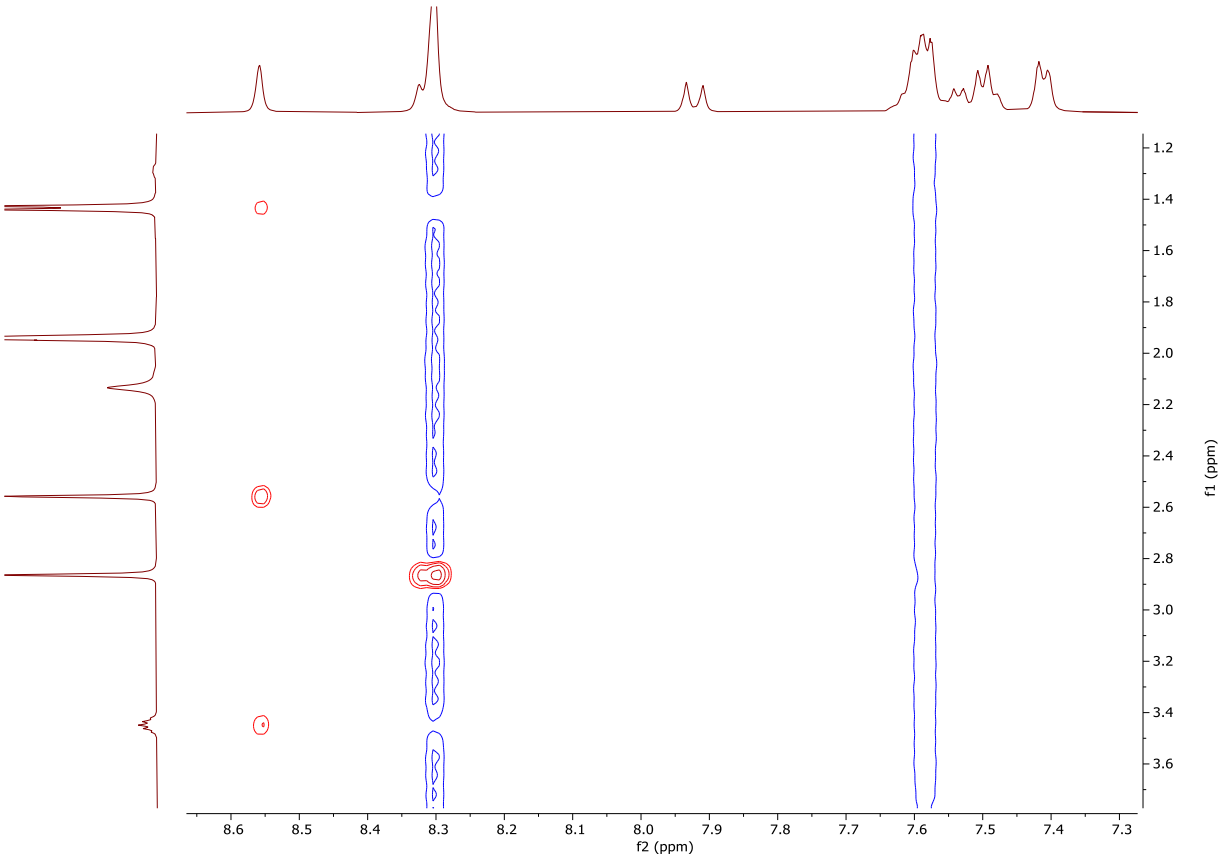

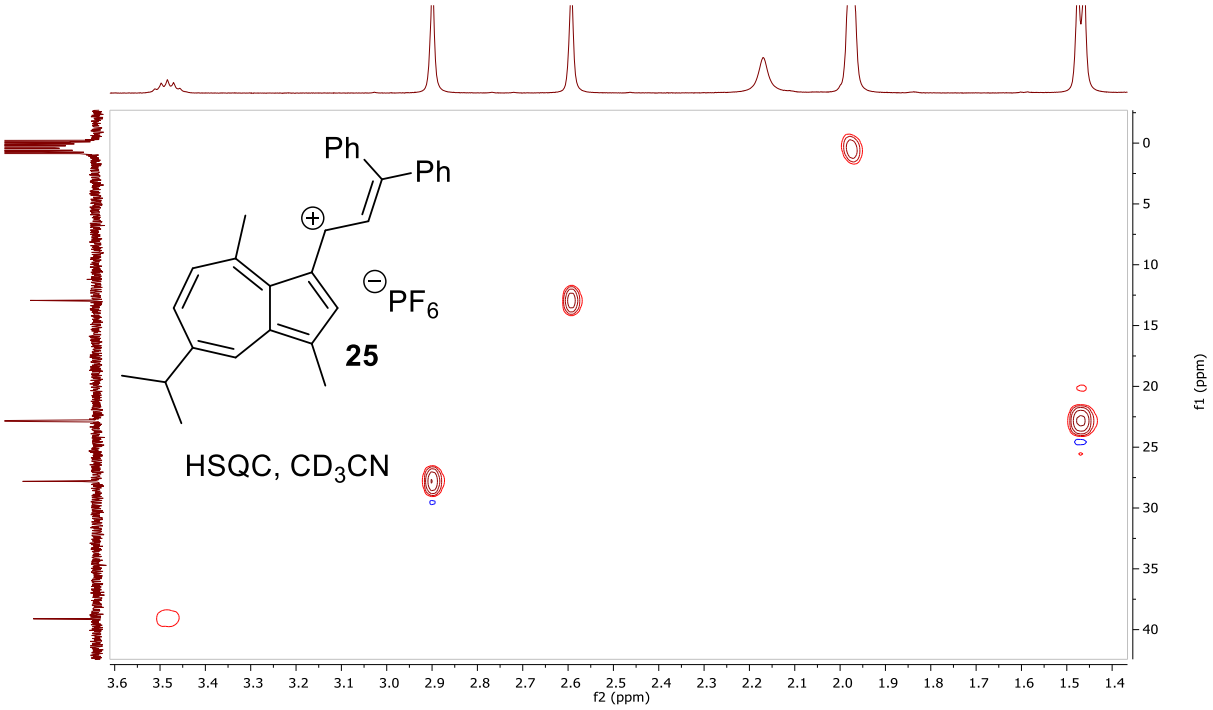
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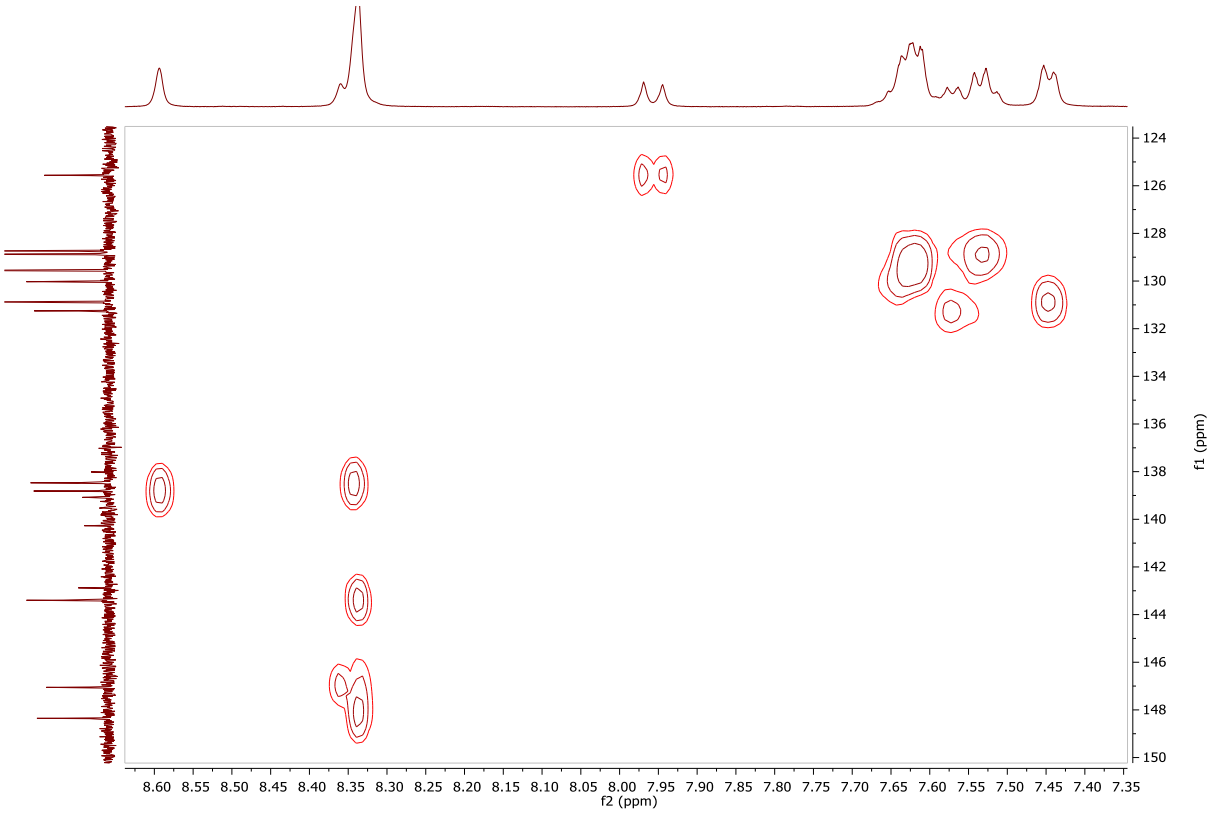
HSQC, CD3CN
f2 (ppm)
f1 (ppm)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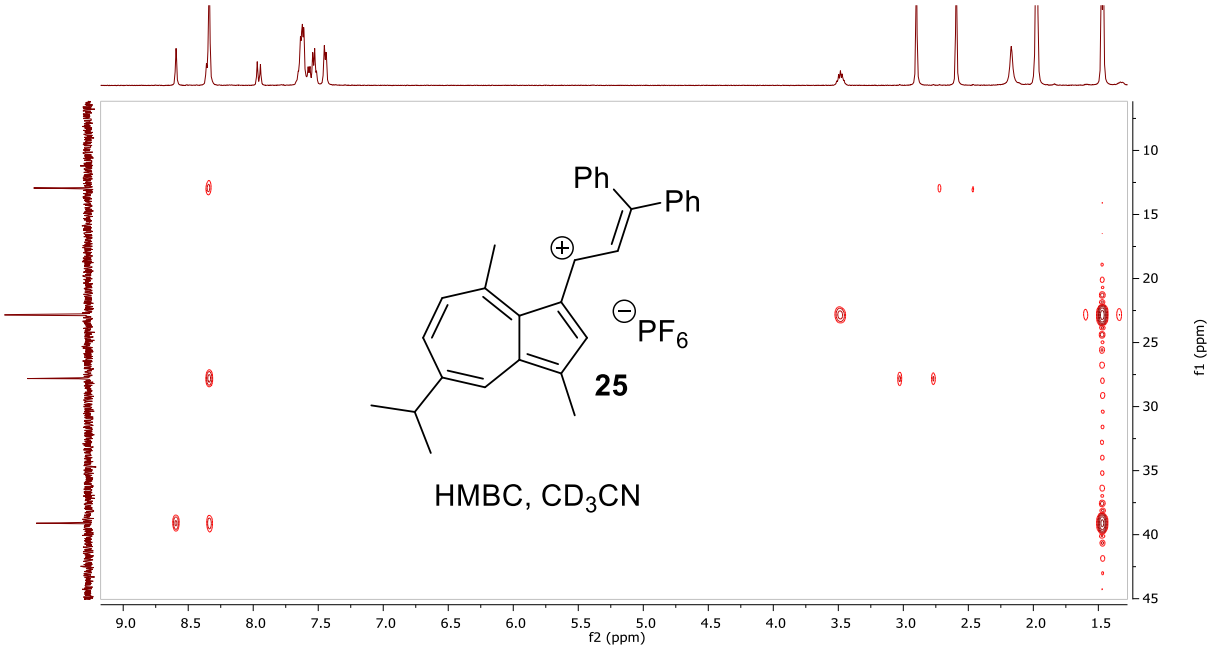
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HMBC, CD3CN
f2 (ppm)
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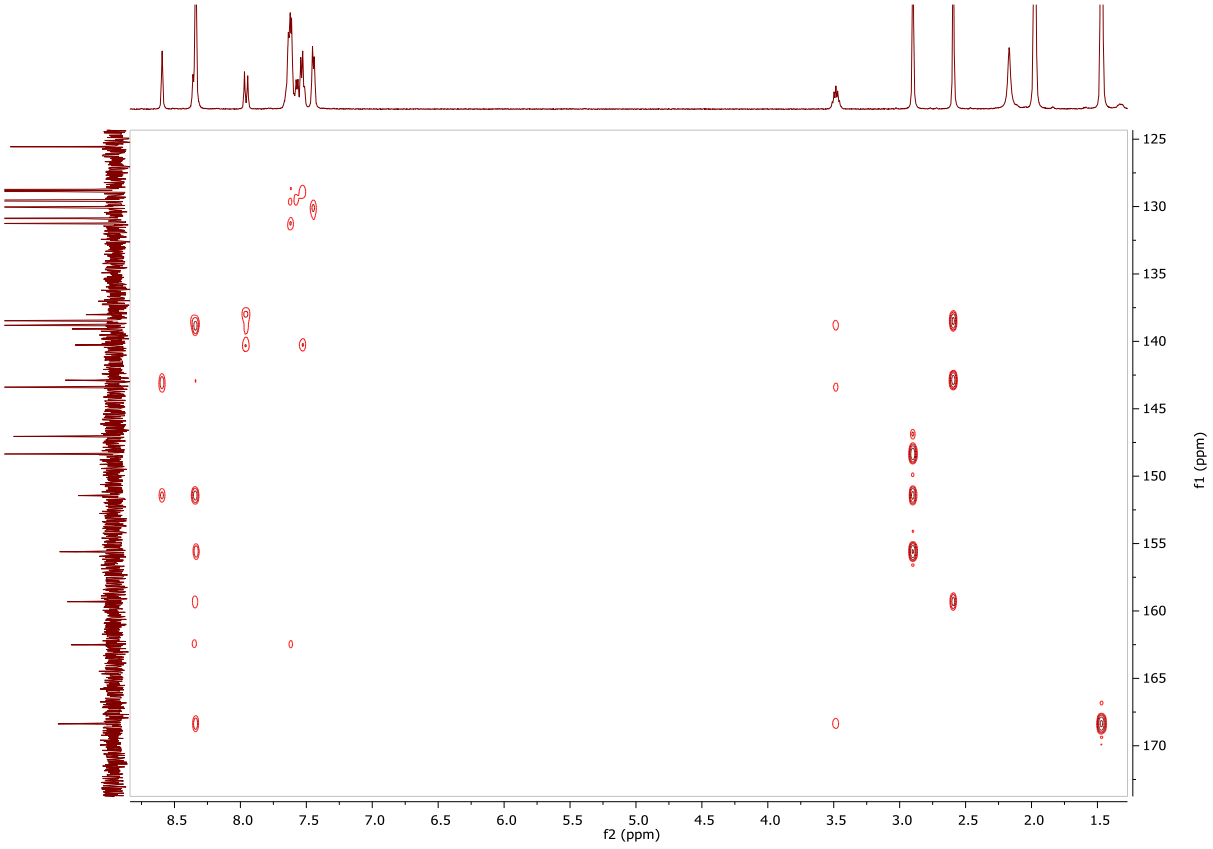
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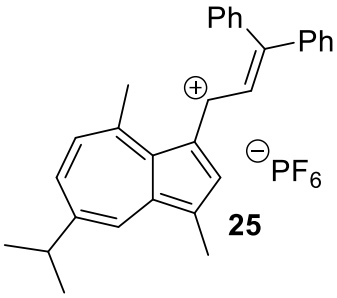
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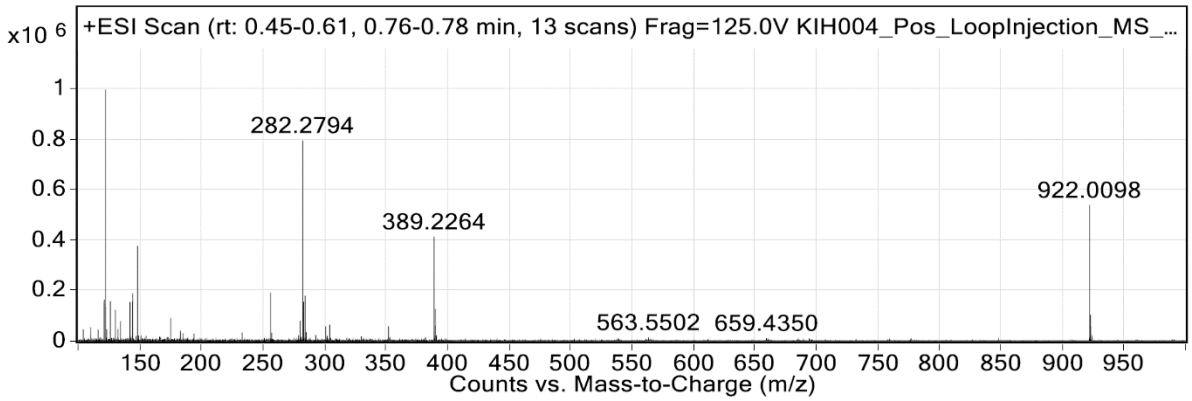
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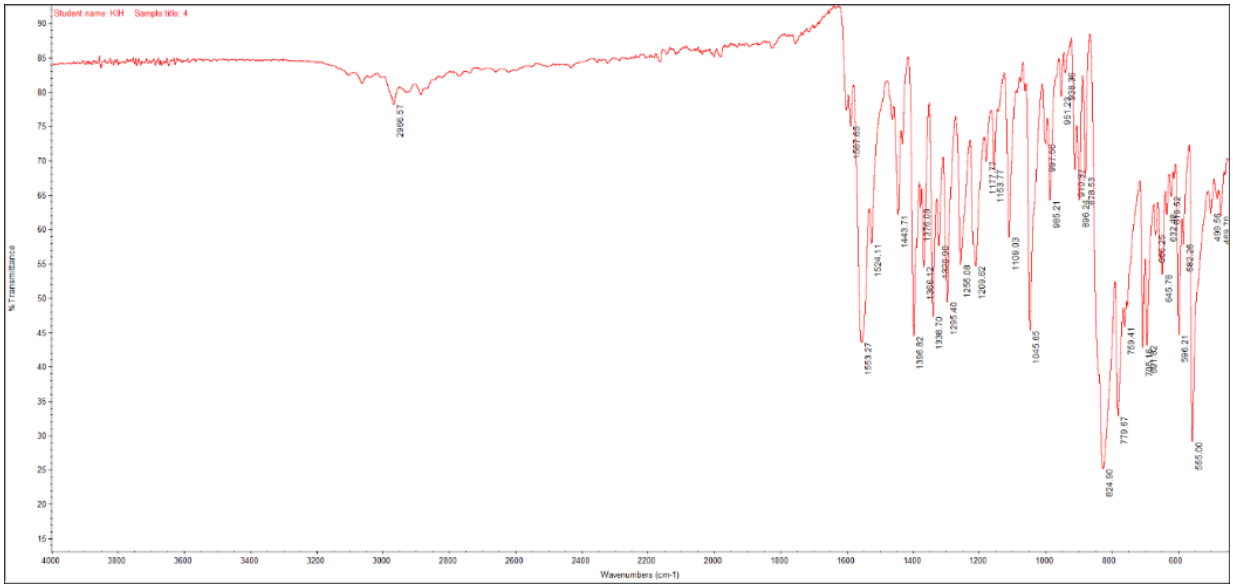
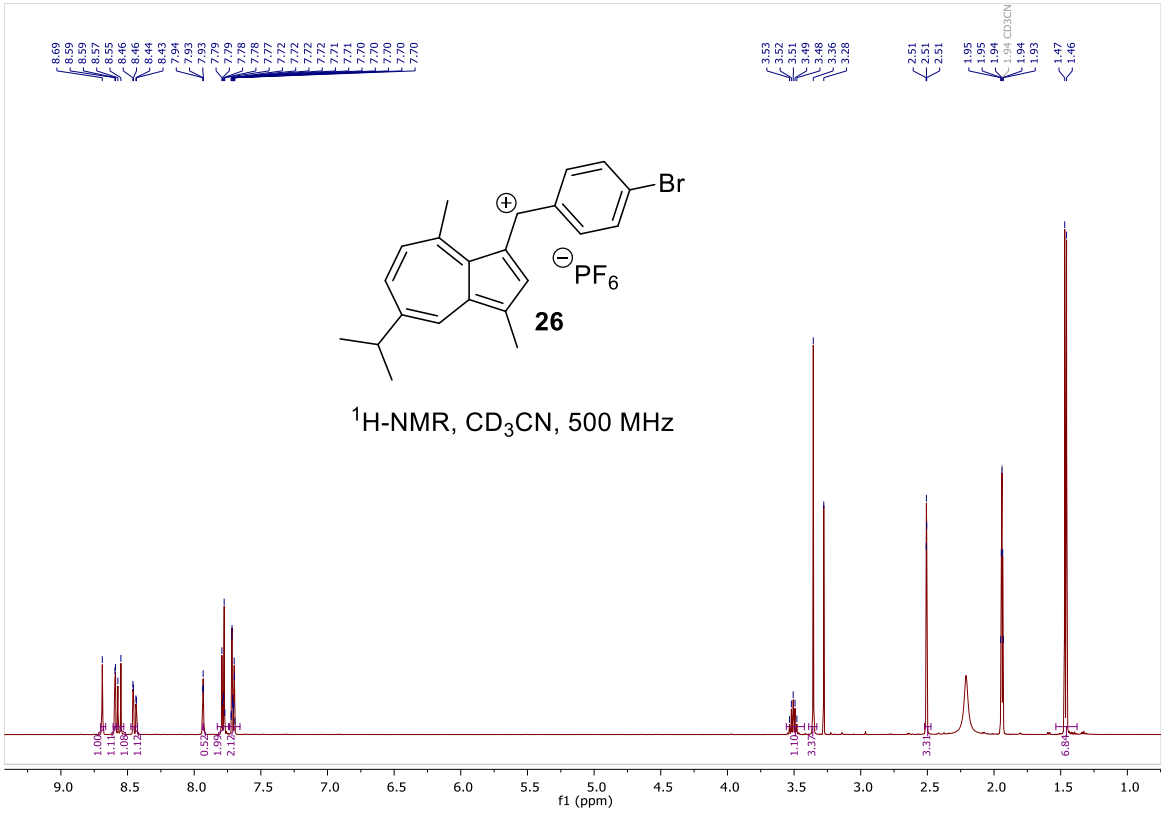
Counts vs. Mass-to-Charge (m/z)


% Transmittance
Wavenumbers (cm-1)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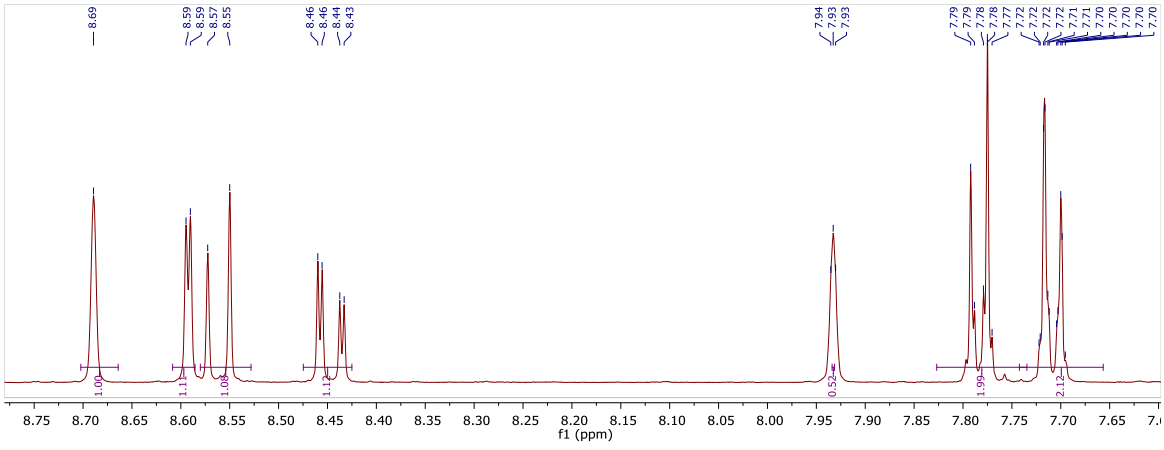
f1 (ppm)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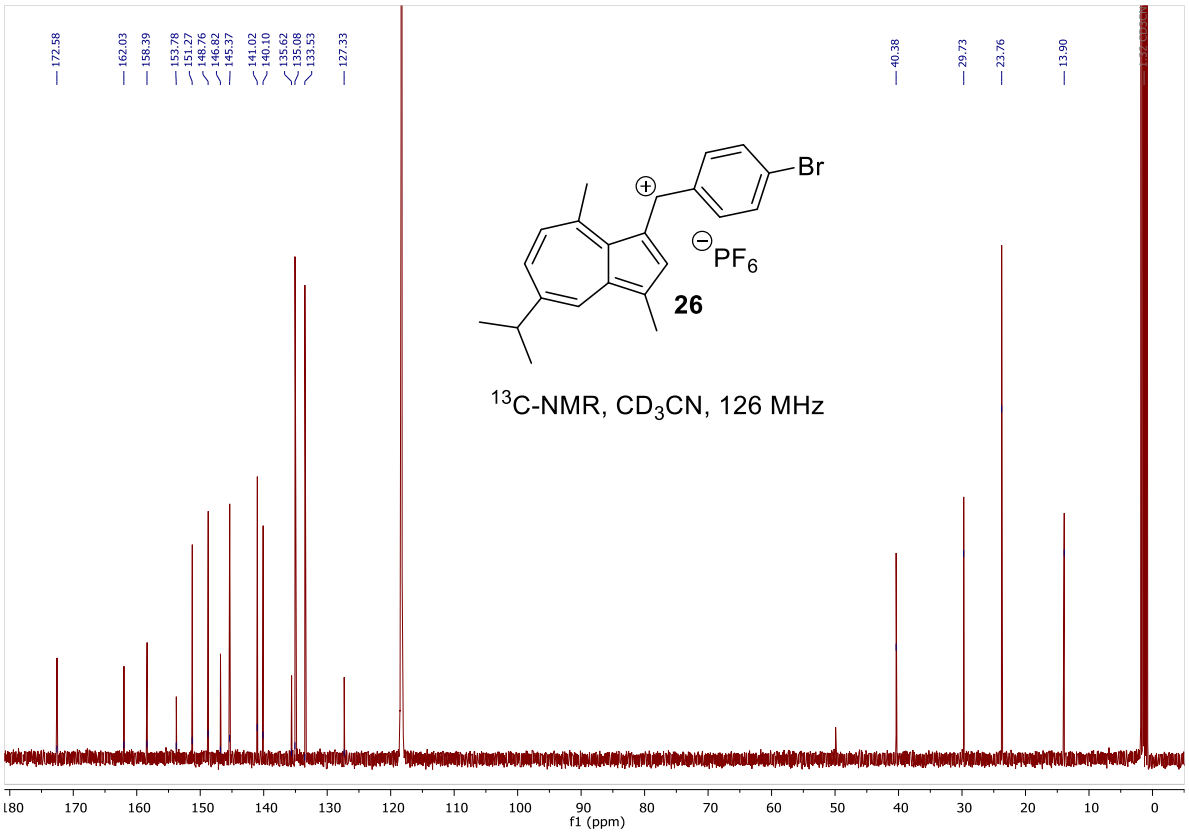
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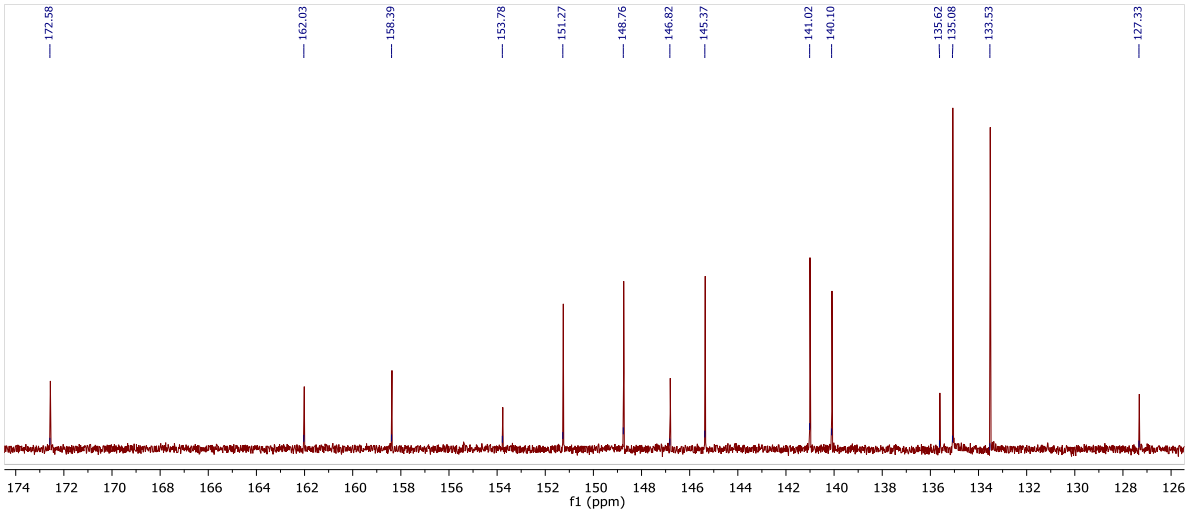
13C-NMR, CD3CN, 126 MHz
f1 (ppm)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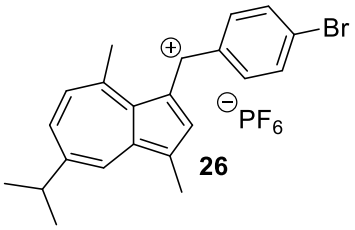
f1 (ppm)



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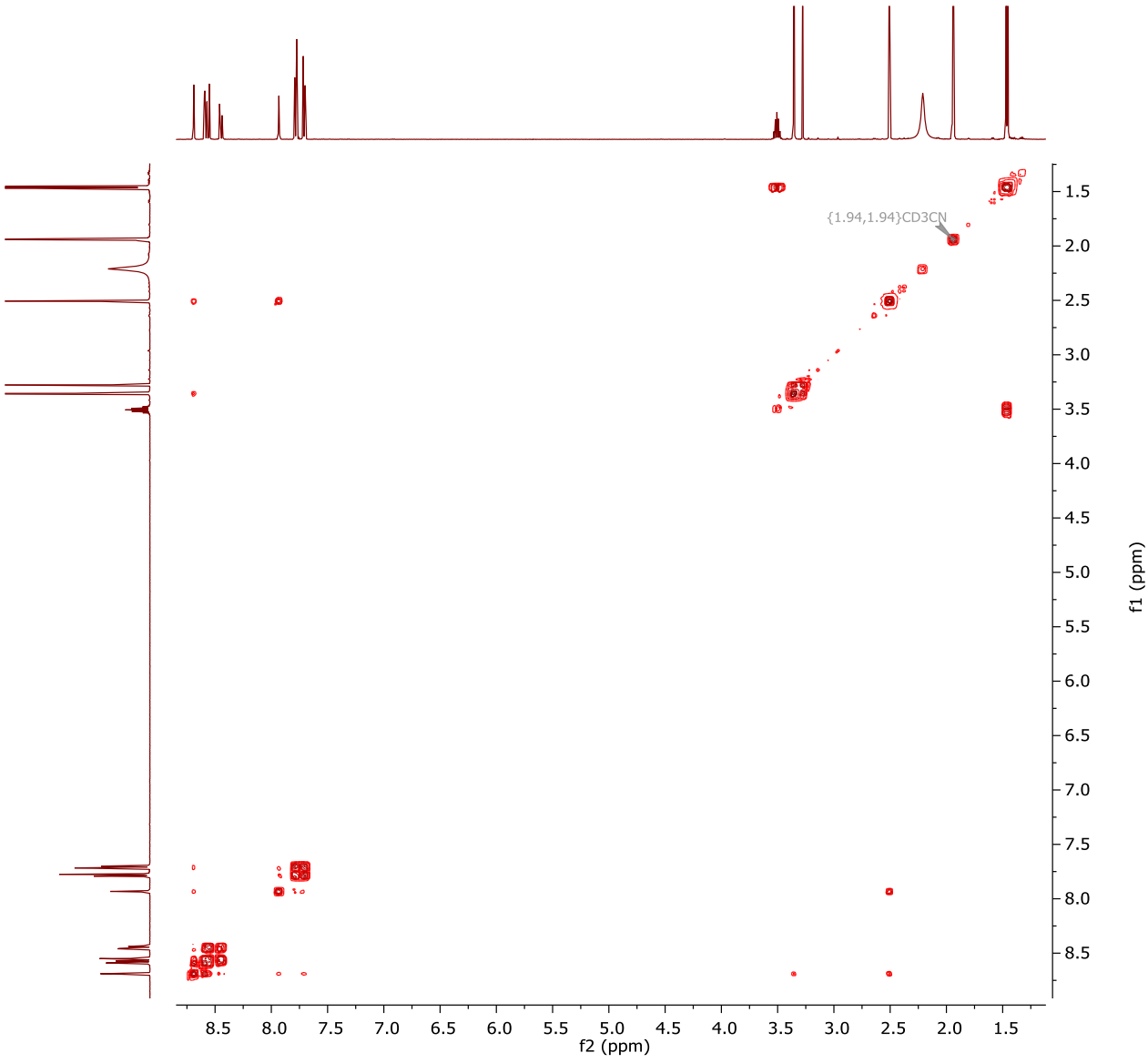

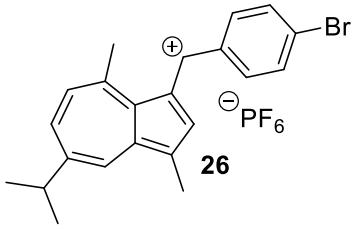

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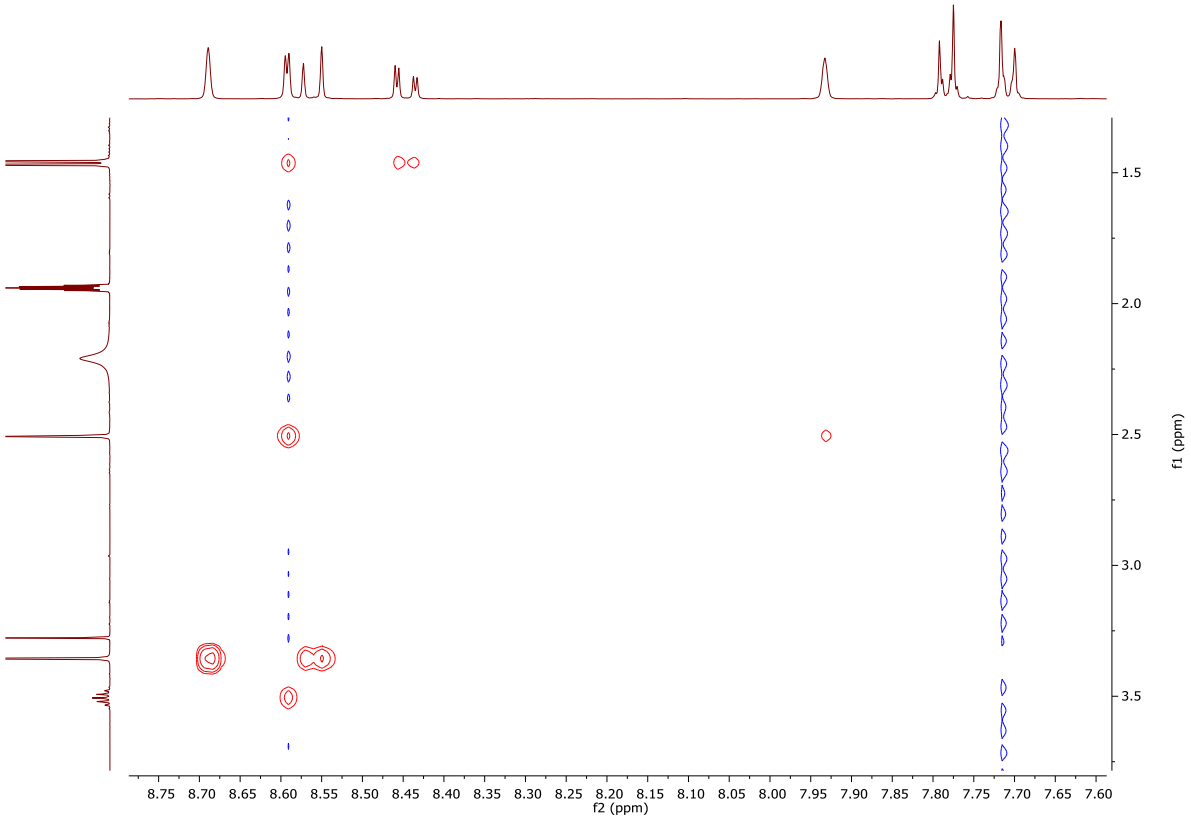

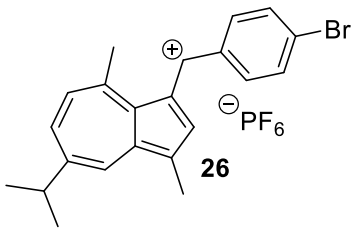

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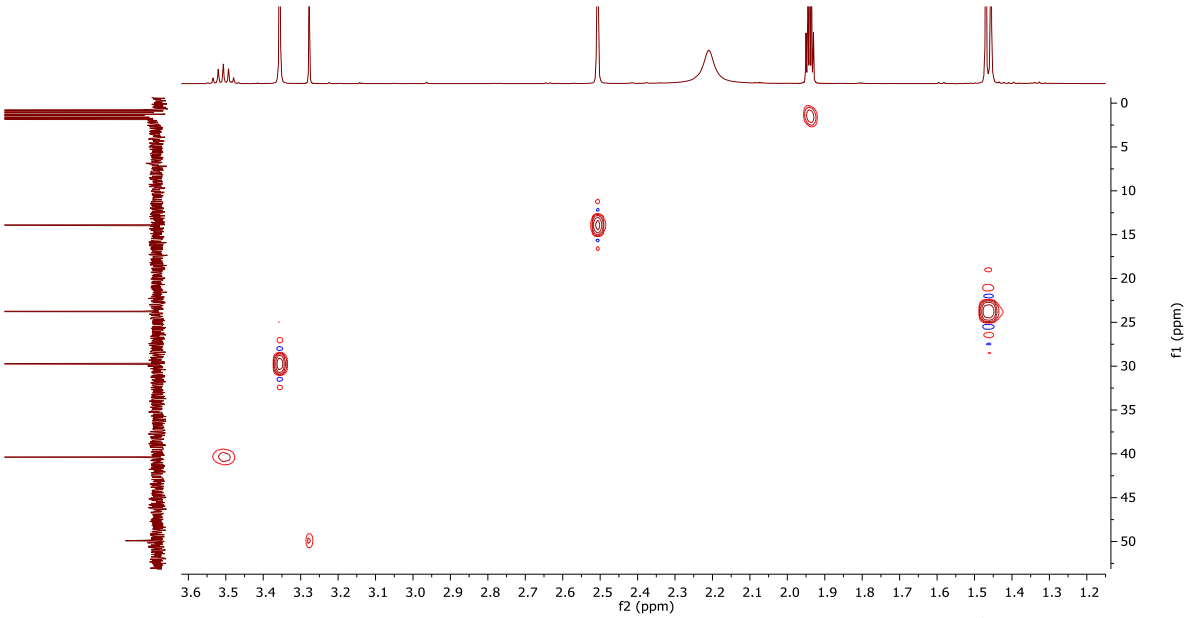

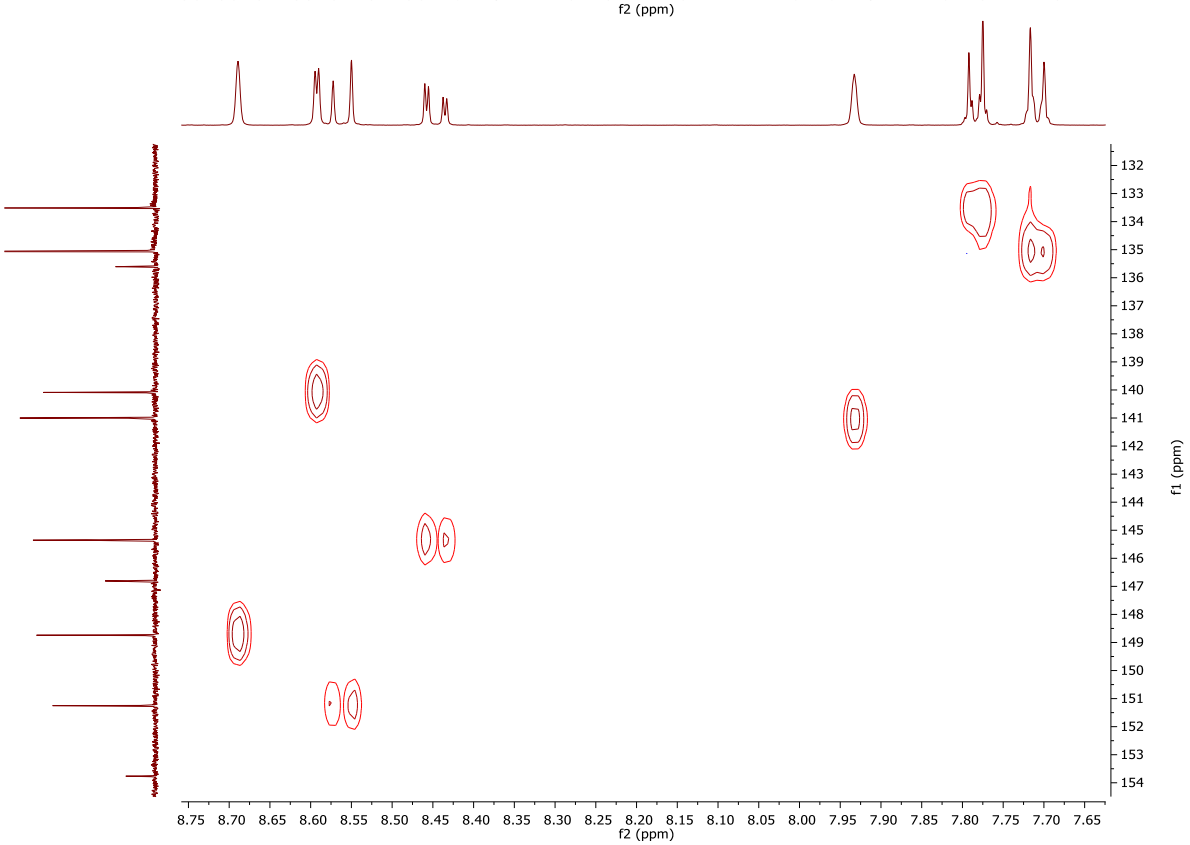

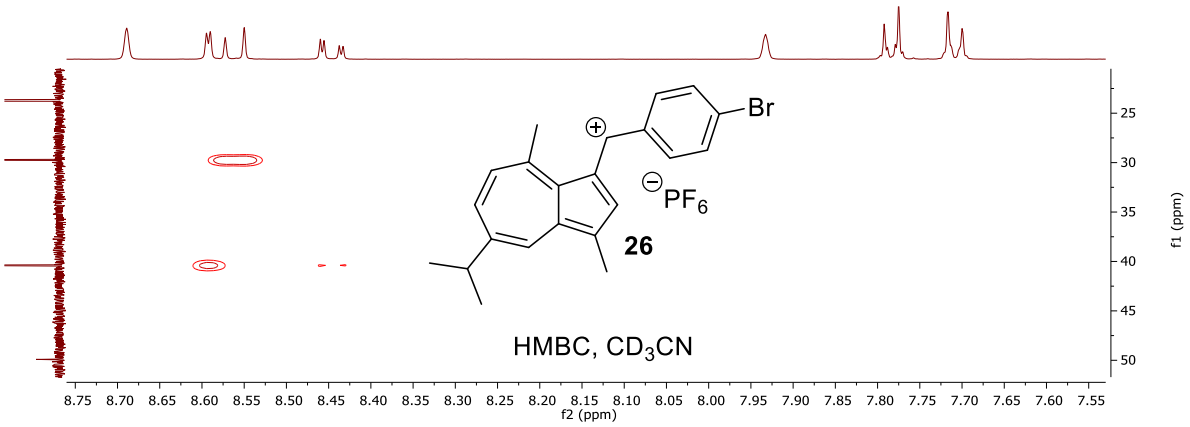
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PF6
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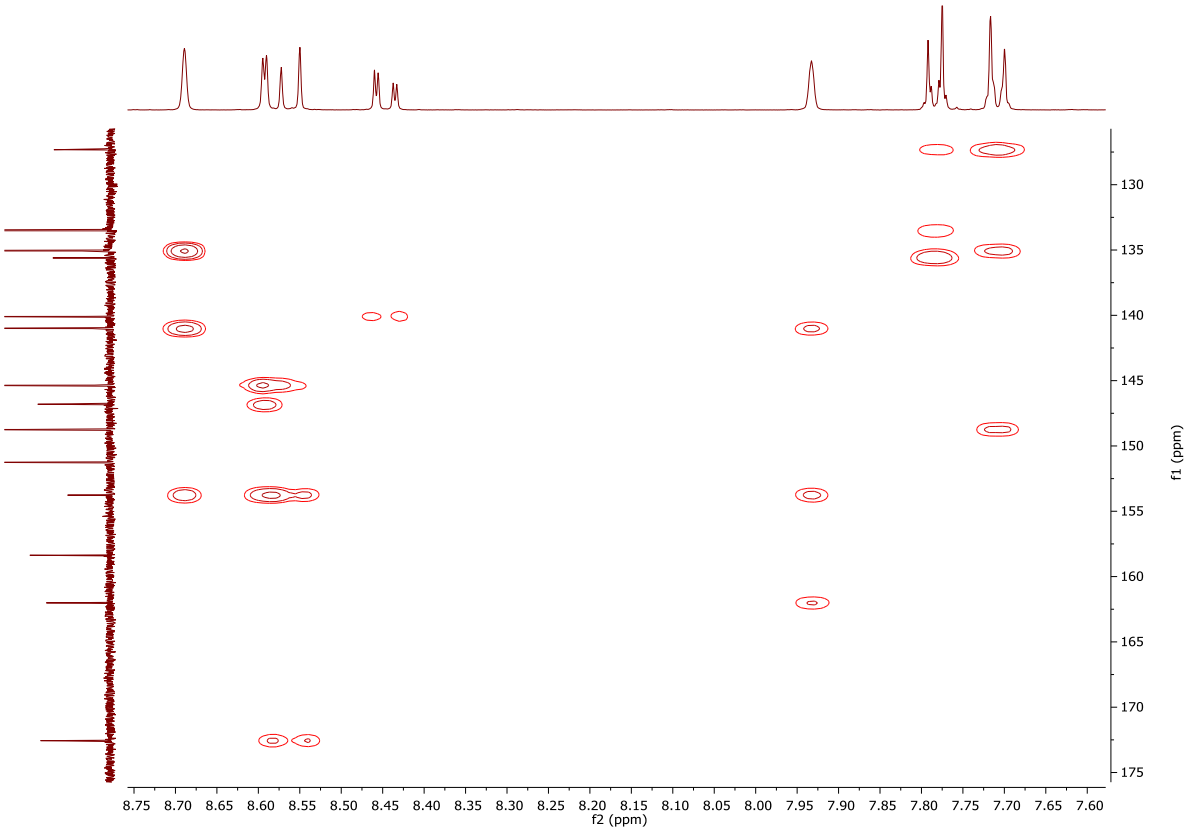
HMBC, CD3CN
f2 (ppm)
f1 (ppm)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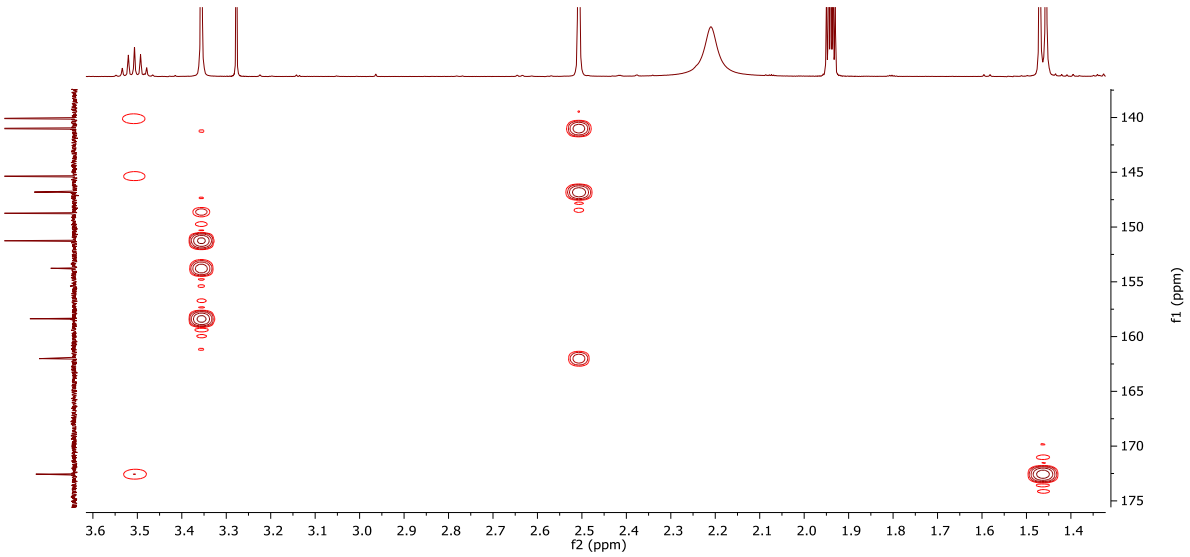
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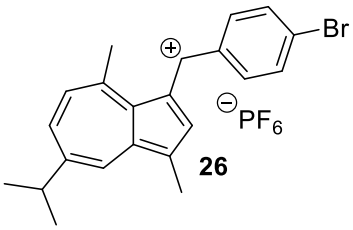
Br
PF6

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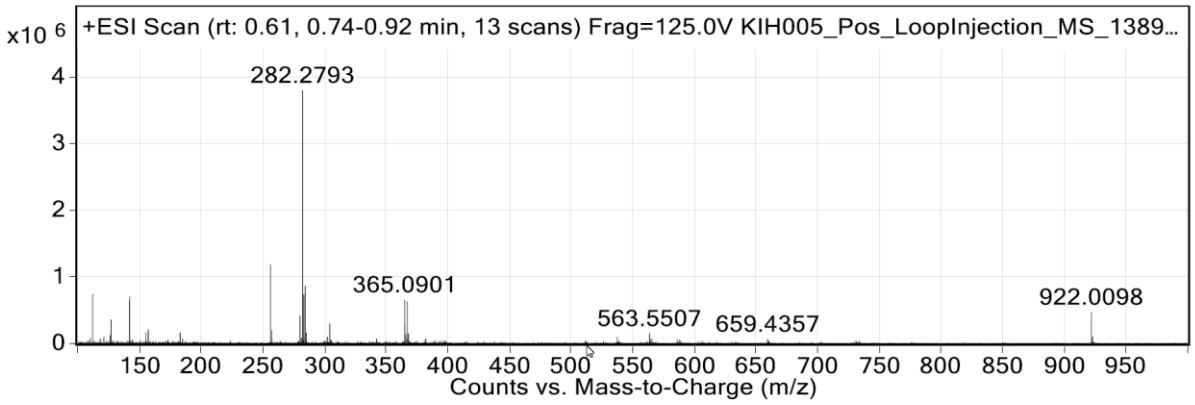
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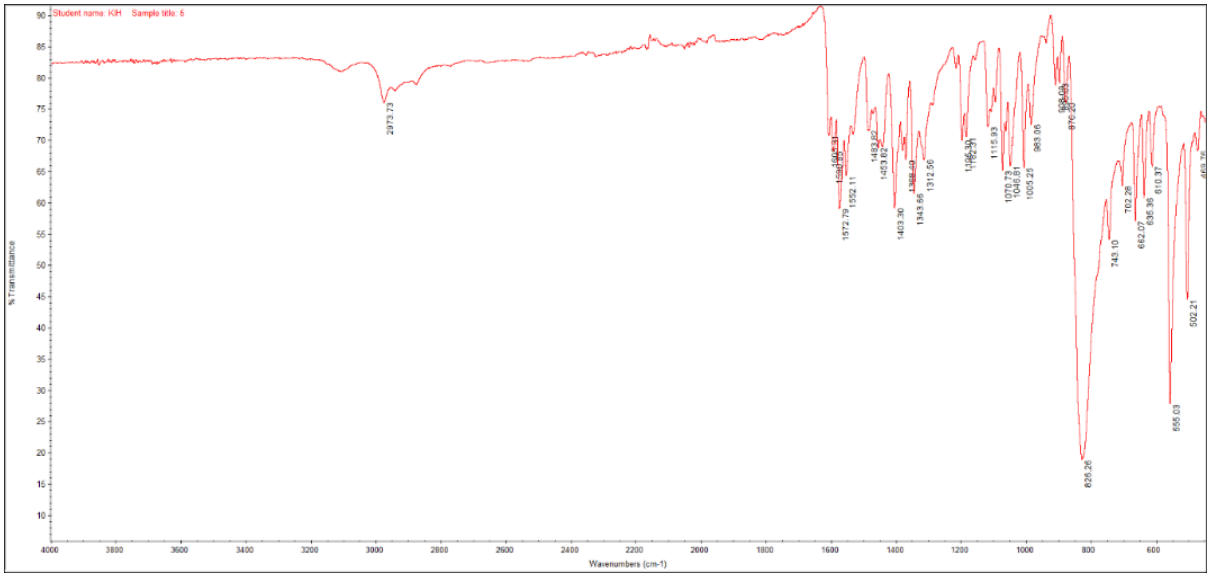
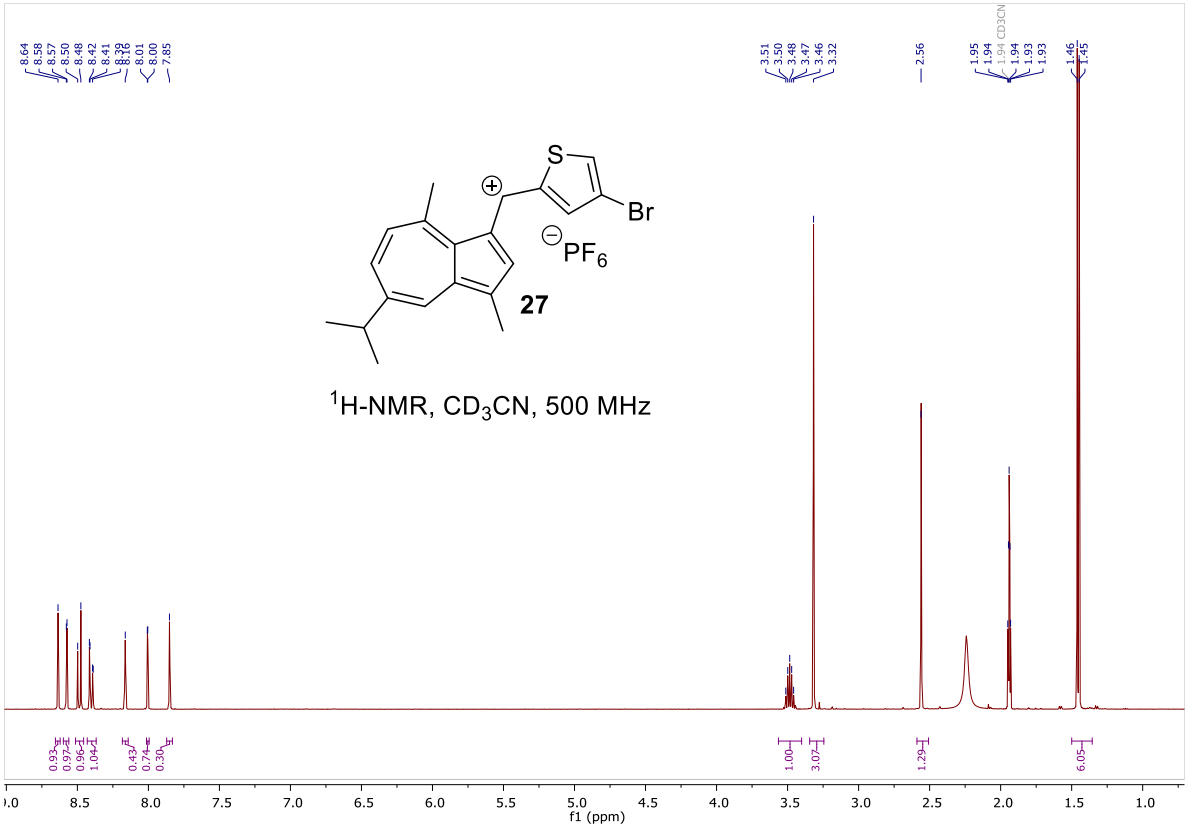
365.0901
563.5507
659.4357
922.0098
Counts vs. Mass-to-Charge (m/z)


% Transmittance
Wavenumbers (cm-1)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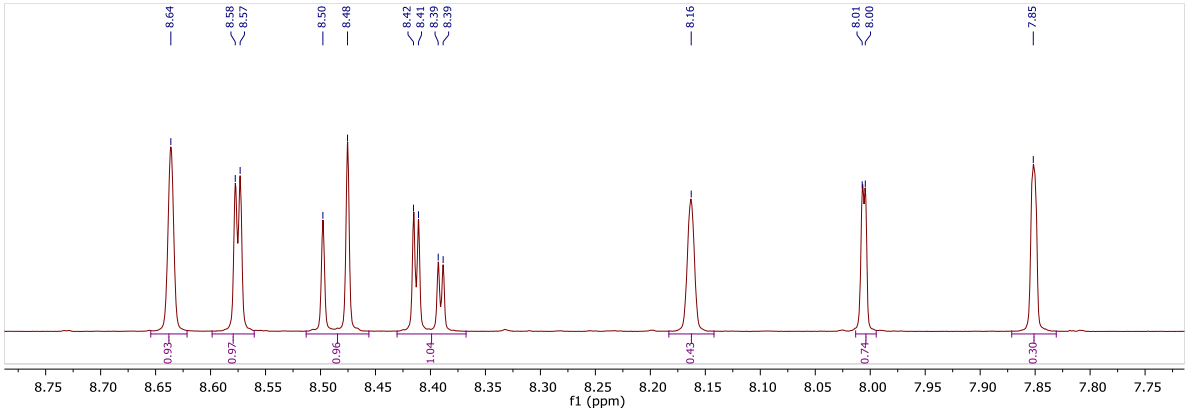
1H-NMR, CD3CN, 500 MHz
f1 (ppm)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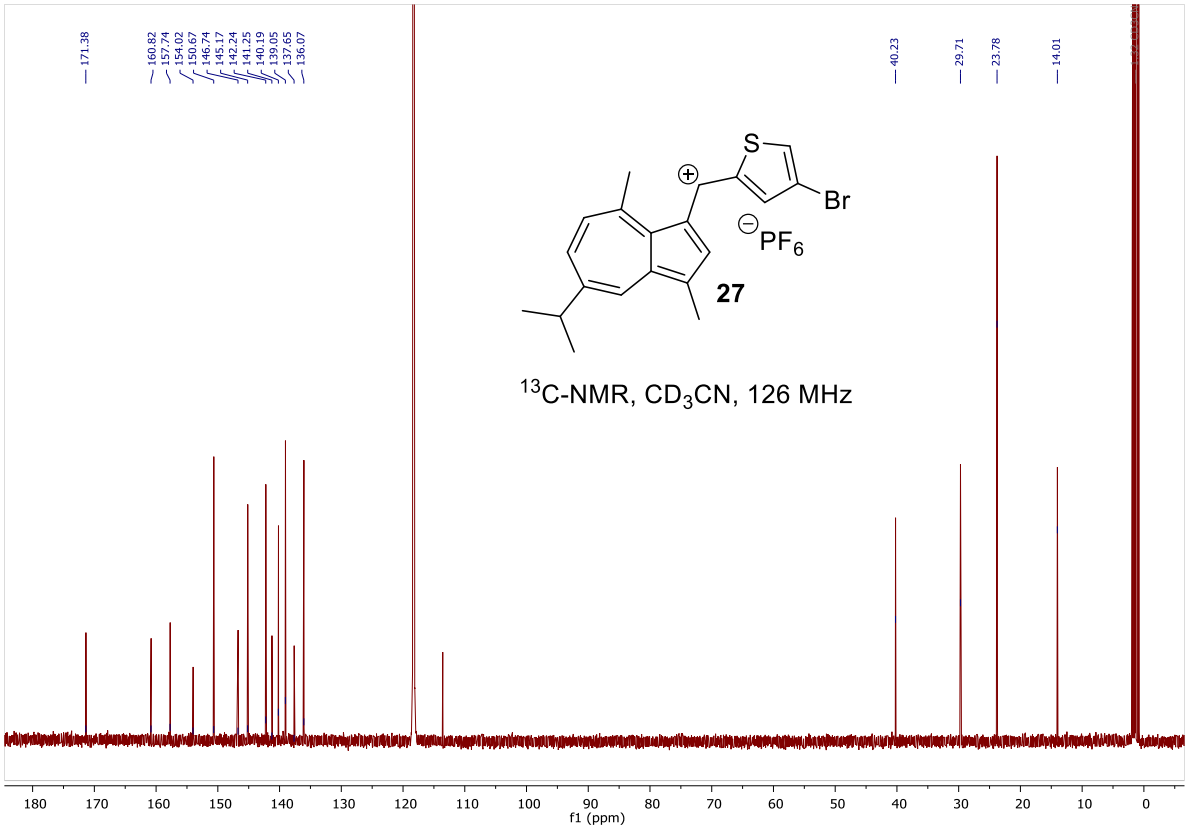
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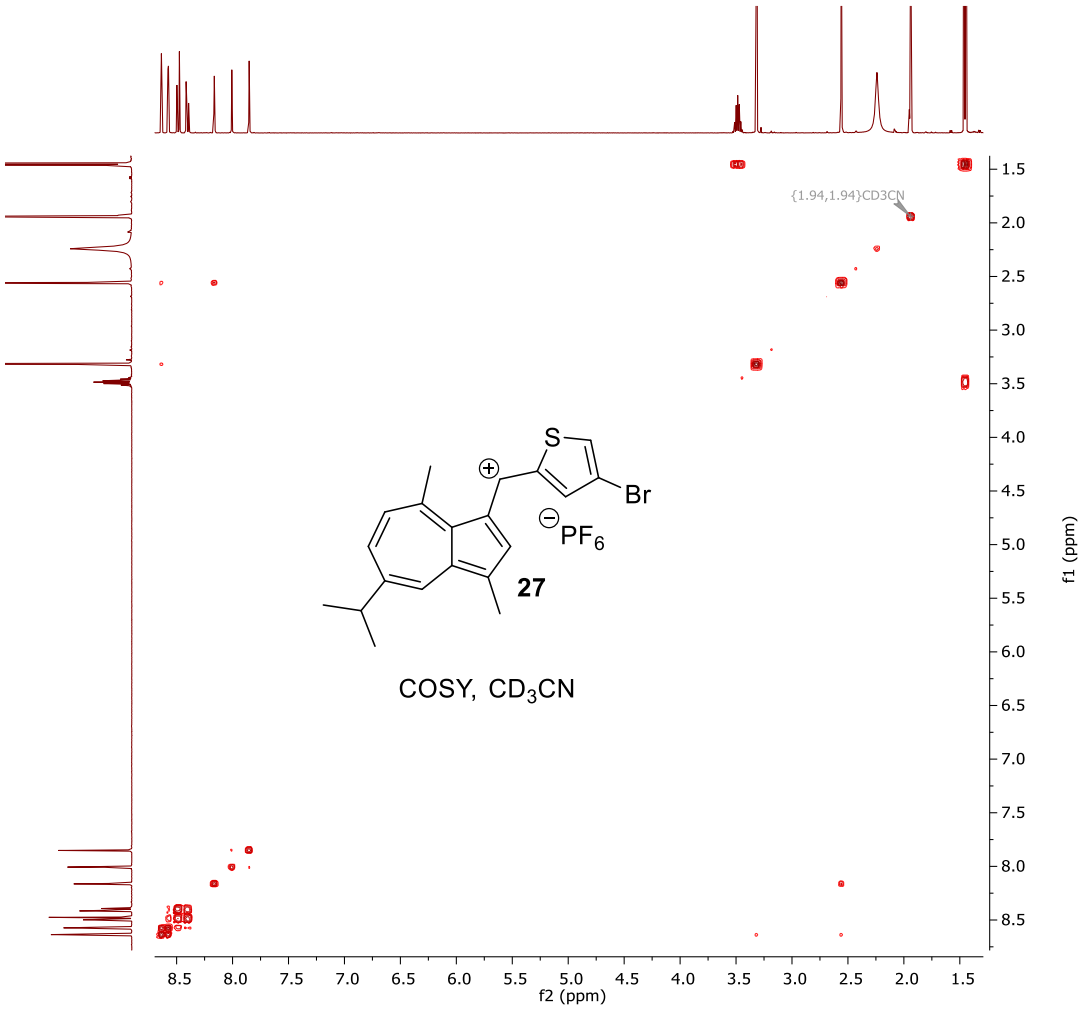
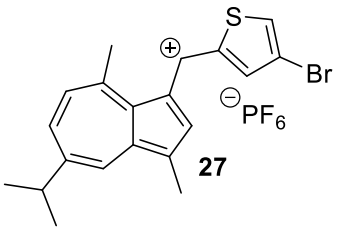
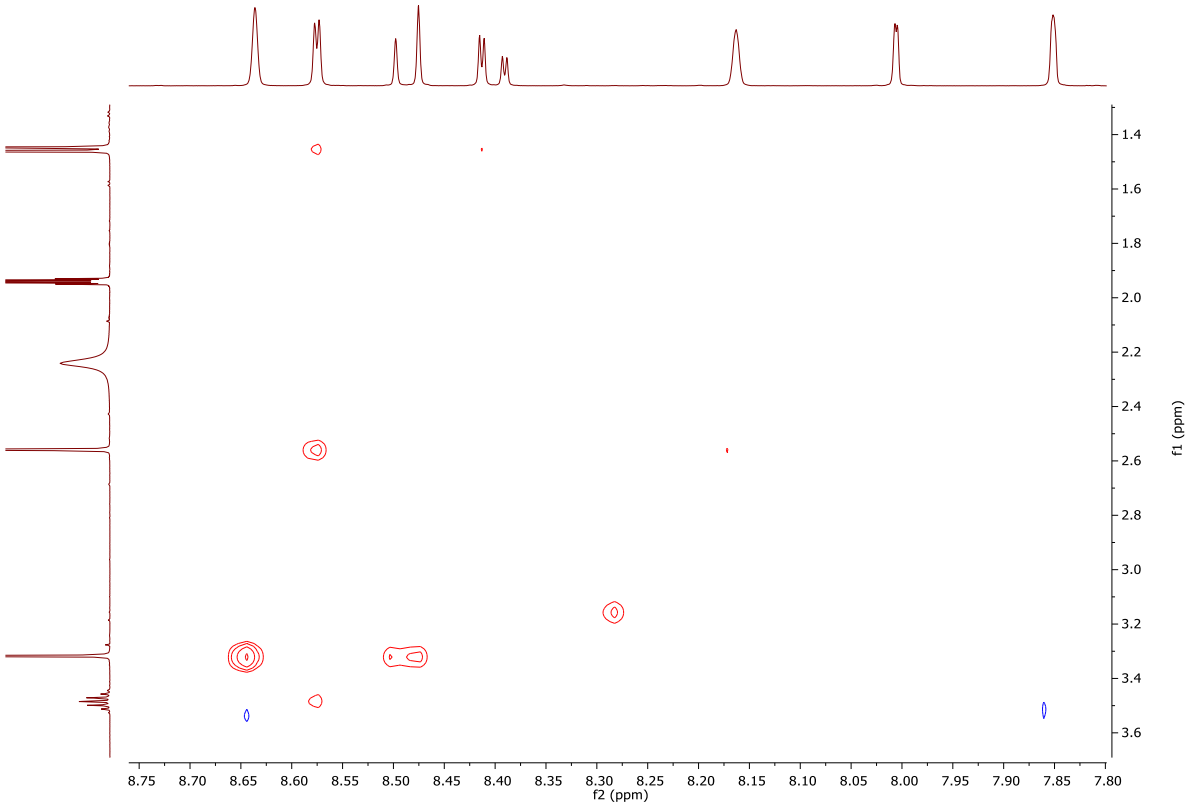
23.78
14.01
S
Br
PF6
27
13C-NMR, CD3CN, 126 MHz
f1 (ppm)

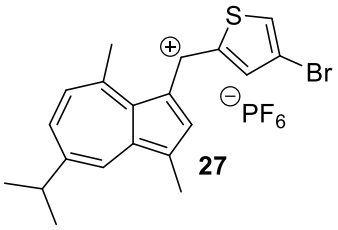

{1.94,1.94}CD3CN
S
Br
PF6
27
COSY, CD3CN
f1 (ppm)
f2 (ppm)



27

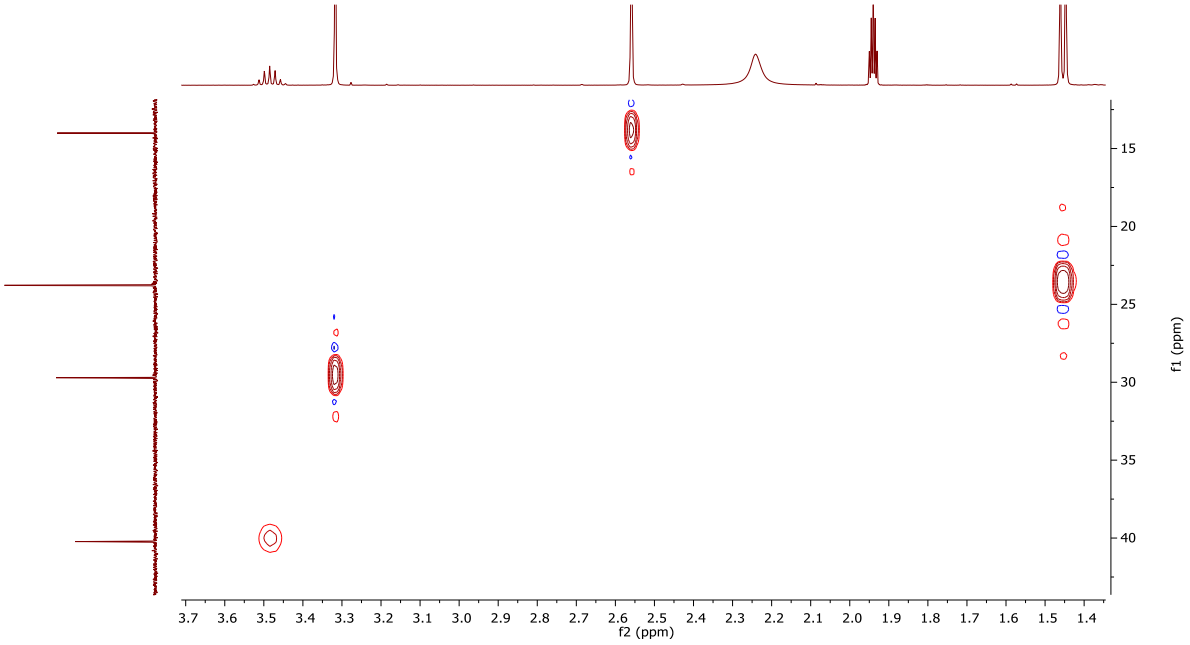
NOESY, CD_3CN

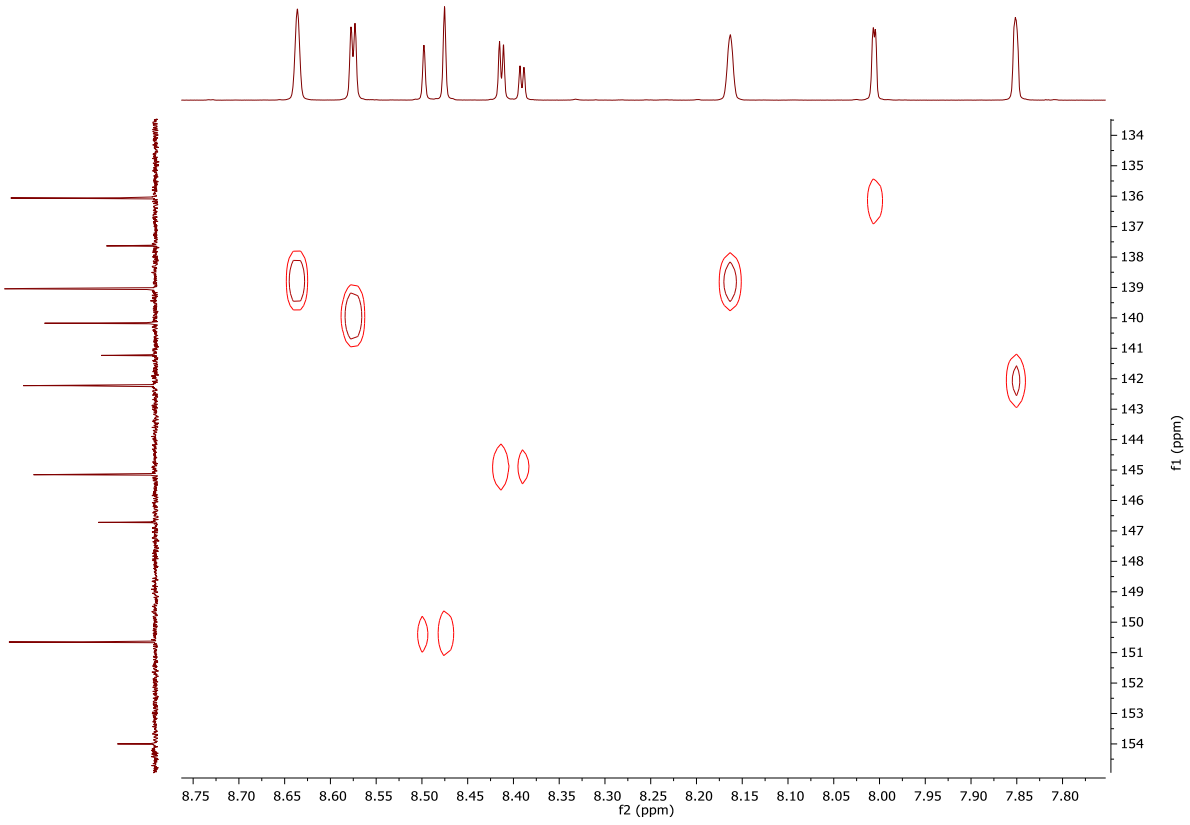


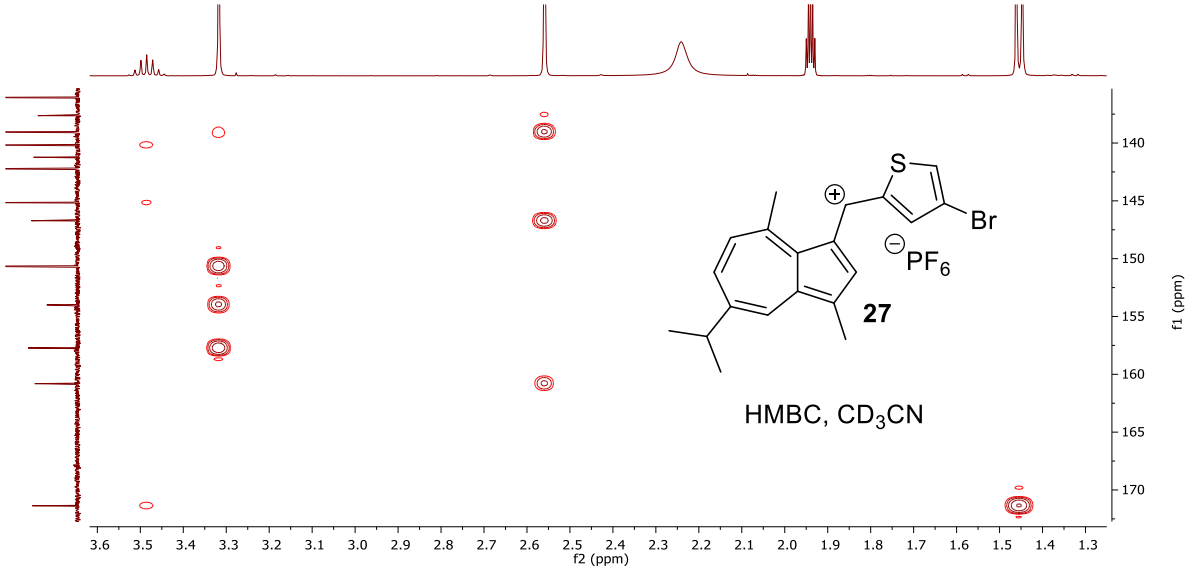


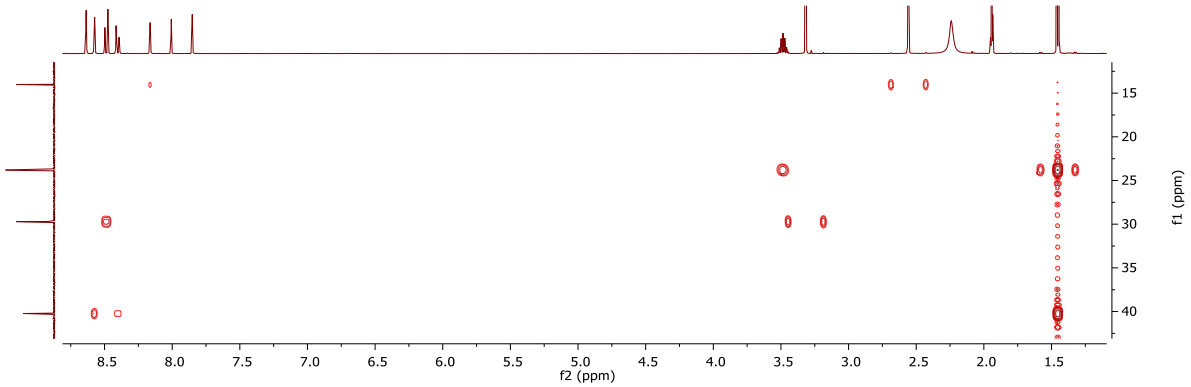
27

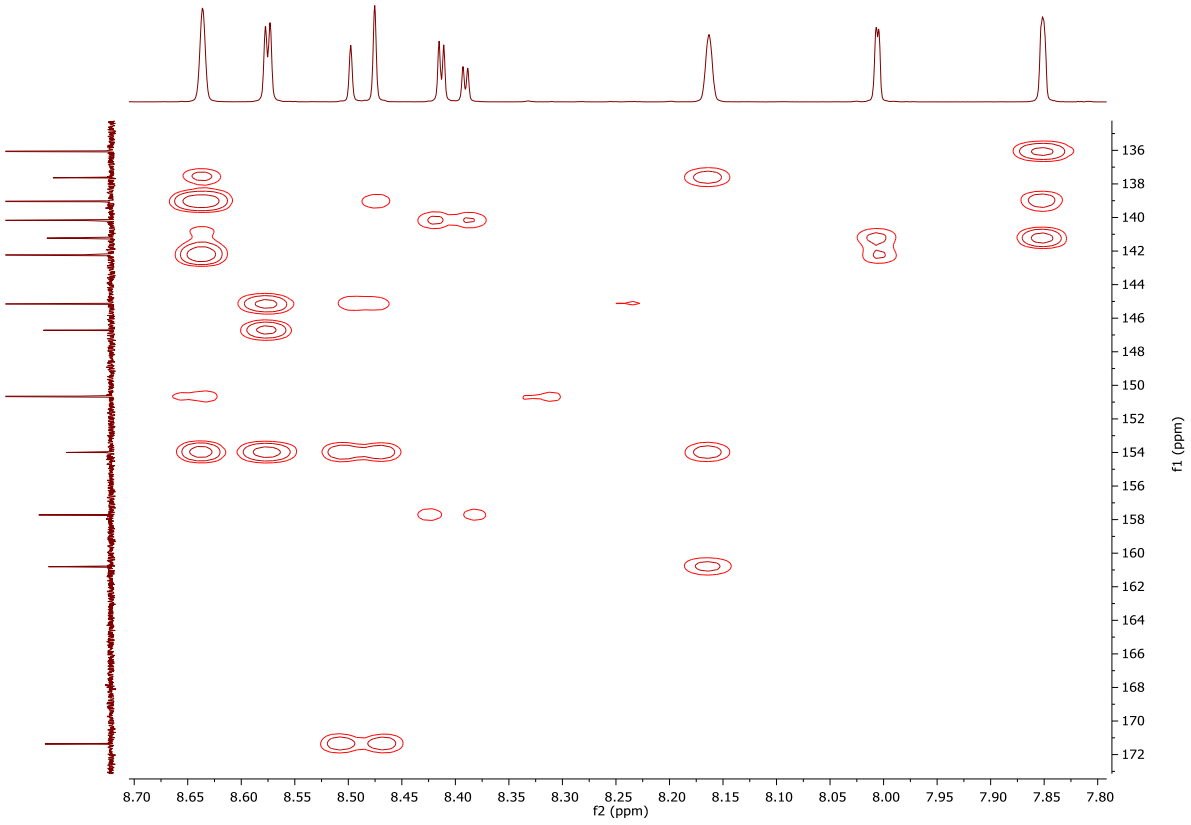
HSQC, CD_3CN

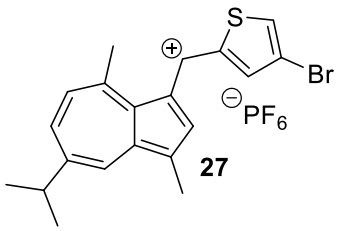




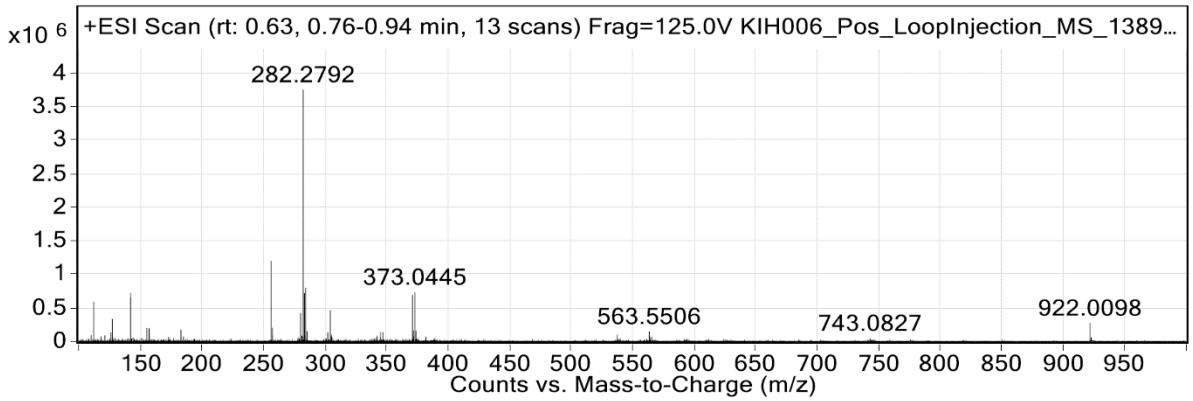

S
Br
PF6
27
HMBC, CD3CN
f2 (ppm)
f1 (ppm)

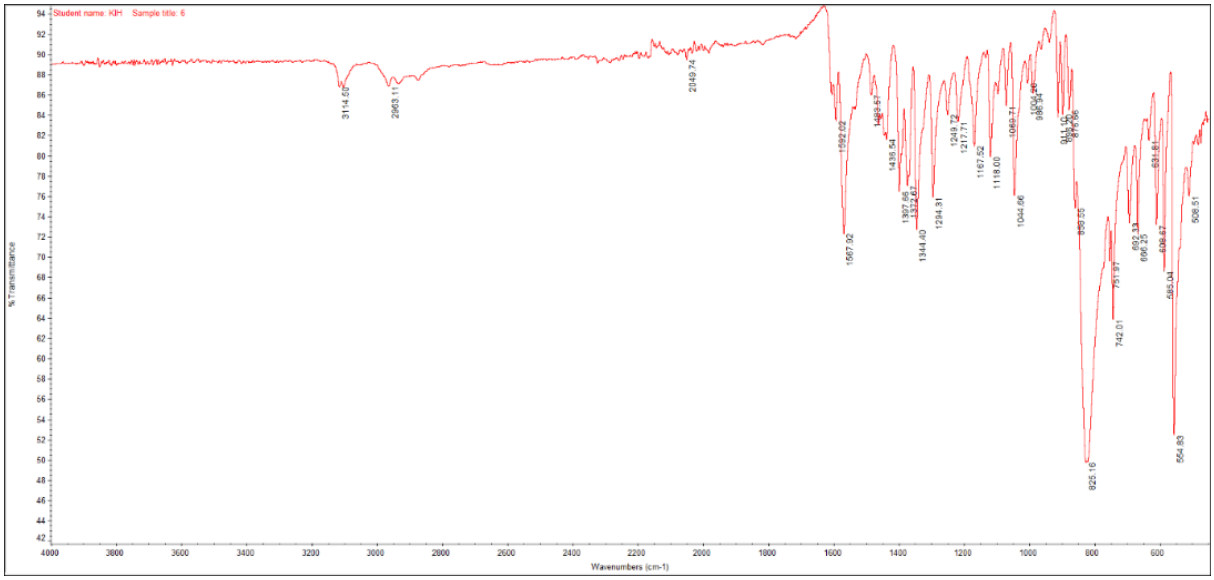

f2 (ppm)
f1 (ppm)

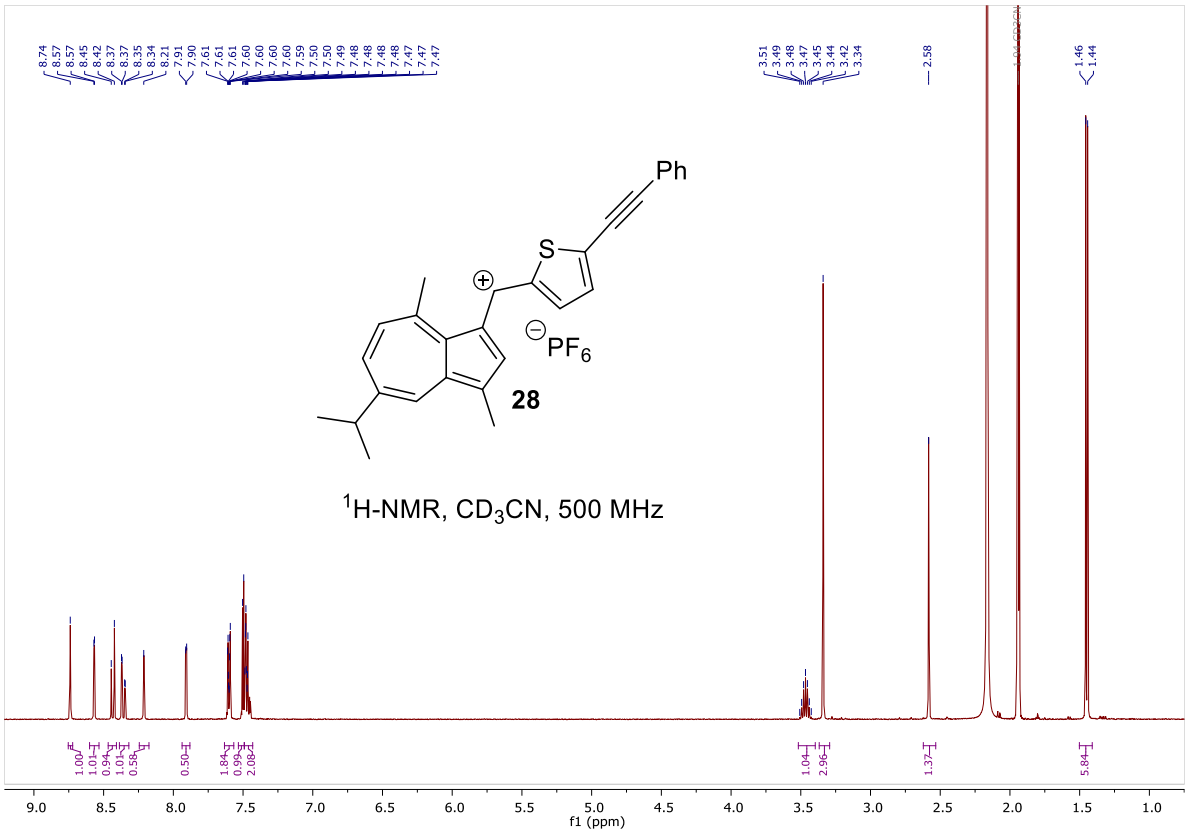

f2 (ppm)
f1 (ppm)

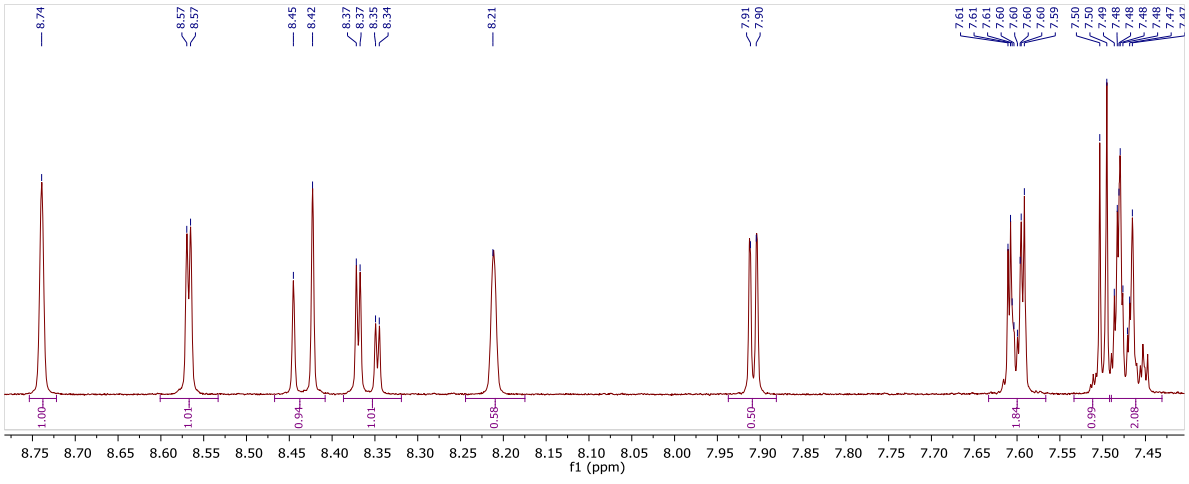

S
Br
PF6

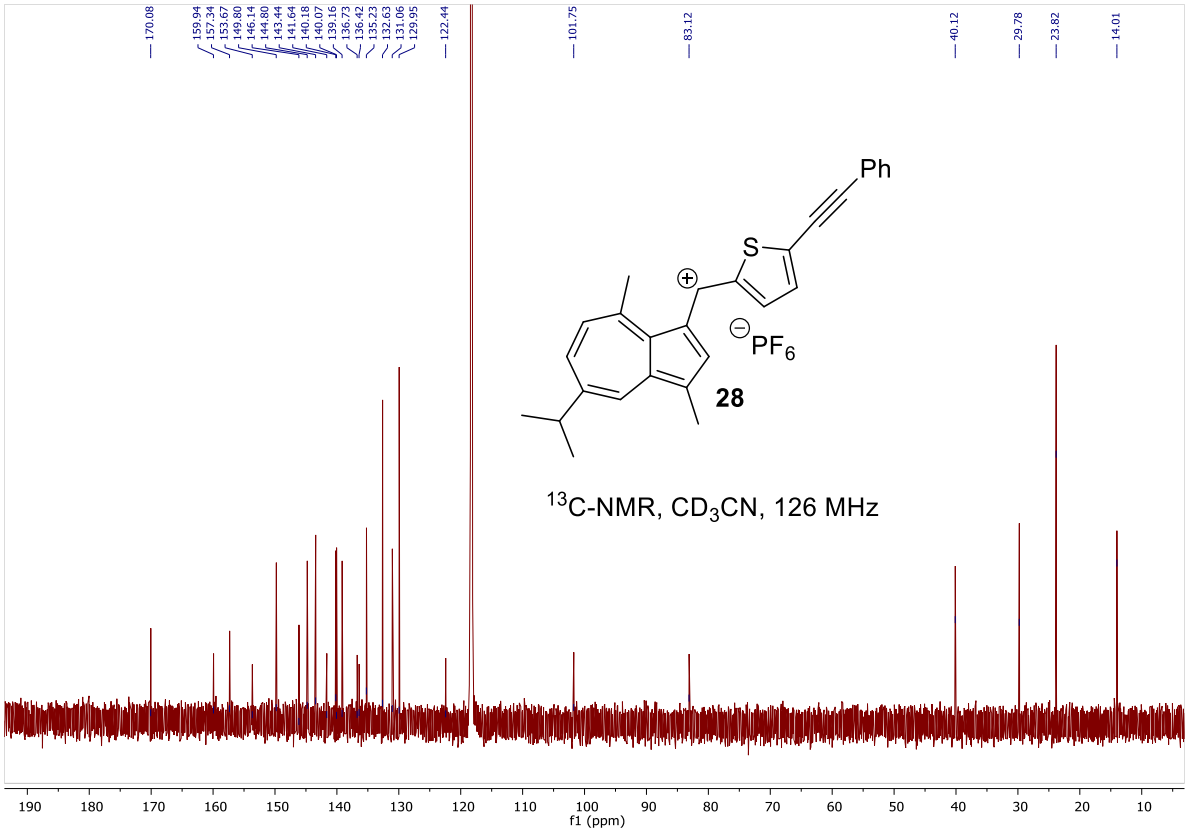
27

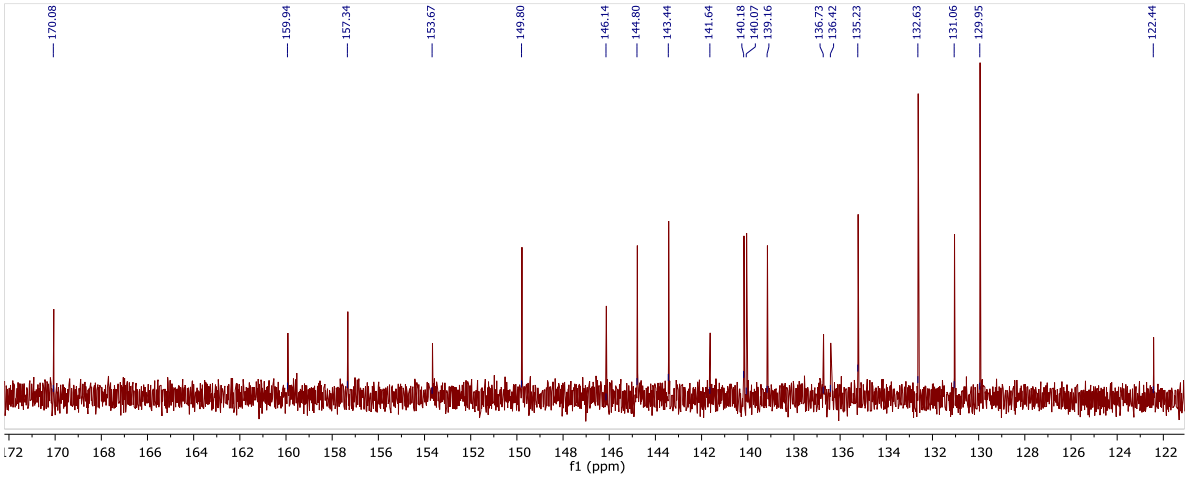

x10 6
+ESI Scan (rt: 0.63, 0.76-0.94 min, 13 scans) Frag=125.0V KIH006_Pos_LoopInjection_MS_1389...
282.2792
373.0445
563.5506
743.0827
922.0098
Counts vs. Mass-to-Charge (m/z)


Student name: KIH Sample title: 6
%Transmittance
Wavenumbers (cm-1)


Ph
S
PF6
28
1H-NMR, CD3CN, 500 MHz
f1 (ppm)


f1 (ppm)


170.08
159.94
157.34
153.67
149.80
146.14
144.80
143.44
141.64
140.18
140.07
139.16
136.73
136.42
135.23
132.63
131.06
129.95
122.44
101.75
83.12
40.12
29.78
23.82
14.01
Ph
S
PF6
28
13C-NMR, CD3CN, 126 MHz
f1 (ppm)


170.08
159.94
157.34
153.67
149.80
146.14
144.80
143.44
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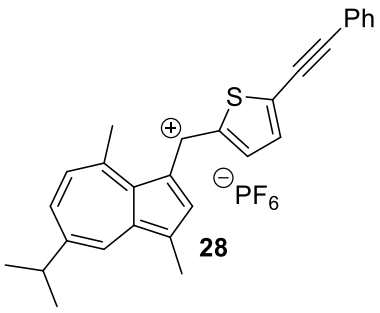
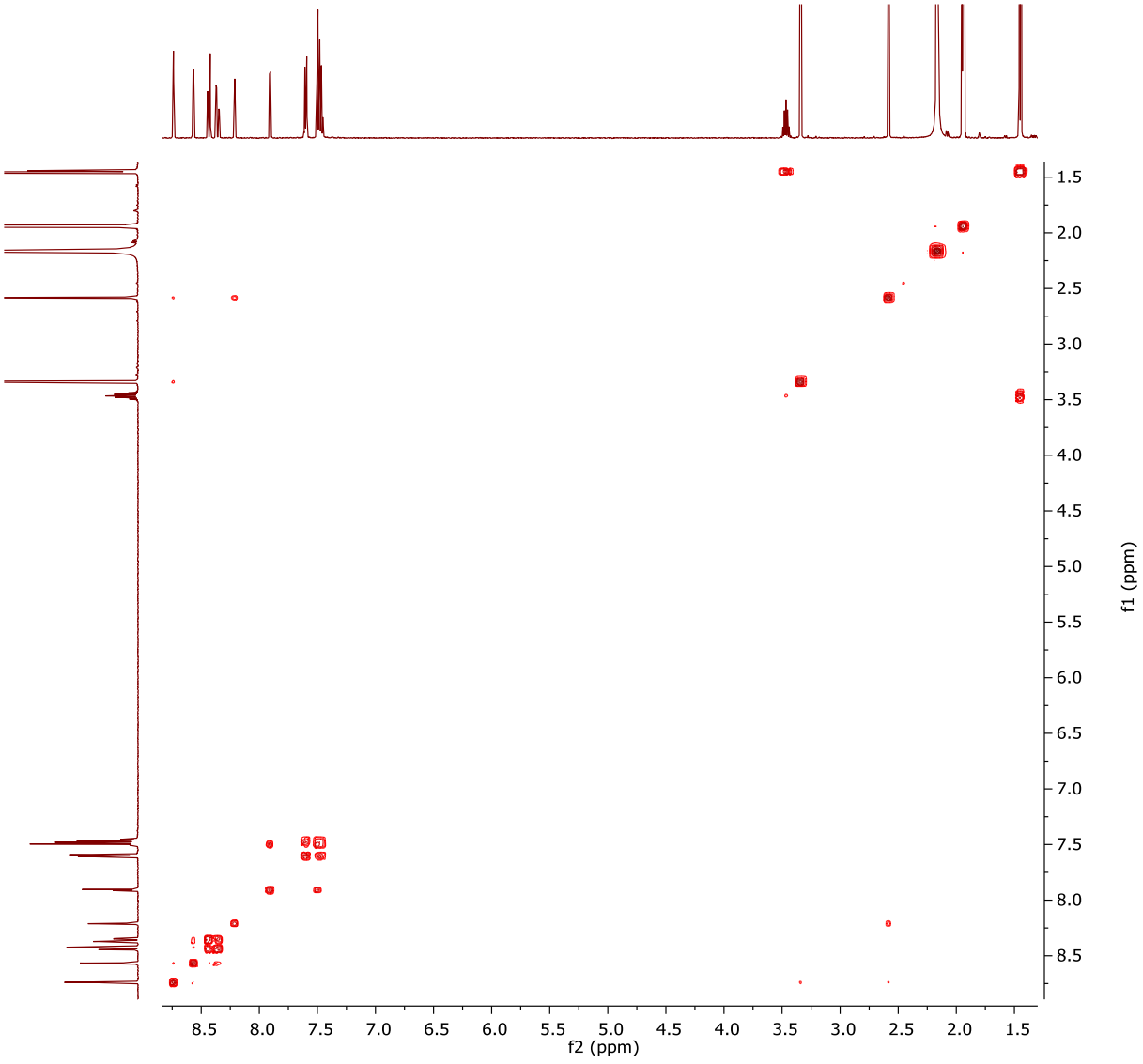
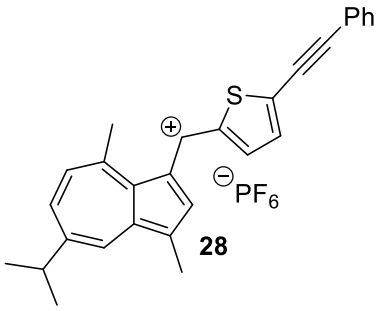
139.16
136.73
136.42
135.23
132.63
131.06
129.95
122.44
f1 (ppm)



28

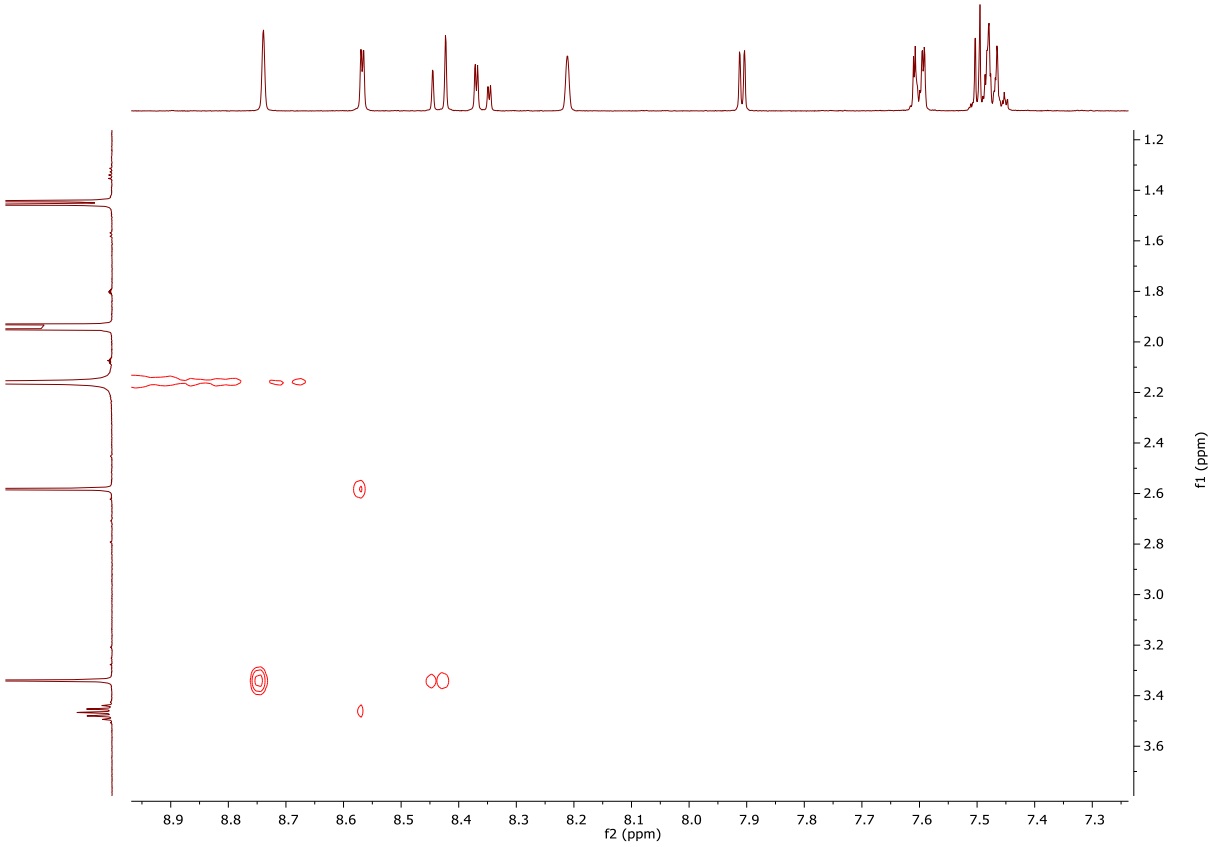
COSY, CD_3CN

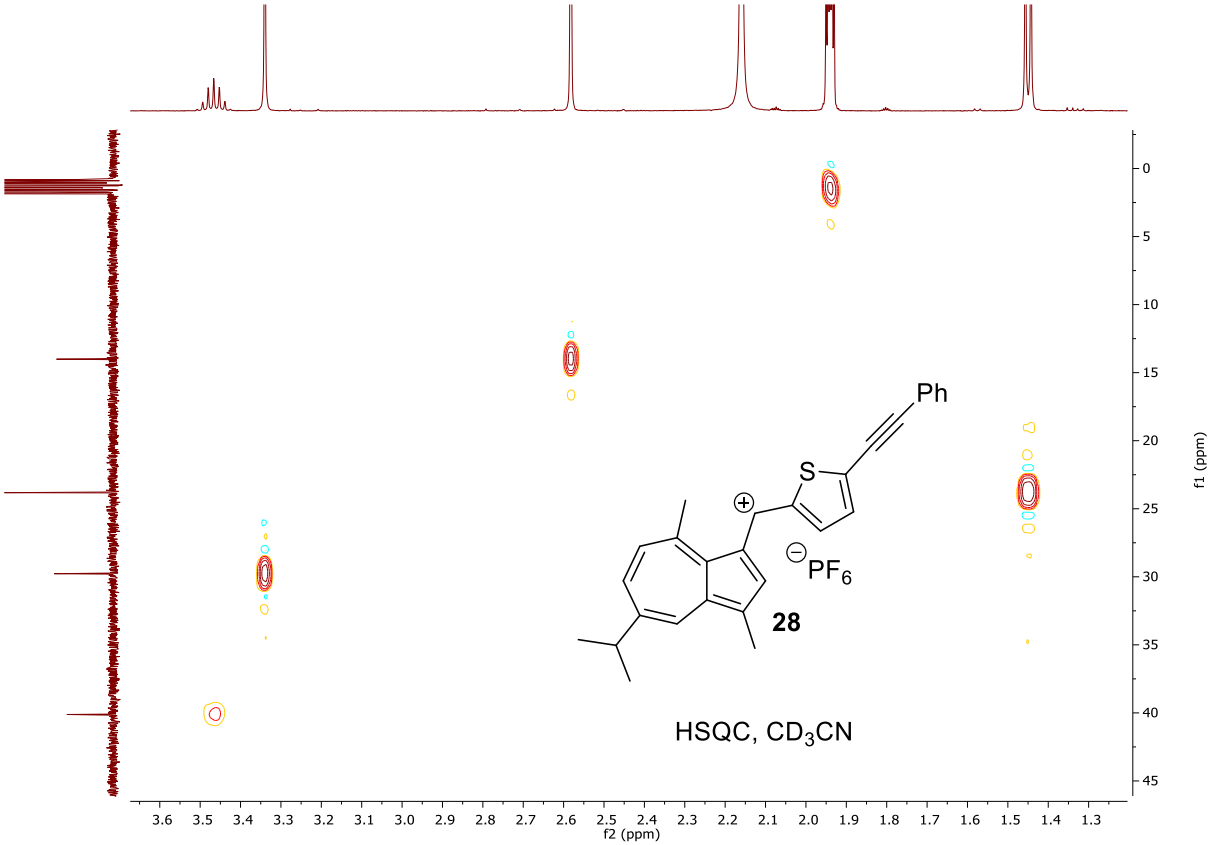


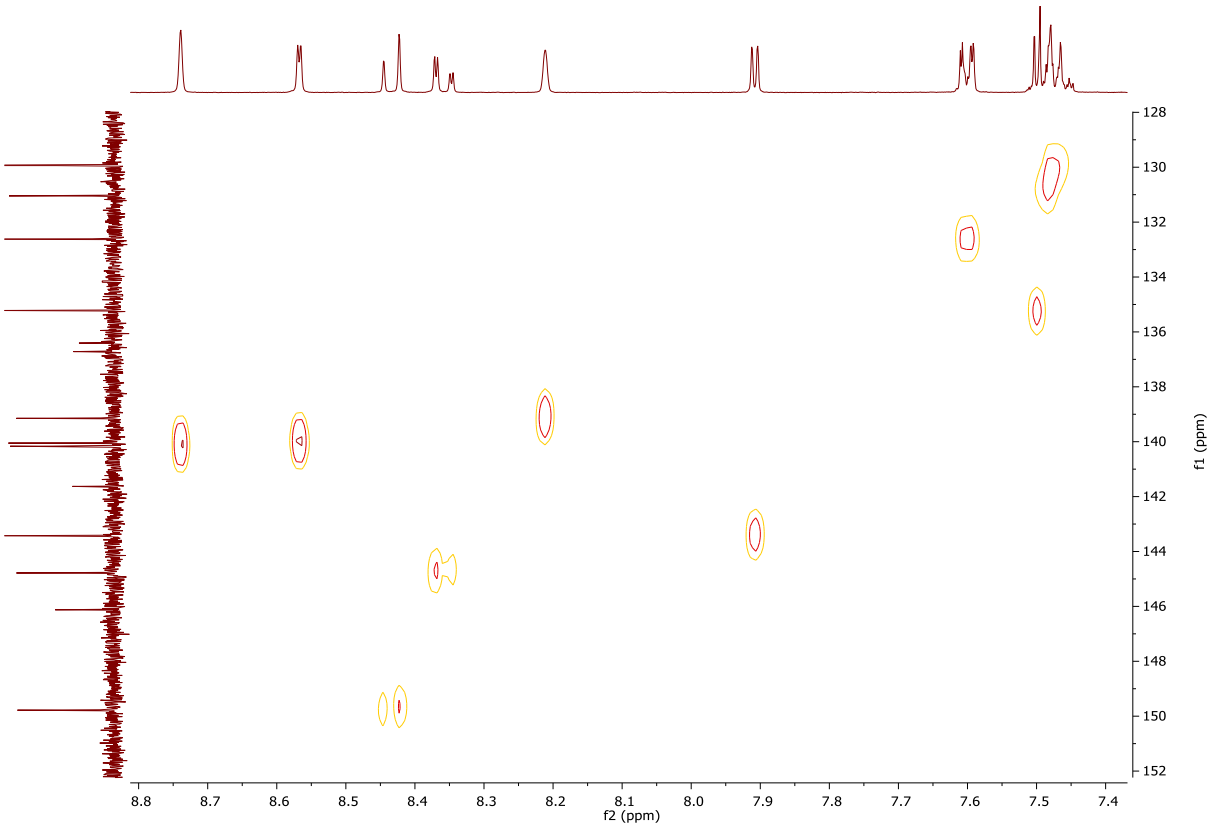


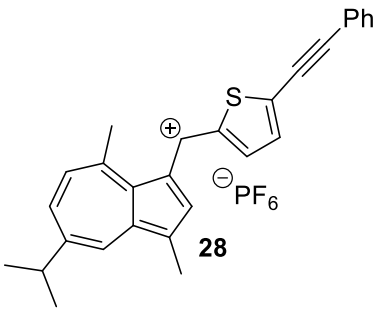
28

NOESY, CD_3CN



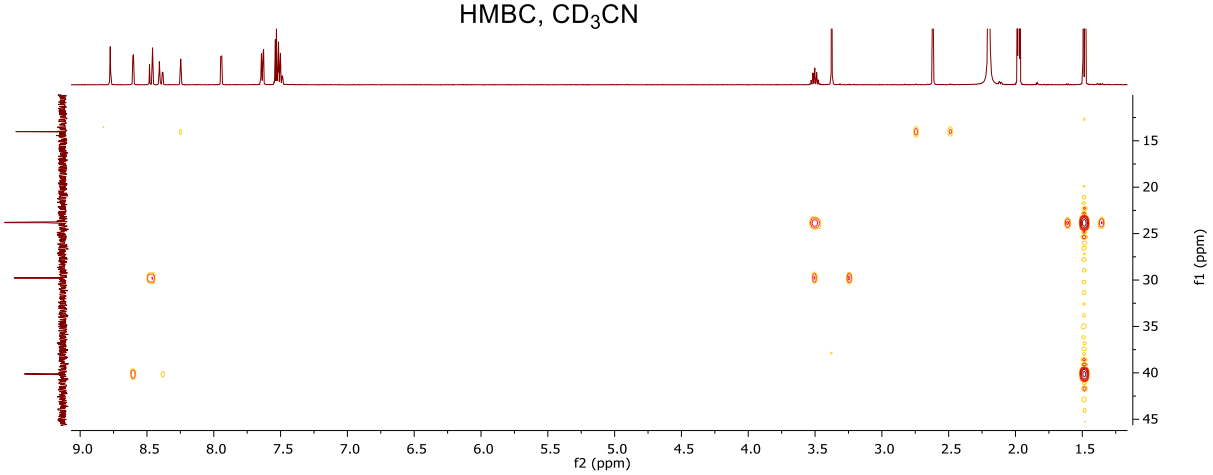

Ph
S
PF6
28
HSQC, CD3CN
f2 (ppm)
f1 (ppm)

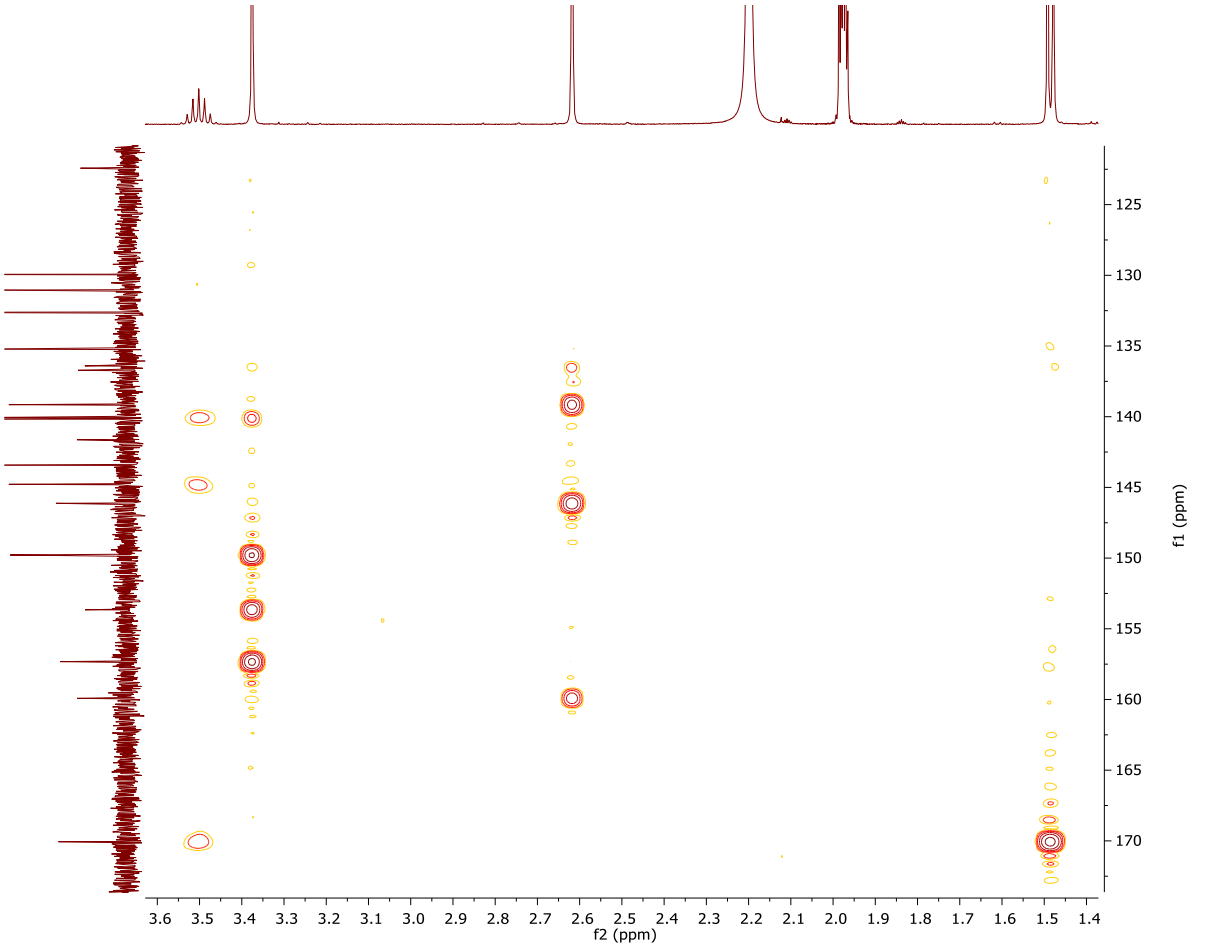

f2 (ppm)
f1 (ppm)

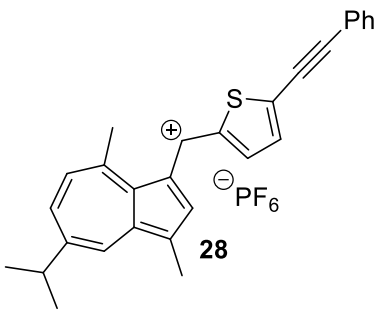


28

HMBC, CD_3CN

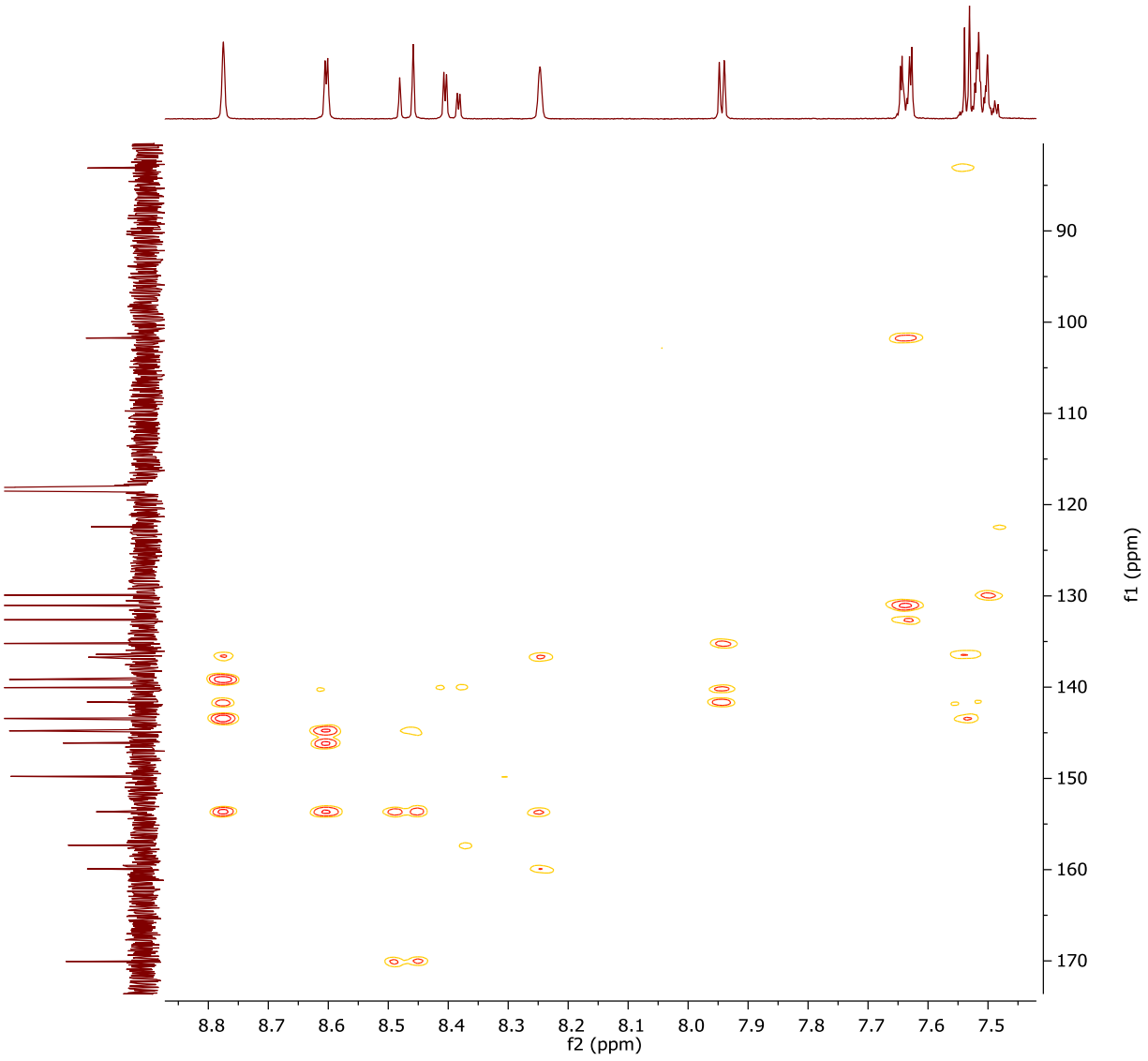


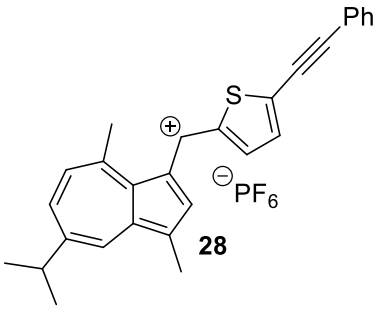




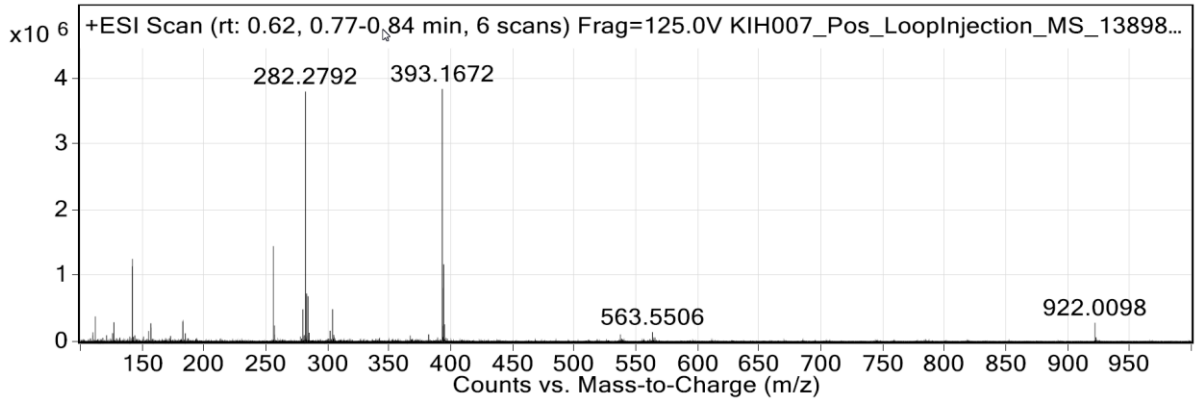
28

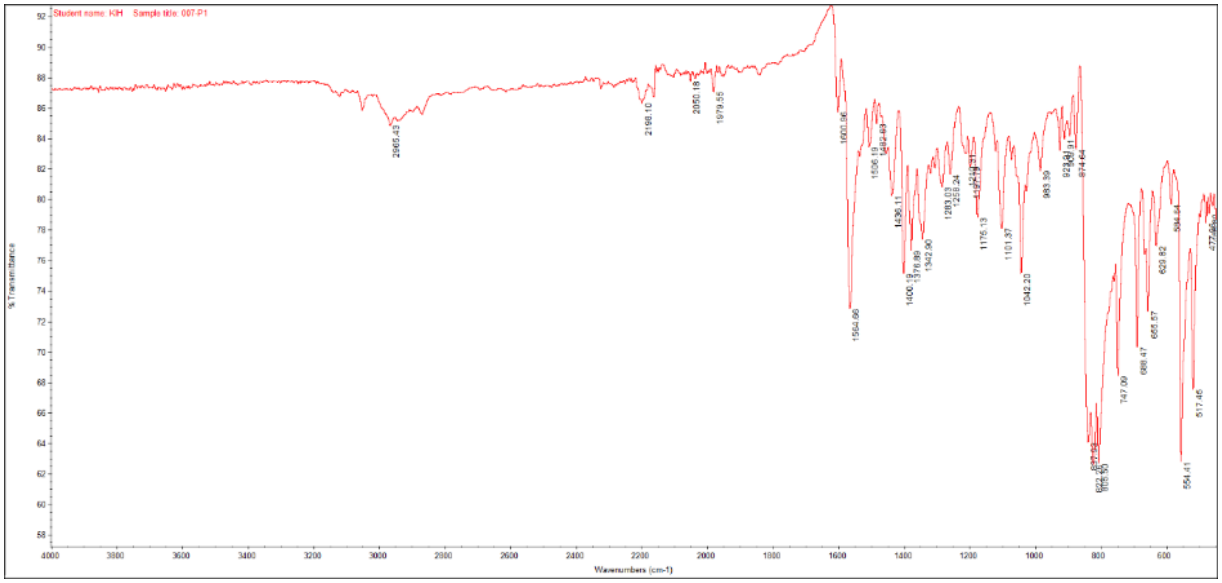
HMBC, CD_3CN

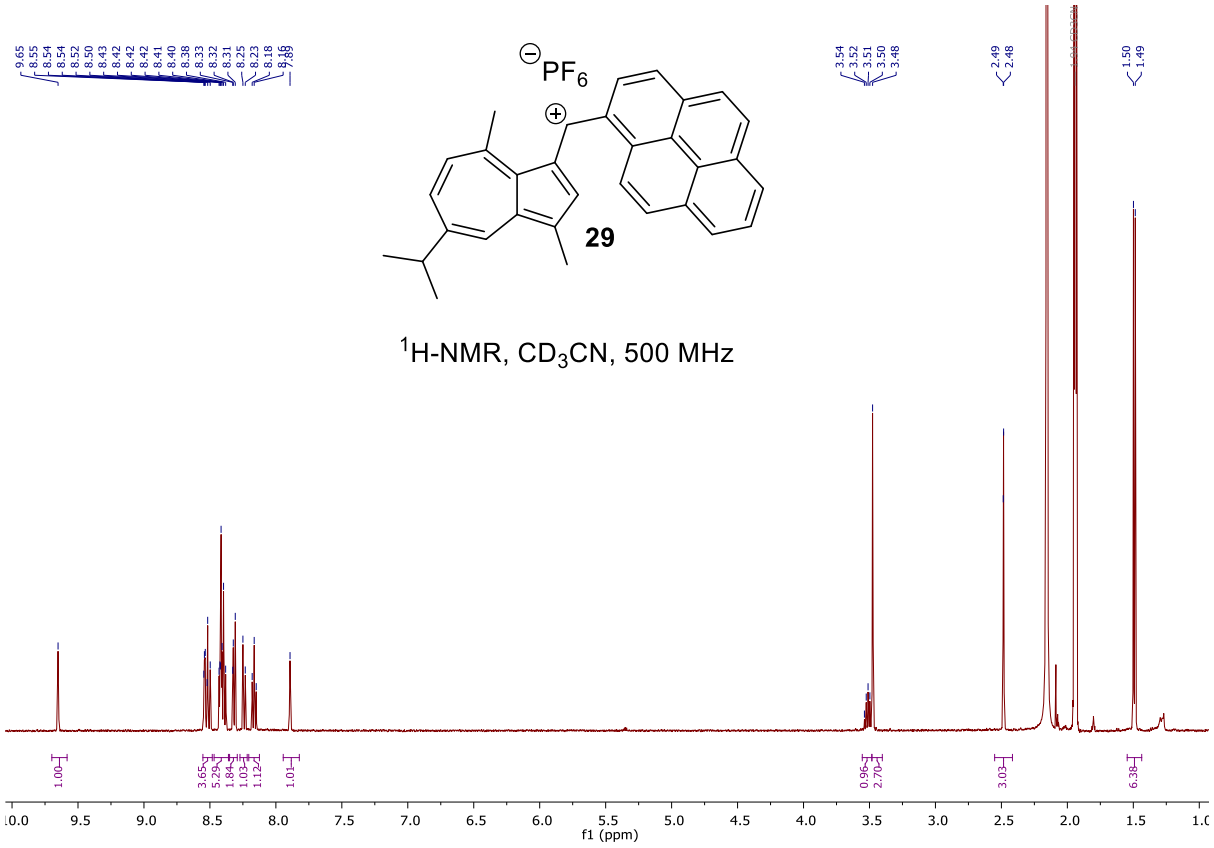


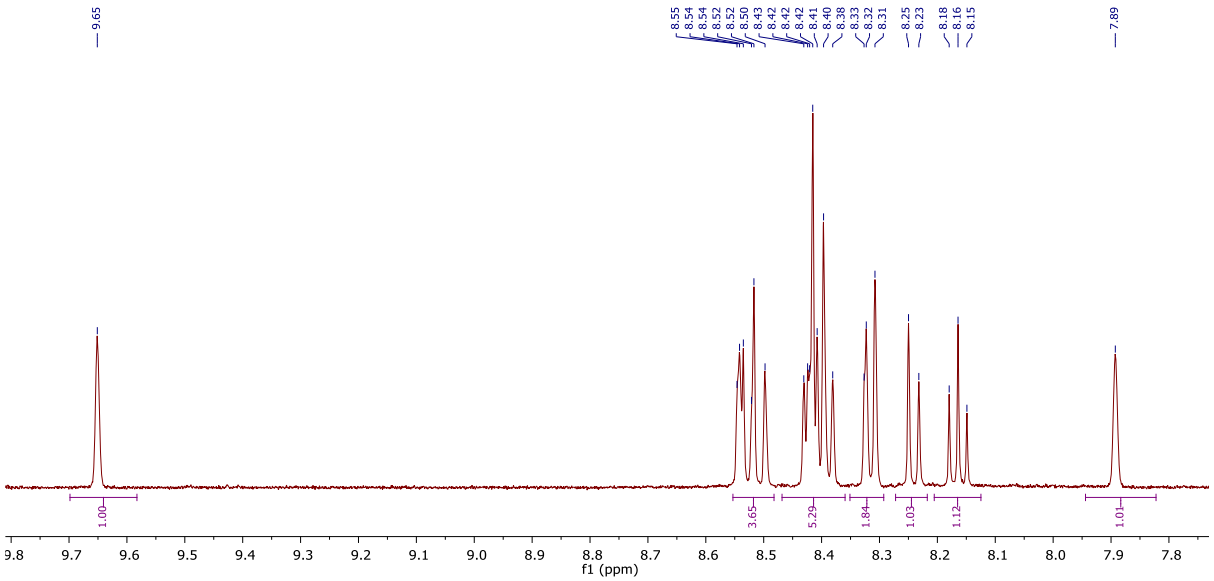

Ph
S
PF6

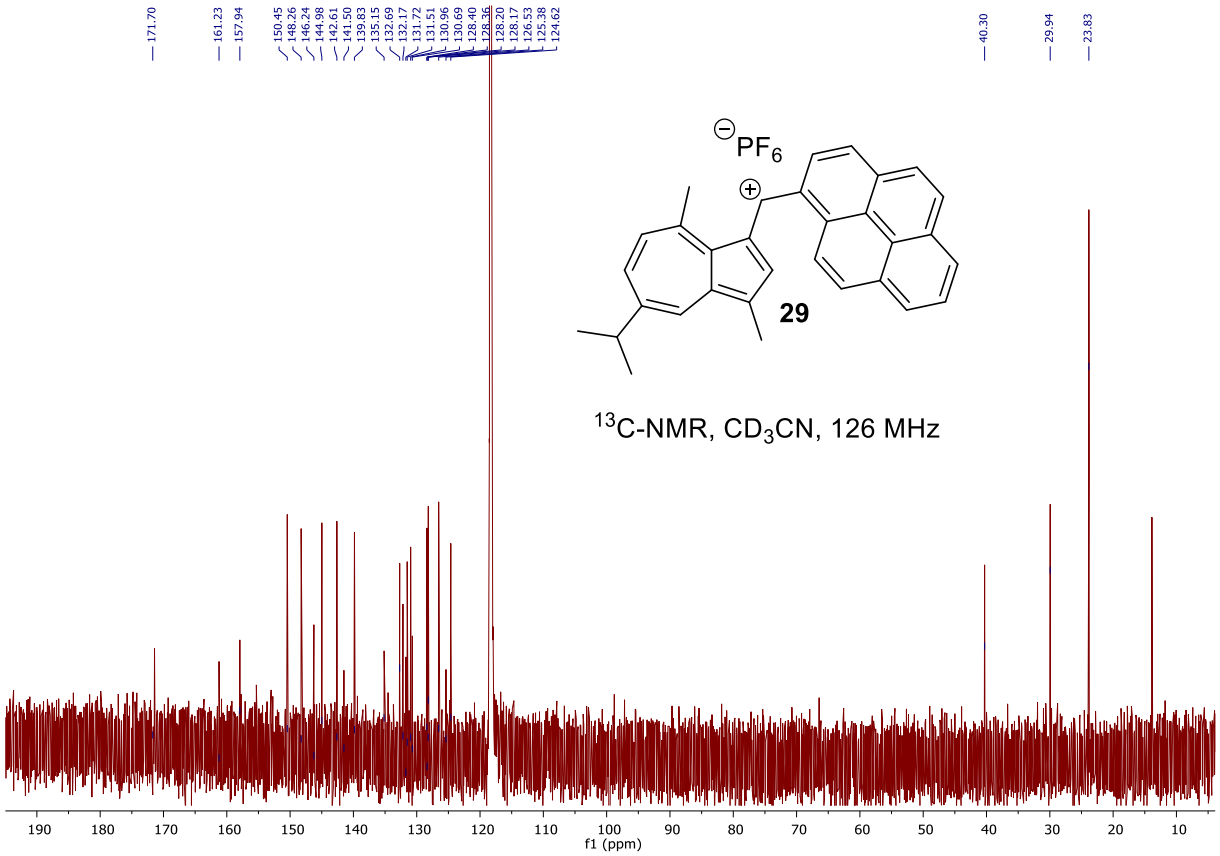
28

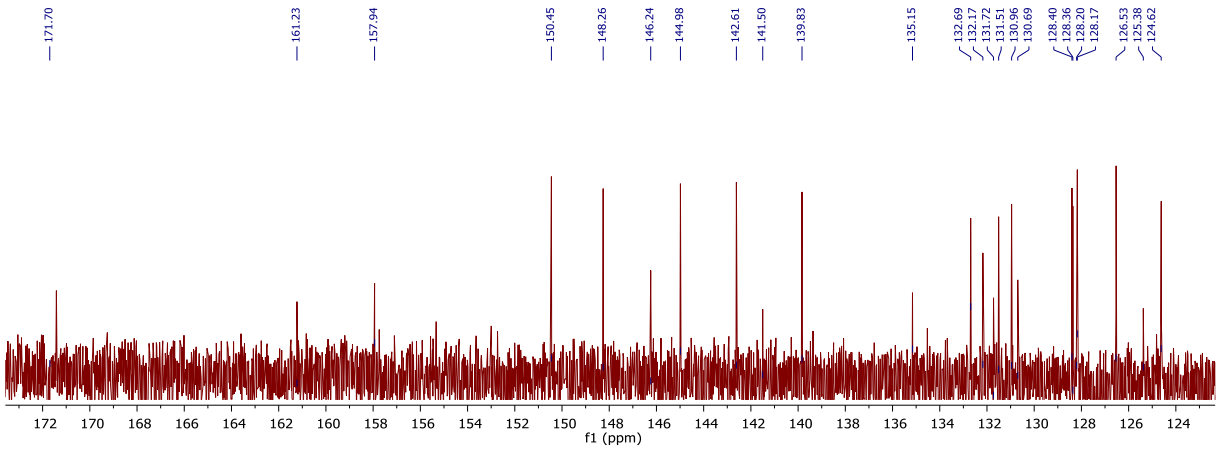

x10 6
+ESI Scan (rt: 0.62, 0.77-0.84 min, 6 scans) Frag=125.0V KIH007_Pos_LoopInjection_MS_13898...
282.2792
393.1672
563.5506
922.0098
Counts vs. Mass-to-Charge (m/z)


Student name: KIH Sample title: 007-P1
% Transmittance
Wavenumbers (cm-1)


PF6
29
1H-NMR, CD3CN, 500 MHz
f1 (ppm)


f1 (ppm)


171.70
161.23
157.94
150.45
148.26
146.24
144.98
142.61
141.50
139.83
135.15
132.69
132.17
131.72
131.51
130.96
130.69
128.40
128.36
128.20
128.17
126.53
125.38
124.62
40.30
29.94
23.83
PF6
29
13C-NMR, CD3CN, 126 MHz
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


171.70
161.23
157.94
150.45
148.26
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142.61
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139.83
135.15
132.69
132.17
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131.51
130.96
130.69
128.40
128.36
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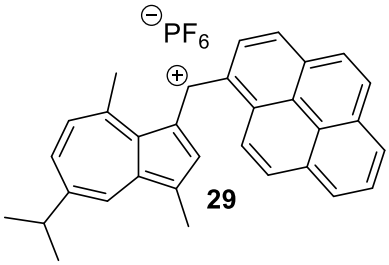
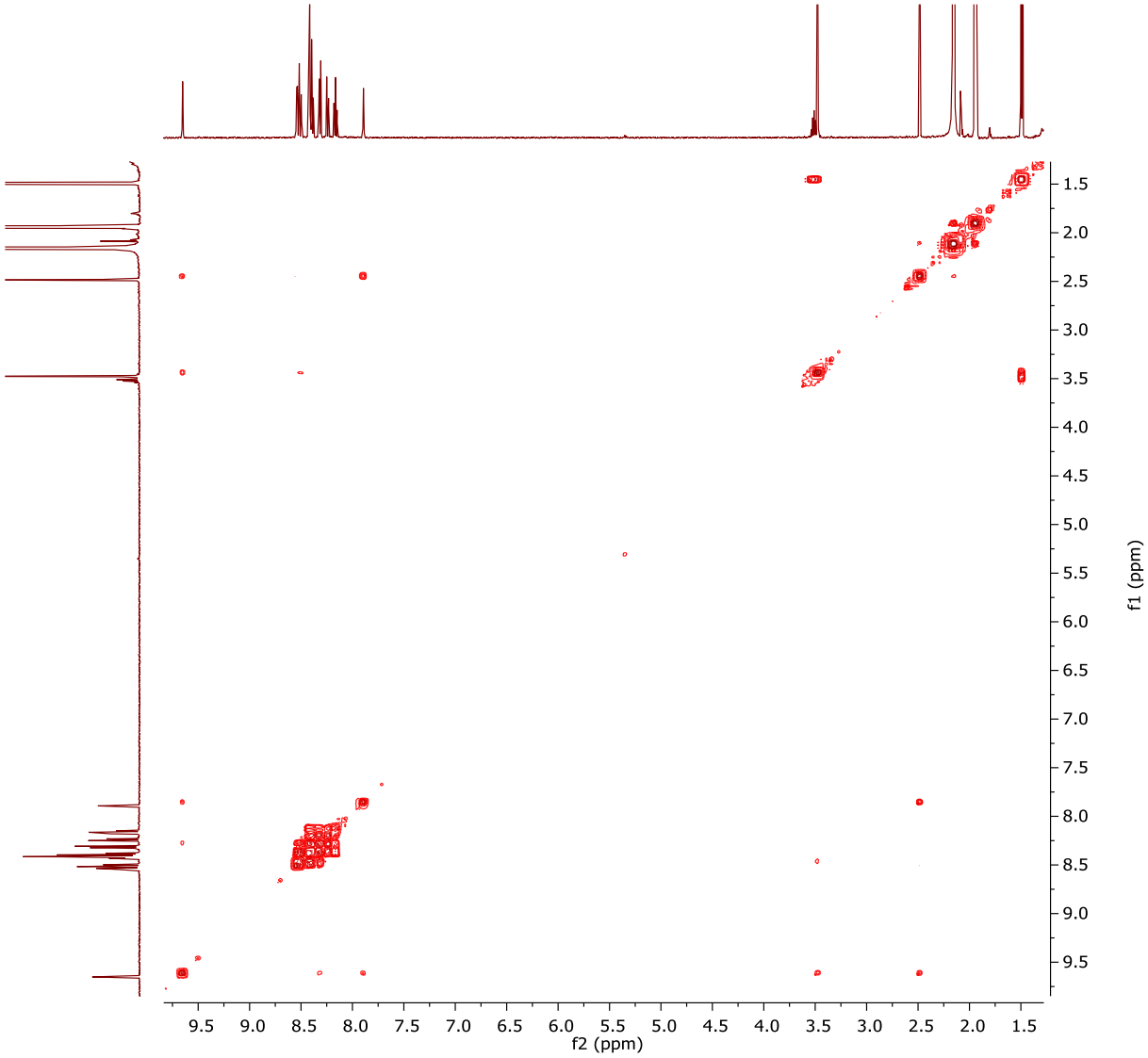
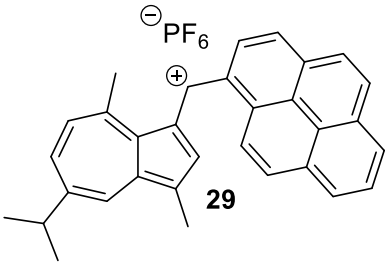
126.53
125.38
124.62
172 170 168 166 164 162 160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124
f1 (ppm)



29

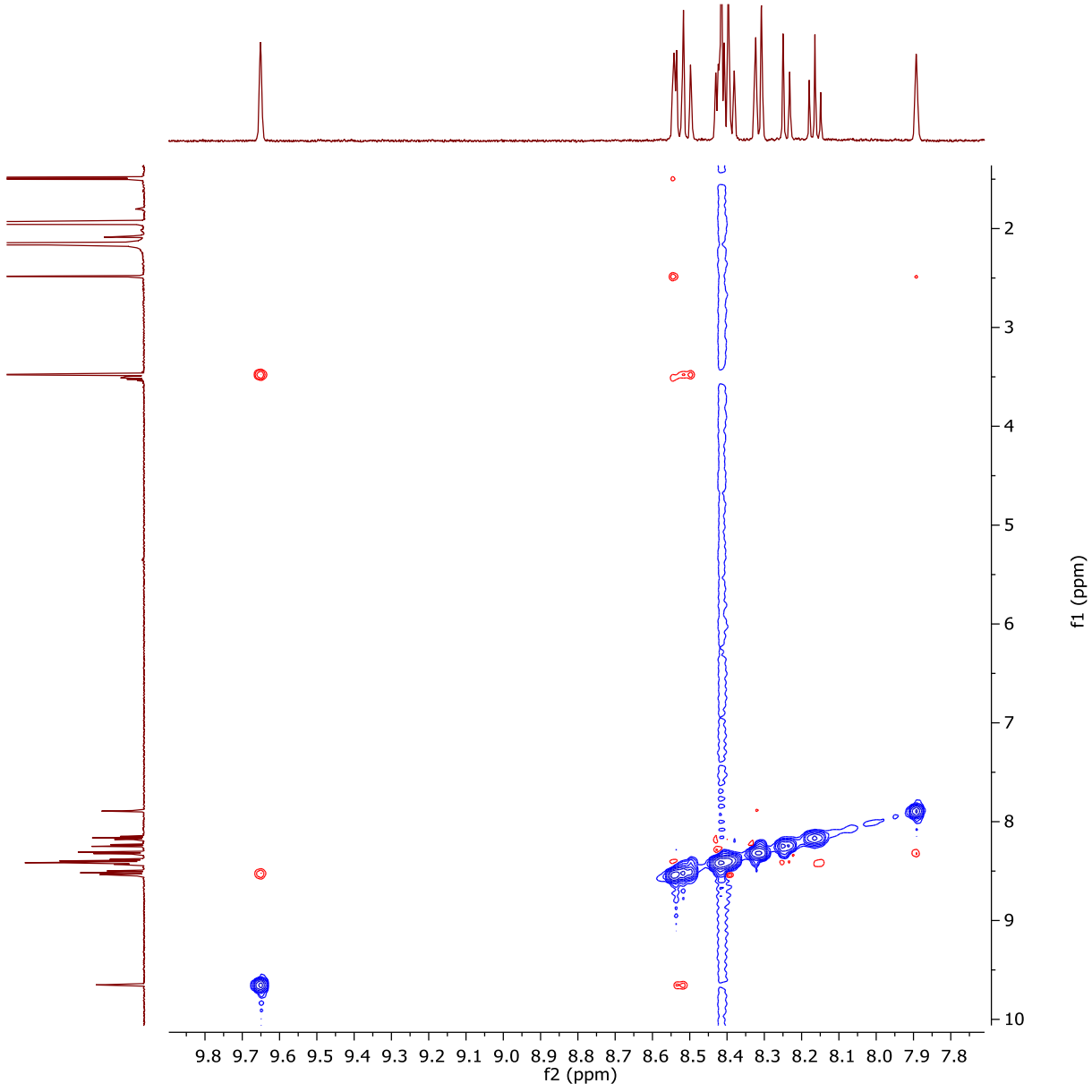
COSY, CD_3CN

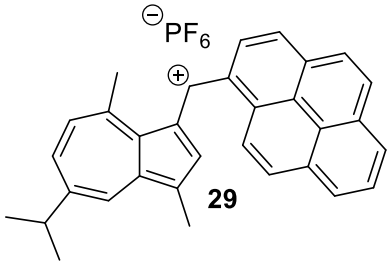




29

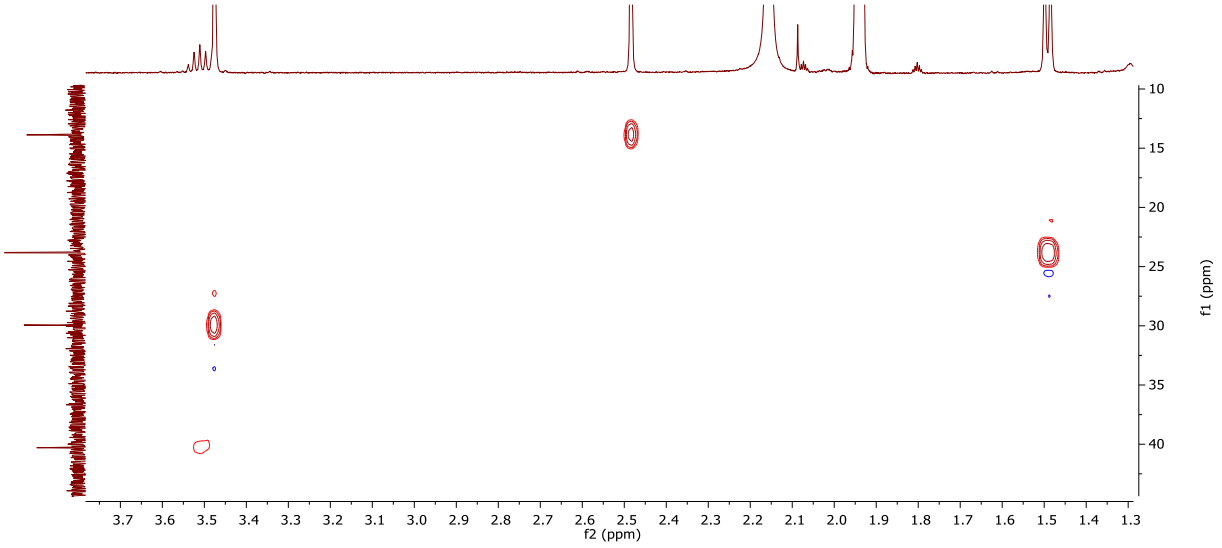
NOESY, CD_3CN

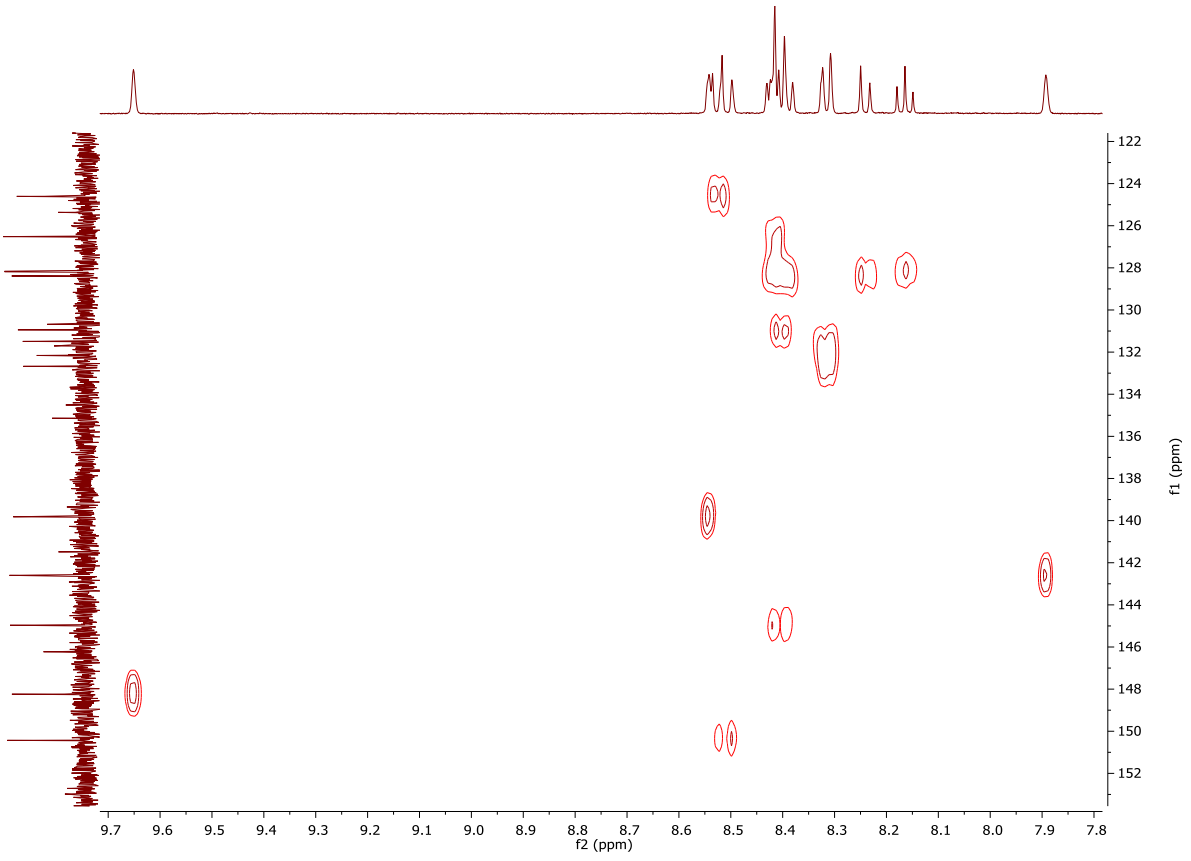


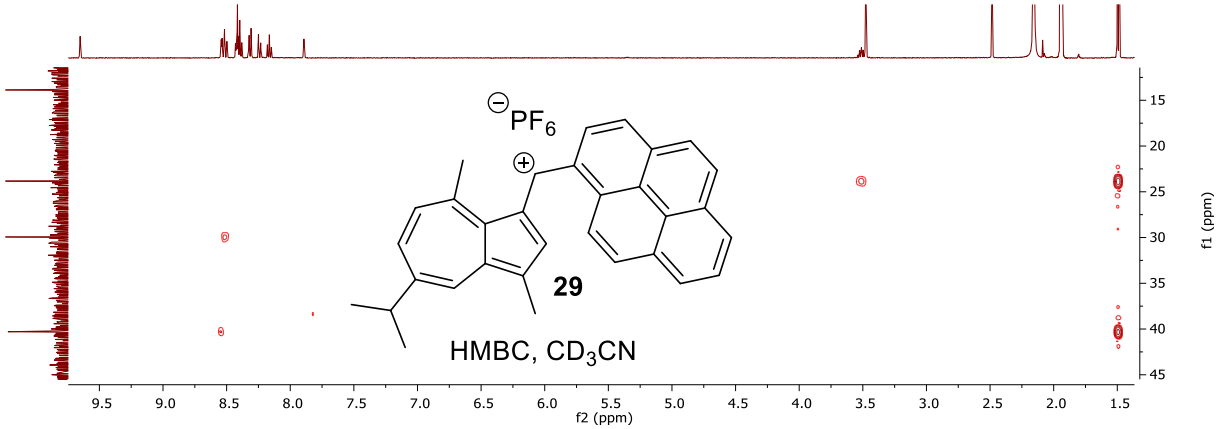


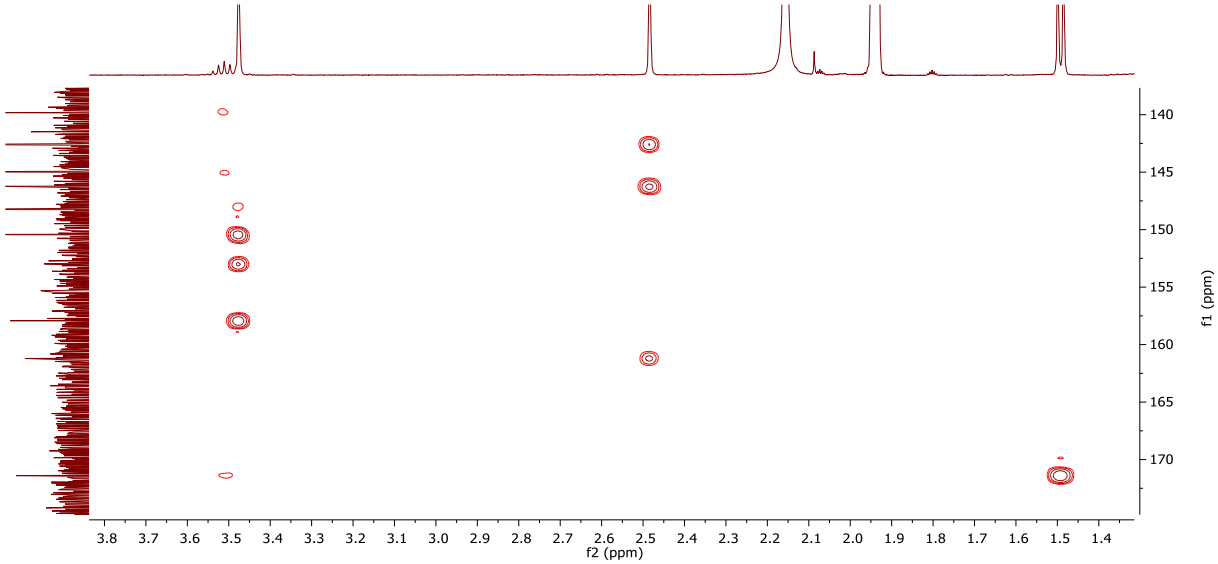
29

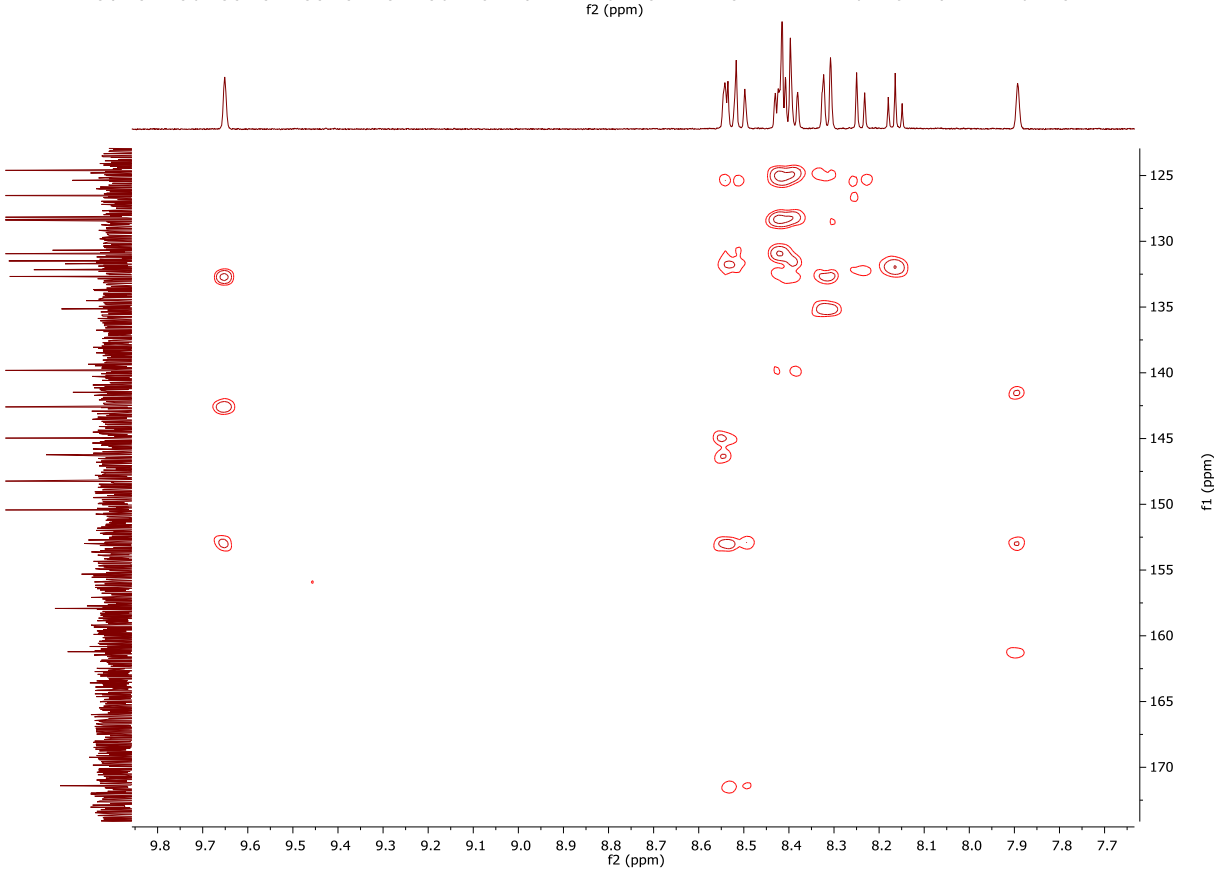
HSQC, CD_3CN

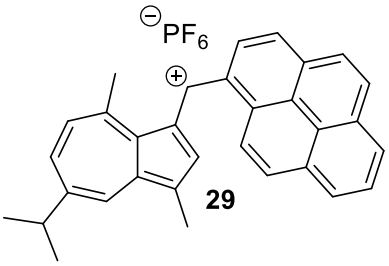




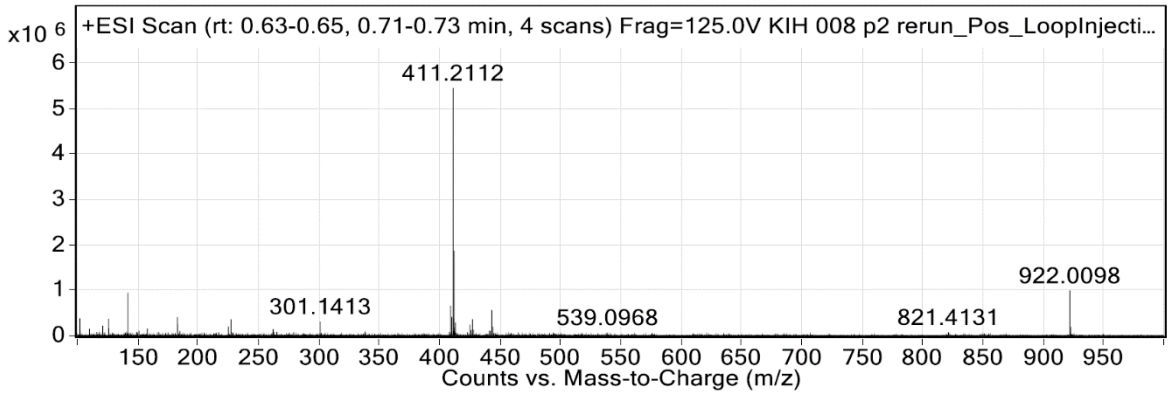

PF6
29
HMBC, CD3CN
f2 (ppm)
f1 (ppm)

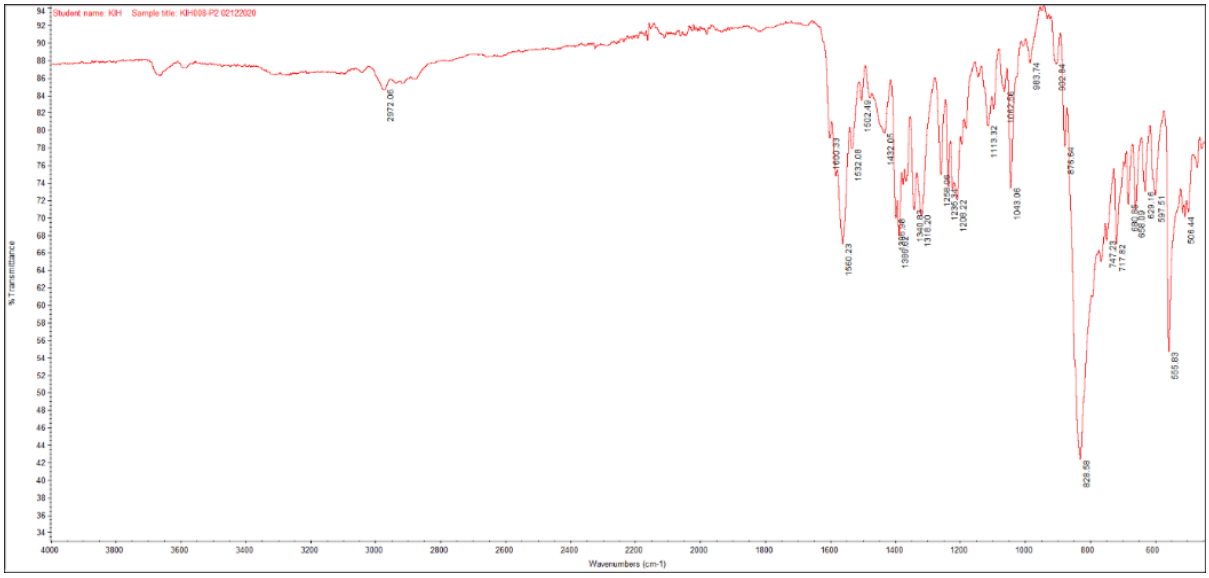

f2 (ppm)
f1 (ppm)

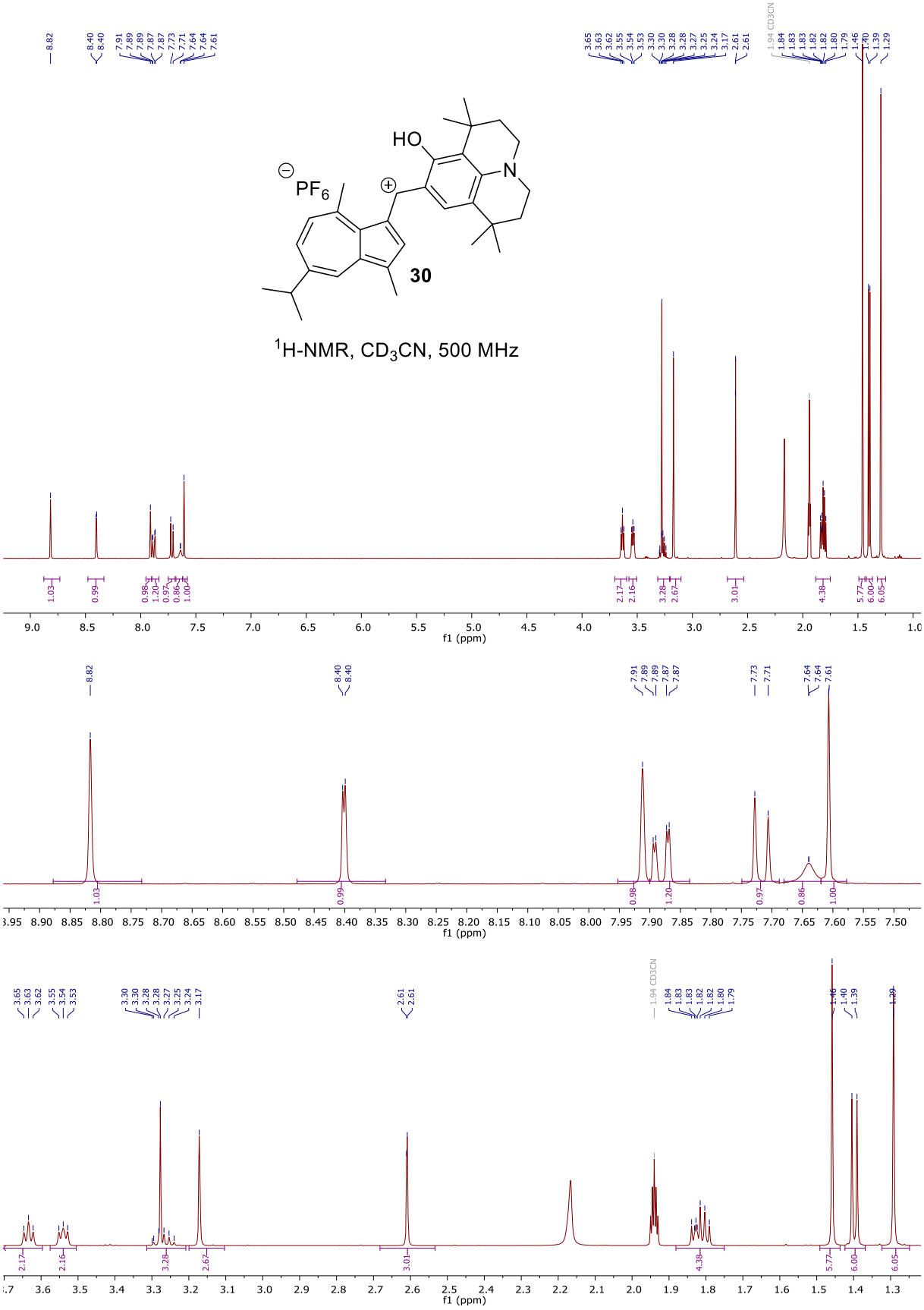

f2 (ppm)
f1 (ppm)

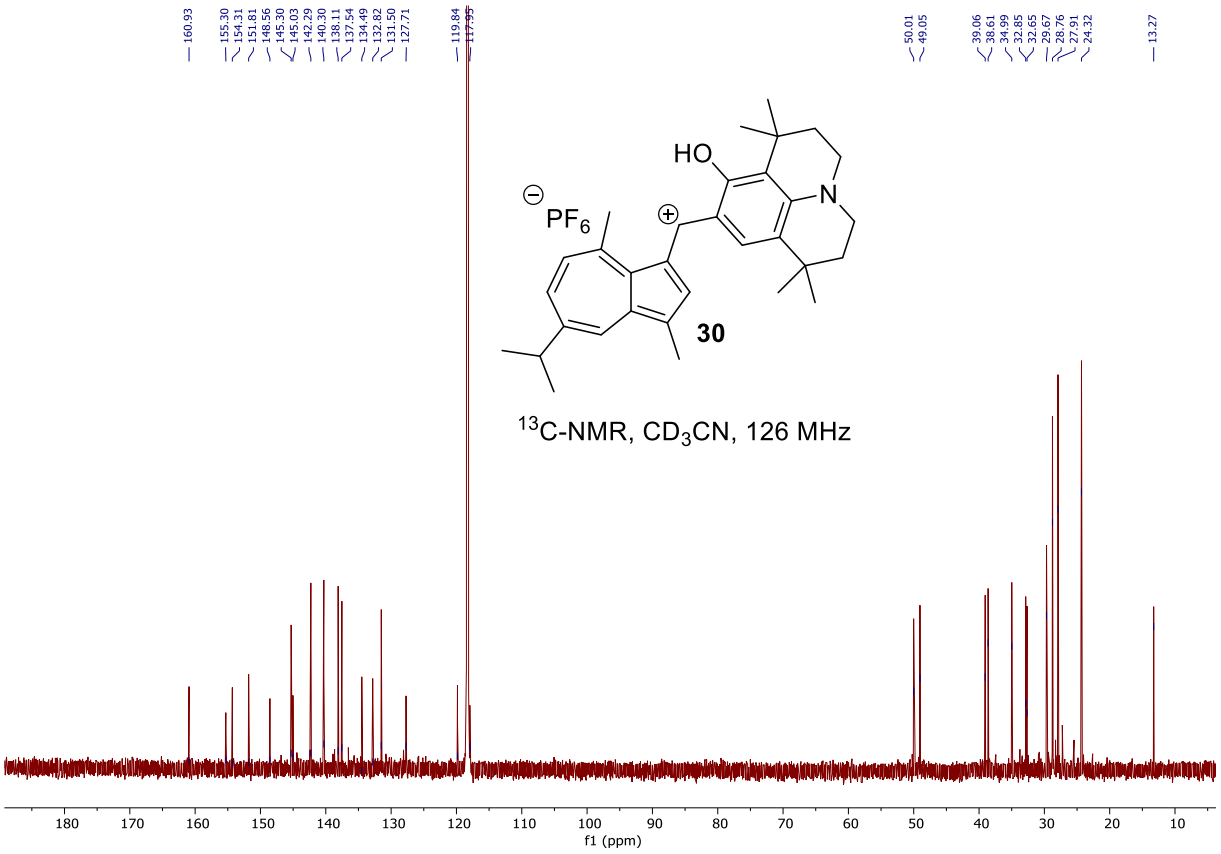

PF6

29


x10 6
+ESI Scan (rt: 0.63-0.65, 0.71-0.73 min, 4 scans) Frag=125.0V KIH 008 p2 rerun_Pos_LoopInjecti...
411.2112
301.1413
539.0968
821.4131
922.0098
Counts vs. Mass-to-Charge (m/z)


% Transmittance
Wavenumbers (cm-1)


HO
N
PF6
30
1H-NMR, CD3CN, 500 MHz
f1 (ppm)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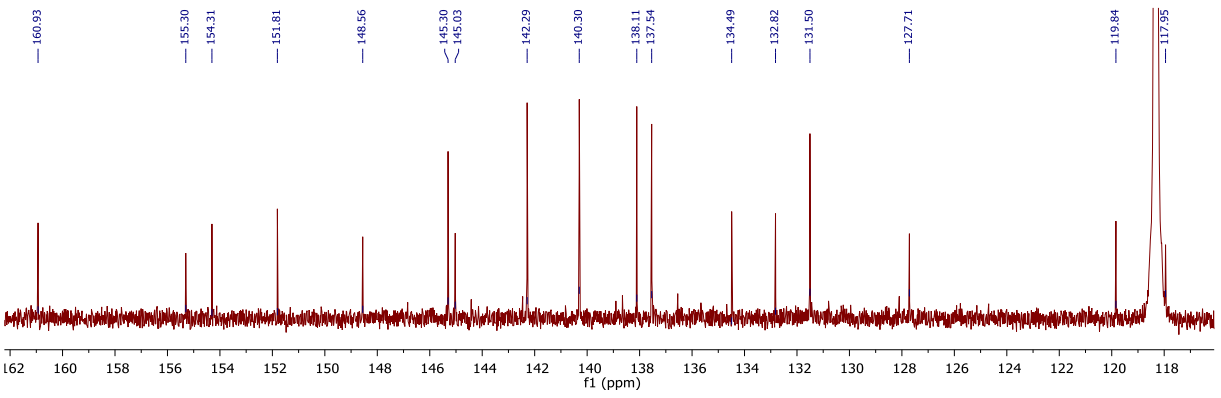
142.29
140.30
138.11
137.54
134.49
132.82
131.50
127.71
119.84
117.95
50.01
49.05
39.06
38.61
34.99
32.85
32.65
29.67
28.76
27.91
24.32
13.27
HO
N
PF6
30
13C-NMR, CD3CN, 126 MHz
f1 (ppm)


160.93
155.30
154.31
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145.03
142.29
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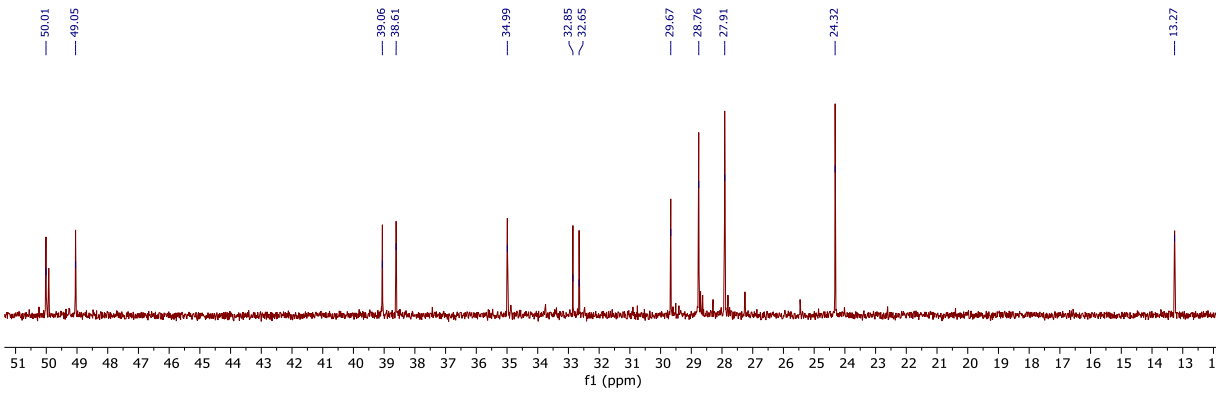
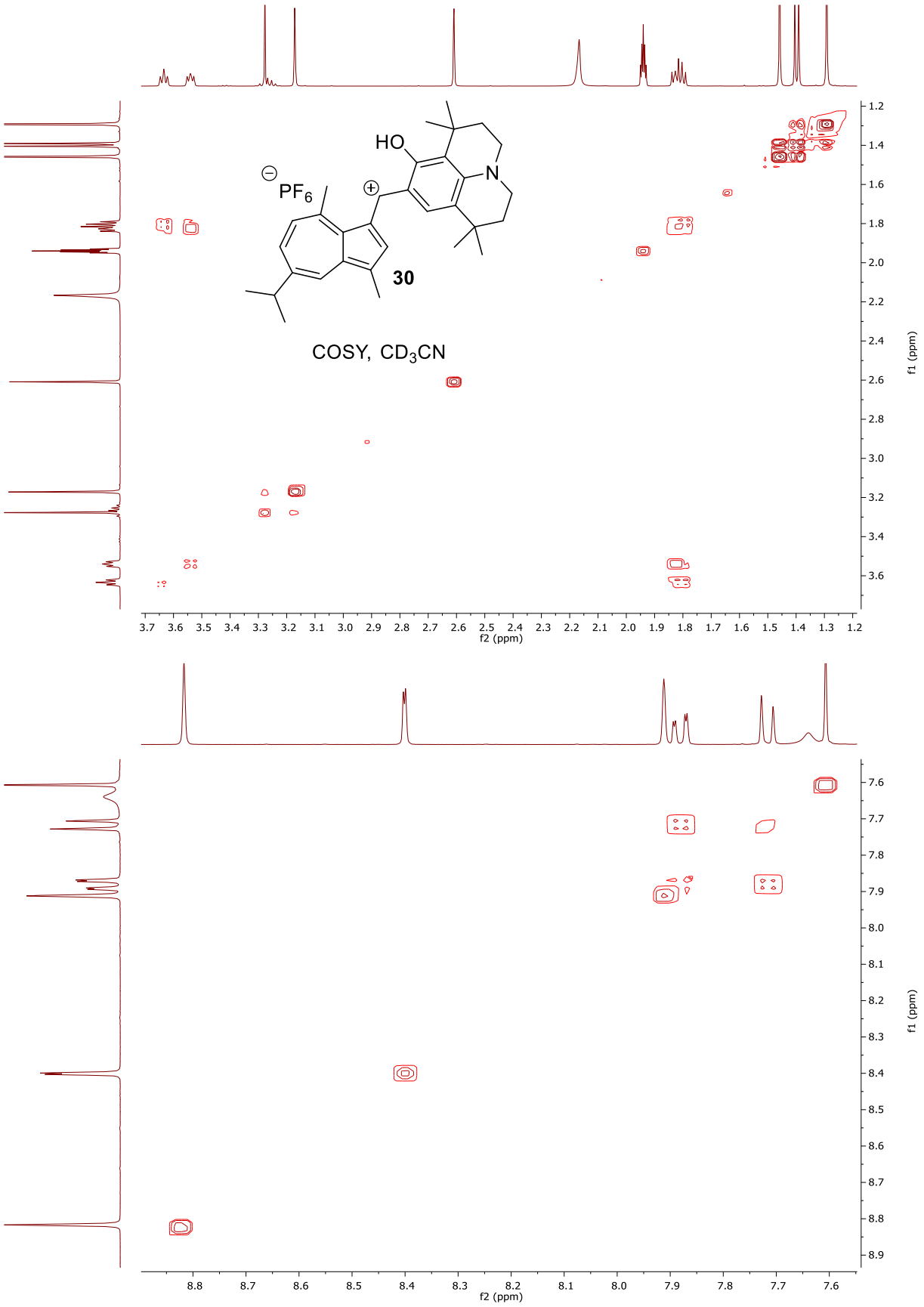
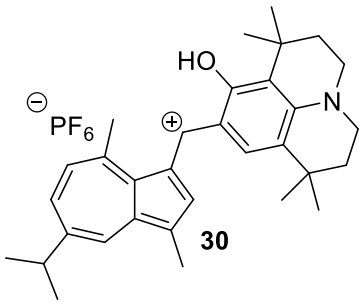
138.11
137.54
134.49
132.82
131.50
127.71
119.84
117.95
f1 (ppm)

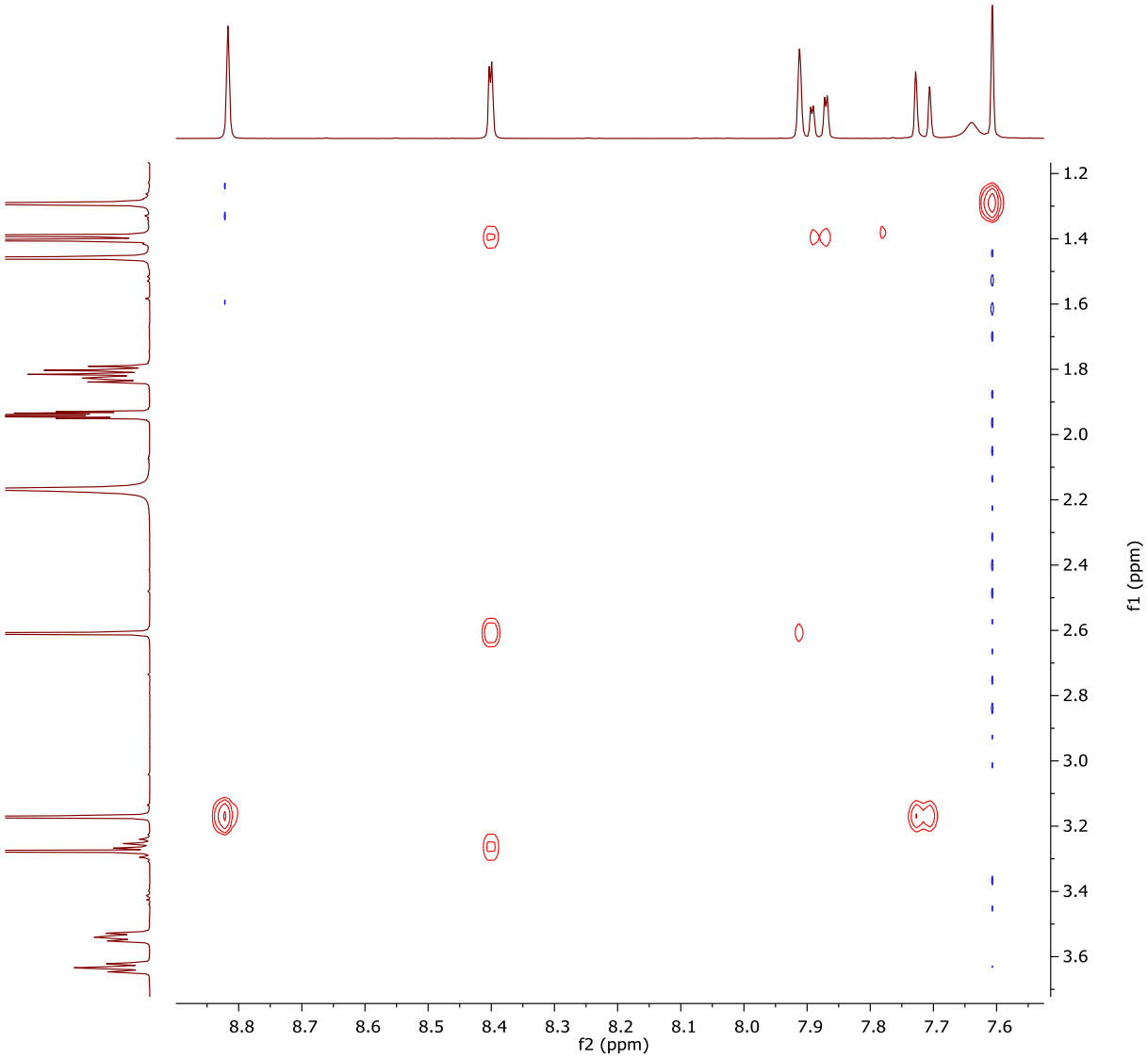

50.01
49.05
39.06
38.61
34.99
32.85
32.65
29.67
28.76
27.91
24.32
13.27
f1 (ppm)

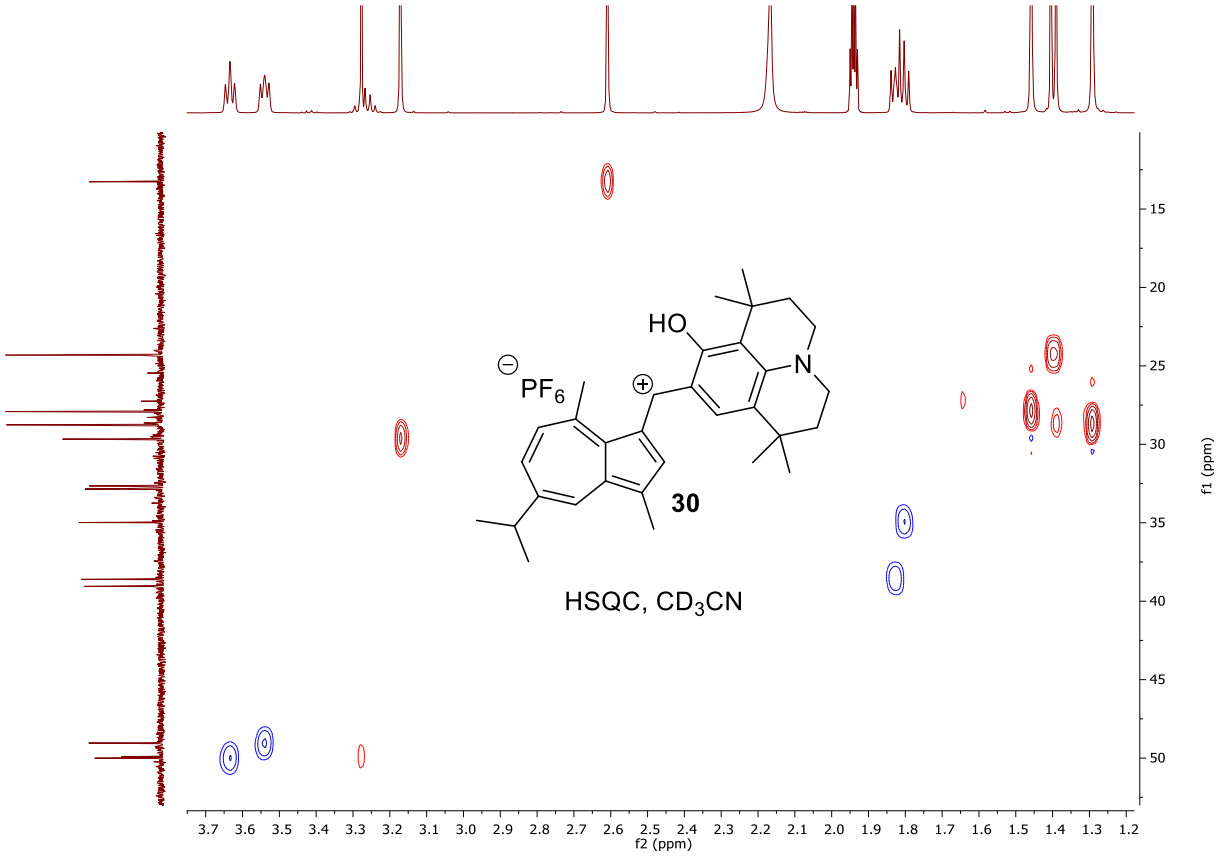

HO
N
PF6
30
COSY, CD3CN
f1 (ppm)
f2 (ppm)
f1 (ppm)
f2 (ppm)

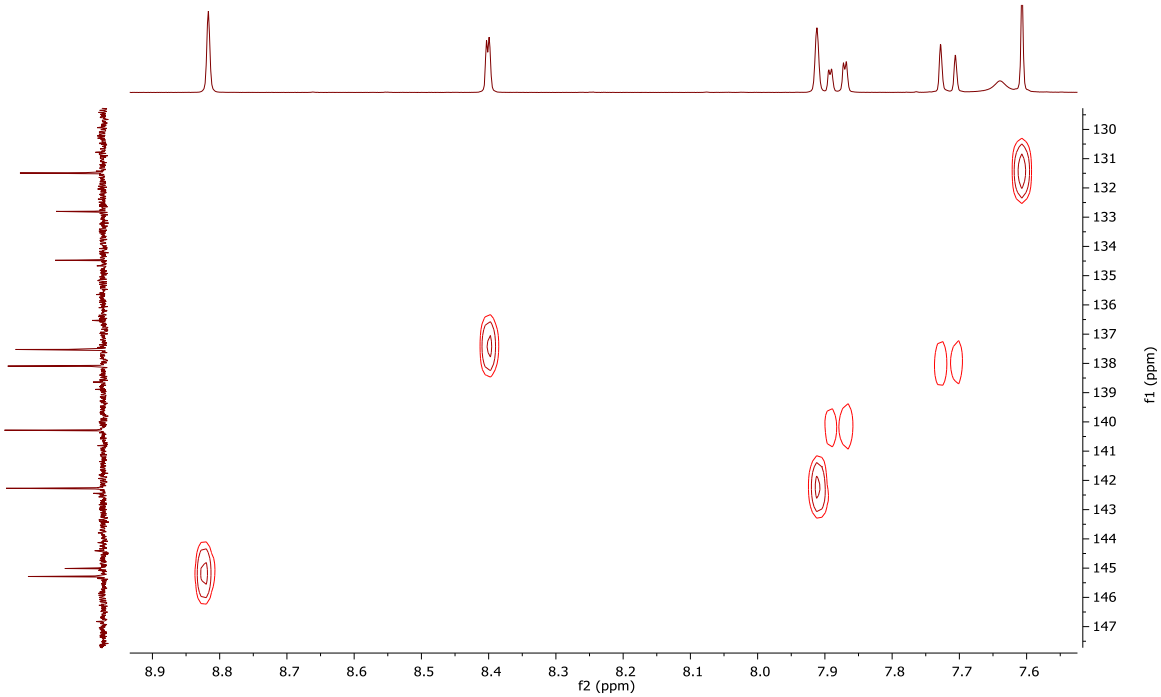


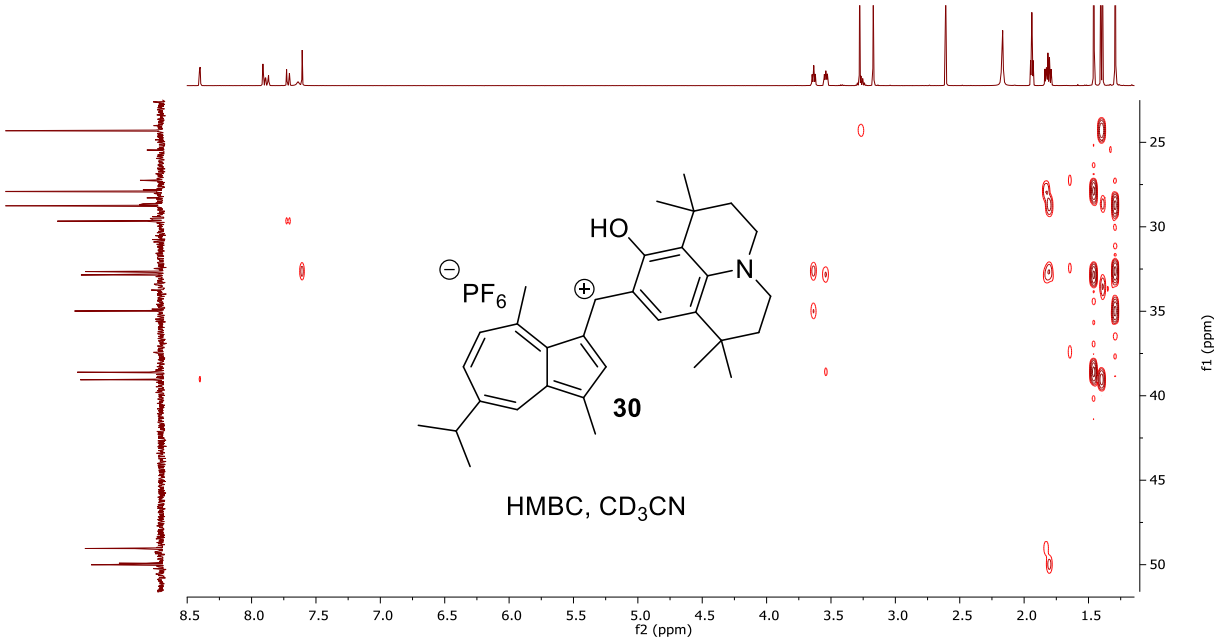
30

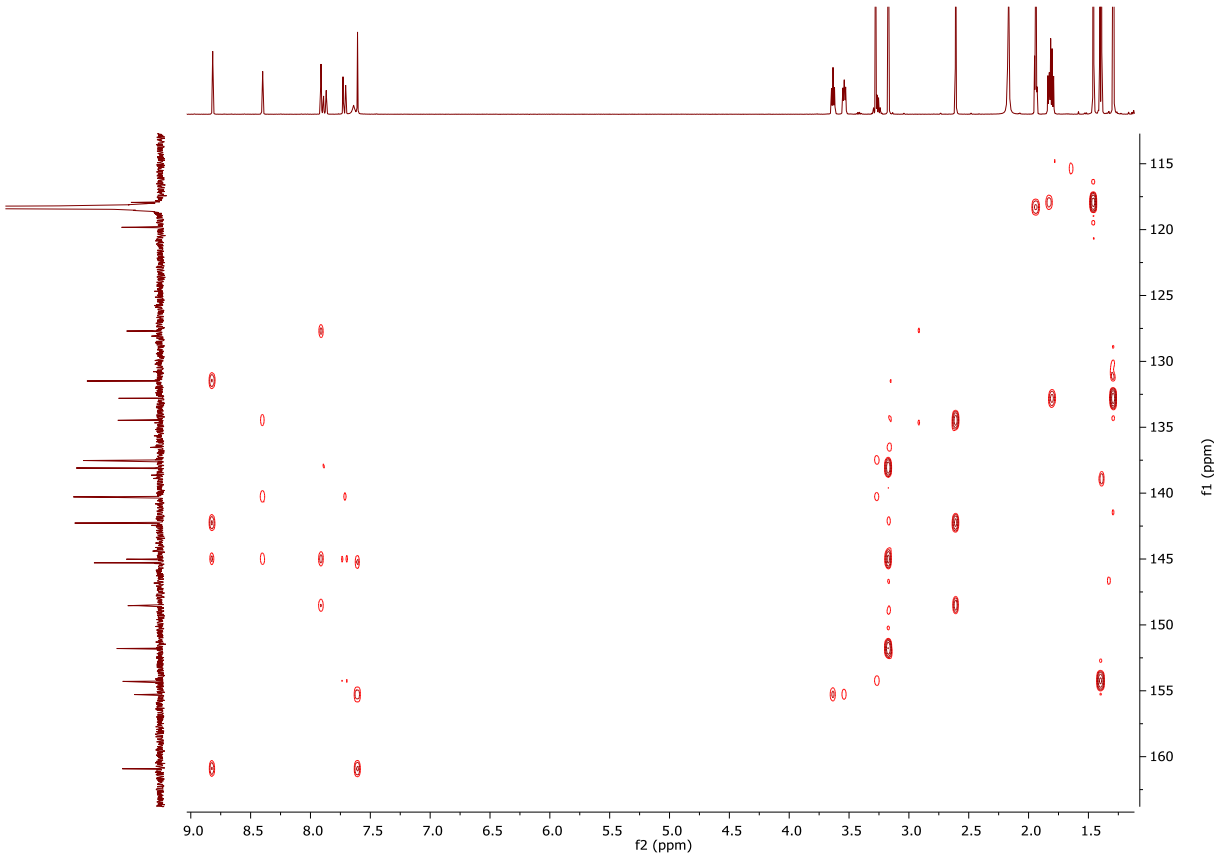
NOESY, CD_3CN

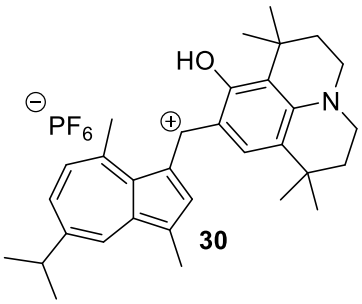



HO
N
PF6
30
HSQC, CD3CN
f2 (ppm)
f1 (ppm)

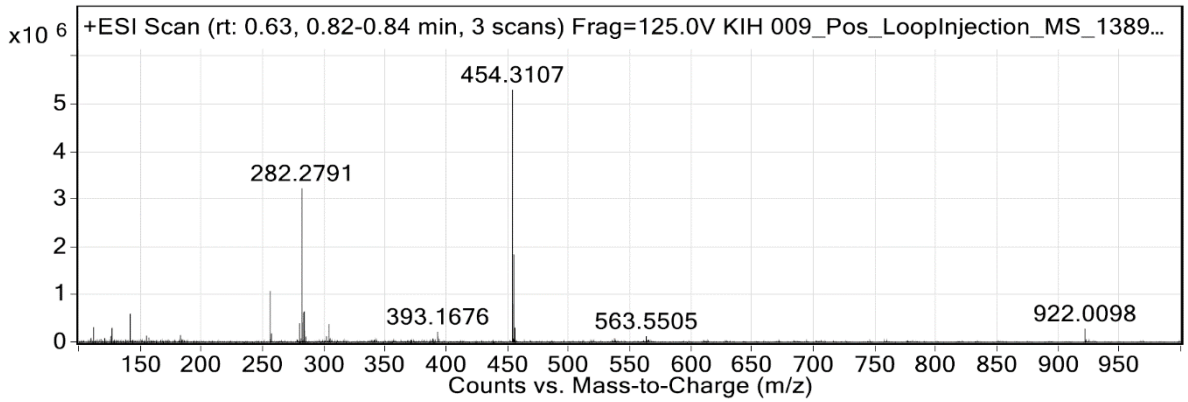

f2 (ppm)
f1 (ppm)

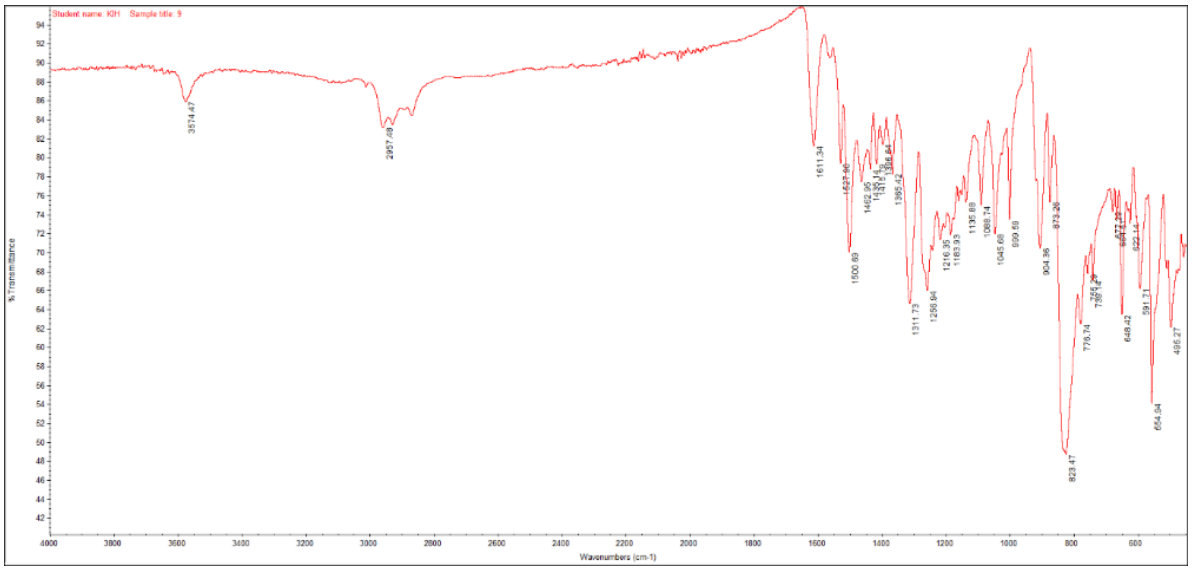

HO
N
PF6
30
HMBC, CD3CN
f2 (ppm)
f1 (ppm)

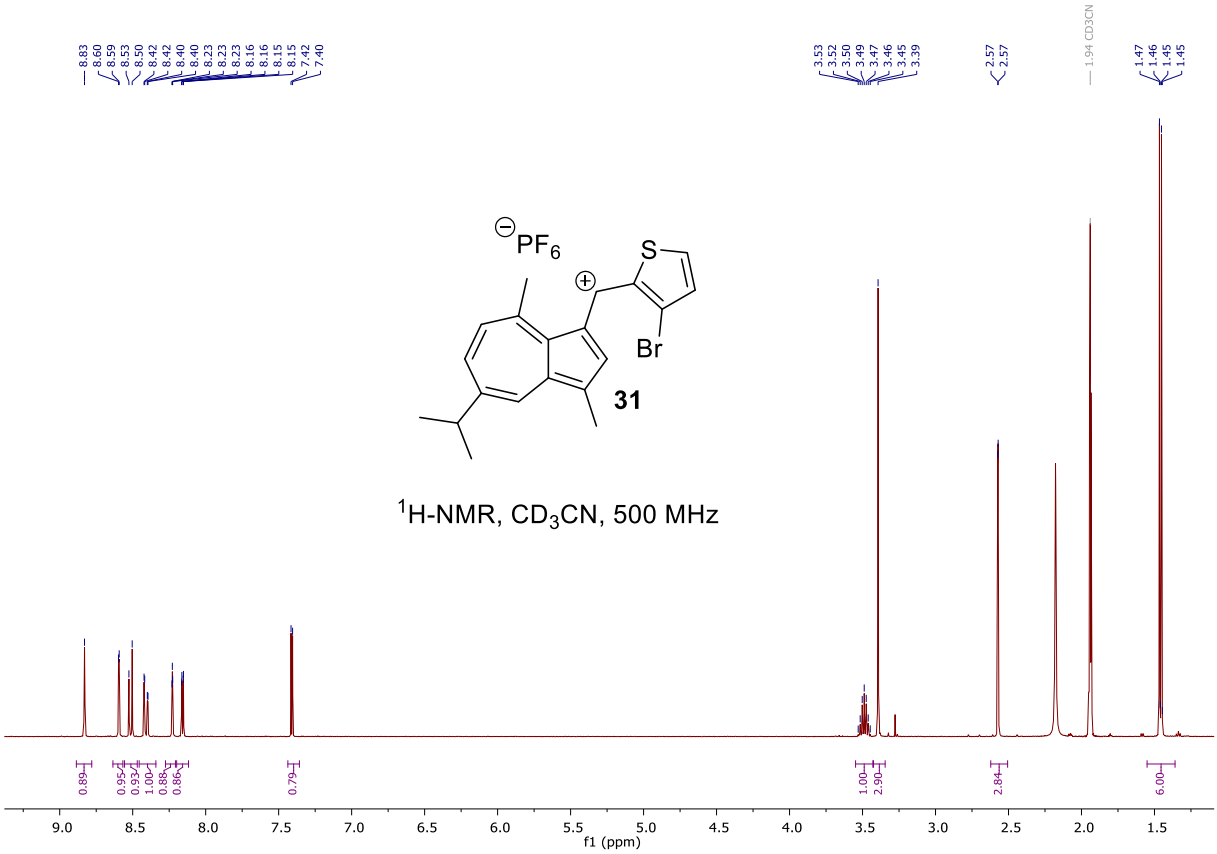

f2 (ppm)
f1 (ppm)


HO
N
PF6

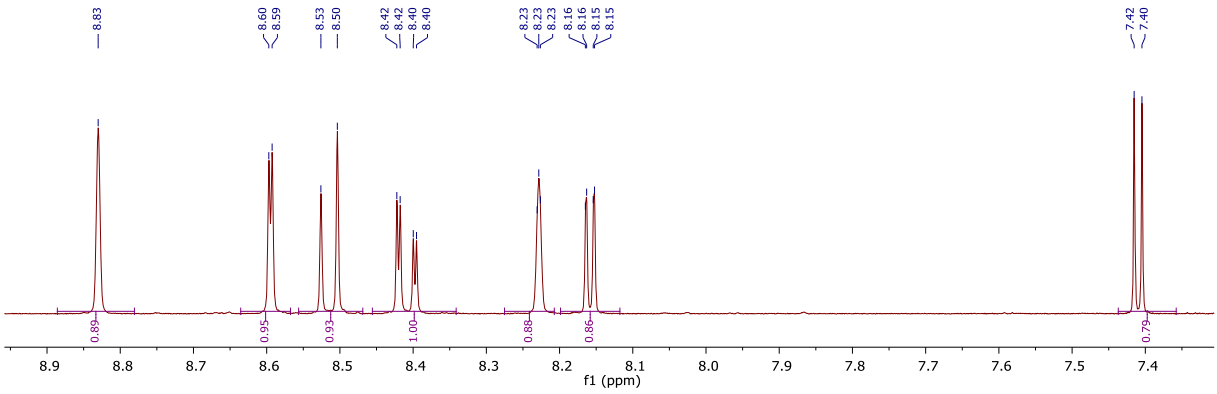
30

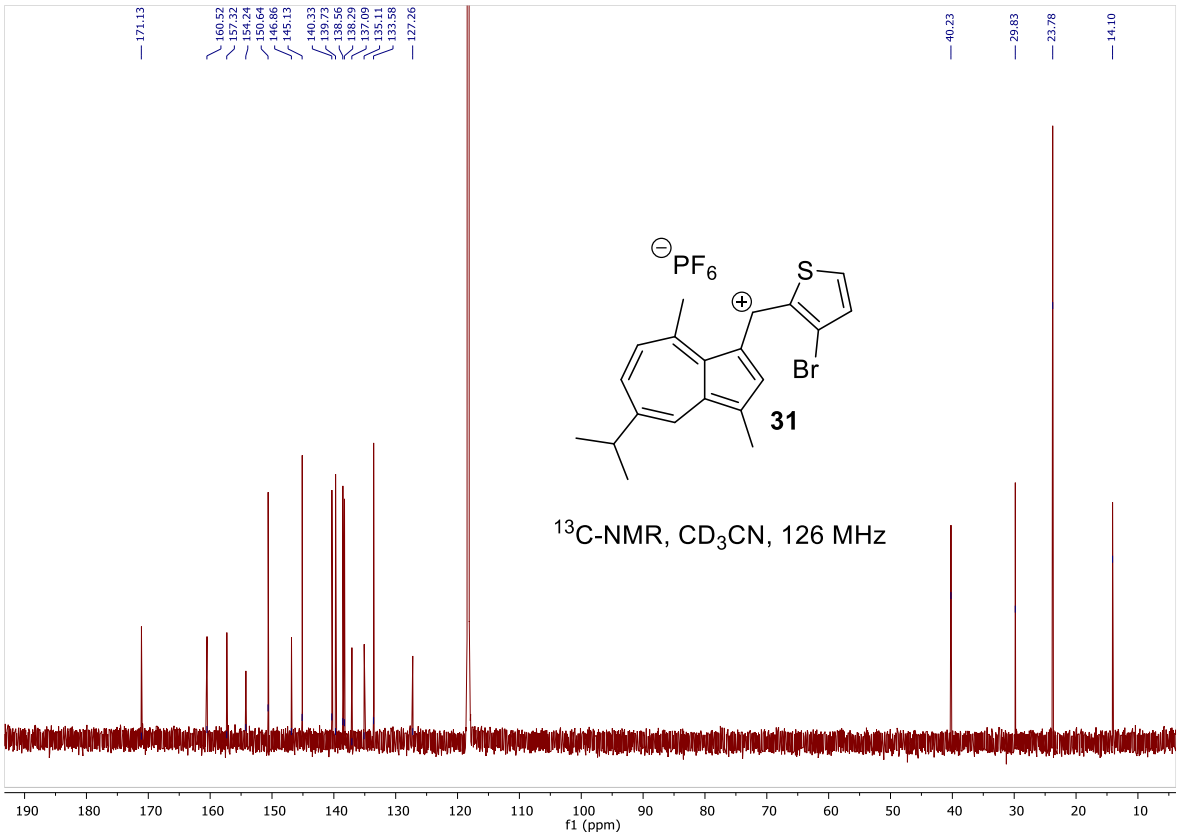

x10 6
+ESI Scan (rt: 0.63, 0.82-0.84 min, 3 scans) Frag=125.0V KIH 009_Pos_LoopInjection_MS_1389...
454.3107
282.2791
393.1676
563.5505
922.0098
Counts vs. Mass-to-Charge (m/z)

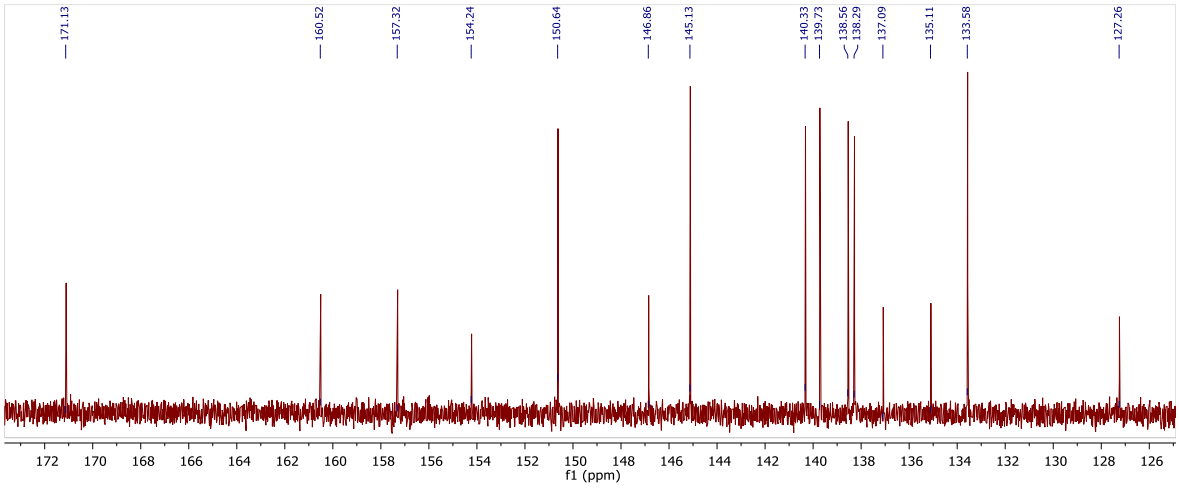

%Transmittance
Wavenumbers (cm-1)

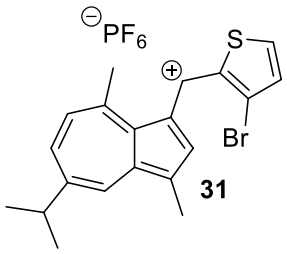


^{1}H-NMR, CD_3CN, 500 MHz



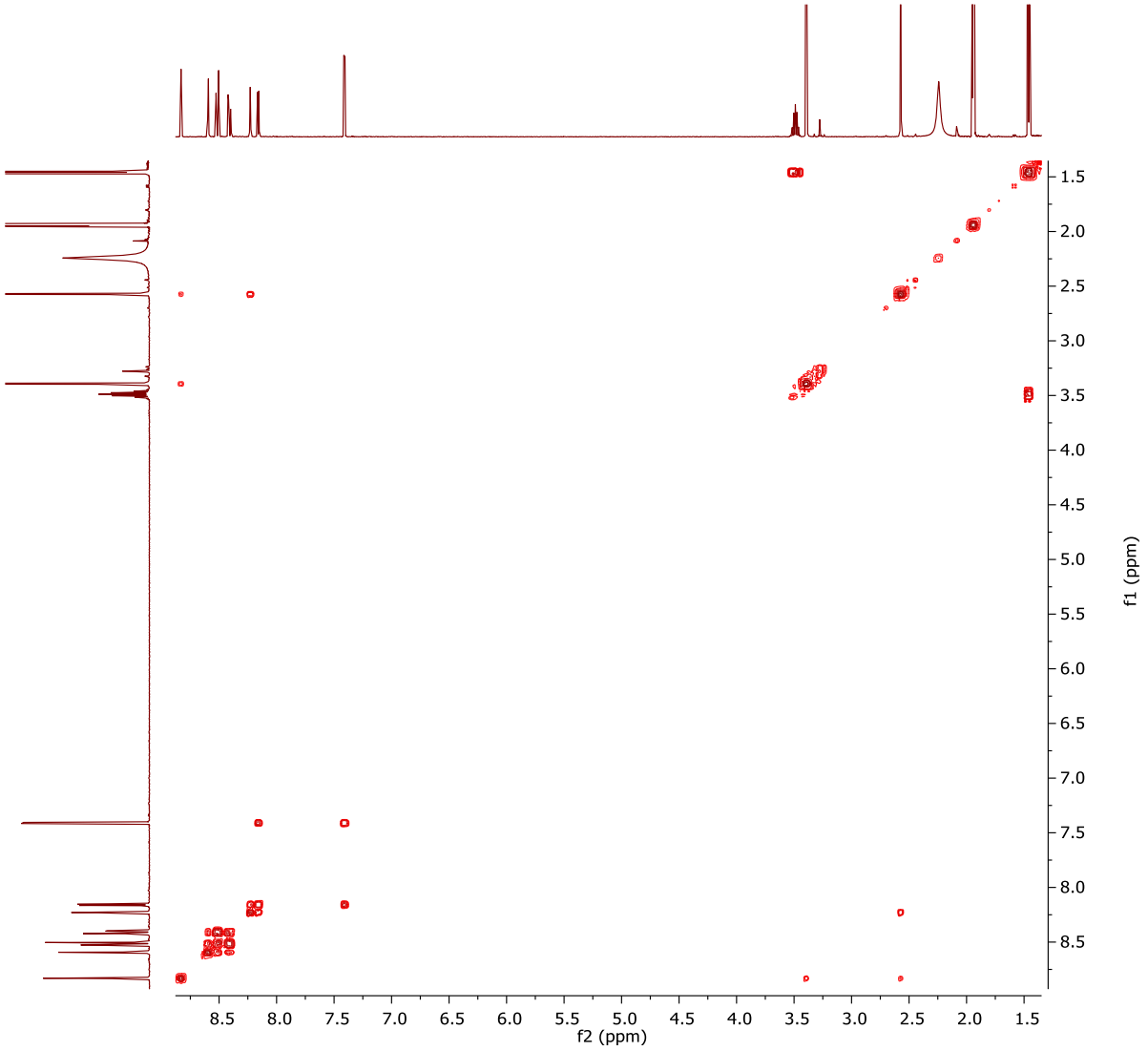

171.13
160.52
157.32
154.24
150.64
146.86
145.13
140.33
139.73
138.56
138.29
137.09
135.11
133.58
127.26
40.23
29.83
23.78
14.10
PF6
S
Br
31
13C-NMR, CD3CN, 126 MHz
f1 (ppm)

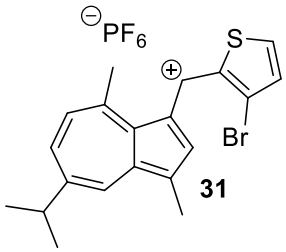

171.13
160.52
157.32
154.24
150.64
146.86
145.13
140.33
139.73
138.56
138.29
137.09
135.11
133.58
127.26
f1 (ppm)



31

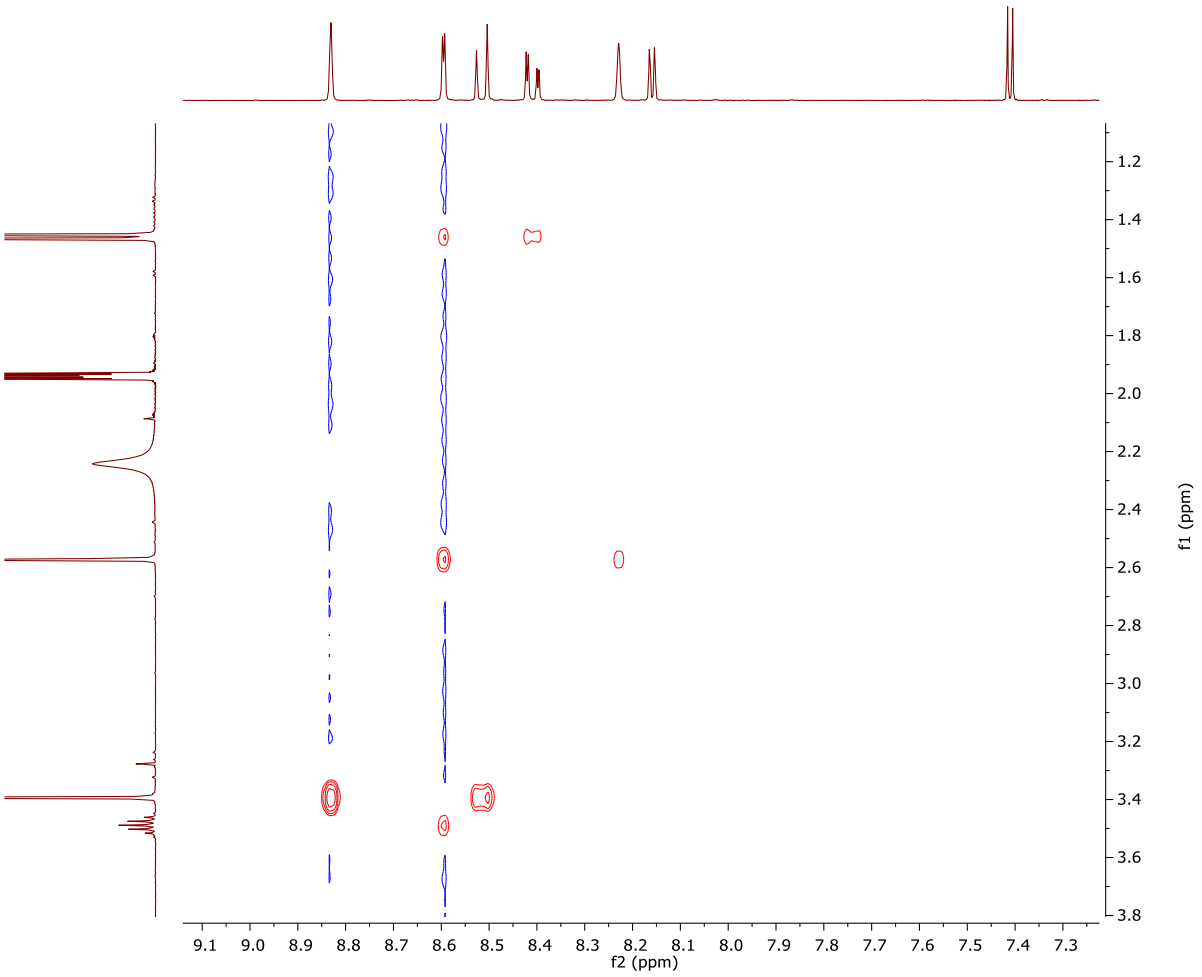
COSY, CD_3CN

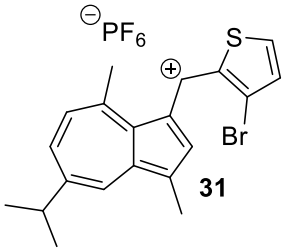




31

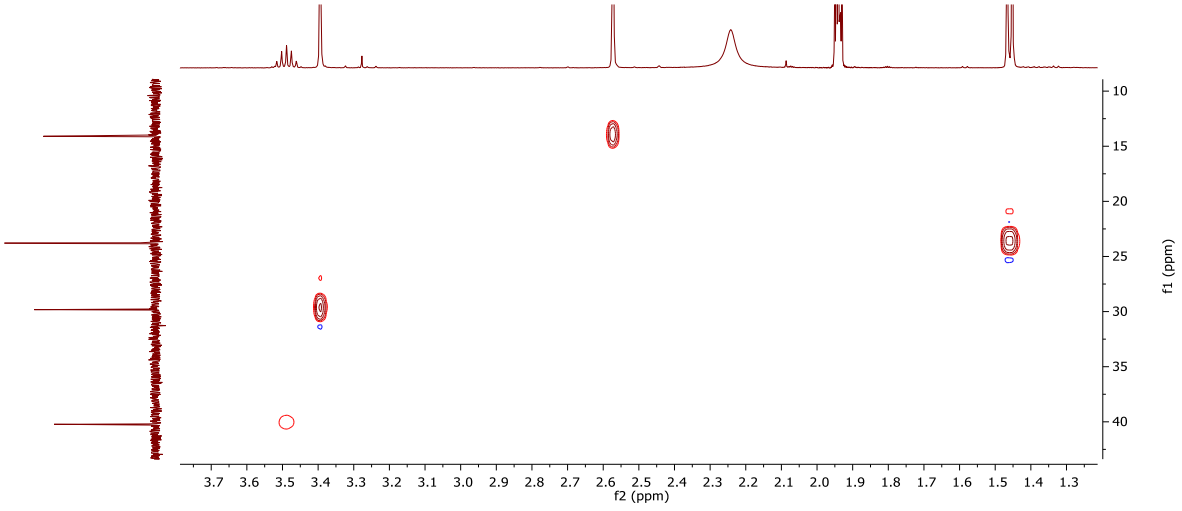
NOESY, CD_3CN

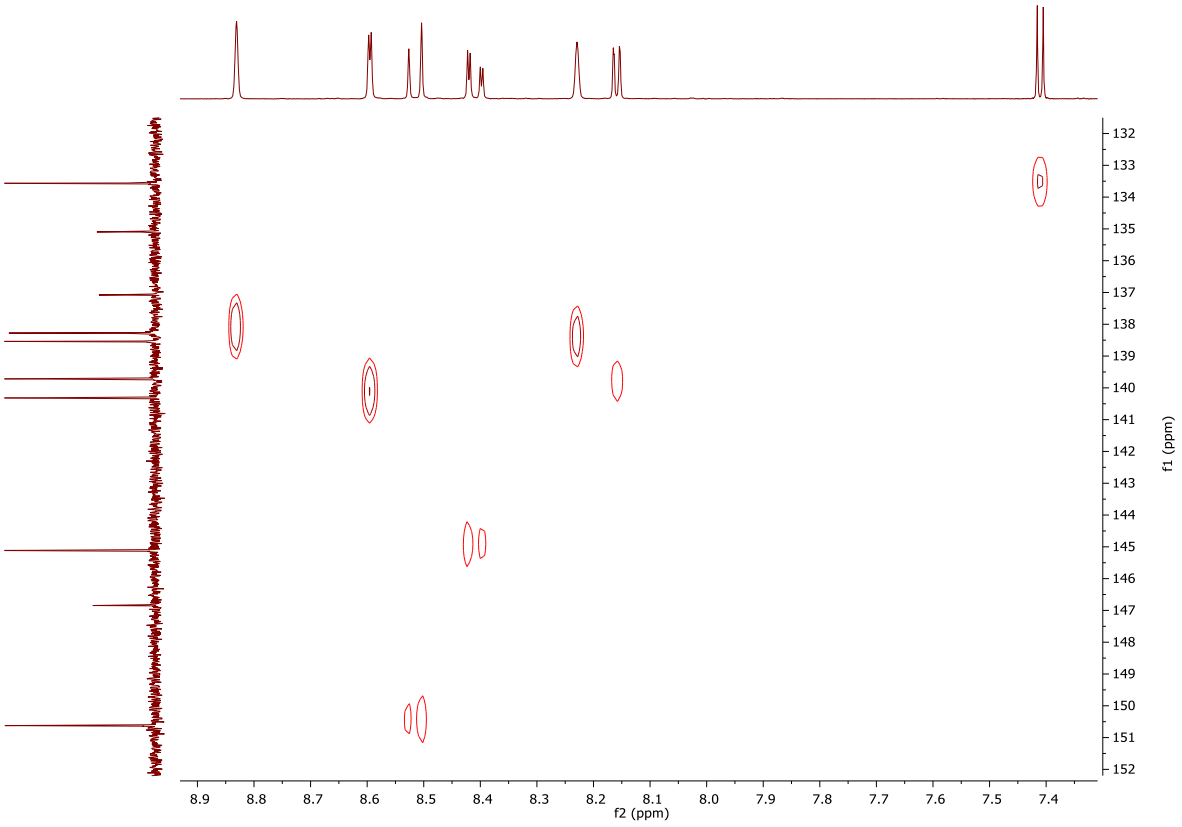


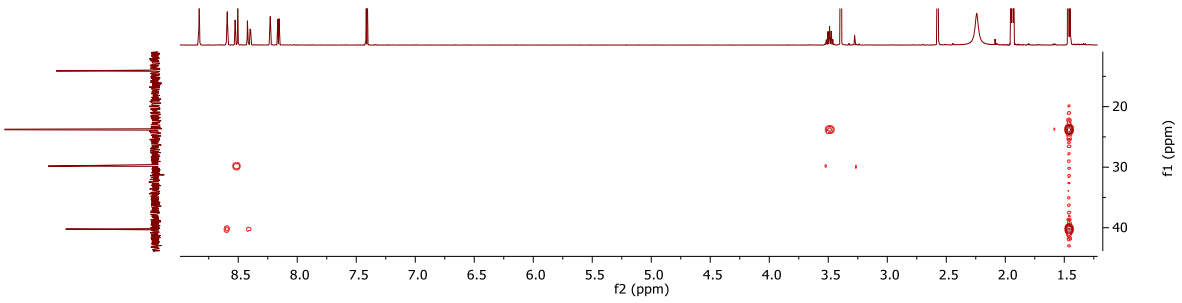


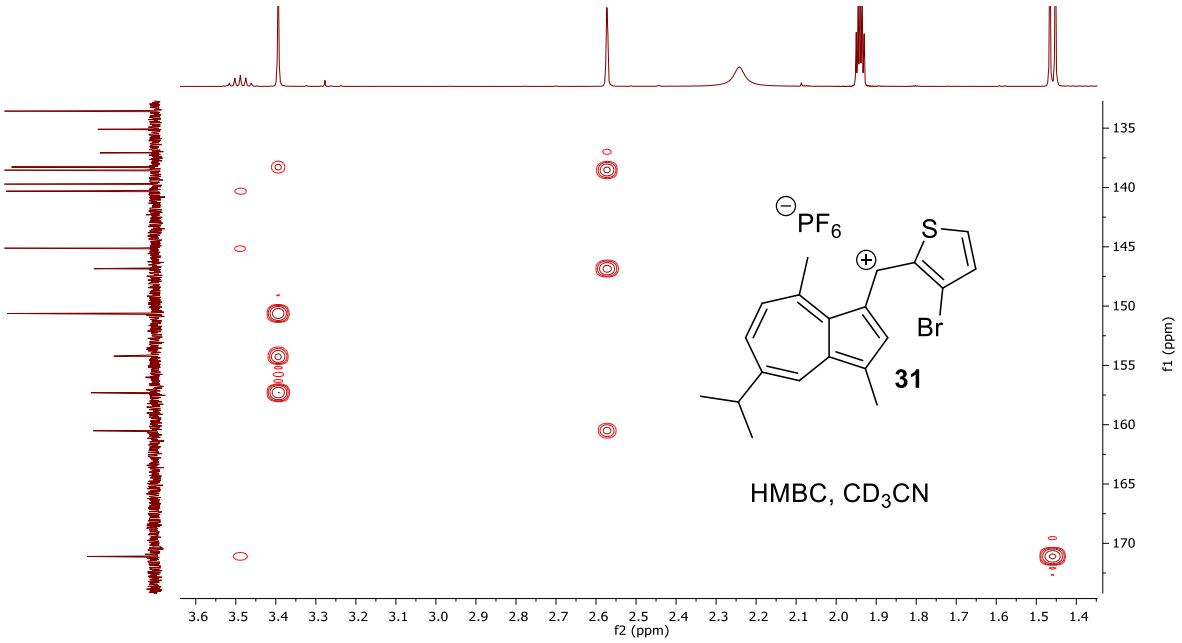
31

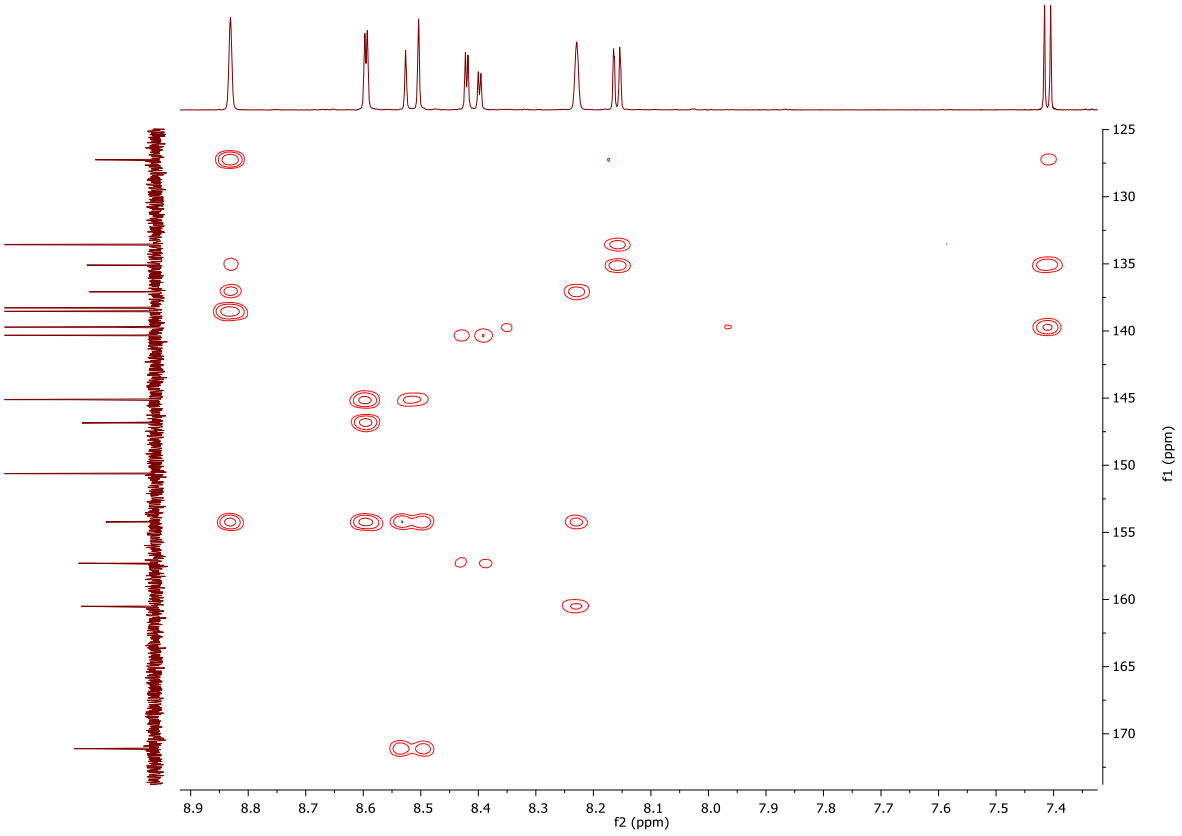
HSQC, CD_3CN

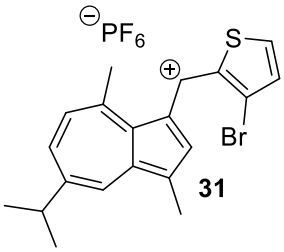




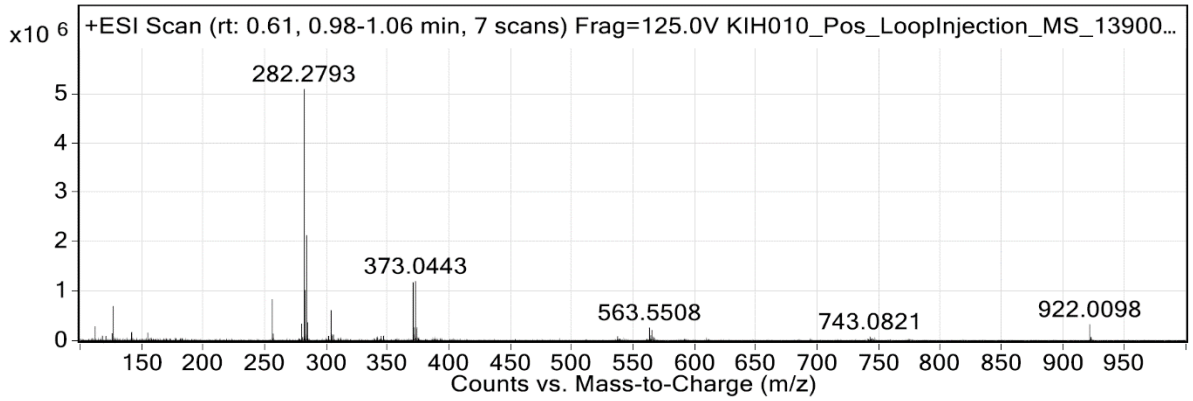

f1 (ppm)
f2 (ppm)

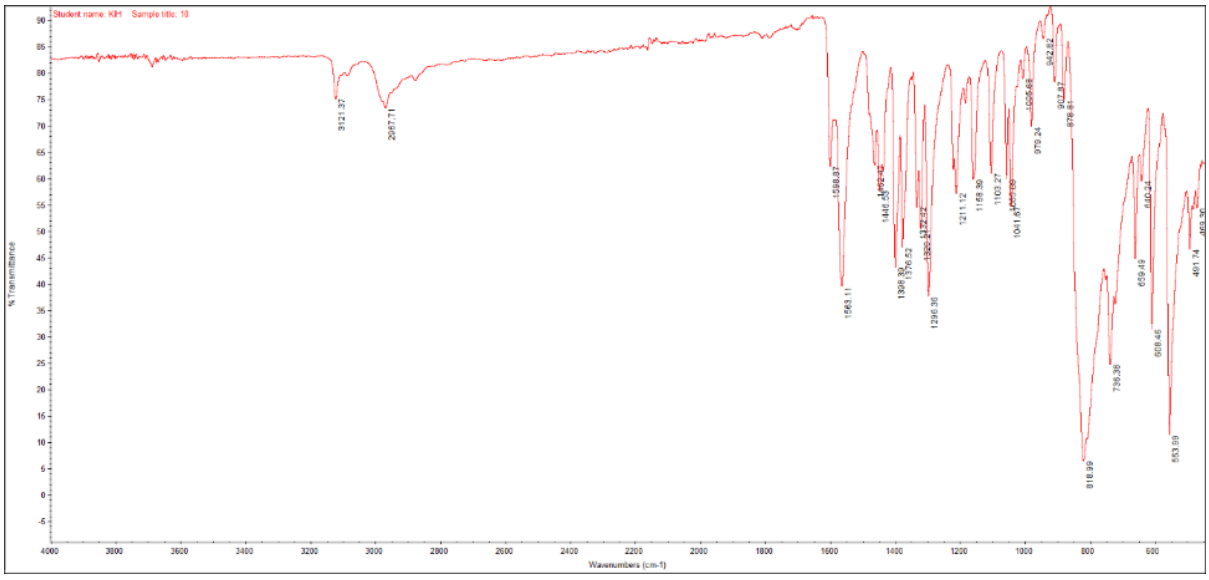

PF6
S
Br
31
HMBC, CD3CN
f1 (ppm)
f2 (ppm)

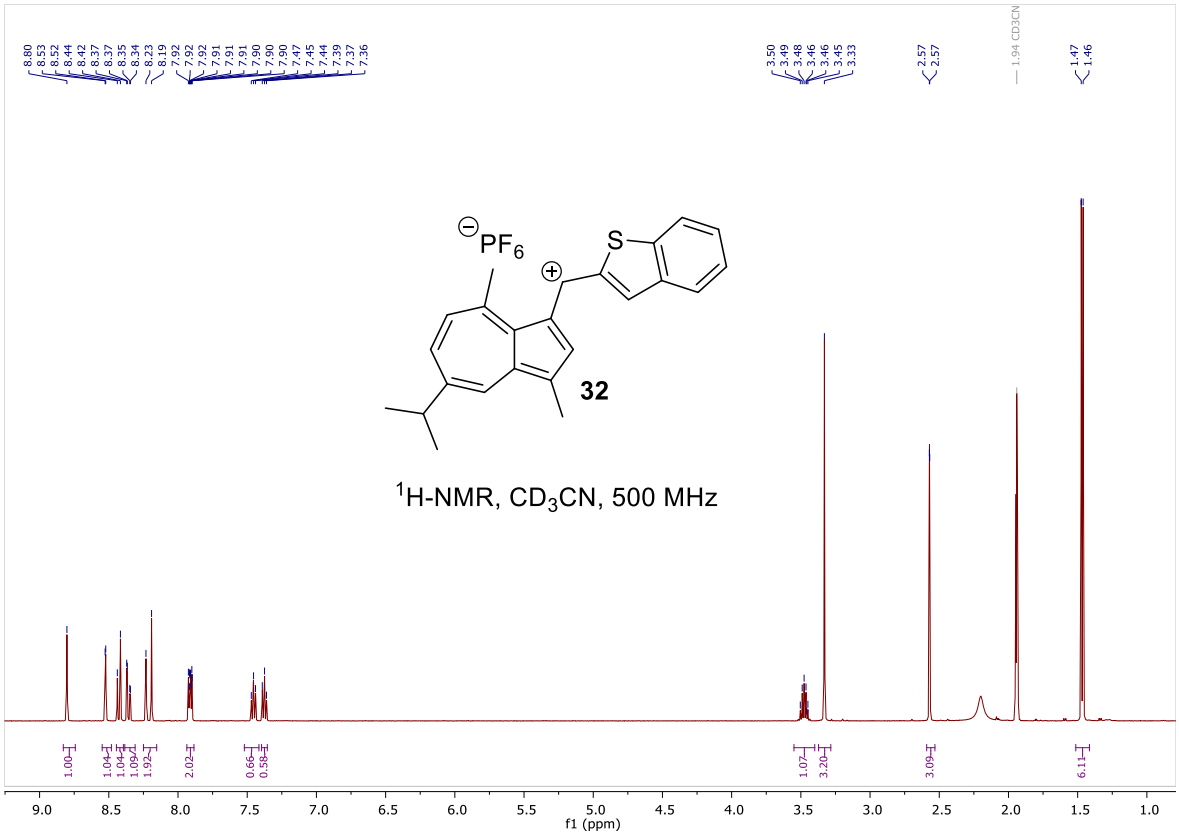

f1 (ppm)
f2 (ppm)

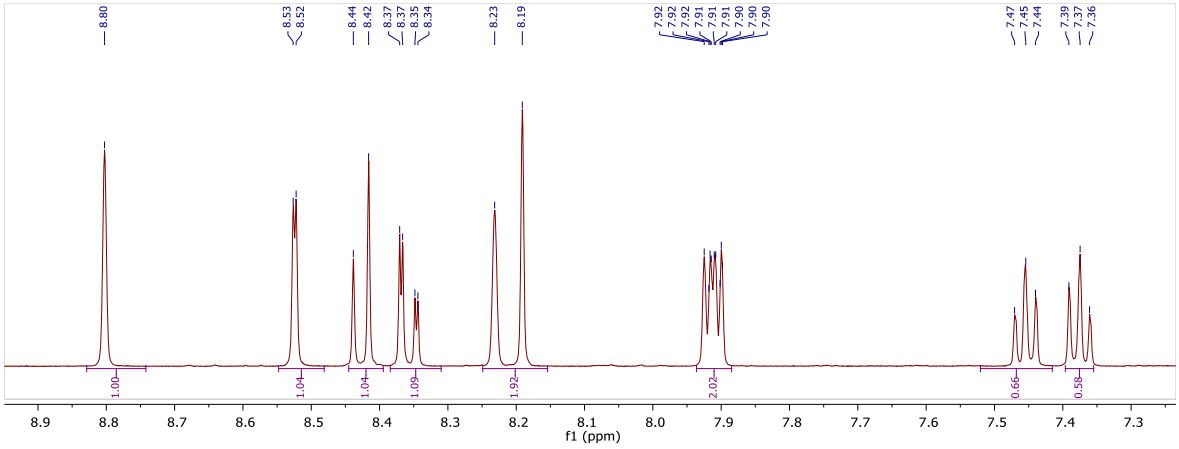

PF6
S
Br

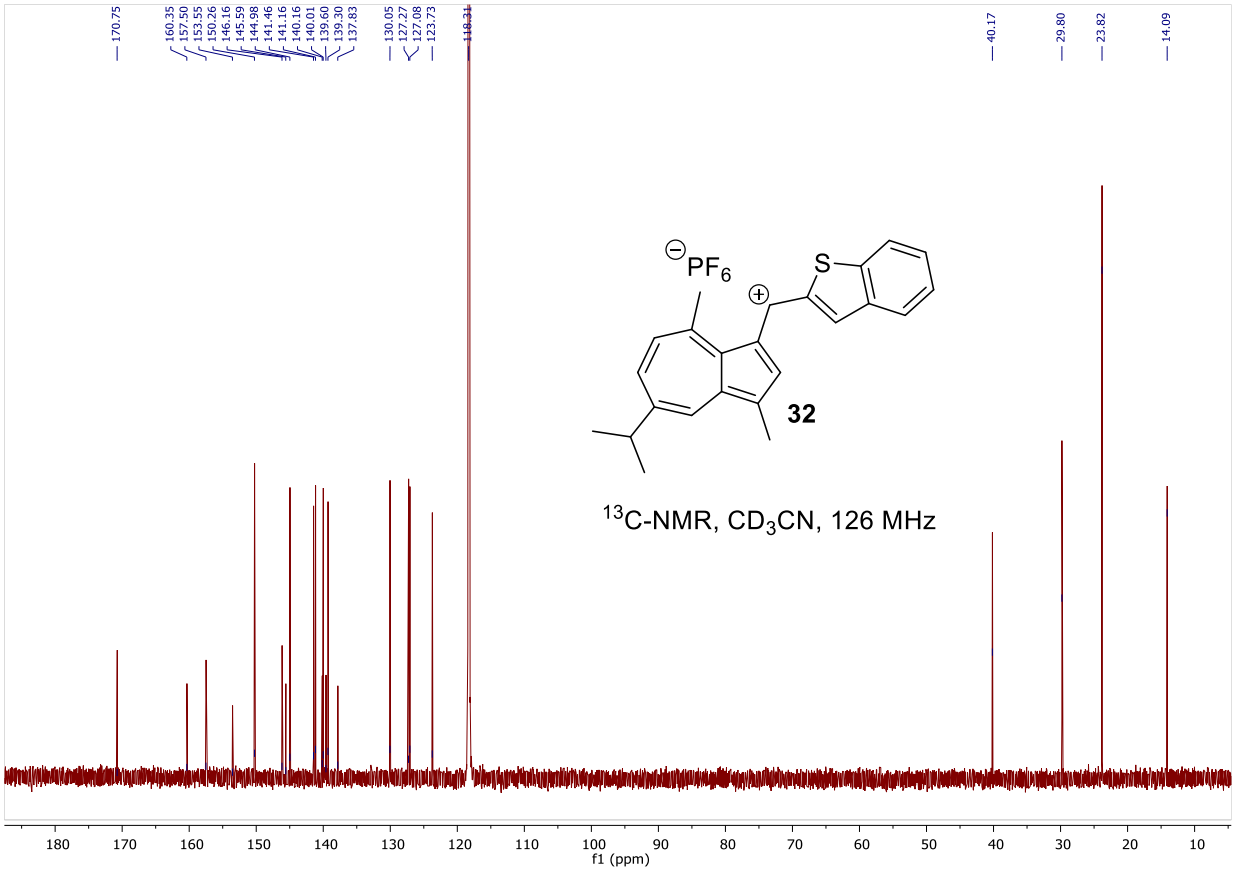
31

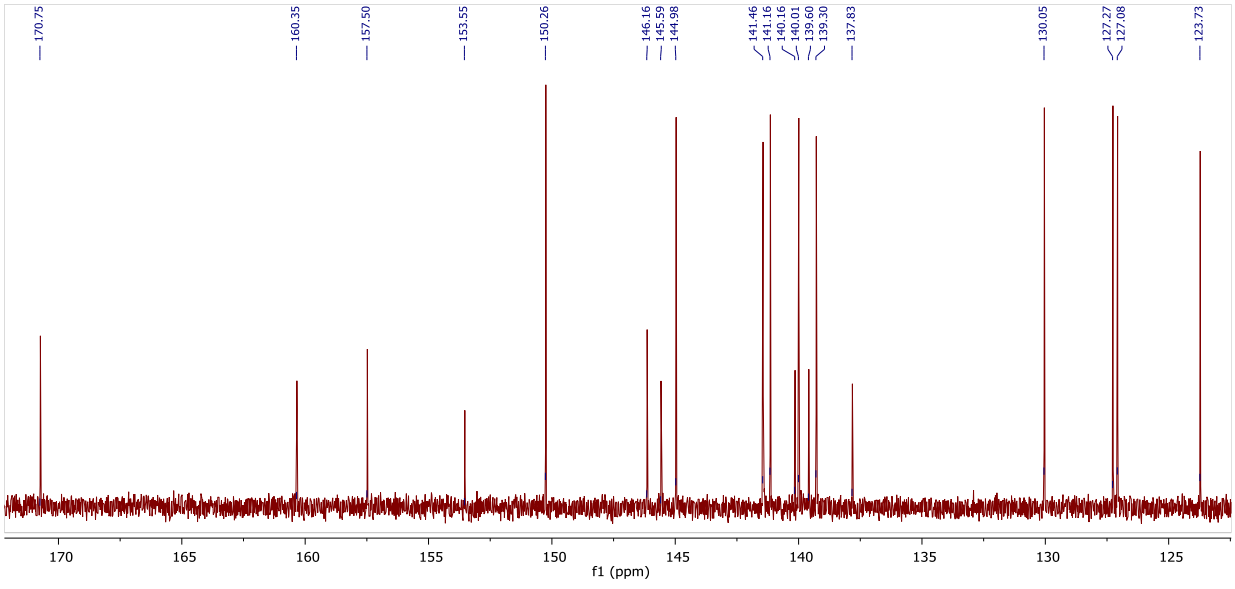

x10 6
+ESI Scan (rt: 0.61, 0.98-1.06 min, 7 scans) Frag=125.0V KIH010_Pos_LoopInjection_MS_13900...
282.2793
373.0443
563.5508
743.0821
922.0098
Counts vs. Mass-to-Charge (m/z)

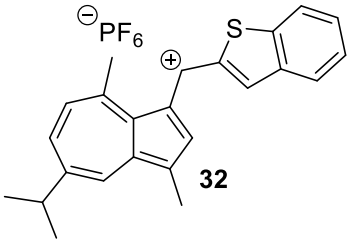

% Transmittance
Wavenumbers (cm-1)


8.80
8.53
8.52
8.44
8.42
8.37
8.37
8.35
8.34
8.23
8.19
7.92
7.92
7.91
7.91
7.91
7.90
7.90
7.90
7.47
7.45
7.44
7.39
7.37
7.36
3.50
3.49
3.48
3.46
3.46
3.45
3.33
2.57
2.57
1.94 CD3CN
1.47
1.46
PF6
S
32
1H-NMR, CD3CN, 500 MHz
1.00
1.04
1.04
1.09
1.92
2.02
0.66
0.58
1.07
3.20
3.09
6.11
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)


8.80
8.53
8.52
8.44
8.42
8.37
8.37
8.35
8.34
8.23
8.19
7.92
7.92
7.92
7.91
7.91
7.90
7.90
7.90
7.47
7.45
7.44
7.39
7.37
7.36
1.00
1.04
1.04
1.09
1.92
2.02
0.66
0.58
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
f1 (ppm)

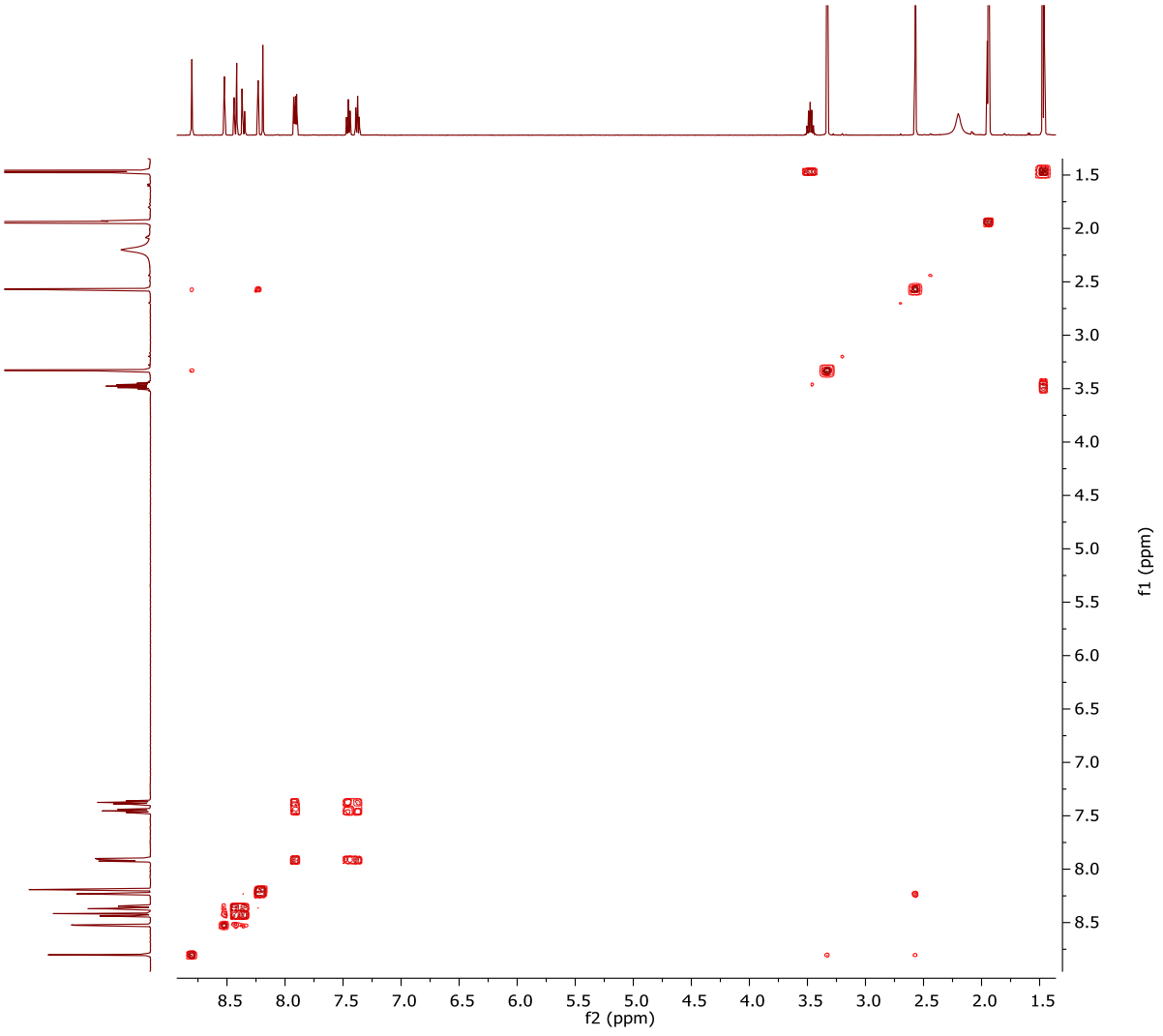

170.75
160.35
157.50
153.55
150.26
146.16
145.59
144.98
141.46
141.16
140.16
140.01
139.60
139.30
137.83
130.05
127.27
127.08
123.73
118.31
40.17
29.80
23.82
14.09
PF6
S
32
13C-NMR, CD3CN, 126 MHz
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

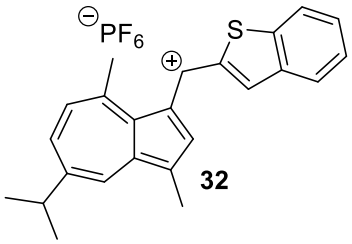

170.75
160.35
157.50
153.55
150.26
146.16
145.59
144.98
141.46
141.16
140.16
140.01
139.60
139.30
137.83
130.05
127.27
127.08
123.73
170
165
160
155
150
145
140
135
130
125
f1 (ppm)



32

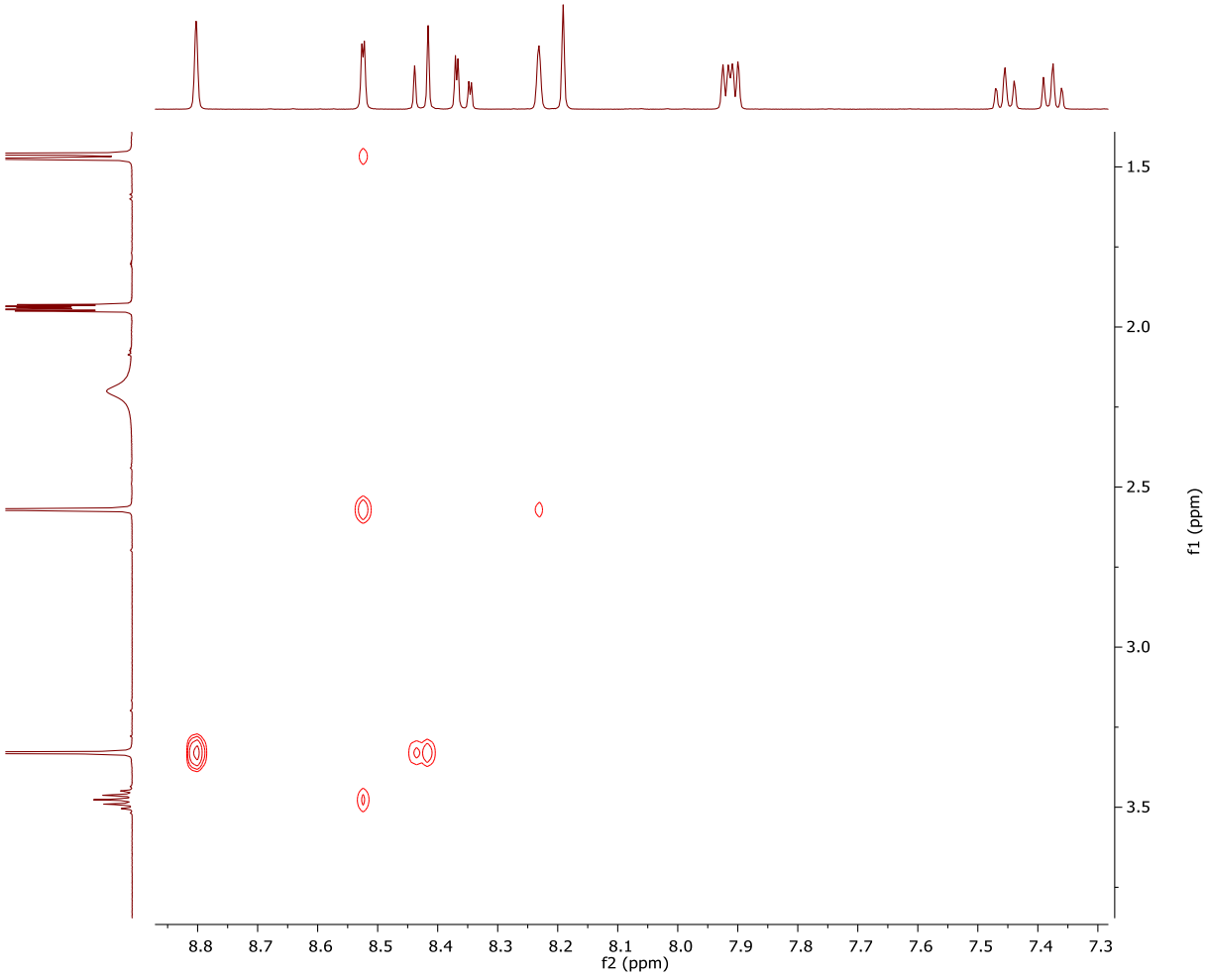
COSY, CD_3CN,

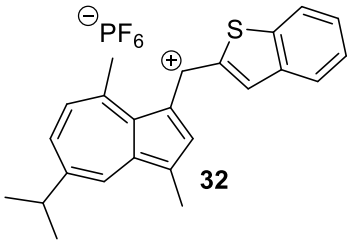




32

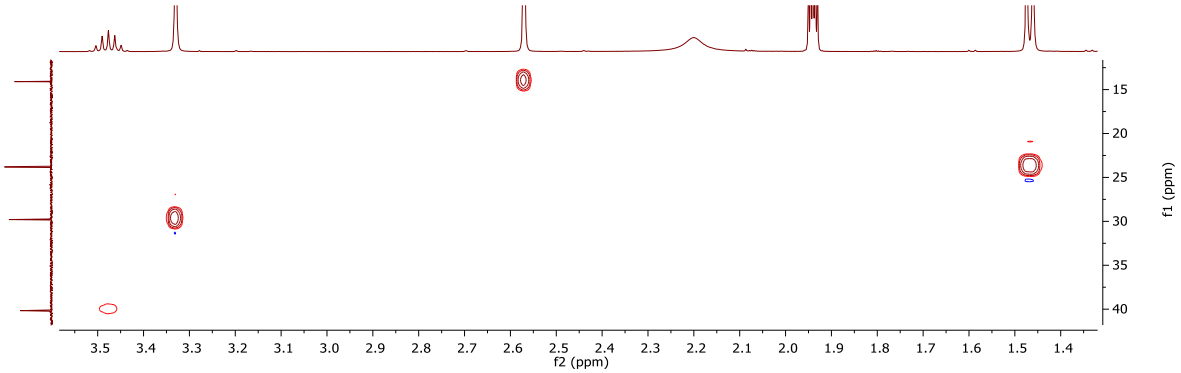
NOESY, CD_3CN,

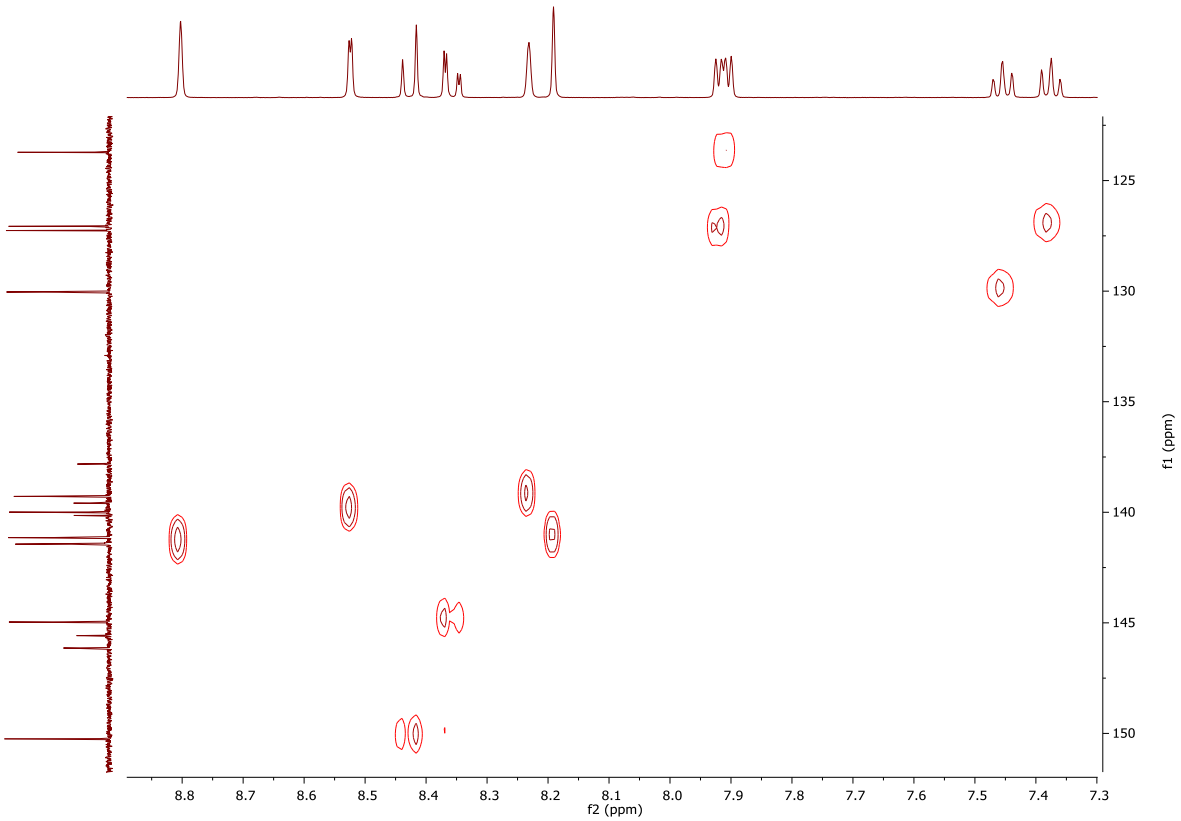


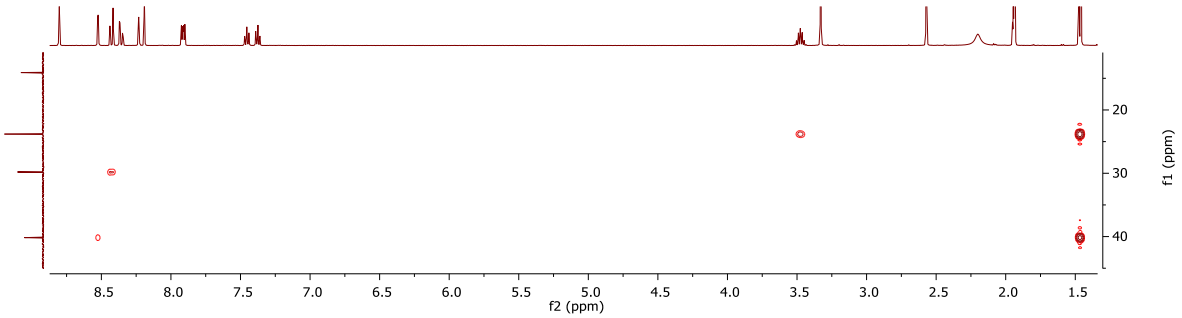


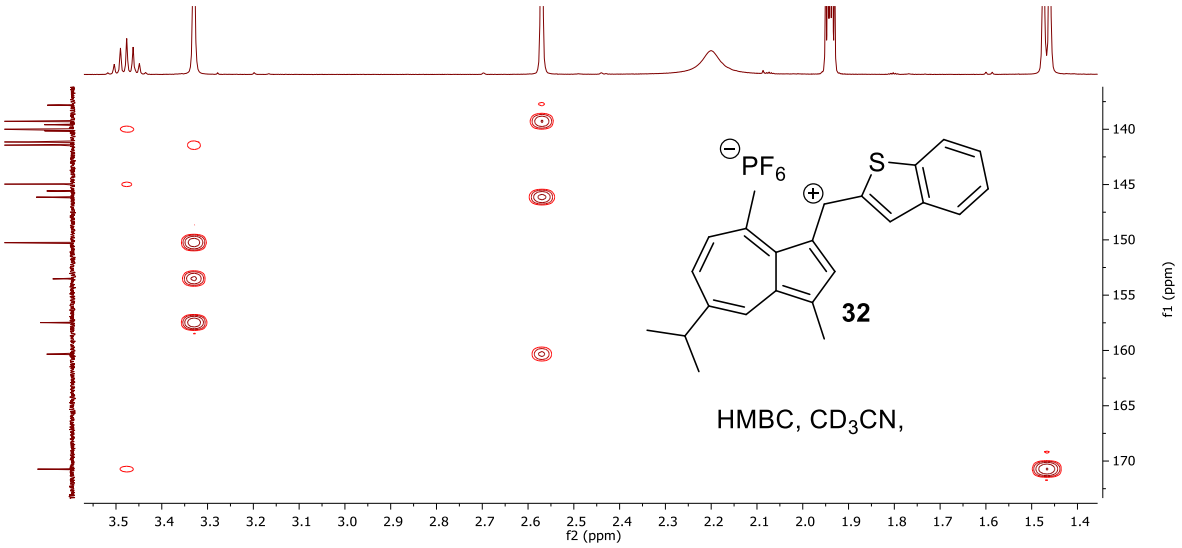
32

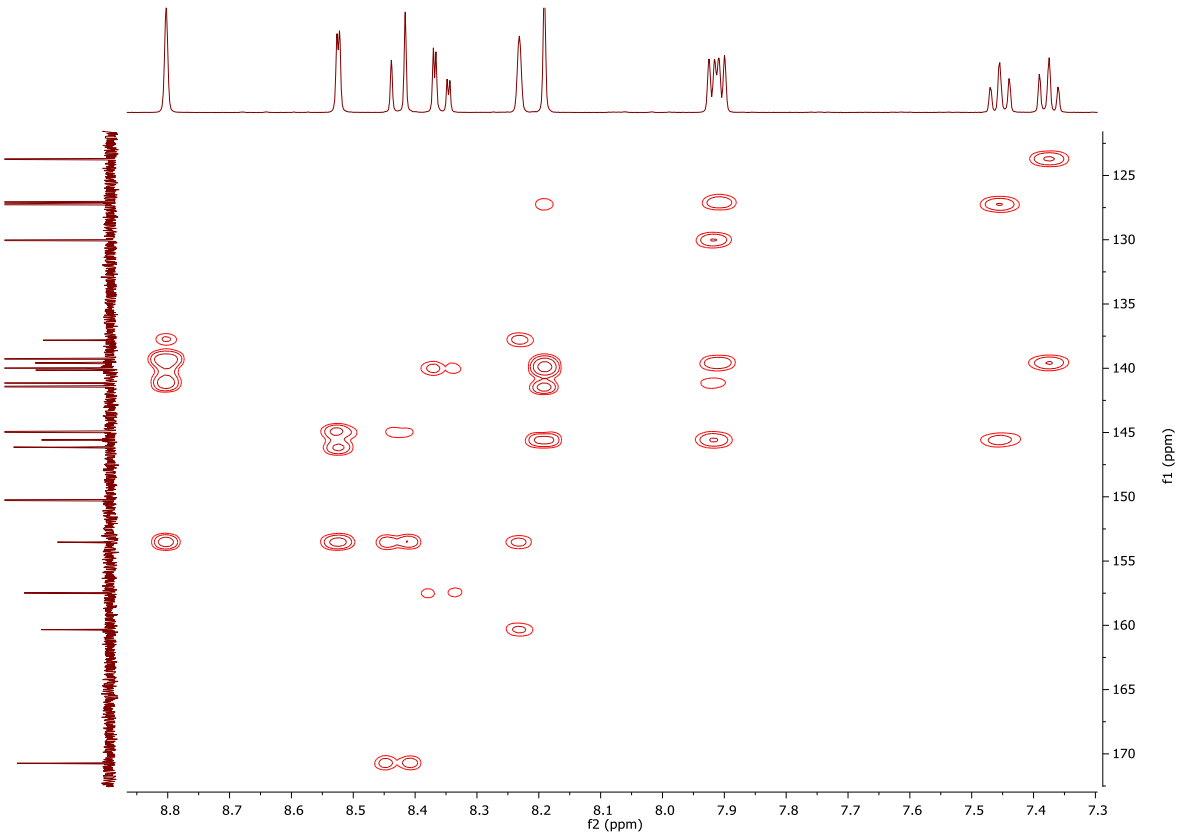
HSQC, CD_3CN,

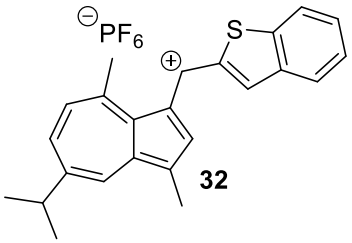




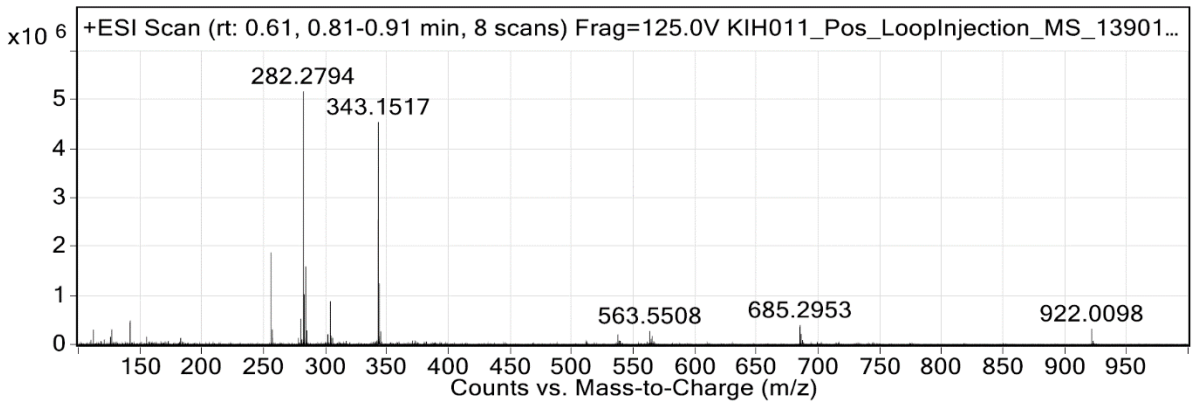

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)
20
30
40
f1 (ppm)

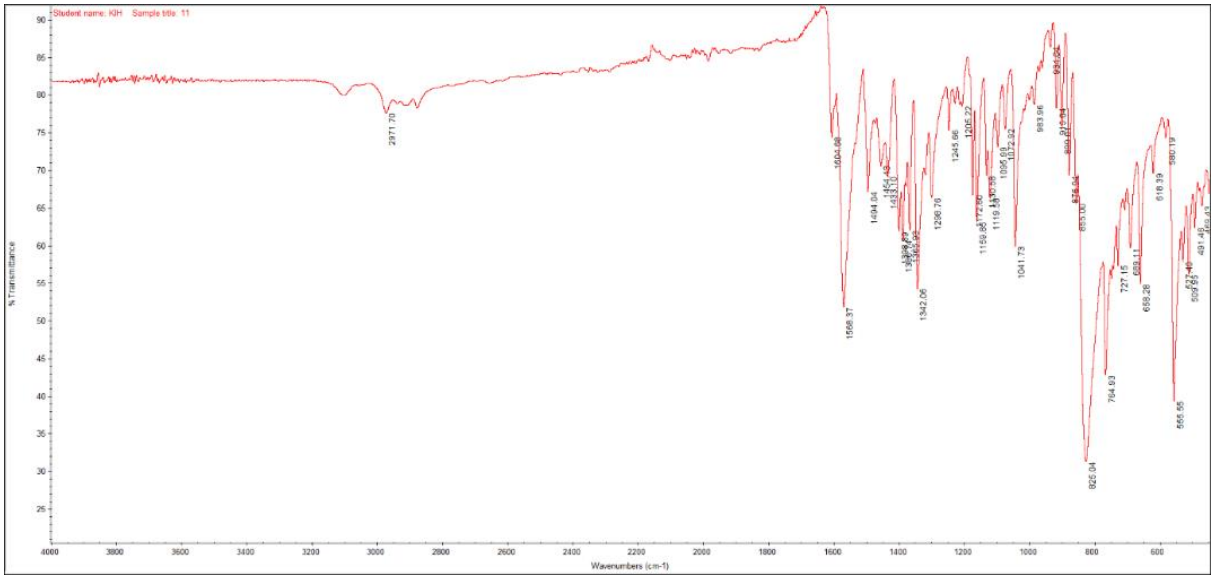

PF6
S
32
HMBC, CD3CN,
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
f2 (ppm)
140
145
150
155
160
165
170
f1 (ppm)

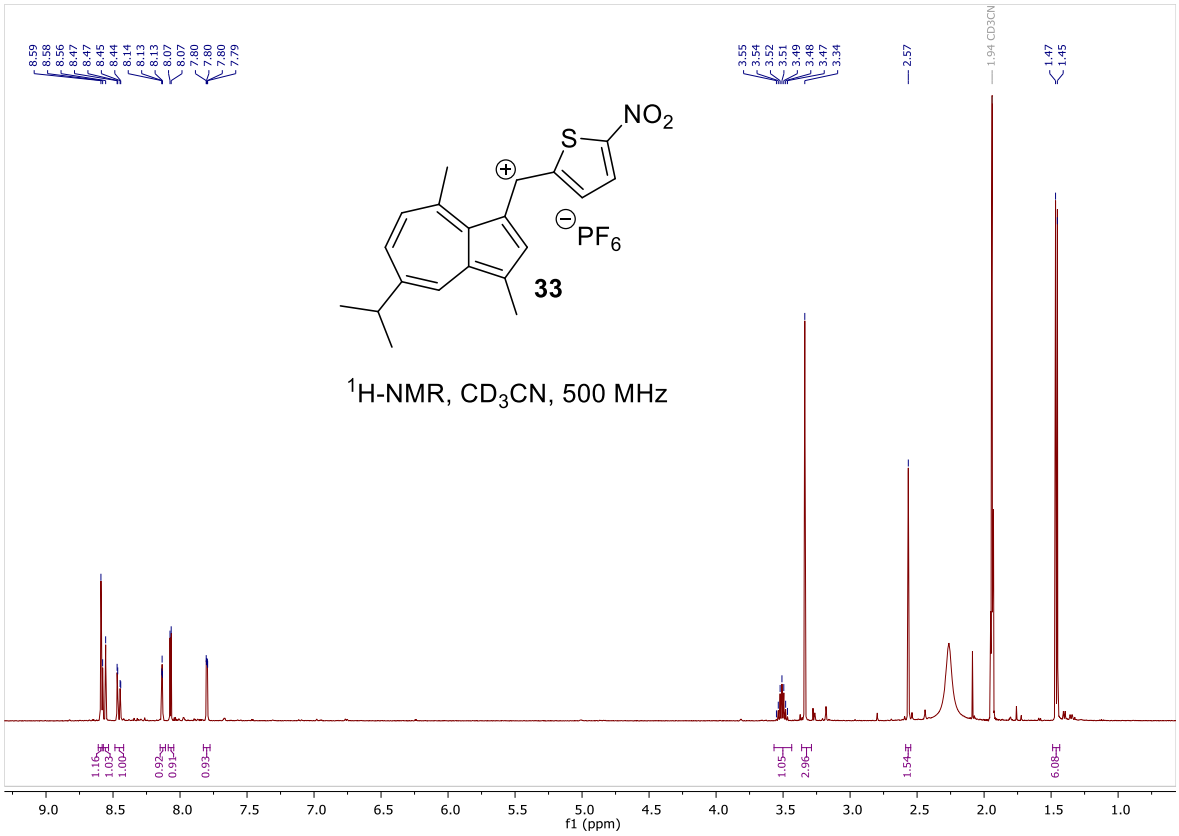

8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
f2 (ppm)
125
130
135
140
145
150
155
160
165
170
f1 (ppm)

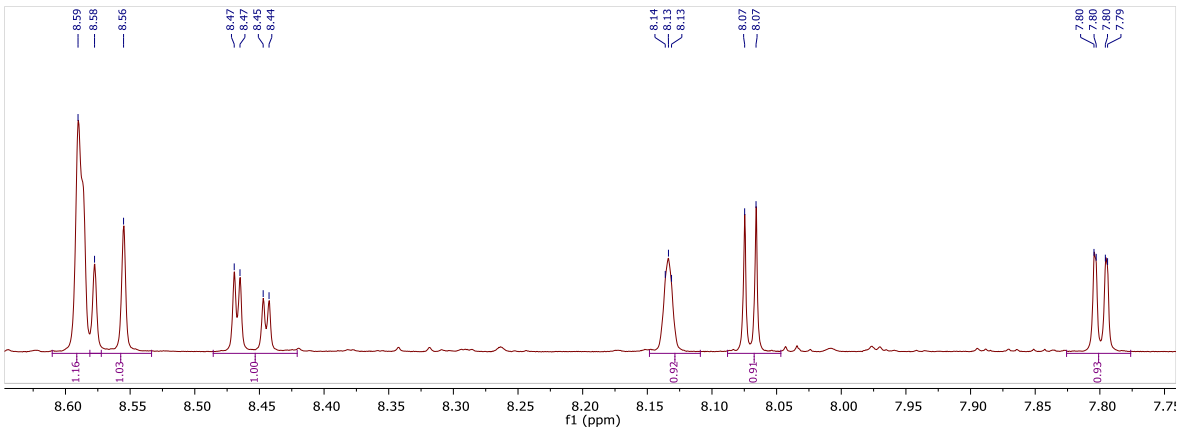

PF6
S

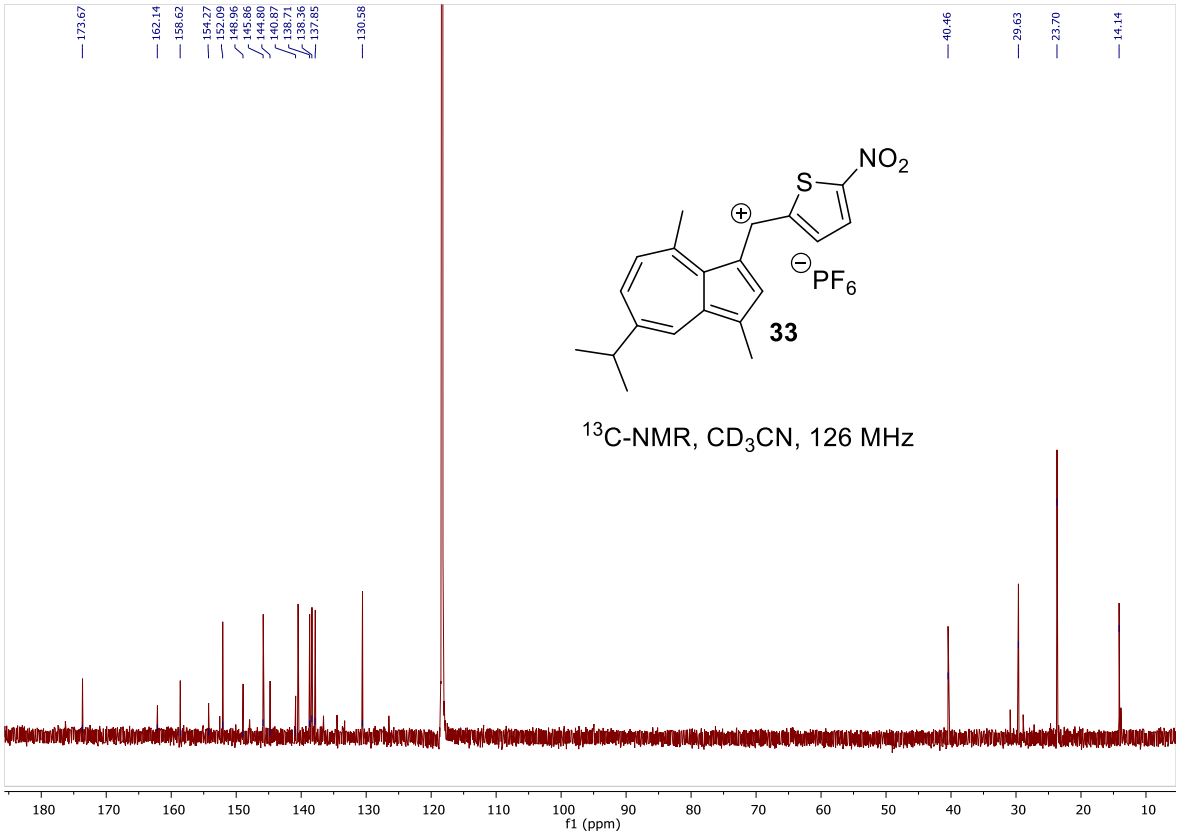
32

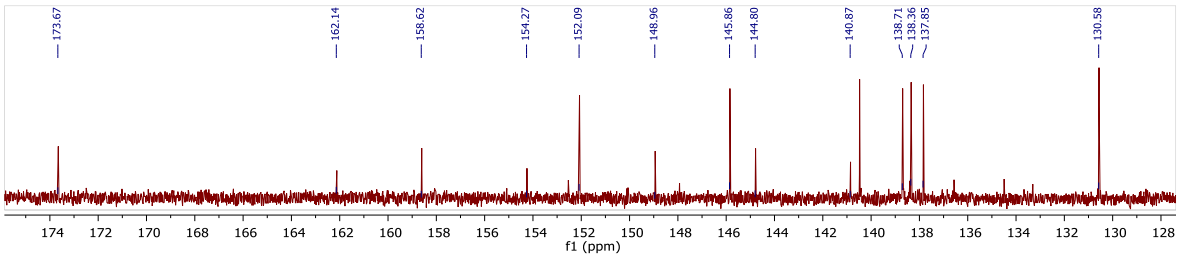

x10 6
+ESI Scan (rt: 0.61, 0.81-0.91 min, 8 scans) Frag=125.0V KIH011_Pos_LoopInjection_MS_13901...
282.2794
343.1517
563.5508
685.2953
922.0098
Counts vs. Mass-to-Charge (m/z)

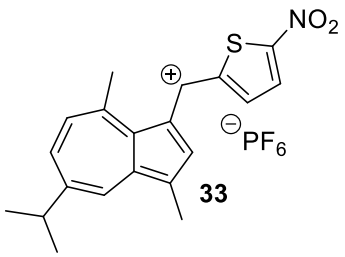

% Transmittance
Wavenumbers (cm-1)


NO2
S
PF6
33
1H-NMR, CD3CN, 500 MHz
f1 (ppm)


f1 (ppm)

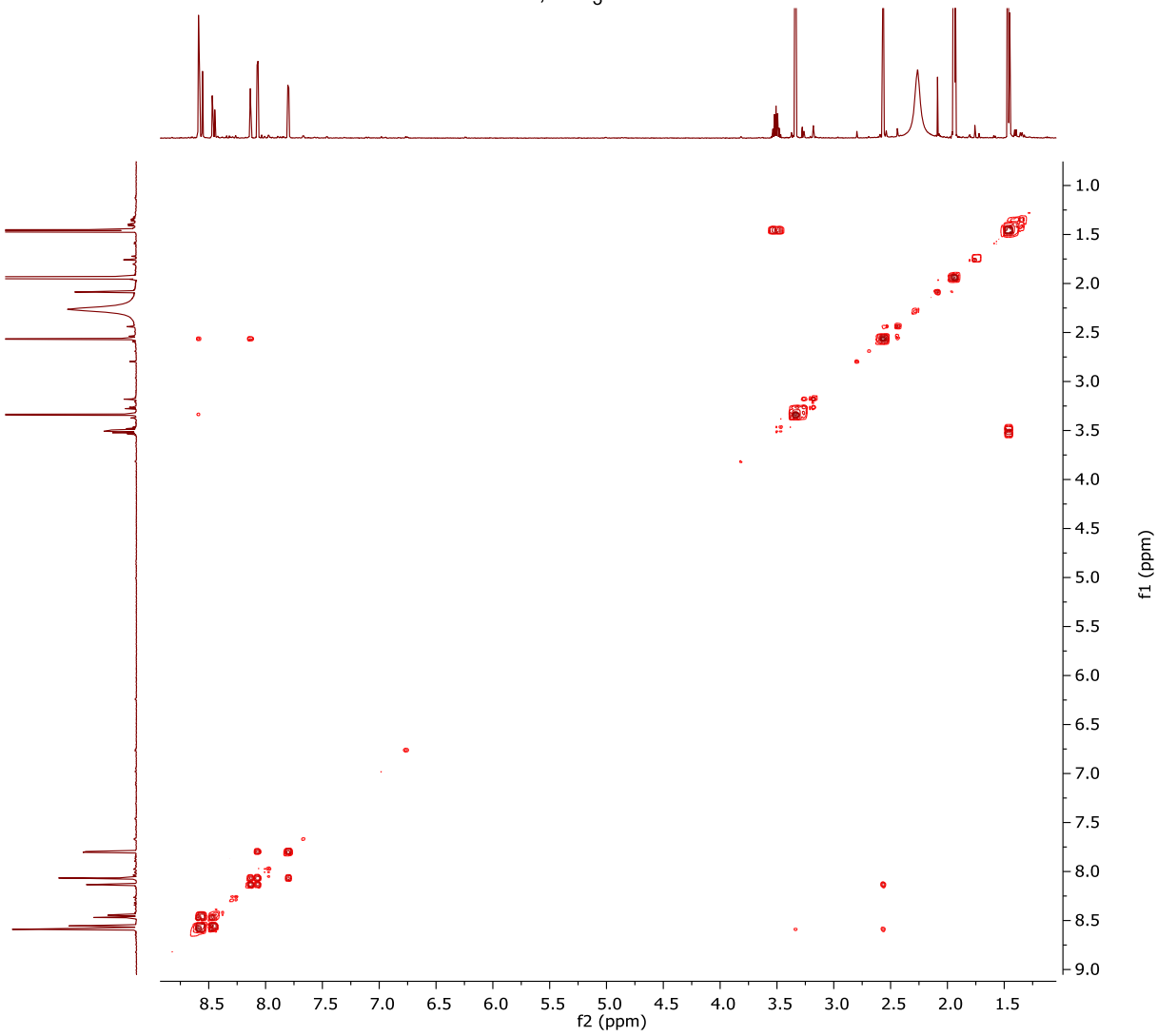

173.67
162.14
158.62
154.27
152.09
148.96
145.86
144.80
140.87
138.71
138.36
137.85
130.58
40.46
29.63
23.70
14.14
NO2
S
PF6
33
13C-NMR, CD3CN, 126 MHz
f1 (ppm)

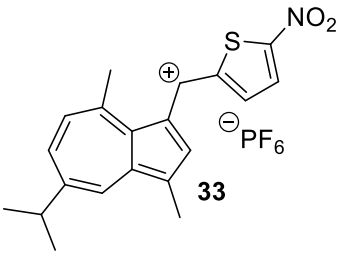

173.67
162.14
158.62
154.27
152.09
148.96
145.86
144.80
140.87
138.71
138.36
137.85
130.58
f1 (ppm)



33

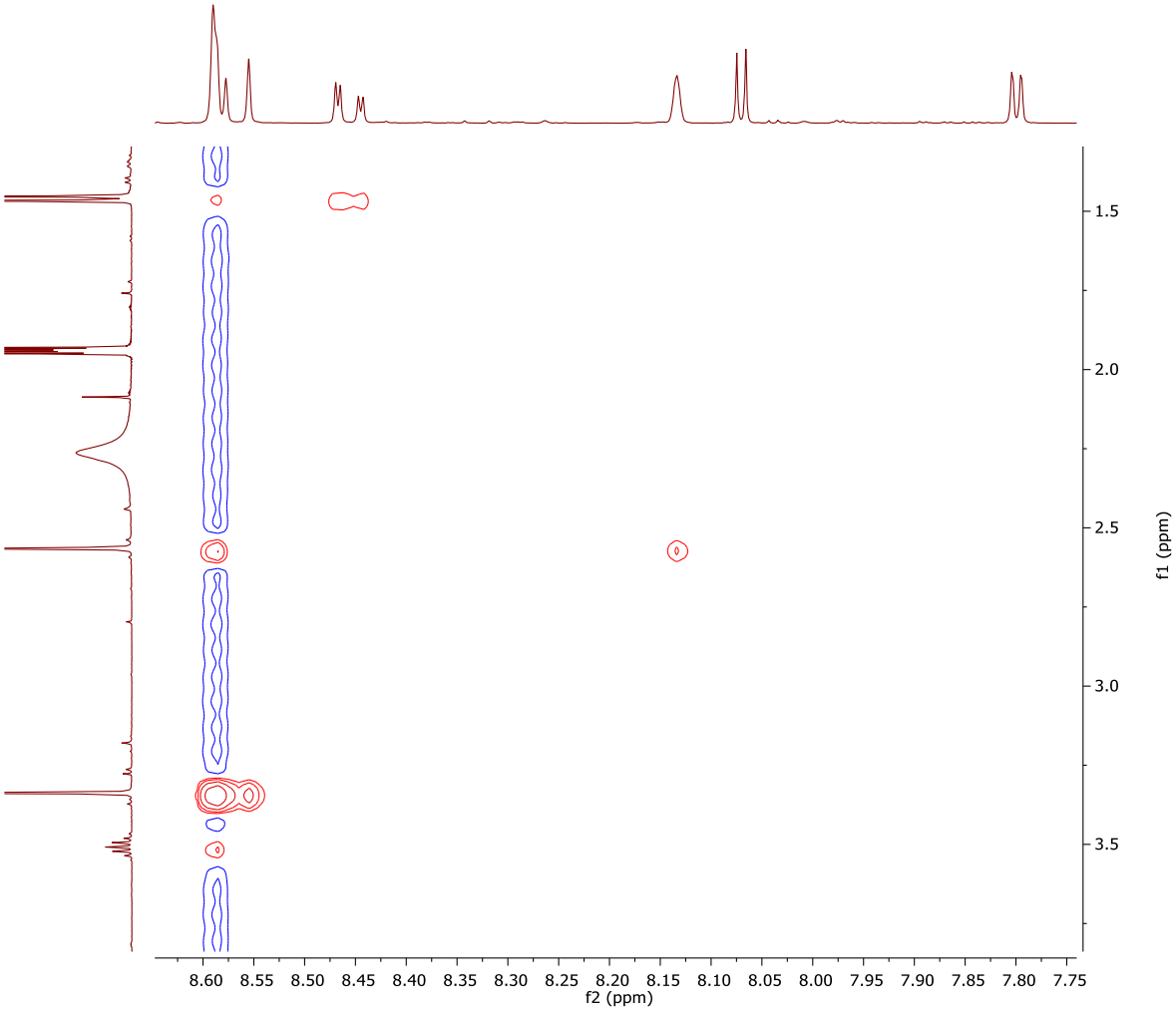
COSY, CD_3CN

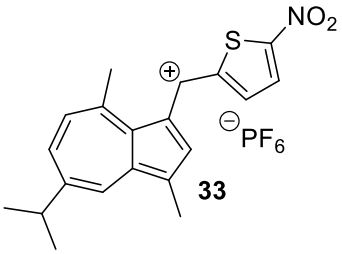




33

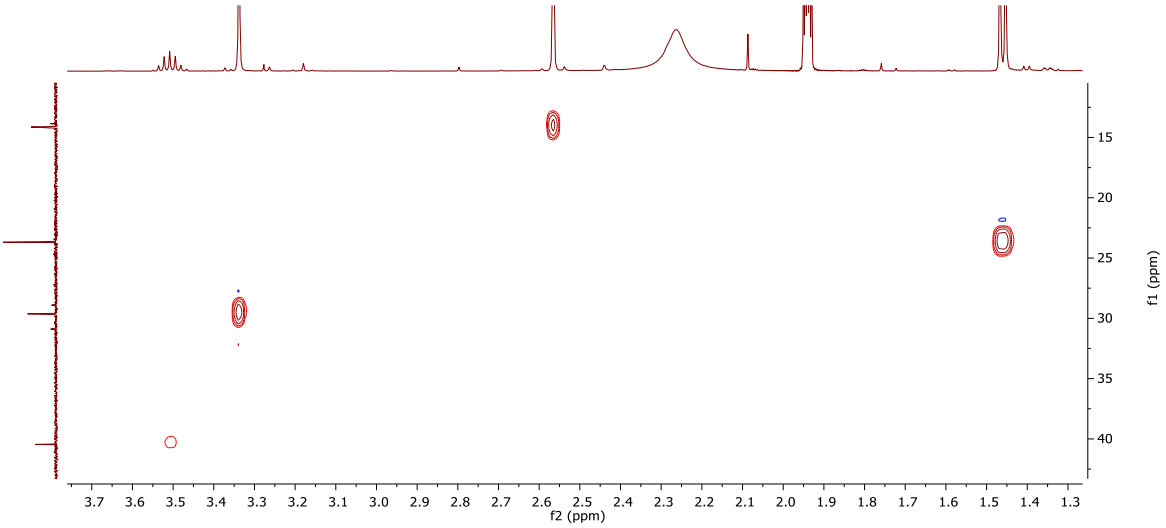
NOESY, CD_3CN

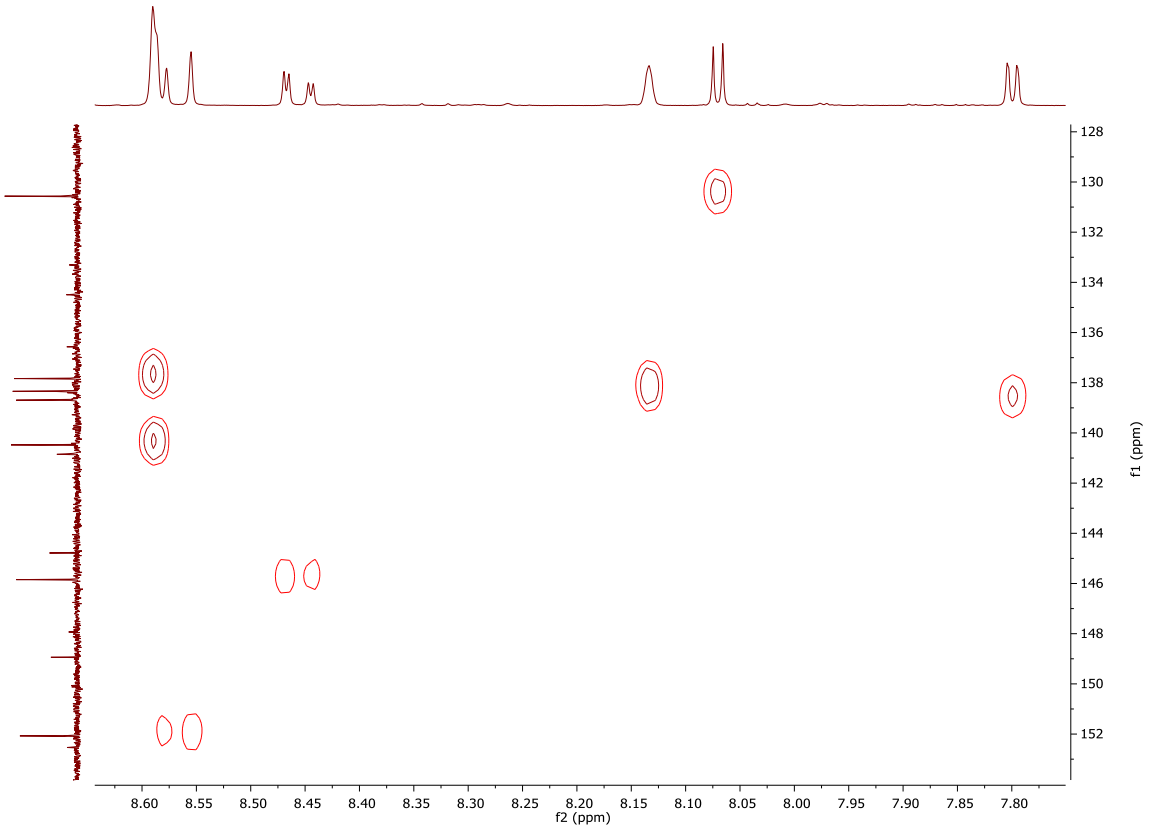


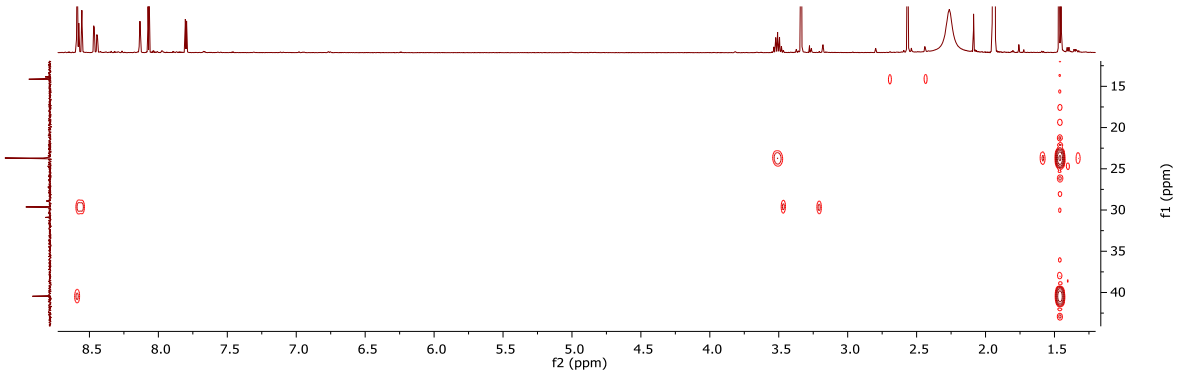


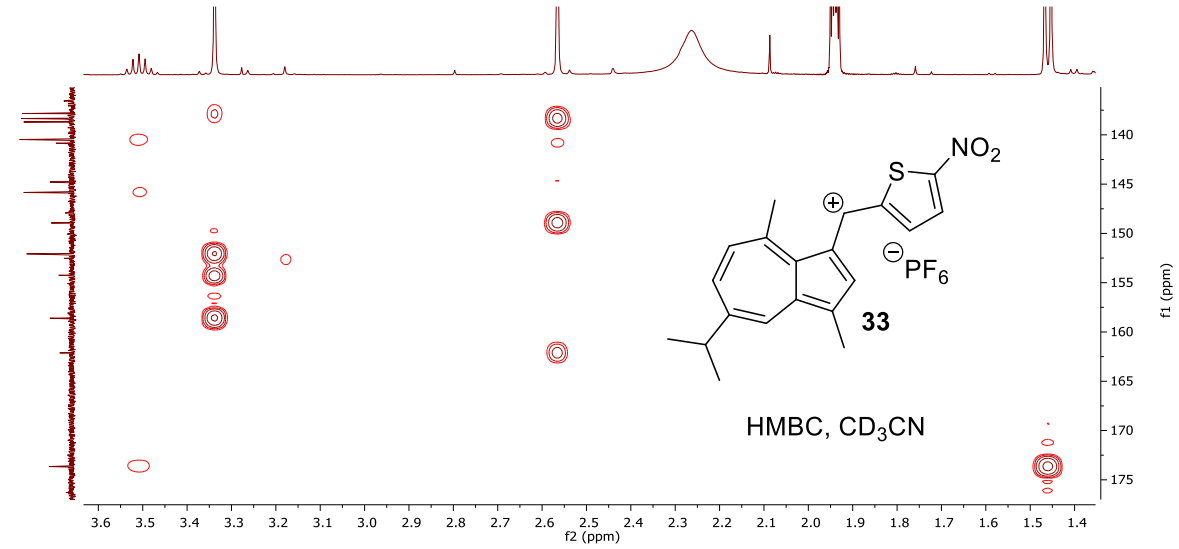
33

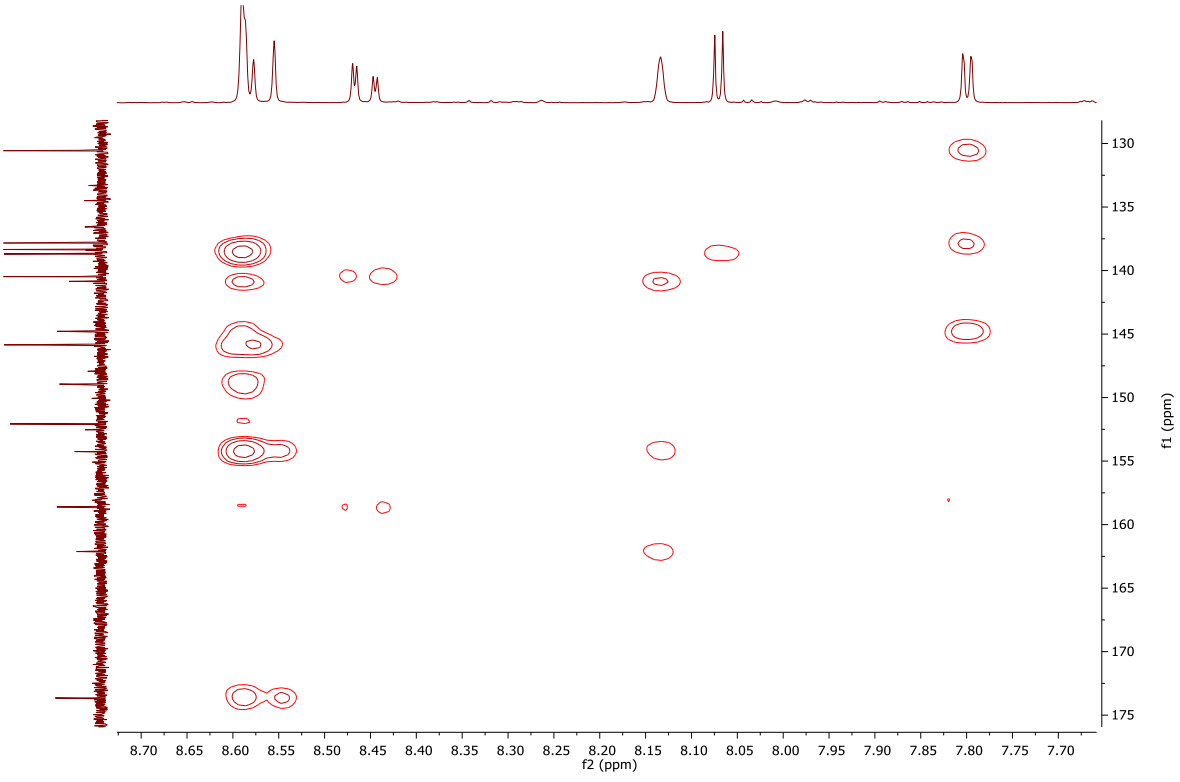
HSQC, CD_3CN

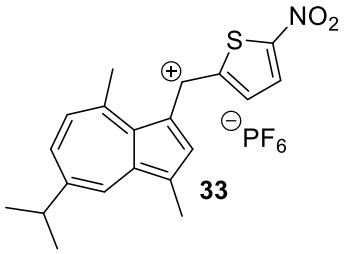




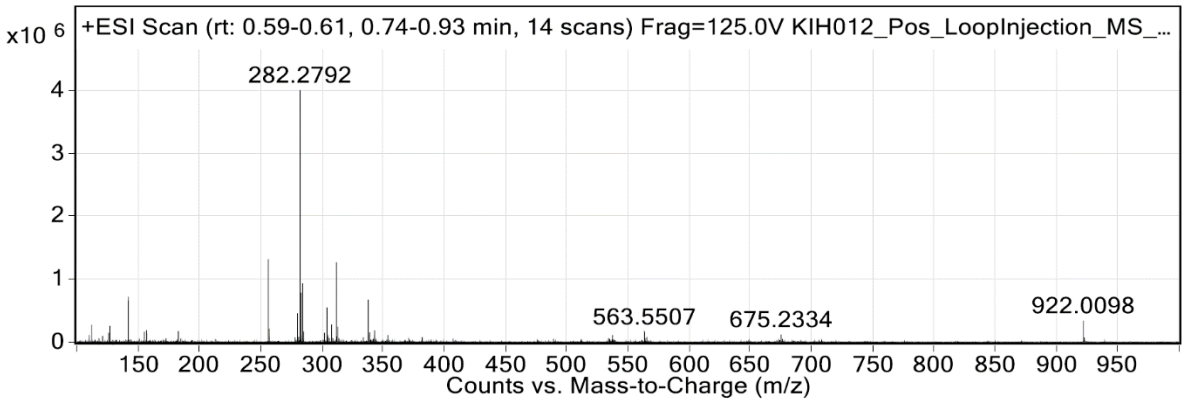

f2 (ppm)
f1 (ppm)

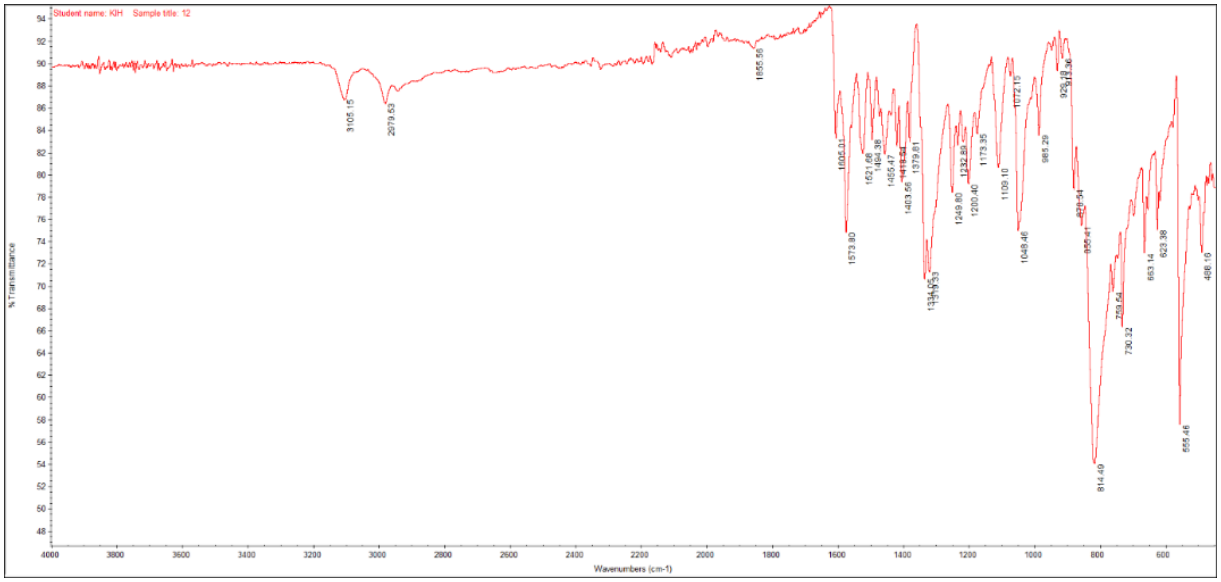

NO2
S
PF6
33
HMBC, CD3CN
f2 (ppm)
f1 (ppm)

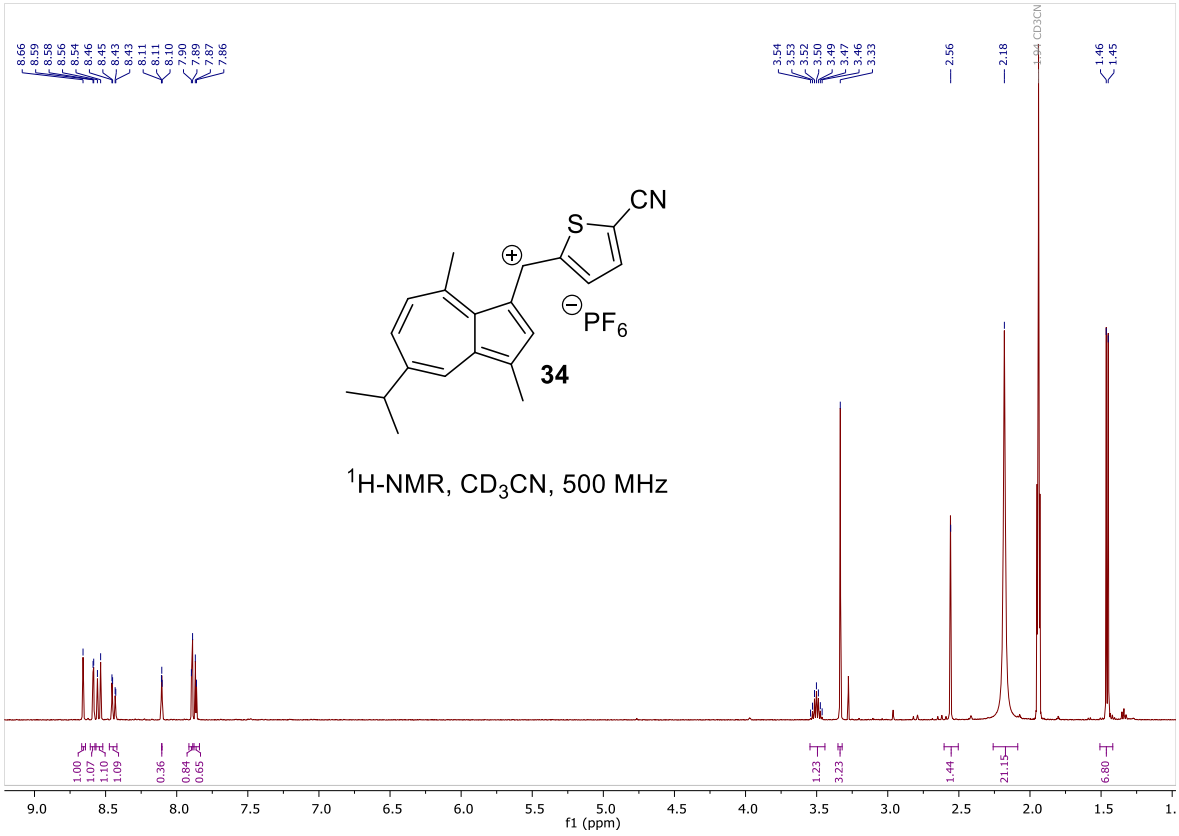

f2 (ppm)
f1 (ppm)

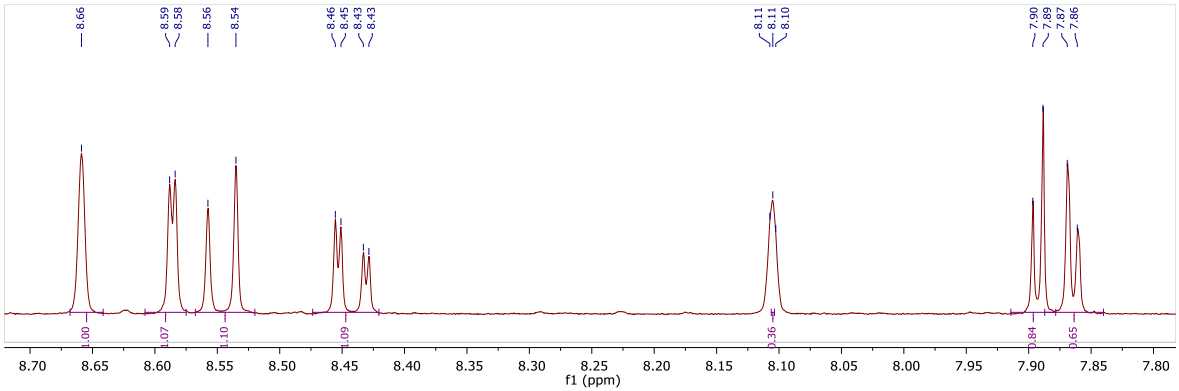

NO2
S
PF6

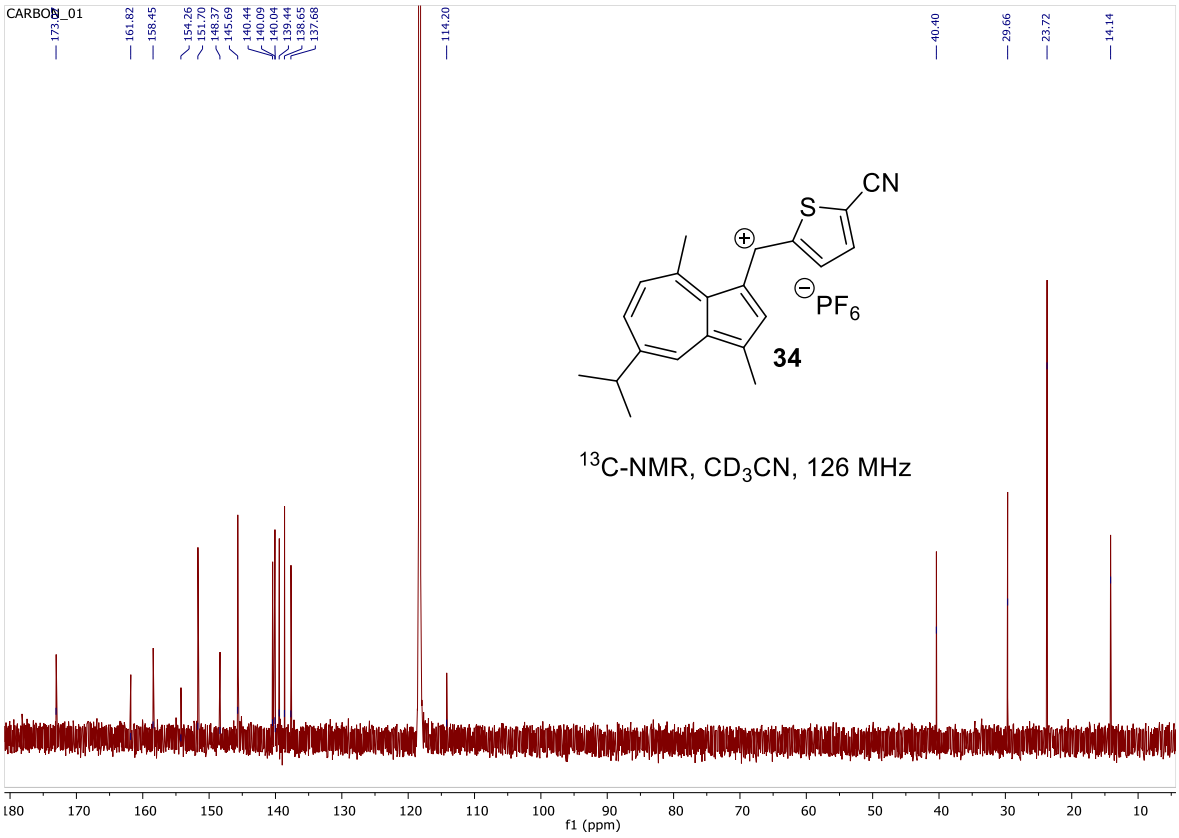
33

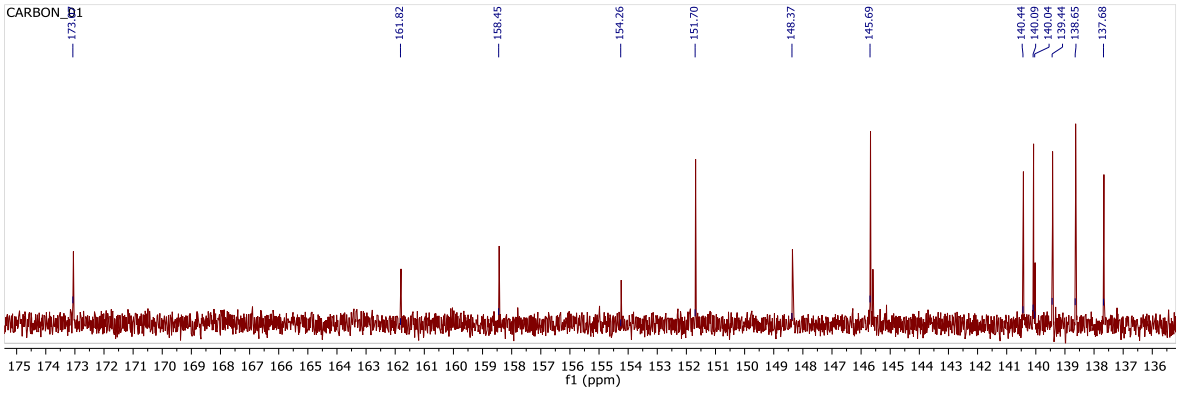

x10 6
+ESI Scan (rt: 0.59-0.61, 0.74-0.93 min, 14 scans) Frag=125.0V KIH012_Pos_LoopInjection_MS_...
282.2792
563.5507
675.2334
922.0098
Counts vs. Mass-to-Charge (m/z)

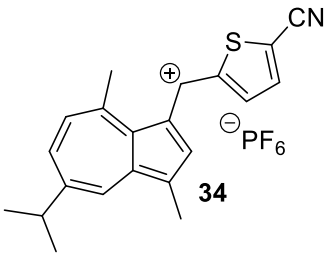

% Transmittance
Wavenumbers (cm-1)


8.66
8.59
8.58
8.56
8.54
8.46
8.45
8.43
8.43
8.11
8.10
7.90
7.89
7.87
7.86
3.54
3.53
3.52
3.50
3.49
3.47
3.46
3.33
2.56
2.18
1.94 CD3CN
1.46
1.45
CN
S
PF6
34
1H-NMR, CD3CN, 500 MHz
1.00
1.07
1.10
1.09
0.36
0.84
0.65
1.23
3.23
1.44
21.15
6.80
f1 (ppm)


8.66
8.59
8.58
8.56
8.54
8.46
8.45
8.43
8.43
8.11
8.11
8.10
7.90
7.89
7.87
7.86
1.00
1.07
1.10
1.09
0.36
0.84
0.65
f1 (ppm)

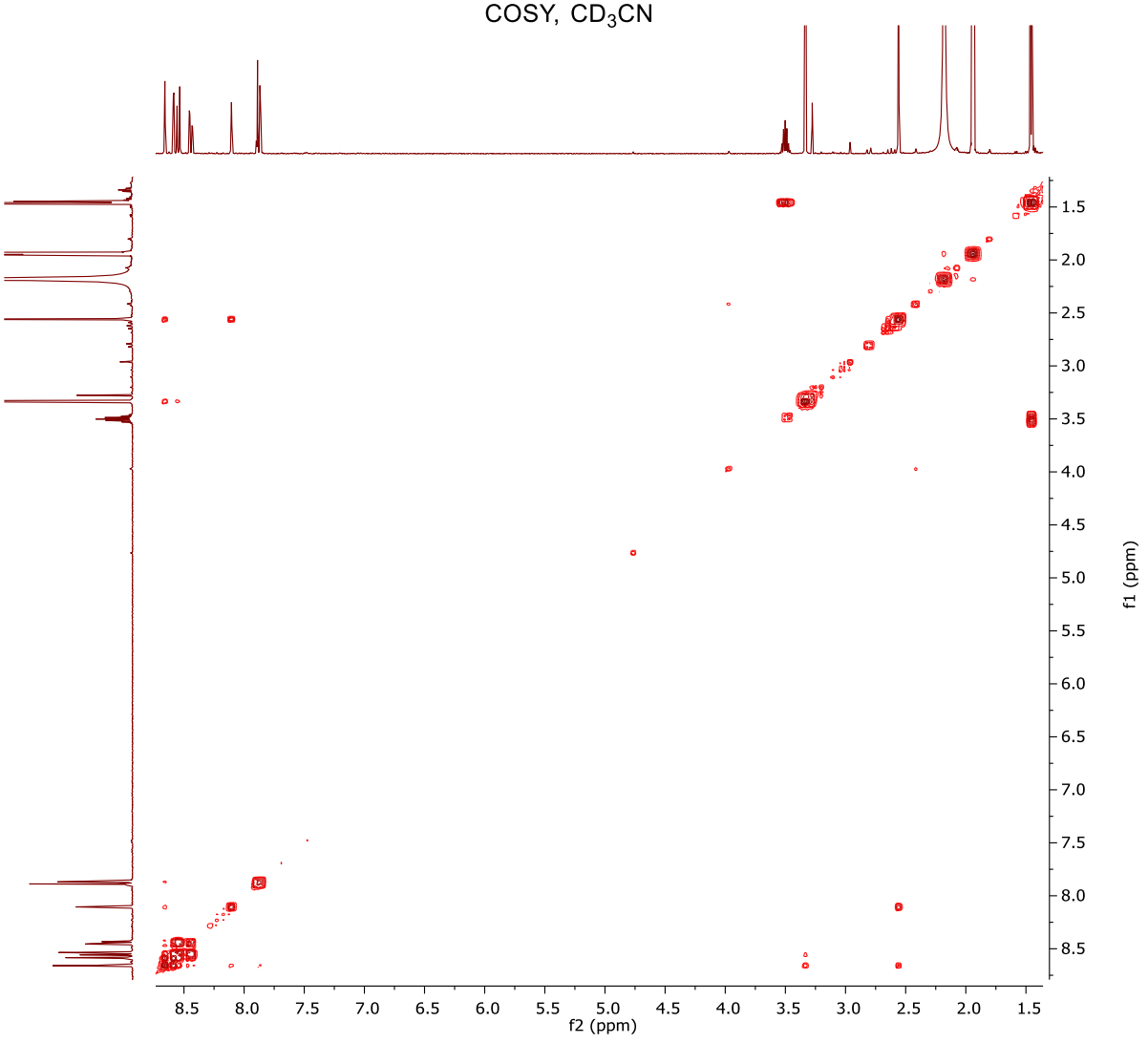

CARBON_01
173.21
161.82
158.45
154.26
151.70
148.37
145.69
140.44
140.09
140.04
139.44
138.65
137.68
114.20
40.40
29.66
23.72
14.14
CN
S
PF6
34
13C-NMR, CD3CN, 126 MHz
f1 (ppm)

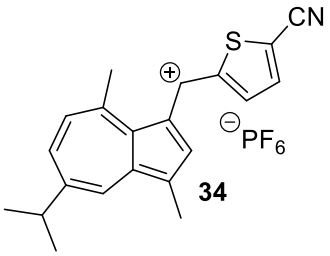

CARBON_01
173.21
161.82
158.45
154.26
151.70
148.37
145.69
140.44
140.09
140.04
139.44
138.65
137.68
f1 (ppm)



34

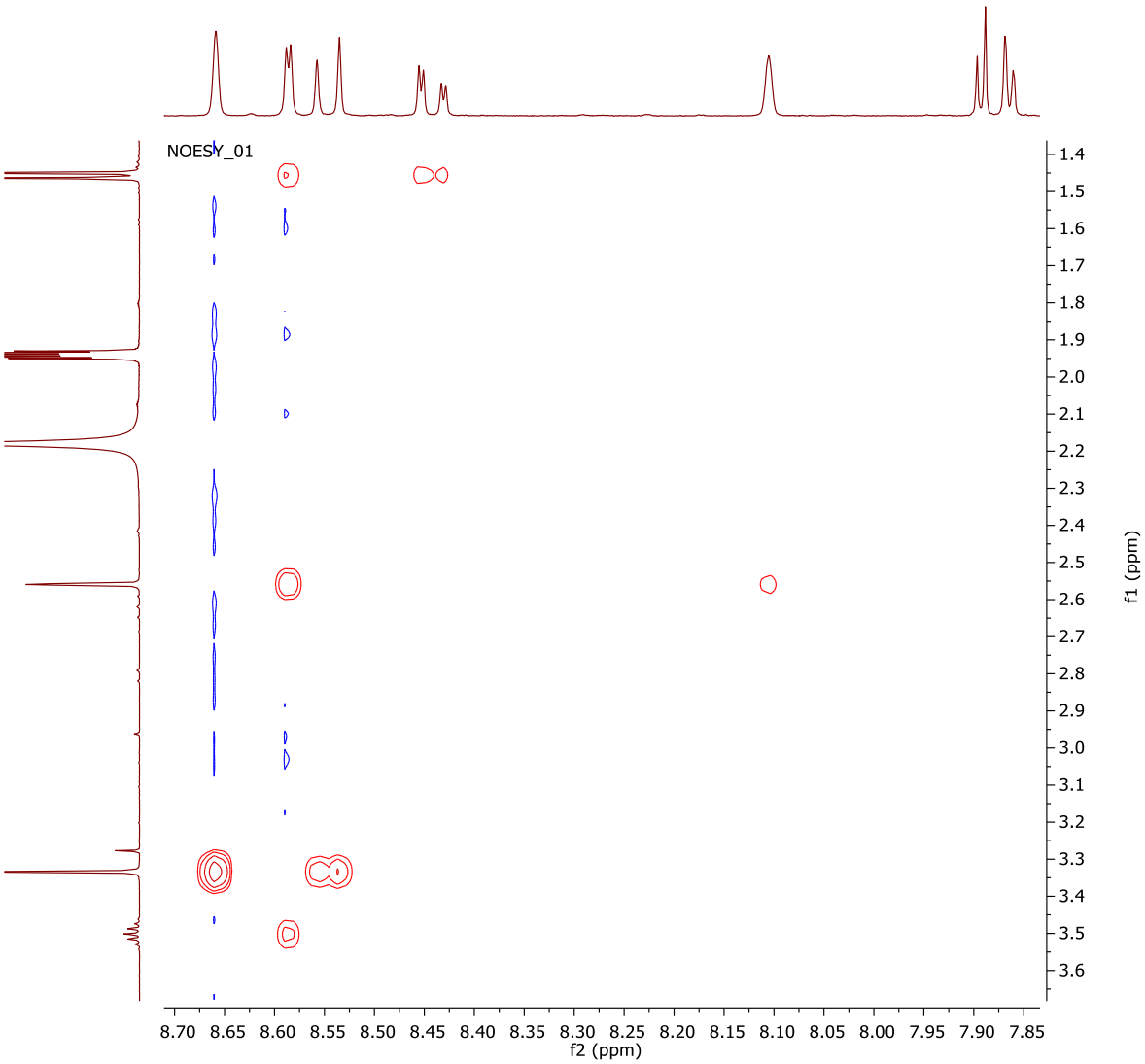
COSY, CD_3CN

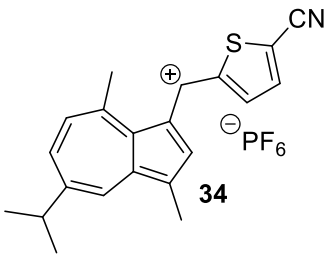




34

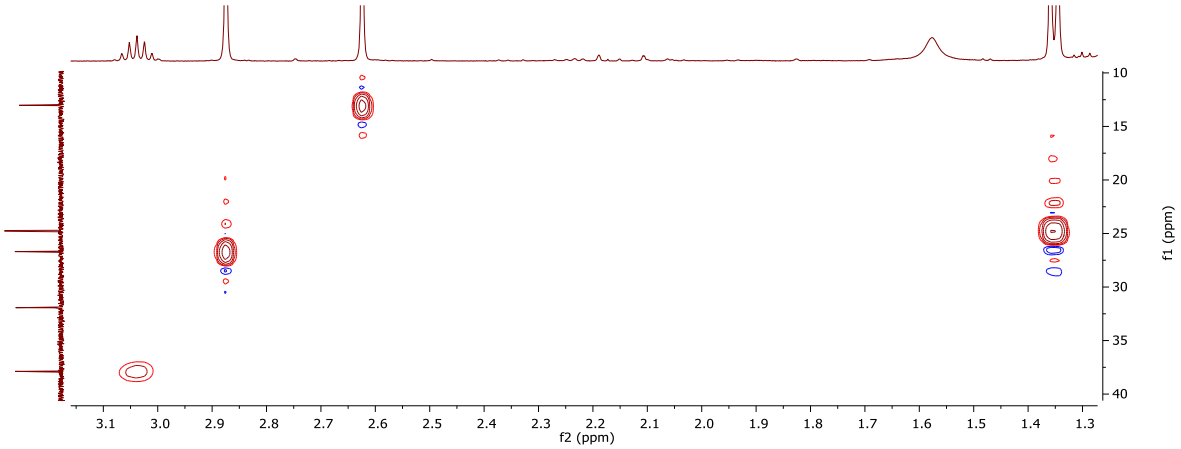
NOESY, CD_3CN

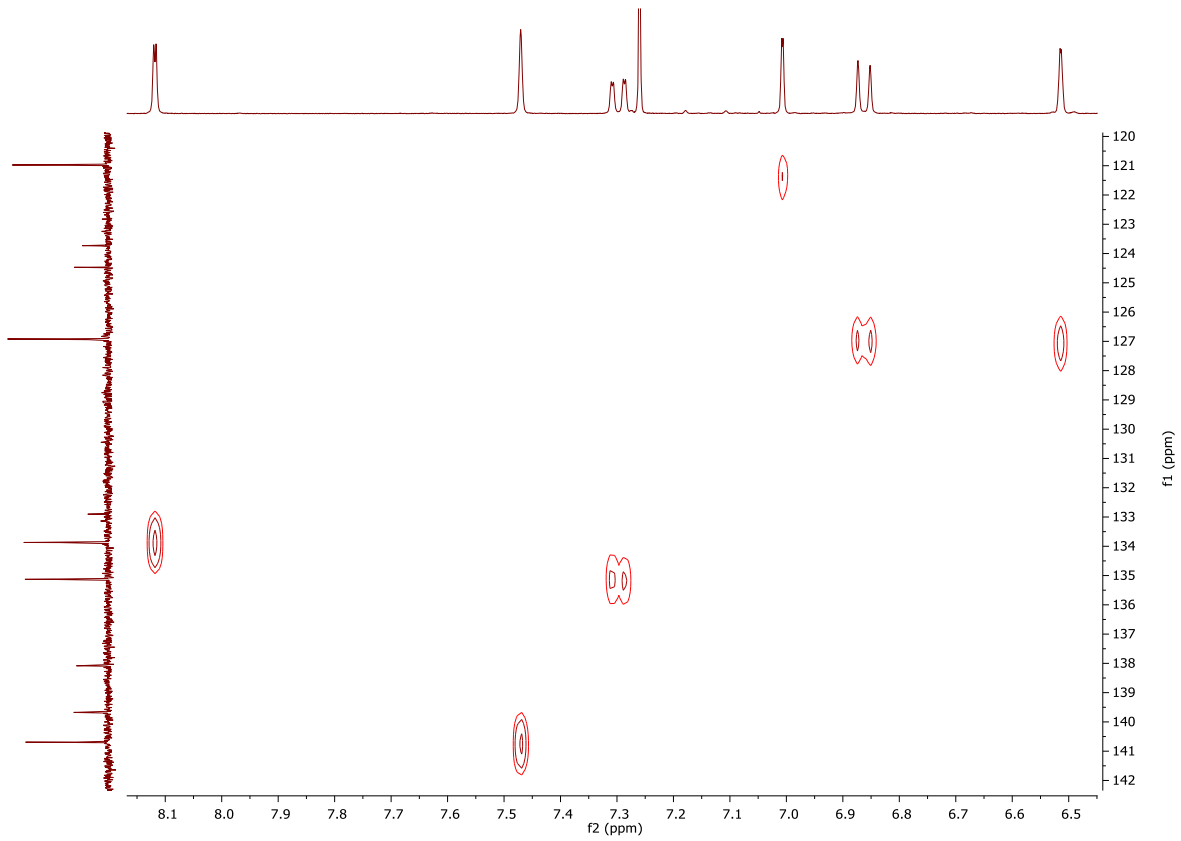


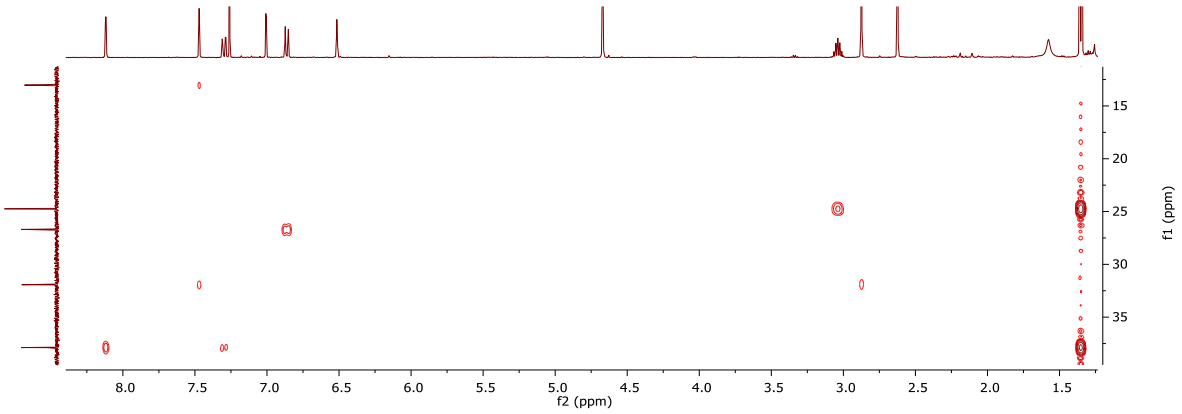


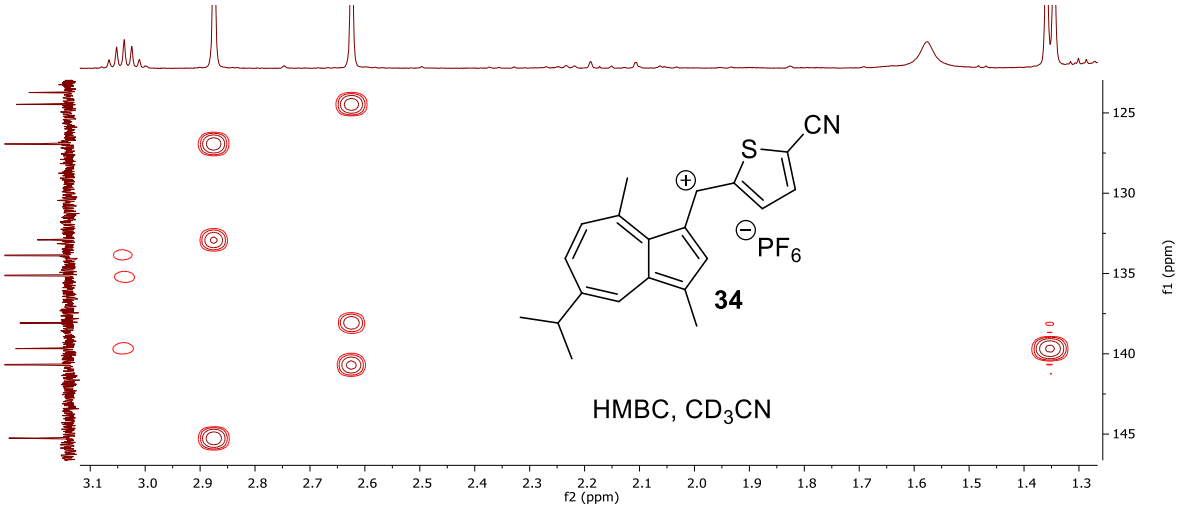
34

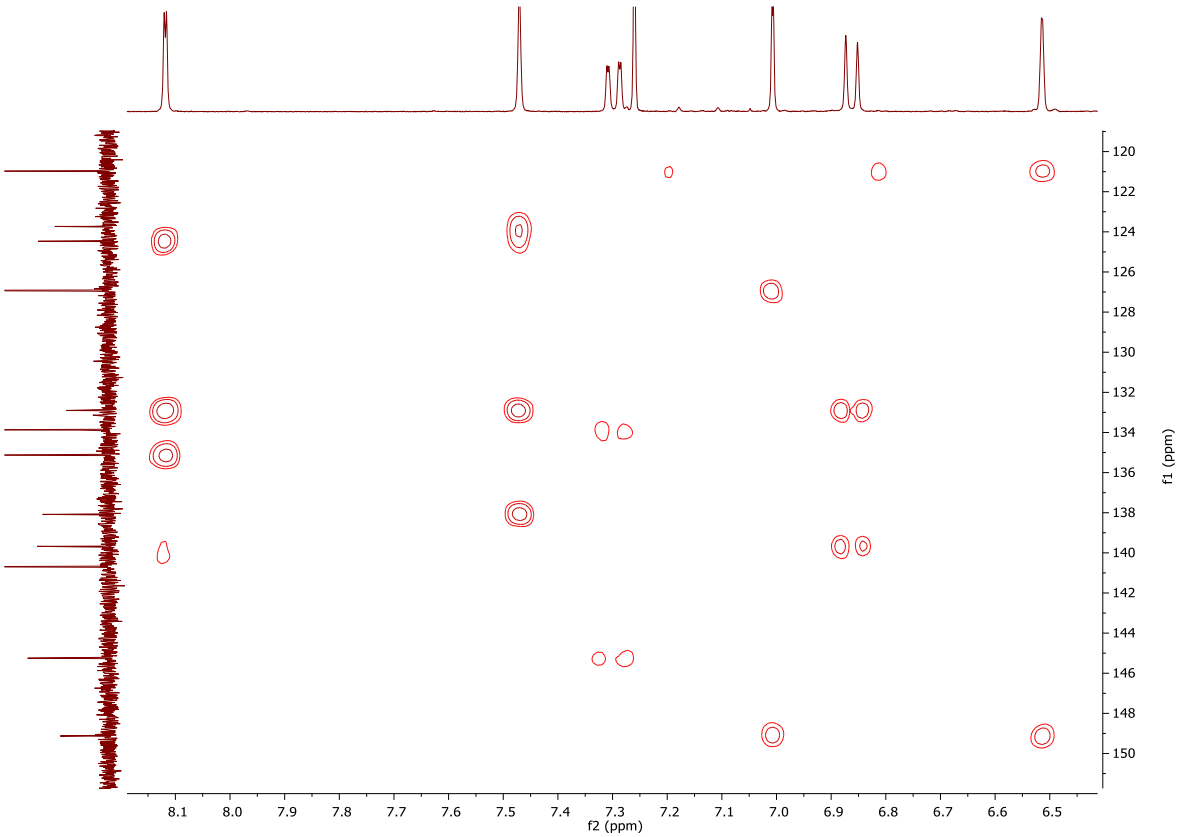
HSQC, CD_3CN

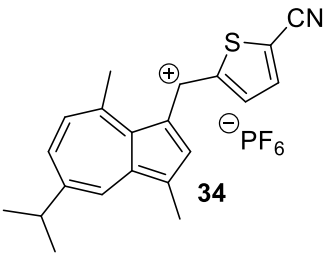




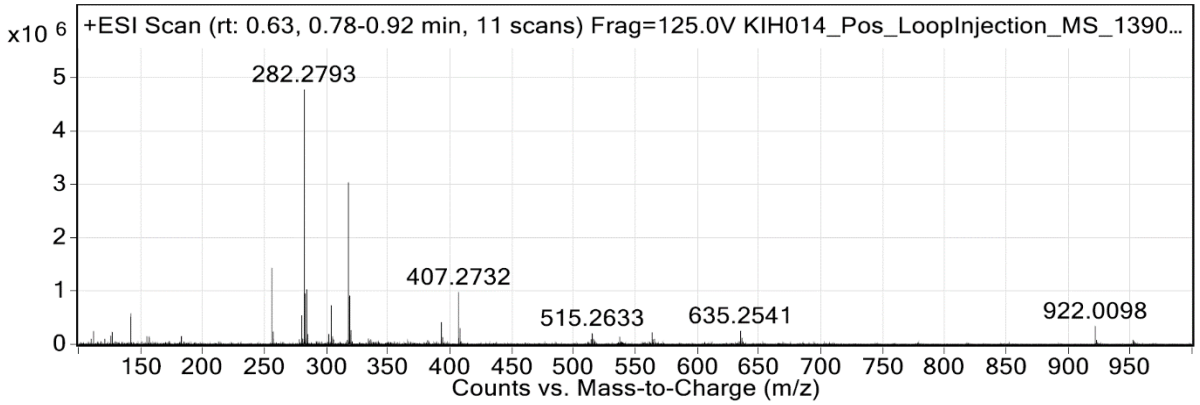

f2 (ppm)
f1 (ppm)

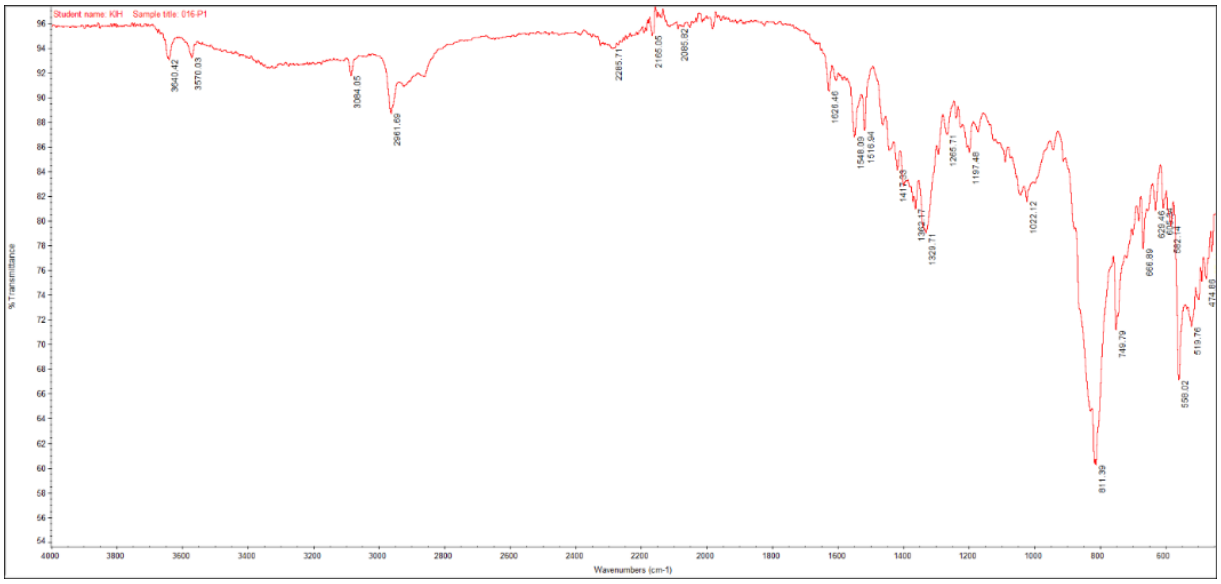

CN
S
PF6
34
HMBC, CD3CN
f2 (ppm)
f1 (ppm)

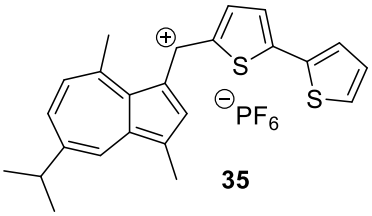

f2 (ppm)
f1 (ppm)


CN
S
PF6

34

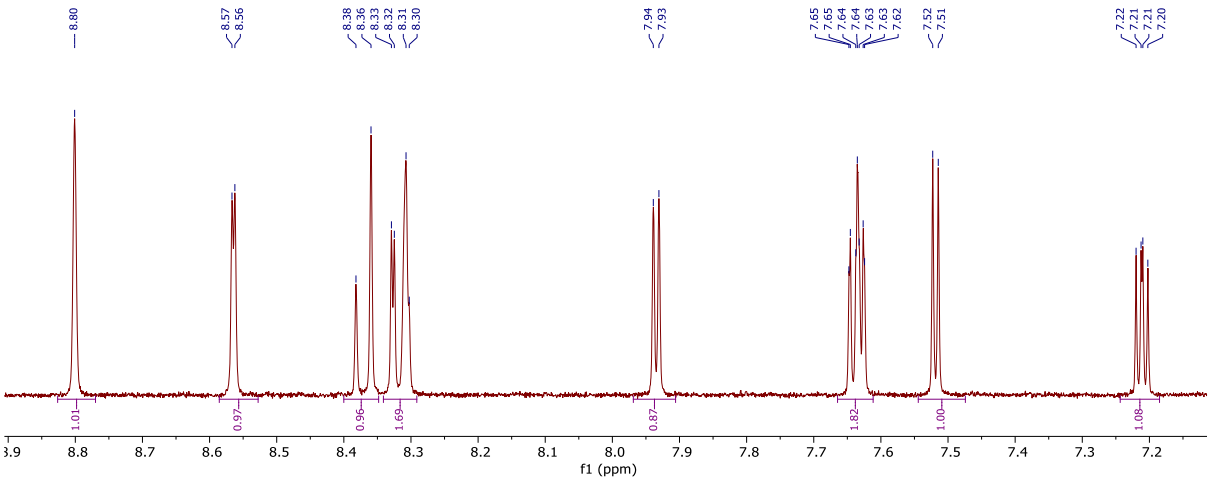

x10 6
+ESI Scan (rt: 0.63, 0.78-0.92 min, 11 scans) Frag=125.0V KIH014_Pos_LoopInjection_MS_1390...
282.2793
407.2732
515.2633
635.2541
922.0098
Counts vs. Mass-to-Charge (m/z)

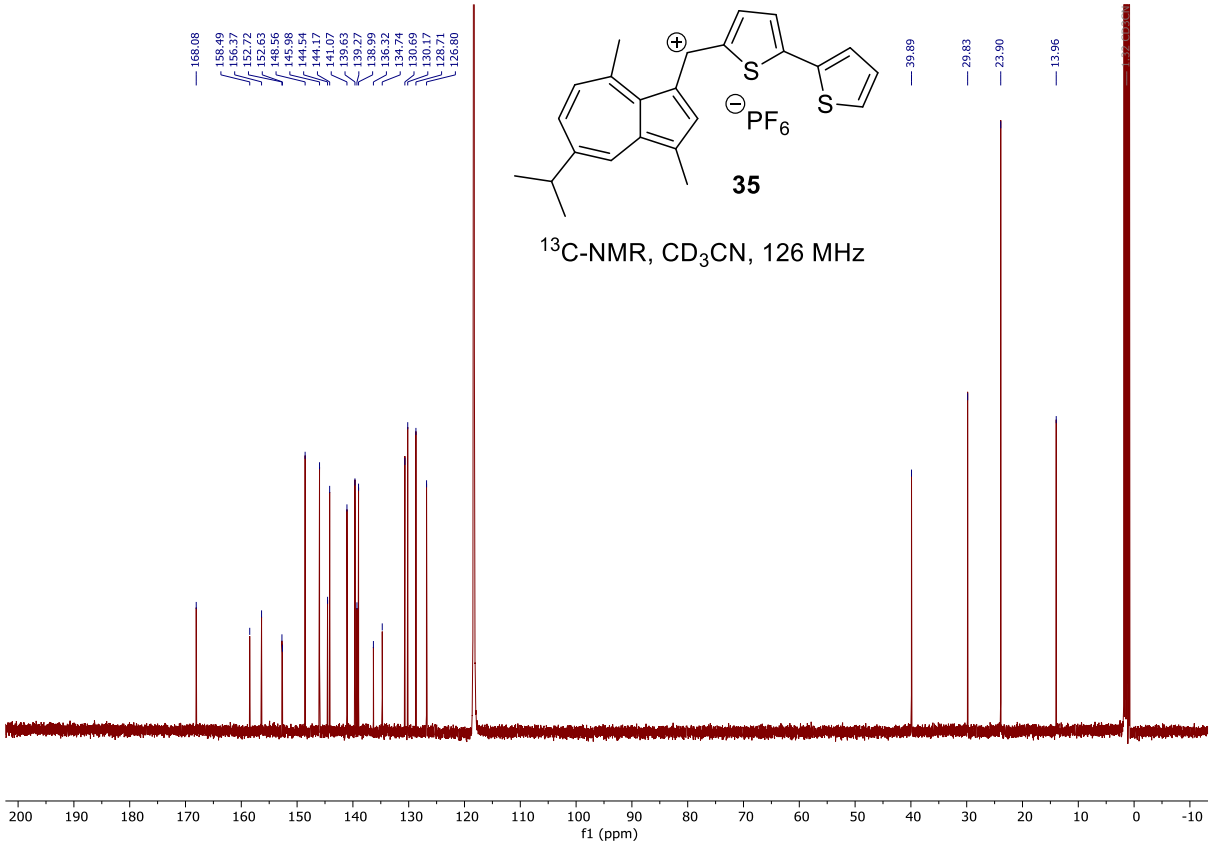

Student name: KIH Sample title: 016-P1
%Transmittance
Wavenumbers (cm-1)

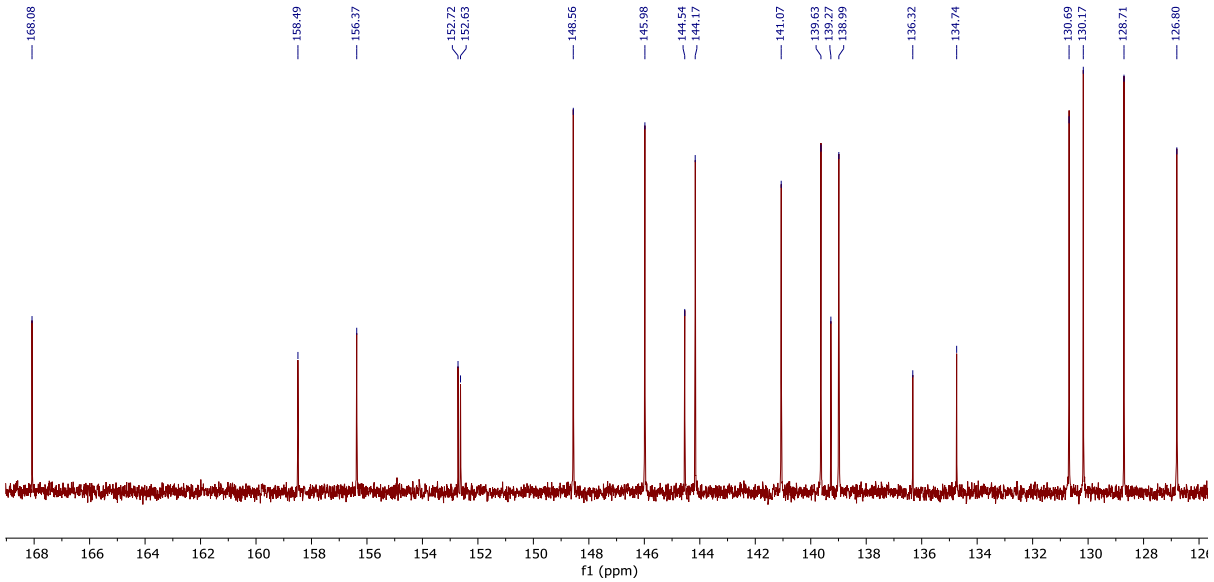


35

^{1}H-NMR, CD_3CN, 500 MHz




168.08
158.49
156.37
152.72
152.63
148.56
145.98
144.54
144.17
141.07
139.63
139.27
138.99
136.32
134.74
130.69
130.17
128.71
126.80
39.89
29.83
23.90
13.96
S
S
PF6
35
13C-NMR, CD3CN, 126 MHz
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


168.08
158.49
156.37
152.72
152.63
148.56
145.98
144.54
144.17
141.07
139.63
139.27
138.99
136.32
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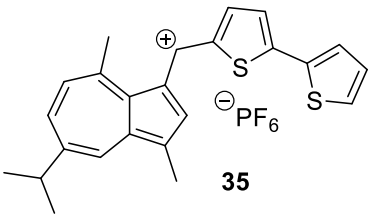
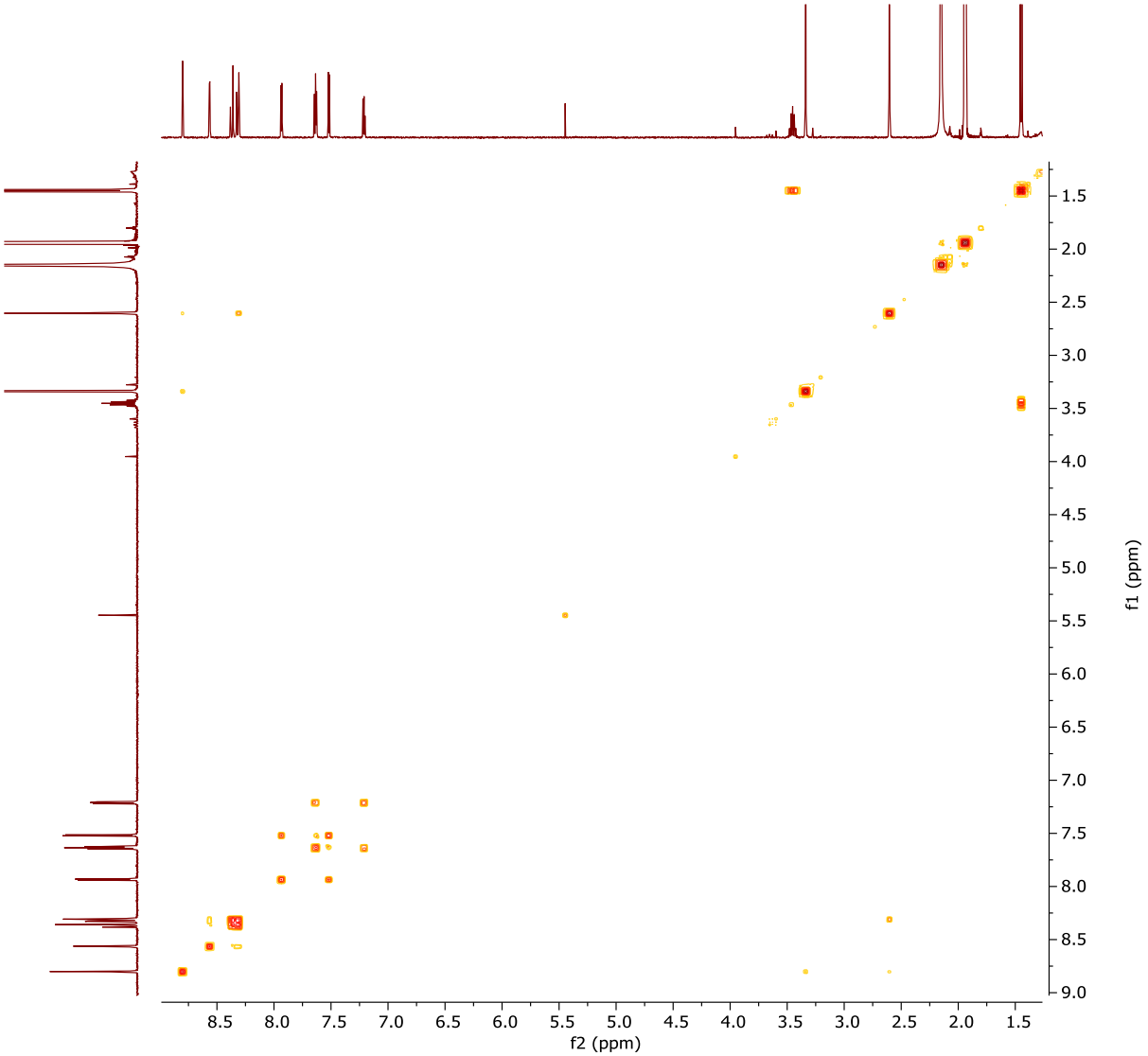
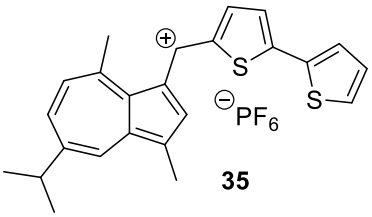
130.69
130.17
128.71
126.80
168 166 164 162 160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128
f1 (ppm)



35

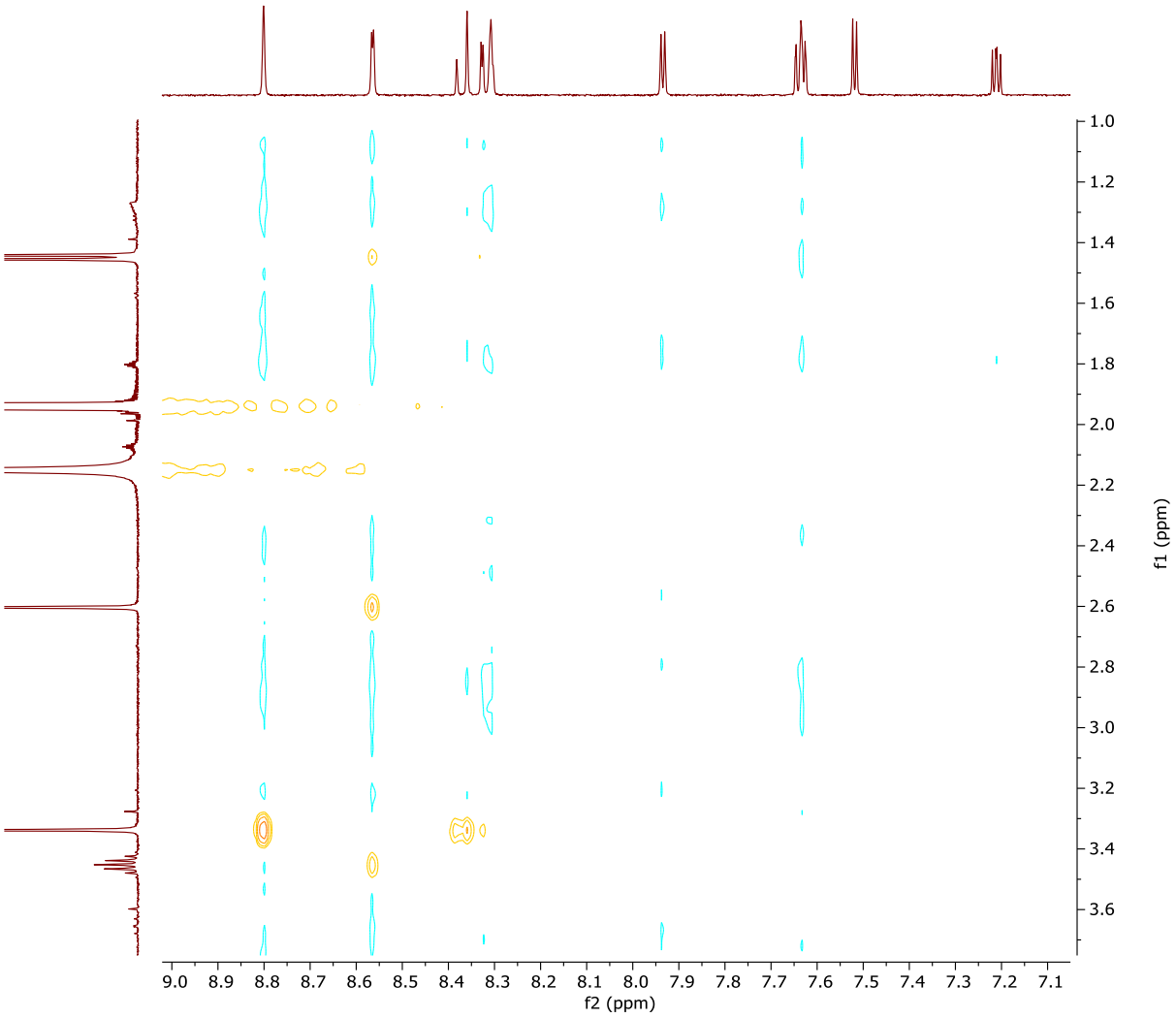
COSY, CD_3CN

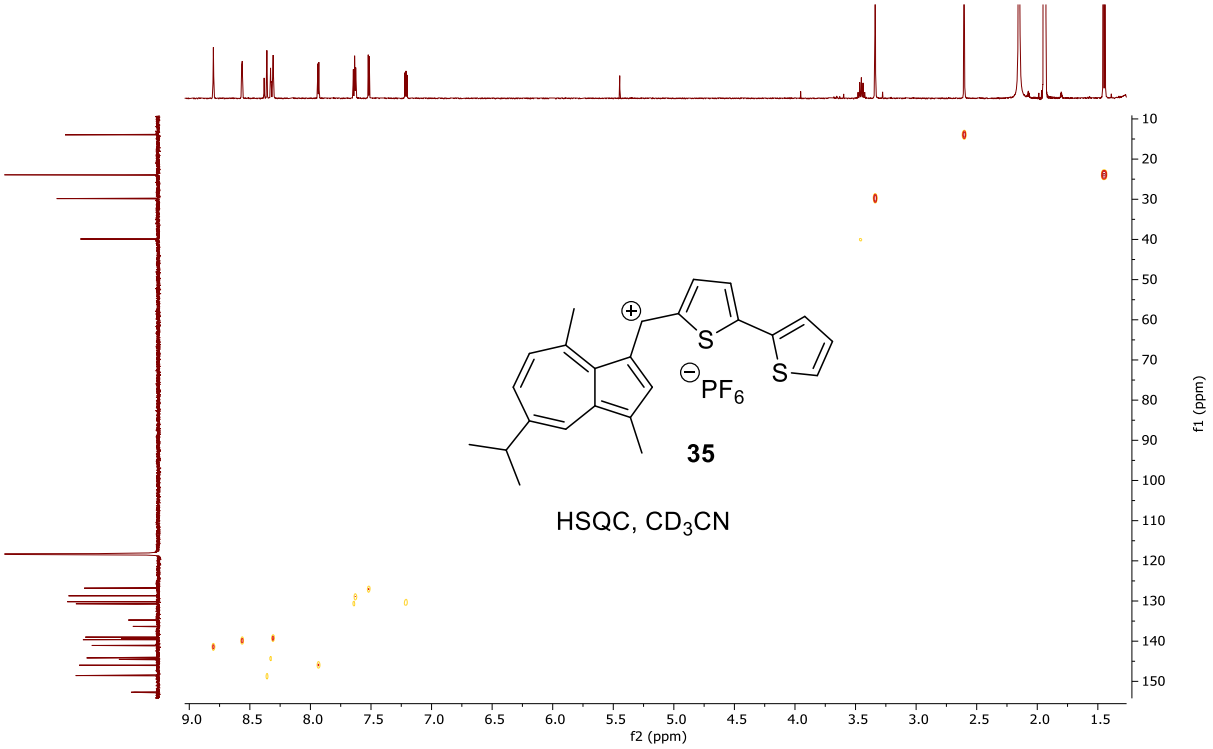


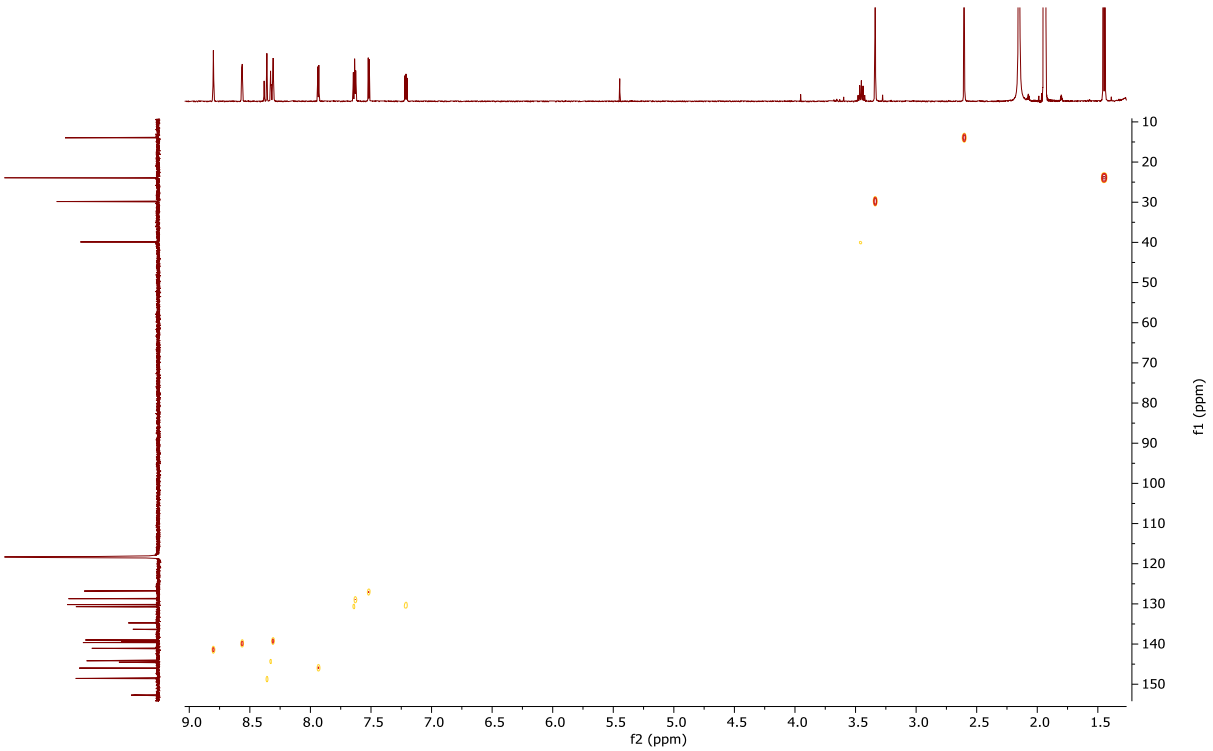


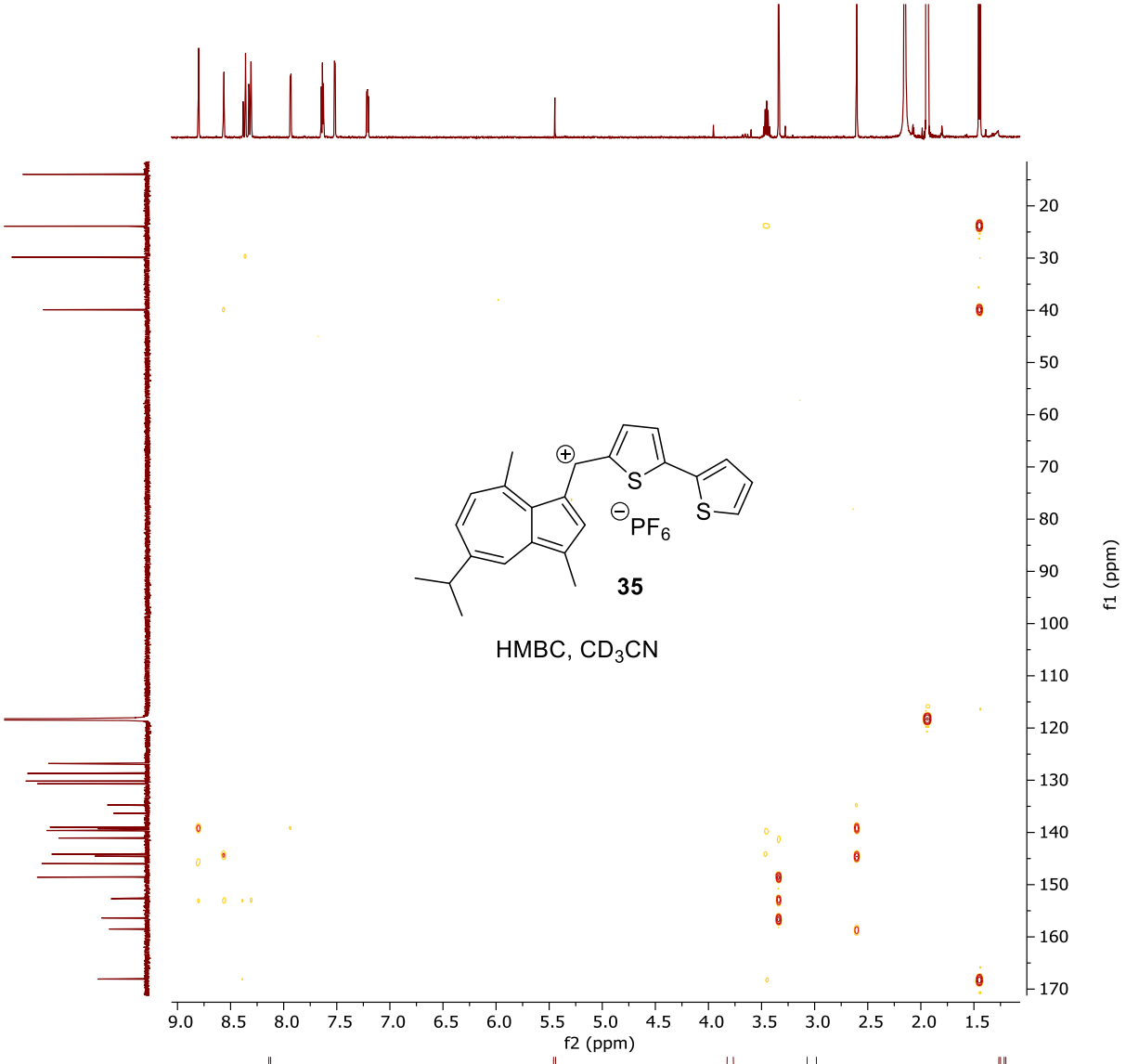
35

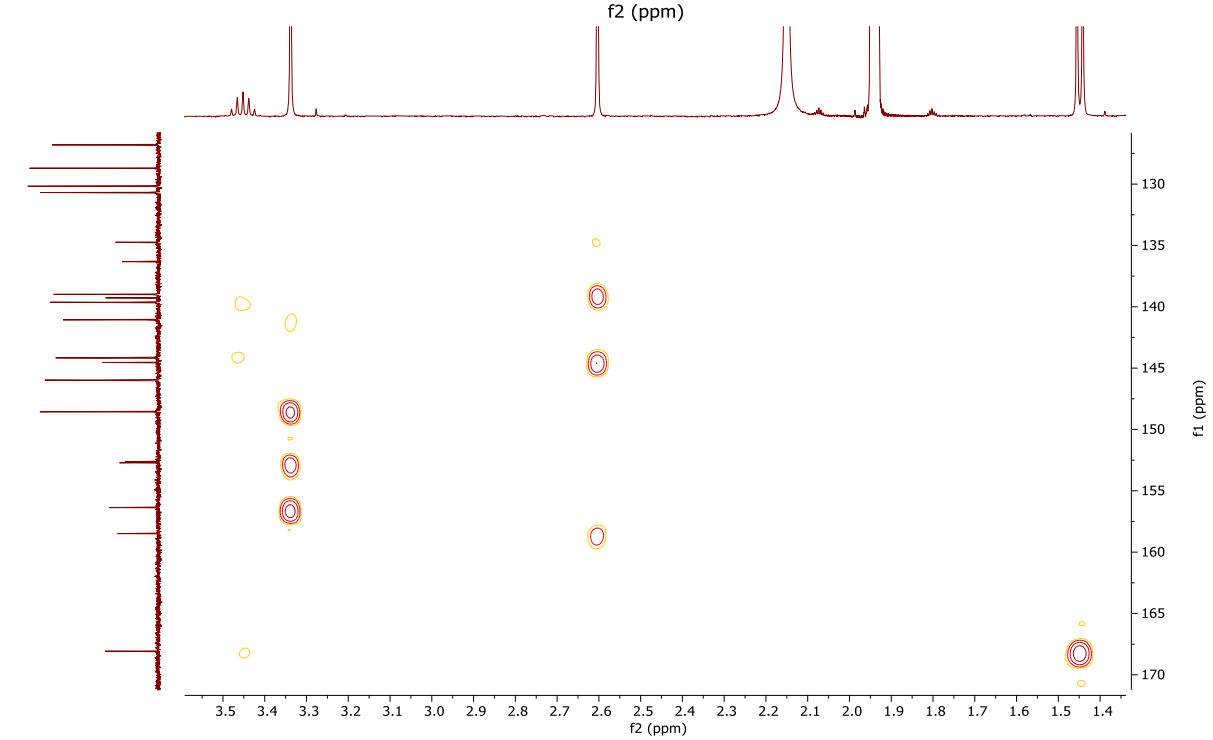
NOESY, CD_3CN

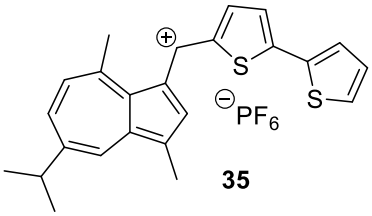



S
S
PF6
35
HSQC, CD3CN
f1 (ppm)
f2 (ppm)


f1 (ppm)
f2 (ppm)

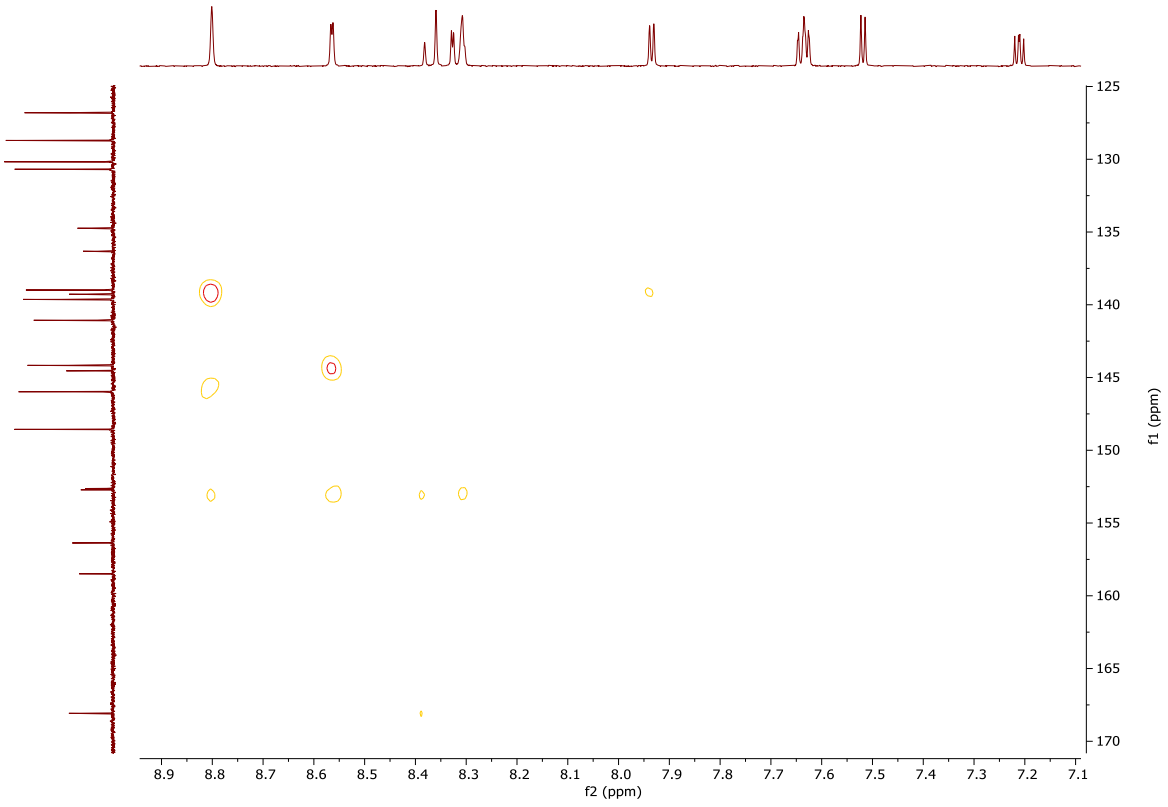

S
S
PF6
35
HMBC, CD3CN
f1 (ppm)
f2 (ppm)

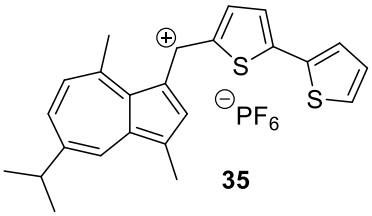

f1 (ppm)
f2 (ppm)



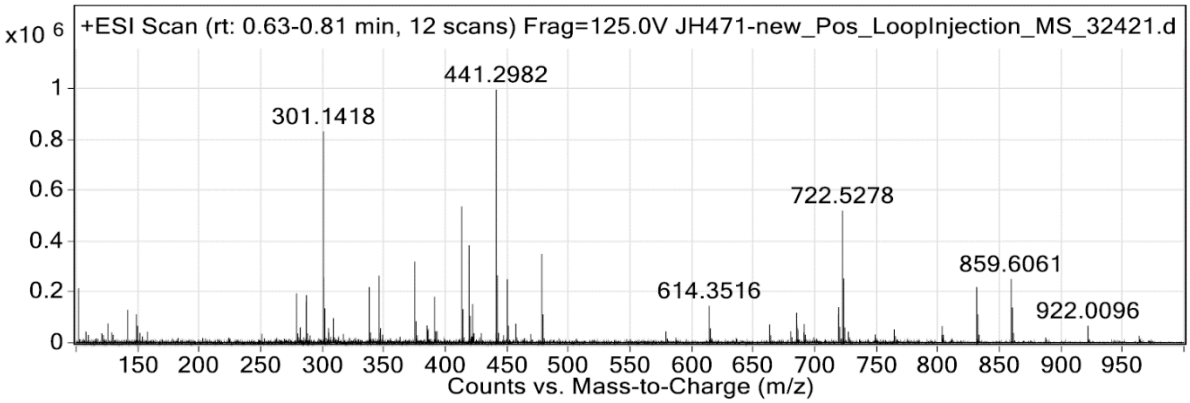
35

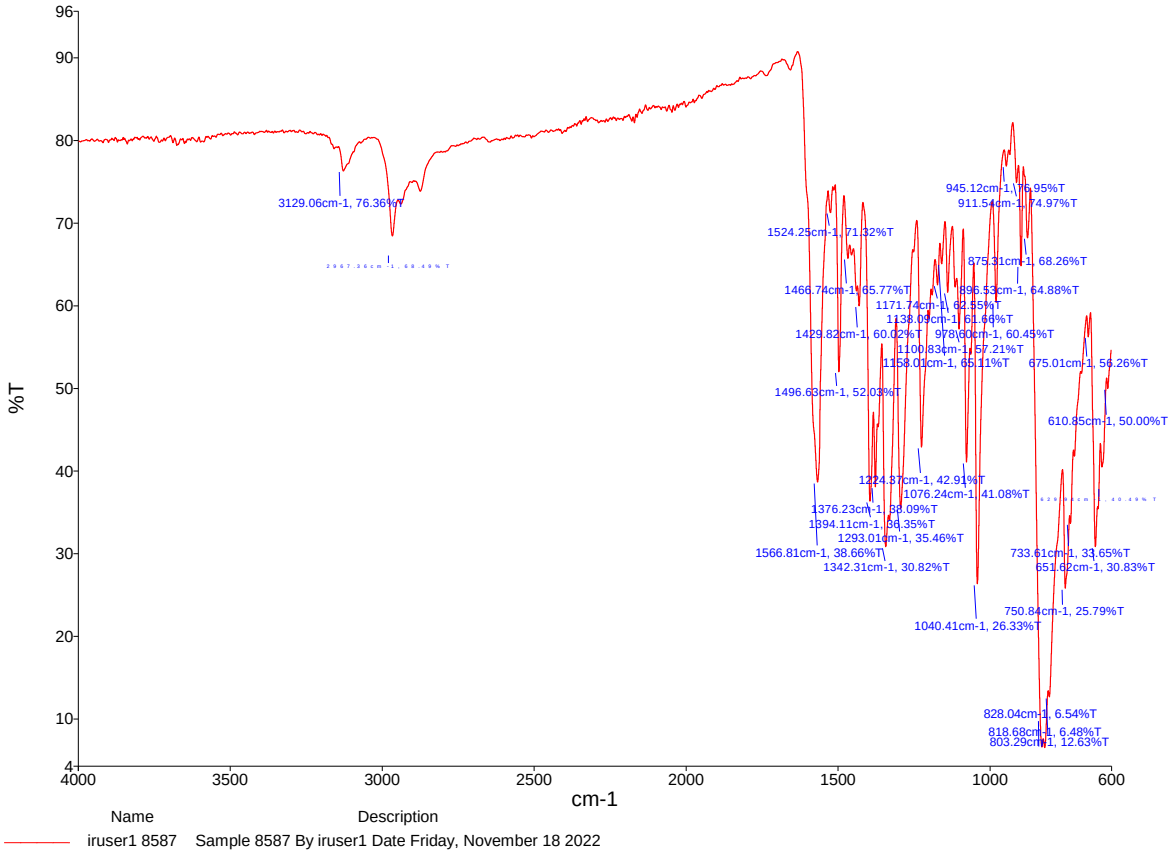
HMBC, CD_3CN

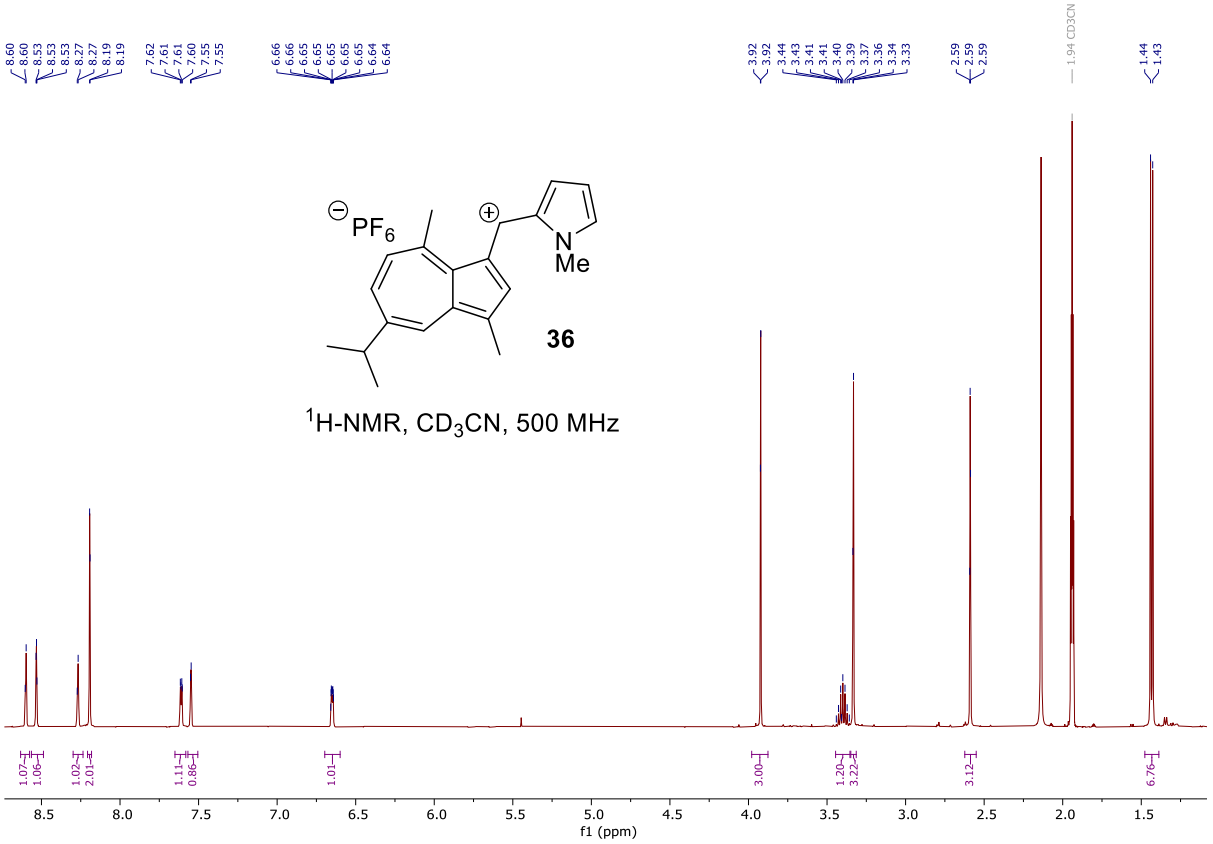


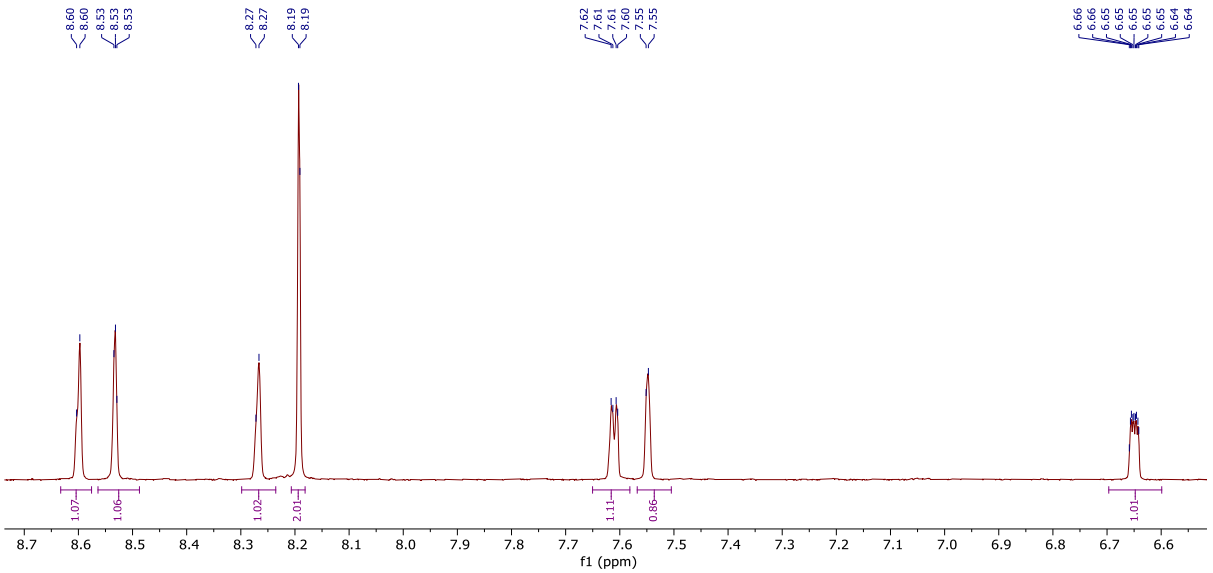

S
S
PF6

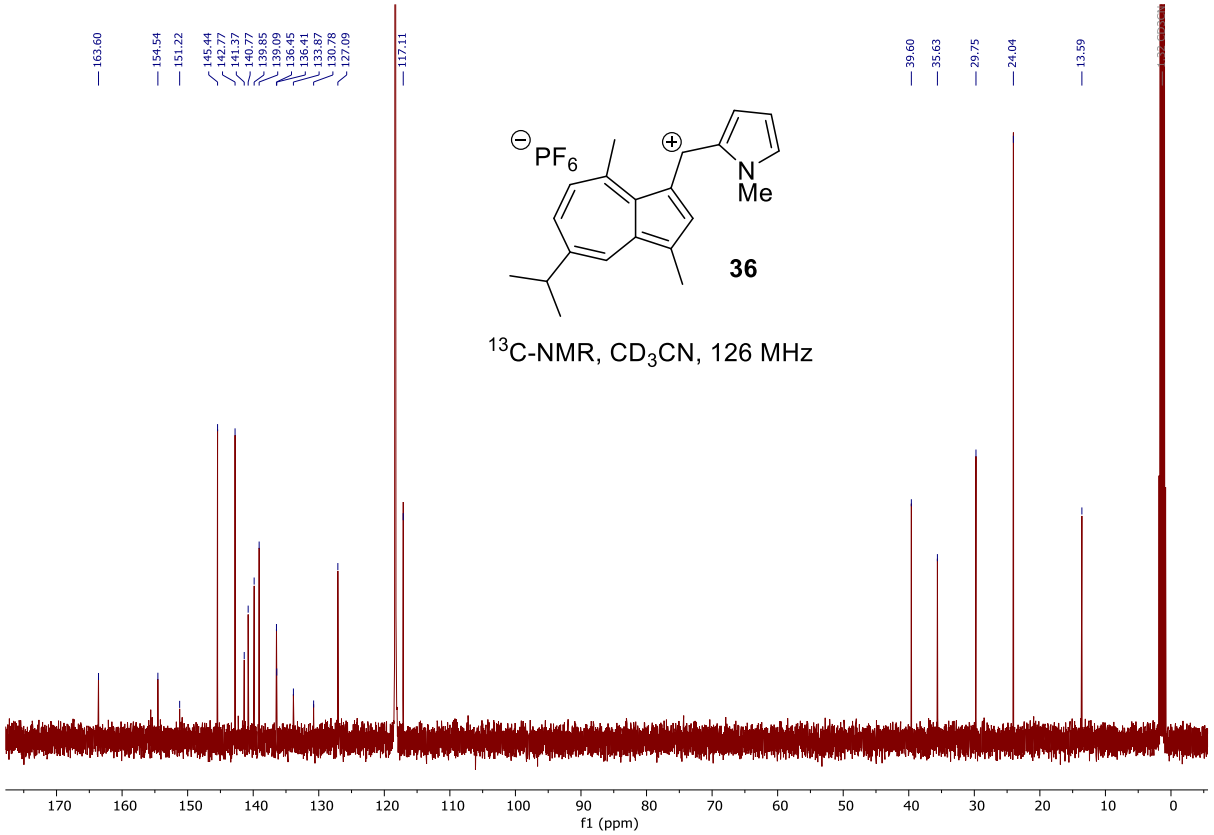
35

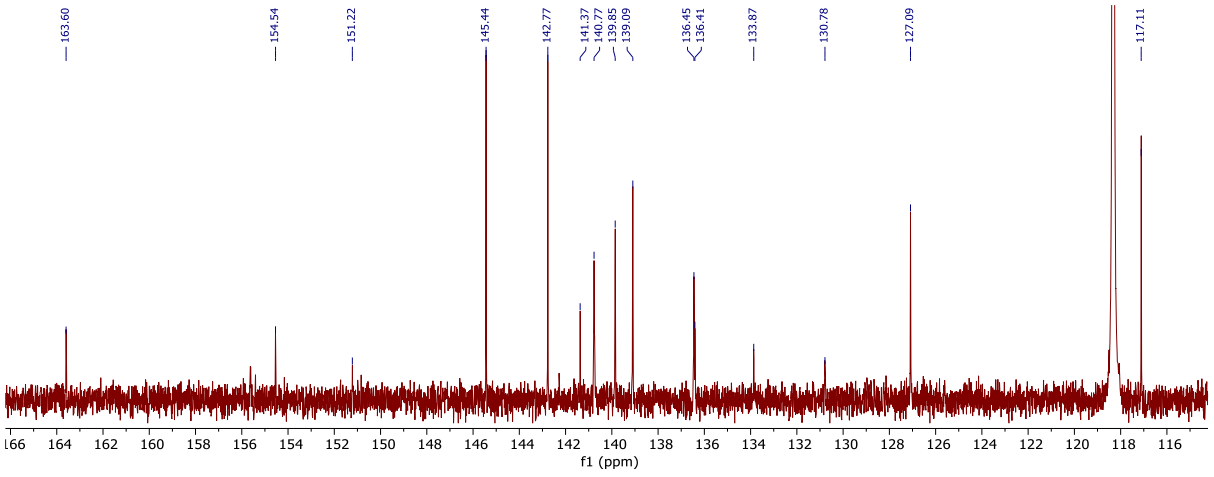

x10 6
+ESI Scan (rt: 0.63-0.81 min, 12 scans) Frag=125.0V JH471-new_Pos_LoopInjection_MS_32421.d
441.2982
301.1418
722.5278
859.6061
614.3516
922.0096
Counts vs. Mass-to-Charge (m/z)

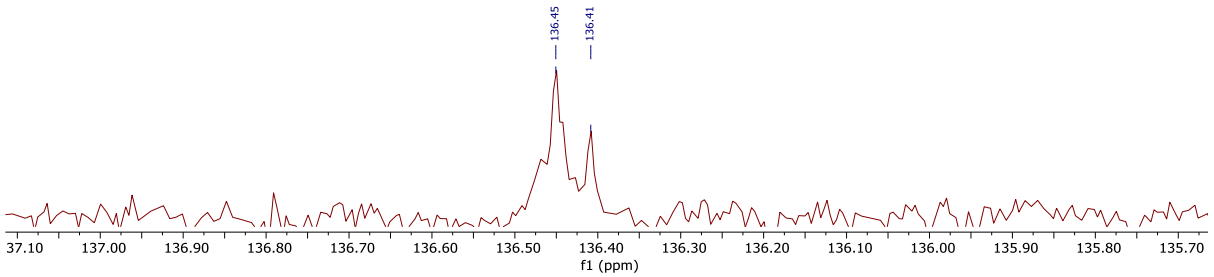

%T
cm-1
3129.06cm-1, 76.36%T
945.12cm-1, 76.95%T
911.54cm-1, 74.97%T
1524.25cm-1, 71.32%T
875.31cm-1, 68.26%T
1466.74cm-1, 65.77%T
896.53cm-1, 64.88%T
1171.74cm-1, 62.55%T
1138.09cm-1, 61.66%T
1429.82cm-1, 60.02%T
978.60cm-1, 60.45%T
1100.83cm-1, 57.21%T
1158.01cm-1, 65.11%T
675.01cm-1, 56.26%T
1496.63cm-1, 52.03%T
610.85cm-1, 50.00%T
1224.57cm-1, 42.91%T
1076.24cm-1, 41.08%T
1376.23cm-1, 38.09%T
1394.11cm-1, 36.35%T
1293.01cm-1, 35.46%T
1566.81cm-1, 38.66%T
733.61cm-1, 33.65%T
1342.31cm-1, 30.82%T
651.82cm-1, 30.83%T
750.84cm-1, 25.79%T
1040.41cm-1, 26.33%T
828.04cm-1, 6.54%T
818.68cm-1, 6.48%T
803.29cm-1, 12.63%T
Name
Description
iruser1 8587
Sample 8587 By iruser1 Date Friday, November 18 2022

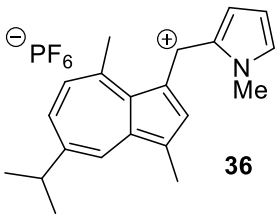

8.60
8.60
8.53
8.53
8.53
8.27
8.27
8.19
8.19
7.62
7.61
7.61
7.60
7.55
7.55
6.66
6.66
6.65
6.65
6.65
6.65
6.64
6.64
3.92
3.92
3.44
3.43
3.41
3.41
3.40
3.39
3.37
3.36
3.34
3.33
2.59
2.59
2.59
1.94 CD3CN
1.44
1.43
PF6
N
Me
36
1H-NMR, CD3CN, 500 MHz
1.07
1.06
1.02
2.01
1.11
0.86
1.01
3.00
1.20
3.22
3.12
6.76
f1 (ppm)


8.60
8.60
8.53
8.53
8.53
8.27
8.27
8.19
8.19
7.62
7.61
7.61
7.60
7.55
7.55
6.66
6.66
6.65
6.65
6.65
6.65
6.64
6.64
1.07
1.06
1.02
2.01
1.11
0.86
1.01
f1 (ppm)


163.60
154.54
151.22
145.44
142.77
141.37
140.77
139.85
139.09
136.45
136.41
133.87
130.78
127.09
117.11
39.60
35.63
29.75
24.04
13.59
PF6
N
Me
36
13C-NMR, CD3CN, 126 MHz
f1 (ppm)

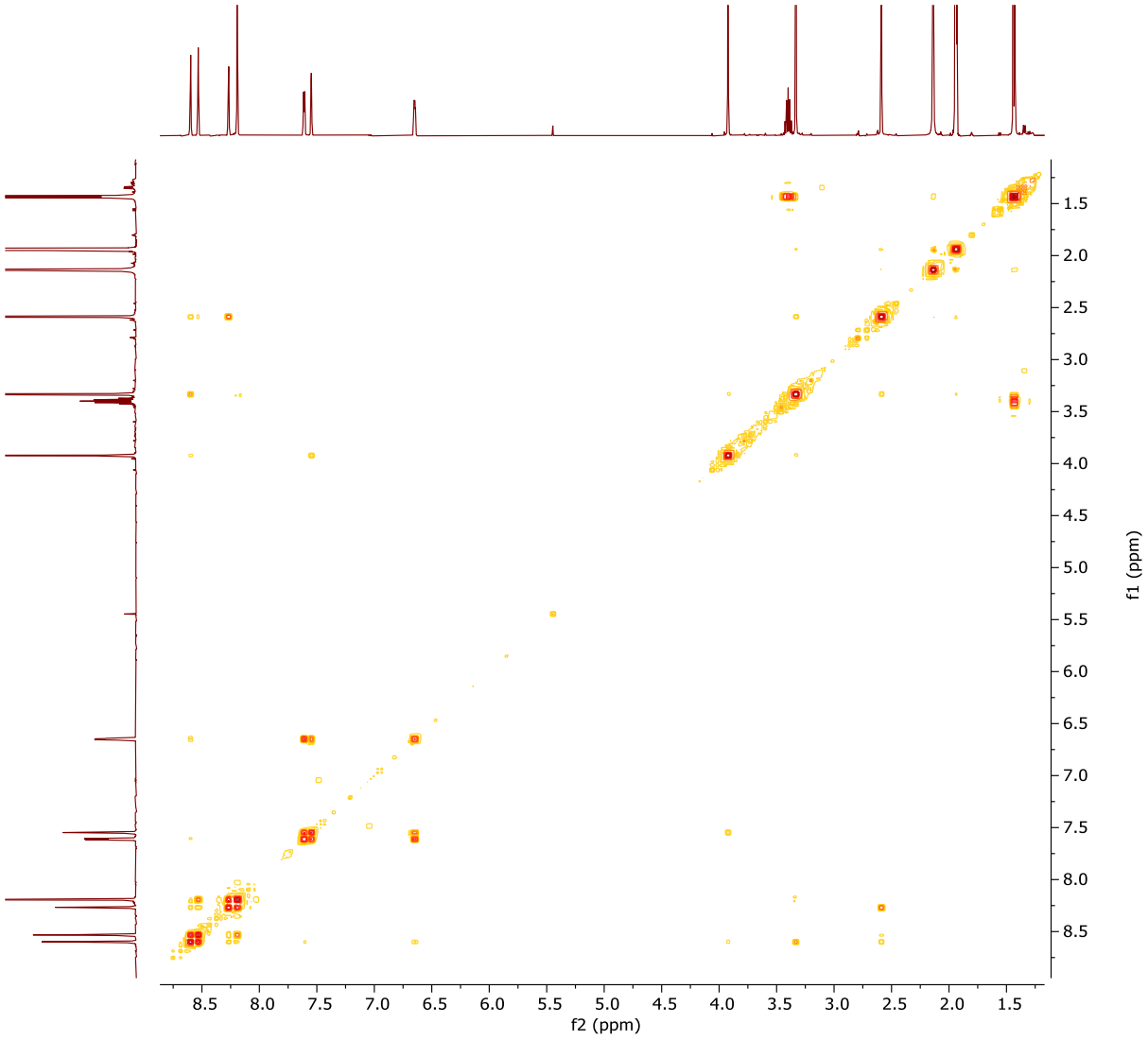

163.60
154.54
151.22
145.44
142.77
141.37
140.77
139.85
139.09
136.45
136.41
133.87
130.78
127.09
117.11
f1 (ppm)

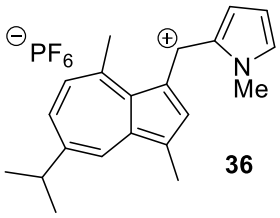

136.45
136.41
f1 (ppm)



36

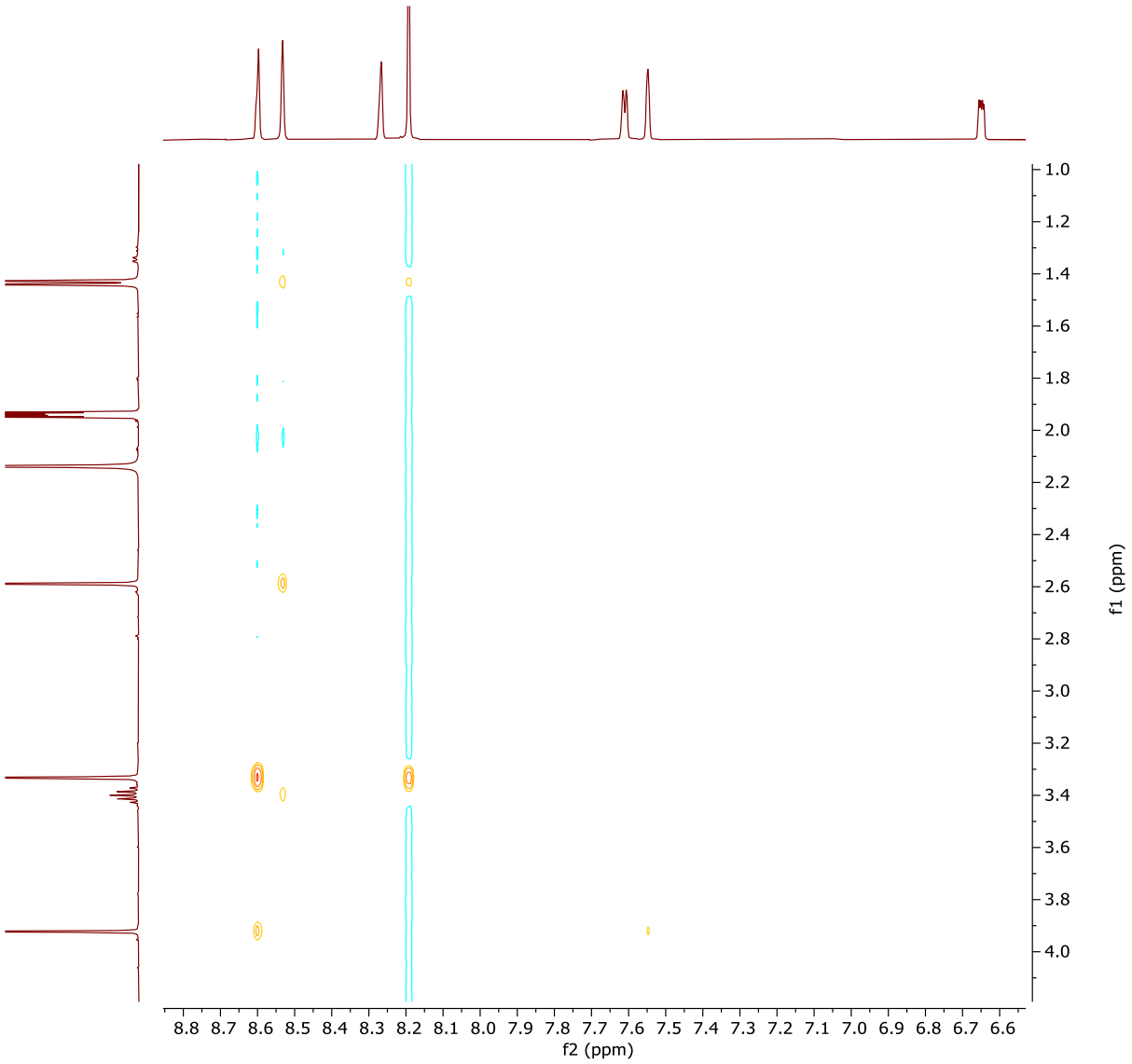
COSY, CD_3CN

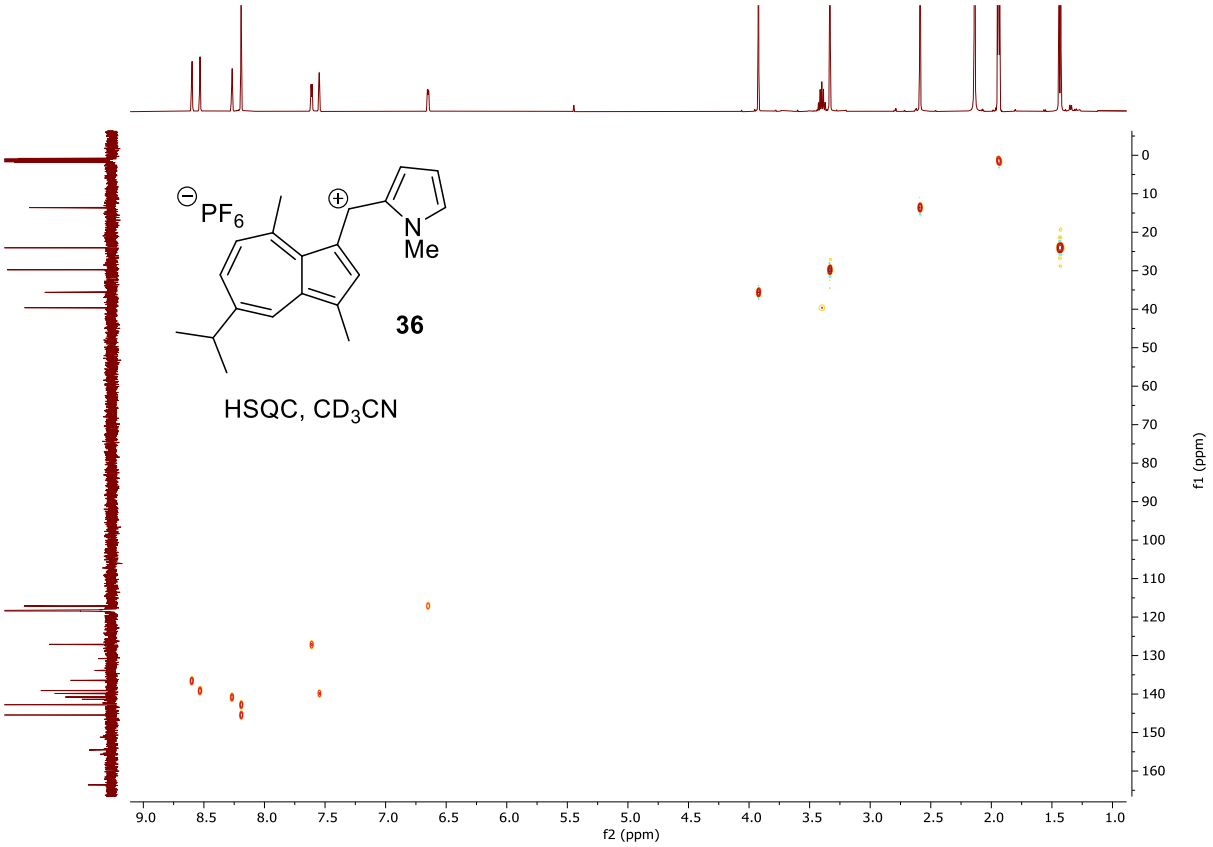


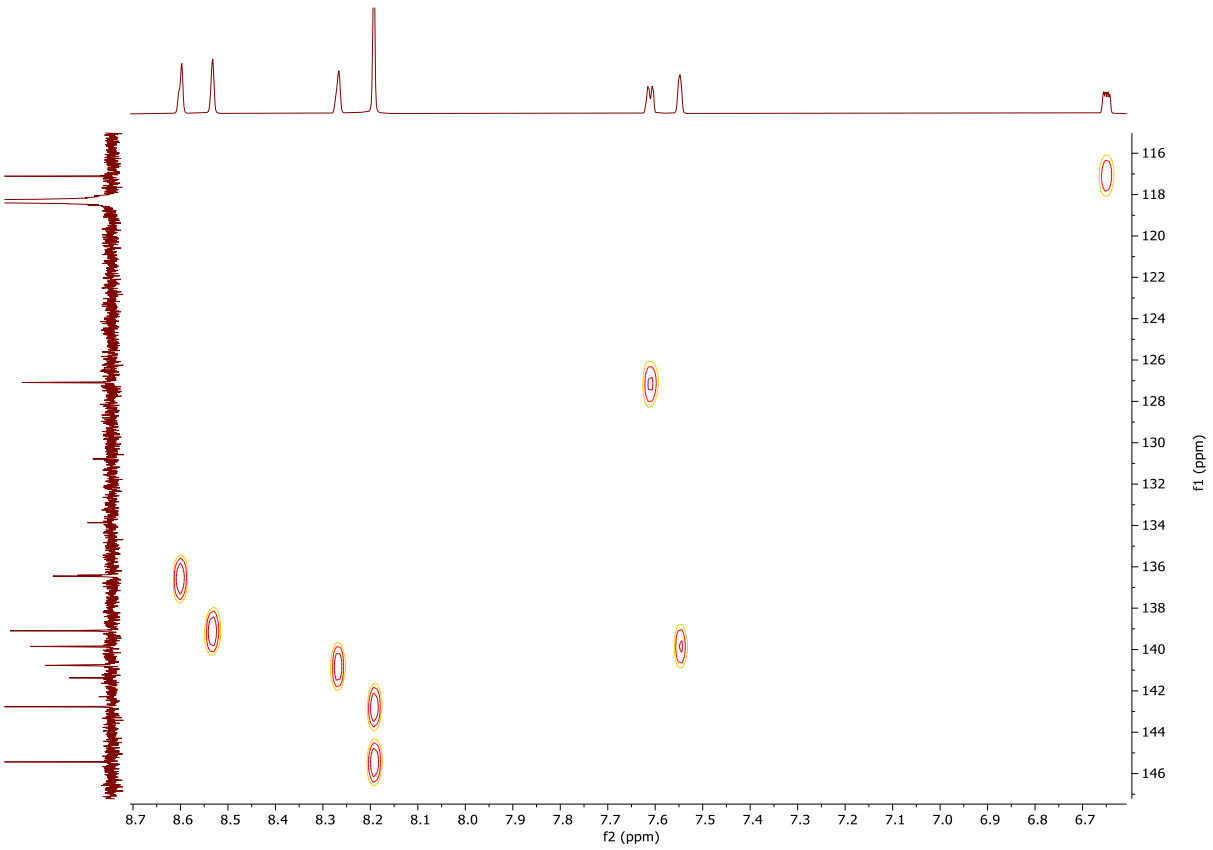


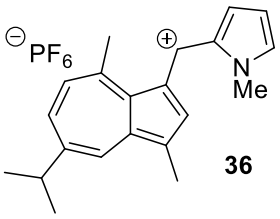
36

NOESY, CD_3CN



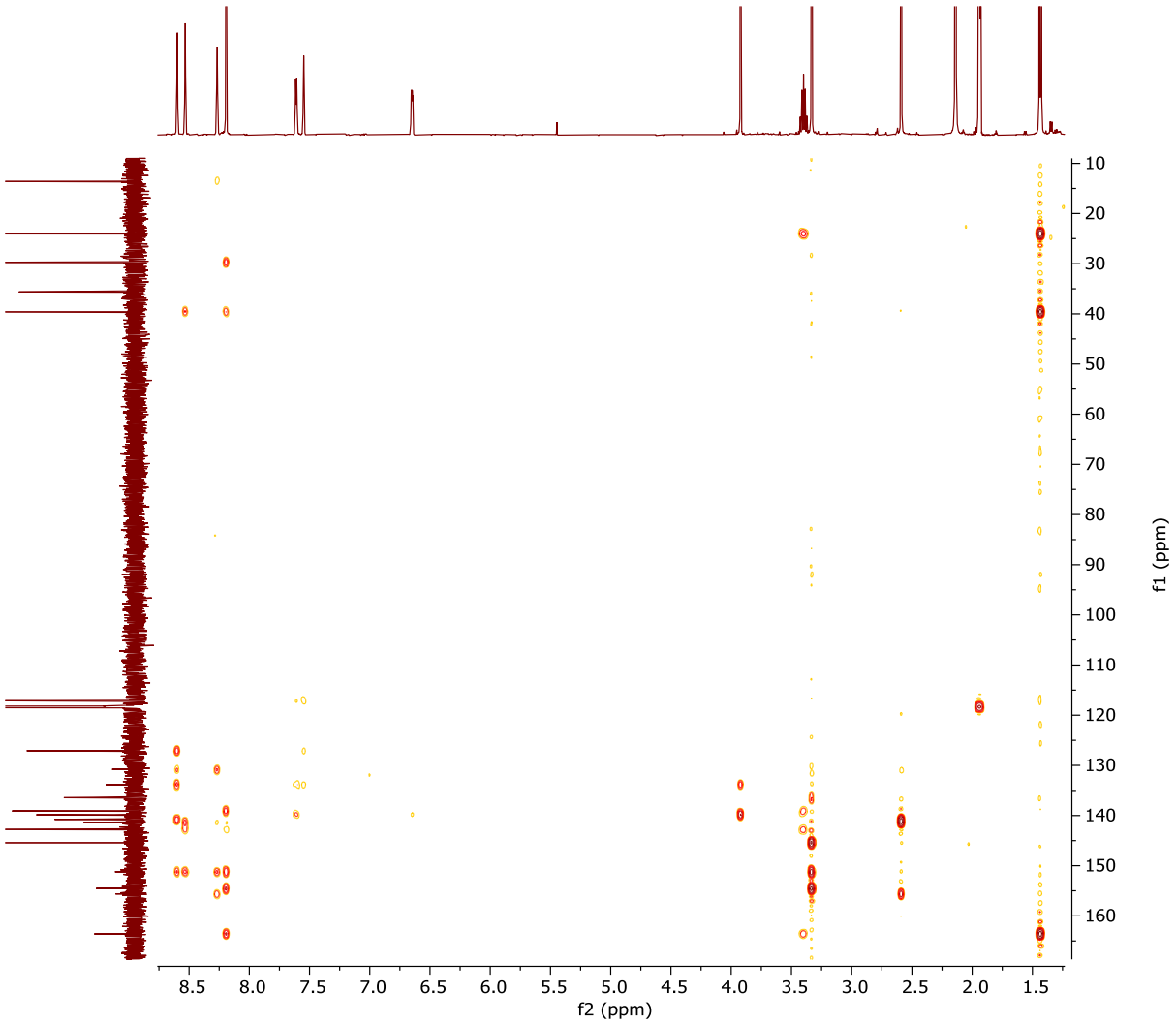

PF6
N
Me
36
HSQC, CD3CN
f2 (ppm)
f1 (ppm)

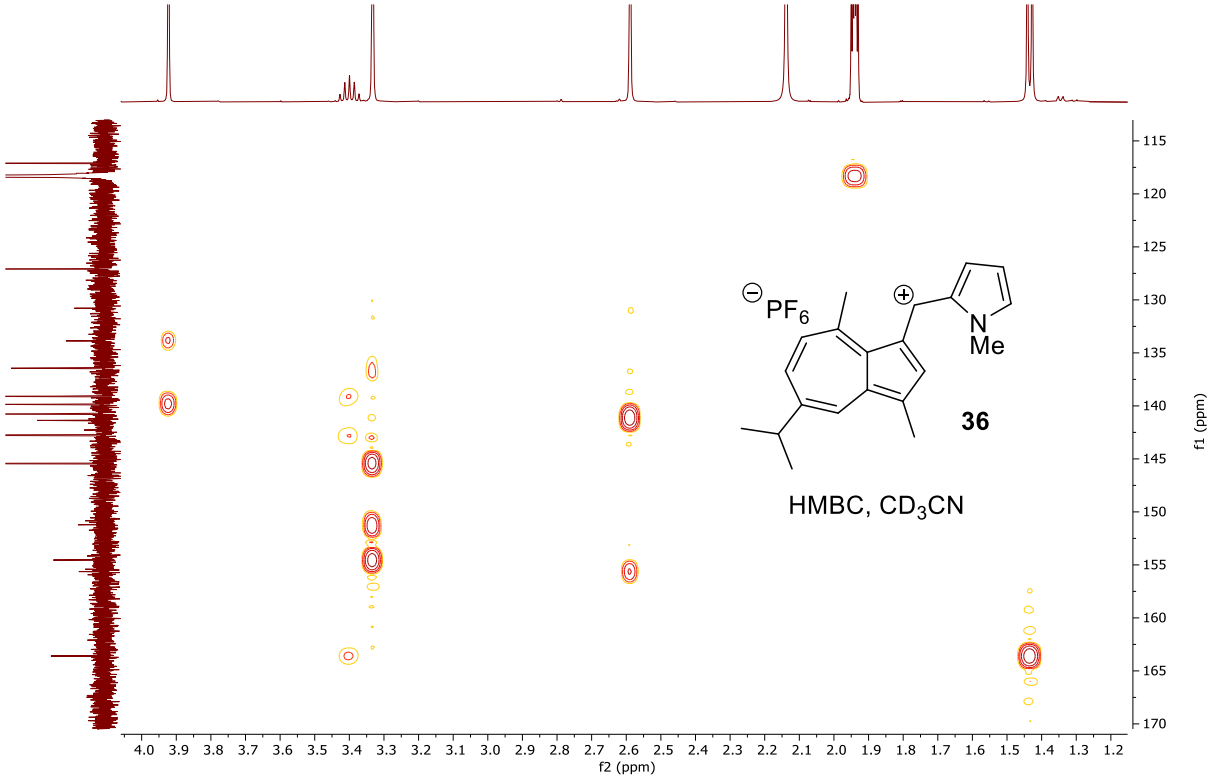

f2 (ppm)
f1 (ppm)

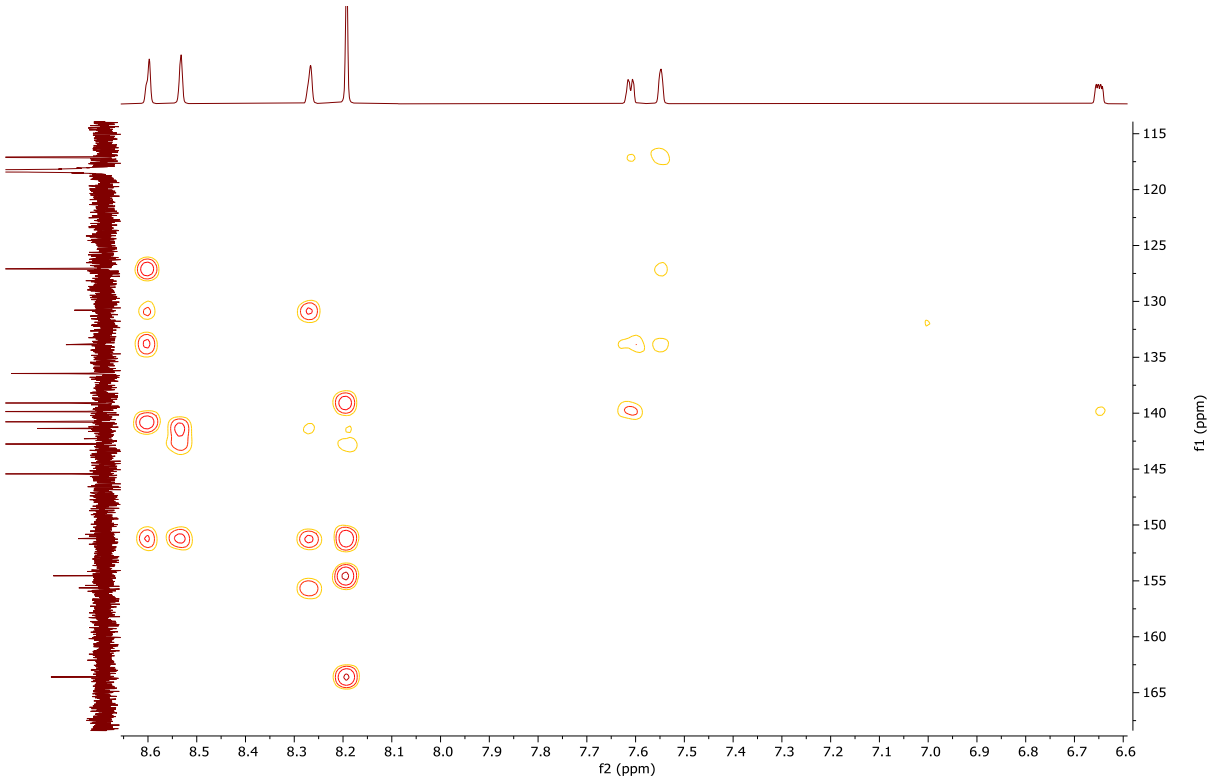


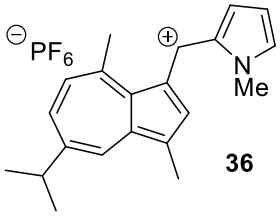
36

HMBC, CD_3CN

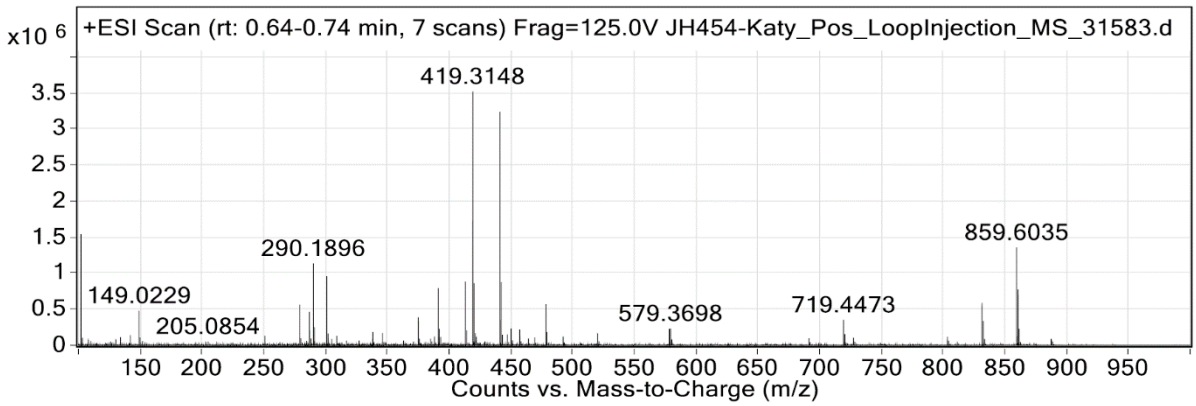


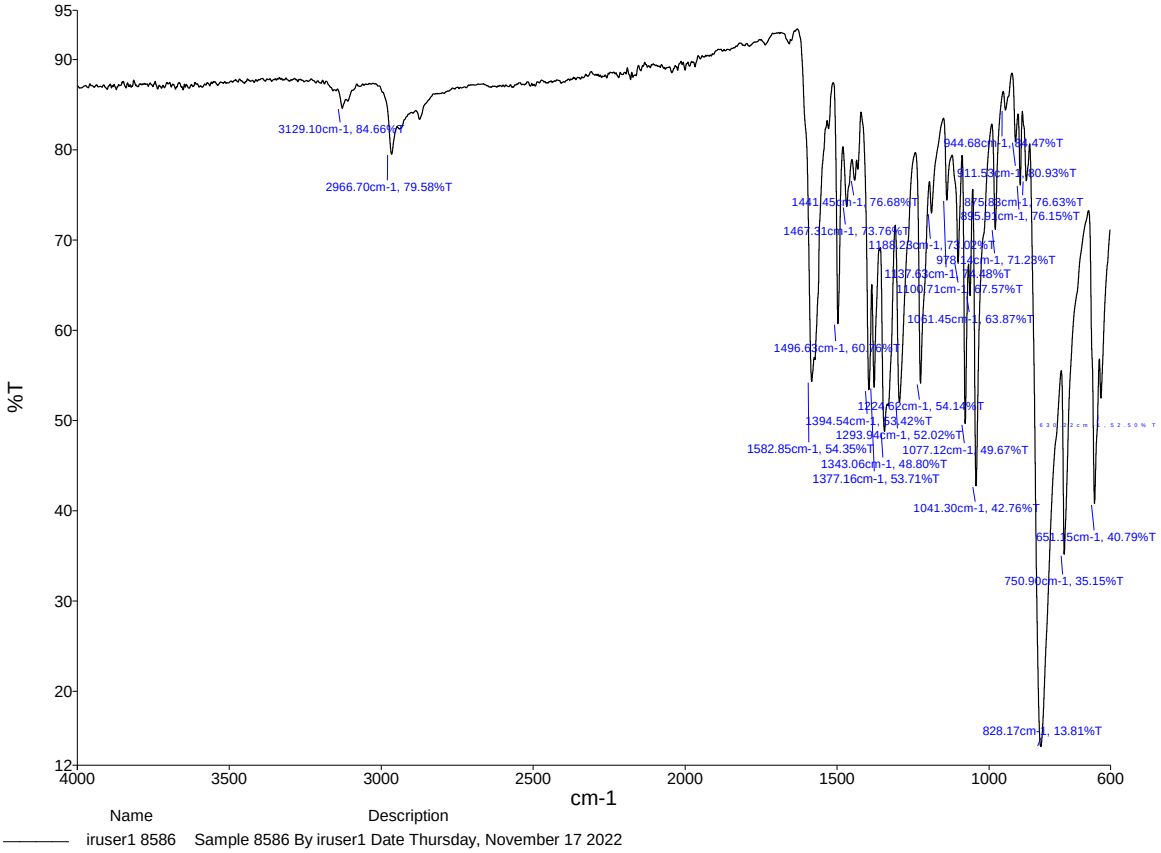

PF6
N
Me
36
HMBC, CD3CN
f1 (ppm)
f2 (ppm)


f1 (ppm)
f2 (ppm)



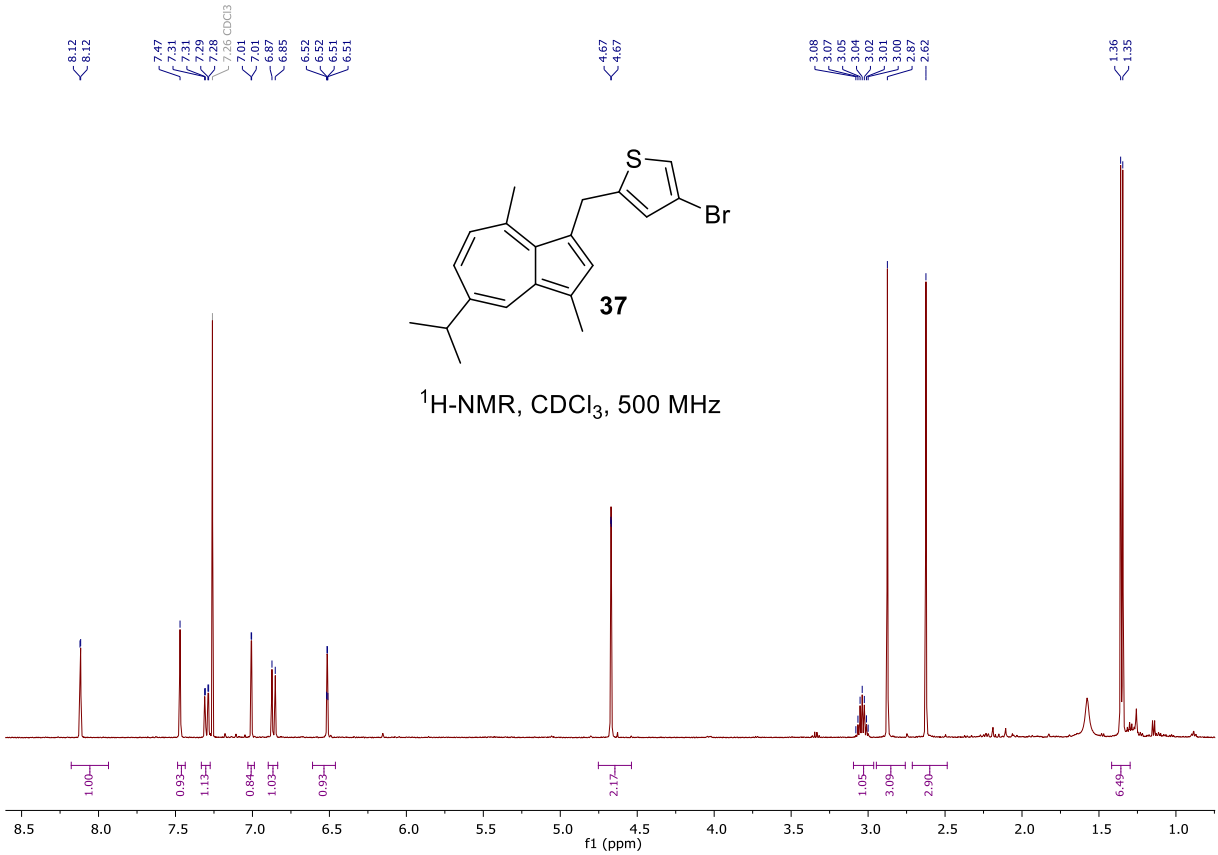
36

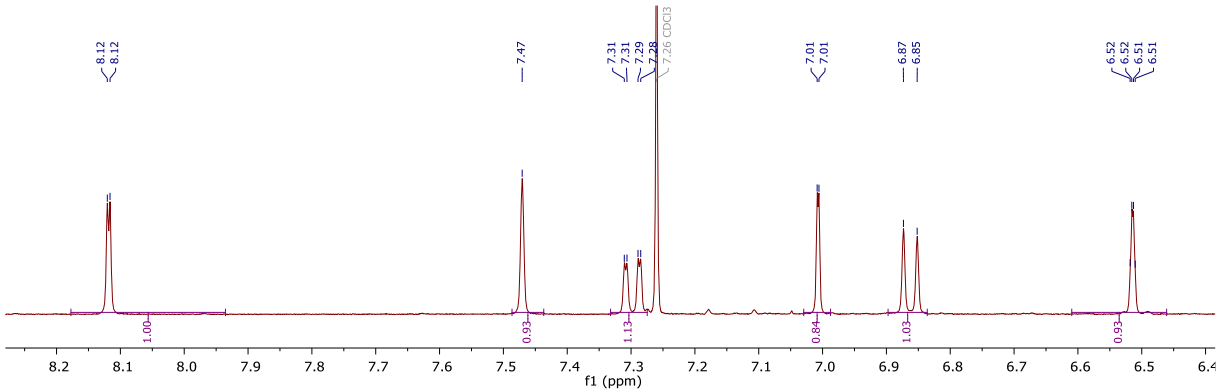


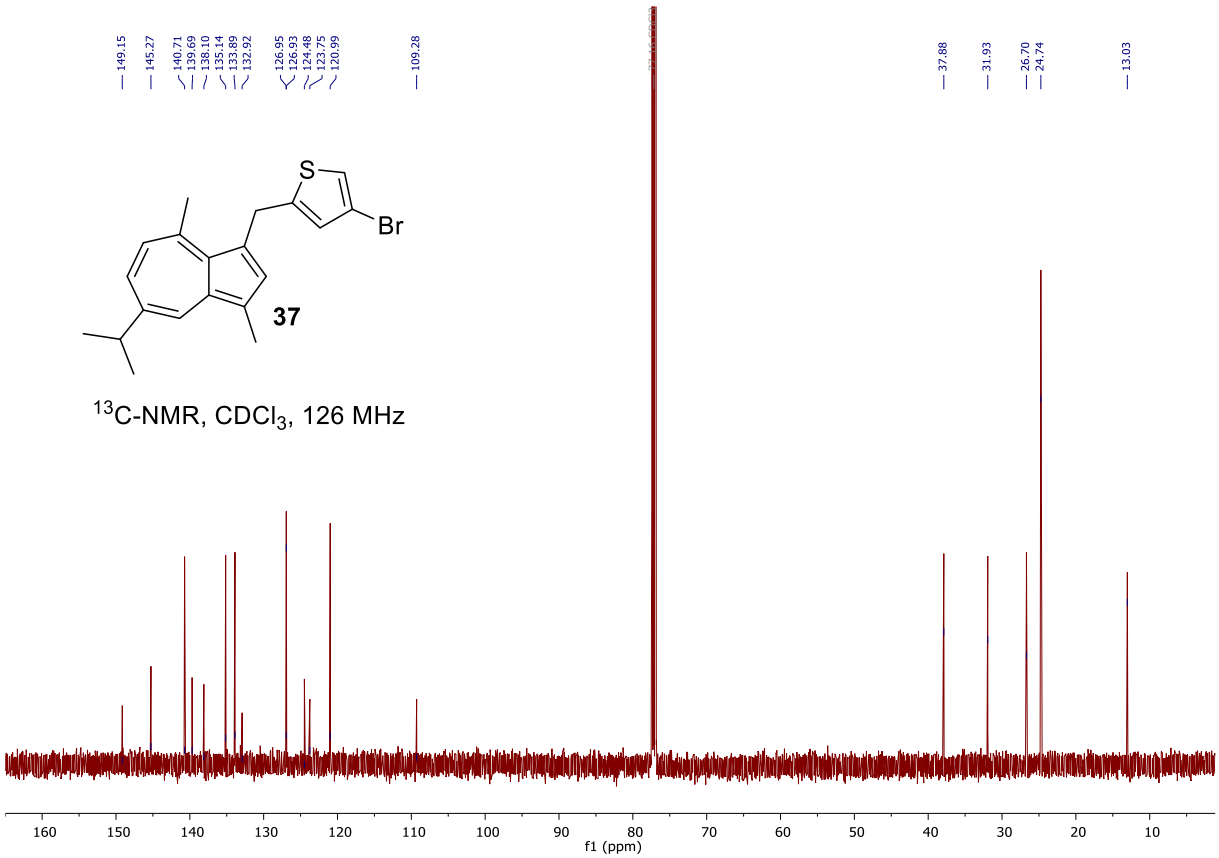


Name Description

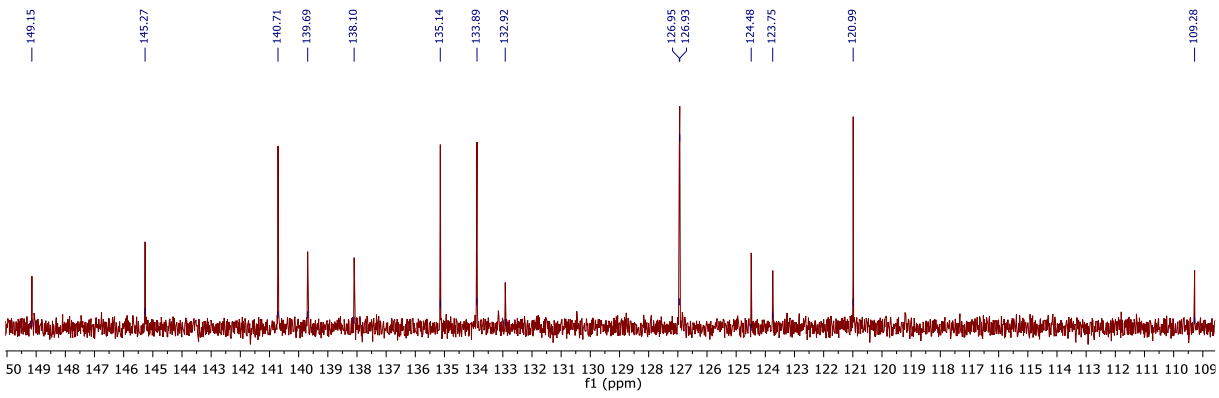
iruser1 8586 Sample 8586 By iruser1 Date Thursday, November 17 2022

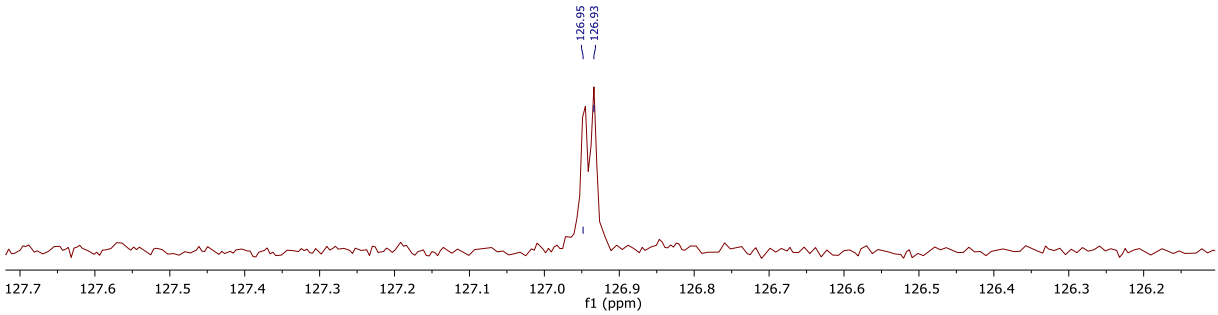

8.12
8.12
7.47
7.31
7.31
7.29
7.28
7.26 CDCl3
7.01
7.01
6.87
6.85
6.52
6.52
6.51
6.51
4.67
4.67
3.08
3.07
3.05
3.04
3.02
3.01
3.00
2.87
2.62
1.36
1.35
S
Br
37
1H-NMR, CDCl3, 500 MHz
1.00
0.93
1.13
0.84
1.03
0.93
2.17
1.05
3.09
2.90
6.49
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

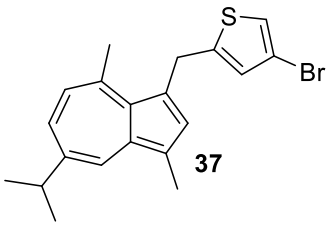

8.12
8.12
7.47
7.31
7.31
7.29
7.28
7.26 CDCl3
7.01
7.01
6.87
6.85
6.52
6.52
6.51
6.51
1.00
0.93
1.13
0.84
1.03
0.93
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
f1 (ppm)



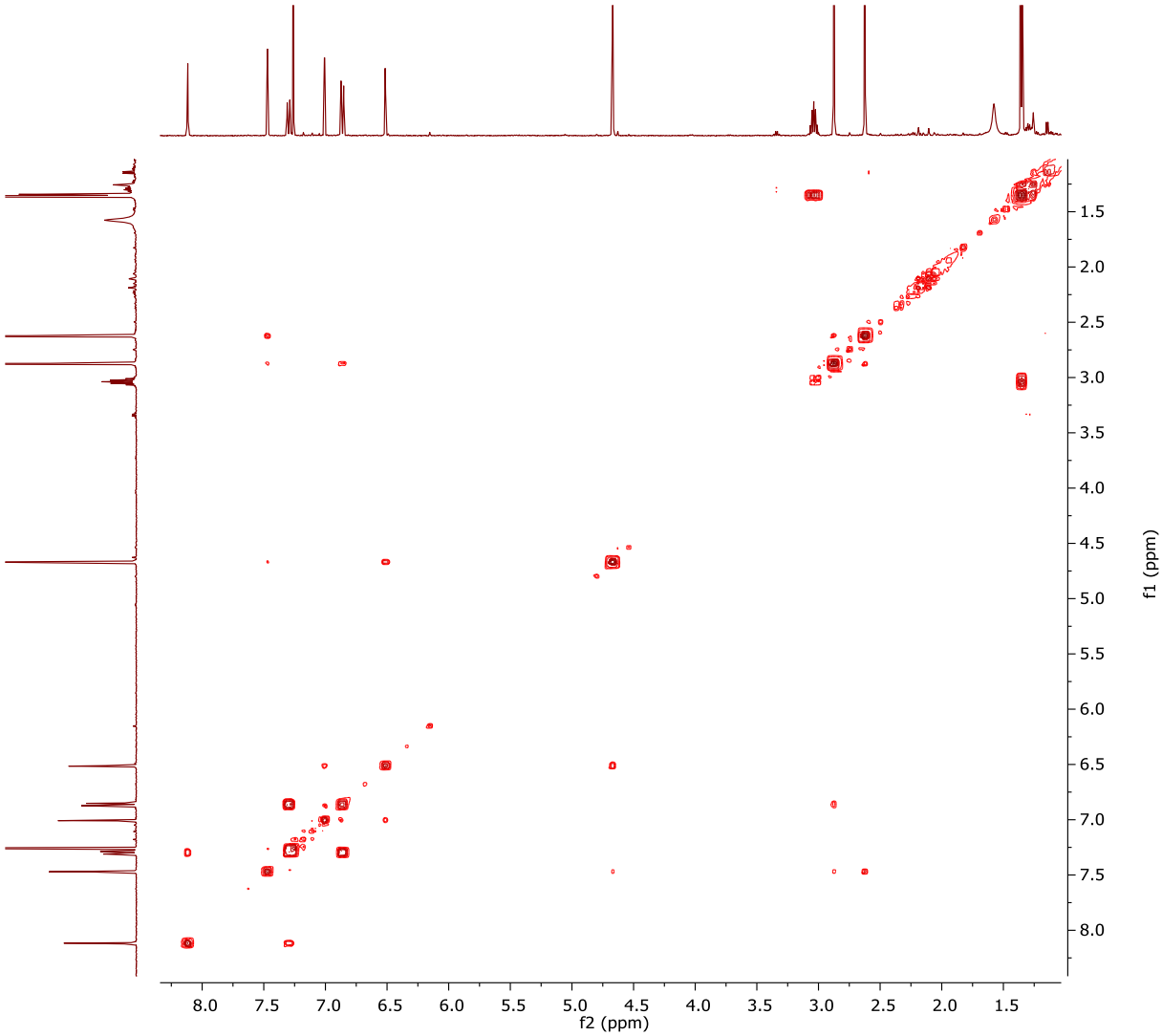
^{13}C-NMR, $CDCl_3$, 126 MHz

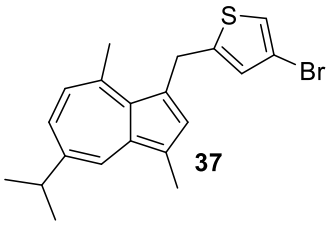





S
Br
37

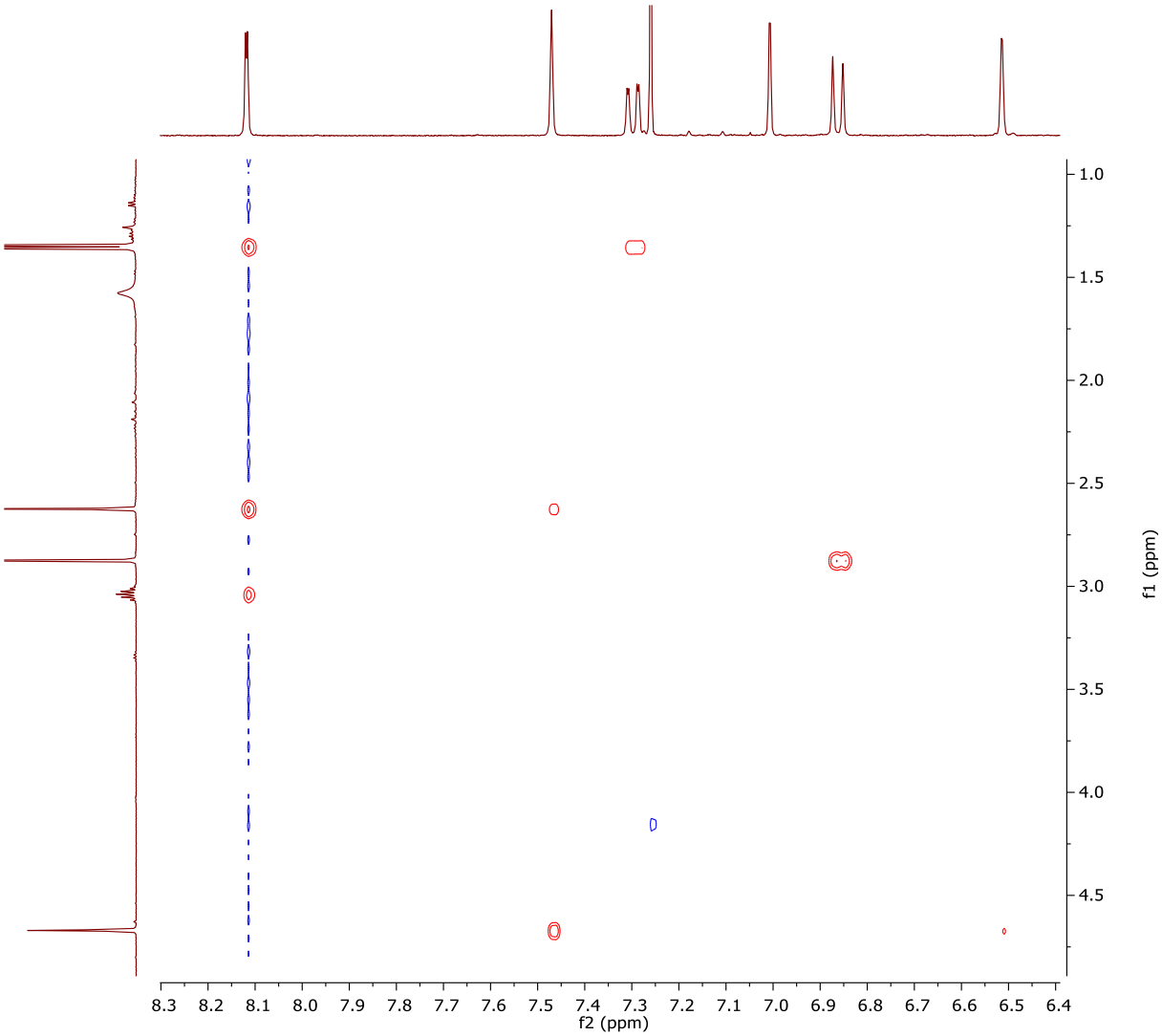
COSY, $CDCl_3$

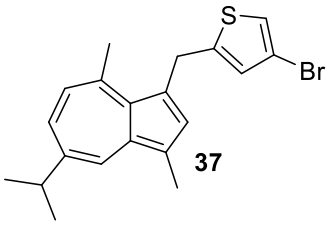

8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
f1 (ppm)



37

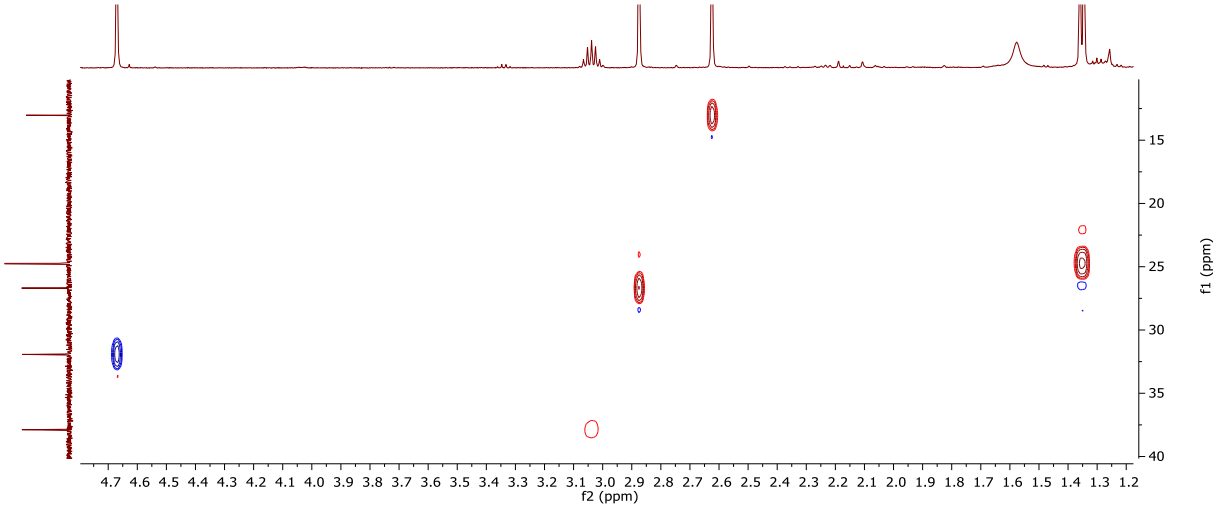
NOESY, $CDCl_3$

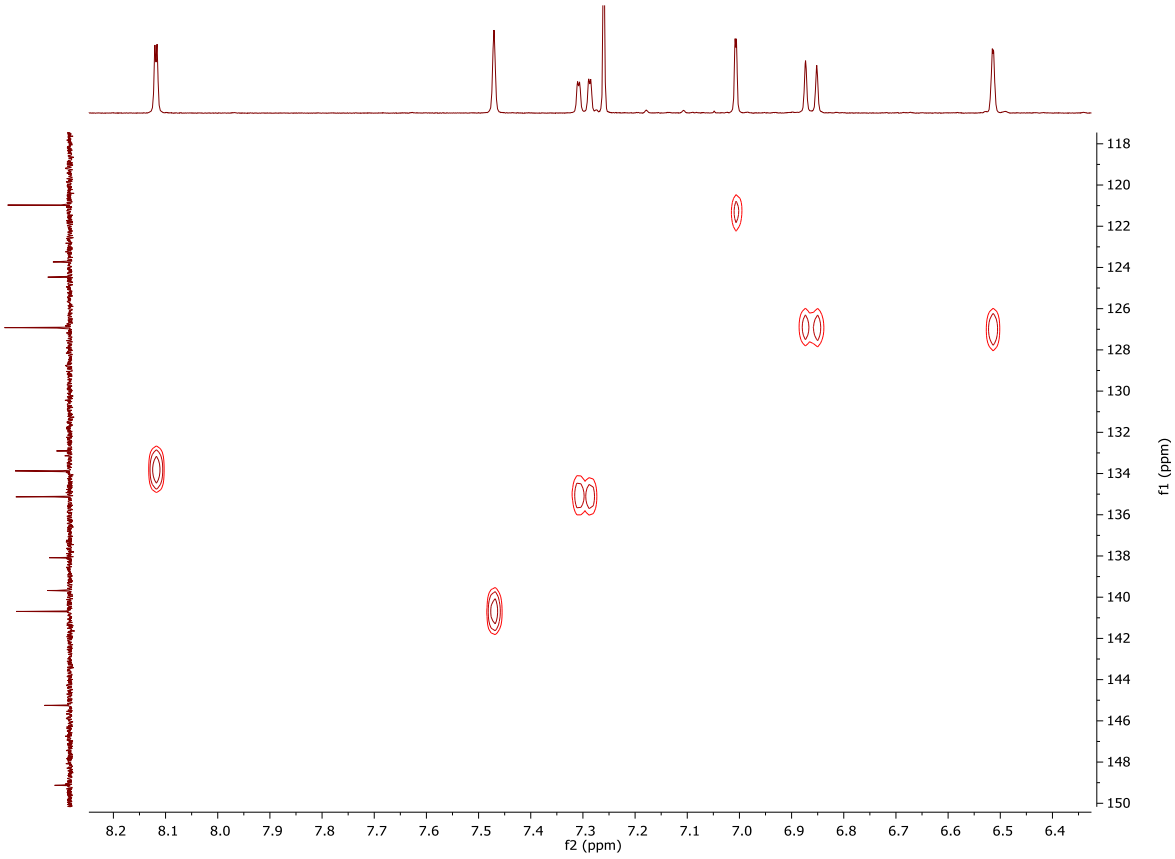


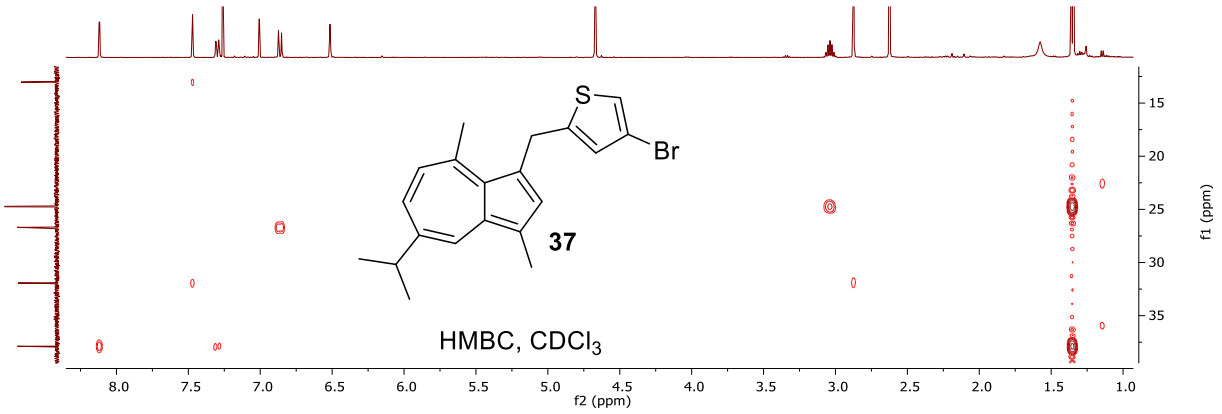


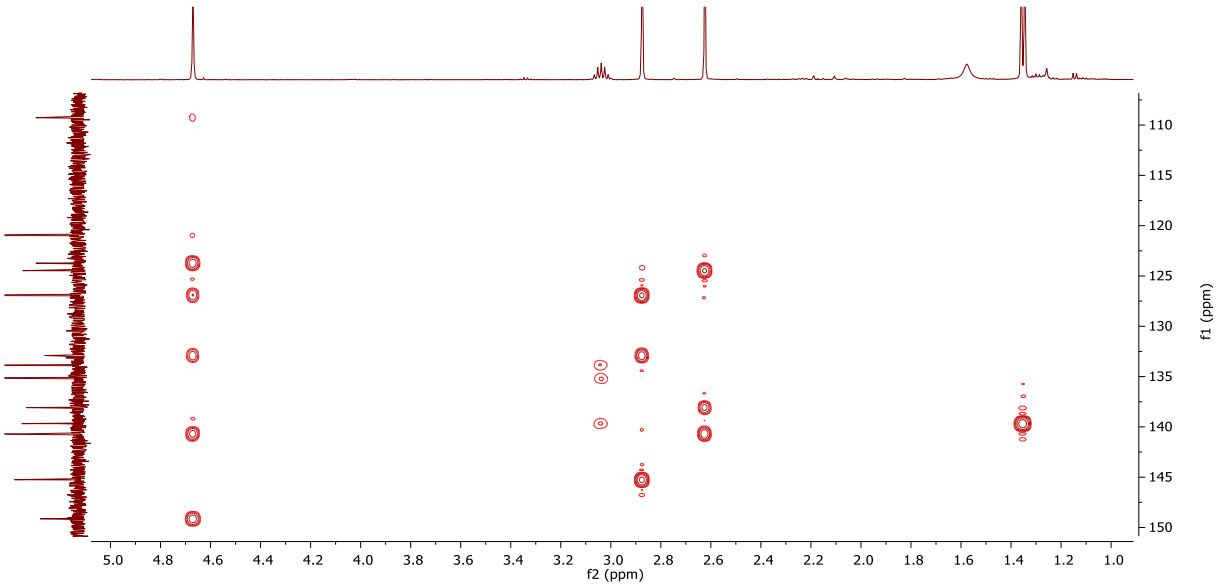
37

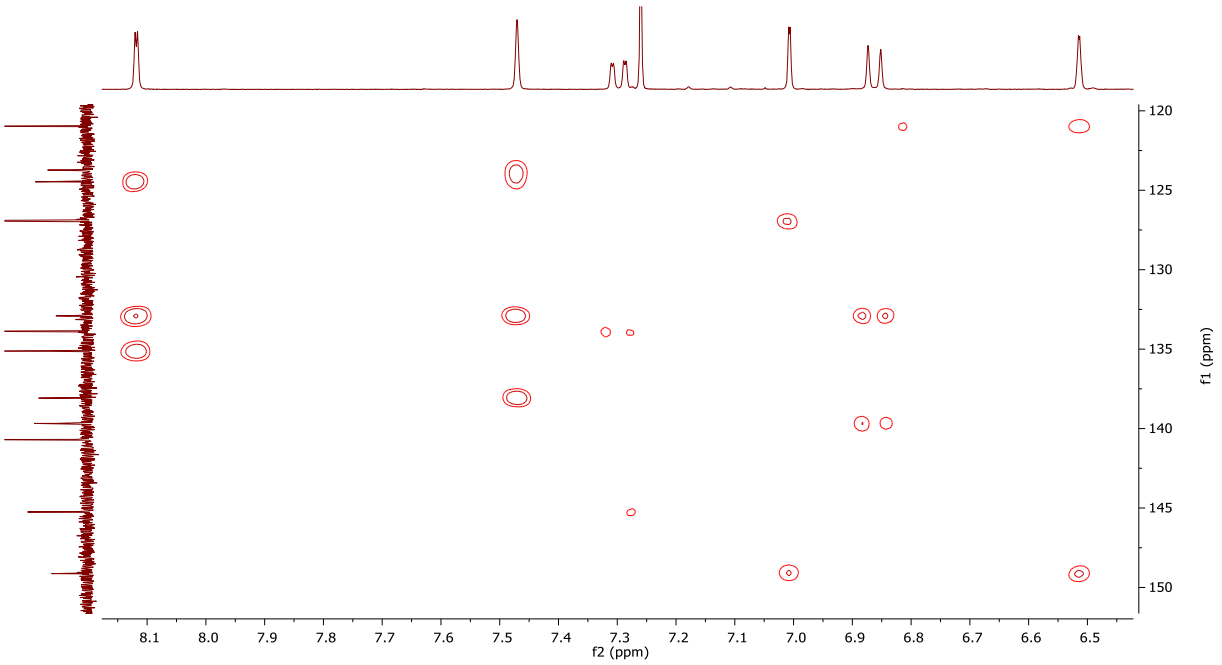
HSQC, $CDCl_3$

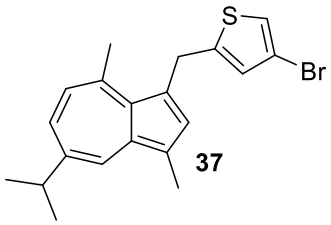




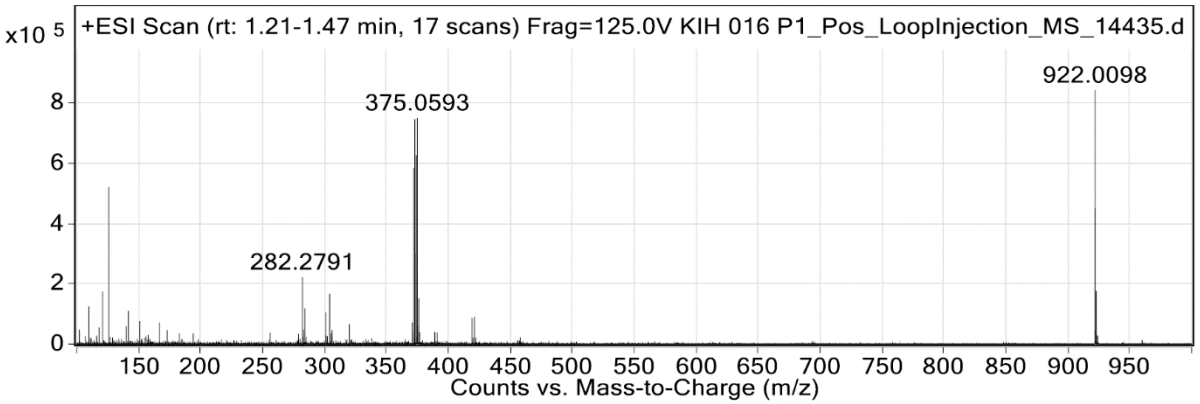

S
Br
37
HMBC, CDCl3
f2 (ppm)
f1 (ppm)

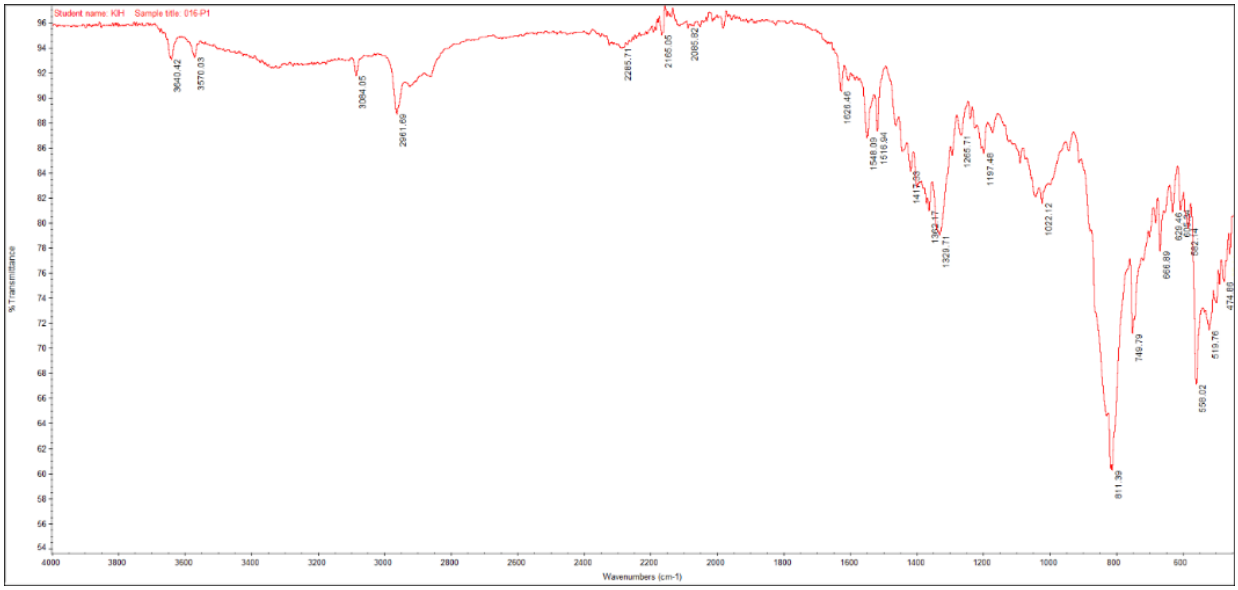

f2 (ppm)
f1 (ppm)

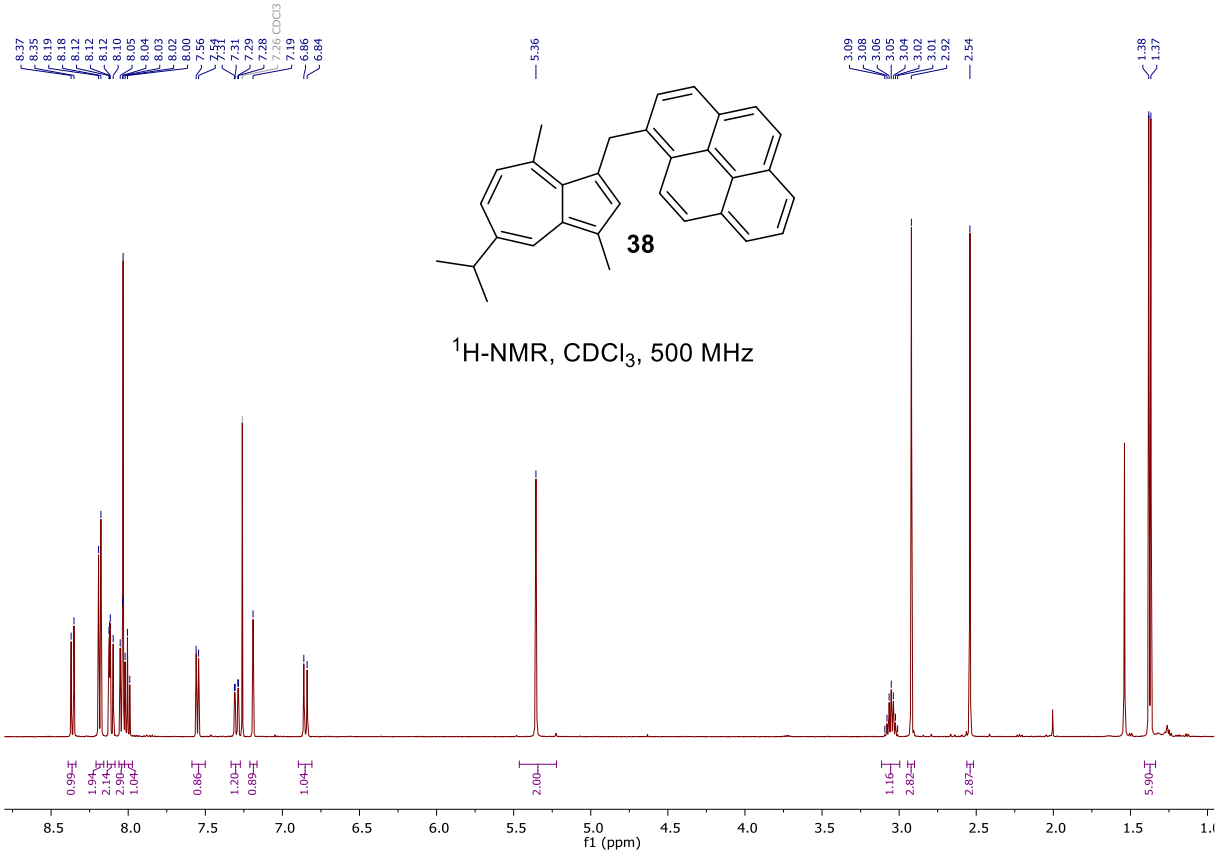

f2 (ppm)
f1 (ppm)

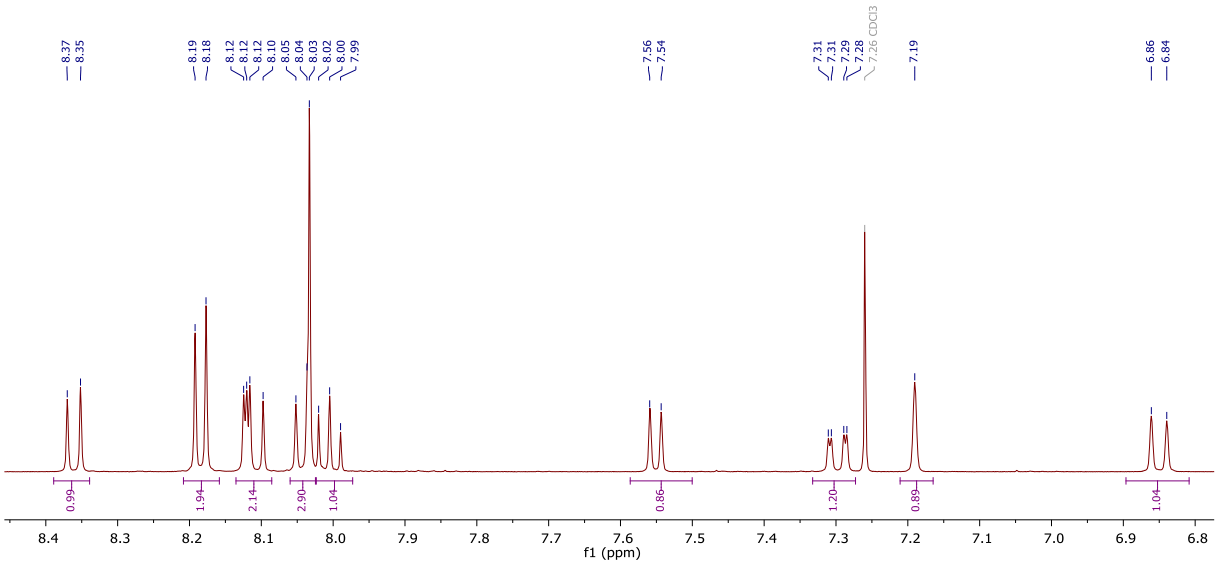

S
Br

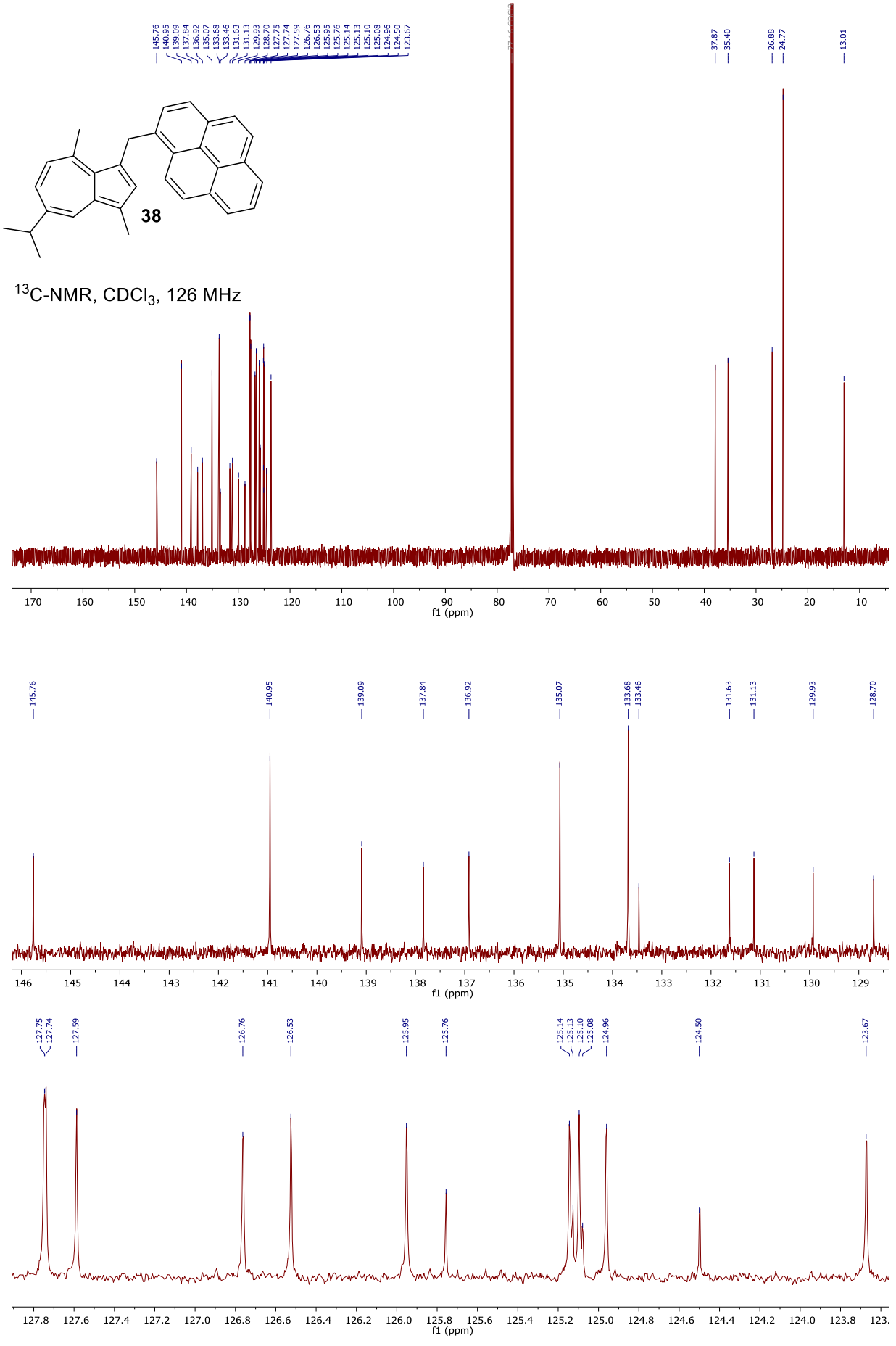
37

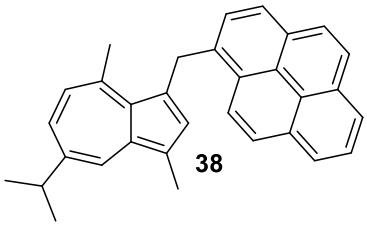

x10 5
+ESI Scan (rt: 1.21-1.47 min, 17 scans) Frag=125.0V KIH 016 P1_Pos_LoopInjection_MS_14435.d
922.0098
375.0593
282.2791
Counts vs. Mass-to-Charge (m/z)


% Transmittance
Wavenumbers (cm-1)


38
^{1}H-NMR, $CDCl_3$, 500 MHz
f1 (ppm)

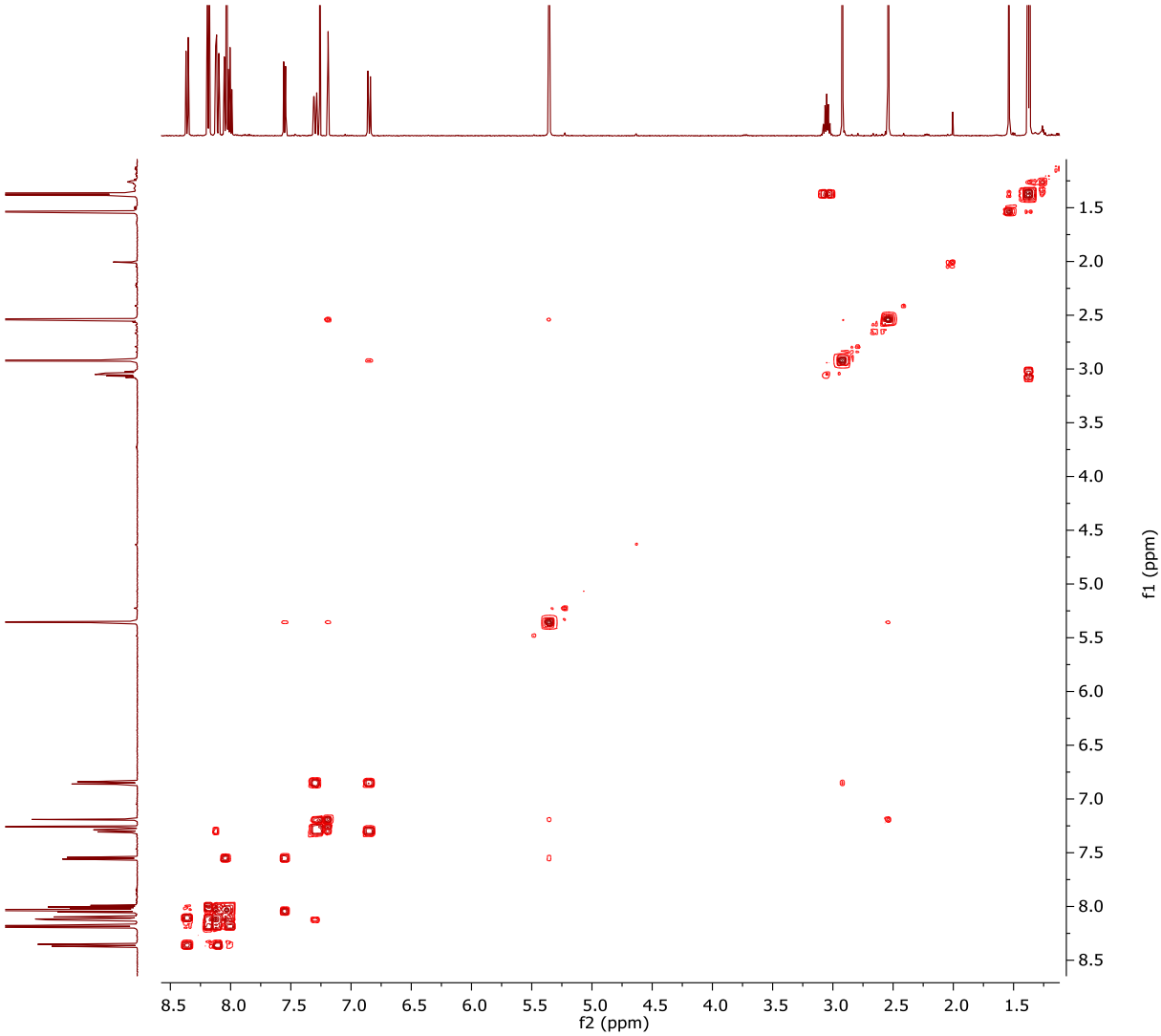

f1 (ppm)

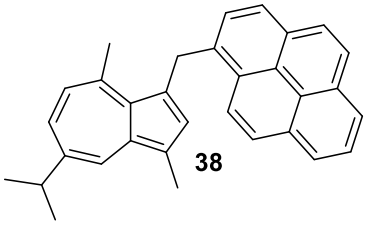

145.76
140.95
139.09
137.84
136.92
135.07
133.68
133.46
131.63
131.13
129.93
128.70
127.75
127.74
127.59
126.76
126.53
125.95
125.76
125.14
125.13
125.10
125.08
124.96
124.50
123.67
37.87
35.40
26.88
24.77
13.01
38
13C-NMR, CDCl3, 126 MHz
f1 (ppm)



38

COSY, $CDCl_3$





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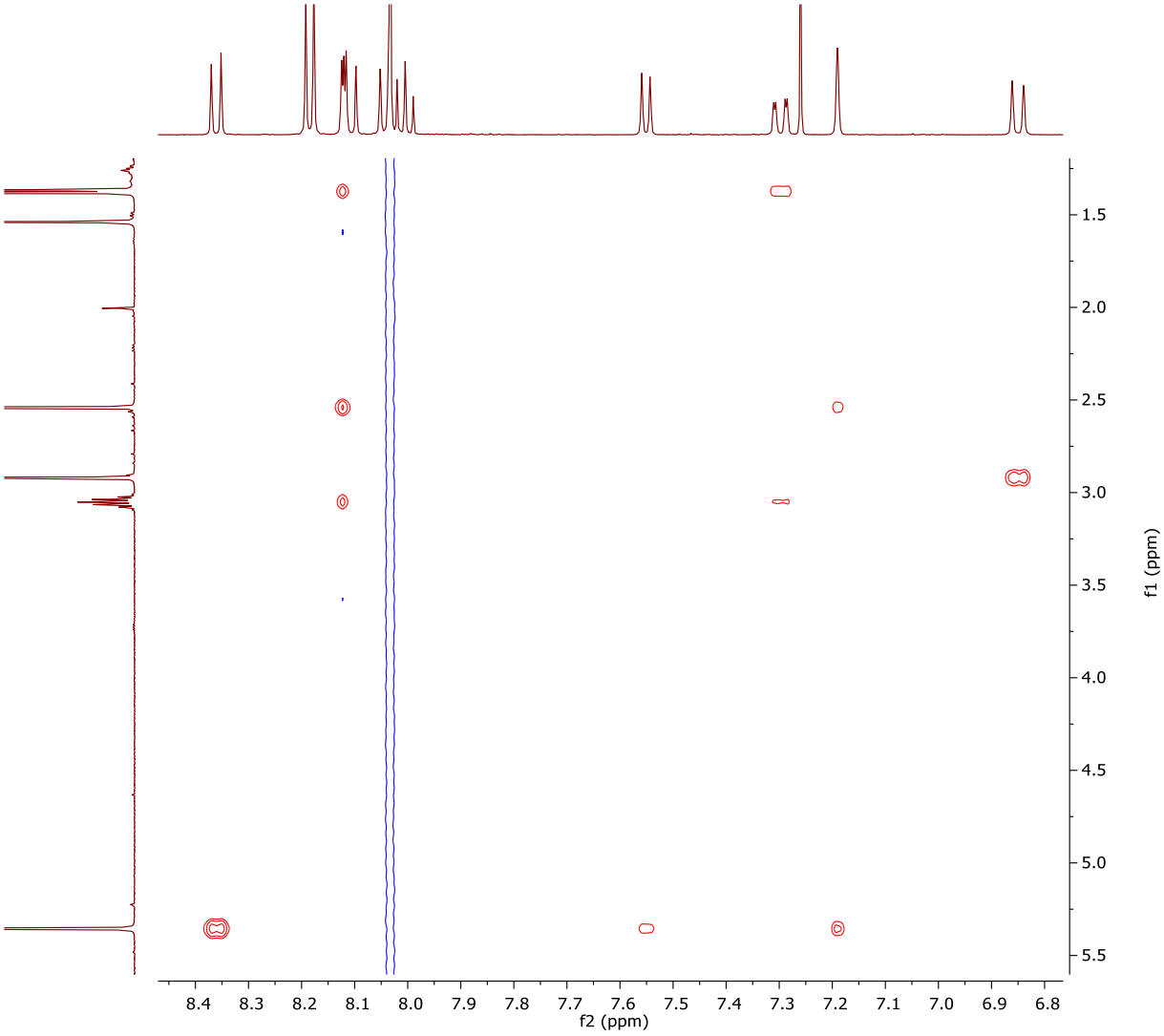
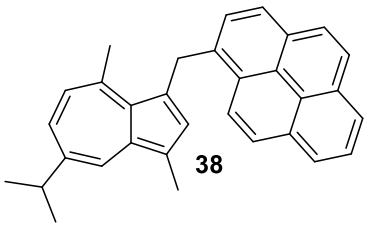
NOESY, $CDCl_3$





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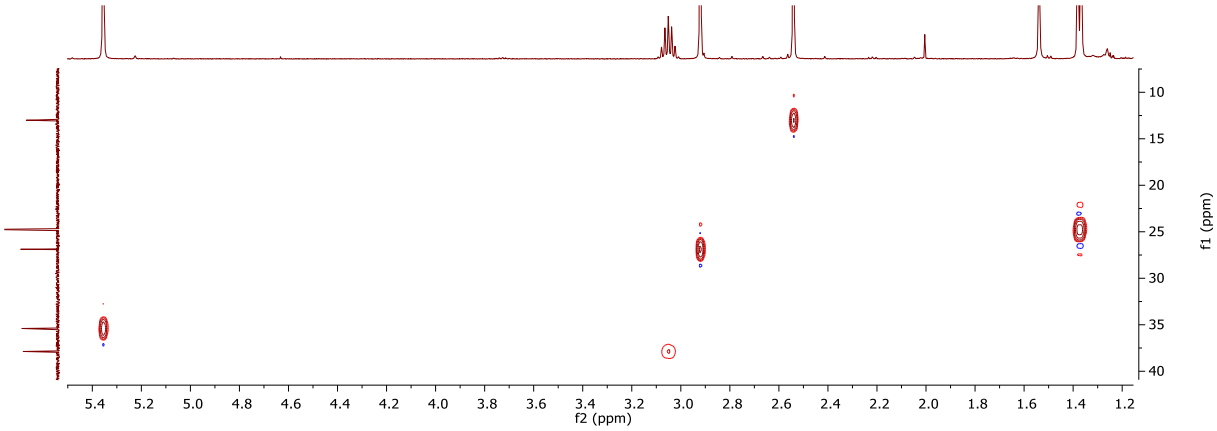
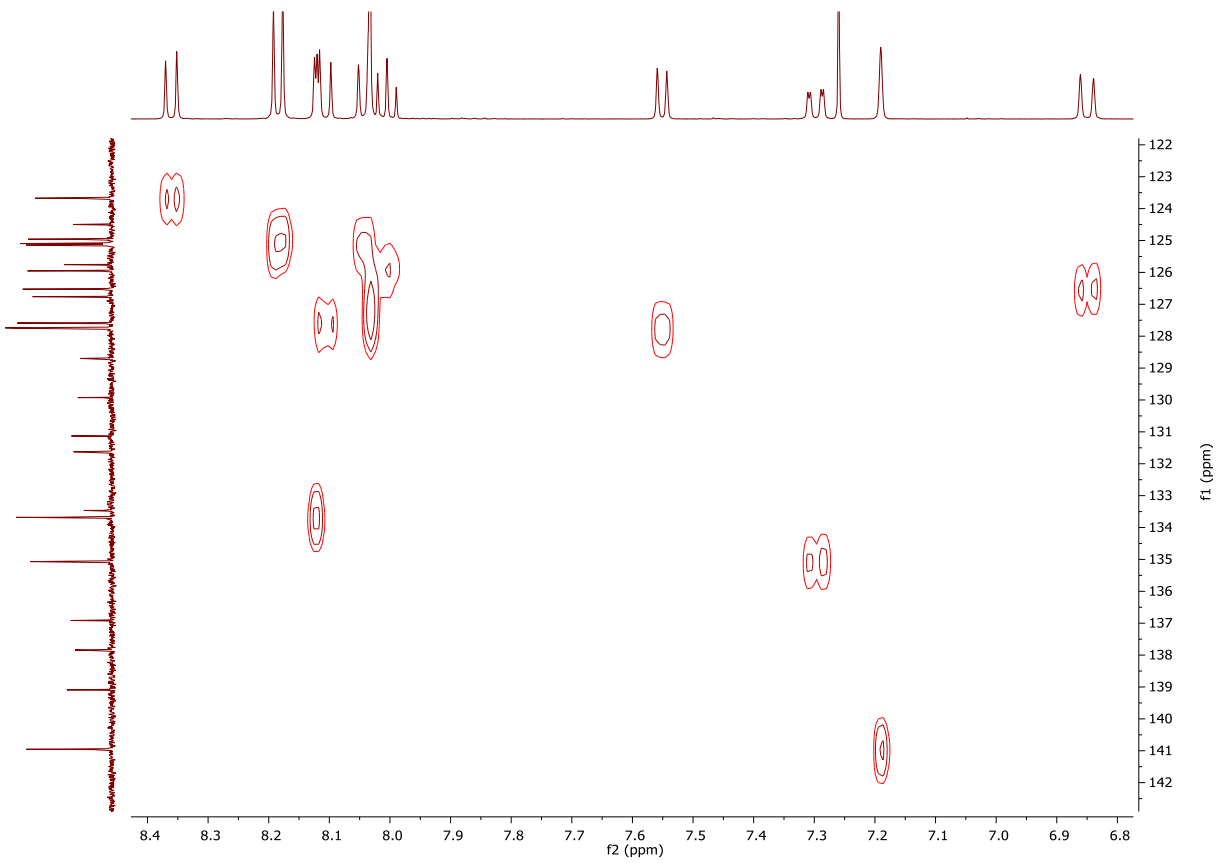
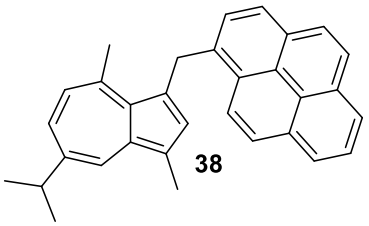
HSQC, $CDCl_3$







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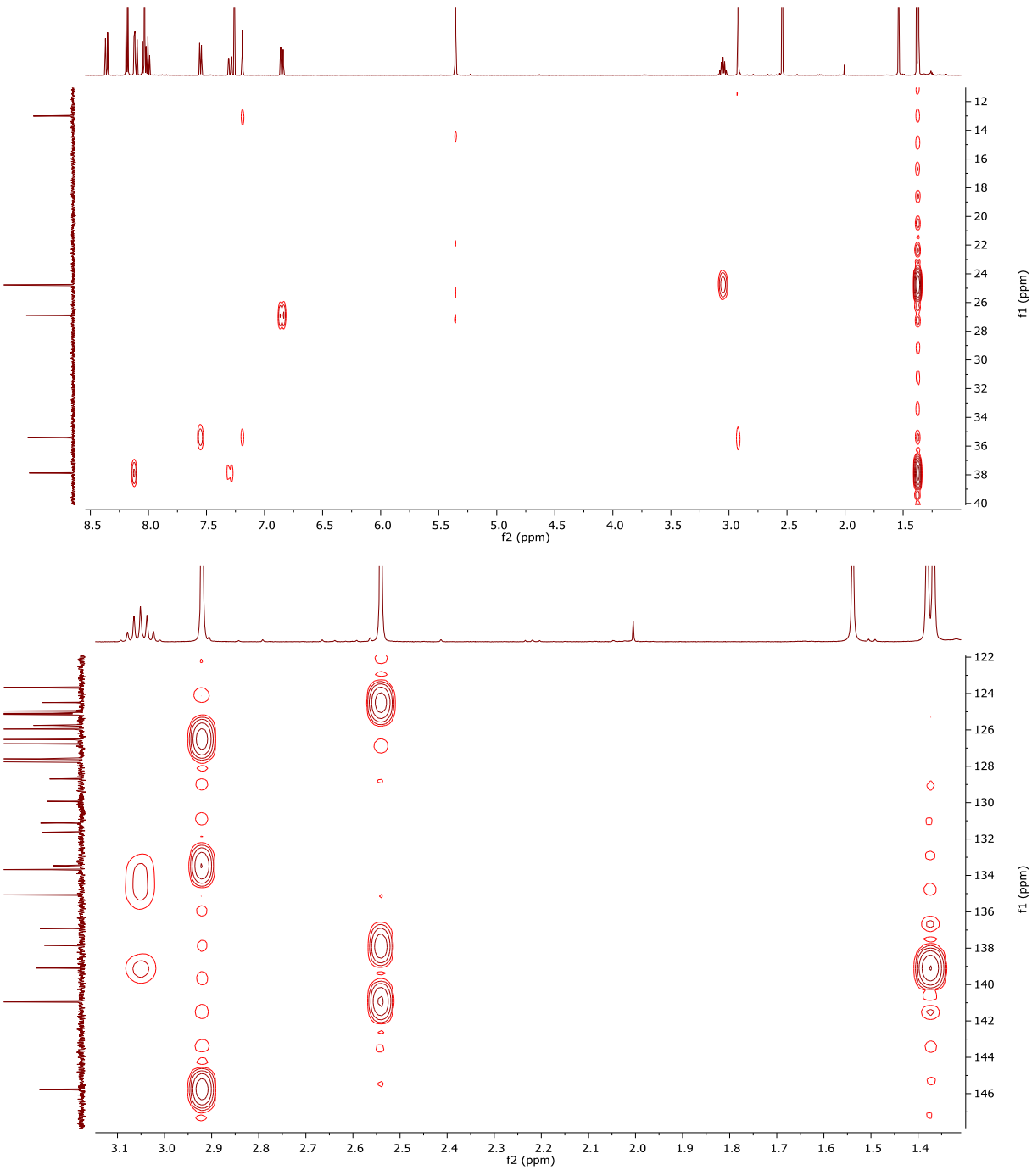
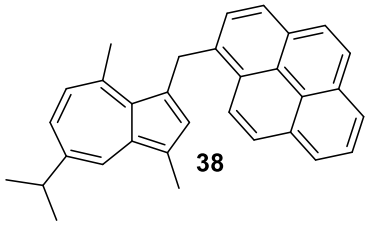
HMBC, $CDCl_3$





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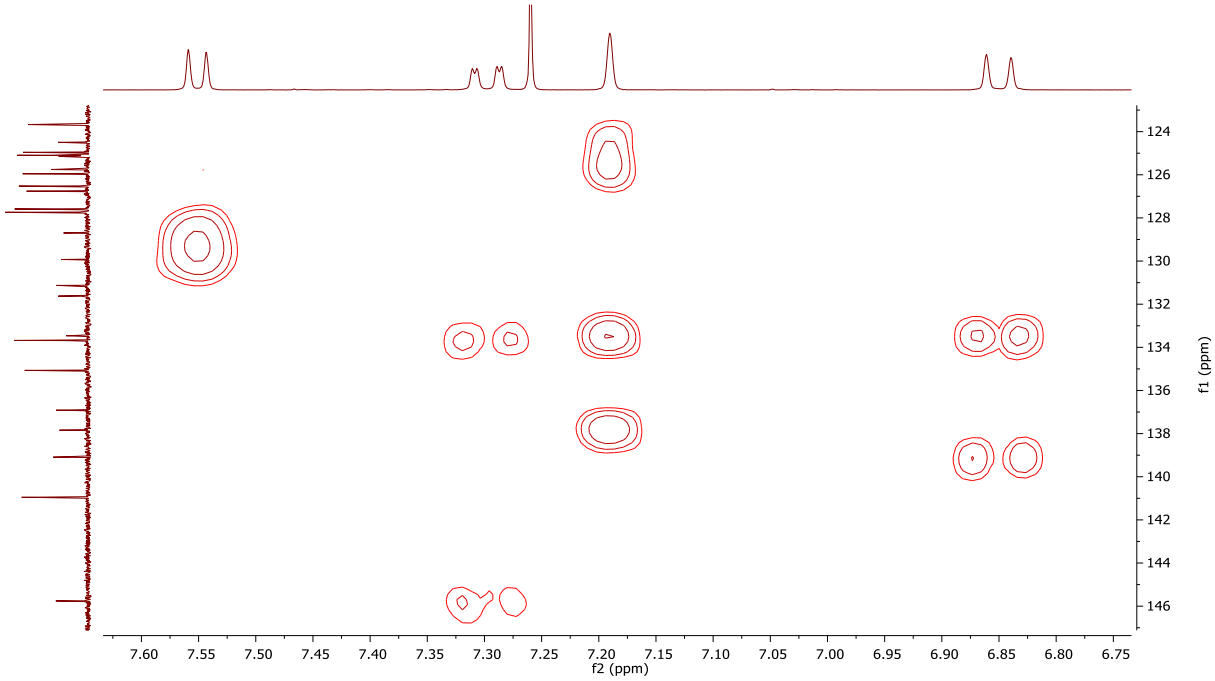

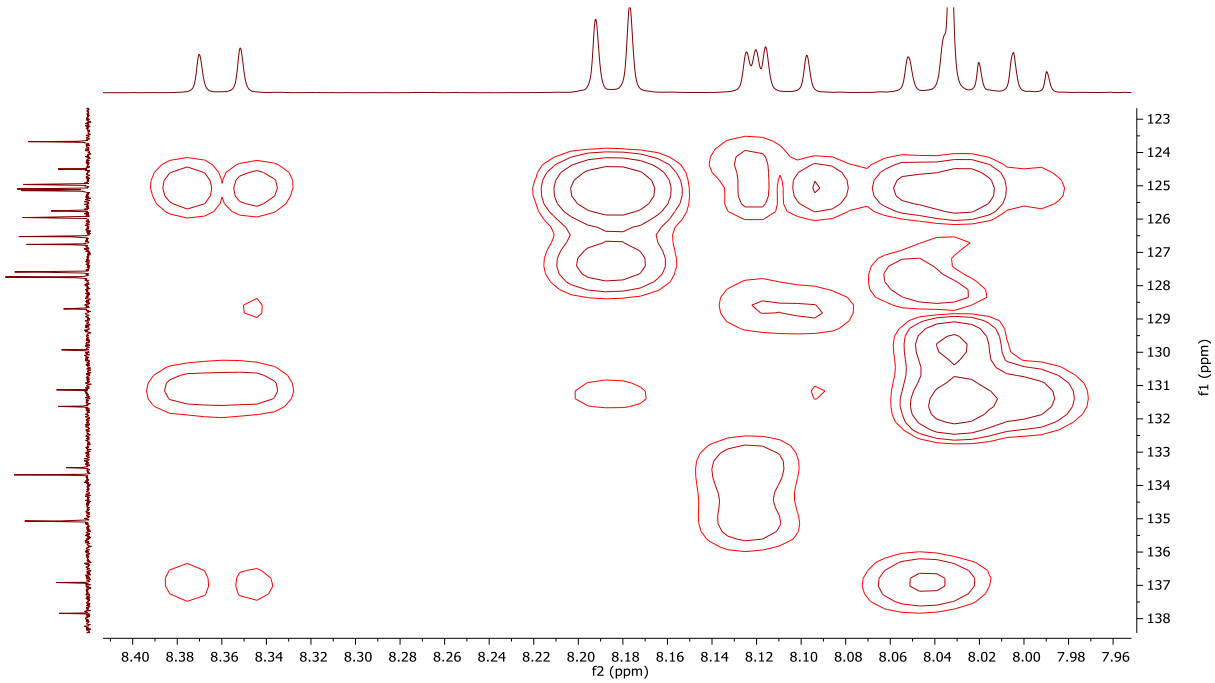

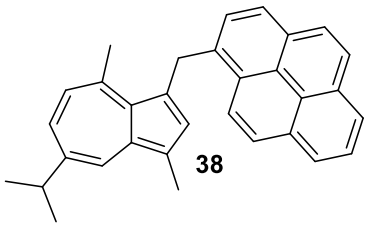

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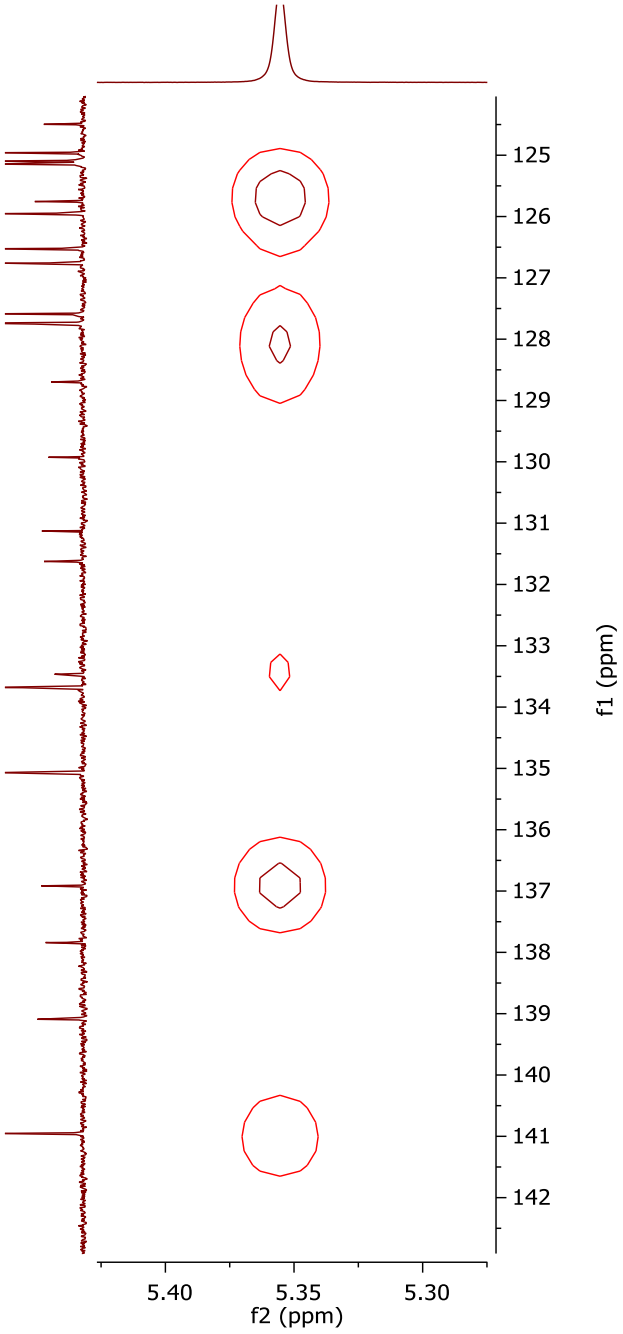
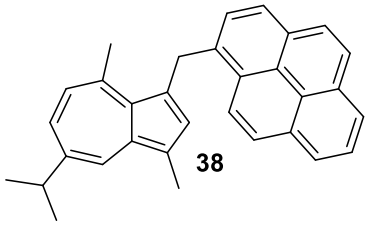




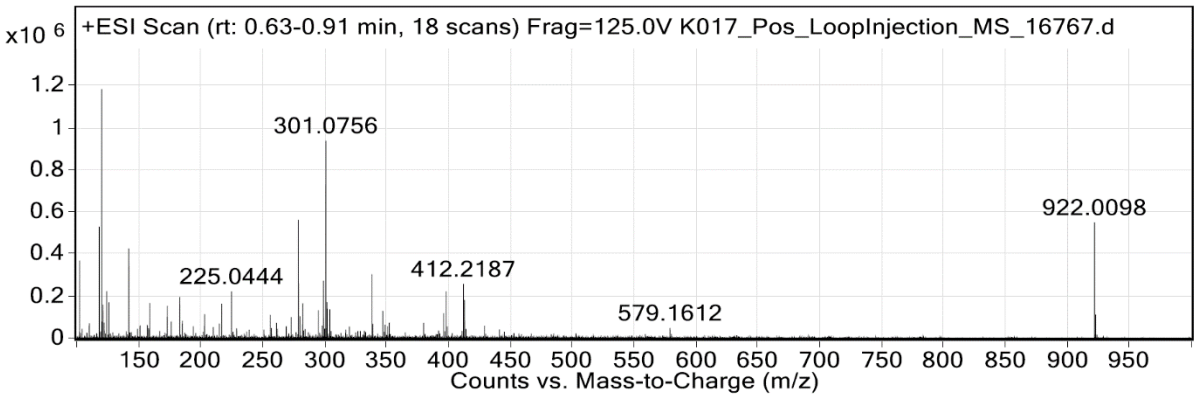


Figure: Extracted ion chromatogram (EIC) of compound.

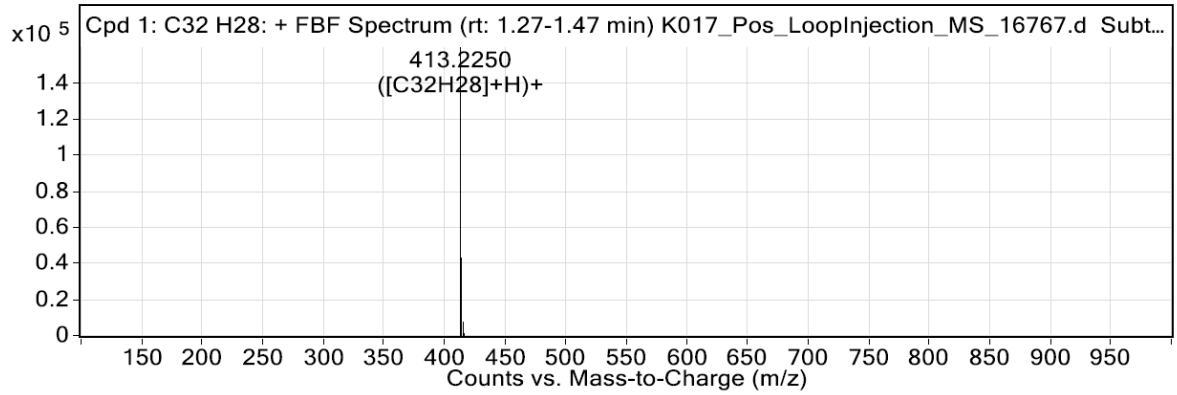
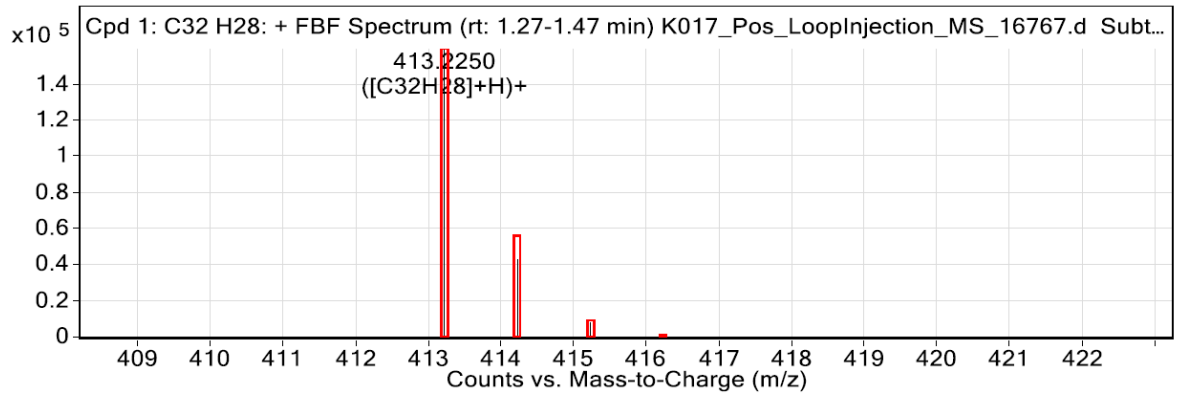
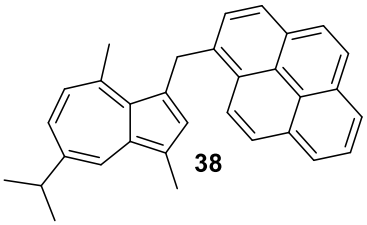


Figure: Full range view of Compound spectra and potential adducts.





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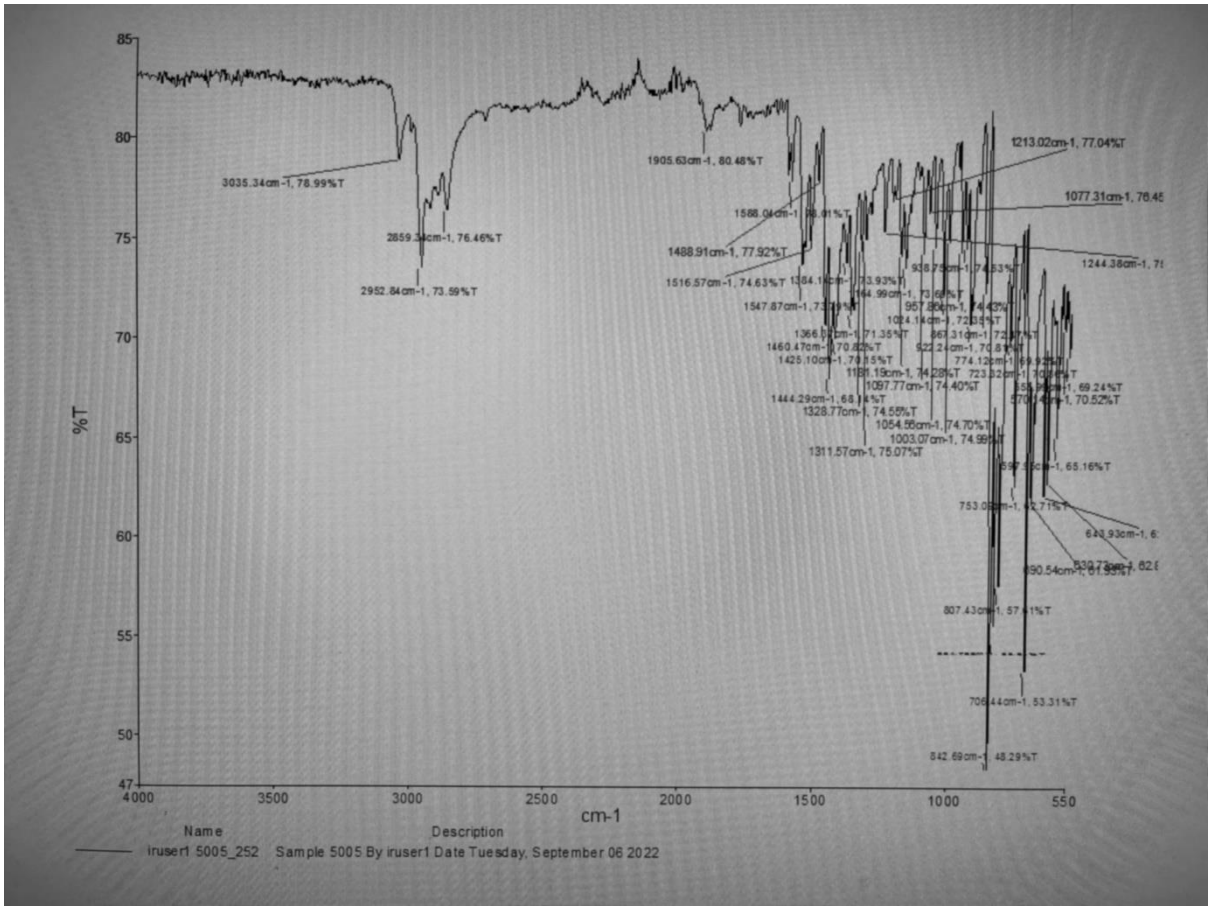
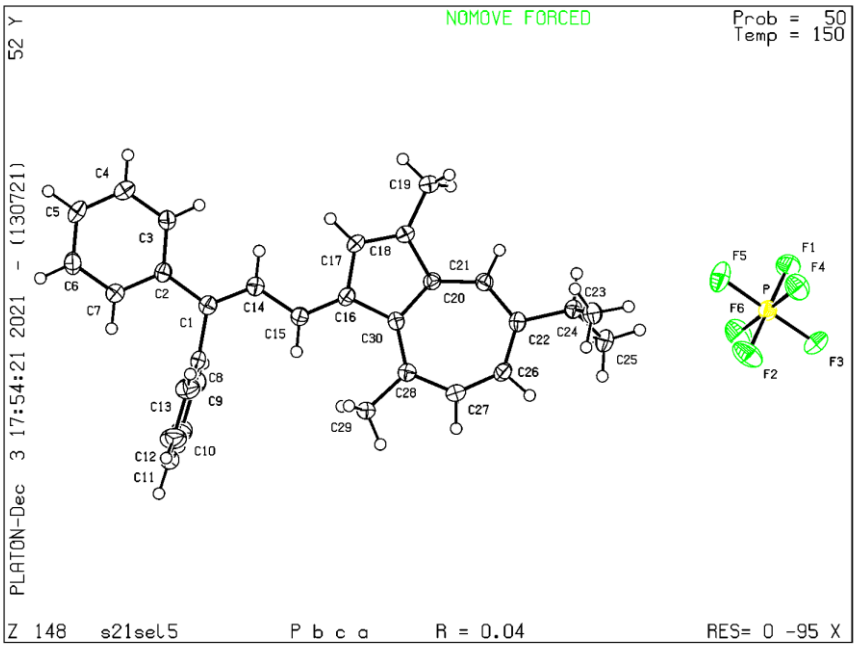
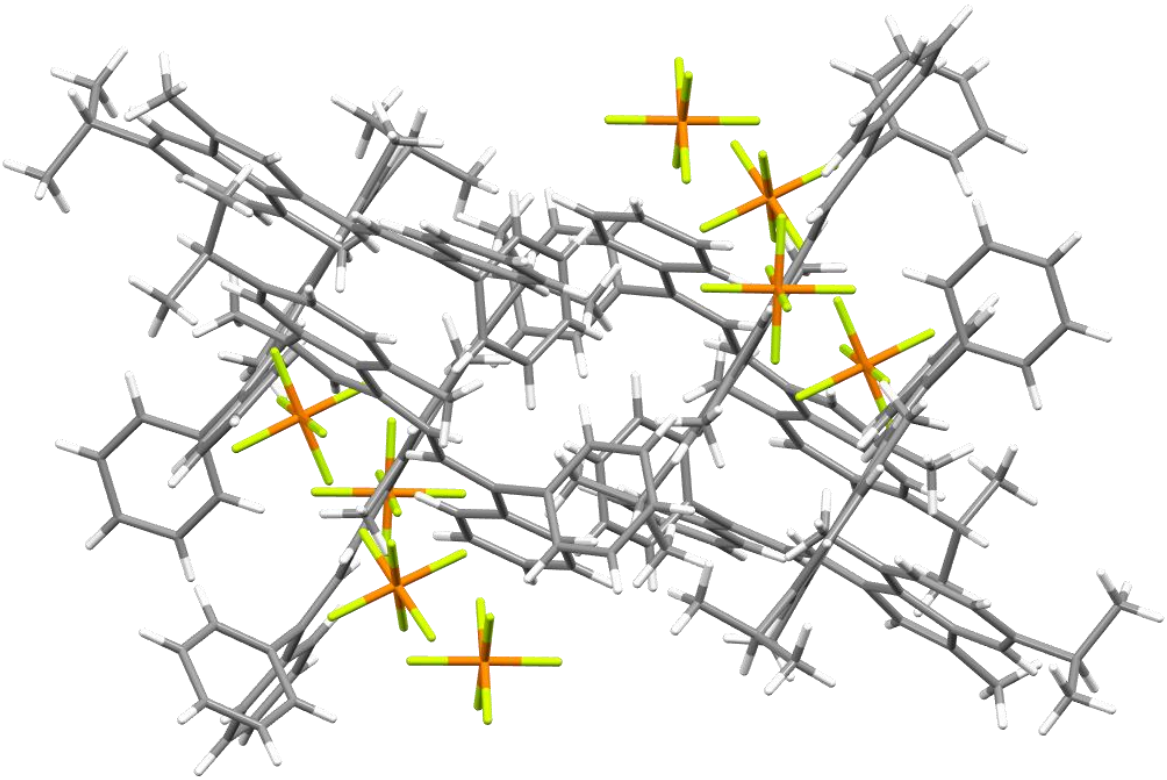

%T
cm-1
3035.34cm-1, 78.99%T
2952.84cm-1, 73.59%T
2859.34cm-1, 76.46%T
1905.63cm-1, 80.48%T
1588.04cm-1, 78.91%T
1516.57cm-1, 74.63%T
1488.91cm-1, 77.92%T
1547.87cm-1, 77.19%T
1460.47cm-1, 79.42%T
1425.10cm-1, 79.15%T
1444.29cm-1, 68.14%T
1328.77cm-1, 74.55%T
1311.57cm-1, 75.07%T
1213.02cm-1, 77.04%T
1077.31cm-1, 76.45
1244.38cm-1, 71
1097.77cm-1, 74.40%T
1054.55cm-1, 74.70%T
1003.07cm-1, 74.99%T
807.43cm-1, 57.61%T
706.44cm-1, 53.31%T
842.69cm-1, 48.29%T
Name
Description
iruser1 5005_252 Sample 5005 By iruser1 Date Tuesday, September 06 2022

X-ray crystallographic data

Table S1: Crystal data and structure refinement for **25**.

CCDC code	2129313	
Empirical formula	$C_{30}H_{29}F_6P$	
Formula weight	534.50	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 10.5171(3) Å	α= 90°.
	b = 19.2813(6) Å	β= 90°.
	c = 25.1199(8) Å	γ = 90°.
Volume	5093.9(3) $Å^3$	
Z	8	
Density (calculated)	1.394 Mg/m^3	
Absorption coefficient	1.505 mm^{-1}	
F(000)	2224	
Crystal size	0.374 x 0.068 x 0.015 mm^3	
Theta range for data collection	3.519 to 68.440°.	
Index ranges	-8<=h<=12, -23<=k<=23, -29<=l<=30	
Reflections collected	32580	
Independent reflections	4677 [R(int) = 0.0768]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.67944	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4677 / 0 / 338	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.0983	
R indices (all data)	R1 = 0.0630, wR2 = 0.1093	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.258 and -0.357 $e.Å^{-3}$	





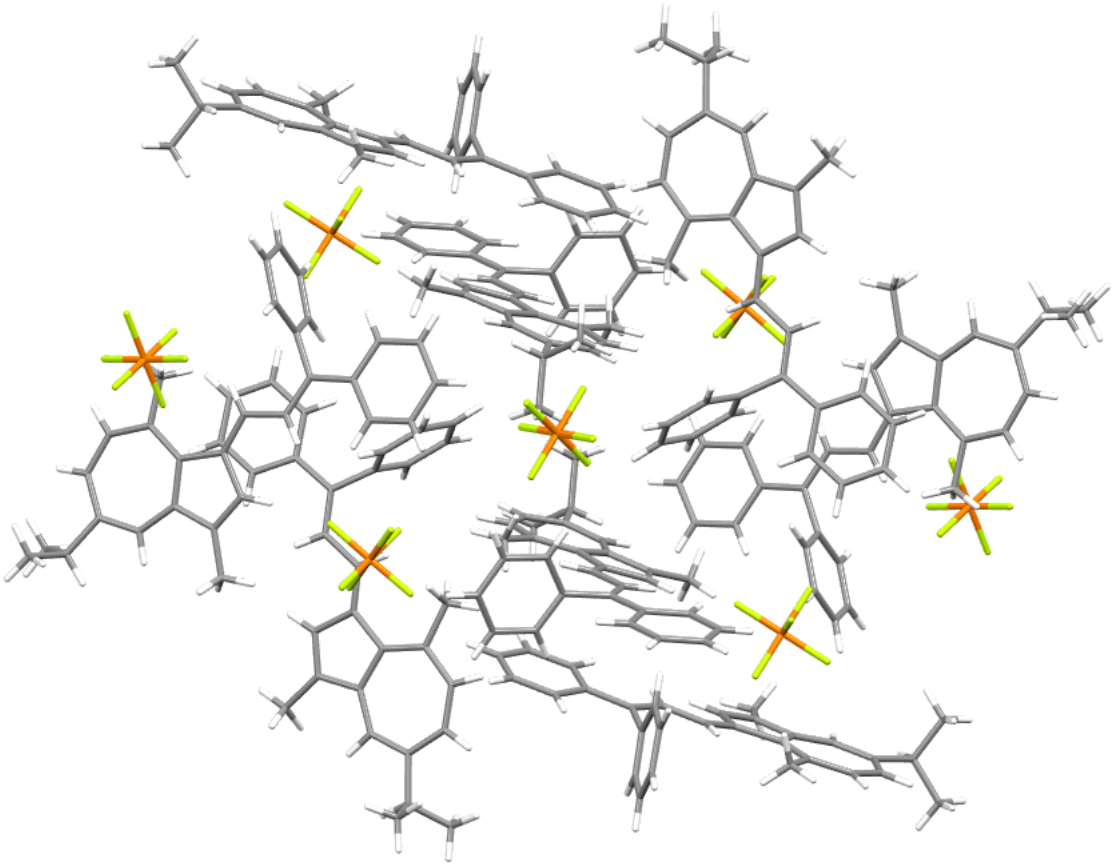


Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **25**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7550(2)	1749(1)	7479(1)	24(1)
C(2)	7915(2)	1601(1)	8036(1)	24(1)
C(3)	7518(2)	2021(1)	8460(1)	26(1)
C(4)	7854(2)	1862(1)	8979(1)	28(1)
C(5)	8606(2)	1290(1)	9088(1)	29(1)
C(6)	9013(2)	869(1)	8674(1)	32(1)
C(7)	8665(2)	1022(1)	8155(1)	27(1)
C(8)	8050(2)	1261(1)	7067(1)	24(1)
C(9)	7334(2)	688(1)	6919(1)	34(1)
C(10)	7831(3)	189(1)	6583(1)	40(1)
C(11)	9055(3)	263(1)	6392(1)	41(1)
C(12)	9768(2)	838(2)	6523(1)	43(1)
C(13)	9262(2)	1337(1)	6862(1)	35(1)
C(14)	6750(2)	2276(1)	7348(1)	27(1)
C(15)	6359(2)	2437(1)	6817(1)	25(1)
C(16)	5429(2)	2914(1)	6702(1)	24(1)
C(17)	4716(2)	3283(1)	7106(1)	27(1)
C(18)	3877(2)	3726(1)	6886(1)	27(1)
C(19)	2967(2)	4186(1)	7174(1)	38(1)
C(20)	3998(2)	3680(1)	6312(1)	22(1)
C(21)	3267(2)	4104(1)	5983(1)	23(1)
C(22)	3215(2)	4151(1)	5433(1)	23(1)
C(23)	2386(2)	4721(1)	5198(1)	25(1)
C(24)	3238(2)	5318(1)	5014(1)	30(1)
C(25)	1512(2)	4473(1)	4752(1)	31(1)
C(26)	3902(2)	3722(1)	5090(1)	27(1)
C(27)	4773(2)	3206(1)	5198(1)	25(1)
C(28)	5296(2)	2945(1)	5674(1)	22(1)
C(29)	6265(2)	2381(1)	5596(1)	29(1)
C(30)	4951(2)	3165(1)	6186(1)	20(1)
P	362(1)	6623(1)	3972(1)	26(1)
F(1)	-962(1)	6804(1)	4249(1)	40(1)
F(2)	1683(1)	6451(1)	3699(1)	53(1)
F(3)	-299(2)	6698(1)	3402(1)	50(1)
F(4)	704(1)	7430(1)	3965(1)	43(1)
F(5)	1000(2)	6558(1)	4546(1)	53(1)
F(6)	8(1)	5820(1)	3982(1)	49(1)

Table S3: Bond lengths [Å] for **25**.

C(1)-C(14)	1.360(3)	C(18)-C(19)	1.492(3)
C(1)-C(2)	1.478(3)	C(19)-H(19A)	0.9800
C(1)-C(8)	1.494(3)	C(19)-H(19B)	0.9800
C(2)-C(7)	1.400(3)	C(19)-H(19C)	0.9800
C(2)-C(3)	1.403(3)	C(20)-C(21)	1.393(3)
C(3)-C(4)	1.383(3)	C(20)-C(30)	1.445(3)
C(3)-H(3)	0.9500	C(21)-C(22)	1.387(3)
C(4)-C(5)	1.386(3)	C(21)-H(21)	0.9500
C(4)-H(4)	0.9500	C(22)-C(26)	1.396(3)
C(5)-C(6)	1.387(3)	C(22)-C(23)	1.521(3)
C(5)-H(5)	0.9500	C(23)-C(25)	1.526(3)
C(6)-C(7)	1.386(3)	C(23)-C(24)	1.532(3)
C(6)-H(6)	0.9500	C(23)-H(23)	1.0000
C(7)-H(7)	0.9500	C(24)-H(24A)	0.9800
C(8)-C(13)	1.382(3)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.388(3)	C(24)-H(24C)	0.9800
C(9)-C(10)	1.382(3)	C(25)-H(25A)	0.9800
C(9)-H(9)	0.9500	C(25)-H(25B)	0.9800
C(10)-C(11)	1.383(4)	C(25)-H(25C)	0.9800
C(10)-H(10)	0.9500	C(26)-C(27)	1.379(3)
C(11)-C(12)	1.377(4)	C(26)-H(26)	0.9500
C(11)-H(11)	0.9500	C(27)-C(28)	1.409(3)
C(12)-C(13)	1.392(4)	C(27)-H(27)	0.9500
C(12)-H(12)	0.9500	C(28)-C(30)	1.402(3)
C(13)-H(13)	0.9500	C(28)-C(29)	1.503(3)
C(14)-C(15)	1.430(3)	C(29)-H(29A)	0.9800
C(14)-H(14)	0.9500	C(29)-H(29B)	0.9800
C(15)-C(16)	1.372(3)	C(29)-H(29C)	0.9800
C(15)-H(15)	0.9500	P-F(2)	1.5839(15)
C(16)-C(17)	1.450(3)	P-F(6)	1.5927(15)
C(16)-C(30)	1.473(3)	P-F(5)	1.5945(15)
C(17)-C(18)	1.346(3)	P-F(1)	1.5957(14)
C(17)-H(17)	0.9500	P-F(4)	1.5986(14)
C(18)-C(20)	1.452(3)	P-F(3)	1.5999(15)

Table S4: Bond angles [°] for **25**

C(14)-C(1)-C(2)	122.2(2)	C(21)-C(20)-C(30)	131.1(2)
C(14)-C(1)-C(8)	121.4(2)	C(21)-C(20)-C(18)	120.27(19)
C(2)-C(1)-C(8)	116.27(18)	C(30)-C(20)-C(18)	108.66(18)
C(7)-C(2)-C(3)	117.8(2)	C(22)-C(21)-C(20)	130.5(2)
C(7)-C(2)-C(1)	120.2(2)	C(22)-C(21)-H(21)	114.7
C(3)-C(2)-C(1)	122.06(19)	C(20)-C(21)-H(21)	114.7
C(4)-C(3)-C(2)	120.8(2)	C(21)-C(22)-C(26)	123.79(19)
C(4)-C(3)-H(3)	119.6	C(21)-C(22)-C(23)	117.12(19)
C(2)-C(3)-H(3)	119.6	C(26)-C(22)-C(23)	119.06(19)
C(3)-C(4)-C(5)	120.6(2)	C(22)-C(23)-C(25)	113.82(18)
C(3)-C(4)-H(4)	119.7	C(22)-C(23)-C(24)	108.94(17)
C(5)-C(4)-H(4)	119.7	C(25)-C(23)-C(24)	111.43(18)
C(4)-C(5)-C(6)	119.5(2)	C(22)-C(23)-H(23)	107.5
C(4)-C(5)-H(5)	120.2	C(25)-C(23)-H(23)	107.5
C(6)-C(5)-H(5)	120.2	C(24)-C(23)-H(23)	107.5
C(7)-C(6)-C(5)	120.1(2)	C(23)-C(24)-H(24A)	109.5
C(7)-C(6)-H(6)	120.0	C(23)-C(24)-H(24B)	109.5
C(5)-C(6)-H(6)	120.0	H(24A)-C(24)-H(24B)	109.5
C(6)-C(7)-C(2)	121.3(2)	C(23)-C(24)-H(24C)	109.5
C(6)-C(7)-H(7)	119.4	H(24A)-C(24)-H(24C)	109.5
C(2)-C(7)-H(7)	119.4	H(24B)-C(24)-H(24C)	109.5
C(13)-C(8)-C(9)	119.0(2)	C(23)-C(25)-H(25A)	109.5
C(13)-C(8)-C(1)	121.0(2)	C(23)-C(25)-H(25B)	109.5
C(9)-C(8)-C(1)	119.73(19)	H(25A)-C(25)-H(25B)	109.5
C(10)-C(9)-C(8)	120.8(2)	C(23)-C(25)-H(25C)	109.5
C(10)-C(9)-H(9)	119.6	H(25A)-C(25)-H(25C)	109.5
C(8)-C(9)-H(9)	119.6	H(25B)-C(25)-H(25C)	109.5
C(9)-C(10)-C(11)	119.5(2)	C(27)-C(26)-C(22)	130.6(2)
C(9)-C(10)-H(10)	120.2	C(27)-C(26)-H(26)	114.7
C(11)-C(10)-H(10)	120.2	C(22)-C(26)-H(26)	114.7
C(12)-C(11)-C(10)	120.4(2)	C(26)-C(27)-C(28)	133.1(2)
C(12)-C(11)-H(11)	119.8	C(26)-C(27)-H(27)	113.5
C(10)-C(11)-H(11)	119.8	C(28)-C(27)-H(27)	113.5
C(11)-C(12)-C(13)	119.7(2)	C(30)-C(28)-C(27)	124.68(19)
C(11)-C(12)-H(12)	120.2	C(30)-C(28)-C(29)	120.92(19)
C(13)-C(12)-H(12)	120.2	C(27)-C(28)-C(29)	114.38(19)
C(8)-C(13)-C(12)	120.5(2)	C(28)-C(29)-H(29A)	109.5
C(8)-C(13)-H(13)	119.8	C(28)-C(29)-H(29B)	109.5
C(12)-C(13)-H(13)	119.8	H(29A)-C(29)-H(29B)	109.5
C(1)-C(14)-C(15)	124.4(2)	C(28)-C(29)-H(29C)	109.5
C(1)-C(14)-H(14)	117.8	H(29A)-C(29)-H(29C)	109.5
C(15)-C(14)-H(14)	117.8	H(29B)-C(29)-H(29C)	109.5
C(16)-C(15)-C(14)	123.2(2)	C(28)-C(30)-C(20)	126.02(19)
C(16)-C(15)-H(15)	118.4	C(28)-C(30)-C(16)	128.26(19)
C(14)-C(15)-H(15)	118.4	C(20)-C(30)-C(16)	105.69(18)
C(15)-C(16)-C(17)	123.3(2)	F(2)-P-F(6)	90.49(9)
C(15)-C(16)-C(30)	130.5(2)	F(2)-P-F(5)	90.36(10)
C(17)-C(16)-C(30)	106.15(18)	F(6)-P-F(5)	90.47(9)
C(18)-C(17)-C(16)	111.29(19)	F(2)-P-F(1)	179.34(10)
C(18)-C(17)-H(17)	124.4	F(6)-P-F(1)	90.16(8)
C(16)-C(17)-H(17)	124.4	F(5)-P-F(1)	89.49(9)
C(17)-C(18)-C(20)	108.19(19)	F(2)-P-F(4)	90.08(9)
C(17)-C(18)-C(19)	126.8(2)	F(6)-P-F(4)	179.42(9)
C(20)-C(18)-C(19)	125.0(2)	F(5)-P-F(4)	89.57(9)
C(18)-C(19)-H(19A)	109.5	F(1)-P-F(4)	89.27(8)
C(18)-C(19)-H(19B)	109.5	F(2)-P-F(3)	90.70(10)
H(19A)-C(19)-H(19B)	109.5	F(6)-P-F(3)	90.04(9)
C(18)-C(19)-H(19C)	109.5	F(5)-P-F(3)	178.82(10)
H(19A)-C(19)-H(19C)	109.5	F(1)-P-F(3)	89.44(8)
H(19B)-C(19)-H(19C)	109.5	F(4)-P-F(3)	89.91(9)

Table S5: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **25**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	26(1)	24(1)	2(1)	-1(1)	-2(1)
C(2)	21(1)	26(1)	24(1)	3(1)	-2(1)	-2(1)
C(3)	26(1)	27(1)	26(1)	1(1)	-3(1)	3(1)
C(4)	30(1)	33(1)	22(1)	-1(1)	-1(1)	-4(1)
C(5)	29(1)	38(1)	21(1)	6(1)	-6(1)	-5(1)
C(6)	31(1)	31(1)	32(1)	7(1)	-4(1)	6(1)
C(7)	28(1)	29(1)	24(1)	0(1)	-1(1)	3(1)
C(8)	27(1)	27(1)	19(1)	4(1)	-4(1)	5(1)
C(9)	32(1)	35(1)	34(1)	0(1)	-1(1)	-2(1)
C(10)	56(2)	31(1)	34(1)	-3(1)	-9(1)	-2(1)
C(11)	53(2)	43(2)	28(1)	-5(1)	-7(1)	21(1)
C(12)	34(1)	60(2)	36(2)	-8(1)	7(1)	4(1)
C(13)	29(1)	43(1)	33(1)	-5(1)	3(1)	-3(1)
C(14)	27(1)	29(1)	24(1)	1(1)	-2(1)	4(1)
C(15)	26(1)	25(1)	24(1)	1(1)	-1(1)	1(1)
C(16)	27(1)	26(1)	20(1)	2(1)	-1(1)	1(1)
C(17)	32(1)	32(1)	17(1)	0(1)	-3(1)	4(1)
C(18)	30(1)	30(1)	20(1)	-2(1)	-1(1)	4(1)
C(19)	47(1)	45(2)	23(1)	-4(1)	0(1)	18(1)
C(20)	25(1)	22(1)	21(1)	-1(1)	-2(1)	-1(1)
C(21)	22(1)	23(1)	24(1)	-2(1)	-2(1)	1(1)
C(22)	21(1)	22(1)	26(1)	2(1)	-3(1)	-2(1)
C(23)	24(1)	27(1)	24(1)	1(1)	-2(1)	2(1)
C(24)	31(1)	27(1)	33(1)	3(1)	-1(1)	0(1)
C(25)	30(1)	33(1)	29(1)	4(1)	-7(1)	-1(1)
C(26)	31(1)	30(1)	19(1)	1(1)	-3(1)	1(1)
C(27)	27(1)	28(1)	21(1)	-2(1)	2(1)	-1(1)
C(28)	21(1)	23(1)	24(1)	-1(1)	-1(1)	-2(1)
C(29)	31(1)	33(1)	22(1)	-2(1)	0(1)	9(1)
C(30)	19(1)	18(1)	24(1)	0(1)	-3(1)	-1(1)
P	26(1)	27(1)	26(1)	4(1)	1(1)	1(1)
F(1)	33(1)	49(1)	40(1)	1(1)	7(1)	2(1)
F(2)	37(1)	47(1)	76(1)	-2(1)	24(1)	5(1)
F(3)	65(1)	60(1)	24(1)	-3(1)	-9(1)	8(1)
F(4)	47(1)	28(1)	54(1)	4(1)	2(1)	-2(1)
F(5)	54(1)	62(1)	42(1)	11(1)	-21(1)	2(1)
F(6)	50(1)	28(1)	68(1)	3(1)	4(1)	-4(1)

Table S6: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **25**.

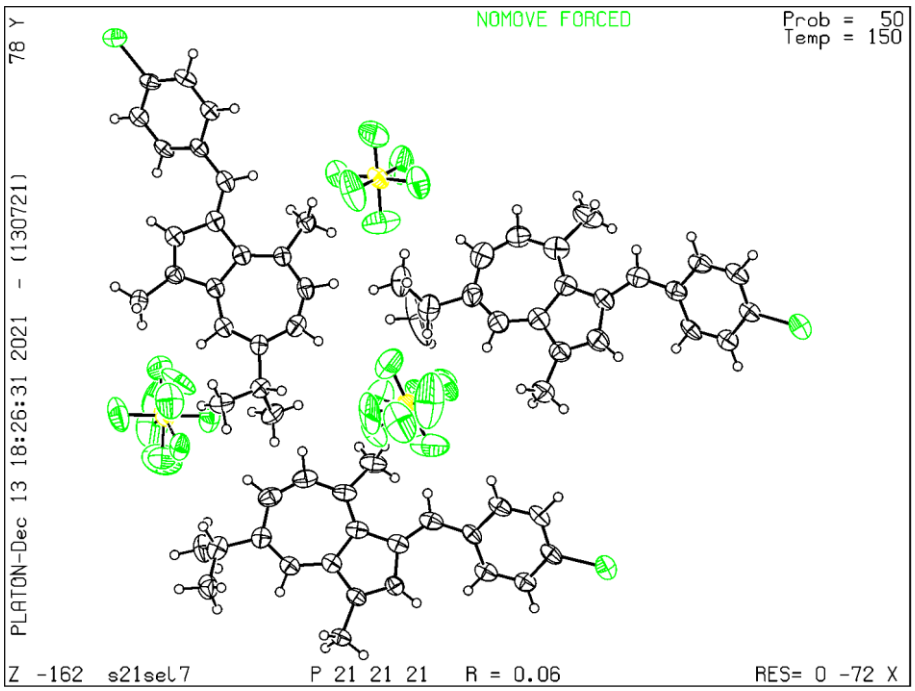
	x	y	z	U(eq)
H(3)	7012	2419	8391	32
H(4)	7568	2149	9262	34
H(5)	8842	1186	9444	35
H(6)	9530	476	8746	38
H(7)	8942	727	7874	33
H(9)	6491	638	7050	40
H(10)	7334	-202	6485	49
H(11)	9408	-84	6167	50
H(12)	10601	892	6383	52
H(13)	9753	1733	6954	42
H(14)	6430	2557	7629	32
H(15)	6762	2203	6530	30
H(17)	4827	3221	7478	33
H(19A)	3202	4672	7114	57
H(19B)	2999	4084	7556	57
H(19C)	2104	4106	7041	57
H(21)	2713	4412	6167	28
H(23)	1834	4902	5491	30
H(24A)	3855	5145	4753	45
H(24B)	3691	5512	5320	45
H(24C)	2714	5680	4849	45
H(25A)	986	4861	4628	46
H(25B)	963	4101	4885	46
H(25C)	2027	4299	4455	46
H(26)	3744	3798	4722	32
H(27)	5084	2981	4887	30
H(29A)	6323	2265	5217	43
H(29B)	6008	1968	5797	43
H(29C)	7095	2541	5723	43

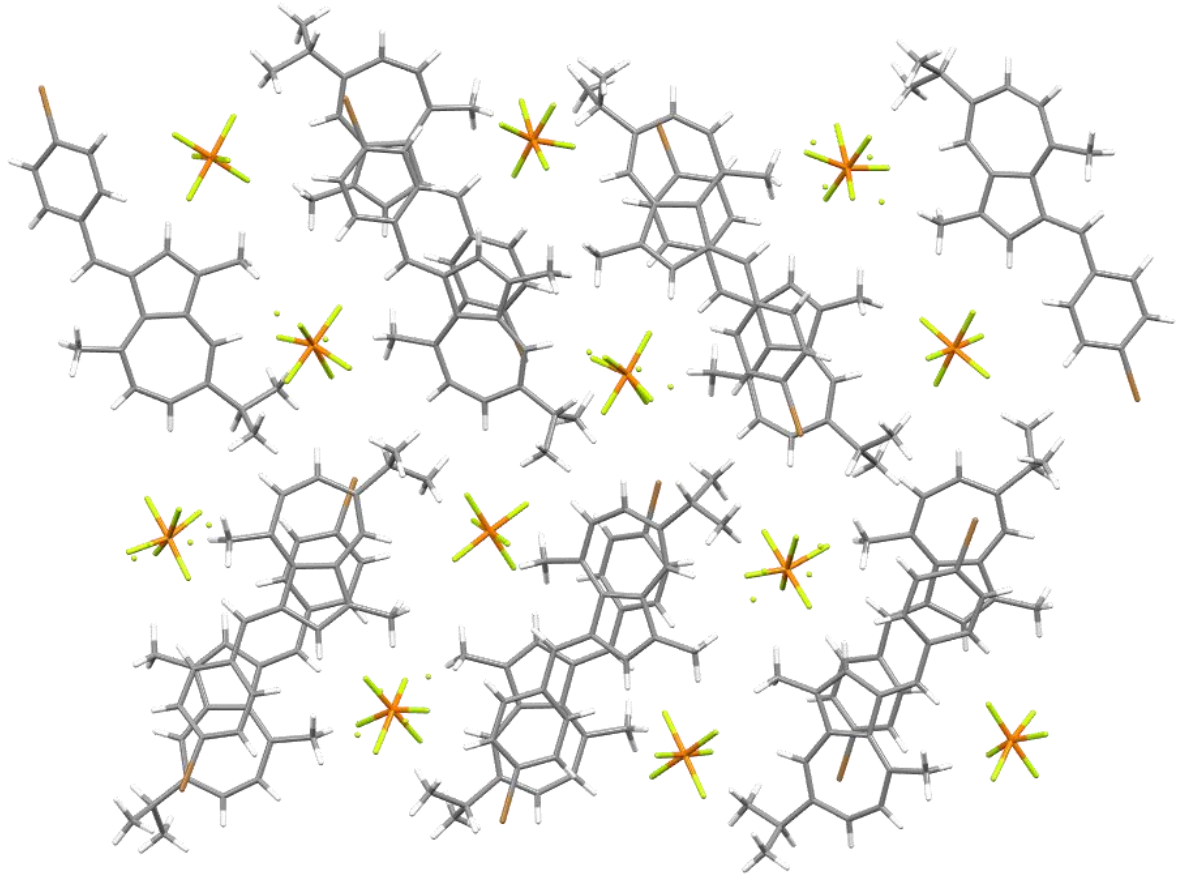
Table S7: Torsion angles [°] for **25**.

C(14)-C(1)-C(2)-C(7)	175.3(2)	C(16)-C(17)-C(18)-C(20)	-0.7(3)
C(8)-C(1)-C(2)-C(7)	-1.4(3)	C(16)-C(17)-C(18)-C(19)	179.1(2)
C(14)-C(1)-C(2)-C(3)	-3.8(3)	C(17)-C(18)-C(20)-C(21)	-177.7(2)
C(8)-C(1)-C(2)-C(3)	179.54(19)	C(19)-C(18)-C(20)-C(21)	2.5(3)
C(7)-C(2)-C(3)-C(4)	-0.3(3)	C(17)-C(18)-C(20)-C(30)	1.4(2)
C(1)-C(2)-C(3)-C(4)	178.78(19)	C(19)-C(18)-C(20)-C(30)	-178.4(2)
C(2)-C(3)-C(4)-C(5)	0.9(3)	C(30)-C(20)-C(21)-C(22)	1.5(4)
C(3)-C(4)-C(5)-C(6)	-0.6(3)	C(18)-C(20)-C(21)-C(22)	-179.7(2)
C(4)-C(5)-C(6)-C(7)	-0.1(3)	C(20)-C(21)-C(22)-C(26)	3.4(4)
C(5)-C(6)-C(7)-C(2)	0.6(3)	C(20)-C(21)-C(22)-C(23)	-174.7(2)
C(3)-C(2)-C(7)-C(6)	-0.4(3)	C(21)-C(22)-C(23)-C(25)	-132.7(2)
C(1)-C(2)-C(7)-C(6)	-179.5(2)	C(26)-C(22)-C(23)-C(25)	49.1(3)
C(14)-C(1)-C(8)-C(13)	100.5(3)	C(21)-C(22)-C(23)-C(24)	102.3(2)
C(2)-C(1)-C(8)-C(13)	-82.8(3)	C(26)-C(22)-C(23)-C(24)	-75.9(2)
C(14)-C(1)-C(8)-C(9)	-85.1(3)	C(21)-C(22)-C(26)-C(27)	-2.8(4)
C(2)-C(1)-C(8)-C(9)	91.5(2)	C(23)-C(22)-C(26)-C(27)	175.2(2)
C(13)-C(8)-C(9)-C(10)	1.6(4)	C(22)-C(26)-C(27)-C(28)	-2.0(4)
C(1)-C(8)-C(9)-C(10)	-172.9(2)	C(26)-C(27)-C(28)-C(30)	3.2(4)
C(8)-C(9)-C(10)-C(11)	-0.2(4)	C(26)-C(27)-C(28)-C(29)	-178.2(2)
C(9)-C(10)-C(11)-C(12)	-1.5(4)	C(27)-C(28)-C(30)-C(20)	1.3(3)
C(10)-C(11)-C(12)-C(13)	1.6(4)	C(29)-C(28)-C(30)-C(20)	-177.26(19)
C(9)-C(8)-C(13)-C(12)	-1.5(4)	C(27)-C(28)-C(30)-C(16)	178.8(2)
C(1)-C(8)-C(13)-C(12)	172.9(2)	C(29)-C(28)-C(30)-C(16)	0.3(3)
C(11)-C(12)-C(13)-C(8)	-0.1(4)	C(21)-C(20)-C(30)-C(28)	-4.5(4)
C(2)-C(1)-C(14)-C(15)	-179.44(19)	C(18)-C(20)-C(30)-C(28)	176.49(19)
C(8)-C(1)-C(14)-C(15)	-3.0(3)	C(21)-C(20)-C(30)-C(16)	177.5(2)
C(1)-C(14)-C(15)-C(16)	171.4(2)	C(18)-C(20)-C(30)-C(16)	-1.5(2)
C(14)-C(15)-C(16)-C(17)	-2.3(3)	C(15)-C(16)-C(30)-C(28)	3.8(4)
C(14)-C(15)-C(16)-C(30)	176.8(2)	C(17)-C(16)-C(30)-C(28)	-176.9(2)
C(15)-C(16)-C(17)-C(18)	179.1(2)	C(15)-C(16)-C(30)-C(20)	-178.2(2)
C(30)-C(16)-C(17)-C(18)	-0.2(3)	C(17)-C(16)-C(30)-C(20)	1.1(2)

Table S8: Crystal data and structure refinement for **26**.

CCDC code	#2129312	
Empirical formula	$C_{22}H_{22}BrF_6P$	
Formula weight	511.27	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.5877(2) Å	α= 90°.
	b = 26.8100(12) Å	β= 90°.
	c = 31.9061(9) Å	γ = 90°.
Volume	6490.5(4) $Å^3$	
Z	12	
Density (calculated)	1.570 Mg/m^3	
Absorption coefficient	3.820 mm^{-1}	
F(000)	3096	
Crystal size	0.234 x 0.101 x 0.025 mm^3	
Theta range for data collection	4.308 to 68.808°.	
Index ranges	-8<=h<=9, -32<=k<=32, -28<=l<=38	
Reflections collected	44869	
Independent reflections	11920 [R(int) = 0.0738]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.63398	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11920 / 0 / 897	
Goodness-of-fit on F^2	1.008	
Final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1239	
R indices (all data)	R1 = 0.0841, wR2 = 0.1370	
Absolute structure parameter	0.003(13)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.906 and -0.689 e.$Å^{-3}$	





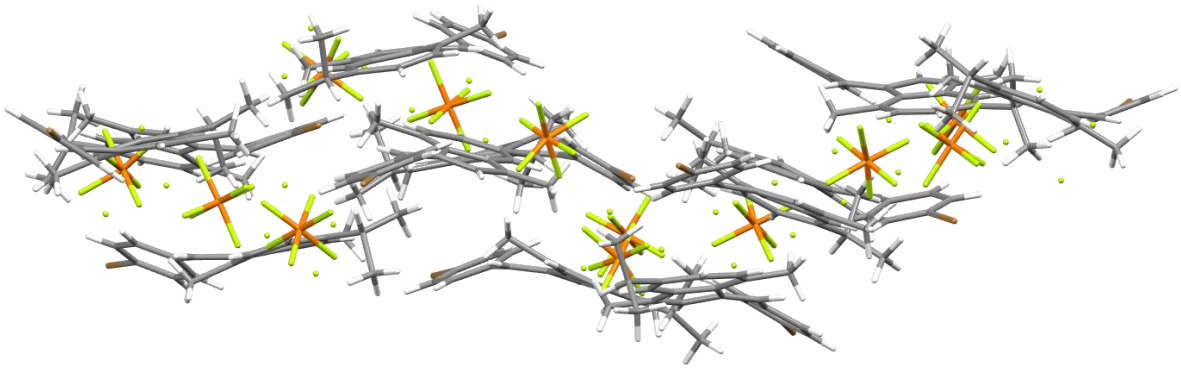


Table S9: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **26**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	10063(1)	441(1)	5786(1)	51(1)
C(1)	9331(11)	2614(3)	5228(2)	40(2)
C(2)	9391(10)	2096(3)	5356(2)	36(2)
C(3)	10139(10)	1977(3)	5750(2)	37(2)
C(4)	10305(10)	1492(4)	5880(2)	42(2)
C(5)	9724(10)	1115(3)	5624(2)	37(2)
C(6)	8923(10)	1213(3)	5242(2)	38(2)
C(7)	8749(10)	1699(3)	5121(2)	36(2)
C(8)	9391(10)	2802(3)	4826(3)	38(2)
C(9)	9749(11)	2511(3)	4450(3)	41(2)
C(10)	10055(12)	2811(3)	4128(2)	40(2)
C(11)	10527(15)	2657(4)	3690(3)	54(3)
C(12)	9911(11)	3324(3)	4262(2)	38(2)
C(13)	10242(10)	3722(3)	3986(2)	37(2)
C(14)	10274(10)	4223(3)	4053(2)	36(2)
C(15)	10709(11)	4577(3)	3697(3)	42(2)
C(16)	11775(13)	4346(4)	3346(3)	55(3)
C(17)	8994(13)	4798(3)	3523(3)	50(2)
C(18)	9854(11)	4446(3)	4439(3)	45(2)
C(19)	9250(11)	4238(3)	4808(3)	42(2)
C(20)	8969(10)	3741(3)	4934(2)	36(2)
C(21)	8072(12)	3689(4)	5361(3)	44(2)
C(22)	9417(10)	3332(3)	4700(2)	35(2)
Br(2)	6129(1)	9512(1)	7492(1)	58(1)
C(31)	4774(12)	7379(4)	6893(3)	51(2)
C(32)	5066(12)	7894(4)	7016(3)	46(2)
C(33)	5781(13)	7983(4)	7412(3)	51(2)
C(34)	6114(12)	8463(4)	7553(3)	51(2)
C(35)	5664(11)	8854(4)	7300(2)	42(2)
C(36)	4888(12)	8785(4)	6910(3)	46(2)
C(37)	4593(10)	8311(4)	6773(2)	44(2)
C(38)	4729(11)	7184(4)	6491(3)	45(2)
C(39)	4405(11)	6662(4)	6370(3)	47(2)
C(40)	3896(12)	6262(4)	6623(3)	55(3)
C(41)	3448(17)	6333(5)	7084(3)	81(4)
C(42)	3759(14)	5771(4)	6485(3)	58(3)
C(43)	3929(14)	5542(5)	6102(4)	66(3)
C(44)	4291(14)	5748(4)	5709(3)	59(3)
C(45)	4390(20)	5396(5)	5331(4)	85(4)
C(46)	2750(20)	5274(9)	5161(5)	191(13)
C(47)	5659(15)	4980(4)	5406(4)	72(3)
C(48)	4658(12)	6240(4)	5643(3)	53(2)
C(49)	4724(12)	6645(4)	5921(3)	50(2)
C(50)	5180(13)	7135(4)	5780(3)	52(2)
C(51)	5589(17)	7272(4)	5338(3)	70(3)
C(52)	5178(13)	7446(4)	6113(3)	55(2)
Br(3)	4237(2)	9148(1)	4201(1)	59(1)
C(61)	4963(12)	7022(4)	3530(3)	45(2)
C(62)	4831(11)	7537(3)	3666(2)	41(2)
C(63)	5323(11)	7653(4)	4086(3)	48(2)
C(64)	5142(12)	8125(4)	4245(3)	45(2)
C(65)	4505(11)	8493(4)	3983(2)	46(2)
C(66)	3996(12)	8399(4)	3573(2)	45(2)
C(67)	4134(11)	7921(4)	3423(3)	45(2)
C(68)	5116(11)	6850(3)	3132(2)	40(2)

C(69)	5277(10)	6327(3)	3001(2)	40(2)
C(70)	4854(11)	5899(4)	3233(2)	44(2)
C(71)	3885(14)	5928(4)	3649(3)	58(3)
C(72)	5306(12)	5408(4)	3117(3)	50(2)
C(73)	5961(13)	5214(4)	2753(3)	52(2)
C(74)	6301(10)	5441(4)	2357(3)	42(2)
C(75)	6695(13)	5082(4)	2000(3)	52(2)
C(76)	7570(14)	5316(4)	1623(3)	60(3)
C(77)	4937(14)	4834(4)	1883(3)	63(3)
C(78)	6178(10)	5940(3)	2290(2)	37(2)
C(79)	5810(10)	6337(3)	2565(2)	36(2)
C(80)	5858(11)	6845(3)	2431(2)	37(2)
C(81)	6342(14)	7009(4)	1997(2)	49(2)
C(82)	5463(11)	7140(3)	2757(2)	39(2)
P(1)	2581(3)	3806(1)	6103(1)	52(1)
F(1)	1860(8)	3310(2)	5875(2)	69(2)
F(2)	3302(10)	4300(3)	6321(2)	88(2)
F(3)	3329(16)	3480(4)	6460(2)	136(4)
F(4)	764(12)	3853(3)	6329(3)	119(3)
F(5)	1871(11)	4125(3)	5730(3)	110(3)
F(6)	4384(9)	3734(3)	5863(2)	111(3)
P(2)	8513(4)	6122(1)	4437(1)	60(1)
F(7)	7855(12)	6610(4)	4213(3)	127(3)
F(8)	9048(17)	5651(3)	4677(3)	134(4)
F(9)	7070(30)	5696(8)	4279(10)	119(12)
F(10)	7370(60)	6258(12)	4834(8)	157(19)
F(11)	10100(40)	6401(12)	4624(16)	186(18)
F(12)	9950(30)	5865(10)	4146(7)	134(12)
F(9A)	7990(19)	5933(6)	3988(4)	88(5)
F(10A)	6530(20)	6119(9)	4574(5)	127(9)
F(11A)	9060(30)	6418(6)	4826(4)	94(6)
F(12A)	10368(17)	6269(9)	4259(6)	128(8)
P(3)	6612(4)	3541(1)	2805(1)	53(1)
F(13)	5757(10)	3974(3)	3066(2)	89(2)
F(14)	7472(11)	3104(3)	2544(2)	102(3)
F(15)	5550(40)	3785(17)	2400(9)	129(13)
F(16)	5130(40)	3231(9)	2897(13)	112(13)
F(17)	7620(40)	3499(12)	3202(5)	99(10)
F(18)	8050(20)	4015(7)	2657(7)	65(7)
F(15A)	4760(20)	3386(9)	2618(8)	137(11)
F(16A)	6240(30)	3128(5)	3179(4)	93(6)
F(17A)	8473(18)	3597(6)	2992(6)	98(6)
F(18A)	6940(30)	3852(6)	2432(4)	110(7)

Table S10: Bond lengths [Å] for **26**.

Br(1)-C(5)	1.897(9)	C(36)-C(37)	1.364(13)
C(1)-C(8)	1.381(11)	C(36)-H(36)	0.9500
C(1)-C(2)	1.449(12)	C(37)-H(37)	0.9500
C(1)-H(1)	0.9500	C(38)-C(52)	1.436(13)
C(2)-C(7)	1.391(11)	C(38)-C(39)	1.472(14)
C(2)-C(3)	1.415(11)	C(39)-C(40)	1.398(13)
C(3)-C(4)	1.373(12)	C(39)-C(49)	1.454(12)
C(3)-H(3)	0.9500	C(40)-C(42)	1.393(15)
C(4)-C(5)	1.373(12)	C(40)-C(41)	1.520(14)
C(4)-H(4)	0.9500	C(41)-H(41A)	0.9800
C(5)-C(6)	1.388(11)	C(41)-H(41B)	0.9800
C(6)-C(7)	1.365(12)	C(41)-H(41C)	0.9800
C(6)-H(6)	0.9500	C(42)-C(43)	1.374(14)
C(7)-H(7)	0.9500	C(42)-H(42)	0.9500
C(8)-C(9)	1.457(11)	C(43)-C(44)	1.398(15)
C(8)-C(22)	1.475(12)	C(43)-H(43)	0.9500
C(9)-C(10)	1.324(11)	C(44)-C(48)	1.362(14)
C(9)-H(9)	0.9500	C(44)-C(45)	1.533(14)
C(10)-C(12)	1.446(12)	C(45)-C(46)	1.40(2)
C(10)-C(11)	1.502(11)	C(45)-C(47)	1.492(16)
C(11)-H(11A)	0.9800	C(45)-H(45)	1.0000
C(11)-H(11B)	0.9800	C(46)-H(46A)	0.9800
C(11)-H(11C)	0.9800	C(46)-H(46B)	0.9800
C(12)-C(13)	1.406(11)	C(46)-H(46C)	0.9800
C(12)-C(22)	1.445(11)	C(47)-H(47A)	0.9800
C(13)-C(14)	1.362(11)	C(47)-H(47B)	0.9800
C(13)-H(13)	0.9500	C(47)-H(47C)	0.9800
C(14)-C(18)	1.407(11)	C(48)-C(49)	1.403(13)
C(14)-C(15)	1.516(11)	C(48)-H(48)	0.9500
C(15)-C(16)	1.514(12)	C(49)-C(50)	1.431(14)
C(15)-C(17)	1.533(12)	C(50)-C(52)	1.350(13)
C(15)-H(15)	1.0000	C(50)-C(51)	1.490(13)
C(16)-H(16A)	0.9800	C(51)-H(51A)	0.9800
C(16)-H(16B)	0.9800	C(51)-H(51B)	0.9800
C(16)-H(16C)	0.9800	C(51)-H(51C)	0.9800
C(17)-H(17A)	0.9800	C(52)-H(52)	0.9500
C(17)-H(17B)	0.9800	Br(3)-C(65)	1.900(10)
C(17)-H(17C)	0.9800	C(61)-C(68)	1.356(11)
C(18)-C(19)	1.381(12)	C(61)-C(62)	1.453(12)
C(18)-H(18)	0.9500	C(61)-H(61)	0.9500
C(19)-C(20)	1.408(12)	C(62)-C(67)	1.393(12)
C(19)-H(19)	0.9500	C(62)-C(63)	1.424(11)
C(20)-C(22)	1.371(11)	C(63)-C(64)	1.370(13)
C(20)-C(21)	1.530(11)	C(63)-H(63)	0.9500
C(21)-H(21A)	0.9800	C(64)-C(65)	1.379(13)
C(21)-H(21B)	0.9800	C(64)-H(64)	0.9500
C(21)-H(21C)	0.9800	C(65)-C(66)	1.388(11)
Br(2)-C(35)	1.899(10)	C(66)-C(67)	1.372(13)
C(31)-C(38)	1.386(12)	C(66)-H(66)	0.9500
C(31)-C(32)	1.454(14)	C(67)-H(67)	0.9500
C(31)-H(31)	0.9500	C(68)-C(82)	1.450(11)
C(32)-C(33)	1.395(12)	C(68)-C(69)	1.467(13)
C(32)-C(37)	1.407(13)	C(69)-C(70)	1.403(12)
C(33)-C(34)	1.387(14)	C(69)-C(79)	1.451(11)
C(33)-H(33)	0.9500	C(70)-C(72)	1.408(14)
C(34)-C(35)	1.366(13)	C(70)-C(71)	1.520(12)
C(34)-H(34)	0.9500	C(71)-H(71A)	0.9800
C(35)-C(36)	1.389(11)	C(71)-H(71B)	0.9800

C(71)-H(71C)	0.9800	P(1)-F(4)	1.561(8)
C(72)-C(73)	1.367(13)	P(1)-F(5)	1.562(7)
C(72)-H(72)	0.9500	P(1)-F(6)	1.580(7)
C(73)-C(74)	1.427(12)	P(1)-F(2)	1.595(7)
C(73)-H(73)	0.9500	P(1)-F(1)	1.611(7)
C(74)-C(78)	1.358(13)	P(2)-F(11A)	1.529(13)
C(74)-C(75)	1.521(12)	P(2)-F(8)	1.532(9)
C(75)-C(76)	1.509(13)	P(2)-F(11)	1.54(3)
C(75)-C(77)	1.537(13)	P(2)-F(10A)	1.567(15)
C(75)-H(75)	1.0000	P(2)-F(12A)	1.568(17)
C(76)-H(76A)	0.9800	P(2)-F(7)	1.570(9)
C(76)-H(76B)	0.9800	P(2)-F(9A)	1.572(11)
C(76)-H(76C)	0.9800	P(2)-F(10)	1.58(2)
C(77)-H(77A)	0.9800	P(2)-F(12)	1.588(17)
C(77)-H(77B)	0.9800	P(2)-F(9)	1.663(19)
C(77)-H(77C)	0.9800	P(3)-F(16)	1.43(2)
C(78)-C(79)	1.406(11)	P(3)-F(18A)	1.475(13)
C(78)-H(78)	0.9500	P(3)-F(17)	1.483(19)
C(79)-C(80)	1.427(12)	P(3)-F(17A)	1.540(11)
C(80)-C(82)	1.342(11)	P(3)-F(13)	1.568(7)
C(80)-C(81)	1.498(10)	P(3)-F(14)	1.579(7)
C(81)-H(81A)	0.9800	P(3)-F(15A)	1.583(15)
C(81)-H(81B)	0.9800	P(3)-F(16A)	1.652(12)
C(81)-H(81C)	0.9800	P(3)-F(15)	1.66(3)
C(82)-H(82)	0.9500	P(3)-F(18)	1.740(17)
P(1)-F(3)	1.545(8)		

Table S11: Bond angles [°] for **26**.

C(8)-C(1)-C(2)	127.7(8)	C(15)-C(17)-H(17B)	109.5
C(8)-C(1)-H(1)	116.2	H(17A)-C(17)-H(17B)	109.5
C(2)-C(1)-H(1)	116.2	C(15)-C(17)-H(17C)	109.5
C(7)-C(2)-C(3)	116.7(8)	H(17A)-C(17)-H(17C)	109.5
C(7)-C(2)-C(1)	124.8(7)	H(17B)-C(17)-H(17C)	109.5
C(3)-C(2)-C(1)	118.5(8)	C(19)-C(18)-C(14)	130.6(8)
C(4)-C(3)-C(2)	121.3(8)	C(19)-C(18)-H(18)	114.7
C(4)-C(3)-H(3)	119.4	C(14)-C(18)-H(18)	114.7
C(2)-C(3)-H(3)	119.4	C(18)-C(19)-C(20)	132.6(8)
C(3)-C(4)-C(5)	119.2(7)	C(18)-C(19)-H(19)	113.7
C(3)-C(4)-H(4)	120.4	C(20)-C(19)-H(19)	113.7
C(5)-C(4)-H(4)	120.4	C(22)-C(20)-C(19)	124.3(8)
C(4)-C(5)-C(6)	121.6(8)	C(22)-C(20)-C(21)	121.6(8)
C(4)-C(5)-Br(1)	119.6(6)	C(19)-C(20)-C(21)	114.1(7)
C(6)-C(5)-Br(1)	118.7(7)	C(20)-C(21)-H(21A)	109.5
C(7)-C(6)-C(5)	118.2(8)	C(20)-C(21)-H(21B)	109.5
C(7)-C(6)-H(6)	120.9	H(21A)-C(21)-H(21B)	109.5
C(5)-C(6)-H(6)	120.9	C(20)-C(21)-H(21C)	109.5
C(6)-C(7)-C(2)	122.9(7)	H(21A)-C(21)-H(21C)	109.5
C(6)-C(7)-H(7)	118.5	H(21B)-C(21)-H(21C)	109.5
C(2)-C(7)-H(7)	118.5	C(20)-C(22)-C(12)	127.1(8)
C(1)-C(8)-C(9)	125.1(8)	C(20)-C(22)-C(8)	128.1(8)
C(1)-C(8)-C(22)	127.3(8)	C(12)-C(22)-C(8)	104.7(7)
C(9)-C(8)-C(22)	106.8(7)	C(38)-C(31)-C(32)	127.7(9)
C(10)-C(9)-C(8)	110.1(8)	C(38)-C(31)-H(31)	116.2
C(10)-C(9)-H(9)	124.9	C(32)-C(31)-H(31)	116.2
C(8)-C(9)-H(9)	124.9	C(33)-C(32)-C(37)	117.5(9)
C(9)-C(10)-C(12)	109.7(8)	C(33)-C(32)-C(31)	117.8(9)
C(9)-C(10)-C(11)	126.6(8)	C(37)-C(32)-C(31)	124.6(8)
C(12)-C(10)-C(11)	123.7(8)	C(34)-C(33)-C(32)	121.6(9)
C(10)-C(11)-H(11A)	109.5	C(34)-C(33)-H(33)	119.2
C(10)-C(11)-H(11B)	109.5	C(32)-C(33)-H(33)	119.2
H(11A)-C(11)-H(11B)	109.5	C(35)-C(34)-C(33)	118.4(8)
C(10)-C(11)-H(11C)	109.5	C(35)-C(34)-H(34)	120.8
H(11A)-C(11)-H(11C)	109.5	C(33)-C(34)-H(34)	120.8
H(11B)-C(11)-H(11C)	109.5	C(34)-C(35)-C(36)	122.1(9)
C(13)-C(12)-C(22)	129.9(8)	C(34)-C(35)-Br(2)	118.5(7)
C(13)-C(12)-C(10)	121.5(7)	C(36)-C(35)-Br(2)	119.4(7)
C(22)-C(12)-C(10)	108.5(8)	C(37)-C(36)-C(35)	118.9(9)
C(14)-C(13)-C(12)	130.8(8)	C(37)-C(36)-H(36)	120.6
C(14)-C(13)-H(13)	114.6	C(35)-C(36)-H(36)	120.6
C(12)-C(13)-H(13)	114.6	C(36)-C(37)-C(32)	121.4(8)
C(13)-C(14)-C(18)	123.6(8)	C(36)-C(37)-H(37)	119.3
C(13)-C(14)-C(15)	120.2(7)	C(32)-C(37)-H(37)	119.3
C(18)-C(14)-C(15)	116.2(8)	C(31)-C(38)-C(52)	126.0(10)
C(16)-C(15)-C(14)	114.5(8)	C(31)-C(38)-C(39)	127.2(9)
C(16)-C(15)-C(17)	110.2(7)	C(52)-C(38)-C(39)	106.5(8)
C(14)-C(15)-C(17)	109.1(7)	C(40)-C(39)-C(49)	126.3(10)
C(16)-C(15)-H(15)	107.6	C(40)-C(39)-C(38)	128.6(9)
C(14)-C(15)-H(15)	107.6	C(49)-C(39)-C(38)	105.1(8)
C(17)-C(15)-H(15)	107.6	C(42)-C(40)-C(39)	124.3(10)
C(15)-C(16)-H(16A)	109.5	C(42)-C(40)-C(41)	114.1(10)
C(15)-C(16)-H(16B)	109.5	C(39)-C(40)-C(41)	121.6(10)
H(16A)-C(16)-H(16B)	109.5	C(40)-C(41)-H(41A)	109.5
C(15)-C(16)-H(16C)	109.5	C(40)-C(41)-H(41B)	109.5
H(16A)-C(16)-H(16C)	109.5	H(41A)-C(41)-H(41B)	109.5
H(16B)-C(16)-H(16C)	109.5	C(40)-C(41)-H(41C)	109.5
C(15)-C(17)-H(17A)	109.5	H(41A)-C(41)-H(41C)	109.5

H(41B)-C(41)-H(41C)	109.5	C(66)-C(65)-Br(3)	118.9(8)
C(43)-C(42)-C(40)	134.1(11)	C(67)-C(66)-C(65)	118.6(9)
C(43)-C(42)-H(42)	112.9	C(67)-C(66)-H(66)	120.7
C(40)-C(42)-H(42)	112.9	C(65)-C(66)-H(66)	120.7
C(42)-C(43)-C(44)	129.9(11)	C(66)-C(67)-C(62)	121.5(8)
C(42)-C(43)-H(43)	115.1	C(66)-C(67)-H(67)	119.2
C(44)-C(43)-H(43)	115.1	C(62)-C(67)-H(67)	119.2
C(48)-C(44)-C(43)	124.1(10)	C(61)-C(68)-C(82)	127.2(9)
C(48)-C(44)-C(45)	117.7(10)	C(61)-C(68)-C(69)	126.6(8)
C(43)-C(44)-C(45)	118.1(10)	C(82)-C(68)-C(69)	105.4(7)
C(46)-C(45)-C(47)	117.5(14)	C(70)-C(69)-C(79)	125.7(9)
C(46)-C(45)-C(44)	113.9(12)	C(70)-C(69)-C(68)	127.9(8)
C(47)-C(45)-C(44)	111.5(10)	C(79)-C(69)-C(68)	106.1(7)
C(46)-C(45)-H(45)	104.0	C(69)-C(70)-C(72)	124.9(8)
C(47)-C(45)-H(45)	104.0	C(69)-C(70)-C(71)	121.8(9)
C(44)-C(45)-H(45)	104.0	C(72)-C(70)-C(71)	113.3(8)
C(45)-C(46)-H(46A)	109.5	C(70)-C(71)-H(71A)	109.5
C(45)-C(46)-H(46B)	109.5	C(70)-C(71)-H(71B)	109.5
H(46A)-C(46)-H(46B)	109.5	H(71A)-C(71)-H(71B)	109.5
C(45)-C(46)-H(46C)	109.5	C(70)-C(71)-H(71C)	109.5
H(46A)-C(46)-H(46C)	109.5	H(71A)-C(71)-H(71C)	109.5
H(46B)-C(46)-H(46C)	109.5	H(71B)-C(71)-H(71C)	109.5
C(45)-C(47)-H(47A)	109.5	C(73)-C(72)-C(70)	131.8(9)
C(45)-C(47)-H(47B)	109.5	C(73)-C(72)-H(72)	114.1
H(47A)-C(47)-H(47B)	109.5	C(70)-C(72)-H(72)	114.1
C(45)-C(47)-H(47C)	109.5	C(72)-C(73)-C(74)	131.0(10)
H(47A)-C(47)-H(47C)	109.5	C(72)-C(73)-H(73)	114.5
H(47B)-C(47)-H(47C)	109.5	C(74)-C(73)-H(73)	114.5
C(44)-C(48)-C(49)	131.2(10)	C(78)-C(74)-C(73)	123.1(9)
C(44)-C(48)-H(48)	114.4	C(78)-C(74)-C(75)	121.4(8)
C(49)-C(48)-H(48)	114.4	C(73)-C(74)-C(75)	115.4(9)
C(48)-C(49)-C(50)	121.5(9)	C(76)-C(75)-C(74)	114.8(8)
C(48)-C(49)-C(39)	129.8(10)	C(76)-C(75)-C(77)	111.6(9)
C(50)-C(49)-C(39)	108.7(9)	C(74)-C(75)-C(77)	106.6(8)
C(52)-C(50)-C(49)	108.7(9)	C(76)-C(75)-H(75)	107.9
C(52)-C(50)-C(51)	126.4(10)	C(74)-C(75)-H(75)	107.9
C(49)-C(50)-C(51)	124.9(10)	C(77)-C(75)-H(75)	107.9
C(50)-C(51)-H(51A)	109.5	C(75)-C(76)-H(76A)	109.5
C(50)-C(51)-H(51B)	109.5	C(75)-C(76)-H(76B)	109.5
H(51A)-C(51)-H(51B)	109.5	H(76A)-C(76)-H(76B)	109.5
C(50)-C(51)-H(51C)	109.5	C(75)-C(76)-H(76C)	109.5
H(51A)-C(51)-H(51C)	109.5	H(76A)-C(76)-H(76C)	109.5
H(51B)-C(51)-H(51C)	109.5	H(76B)-C(76)-H(76C)	109.5
C(50)-C(52)-C(38)	111.0(10)	C(75)-C(77)-H(77A)	109.5
C(50)-C(52)-H(52)	124.5	C(75)-C(77)-H(77B)	109.5
C(38)-C(52)-H(52)	124.5	H(77A)-C(77)-H(77B)	109.5
C(68)-C(61)-C(62)	127.6(8)	C(75)-C(77)-H(77C)	109.5
C(68)-C(61)-H(61)	116.2	H(77A)-C(77)-H(77C)	109.5
C(62)-C(61)-H(61)	116.2	H(77B)-C(77)-H(77C)	109.5
C(67)-C(62)-C(63)	117.6(9)	C(74)-C(78)-C(79)	131.5(8)
C(67)-C(62)-C(61)	124.1(8)	C(74)-C(78)-H(78)	114.3
C(63)-C(62)-C(61)	118.2(8)	C(79)-C(78)-H(78)	114.3
C(64)-C(63)-C(62)	121.6(9)	C(78)-C(79)-C(80)	122.1(7)
C(64)-C(63)-H(63)	119.2	C(78)-C(79)-C(69)	129.7(8)
C(62)-C(63)-H(63)	119.2	C(80)-C(79)-C(69)	108.2(7)
C(63)-C(64)-C(65)	118.1(8)	C(82)-C(80)-C(79)	109.0(7)
C(63)-C(64)-H(64)	120.9	C(82)-C(80)-C(81)	126.7(8)
C(65)-C(64)-H(64)	120.9	C(79)-C(80)-C(81)	124.3(8)
C(64)-C(65)-C(66)	122.5(9)	C(80)-C(81)-H(81A)	109.5
C(64)-C(65)-Br(3)	118.5(6)	C(80)-C(81)-H(81B)	109.5

H(81A)-C(81)-H(81B)	109.5	F(11)-P(2)-F(10)	90(2)
C(80)-C(81)-H(81C)	109.5	F(7)-P(2)-F(10)	89.9(10)
H(81A)-C(81)-H(81C)	109.5	F(8)-P(2)-F(12)	75.7(11)
H(81B)-C(81)-H(81C)	109.5	F(11)-P(2)-F(12)	84.3(16)
C(80)-C(82)-C(68)	111.3(8)	F(7)-P(2)-F(12)	108.2(11)
C(80)-C(82)-H(82)	124.4	F(10)-P(2)-F(12)	161.2(15)
C(68)-C(82)-H(82)	124.4	F(8)-P(2)-F(9)	76.1(10)
F(3)-P(1)-F(4)	91.7(6)	F(11)-P(2)-F(9)	165.6(17)
F(3)-P(1)-F(5)	177.8(6)	F(7)-P(2)-F(9)	103.0(9)
F(4)-P(1)-F(5)	90.1(5)	F(10)-P(2)-F(9)	92(2)
F(3)-P(1)-F(6)	88.3(6)	F(12)-P(2)-F(9)	88.7(13)
F(4)-P(1)-F(6)	177.1(5)	F(16)-P(3)-F(17)	100.7(18)
F(5)-P(1)-F(6)	89.8(5)	F(18A)-P(3)-F(17A)	95.9(11)
F(3)-P(1)-F(2)	91.3(5)	F(16)-P(3)-F(13)	89.8(12)
F(4)-P(1)-F(2)	92.0(4)	F(18A)-P(3)-F(13)	94.5(7)
F(5)-P(1)-F(2)	89.8(5)	F(17)-P(3)-F(13)	79.5(11)
F(6)-P(1)-F(2)	90.9(4)	F(17A)-P(3)-F(13)	95.8(7)
F(3)-P(1)-F(1)	89.5(5)	F(16)-P(3)-F(14)	90.1(12)
F(4)-P(1)-F(1)	88.6(4)	F(18A)-P(3)-F(14)	85.7(7)
F(5)-P(1)-F(1)	89.4(4)	F(17)-P(3)-F(14)	100.4(11)
F(6)-P(1)-F(1)	88.5(4)	F(17A)-P(3)-F(14)	84.1(7)
F(2)-P(1)-F(1)	179.0(4)	F(13)-P(3)-F(14)	179.8(5)
F(11A)-P(2)-F(8)	87.1(7)	F(18A)-P(3)-F(15A)	89.6(12)
F(8)-P(2)-F(11)	89.9(17)	F(17A)-P(3)-F(15A)	170.4(10)
F(11A)-P(2)-F(10A)	92.1(10)	F(13)-P(3)-F(15A)	91.5(8)
F(8)-P(2)-F(10A)	96.3(10)	F(14)-P(3)-F(15A)	88.5(8)
F(11A)-P(2)-F(12A)	85.4(11)	F(18A)-P(3)-F(16A)	172.3(8)
F(8)-P(2)-F(12A)	98.7(9)	F(17A)-P(3)-F(16A)	86.7(9)
F(10A)-P(2)-F(12A)	164.7(12)	F(13)-P(3)-F(16A)	92.5(5)
F(11A)-P(2)-F(7)	91.4(8)	F(14)-P(3)-F(16A)	87.3(6)
F(8)-P(2)-F(7)	176.0(6)	F(15A)-P(3)-F(16A)	86.9(11)
F(11)-P(2)-F(7)	91.2(16)	F(16)-P(3)-F(15)	90.4(17)
F(10A)-P(2)-F(7)	80.0(9)	F(17)-P(3)-F(15)	161(2)
F(12A)-P(2)-F(7)	84.9(8)	F(13)-P(3)-F(15)	85.4(14)
F(11A)-P(2)-F(9A)	167.4(9)	F(14)-P(3)-F(15)	94.7(14)
F(8)-P(2)-F(9A)	104.9(7)	F(16)-P(3)-F(18)	166.8(15)
F(10A)-P(2)-F(9A)	90.6(9)	F(17)-P(3)-F(18)	88.1(13)
F(12A)-P(2)-F(9A)	88.7(8)	F(13)-P(3)-F(18)	82.1(6)
F(7)-P(2)-F(9A)	76.9(7)	F(14)-P(3)-F(18)	98.1(6)
F(8)-P(2)-F(10)	86.2(10)	F(15)-P(3)-F(18)	78.7(14)

Symmetry transformations used to generate equivalent atoms:

Table S12: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **26**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	44(1)	58(1)	50(1)	15(1)	2(1)	4(1)
C(1)	28(4)	53(6)	38(4)	-10(4)	-2(3)	-4(4)
C(2)	27(4)	51(5)	30(4)	-3(4)	3(3)	0(4)
C(3)	29(4)	49(5)	33(4)	-3(4)	-1(4)	-2(4)
C(4)	32(4)	67(6)	26(4)	4(4)	-1(3)	-3(4)
C(5)	29(4)	53(5)	30(4)	8(4)	-1(3)	3(4)
C(6)	27(4)	51(5)	38(4)	-1(4)	6(3)	-3(4)
C(7)	27(4)	59(6)	23(4)	-2(3)	-2(3)	-2(4)
C(8)	22(4)	50(5)	43(5)	-5(4)	0(3)	2(4)
C(9)	32(4)	49(5)	41(5)	-3(4)	1(4)	-2(4)
C(10)	38(4)	47(5)	35(4)	0(4)	-6(4)	2(4)
C(11)	69(7)	40(5)	54(6)	-8(4)	7(5)	3(5)
C(12)	29(4)	49(5)	36(4)	-6(4)	-4(4)	2(4)
C(13)	26(4)	47(5)	38(4)	-5(4)	-4(3)	-4(4)
C(14)	23(4)	40(5)	43(4)	-6(4)	-8(3)	2(3)
C(15)	38(4)	42(5)	48(5)	1(4)	-4(4)	-1(4)
C(16)	45(5)	60(7)	59(6)	12(5)	-1(4)	-3(5)
C(17)	41(5)	43(5)	67(6)	9(5)	-4(5)	4(4)
C(18)	38(4)	40(5)	59(5)	-4(4)	-12(4)	-2(4)
C(19)	35(4)	49(6)	42(5)	-14(4)	-4(4)	3(4)
C(20)	28(4)	43(5)	36(4)	-6(3)	-8(3)	5(4)
C(21)	38(5)	49(6)	46(5)	-4(4)	0(4)	6(4)
C(22)	21(4)	48(5)	37(4)	-6(4)	-9(3)	1(3)
Br(2)	45(1)	78(1)	53(1)	-14(1)	1(1)	-7(1)
C(31)	37(5)	68(7)	49(5)	8(5)	4(4)	12(5)
C(32)	35(4)	64(6)	40(5)	4(4)	8(4)	6(5)
C(33)	37(5)	74(7)	41(5)	8(5)	-6(4)	9(5)
C(34)	37(4)	83(7)	34(5)	-1(5)	-1(4)	3(5)
C(35)	29(4)	62(6)	36(4)	0(4)	-3(3)	3(4)
C(36)	34(4)	61(6)	44(5)	0(4)	1(4)	7(5)
C(37)	26(4)	79(7)	26(4)	-7(4)	-1(3)	3(4)
C(38)	31(4)	63(6)	41(5)	-5(4)	5(4)	1(4)
C(39)	31(4)	61(6)	50(5)	5(4)	-4(4)	9(4)
C(40)	27(4)	74(7)	65(6)	9(5)	6(4)	-6(5)
C(41)	80(9)	104(11)	58(7)	14(7)	18(6)	-31(8)
C(42)	51(6)	61(7)	61(6)	10(5)	3(5)	-7(5)
C(43)	46(5)	66(7)	84(7)	-4(6)	-2(5)	8(6)
C(44)	58(6)	58(7)	60(6)	-9(5)	-14(5)	20(5)
C(45)	112(12)	65(8)	77(8)	-14(6)	-7(8)	13(8)
C(46)	90(12)	320(30)	164(16)	-174(19)	-75(12)	109(16)
C(47)	55(6)	69(8)	91(8)	-29(6)	1(6)	7(6)
C(48)	47(6)	63(7)	50(5)	-3(5)	-8(4)	17(5)
C(49)	36(5)	64(6)	50(5)	-3(5)	-5(4)	5(5)
C(50)	48(5)	63(6)	45(5)	3(5)	-4(5)	16(5)
C(51)	88(9)	70(8)	51(6)	4(5)	12(6)	12(7)
C(52)	49(6)	69(7)	47(5)	-1(5)	11(5)	0(5)
Br(3)	58(1)	66(1)	53(1)	-11(1)	6(1)	-5(1)
C(61)	29(4)	68(6)	38(4)	10(4)	-7(4)	5(4)
C(62)	33(4)	60(6)	29(4)	-5(4)	5(3)	1(4)
C(63)	38(5)	74(7)	33(4)	3(4)	-2(3)	4(5)
C(64)	38(4)	72(6)	27(4)	-7(4)	1(4)	-1(4)
C(65)	34(5)	74(7)	30(4)	-3(4)	8(3)	1(4)
C(66)	34(4)	60(6)	40(5)	4(4)	-2(4)	7(4)
C(67)	28(4)	68(6)	38(4)	5(4)	-3(4)	5(4)
C(68)	25(4)	55(5)	38(4)	3(4)	-6(4)	-3(4)

C(69)	25(4)	54(6)	39(4)	10(4)	-5(3)	-5(4)
C(70)	31(4)	62(6)	39(4)	13(4)	-16(4)	-2(4)
C(71)	51(6)	73(7)	51(5)	20(5)	6(4)	-11(5)
C(72)	43(5)	53(6)	54(5)	17(5)	-10(4)	-8(5)
C(73)	48(5)	52(6)	57(6)	11(5)	-17(5)	0(5)
C(74)	27(4)	48(5)	50(5)	-3(4)	-10(3)	5(4)
C(75)	42(5)	46(6)	69(6)	-6(5)	-7(5)	1(4)
C(76)	57(6)	62(7)	59(6)	-13(5)	-1(5)	17(5)
C(77)	57(6)	68(7)	64(6)	-27(5)	-7(5)	3(6)
C(78)	26(4)	49(5)	37(4)	0(4)	-6(3)	0(4)
C(79)	23(3)	48(5)	38(4)	0(4)	-5(3)	-4(3)
C(80)	31(4)	50(5)	30(4)	0(4)	-4(4)	-3(4)
C(81)	64(6)	50(6)	32(4)	5(4)	6(4)	-2(5)
C(82)	33(4)	46(5)	38(4)	0(4)	9(3)	-2(4)
P(1)	48(1)	70(2)	39(1)	-5(1)	7(1)	3(1)
F(1)	58(3)	79(4)	69(4)	-12(3)	0(3)	-3(3)
F(2)	79(5)	98(6)	88(5)	-35(4)	-4(4)	-5(4)
F(3)	214(12)	133(8)	61(4)	-5(5)	-60(6)	47(8)
F(4)	107(6)	94(6)	157(7)	-33(5)	88(6)	-12(5)
F(5)	111(6)	105(6)	114(6)	51(5)	-37(5)	-29(5)
F(6)	53(4)	164(8)	114(6)	-69(6)	27(4)	-22(5)
P(2)	71(2)	67(2)	41(1)	-4(1)	-1(1)	11(2)
F(7)	123(7)	160(9)	97(6)	62(6)	16(6)	31(7)
F(8)	209(12)	67(5)	127(7)	-2(5)	-26(8)	24(6)
F(9)	66(13)	97(16)	190(30)	-38(17)	-45(17)	-8(11)
F(10)	260(50)	140(30)	71(16)	22(16)	90(20)	110(30)
F(11)	100(20)	150(30)	310(50)	-110(30)	60(30)	-51(19)
F(12)	140(20)	125(19)	140(20)	-60(16)	110(18)	-5(17)
F(9A)	82(10)	126(13)	57(7)	-31(7)	1(6)	-18(9)
F(10A)	81(10)	230(20)	73(10)	-3(12)	42(8)	-28(12)
F(11A)	134(16)	103(11)	46(7)	-21(7)	-17(9)	-6(13)
F(12A)	52(8)	210(20)	126(13)	-49(14)	-23(8)	51(10)
P(3)	55(2)	66(2)	39(1)	-12(1)	-6(1)	9(1)
F(13)	90(5)	68(5)	110(5)	-23(4)	37(4)	3(4)
F(14)	104(6)	121(7)	83(5)	-49(5)	0(5)	35(5)
F(15)	75(18)	200(40)	110(20)	30(20)	-10(16)	10(20)
F(16)	90(20)	43(13)	200(40)	-16(17)	10(20)	-32(14)
F(17)	81(17)	190(30)	32(10)	5(12)	-3(9)	14(18)
F(18)	60(11)	55(11)	79(14)	-11(9)	36(10)	-4(8)
F(15A)	62(9)	150(20)	200(30)	-58(17)	-62(14)	21(11)
F(16A)	138(16)	62(8)	79(9)	8(6)	26(9)	-4(9)
F(17A)	56(8)	121(12)	117(14)	-36(10)	-30(8)	-5(8)
F(18A)	190(20)	79(10)	65(9)	20(7)	21(13)	9(13)

Table S13: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **26**.

	x	y	z	U(eq)
H(1)	9239	2853	5447	48
H(3)	10535	2239	5927	44
H(4)	10815	1417	6145	50
H(6)	8508	950	5069	46
H(7)	8164	1769	4864	43
H(9)	9762	2157	4437	49
H(11A)	9733	2821	3491	81
H(11B)	10410	2294	3662	81
H(11C)	11746	2755	3630	81
H(13)	10485	3624	3705	44
H(15)	11417	4858	3816	51
H(16A)	11033	4113	3188	82
H(16B)	12782	4165	3464	82
H(16C)	12201	4609	3158	82
H(17A)	9270	5040	3303	76
H(17B)	8351	4965	3750	76
H(17C)	8264	4530	3407	76
H(18)	10013	4797	4448	54
H(19)	8970	4476	5018	50
H(21A)	7313	3394	5361	66
H(21B)	7358	3987	5417	66
H(21C)	8970	3655	5580	66
H(31)	4594	7148	7115	61
H(33)	6048	7709	7589	61
H(34)	6642	8519	7819	61
H(36)	4567	9063	6743	56
H(37)	4058	8261	6507	52
H(41A)	2813	6040	7187	121
H(41B)	2705	6630	7116	121
H(41C)	4537	6377	7245	121
H(42)	3488	5543	6704	69
H(43)	3778	5191	6104	79
H(45)	4968	5600	5108	102
H(46A)	2879	4989	4971	287
H(46B)	2286	5560	5006	287
H(46C)	1934	5186	5388	287
H(47A)	6843	5117	5449	107
H(47B)	5666	4756	5164	107
H(47C)	5301	4794	5657	107
H(48)	4913	6322	5360	64
H(51A)	5845	7629	5321	105
H(51B)	4574	7193	5160	105
H(51C)	6617	7082	5242	105
H(52)	5439	7792	6099	66
H(61)	4940	6776	3744	54
H(63)	5787	7398	4260	58
H(64)	5447	8197	4527	55
H(66)	3561	8659	3400	54
H(67)	3745	7850	3146	54
H(71A)	3084	6215	3646	87
H(71B)	4741	5968	3877	87
H(71C)	3206	5622	3692	87
H(72)	5123	5168	3332	60
H(73)	6238	4869	2766	63

H(75)	7498	4817	2110	63
H(76A)	7978	5053	1433	89
H(76B)	8578	5517	1715	89
H(76C)	6722	5530	1477	89
H(77A)	4098	5089	1791	95
H(77B)	4460	4659	2128	95
H(77C)	5131	4595	1655	95
H(78)	6377	6039	2008	45
H(81A)	7519	6884	1927	73
H(81B)	6341	7375	1984	73
H(81C)	5483	6877	1797	73
H(82)	5416	7494	2744	47

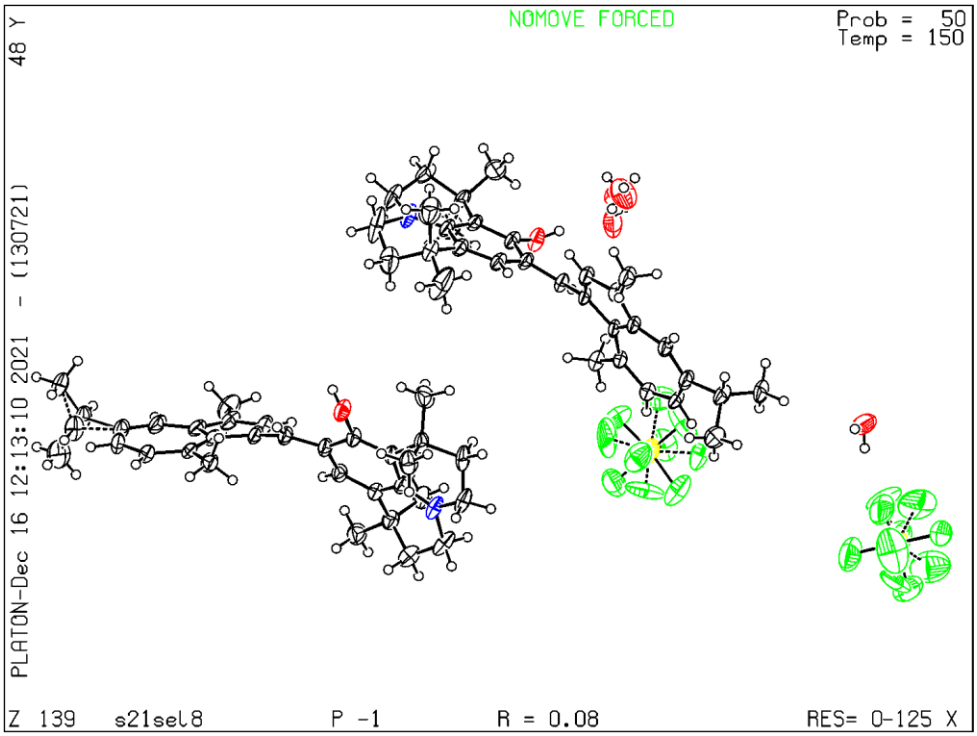
Table S14: Torsion angles [°] for **26**.

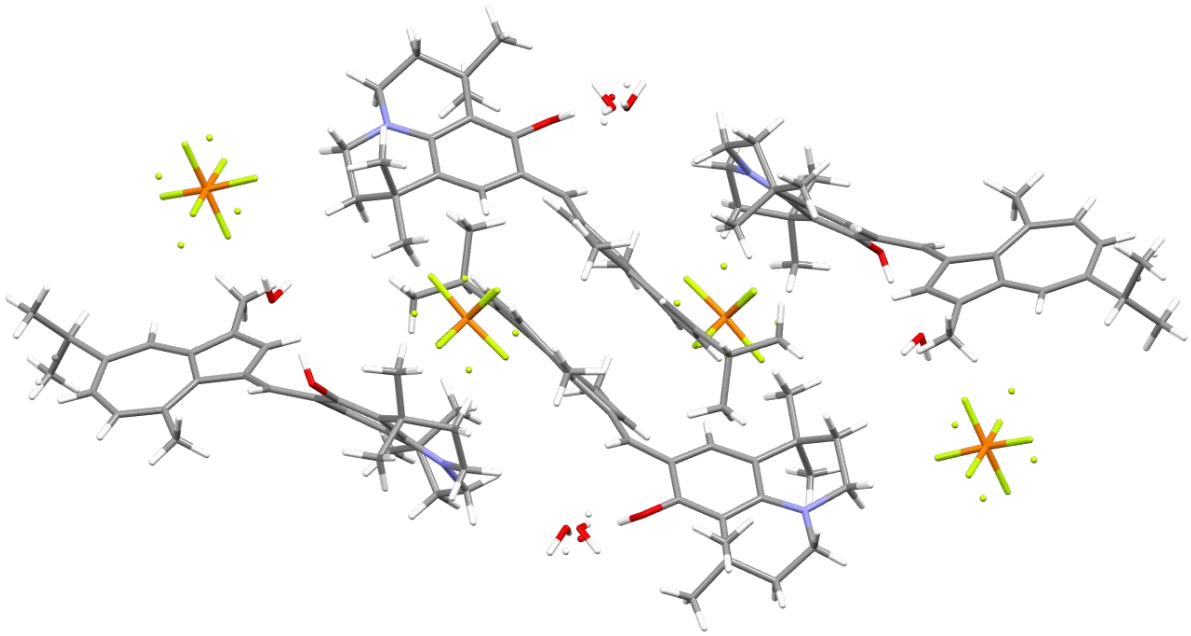
C(8)-C(1)-C(2)-C(7)	-30.4(14)	C(31)-C(32)-C(37)-C(36)	179.2(9)
C(8)-C(1)-C(2)-C(3)	150.1(8)	C(32)-C(31)-C(38)-C(52)	8.2(16)
C(7)-C(2)-C(3)-C(4)	3.4(12)	C(32)-C(31)-C(38)-C(39)	-179.0(9)
C(1)-C(2)-C(3)-C(4)	-177.1(8)	C(31)-C(38)-C(39)-C(40)	7.4(16)
C(2)-C(3)-C(4)-C(5)	-0.3(12)	C(52)-C(38)-C(39)-C(40)	-178.7(9)
C(3)-C(4)-C(5)-C(6)	-2.0(12)	C(31)-C(38)-C(39)-C(49)	-172.8(9)
C(3)-C(4)-C(5)-Br(1)	176.5(6)	C(52)-C(38)-C(39)-C(49)	1.1(10)
C(4)-C(5)-C(6)-C(7)	1.1(12)	C(49)-C(39)-C(40)-C(42)	5.7(15)
Br(1)-C(5)-C(6)-C(7)	-177.5(6)	C(38)-C(39)-C(40)-C(42)	-174.6(9)
C(5)-C(6)-C(7)-C(2)	2.3(12)	C(49)-C(39)-C(40)-C(41)	-174.6(9)
C(3)-C(2)-C(7)-C(6)	-4.4(12)	C(38)-C(39)-C(40)-C(41)	5.1(15)
C(1)-C(2)-C(7)-C(6)	176.1(8)	C(39)-C(40)-C(42)-C(43)	-4.8(19)
C(2)-C(1)-C(8)-C(9)	-8.1(14)	C(41)-C(40)-C(42)-C(43)	175.5(12)
C(2)-C(1)-C(8)-C(22)	-176.7(8)	C(40)-C(42)-C(43)-C(44)	-1(2)
C(1)-C(8)-C(9)-C(10)	-167.8(8)	C(42)-C(43)-C(44)-C(48)	4.2(19)
C(22)-C(8)-C(9)-C(10)	2.8(10)	C(42)-C(43)-C(44)-C(45)	-179.6(11)
C(8)-C(9)-C(10)-C(12)	-0.5(10)	C(48)-C(44)-C(45)-C(46)	-101.4(18)
C(8)-C(9)-C(10)-C(11)	178.1(9)	C(43)-C(44)-C(45)-C(46)	82.1(18)
C(9)-C(10)-C(12)-C(13)	177.4(7)	C(48)-C(44)-C(45)-C(47)	122.7(12)
C(11)-C(10)-C(12)-C(13)	-1.2(14)	C(43)-C(44)-C(45)-C(47)	-53.7(16)
C(9)-C(10)-C(12)-C(22)	-2.0(10)	C(43)-C(44)-C(48)-C(49)	-1.9(18)
C(11)-C(10)-C(12)-C(22)	179.3(8)	C(45)-C(44)-C(48)-C(49)	-178.1(10)
C(22)-C(12)-C(13)-C(14)	3.3(15)	C(44)-C(48)-C(49)-C(50)	178.7(10)
C(10)-C(12)-C(13)-C(14)	-176.0(8)	C(44)-C(48)-C(49)-C(39)	-0.3(18)
C(12)-C(13)-C(14)-C(18)	-3.6(14)	C(40)-C(39)-C(49)-C(48)	-2.1(16)
C(12)-C(13)-C(14)-C(15)	178.8(8)	C(38)-C(39)-C(49)-C(48)	178.1(9)
C(13)-C(14)-C(15)-C(16)	-23.7(11)	C(40)-C(39)-C(49)-C(50)	178.7(9)
C(18)-C(14)-C(15)-C(16)	158.5(8)	C(38)-C(39)-C(49)-C(50)	-1.1(10)
C(13)-C(14)-C(15)-C(17)	100.3(9)	C(48)-C(49)-C(50)-C(52)	-178.6(9)
C(18)-C(14)-C(15)-C(17)	-77.4(9)	C(39)-C(49)-C(50)-C(52)	0.6(11)
C(13)-C(14)-C(18)-C(19)	-4.4(14)	C(48)-C(49)-C(50)-C(51)	1.3(15)
C(15)-C(14)-C(18)-C(19)	173.3(8)	C(39)-C(49)-C(50)-C(51)	-179.5(9)
C(14)-C(18)-C(19)-C(20)	5.2(17)	C(49)-C(50)-C(52)-C(38)	0.2(12)
C(18)-C(19)-C(20)-C(22)	5.7(15)	C(51)-C(50)-C(52)-C(38)	-179.8(10)
C(18)-C(19)-C(20)-C(21)	-173.2(9)	C(31)-C(38)-C(52)-C(50)	173.2(9)
C(19)-C(20)-C(22)-C(12)	-13.2(13)	C(39)-C(38)-C(52)-C(50)	-0.8(11)
C(21)-C(20)-C(22)-C(12)	165.7(8)	C(68)-C(61)-C(62)-C(67)	27.5(15)
C(19)-C(20)-C(22)-C(8)	171.3(8)	C(68)-C(61)-C(62)-C(63)	-157.3(9)
C(21)-C(20)-C(22)-C(8)	-9.8(13)	C(67)-C(62)-C(63)-C(64)	-0.8(13)
C(13)-C(12)-C(22)-C(20)	7.8(14)	C(61)-C(62)-C(63)-C(64)	-176.3(8)
C(10)-C(12)-C(22)-C(20)	-172.8(8)	C(62)-C(63)-C(64)-C(65)	-1.5(13)
C(13)-C(12)-C(22)-C(8)	-175.8(8)	C(63)-C(64)-C(65)-C(66)	2.0(13)
C(10)-C(12)-C(22)-C(8)	3.6(9)	C(63)-C(64)-C(65)-Br(3)	179.7(7)
C(1)-C(8)-C(22)-C(20)	-17.2(13)	C(64)-C(65)-C(66)-C(67)	0.0(13)
C(9)-C(8)-C(22)-C(20)	172.5(8)	Br(3)-C(65)-C(66)-C(67)	-177.7(7)
C(1)-C(8)-C(22)-C(12)	166.5(8)	C(65)-C(66)-C(67)-C(62)	-2.5(13)
C(9)-C(8)-C(22)-C(12)	-3.9(8)	C(63)-C(62)-C(67)-C(66)	2.9(13)
C(38)-C(31)-C(32)-C(33)	-153.6(9)	C(61)-C(62)-C(67)-C(66)	178.1(9)
C(38)-C(31)-C(32)-C(37)	29.8(15)	C(62)-C(61)-C(68)-C(82)	10.6(15)
C(37)-C(32)-C(33)-C(34)	-3.6(14)	C(62)-C(61)-C(68)-C(69)	178.9(8)
C(31)-C(32)-C(33)-C(34)	179.5(9)	C(61)-C(68)-C(69)-C(70)	18.4(14)
C(32)-C(33)-C(34)-C(35)	2.3(14)	C(82)-C(68)-C(69)-C(70)	-171.3(8)
C(33)-C(34)-C(35)-C(36)	0.1(13)	C(61)-C(68)-C(69)-C(79)	-167.1(8)
C(33)-C(34)-C(35)-Br(2)	-179.7(7)	C(82)-C(68)-C(69)-C(79)	3.2(9)
C(34)-C(35)-C(36)-C(37)	-1.1(13)	C(79)-C(69)-C(70)-C(72)	17.5(13)
Br(2)-C(35)-C(36)-C(37)	178.7(6)	C(68)-C(69)-C(70)-C(72)	-169.0(8)
C(35)-C(36)-C(37)-C(32)	-0.3(13)	C(79)-C(69)-C(70)-C(71)	-164.5(8)
C(33)-C(32)-C(37)-C(36)	2.6(13)	C(68)-C(69)-C(70)-C(71)	9.0(13)

C(69)-C(70)-C(72)-C(73)	-11.5(15)	C(70)-C(69)-C(79)-C(78)	-6.5(13)
C(71)-C(70)-C(72)-C(73)	170.4(10)	C(68)-C(69)-C(79)-C(78)	178.8(8)
C(70)-C(72)-C(73)-C(74)	-4.6(18)	C(70)-C(69)-C(79)-C(80)	171.3(8)
C(72)-C(73)-C(74)-C(78)	7.6(16)	C(68)-C(69)-C(79)-C(80)	-3.4(8)
C(72)-C(73)-C(74)-C(75)	-168.4(10)	C(78)-C(79)-C(80)-C(82)	-179.7(7)
C(78)-C(74)-C(75)-C(76)	21.3(12)	C(69)-C(79)-C(80)-C(82)	2.3(9)
C(73)-C(74)-C(75)-C(76)	-162.6(8)	C(78)-C(79)-C(80)-C(81)	-1.7(13)
C(78)-C(74)-C(75)-C(77)	-102.8(10)	C(69)-C(79)-C(80)-C(81)	-179.7(8)
C(73)-C(74)-C(75)-C(77)	73.3(10)	C(79)-C(80)-C(82)-C(68)	-0.2(10)
C(73)-C(74)-C(78)-C(79)	3.2(14)	C(81)-C(80)-C(82)-C(68)	-178.2(8)
C(75)-C(74)-C(78)-C(79)	179.0(8)	C(61)-C(68)-C(82)-C(80)	168.3(9)
C(74)-C(78)-C(79)-C(80)	175.9(8)	C(69)-C(68)-C(82)-C(80)	-1.9(10)
C(74)-C(78)-C(79)-C(69)	-6.6(14)		

Table S15: Crystal data and structure refinement for **30**.

CCDC code	#2129314	
Empirical formula	$C_{128}H_{171}F_{24}N_4O_{9.50}P_4$	
Formula weight	2497.56	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.3599(10) Å	α= 75.138(5)°.
	b = 12.9645(7) Å	β= 74.245(6)°.
	c = 20.9049(12) Å	γ = 83.084(6)°.
Volume	3111.5(4) $Å^3$	
Z	1	
Density (calculated)	1.333 Mg/m^3	
Absorption coefficient	1.371 mm^{-1}	
F(000)	1319	
Crystal size	0.250 x 0.200 x 0.150 mm^3	
Theta range for data collection	4.521 to 68.847°.	
Index ranges	-14<=h<=14, -15<=k<=15, -25<=l<=25	
Reflections collected	20034	
Independent reflections	20034 [R(int) = ?]	
Completeness to theta = 67.684°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.90720	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20034 / 110 / 890	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0807, wR2 = 0.2207	
R indices (all data)	R1 = 0.1176, wR2 = 0.2420	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.023 and -0.489 $e.Å^{-3}$	





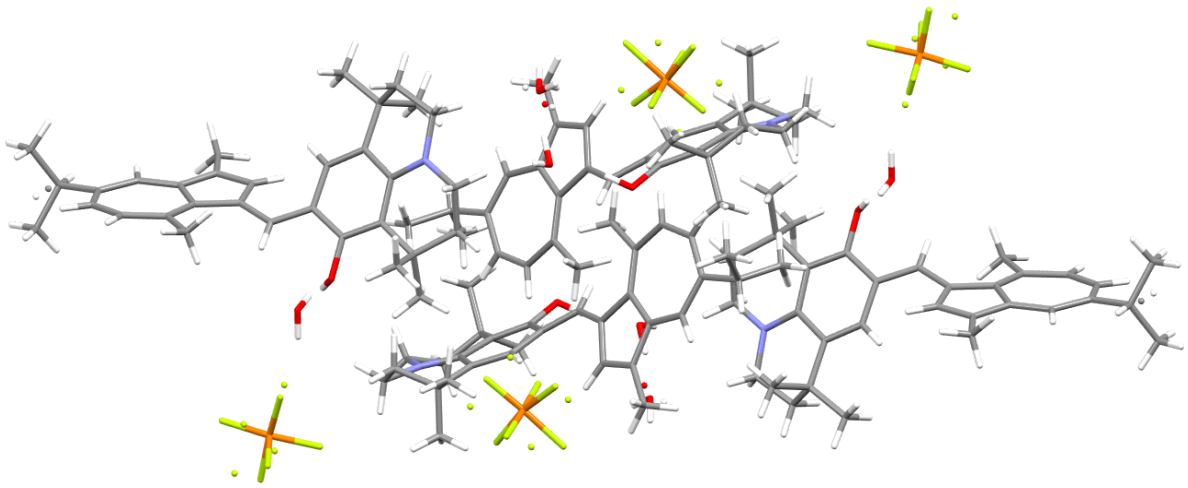


Table S16: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **30**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	2714(3)	6359(3)	8771(2)	45(1)
O(1)	879(3)	5854(3)	7169(1)	45(1)
C(1)	2813(3)	6312(3)	6114(2)	34(1)
C(2)	2753(3)	6490(3)	6751(2)	33(1)
C(3)	1753(3)	6200(3)	7301(2)	33(1)
C(4)	1701(3)	6225(3)	7966(2)	32(1)
C(5)	602(4)	5976(3)	8527(2)	38(1)
C(6)	459(4)	4768(4)	8742(2)	47(1)
C(7)	-428(4)	6558(5)	8302(2)	62(1)
C(8)	685(4)	6383(4)	9135(2)	47(1)
C(9)	1743(4)	6028(4)	9343(2)	50(1)
C(10)	3741(5)	6444(6)	8985(2)	80(2)
C(11)	4818(5)	6298(5)	8422(3)	68(1)
C(12)	4703(4)	7076(3)	7760(2)	40(1)
C(13)	4504(6)	8217(5)	7845(3)	70(2)
C(14)	5789(5)	7022(8)	7213(3)	97(3)
C(15)	3688(3)	6792(3)	7576(2)	35(1)
C(16)	3670(3)	6824(3)	6925(2)	34(1)
C(17)	2684(3)	6458(3)	8123(2)	34(1)
C(18)	3558(3)	6769(3)	5480(2)	33(1)
C(19)	3995(3)	7792(3)	5319(2)	38(1)
C(20)	4543(4)	8100(3)	4639(2)	39(1)
C(21)	5074(4)	9142(4)	4285(2)	50(1)
C(22)	4515(3)	7247(3)	4335(2)	33(1)
C(23)	4987(3)	7326(3)	3641(2)	40(1)
C(24)	5066(4)	6595(3)	3249(2)	39(1)
C(25)	5565(4)	6969(4)	2478(2)	48(1)
C(26)	4705(4)	6935(4)	2088(2)	56(1)
C(27)	6664(5)	6364(5)	2239(2)	62(1)
C(28)	4748(4)	5551(4)	3516(2)	44(1)
C(29)	4213(3)	5017(3)	4173(2)	39(1)
C(30)	3784(3)	5359(3)	4787(2)	34(1)
C(31)	3184(4)	4525(3)	5378(2)	39(1)
C(32)	3894(3)	6378(3)	4865(2)	33(1)
N(2)	8655(3)	1854(3)	6353(2)	45(1)
O(2)	8790(3)	3897(2)	7913(1)	45(1)
C(41)	8496(3)	2078(3)	8967(2)	34(1)
C(42)	8296(3)	2076(3)	8346(2)	34(1)
C(43)	8561(3)	2995(3)	7782(2)	34(1)
C(44)	8611(3)	2971(3)	7122(2)	32(1)
C(45)	8873(3)	3974(3)	6533(2)	38(1)
C(46)	8187(4)	4970(4)	6709(2)	51(1)
C(47)	10137(4)	4157(4)	6342(2)	49(1)
C(48)	8535(4)	3766(4)	5926(2)	51(1)
C(49)	9003(4)	2739(4)	5759(2)	53(1)
C(50)	8652(5)	815(4)	6184(2)	57(1)
C(51)	8590(5)	-120(4)	6792(2)	53(1)
C(52)	7686(4)	101(3)	7404(2)	39(1)
C(53)	6546(4)	370(4)	7226(2)	47(1)
C(54)	7597(5)	-877(3)	8000(2)	51(1)
C(55)	8026(3)	1089(3)	7563(2)	35(1)
C(56)	7958(3)	1166(3)	8202(2)	33(1)
C(57)	8439(3)	1986(3)	6991(2)	32(1)
C(58)	8070(4)	1363(3)	9609(2)	35(1)
C(59)	6985(4)	953(3)	9795(2)	41(1)

C(60)	6707(4)	418(3)	10474(2)	43(1)
C(61)	5590(5)	-43(4)	10846(2)	59(1)
C(62)	7615(4)	449(3)	10748(2)	39(1)
C(63)	7581(4)	8(3)	11436(2)	47(1)
C(64)	8353(5)	-32(3)	11803(2)	47(1)
C(65)	7934(12)	-486(5)	12585(3)	46(3)
C(65A)	8580(50)	-460(20)	12532(13)	45(10)
C(66)	8027(5)	347(5)	12961(2)	65(1)
C(67)	8550(7)	-1530(5)	12797(3)	90(2)
C(68)	9428(5)	304(4)	11518(2)	54(1)
C(69)	9986(4)	799(3)	10846(2)	46(1)
C(70)	9599(4)	1170(3)	10243(2)	37(1)
C(71)	10459(4)	1728(3)	9629(2)	41(1)
C(72)	8512(4)	1048(3)	10200(2)	35(1)
P(1)	2253(1)	1571(1)	4729(1)	60(1)
F(1)	3412(3)	2116(4)	4563(2)	87(1)
F(2)	1084(3)	1034(3)	4866(2)	88(1)
F(3)	1776(8)	1849(8)	5442(4)	119(3)
F(4)	2747(5)	1049(6)	4089(3)	84(2)
F(5)	1791(7)	2556(5)	4326(6)	115(4)
F(6)	2728(5)	427(5)	5178(4)	82(2)
F(3A)	1569(12)	2871(11)	4809(9)	90(5)
F(4A)	2834(11)	672(10)	4617(12)	109(7)
F(5A)	2112(12)	2062(14)	3921(6)	80(5)
F(6A)	2295(17)	1460(20)	5450(7)	124(8)
P(2)	3736(2)	3047(1)	31(1)	65(1)
F(7)	3467(5)	3755(4)	-629(2)	132(2)
F(8)	4180(5)	2412(3)	679(2)	107(2)
F(9)	3112(8)	3821(7)	466(4)	123(3)
F(10)	4242(10)	2114(5)	-332(3)	116(3)
F(11)	4862(7)	3629(8)	-250(4)	135(4)
F(12)	2673(6)	2304(7)	374(4)	123(3)
F(9A)	3960(30)	4124(12)	228(12)	133(9)
F(10A)	3340(20)	2420(20)	-418(14)	141(9)
F(11A)	4900(18)	2699(16)	-324(12)	122(7)
F(12A)	2281(17)	3442(17)	160(9)	131(9)
O(3)	2761(5)	5719(3)	943(2)	78(1)
O(4)	353(4)	7017(4)	6043(2)	80(1)
O(5)	1298(10)	8859(8)	5573(6)	81(4)
O(6)	886(19)	8490(20)	5812(12)	103(10)

Table S17: Bond lengths [Å] for **30**.

N(1)-C(17)	1.338(5)	C(24)-C(28)	1.386(6)
N(1)-C(9)	1.461(5)	C(24)-C(25)	1.532(5)
N(1)-C(10)	1.481(7)	C(25)-C(27)	1.511(7)
O(1)-C(3)	1.337(5)	C(25)-C(26)	1.515(7)
O(1)-H(1A)	0.8400	C(25)-H(25)	1.0000
C(1)-C(2)	1.391(5)	C(26)-H(26A)	0.9800
C(1)-C(18)	1.421(5)	C(26)-H(26B)	0.9800
C(1)-H(1)	0.9500	C(26)-H(26C)	0.9800
C(2)-C(16)	1.424(6)	C(27)-H(27A)	0.9800
C(2)-C(3)	1.452(5)	C(27)-H(27B)	0.9800
C(3)-C(4)	1.383(5)	C(27)-H(27C)	0.9800
C(4)-C(17)	1.425(6)	C(28)-C(29)	1.390(6)
C(4)-C(5)	1.540(5)	C(28)-H(28)	0.9500
C(5)-C(7)	1.524(7)	C(29)-C(30)	1.411(5)
C(5)-C(8)	1.527(6)	C(29)-H(29)	0.9500
C(5)-C(6)	1.533(6)	C(30)-C(32)	1.399(6)
C(6)-H(6A)	0.9800	C(30)-C(31)	1.502(5)
C(6)-H(6B)	0.9800	C(31)-H(31A)	0.9800
C(6)-H(6C)	0.9800	C(31)-H(31B)	0.9800
C(7)-H(7A)	0.9800	C(31)-H(31C)	0.9800
C(7)-H(7B)	0.9800	N(2)-C(57)	1.339(5)
C(7)-H(7C)	0.9800	N(2)-C(49)	1.465(6)
C(8)-C(9)	1.473(7)	N(2)-C(50)	1.478(6)
C(8)-H(8A)	0.9900	O(2)-C(43)	1.345(5)
C(8)-H(8B)	0.9900	O(2)-H(2)	0.87(3)
C(9)-H(9A)	0.9900	C(41)-C(42)	1.385(5)
C(9)-H(9B)	0.9900	C(41)-C(58)	1.426(5)
C(10)-C(11)	1.548(9)	C(41)-H(41)	0.9500
C(10)-H(10A)	0.9900	C(42)-C(56)	1.424(6)
C(10)-H(10B)	0.9900	C(42)-C(43)	1.442(5)
C(11)-C(12)	1.520(7)	C(43)-C(44)	1.372(5)
C(11)-H(11A)	0.9900	C(44)-C(57)	1.424(6)
C(11)-H(11B)	0.9900	C(44)-C(45)	1.542(5)
C(12)-C(14)	1.517(7)	C(45)-C(46)	1.527(6)
C(12)-C(13)	1.517(7)	C(45)-C(48)	1.531(6)
C(12)-C(15)	1.518(6)	C(45)-C(47)	1.536(6)
C(13)-H(13A)	0.9800	C(46)-H(46A)	0.9800
C(13)-H(13B)	0.9800	C(46)-H(46B)	0.9800
C(13)-H(13C)	0.9800	C(46)-H(46C)	0.9800
C(14)-H(14A)	0.9800	C(47)-H(47A)	0.9800
C(14)-H(14B)	0.9800	C(47)-H(47B)	0.9800
C(14)-H(14C)	0.9800	C(47)-H(47C)	0.9800
C(15)-C(16)	1.358(5)	C(48)-C(49)	1.474(7)
C(15)-C(17)	1.463(5)	C(48)-H(48A)	0.9900
C(16)-H(16)	0.9500	C(48)-H(48B)	0.9900
C(18)-C(19)	1.417(6)	C(49)-H(49A)	0.9900
C(18)-C(32)	1.442(5)	C(49)-H(49B)	0.9900
C(19)-C(20)	1.376(5)	C(50)-C(51)	1.506(7)
C(19)-H(19)	0.9500	C(50)-H(50A)	0.9900
C(20)-C(22)	1.418(6)	C(50)-H(50B)	0.9900
C(20)-C(21)	1.497(6)	C(51)-C(52)	1.518(6)
C(21)-H(21A)	0.9800	C(51)-H(51A)	0.9900
C(21)-H(21B)	0.9800	C(51)-H(51B)	0.9900
C(21)-H(21C)	0.9800	C(52)-C(54)	1.522(6)
C(22)-C(23)	1.390(5)	C(52)-C(53)	1.531(6)
C(22)-C(32)	1.480(5)	C(52)-C(55)	1.534(5)
C(23)-C(24)	1.382(6)	C(53)-H(53A)	0.9800
C(23)-H(23)	0.9500	C(53)-H(53B)	0.9800

C(53)-H(53C)	0.9800	C(69)-C(70)	1.418(6)
C(54)-H(54A)	0.9800	C(69)-H(69)	0.9500
C(54)-H(54B)	0.9800	C(70)-C(72)	1.401(6)
C(54)-H(54C)	0.9800	C(70)-C(71)	1.506(6)
C(55)-C(56)	1.344(5)	C(71)-H(71A)	0.9800
C(55)-C(57)	1.463(5)	C(71)-H(71B)	0.9800
C(56)-H(56)	0.9500	C(71)-H(71C)	0.9800
C(58)-C(59)	1.420(6)	P(1)-F(4A)	1.334(11)
C(58)-C(72)	1.430(5)	P(1)-F(5)	1.483(5)
C(59)-C(60)	1.379(6)	P(1)-F(6A)	1.492(16)
C(59)-H(59)	0.9500	P(1)-F(3)	1.563(7)
C(60)-C(62)	1.400(7)	P(1)-F(1)	1.587(4)
C(60)-C(61)	1.499(6)	P(1)-F(4)	1.596(5)
C(61)-H(61A)	0.9800	P(1)-F(2)	1.603(4)
C(61)-H(61B)	0.9800	P(1)-F(6)	1.674(6)
C(61)-H(61C)	0.9800	P(1)-F(5A)	1.694(12)
C(62)-C(63)	1.397(5)	P(1)-F(3A)	1.818(13)
C(62)-C(72)	1.485(5)	P(2)-F(11A)	1.50(2)
C(63)-C(64)	1.365(7)	P(2)-F(9)	1.524(6)
C(63)-H(63)	0.9500	P(2)-F(7)	1.543(4)
C(64)-C(68)	1.374(8)	P(2)-F(11)	1.560(6)
C(64)-C(65)	1.552(7)	P(2)-F(10)	1.569(6)
C(64)-C(65A)	1.57(3)	P(2)-F(10A)	1.58(2)
C(65)-C(67)	1.495(10)	P(2)-F(8)	1.594(4)
C(65)-C(66)	1.519(9)	P(2)-F(12)	1.615(7)
C(65)-H(65)	1.0000	P(2)-F(9A)	1.627(17)
C(65A)-C(67)	1.36(3)	P(2)-F(12A)	1.77(2)
C(65A)-C(66)	1.52(4)	F(7)-F(10A)	1.68(2)
C(65A)-H(65A)	1.0000	O(3)-H(3A)	0.90(2)
C(66)-H(66A)	0.9800	O(3)-H(3B)	0.86(3)
C(66)-H(66B)	0.9800	O(4)-H(4A)	0.9057
C(66)-H(66C)	0.9800	O(4)-H(4B)	0.8575
C(67)-H(67A)	0.9800	O(5)-H(5A)	0.8483
C(67)-H(67B)	0.9800	O(5)-H(5B)	0.8599
C(67)-H(67C)	0.9800	O(6)-H(4A)	1.1016
C(68)-C(69)	1.407(6)	O(6)-H(6D)	0.7950
C(68)-H(68)	0.9500	O(6)-H(6E)	0.7806

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Table S18: Bond angles [°] for **30**.

C(17)-N(1)-C(9)	121.7(4)	C(14)-C(12)-C(13)	107.5(5)
C(17)-N(1)-C(10)	124.3(4)	C(14)-C(12)-C(15)	113.1(4)
C(9)-N(1)-C(10)	113.6(4)	C(13)-C(12)-C(15)	108.1(4)
C(3)-O(1)-H(1A)	109.5	C(14)-C(12)-C(11)	109.1(5)
C(2)-C(1)-C(18)	127.1(4)	C(13)-C(12)-C(11)	111.1(4)
C(2)-C(1)-H(1)	116.5	C(15)-C(12)-C(11)	108.0(4)
C(18)-C(1)-H(1)	116.5	C(12)-C(13)-H(13A)	109.5
C(1)-C(2)-C(16)	123.8(3)	C(12)-C(13)-H(13B)	109.5
C(1)-C(2)-C(3)	118.8(4)	H(13A)-C(13)-H(13B)	109.5
C(16)-C(2)-C(3)	117.0(3)	C(12)-C(13)-H(13C)	109.5
O(1)-C(3)-C(4)	118.9(3)	H(13A)-C(13)-H(13C)	109.5
O(1)-C(3)-C(2)	119.4(3)	H(13B)-C(13)-H(13C)	109.5
C(4)-C(3)-C(2)	121.6(4)	C(12)-C(14)-H(14A)	109.5
C(3)-C(4)-C(17)	118.9(3)	C(12)-C(14)-H(14B)	109.5
C(3)-C(4)-C(5)	120.1(4)	H(14A)-C(14)-H(14B)	109.5
C(17)-C(4)-C(5)	121.0(3)	C(12)-C(14)-H(14C)	109.5
C(7)-C(5)-C(8)	106.8(4)	H(14A)-C(14)-H(14C)	109.5
C(7)-C(5)-C(6)	110.1(4)	H(14B)-C(14)-H(14C)	109.5
C(8)-C(5)-C(6)	110.1(3)	C(16)-C(15)-C(17)	118.1(4)
C(7)-C(5)-C(4)	112.4(3)	C(16)-C(15)-C(12)	123.0(3)
C(8)-C(5)-C(4)	107.5(3)	C(17)-C(15)-C(12)	118.9(3)
C(6)-C(5)-C(4)	109.9(3)	C(15)-C(16)-C(2)	123.5(3)
C(5)-C(6)-H(6A)	109.5	C(15)-C(16)-H(16)	118.3
C(5)-C(6)-H(6B)	109.5	C(2)-C(16)-H(16)	118.3
H(6A)-C(6)-H(6B)	109.5	N(1)-C(17)-C(4)	120.8(3)
C(5)-C(6)-H(6C)	109.5	N(1)-C(17)-C(15)	118.7(4)
H(6A)-C(6)-H(6C)	109.5	C(4)-C(17)-C(15)	120.4(3)
H(6B)-C(6)-H(6C)	109.5	C(19)-C(18)-C(1)	124.3(4)
C(5)-C(7)-H(7A)	109.5	C(19)-C(18)-C(32)	107.1(3)
C(5)-C(7)-H(7B)	109.5	C(1)-C(18)-C(32)	128.1(4)
H(7A)-C(7)-H(7B)	109.5	C(20)-C(19)-C(18)	111.7(4)
C(5)-C(7)-H(7C)	109.5	C(20)-C(19)-H(19)	124.1
H(7A)-C(7)-H(7C)	109.5	C(18)-C(19)-H(19)	124.1
H(7B)-C(7)-H(7C)	109.5	C(19)-C(20)-C(22)	107.3(4)
C(9)-C(8)-C(5)	113.4(4)	C(19)-C(20)-C(21)	126.3(4)
C(9)-C(8)-H(8A)	108.9	C(22)-C(20)-C(21)	126.4(3)
C(5)-C(8)-H(8A)	108.9	C(20)-C(21)-H(21A)	109.5
C(9)-C(8)-H(8B)	108.9	C(20)-C(21)-H(21B)	109.5
C(5)-C(8)-H(8B)	108.9	H(21A)-C(21)-H(21B)	109.5
H(8A)-C(8)-H(8B)	107.7	C(20)-C(21)-H(21C)	109.5
N(1)-C(9)-C(8)	110.7(3)	H(21A)-C(21)-H(21C)	109.5
N(1)-C(9)-H(9A)	109.5	H(21B)-C(21)-H(21C)	109.5
C(8)-C(9)-H(9A)	109.5	C(23)-C(22)-C(20)	121.1(4)
N(1)-C(9)-H(9B)	109.5	C(23)-C(22)-C(32)	130.3(4)
C(8)-C(9)-H(9B)	109.5	C(20)-C(22)-C(32)	108.5(3)
H(9A)-C(9)-H(9B)	108.1	C(24)-C(23)-C(22)	130.5(4)
N(1)-C(10)-C(11)	111.3(4)	C(24)-C(23)-H(23)	114.8
N(1)-C(10)-H(10A)	109.4	C(22)-C(23)-H(23)	114.8
C(11)-C(10)-H(10A)	109.4	C(23)-C(24)-C(28)	123.9(3)
N(1)-C(10)-H(10B)	109.4	C(23)-C(24)-C(25)	117.3(4)
C(11)-C(10)-H(10B)	109.4	C(28)-C(24)-C(25)	118.9(4)
H(10A)-C(10)-H(10B)	108.0	C(27)-C(25)-C(26)	113.1(4)
C(12)-C(11)-C(10)	107.9(5)	C(27)-C(25)-C(24)	112.0(4)
C(12)-C(11)-H(11A)	110.1	C(26)-C(25)-C(24)	110.6(4)
C(10)-C(11)-H(11A)	110.1	C(27)-C(25)-H(25)	106.9
C(12)-C(11)-H(11B)	110.1	C(26)-C(25)-H(25)	106.9
C(10)-C(11)-H(11B)	110.1	C(24)-C(25)-H(25)	106.9
H(11A)-C(11)-H(11B)	108.4	C(25)-C(26)-H(26A)	109.5

C(25)-C(26)-H(26B)	109.5	C(45)-C(47)-H(47C)	109.5
H(26A)-C(26)-H(26B)	109.5	H(47A)-C(47)-H(47C)	109.5
C(25)-C(26)-H(26C)	109.5	H(47B)-C(47)-H(47C)	109.5
H(26A)-C(26)-H(26C)	109.5	C(49)-C(48)-C(45)	113.7(4)
H(26B)-C(26)-H(26C)	109.5	C(49)-C(48)-H(48A)	108.8
C(25)-C(27)-H(27A)	109.5	C(45)-C(48)-H(48A)	108.8
C(25)-C(27)-H(27B)	109.5	C(49)-C(48)-H(48B)	108.8
H(27A)-C(27)-H(27B)	109.5	C(45)-C(48)-H(48B)	108.8
C(25)-C(27)-H(27C)	109.5	H(48A)-C(48)-H(48B)	107.7
H(27A)-C(27)-H(27C)	109.5	N(2)-C(49)-C(48)	110.2(3)
H(27B)-C(27)-H(27C)	109.5	N(2)-C(49)-H(49A)	109.6
C(24)-C(28)-C(29)	131.7(4)	C(48)-C(49)-H(49A)	109.6
C(24)-C(28)-H(28)	114.2	N(2)-C(49)-H(49B)	109.6
C(29)-C(28)-H(28)	114.2	C(48)-C(49)-H(49B)	109.6
C(28)-C(29)-C(30)	132.1(4)	H(49A)-C(49)-H(49B)	108.1
C(28)-C(29)-H(29)	113.9	N(2)-C(50)-C(51)	113.1(4)
C(30)-C(29)-H(29)	113.9	N(2)-C(50)-H(50A)	109.0
C(32)-C(30)-C(29)	124.7(4)	C(51)-C(50)-H(50A)	109.0
C(32)-C(30)-C(31)	120.8(3)	N(2)-C(50)-H(50B)	109.0
C(29)-C(30)-C(31)	114.4(4)	C(51)-C(50)-H(50B)	109.0
C(30)-C(31)-H(31A)	109.5	H(50A)-C(50)-H(50B)	107.8
C(30)-C(31)-H(31B)	109.5	C(50)-C(51)-C(52)	110.7(4)
H(31A)-C(31)-H(31B)	109.5	C(50)-C(51)-H(51A)	109.5
C(30)-C(31)-H(31C)	109.5	C(52)-C(51)-H(51A)	109.5
H(31A)-C(31)-H(31C)	109.5	C(50)-C(51)-H(51B)	109.5
H(31B)-C(31)-H(31C)	109.5	C(52)-C(51)-H(51B)	109.5
C(30)-C(32)-C(18)	128.4(3)	H(51A)-C(51)-H(51B)	108.1
C(30)-C(32)-C(22)	126.0(3)	C(51)-C(52)-C(54)	109.7(4)
C(18)-C(32)-C(22)	105.3(3)	C(51)-C(52)-C(53)	110.5(4)
C(57)-N(2)-C(49)	121.3(4)	C(54)-C(52)-C(53)	109.4(4)
C(57)-N(2)-C(50)	124.2(4)	C(51)-C(52)-C(55)	106.3(3)
C(49)-N(2)-C(50)	114.3(4)	C(54)-C(52)-C(55)	112.8(3)
C(43)-O(2)-H(2)	106(6)	C(53)-C(52)-C(55)	108.1(3)
C(42)-C(41)-C(58)	126.6(4)	C(52)-C(53)-H(53A)	109.5
C(42)-C(41)-H(41)	116.7	C(52)-C(53)-H(53B)	109.5
C(58)-C(41)-H(41)	116.7	H(53A)-C(53)-H(53B)	109.5
C(41)-C(42)-C(56)	123.6(3)	C(52)-C(53)-H(53C)	109.5
C(41)-C(42)-C(43)	119.3(4)	H(53A)-C(53)-H(53C)	109.5
C(56)-C(42)-C(43)	116.6(3)	H(53B)-C(53)-H(53C)	109.5
O(2)-C(43)-C(44)	119.4(3)	C(52)-C(54)-H(54A)	109.5
O(2)-C(43)-C(42)	118.1(3)	C(52)-C(54)-H(54B)	109.5
C(44)-C(43)-C(42)	122.5(4)	H(54A)-C(54)-H(54B)	109.5
C(43)-C(44)-C(57)	118.2(3)	C(52)-C(54)-H(54C)	109.5
C(43)-C(44)-C(45)	121.2(4)	H(54A)-C(54)-H(54C)	109.5
C(57)-C(44)-C(45)	120.5(3)	H(54B)-C(54)-H(54C)	109.5
C(46)-C(45)-C(48)	107.3(4)	C(56)-C(55)-C(57)	118.8(4)
C(46)-C(45)-C(47)	110.2(4)	C(56)-C(55)-C(52)	122.9(3)
C(48)-C(45)-C(47)	110.3(3)	C(57)-C(55)-C(52)	118.3(3)
C(46)-C(45)-C(44)	112.4(3)	C(55)-C(56)-C(42)	122.7(3)
C(48)-C(45)-C(44)	107.0(3)	C(55)-C(56)-H(56)	118.6
C(47)-C(45)-C(44)	109.6(3)	C(42)-C(56)-H(56)	118.6
C(45)-C(46)-H(46A)	109.5	N(2)-C(57)-C(44)	121.6(3)
C(45)-C(46)-H(46B)	109.5	N(2)-C(57)-C(55)	118.7(4)
H(46A)-C(46)-H(46B)	109.5	C(44)-C(57)-C(55)	119.8(3)
C(45)-C(46)-H(46C)	109.5	C(59)-C(58)-C(41)	122.3(4)
H(46A)-C(46)-H(46C)	109.5	C(59)-C(58)-C(72)	107.3(3)
H(46B)-C(46)-H(46C)	109.5	C(41)-C(58)-C(72)	129.7(4)
C(45)-C(47)-H(47A)	109.5	C(60)-C(59)-C(58)	110.9(4)
C(45)-C(47)-H(47B)	109.5	C(60)-C(59)-H(59)	124.5
H(47A)-C(47)-H(47B)	109.5	C(58)-C(59)-H(59)	124.5

C(59)-C(60)-C(62)	108.0(4)	C(70)-C(72)-C(62)	126.5(4)
C(59)-C(60)-C(61)	124.6(5)	C(58)-C(72)-C(62)	105.4(4)
C(62)-C(60)-C(61)	127.3(4)	F(4A)-P(1)-F(6A)	99.4(15)
C(60)-C(61)-H(61A)	109.5	F(5)-P(1)-F(3)	96.5(6)
C(60)-C(61)-H(61B)	109.5	F(4A)-P(1)-F(1)	88.6(7)
H(61A)-C(61)-H(61B)	109.5	F(5)-P(1)-F(1)	89.8(3)
C(60)-C(61)-H(61C)	109.5	F(6A)-P(1)-F(1)	82.7(8)
H(61A)-C(61)-H(61C)	109.5	F(3)-P(1)-F(1)	95.2(4)
H(61B)-C(61)-H(61C)	109.5	F(5)-P(1)-F(4)	94.1(6)
C(63)-C(62)-C(60)	122.1(4)	F(3)-P(1)-F(4)	168.6(5)
C(63)-C(62)-C(72)	129.4(4)	F(1)-P(1)-F(4)	89.1(2)
C(60)-C(62)-C(72)	108.4(3)	F(4A)-P(1)-F(2)	91.2(7)
C(64)-C(63)-C(62)	131.4(5)	F(5)-P(1)-F(2)	88.8(3)
C(64)-C(63)-H(63)	114.3	F(6A)-P(1)-F(2)	99.5(8)
C(62)-C(63)-H(63)	114.3	F(3)-P(1)-F(2)	86.8(4)
C(63)-C(64)-C(68)	123.9(4)	F(1)-P(1)-F(2)	177.7(2)
C(63)-C(64)-C(65)	115.3(7)	F(4)-P(1)-F(2)	89.2(3)
C(68)-C(64)-C(65)	120.8(7)	F(5)-P(1)-F(6)	177.3(4)
C(63)-C(64)-C(65A)	143(2)	F(3)-P(1)-F(6)	84.4(4)
C(68)-C(64)-C(65A)	92(2)	F(1)-P(1)-F(6)	92.7(3)
C(67)-C(65)-C(66)	113.9(7)	F(4)-P(1)-F(6)	84.8(4)
C(67)-C(65)-C(64)	110.1(7)	F(2)-P(1)-F(6)	88.7(3)
C(66)-C(65)-C(64)	109.5(6)	F(4A)-P(1)-F(5A)	96.2(12)
C(67)-C(65)-H(65)	107.7	F(6A)-P(1)-F(5A)	163.6(13)
C(66)-C(65)-H(65)	107.7	F(1)-P(1)-F(5A)	92.6(4)
C(64)-C(65)-H(65)	107.7	F(2)-P(1)-F(5A)	85.2(4)
C(67)-C(65A)-C(66)	122(2)	F(4A)-P(1)-F(3A)	174.1(8)
C(67)-C(65A)-C(64)	117(2)	F(6A)-P(1)-F(3A)	83.6(12)
C(66)-C(65A)-C(64)	108(3)	F(1)-P(1)-F(3A)	86.7(5)
C(67)-C(65A)-H(65A)	102.1	F(2)-P(1)-F(3A)	93.3(5)
C(66)-C(65A)-H(65A)	102.1	F(5A)-P(1)-F(3A)	80.4(9)
C(64)-C(65A)-H(65A)	102.1	F(11A)-P(2)-F(7)	94.4(8)
C(65)-C(66)-H(66A)	109.5	F(9)-P(2)-F(7)	93.3(4)
C(65)-C(66)-H(66B)	109.5	F(9)-P(2)-F(11)	96.3(5)
H(66A)-C(66)-H(66B)	109.5	F(7)-P(2)-F(11)	83.1(4)
C(65)-C(66)-H(66C)	109.5	F(9)-P(2)-F(10)	170.7(5)
H(66A)-C(66)-H(66C)	109.5	F(7)-P(2)-F(10)	91.6(3)
H(66B)-C(66)-H(66C)	109.5	F(11)-P(2)-F(10)	92.1(6)
C(65)-C(67)-H(67A)	109.5	F(11A)-P(2)-F(10A)	84.1(12)
C(65)-C(67)-H(67B)	109.5	F(7)-P(2)-F(10A)	65.2(11)
H(67A)-C(67)-H(67B)	109.5	F(11A)-P(2)-F(8)	80.3(8)
C(65)-C(67)-H(67C)	109.5	F(9)-P(2)-F(8)	86.9(4)
H(67A)-C(67)-H(67C)	109.5	F(7)-P(2)-F(8)	171.4(3)
H(67B)-C(67)-H(67C)	109.5	F(11)-P(2)-F(8)	88.4(3)
C(64)-C(68)-C(69)	132.2(5)	F(10)-P(2)-F(8)	89.4(4)
C(64)-C(68)-H(68)	113.9	F(10A)-P(2)-F(8)	120.5(11)
C(69)-C(68)-H(68)	113.9	F(9)-P(2)-F(12)	87.4(5)
C(68)-C(69)-C(70)	131.4(5)	F(7)-P(2)-F(12)	104.1(4)
C(68)-C(69)-H(69)	114.3	F(11)-P(2)-F(12)	171.8(5)
C(70)-C(69)-H(69)	114.3	F(10)-P(2)-F(12)	83.8(5)
C(72)-C(70)-C(69)	124.4(4)	F(8)-P(2)-F(12)	84.5(4)
C(72)-C(70)-C(71)	121.0(3)	F(11A)-P(2)-F(9A)	102.3(16)
C(69)-C(70)-C(71)	114.6(4)	F(7)-P(2)-F(9A)	88.7(6)
C(70)-C(71)-H(71A)	109.5	F(10A)-P(2)-F(9A)	153.7(13)
C(70)-C(71)-H(71B)	109.5	F(8)-P(2)-F(9A)	85.8(6)
H(71A)-C(71)-H(71B)	109.5	F(11A)-P(2)-F(12A)	159.0(11)
C(70)-C(71)-H(71C)	109.5	F(7)-P(2)-F(12A)	68.4(6)
H(71A)-C(71)-H(71C)	109.5	F(10A)-P(2)-F(12A)	77.8(14)
H(71B)-C(71)-H(71C)	109.5	F(8)-P(2)-F(12A)	118.1(6)
C(70)-C(72)-C(58)	127.8(3)	F(9A)-P(2)-F(12A)	89.8(13)

P(2)-F(7)-F(10A)	58.6(10)	H(5A)-O(5)-H(5B)	106.1
P(2)-F(10A)-F(7)	56.3(7)	H(4A)-O(6)-H(6D)	124.1
H(3A)-O(3)-H(3B)	102(3)	H(4A)-O(6)-H(6E)	102.5
H(4A)-O(4)-H(4B)	101.2	H(6D)-O(6)-H(6E)	111.1

Symmetry transformations used to generate equivalent atoms:

Table S19: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **30**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	60(2)	58(2)	20(2)	-8(1)	-8(2)	-18(2)
O(1)	45(2)	66(2)	25(1)	-10(1)	-6(1)	-15(2)
C(1)	40(2)	45(2)	19(2)	-10(1)	-7(1)	-4(2)
C(2)	41(2)	38(2)	18(2)	-9(1)	-4(1)	-2(2)
C(3)	42(2)	37(2)	20(2)	-9(1)	-3(2)	-5(2)
C(4)	42(2)	34(2)	19(2)	-9(1)	-3(1)	0(2)
C(5)	46(2)	47(2)	17(2)	-10(1)	1(2)	-1(2)
C(6)	59(3)	52(2)	27(2)	-10(2)	1(2)	-17(2)
C(7)	53(3)	82(3)	37(2)	-13(2)	0(2)	19(3)
C(8)	64(3)	49(2)	24(2)	-15(2)	4(2)	-8(2)
C(9)	72(3)	60(3)	18(2)	-11(2)	-4(2)	-18(2)
C(10)	85(4)	138(6)	24(2)	-9(3)	-16(2)	-51(4)
C(11)	80(4)	79(3)	55(3)	-15(3)	-33(3)	-8(3)
C(12)	48(2)	49(2)	26(2)	-12(2)	-9(2)	-9(2)
C(13)	85(4)	71(3)	64(3)	-18(3)	-29(3)	-17(3)
C(14)	58(3)	190(8)	66(4)	-68(5)	-11(3)	-23(4)
C(15)	43(2)	37(2)	24(2)	-10(1)	-6(2)	-3(2)
C(16)	41(2)	40(2)	21(2)	-10(1)	-3(1)	-4(2)
C(17)	49(2)	35(2)	17(2)	-10(1)	-4(2)	-4(2)
C(18)	40(2)	46(2)	16(2)	-10(1)	-9(1)	2(2)
C(19)	44(2)	48(2)	23(2)	-10(2)	-9(2)	-2(2)
C(20)	45(2)	46(2)	26(2)	-9(2)	-12(2)	-1(2)
C(21)	67(3)	53(2)	28(2)	-8(2)	-12(2)	-6(2)
C(22)	36(2)	43(2)	19(2)	-8(1)	-7(1)	1(2)
C(23)	44(2)	52(2)	21(2)	-7(2)	-9(2)	2(2)
C(24)	44(2)	53(2)	20(2)	-11(2)	-6(2)	-2(2)
C(25)	55(3)	65(3)	22(2)	-14(2)	-3(2)	1(2)
C(26)	66(3)	76(3)	21(2)	-9(2)	-12(2)	7(3)
C(27)	61(3)	78(3)	35(2)	-12(2)	1(2)	10(3)
C(28)	49(2)	64(3)	24(2)	-25(2)	-11(2)	11(2)
C(29)	43(2)	47(2)	30(2)	-14(2)	-13(2)	4(2)
C(30)	35(2)	46(2)	24(2)	-12(2)	-12(1)	5(2)
C(31)	45(2)	48(2)	28(2)	-10(2)	-11(2)	-5(2)
C(32)	37(2)	47(2)	16(2)	-8(1)	-10(1)	3(2)
N(2)	53(2)	64(2)	22(2)	-16(2)	-4(1)	-14(2)
O(2)	69(2)	42(1)	25(1)	-5(1)	-12(1)	-11(1)
C(41)	46(2)	37(2)	21(2)	-6(1)	-9(2)	-3(2)
C(42)	44(2)	39(2)	21(2)	-5(1)	-10(1)	-2(2)
C(43)	42(2)	38(2)	22(2)	-5(1)	-9(1)	-6(2)
C(44)	34(2)	42(2)	20(2)	-4(1)	-7(1)	-3(2)
C(45)	43(2)	48(2)	20(2)	0(2)	-8(2)	-5(2)
C(46)	57(3)	48(2)	39(2)	4(2)	-12(2)	0(2)
C(47)	46(2)	60(3)	34(2)	2(2)	-7(2)	-12(2)
C(48)	61(3)	68(3)	18(2)	4(2)	-12(2)	-12(2)
C(49)	65(3)	76(3)	19(2)	-13(2)	-6(2)	-16(3)
C(50)	68(3)	74(3)	36(2)	-31(2)	-2(2)	-22(3)
C(51)	62(3)	58(3)	46(3)	-25(2)	-9(2)	-8(2)
C(52)	46(2)	39(2)	34(2)	-11(2)	-12(2)	-7(2)
C(53)	51(3)	53(2)	43(2)	-12(2)	-16(2)	-11(2)
C(54)	72(3)	40(2)	48(3)	-11(2)	-25(2)	-3(2)
C(55)	38(2)	42(2)	28(2)	-13(2)	-11(2)	3(2)
C(56)	39(2)	33(2)	24(2)	-2(1)	-7(1)	-4(2)
C(57)	33(2)	44(2)	21(2)	-10(1)	-5(1)	-1(2)
C(58)	51(2)	37(2)	19(2)	-9(1)	-8(2)	-3(2)
C(59)	55(2)	45(2)	26(2)	-12(2)	-12(2)	-3(2)

C(60)	57(3)	44(2)	26(2)	-14(2)	1(2)	-8(2)
C(61)	66(3)	68(3)	38(2)	-13(2)	3(2)	-26(3)
C(62)	63(3)	30(2)	22(2)	-9(1)	-3(2)	2(2)
C(63)	76(3)	38(2)	20(2)	-8(2)	-5(2)	1(2)
C(64)	77(3)	38(2)	22(2)	-4(2)	-13(2)	2(2)
C(65)	52(7)	60(3)	22(3)	0(2)	-7(3)	-8(3)
C(65A)	40(30)	58(16)	30(13)	5(11)	0(12)	-21(15)
C(66)	89(4)	79(3)	23(2)	-13(2)	-14(2)	8(3)
C(67)	134(6)	76(4)	37(3)	13(3)	-12(3)	8(4)
C(68)	91(4)	49(2)	33(2)	-14(2)	-36(2)	14(2)
C(69)	67(3)	45(2)	33(2)	-18(2)	-24(2)	12(2)
C(70)	57(2)	33(2)	25(2)	-15(1)	-14(2)	6(2)
C(71)	53(2)	40(2)	35(2)	-12(2)	-16(2)	-4(2)
C(72)	55(2)	32(2)	20(2)	-11(1)	-9(2)	2(2)
P(1)	56(1)	86(1)	40(1)	-19(1)	-15(1)	-2(1)
F(1)	71(2)	122(3)	87(3)	-49(2)	-23(2)	-21(2)
F(2)	63(2)	106(3)	79(2)	7(2)	-10(2)	-20(2)
F(3)	133(7)	157(7)	76(5)	-73(5)	-27(4)	55(6)
F(4)	78(4)	134(6)	56(3)	-50(3)	-1(3)	-37(4)
F(5)	104(5)	71(4)	167(10)	39(5)	-91(6)	-14(4)
F(6)	79(3)	82(4)	77(4)	-2(3)	-30(3)	9(3)
F(3A)	70(7)	73(7)	116(12)	-35(8)	9(7)	-9(6)
F(4A)	75(8)	64(7)	160(20)	-33(9)	1(10)	40(6)
F(5A)	80(8)	128(12)	45(6)	-25(6)	-18(5)	-44(8)
F(6A)	109(12)	197(19)	30(6)	32(9)	-16(7)	-3(12)
P(2)	101(1)	62(1)	32(1)	-23(1)	-14(1)	11(1)
F(7)	193(5)	141(4)	60(2)	-38(2)	-55(3)	87(4)
F(8)	173(5)	95(3)	58(2)	-6(2)	-43(3)	-19(3)
F(9)	142(7)	140(7)	95(5)	-87(5)	5(5)	15(5)
F(10)	197(9)	75(4)	75(4)	-34(3)	-27(5)	22(5)
F(11)	104(5)	155(8)	114(6)	47(6)	-24(4)	-70(6)
F(12)	118(5)	173(8)	104(5)	-50(5)	-30(4)	-58(5)
F(9A)	280(20)	57(7)	103(14)	-39(8)	-106(16)	33(12)
F(10A)	135(13)	120(12)	180(14)	-66(10)	-27(10)	-17(10)
F(11A)	133(13)	88(11)	166(16)	-51(10)	-90(12)	78(11)
F(12A)	116(12)	136(14)	83(11)	-11(9)	53(9)	-1(11)
O(3)	111(4)	68(2)	48(2)	-25(2)	-7(2)	17(3)
O(4)	68(2)	122(3)	48(2)	-10(2)	-27(2)	7(2)
O(5)	93(9)	53(4)	88(8)	15(5)	-32(6)	-18(5)
O(6)	60(13)	190(30)	84(17)	-91(19)	-28(11)	40(16)

Table S20: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **30**.

	x	y	z	U(eq)
H(1A)	689	6299	6843	67
H(1)	2299	5833	6100	15(8)
H(6A)	449	4508	8343	70
H(6B)	-250	4617	9091	70
H(6C)	1088	4406	8929	70
H(7A)	-676	6155	8035	93
H(7B)	-234	7273	8021	93
H(7C)	-1037	6620	8706	93
H(8A)	620	7174	9016	56
H(8B)	44	6130	9528	56
H(9A)	1759	6339	9726	60
H(9B)	1782	5240	9504	60
H(10A)	3758	5891	9409	96
H(10B)	3722	7153	9086	96
H(11A)	5490	6445	8550	81
H(11B)	4905	5555	8365	81
H(13A)	4627	8713	7394	105
H(13B)	5028	8350	8089	105
H(13C)	3729	8324	8108	105
H(14A)	5882	6327	7095	145
H(14B)	6426	7113	7385	145
H(14C)	5762	7592	6805	145
H(16)	4303	7083	6566	41
H(19)	3919	8213	5642	45
H(21A)	5895	9022	4163	74
H(21B)	4861	9633	4592	74
H(21C)	4814	9454	3870	74
H(23)	5307	7988	3397	47
H(25)	5738	7735	2386	58
H(26A)	5033	7190	1597	83
H(26B)	4040	7393	2234	83
H(26C)	4485	6199	2182	83
H(27A)	6524	5614	2295	93
H(27B)	7183	6407	2511	93
H(27C)	6998	6680	1756	93
H(28)	4927	5123	3190	53
H(29)	4119	4283	4216	47
H(31A)	2376	4725	5489	59
H(31B)	3480	4472	5775	59
H(31C)	3304	3833	5254	59
H(2)	8240(60)	4010(70)	8260(30)	130(30)
H(41)	8964	2609	8964	41
H(46A)	8187	5518	6288	76
H(46B)	8522	5243	7003	76
H(46C)	7411	4786	6950	76
H(47A)	10567	3540	6190	73
H(47B)	10351	4246	6743	73
H(47C)	10300	4802	5973	73
H(48A)	7704	3778	6031	61
H(48B)	8792	4352	5520	61
H(49A)	8736	2645	5373	64
H(49B)	9835	2740	5617	64
H(50A)	9345	720	5827	68
H(50B)	8000	824	5993	68

H(51A)	9328	-257	6907	64
H(51B)	8420	-767	6676	64
H(53A)	6597	1011	6851	71
H(53B)	5970	501	7628	71
H(53C)	6343	-230	7085	71
H(54A)	7383	-1484	7871	77
H(54B)	7024	-726	8397	77
H(54C)	8325	-1050	8114	77
H(56)	7672	589	8573	39
H(59)	6513	1037	9492	49
H(61A)	5046	230	10569	88
H(61B)	5322	163	11285	88
H(61C)	5671	-824	10928	88
H(63)	6901	-322	11695	56
H(65)	7119	-624	12686	56
H(65A)	9395	-335	12439	54
H(66A)	8815	524	12852	97
H(66B)	7757	61	13454	97
H(66C)	7568	992	12817	97
H(67A)	9343	-1412	12736	135
H(67B)	8495	-2010	12514	135
H(67C)	8214	-1854	13278	135
H(68)	9881	177	11835	65
H(69)	10758	904	10786	55
H(71A)	10459	1461	9231	62
H(71B)	11207	1587	9720	62
H(71C)	10272	2499	9537	62
H(3A)	3440(30)	5980(30)	880(20)	31(12)
H(3B)	2950(40)	5100(30)	860(30)	76(19)
H(4A)	581	7695	5887	96
H(4B)	-353	7121	6065	96
H(5A)	1715	9387	5438	97
H(5B)	913	8880	5980	97
H(6D)	665	9024	5585	123
H(6E)	1537	8398	5685	123

Table S21: Torsion angles [°] for **30**.

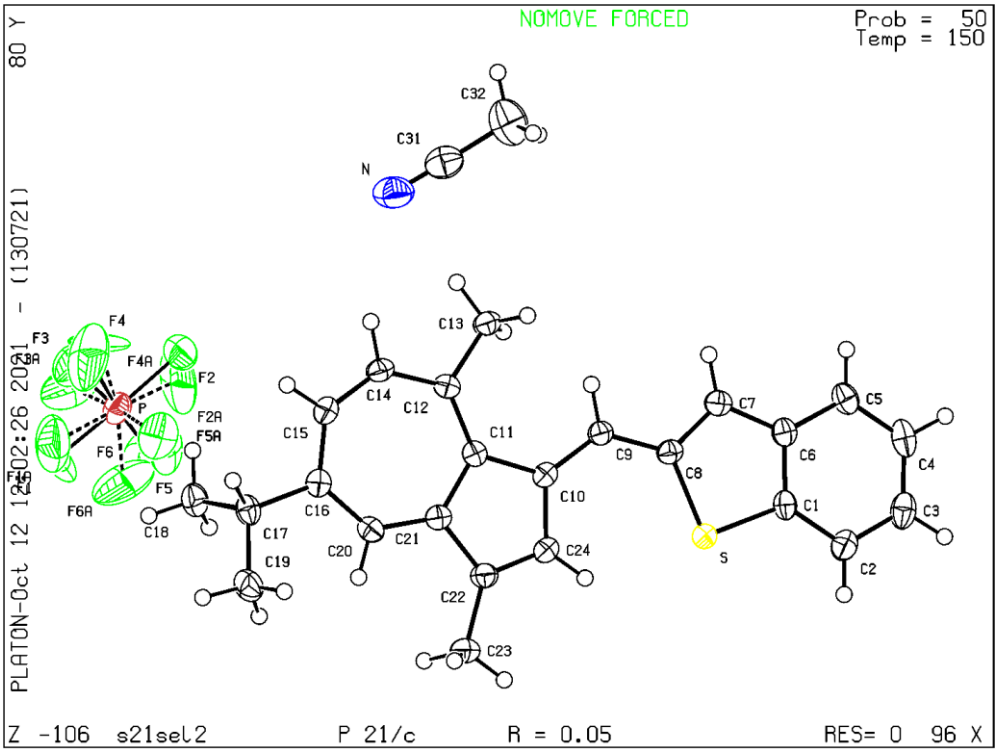
C(18)-C(1)-C(2)-C(16)	-24.9(6)	C(19)-C(20)-C(22)-C(32)	1.0(5)
C(18)-C(1)-C(2)-C(3)	162.9(4)	C(21)-C(20)-C(22)-C(32)	-179.2(4)
C(1)-C(2)-C(3)-O(1)	-5.4(5)	C(20)-C(22)-C(23)-C(24)	178.9(4)
C(16)-C(2)-C(3)-O(1)	-178.2(3)	C(32)-C(22)-C(23)-C(24)	-3.7(8)
C(1)-C(2)-C(3)-C(4)	171.4(4)	C(22)-C(23)-C(24)-C(28)	-6.2(8)
C(16)-C(2)-C(3)-C(4)	-1.3(5)	C(22)-C(23)-C(24)-C(25)	175.4(4)
O(1)-C(3)-C(4)-C(17)	171.8(3)	C(23)-C(24)-C(25)-C(27)	115.2(5)
C(2)-C(3)-C(4)-C(17)	-5.1(5)	C(28)-C(24)-C(25)-C(27)	-63.4(6)
O(1)-C(3)-C(4)-C(5)	-6.7(5)	C(23)-C(24)-C(25)-C(26)	-117.7(5)
C(2)-C(3)-C(4)-C(5)	176.4(3)	C(28)-C(24)-C(25)-C(26)	63.8(6)
C(3)-C(4)-C(5)-C(7)	-46.2(5)	C(23)-C(24)-C(28)-C(29)	6.5(8)
C(17)-C(4)-C(5)-C(7)	135.4(4)	C(25)-C(24)-C(28)-C(29)	-175.1(5)
C(3)-C(4)-C(5)-C(8)	-163.4(4)	C(24)-C(28)-C(29)-C(30)	2.1(9)
C(17)-C(4)-C(5)-C(8)	18.1(5)	C(28)-C(29)-C(30)-C(32)	-4.9(7)
C(3)-C(4)-C(5)-C(6)	76.7(5)	C(28)-C(29)-C(30)-C(31)	175.5(4)
C(17)-C(4)-C(5)-C(6)	-101.7(4)	C(29)-C(30)-C(32)-C(18)	-175.0(4)
C(7)-C(5)-C(8)-C(9)	-170.5(4)	C(31)-C(30)-C(32)-C(18)	4.6(6)
C(6)-C(5)-C(8)-C(9)	70.0(5)	C(29)-C(30)-C(32)-C(22)	-3.0(6)
C(4)-C(5)-C(8)-C(9)	-49.7(4)	C(31)-C(30)-C(32)-C(22)	176.6(4)
C(17)-N(1)-C(9)-C(8)	-30.5(6)	C(19)-C(18)-C(32)-C(30)	171.4(4)
C(10)-N(1)-C(9)-C(8)	156.1(5)	C(1)-C(18)-C(32)-C(30)	-16.2(7)
C(5)-C(8)-C(9)-N(1)	57.0(5)	C(19)-C(18)-C(32)-C(22)	-1.9(4)
C(17)-N(1)-C(10)-C(11)	-18.2(8)	C(1)-C(18)-C(32)-C(22)	170.6(4)
C(9)-N(1)-C(10)-C(11)	155.0(5)	C(23)-C(22)-C(32)-C(30)	9.5(7)
N(1)-C(10)-C(11)-C(12)	52.9(7)	C(20)-C(22)-C(32)-C(30)	-172.9(4)
C(10)-C(11)-C(12)-C(14)	175.0(5)	C(23)-C(22)-C(32)-C(18)	-177.0(4)
C(10)-C(11)-C(12)-C(13)	56.7(6)	C(20)-C(22)-C(32)-C(18)	0.6(4)
C(10)-C(11)-C(12)-C(15)	-61.7(5)	C(58)-C(41)-C(42)-C(56)	-22.1(7)
C(14)-C(12)-C(15)-C(16)	-19.8(7)	C(58)-C(41)-C(42)-C(43)	165.3(4)
C(13)-C(12)-C(15)-C(16)	99.0(5)	C(41)-C(42)-C(43)-O(2)	-12.5(6)
C(11)-C(12)-C(15)-C(16)	-140.6(4)	C(56)-C(42)-C(43)-O(2)	174.4(4)
C(14)-C(12)-C(15)-C(17)	159.5(5)	C(41)-C(42)-C(43)-C(44)	166.1(4)
C(13)-C(12)-C(15)-C(17)	-81.6(5)	C(56)-C(42)-C(43)-C(44)	-7.0(6)
C(11)-C(12)-C(15)-C(17)	38.7(5)	O(2)-C(43)-C(44)-C(57)	175.9(4)
C(17)-C(15)-C(16)-C(2)	-3.8(6)	C(42)-C(43)-C(44)-C(57)	-2.7(6)
C(12)-C(15)-C(16)-C(2)	175.6(4)	O(2)-C(43)-C(44)-C(45)	-2.7(6)
C(1)-C(2)-C(16)-C(15)	-166.4(4)	C(42)-C(43)-C(44)-C(45)	178.8(4)
C(3)-C(2)-C(16)-C(15)	6.0(6)	C(43)-C(44)-C(45)-C(46)	-46.6(5)
C(9)-N(1)-C(17)-C(4)	-1.1(6)	C(57)-C(44)-C(45)-C(46)	134.8(4)
C(10)-N(1)-C(17)-C(4)	171.5(5)	C(43)-C(44)-C(45)-C(48)	-164.2(4)
C(9)-N(1)-C(17)-C(15)	180.0(4)	C(57)-C(44)-C(45)-C(48)	17.3(5)
C(10)-N(1)-C(17)-C(15)	-7.4(7)	C(43)-C(44)-C(45)-C(47)	76.2(5)
C(3)-C(4)-C(17)-N(1)	-171.5(4)	C(57)-C(44)-C(45)-C(47)	-102.4(4)
C(5)-C(4)-C(17)-N(1)	6.9(6)	C(46)-C(45)-C(48)-C(49)	-171.5(4)
C(3)-C(4)-C(17)-C(15)	7.4(5)	C(47)-C(45)-C(48)-C(49)	68.5(5)
C(5)-C(4)-C(17)-C(15)	-174.2(3)	C(44)-C(45)-C(48)-C(49)	-50.7(5)
C(16)-C(15)-C(17)-N(1)	175.9(4)	C(57)-N(2)-C(49)-C(48)	-28.8(6)
C(12)-C(15)-C(17)-N(1)	-3.5(5)	C(50)-N(2)-C(49)-C(48)	155.6(4)
C(16)-C(15)-C(17)-C(4)	-3.0(5)	C(45)-C(48)-C(49)-N(2)	57.6(5)
C(12)-C(15)-C(17)-C(4)	177.6(3)	C(57)-N(2)-C(50)-C(51)	-10.5(7)
C(2)-C(1)-C(18)-C(19)	-30.0(7)	C(49)-N(2)-C(50)-C(51)	164.9(4)
C(2)-C(1)-C(18)-C(32)	158.8(4)	N(2)-C(50)-C(51)-C(52)	46.6(6)
C(1)-C(18)-C(19)-C(20)	-170.1(4)	C(50)-C(51)-C(52)-C(54)	177.0(4)
C(32)-C(18)-C(19)-C(20)	2.6(5)	C(50)-C(51)-C(52)-C(53)	56.3(5)
C(18)-C(19)-C(20)-C(22)	-2.3(5)	C(50)-C(51)-C(52)-C(55)	-60.7(5)
C(18)-C(19)-C(20)-C(21)	178.0(4)	C(51)-C(52)-C(55)-C(56)	-137.0(4)
C(19)-C(20)-C(22)-C(23)	178.9(4)	C(54)-C(52)-C(55)-C(56)	-16.7(6)
C(21)-C(20)-C(22)-C(23)	-1.4(7)	C(53)-C(52)-C(55)-C(56)	104.4(4)

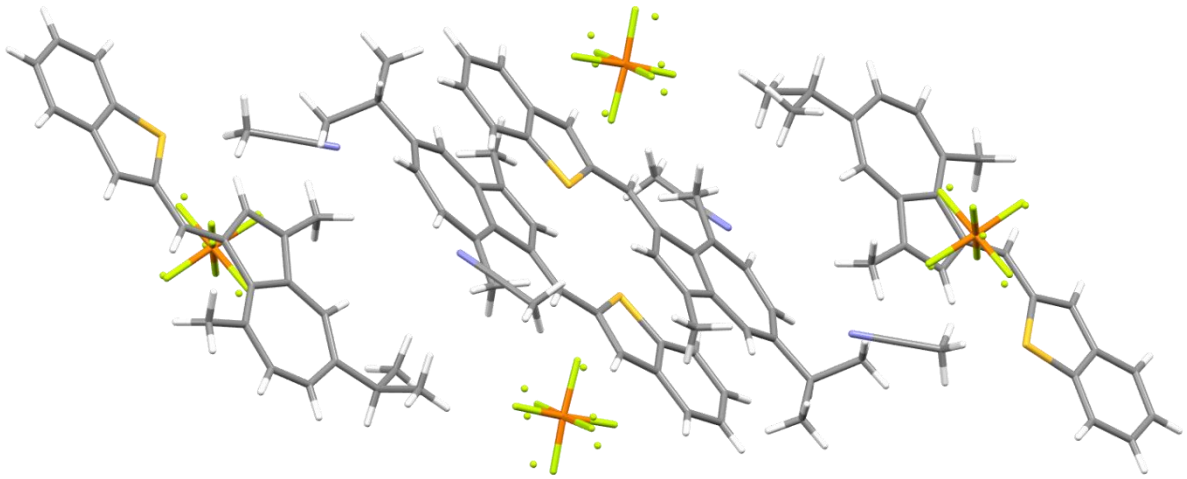
C(51)-C(52)-C(55)-C(57)	43.3(5)	C(63)-C(64)-C(65)-C(67)	112.9(9)
C(54)-C(52)-C(55)-C(57)	163.6(4)	C(68)-C(64)-C(65)-C(67)	-67.4(9)
C(53)-C(52)-C(55)-C(57)	-75.3(4)	C(63)-C(64)-C(65)-C(66)	-121.0(8)
C(57)-C(55)-C(56)-C(42)	-1.6(6)	C(68)-C(64)-C(65)-C(66)	58.7(9)
C(52)-C(55)-C(56)-C(42)	178.7(4)	C(63)-C(64)-C(65A)-C(67)	59(5)
C(41)-C(42)-C(56)-C(55)	-163.6(4)	C(68)-C(64)-C(65A)-C(67)	-114(4)
C(43)-C(42)-C(56)-C(55)	9.2(6)	C(63)-C(64)-C(65A)-C(66)	-84(3)
C(49)-N(2)-C(57)-C(44)	-4.3(6)	C(68)-C(64)-C(65A)-C(66)	103(3)
C(50)-N(2)-C(57)-C(44)	170.8(4)	C(63)-C(64)-C(68)-C(69)	4.3(8)
C(49)-N(2)-C(57)-C(55)	176.3(4)	C(65)-C(64)-C(68)-C(69)	-175.4(5)
C(50)-N(2)-C(57)-C(55)	-8.6(6)	C(65A)-C(64)-C(68)-C(69)	179.5(14)
C(43)-C(44)-C(57)-N(2)	-168.9(4)	C(64)-C(68)-C(69)-C(70)	3.9(9)
C(45)-C(44)-C(57)-N(2)	9.7(6)	C(68)-C(69)-C(70)-C(72)	-3.7(7)
C(43)-C(44)-C(57)-C(55)	10.5(6)	C(68)-C(69)-C(70)-C(71)	176.0(4)
C(45)-C(44)-C(57)-C(55)	-170.9(3)	C(69)-C(70)-C(72)-C(58)	-177.6(4)
C(56)-C(55)-C(57)-N(2)	170.8(4)	C(71)-C(70)-C(72)-C(58)	2.7(6)
C(52)-C(55)-C(57)-N(2)	-9.4(6)	C(69)-C(70)-C(72)-C(62)	-5.1(6)
C(56)-C(55)-C(57)-C(44)	-8.6(6)	C(71)-C(70)-C(72)-C(62)	175.2(3)
C(52)-C(55)-C(57)-C(44)	171.1(4)	C(59)-C(58)-C(72)-C(70)	172.6(4)
C(42)-C(41)-C(58)-C(59)	-34.8(6)	C(41)-C(58)-C(72)-C(70)	-16.1(7)
C(42)-C(41)-C(58)-C(72)	155.1(4)	C(59)-C(58)-C(72)-C(62)	-1.1(4)
C(41)-C(58)-C(59)-C(60)	-170.7(4)	C(41)-C(58)-C(72)-C(62)	170.1(4)
C(72)-C(58)-C(59)-C(60)	1.3(5)	C(63)-C(62)-C(72)-C(70)	9.6(6)
C(58)-C(59)-C(60)-C(62)	-1.0(5)	C(60)-C(62)-C(72)-C(70)	-173.3(4)
C(58)-C(59)-C(60)-C(61)	175.5(4)	C(63)-C(62)-C(72)-C(58)	-176.6(4)
C(59)-C(60)-C(62)-C(63)	177.6(4)	C(60)-C(62)-C(72)-C(58)	0.6(4)
C(61)-C(60)-C(62)-C(63)	1.3(7)	F(11A)-P(2)-F(7)-F(10A)	81.4(13)
C(59)-C(60)-C(62)-C(72)	0.2(5)	F(9A)-P(2)-F(7)-F(10A)	-176.4(16)
C(61)-C(60)-C(62)-C(72)	-176.1(4)	F(12A)-P(2)-F(7)-F(10A)	-86.1(14)
C(60)-C(62)-C(63)-C(64)	-178.8(4)	F(11A)-P(2)-F(10A)-F(7)	-97.6(9)
C(72)-C(62)-C(63)-C(64)	-2.0(7)	F(8)-P(2)-F(10A)-F(7)	-172.7(4)
C(62)-C(63)-C(64)-C(68)	-6.5(8)	F(9A)-P(2)-F(10A)-F(7)	8(4)
C(62)-C(63)-C(64)-C(65)	173.2(5)	F(12A)-P(2)-F(10A)-F(7)	71.7(8)
C(62)-C(63)-C(64)-C(65A)	-178(2)		

Table S22: Crystal data and structure refinement for **32**

.

CCDC code	#2129315	
Empirical formula	$C_{26}H_{26}F_6NPS$	
Formula weight	529.51	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.4072(2) Å	α= 90°.
	b = 15.5867(5) Å	β= 99.378(2)°.
	c = 21.6148(6) Å	γ = 90°.
Volume	2462.16(12) $Å^3$	
Z	4	
Density (calculated)	1.428 Mg/m^3	
Absorption coefficient	2.334 mm^{-1}	
F(000)	1096	
Crystal size	0.250 x 0.050 x 0.020 mm^3	
Theta range for data collection	3.512 to 72.905°.	
Index ranges	-9<=h<=7, -17<=k<=19, -26<=l<=25	
Reflections collected	16632	
Independent reflections	4834 [R(int) = 0.0469]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86900	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4834 / 72 / 376	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1048	
R indices (all data)	R1 = 0.0634, wR2 = 0.1143	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.365 and -0.284 $e.Å^{-3}$	





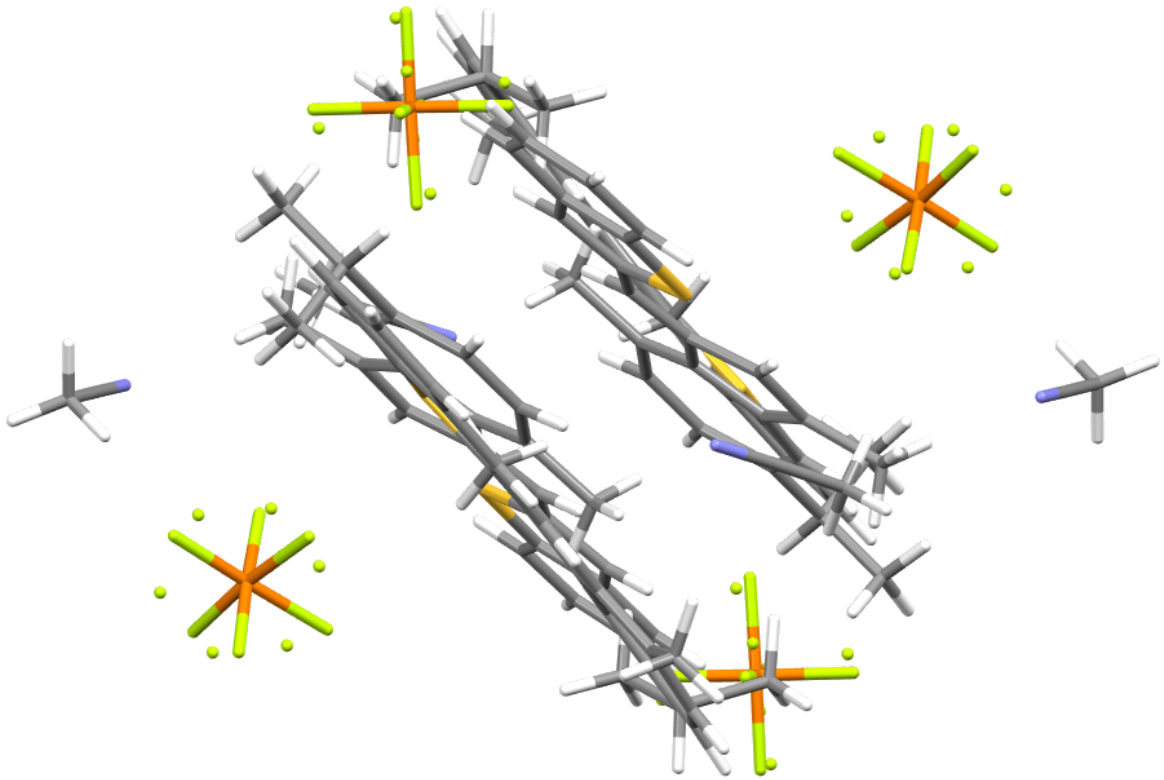


Table S23: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **32**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S	1200(1)	3855(1)	4339(1)	25(1)
C(1)	168(3)	4119(2)	3583(1)	25(1)
C(2)	-630(3)	3545(2)	3122(1)	32(1)
C(3)	-1393(3)	3882(2)	2550(1)	35(1)
C(4)	-1381(3)	4765(2)	2435(1)	35(1)
C(5)	-582(3)	5331(2)	2887(1)	31(1)
C(6)	228(3)	5008(2)	3477(1)	26(1)
C(7)	1146(3)	5454(2)	4013(1)	26(1)
C(8)	1745(3)	4930(1)	4514(1)	24(1)
C(9)	2685(3)	5257(2)	5096(1)	24(1)
C(10)	3289(3)	4835(1)	5648(1)	22(1)
C(11)	4322(3)	5187(2)	6236(1)	22(1)
C(12)	4799(3)	6041(1)	6376(1)	23(1)
C(13)	4154(3)	6762(2)	5926(1)	30(1)
C(14)	5905(3)	6316(2)	6938(1)	27(1)
C(15)	6677(3)	5894(2)	7477(1)	27(1)
C(16)	6568(3)	5034(2)	7654(1)	25(1)
C(17)	7466(3)	4808(2)	8317(1)	28(1)
C(18)	6291(4)	5160(2)	8782(1)	37(1)
C(19)	7826(4)	3855(2)	8426(1)	38(1)
C(20)	5652(3)	4412(2)	7267(1)	26(1)
C(21)	4710(3)	4466(2)	6654(1)	24(1)
C(22)	3885(3)	3707(2)	6341(1)	27(1)
C(23)	3916(4)	2834(2)	6626(1)	38(1)
C(24)	3067(3)	3931(2)	5757(1)	26(1)
N	7486(4)	8328(2)	6537(1)	53(1)
C(31)	7414(4)	8575(2)	6042(2)	44(1)
C(32)	7294(5)	8913(3)	5408(2)	67(1)
P	1651(1)	6852(1)	9359(1)	34(1)
F(1)	2124(15)	6353(6)	9975(4)	94(3)
F(3)	669(12)	7572(5)	9710(3)	68(2)
F(2)	1224(10)	7414(3)	8714(2)	73(2)
F(4)	3470(10)	7401(6)	9525(3)	111(3)
F(5)	2626(13)	6170(9)	8983(5)	85(3)
F(6)	-183(8)	6388(6)	9149(3)	100(2)
F(1A)	2830(30)	6488(18)	9980(11)	95(7)
F(2A)	460(30)	7145(16)	8781(6)	107(7)
F(3A)	360(30)	7335(14)	9758(11)	84(6)
F(4A)	2970(30)	7595(7)	9410(9)	89(5)
F(5A)	2930(20)	6310(20)	9029(14)	56(4)
F(6A)	350(20)	6036(11)	9427(12)	97(6)

Table S24: Bond lengths [Å] for **32**.

S-C(1)	1.738(2)	C(17)-C(18)	1.534(3)
S-C(8)	1.751(2)	C(17)-H(17)	1.0000
C(1)-C(2)	1.396(3)	C(18)-H(18A)	0.9800
C(1)-C(6)	1.406(3)	C(18)-H(18B)	0.9800
C(2)-C(3)	1.377(4)	C(18)-H(18C)	0.9800
C(2)-H(2)	0.9500	C(19)-H(19A)	0.9800
C(3)-C(4)	1.400(4)	C(19)-H(19B)	0.9800
C(3)-H(3)	0.9500	C(19)-H(19C)	0.9800
C(4)-C(5)	1.377(4)	C(20)-C(21)	1.397(3)
C(4)-H(4)	0.9500	C(20)-H(20)	0.9500
C(5)-C(6)	1.411(3)	C(21)-C(22)	1.448(3)
C(5)-H(5)	0.9500	C(22)-C(24)	1.354(3)
C(6)-C(7)	1.425(3)	C(22)-C(23)	1.492(3)
C(7)-C(8)	1.370(3)	C(23)-H(23A)	0.9800
C(7)-H(7)	0.9500	C(23)-H(23B)	0.9800
C(8)-C(9)	1.428(3)	C(23)-H(23C)	0.9800
C(9)-C(10)	1.373(3)	C(24)-H(24)	0.9500
C(9)-H(9)	0.9500	N-C(31)	1.132(4)
C(10)-C(24)	1.442(3)	C(31)-C(32)	1.456(5)
C(10)-C(11)	1.477(3)	C(32)-H(32A)	0.9800
C(11)-C(12)	1.397(3)	C(32)-H(32B)	0.9800
C(11)-C(21)	1.442(3)	C(32)-H(32C)	0.9800
C(12)-C(14)	1.417(3)	P-F(2A)	1.477(11)
C(12)-C(13)	1.512(3)	P-F(4A)	1.509(13)
C(13)-H(13A)	0.9800	P-F(5A)	1.53(2)
C(13)-H(13B)	0.9800	P-F(1)	1.532(7)
C(13)-H(13C)	0.9800	P-F(6)	1.541(5)
C(14)-C(15)	1.378(3)	P-F(3A)	1.577(19)
C(14)-H(14)	0.9500	P-F(1A)	1.58(2)
C(15)-C(16)	1.400(3)	P-F(5)	1.583(11)
C(15)-H(15)	0.9500	P-F(4)	1.587(6)
C(16)-C(20)	1.385(3)	P-F(3)	1.595(7)
C(16)-C(17)	1.519(3)	P-F(6A)	1.618(13)
C(17)-C(19)	1.520(4)	P-F(2)	1.633(5)

Table S25: Bond angles [°] for **32**.

C(1)-S-C(8)	91.56(11)	C(17)-C(18)-H(18A)	109.5
C(2)-C(1)-C(6)	122.4(2)	C(17)-C(18)-H(18B)	109.5
C(2)-C(1)-S	126.1(2)	H(18A)-C(18)-H(18B)	109.5
C(6)-C(1)-S	111.42(17)	C(17)-C(18)-H(18C)	109.5
C(3)-C(2)-C(1)	117.4(3)	H(18A)-C(18)-H(18C)	109.5
C(3)-C(2)-H(2)	121.3	H(18B)-C(18)-H(18C)	109.5
C(1)-C(2)-H(2)	121.3	C(17)-C(19)-H(19A)	109.5
C(2)-C(3)-C(4)	121.5(2)	C(17)-C(19)-H(19B)	109.5
C(2)-C(3)-H(3)	119.3	H(19A)-C(19)-H(19B)	109.5
C(4)-C(3)-H(3)	119.3	C(17)-C(19)-H(19C)	109.5
C(5)-C(4)-C(3)	121.2(2)	H(19A)-C(19)-H(19C)	109.5
C(5)-C(4)-H(4)	119.4	H(19B)-C(19)-H(19C)	109.5
C(3)-C(4)-H(4)	119.4	C(16)-C(20)-C(21)	130.6(2)
C(4)-C(5)-C(6)	118.9(2)	C(16)-C(20)-H(20)	114.7
C(4)-C(5)-H(5)	120.6	C(21)-C(20)-H(20)	114.7
C(6)-C(5)-H(5)	120.6	C(20)-C(21)-C(11)	131.3(2)
C(1)-C(6)-C(5)	118.6(2)	C(20)-C(21)-C(22)	120.1(2)
C(1)-C(6)-C(7)	111.8(2)	C(11)-C(21)-C(22)	108.60(19)
C(5)-C(6)-C(7)	129.5(2)	C(24)-C(22)-C(21)	108.3(2)
C(8)-C(7)-C(6)	113.7(2)	C(24)-C(22)-C(23)	126.5(2)
C(8)-C(7)-H(7)	123.1	C(21)-C(22)-C(23)	125.2(2)
C(6)-C(7)-H(7)	123.1	C(22)-C(23)-H(23A)	109.5
C(7)-C(8)-C(9)	122.2(2)	C(22)-C(23)-H(23B)	109.5
C(7)-C(8)-S	111.45(17)	H(23A)-C(23)-H(23B)	109.5
C(9)-C(8)-S	126.38(18)	C(22)-C(23)-H(23C)	109.5
C(10)-C(9)-C(8)	129.7(2)	H(23A)-C(23)-H(23C)	109.5
C(10)-C(9)-H(9)	115.2	H(23B)-C(23)-H(23C)	109.5
C(8)-C(9)-H(9)	115.2	C(22)-C(24)-C(10)	111.0(2)
C(9)-C(10)-C(24)	125.4(2)	C(22)-C(24)-H(24)	124.5
C(9)-C(10)-C(11)	128.2(2)	C(10)-C(24)-H(24)	124.5
C(24)-C(10)-C(11)	106.30(19)	N-C(31)-C(32)	178.4(4)
C(12)-C(11)-C(21)	126.1(2)	C(31)-C(32)-H(32A)	109.5
C(12)-C(11)-C(10)	128.2(2)	C(31)-C(32)-H(32B)	109.5
C(21)-C(11)-C(10)	105.72(19)	H(32A)-C(32)-H(32B)	109.5
C(11)-C(12)-C(14)	124.4(2)	C(31)-C(32)-H(32C)	109.5
C(11)-C(12)-C(13)	121.8(2)	H(32A)-C(32)-H(32C)	109.5
C(14)-C(12)-C(13)	113.8(2)	H(32B)-C(32)-H(32C)	109.5
C(12)-C(13)-H(13A)	109.5	F(2A)-P-F(4A)	96.6(11)
C(12)-C(13)-H(13B)	109.5	F(2A)-P-F(5A)	96.0(13)
H(13A)-C(13)-H(13B)	109.5	F(4A)-P-F(5A)	91.0(12)
C(12)-C(13)-H(13C)	109.5	F(1)-P-F(6)	94.8(4)
H(13A)-C(13)-H(13C)	109.5	F(2A)-P-F(3A)	89.1(10)
H(13B)-C(13)-H(13C)	109.5	F(4A)-P-F(3A)	92.2(10)
C(15)-C(14)-C(12)	133.1(2)	F(5A)-P-F(3A)	173.6(15)
C(15)-C(14)-H(14)	113.4	F(2A)-P-F(1A)	176.1(13)
C(12)-C(14)-H(14)	113.4	F(4A)-P-F(1A)	87.3(11)
C(14)-C(15)-C(16)	130.8(2)	F(5A)-P-F(1A)	84.3(15)
C(14)-C(15)-H(15)	114.6	F(3A)-P-F(1A)	90.3(13)
C(16)-C(15)-H(15)	114.6	F(1)-P-F(5)	92.7(6)
C(20)-C(16)-C(15)	123.4(2)	F(6)-P-F(5)	89.3(4)
C(20)-C(16)-C(17)	120.2(2)	F(1)-P-F(4)	90.6(4)
C(15)-C(16)-C(17)	116.4(2)	F(6)-P-F(4)	174.3(3)
C(16)-C(17)-C(19)	114.4(2)	F(5)-P-F(4)	92.1(5)
C(16)-C(17)-C(18)	109.01(19)	F(1)-P-F(3)	90.1(4)
C(19)-C(17)-C(18)	110.6(2)	F(6)-P-F(3)	91.2(4)
C(16)-C(17)-H(17)	107.5	F(5)-P-F(3)	177.1(5)
C(19)-C(17)-H(17)	107.5	F(4)-P-F(3)	87.1(4)
C(18)-C(17)-H(17)	107.5	F(2A)-P-F(6A)	92.2(9)

F(4A)-P-F(6A)	170.6(10)	F(6)-P-F(2)	87.8(3)
F(5A)-P-F(6A)	91.6(11)	F(5)-P-F(2)	87.8(5)
F(3A)-P-F(6A)	84.4(9)	F(4)-P-F(2)	86.7(3)
F(1A)-P-F(6A)	83.9(11)	F(3)-P-F(2)	89.4(3)
F(1)-P-F(2)	177.3(4)		

Table S26: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **32**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S	29(1)	23(1)	24(1)	0(1)	3(1)	0(1)
C(1)	22(1)	33(1)	21(1)	-1(1)	4(1)	1(1)
C(2)	31(1)	36(1)	29(1)	-6(1)	6(1)	-5(1)
C(3)	26(1)	52(2)	27(1)	-8(1)	5(1)	-5(1)
C(4)	26(1)	56(2)	21(1)	2(1)	3(1)	5(1)
C(5)	28(1)	39(1)	26(1)	4(1)	7(1)	5(1)
C(6)	23(1)	31(1)	24(1)	0(1)	7(1)	2(1)
C(7)	26(1)	24(1)	29(1)	0(1)	9(1)	2(1)
C(8)	24(1)	22(1)	27(1)	-2(1)	9(1)	0(1)
C(9)	25(1)	22(1)	24(1)	-1(1)	8(1)	-1(1)
C(10)	20(1)	23(1)	25(1)	-3(1)	5(1)	-1(1)
C(11)	18(1)	25(1)	23(1)	0(1)	6(1)	1(1)
C(12)	20(1)	23(1)	27(1)	2(1)	6(1)	1(1)
C(13)	35(1)	21(1)	31(1)	-1(1)	-1(1)	-1(1)
C(14)	28(1)	21(1)	31(1)	-2(1)	6(1)	-4(1)
C(15)	26(1)	28(1)	25(1)	-4(1)	3(1)	-2(1)
C(16)	20(1)	30(1)	25(1)	-2(1)	5(1)	1(1)
C(17)	24(1)	37(1)	23(1)	1(1)	2(1)	-1(1)
C(18)	43(1)	44(2)	26(1)	-1(1)	9(1)	1(1)
C(19)	42(1)	39(2)	31(1)	6(1)	-2(1)	8(1)
C(20)	25(1)	27(1)	26(1)	4(1)	3(1)	0(1)
C(21)	22(1)	23(1)	27(1)	-1(1)	7(1)	1(1)
C(22)	30(1)	23(1)	29(1)	0(1)	6(1)	0(1)
C(23)	54(2)	23(1)	34(1)	3(1)	-1(1)	-5(1)
C(24)	29(1)	23(1)	26(1)	-4(1)	3(1)	-2(1)
N	51(2)	40(1)	65(2)	5(1)	2(1)	-9(1)
C(31)	34(1)	40(2)	58(2)	-2(1)	6(1)	-3(1)
C(32)	64(2)	85(3)	55(2)	7(2)	16(2)	6(2)
P	36(1)	34(1)	33(1)	-8(1)	4(1)	4(1)
F(1)	163(8)	80(4)	45(3)	34(3)	39(4)	57(5)
F(3)	100(5)	54(3)	55(2)	-17(2)	23(2)	24(3)
F(2)	135(4)	42(2)	41(2)	3(1)	15(2)	13(2)
F(4)	71(3)	186(7)	76(3)	-43(4)	11(2)	-64(4)
F(5)	122(6)	89(5)	44(3)	-14(3)	10(4)	63(5)
F(6)	70(3)	107(5)	118(4)	-23(3)	2(3)	-47(3)
F(1A)	116(12)	111(11)	47(8)	-10(7)	-17(8)	39(9)
F(2A)	105(11)	157(14)	47(6)	7(8)	-25(6)	85(10)
F(3A)	66(6)	63(11)	137(11)	-30(7)	61(6)	9(6)
F(4A)	110(11)	24(5)	143(12)	27(5)	47(8)	-19(5)
F(5A)	37(4)	72(8)	64(10)	-15(6)	19(4)	21(5)
F(6A)	66(7)	73(8)	162(14)	-43(8)	47(8)	-39(6)

Table S27: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **32**.

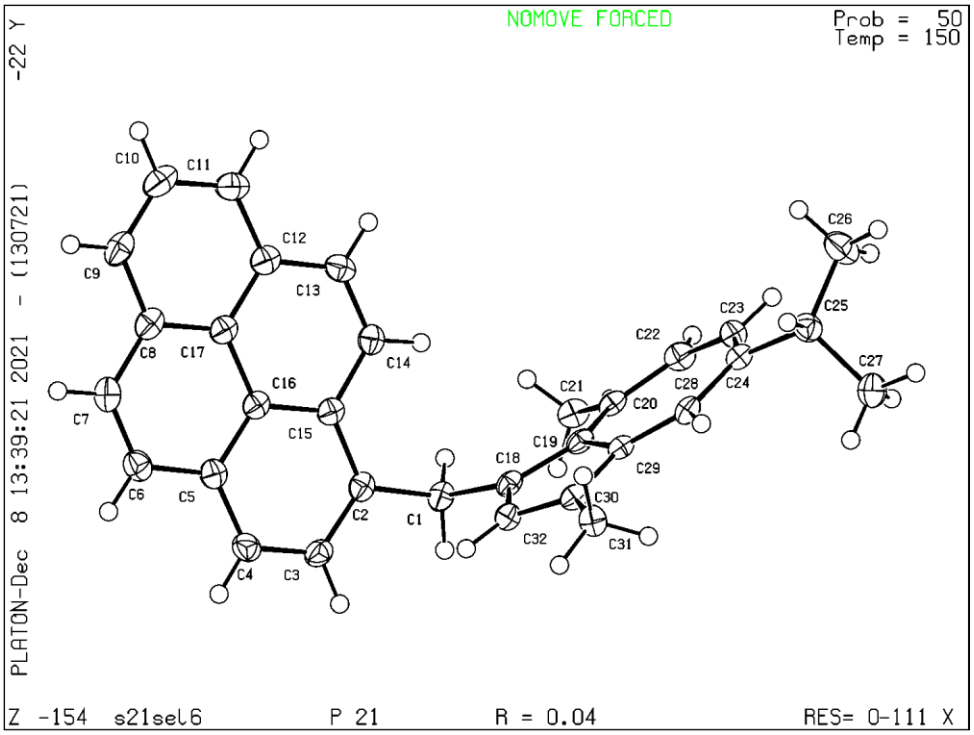
	x	y	z	U(eq)
H(2)	-645	2945	3201	38
H(3)	-1940	3506	2227	42
H(4)	-1935	4978	2037	42
H(5)	-575	5930	2804	37
H(7)	1325	6057	4022	31
H(9)	2930	5855	5101	28
H(13A)	4739	6711	5553	45
H(13B)	4484	7314	6131	45
H(13C)	2823	6729	5804	45
H(14)	6169	6912	6945	32
H(15)	7405	6246	7779	32
H(17)	8673	5109	8399	34
H(18A)	6155	5782	8727	56
H(18B)	6886	5035	9211	56
H(18C)	5082	4889	8704	56
H(19A)	6659	3548	8386	57
H(19B)	8519	3767	8847	57
H(19C)	8534	3636	8114	57
H(20)	5667	3856	7449	31
H(23A)	3213	2437	6327	58
H(23B)	3371	2858	7009	58
H(23C)	5183	2633	6728	58
H(24)	2430	3544	5458	32
H(32A)	8236	8644	5202	101
H(32B)	7485	9535	5427	101
H(32C)	6083	8787	5169	101

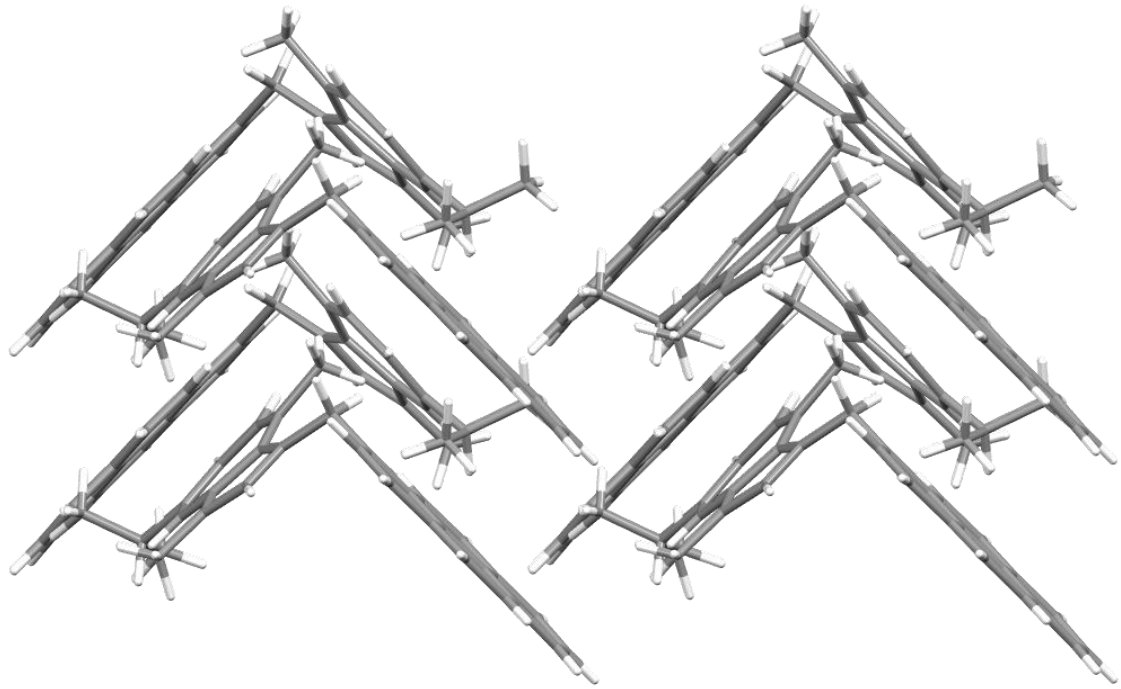
Table S28: Torsion angles [°] for **32**.

C(8)-S-C(1)-C(2)	179.0(2)	C(10)-C(11)-C(12)-C(14)	-175.4(2)
C(8)-S-C(1)-C(6)	-0.77(17)	C(21)-C(11)-C(12)-C(13)	-173.5(2)
C(6)-C(1)-C(2)-C(3)	-0.8(3)	C(10)-C(11)-C(12)-C(13)	4.6(3)
S-C(1)-C(2)-C(3)	179.51(18)	C(11)-C(12)-C(14)-C(15)	-4.3(4)
C(1)-C(2)-C(3)-C(4)	-0.3(4)	C(13)-C(12)-C(14)-C(15)	175.6(2)
C(2)-C(3)-C(4)-C(5)	0.9(4)	C(12)-C(14)-C(15)-C(16)	-2.1(5)
C(3)-C(4)-C(5)-C(6)	-0.3(4)	C(14)-C(15)-C(16)-C(20)	3.4(4)
C(2)-C(1)-C(6)-C(5)	1.3(3)	C(14)-C(15)-C(16)-C(17)	-174.6(2)
S-C(1)-C(6)-C(5)	-178.91(17)	C(20)-C(16)-C(17)-C(19)	19.6(3)
C(2)-C(1)-C(6)-C(7)	-178.7(2)	C(15)-C(16)-C(17)-C(19)	-162.4(2)
S-C(1)-C(6)-C(7)	1.0(2)	C(20)-C(16)-C(17)-C(18)	-104.8(3)
C(4)-C(5)-C(6)-C(1)	-0.8(3)	C(15)-C(16)-C(17)-C(18)	73.2(3)
C(4)-C(5)-C(6)-C(7)	179.3(2)	C(15)-C(16)-C(20)-C(21)	1.0(4)
C(1)-C(6)-C(7)-C(8)	-0.8(3)	C(17)-C(16)-C(20)-C(21)	178.9(2)
C(5)-C(6)-C(7)-C(8)	179.1(2)	C(16)-C(20)-C(21)-C(11)	-2.9(4)
C(6)-C(7)-C(8)-C(9)	-179.6(2)	C(16)-C(20)-C(21)-C(22)	178.8(2)
C(6)-C(7)-C(8)-S	0.2(2)	C(12)-C(11)-C(21)-C(20)	-2.0(4)
C(1)-S-C(8)-C(7)	0.32(17)	C(10)-C(11)-C(21)-C(20)	179.5(2)
C(1)-S-C(8)-C(9)	-179.9(2)	C(12)-C(11)-C(21)-C(22)	176.4(2)
C(7)-C(8)-C(9)-C(10)	176.3(2)	C(10)-C(11)-C(21)-C(22)	-2.1(2)
S-C(8)-C(9)-C(10)	-3.5(4)	C(20)-C(21)-C(22)-C(24)	-179.9(2)
C(8)-C(9)-C(10)-C(24)	-0.6(4)	C(11)-C(21)-C(22)-C(24)	1.4(3)
C(8)-C(9)-C(10)-C(11)	177.5(2)	C(20)-C(21)-C(22)-C(23)	1.1(4)
C(9)-C(10)-C(11)-C(12)	5.2(4)	C(11)-C(21)-C(22)-C(23)	-177.6(2)
C(24)-C(10)-C(11)-C(12)	-176.5(2)	C(21)-C(22)-C(24)-C(10)	-0.2(3)
C(9)-C(10)-C(11)-C(21)	-176.4(2)	C(23)-C(22)-C(24)-C(10)	178.8(2)
C(24)-C(10)-C(11)-C(21)	1.9(2)	C(9)-C(10)-C(24)-C(22)	177.3(2)
C(21)-C(11)-C(12)-C(14)	6.5(3)	C(11)-C(10)-C(24)-C(22)	-1.1(3)

Table S29: Crystal data and structure refinement for **36**.

CCDC code	#2129310	
Empirical formula	$C_{32}H_{28}$	
Formula weight	412.54	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.9223(4) Å	α= 90°.
	b = 4.9868(2) Å	β= 98.446(3)°.
	c = 18.1330(7) Å	γ = 90°.
Volume	1066.39(7) Å^3	
Z	2	
Density (calculated)	1.285 Mg/m^3	
Absorption coefficient	0.543 mm^{-1}	
F(000)	440	
Crystal size	0.210 x 0.040 x 0.030 mm^3	
Theta range for data collection	3.748 to 72.881°.	
Index ranges	-14<=h<=14, -6<=k<=4, -22<=l<=22	
Reflections collected	6420	
Independent reflections	3075 [R(int) = 0.0339]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.85750	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3075 / 1 / 293	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.0943	
R indices (all data)	R1 = 0.0461, wR2 = 0.0986	
Absolute structure parameter	-1.4(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.175 and -0.197 e.Å^{-3}	





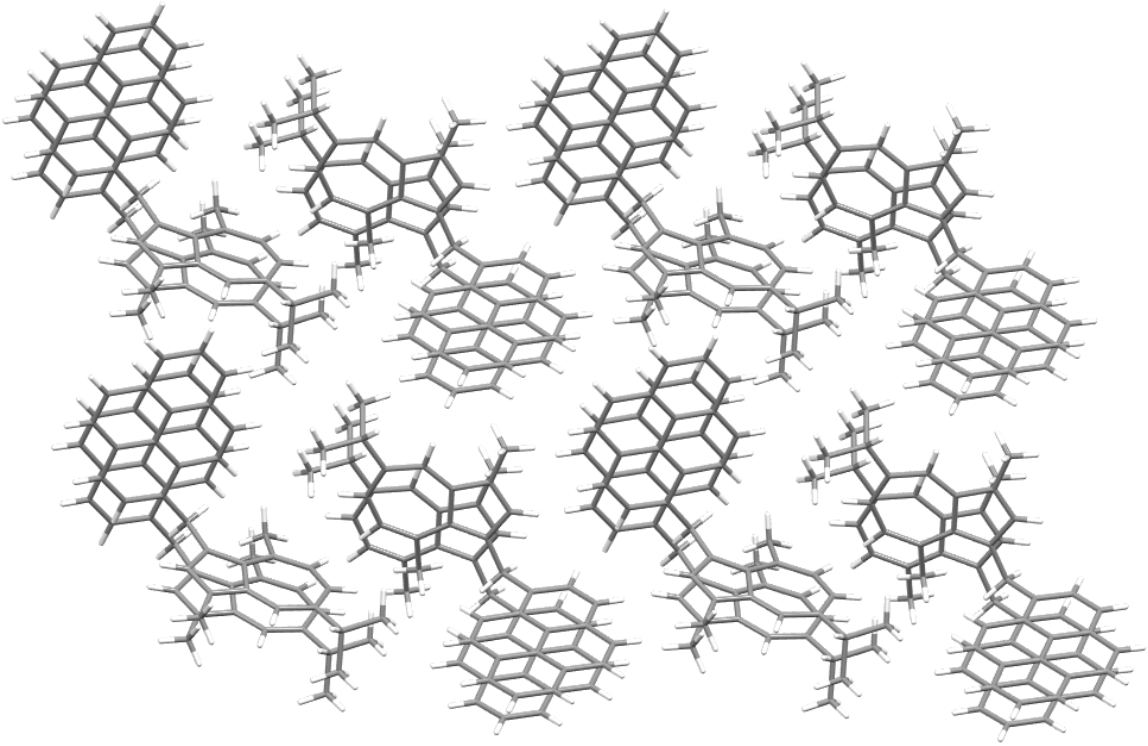


Table S30: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **36**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5548(2)	692(5)	1861(1)	23(1)
C(2)	6230(2)	2453(5)	1406(1)	21(1)
C(3)	6063(2)	2255(6)	631(2)	24(1)
C(4)	6660(2)	3817(6)	193(1)	26(1)
C(5)	7465(2)	5674(5)	514(1)	22(1)
C(6)	8118(2)	7295(6)	76(2)	27(1)
C(7)	8879(2)	9086(6)	396(2)	28(1)
C(8)	9078(2)	9427(6)	1190(2)	24(1)
C(9)	9857(2)	11318(6)	1533(2)	29(1)
C(10)	10051(2)	11572(6)	2303(2)	32(1)
C(11)	9469(2)	9983(6)	2748(2)	29(1)
C(12)	8665(2)	8096(6)	2430(2)	24(1)
C(13)	8033(2)	6454(6)	2866(1)	24(1)
C(14)	7256(2)	4661(5)	2548(1)	22(1)
C(15)	7030(2)	4318(5)	1751(1)	20(1)
C(16)	7651(2)	5925(5)	1304(1)	21(1)
C(17)	8467(2)	7813(5)	1640(2)	22(1)
C(18)	4576(2)	2213(5)	2124(1)	20(1)
C(19)	4180(2)	2298(5)	2816(1)	19(1)
C(20)	4516(2)	769(5)	3468(1)	20(1)
C(21)	5332(2)	-1530(5)	3446(2)	24(1)
C(22)	4148(2)	1164(6)	4157(1)	24(1)
C(23)	3393(2)	2987(6)	4407(1)	24(1)
C(24)	2693(2)	4903(5)	4025(1)	22(1)
C(25)	1878(2)	6513(6)	4426(1)	25(1)
C(26)	2256(3)	6908(7)	5260(2)	35(1)
C(27)	707(2)	5195(7)	4288(2)	36(1)
C(28)	2627(2)	5376(5)	3257(1)	21(1)
C(29)	3230(2)	4316(5)	2732(1)	18(1)
C(30)	3071(2)	5188(5)	1979(1)	20(1)
C(31)	2196(2)	7169(6)	1641(1)	23(1)
C(32)	3885(2)	3961(5)	1632(1)	21(1)

Table S31: Bond lengths [Å] for **36**.

C(1)-C(18)	1.519(3)	C(18)-C(32)	1.421(3)
C(1)-C(2)	1.521(3)	C(19)-C(20)	1.415(3)
C(1)-H(1A)	0.9900	C(19)-C(29)	1.505(3)
C(1)-H(1B)	0.9900	C(20)-C(22)	1.397(4)
C(2)-C(3)	1.393(3)	C(20)-C(21)	1.507(3)
C(2)-C(15)	1.411(4)	C(21)-H(21A)	0.9800
C(3)-C(4)	1.382(4)	C(21)-H(21B)	0.9800
C(3)-H(3)	0.9500	C(21)-H(21C)	0.9800
C(4)-C(5)	1.398(4)	C(22)-C(23)	1.401(4)
C(4)-H(4)	0.9500	C(22)-H(22)	0.9500
C(5)-C(16)	1.424(3)	C(23)-C(24)	1.386(4)
C(5)-C(6)	1.440(4)	C(23)-H(23)	0.9500
C(6)-C(7)	1.342(4)	C(24)-C(28)	1.403(3)
C(6)-H(6)	0.9500	C(24)-C(25)	1.525(3)
C(7)-C(8)	1.435(4)	C(25)-C(26)	1.526(4)
C(7)-H(7)	0.9500	C(25)-C(27)	1.530(4)
C(8)-C(9)	1.403(4)	C(25)-H(25)	1.0000
C(8)-C(17)	1.421(4)	C(26)-H(26A)	0.9800
C(9)-C(10)	1.387(4)	C(26)-H(26B)	0.9800
C(9)-H(9)	0.9500	C(26)-H(26C)	0.9800
C(10)-C(11)	1.387(4)	C(27)-H(27A)	0.9800
C(10)-H(10)	0.9500	C(27)-H(27B)	0.9800
C(11)-C(12)	1.405(4)	C(27)-H(27C)	0.9800
C(11)-H(11)	0.9500	C(28)-C(29)	1.379(3)
C(12)-C(17)	1.424(4)	C(28)-H(28)	0.9500
C(12)-C(13)	1.427(4)	C(29)-C(30)	1.420(3)
C(13)-C(14)	1.354(4)	C(30)-C(32)	1.376(3)
C(13)-H(13)	0.9500	C(30)-C(31)	1.500(3)
C(14)-C(15)	1.440(3)	C(31)-H(31A)	0.9800
C(14)-H(14)	0.9500	C(31)-H(31B)	0.9800
C(15)-C(16)	1.422(3)	C(31)-H(31C)	0.9800
C(16)-C(17)	1.425(3)	C(32)-H(32)	0.9500
C(18)-C(19)	1.406(3)		

Table S32: Bond angles [°] for **36**.

C(18)-C(1)-C(2)	112.1(2)	C(18)-C(19)-C(20)	129.7(2)
C(18)-C(1)-H(1A)	109.2	C(18)-C(19)-C(29)	106.0(2)
C(2)-C(1)-H(1A)	109.2	C(20)-C(19)-C(29)	124.2(2)
C(18)-C(1)-H(1B)	109.2	C(22)-C(20)-C(19)	125.7(2)
C(2)-C(1)-H(1B)	109.2	C(22)-C(20)-C(21)	114.9(2)
H(1A)-C(1)-H(1B)	107.9	C(19)-C(20)-C(21)	119.5(2)
C(3)-C(2)-C(15)	118.8(2)	C(20)-C(21)-H(21A)	109.5
C(3)-C(2)-C(1)	119.9(2)	C(20)-C(21)-H(21B)	109.5
C(15)-C(2)-C(1)	121.3(2)	H(21A)-C(21)-H(21B)	109.5
C(4)-C(3)-C(2)	122.0(2)	C(20)-C(21)-H(21C)	109.5
C(4)-C(3)-H(3)	119.0	H(21A)-C(21)-H(21C)	109.5
C(2)-C(3)-H(3)	119.0	H(21B)-C(21)-H(21C)	109.5
C(3)-C(4)-C(5)	121.0(2)	C(20)-C(22)-C(23)	133.0(2)
C(3)-C(4)-H(4)	119.5	C(20)-C(22)-H(22)	113.5
C(5)-C(4)-H(4)	119.5	C(23)-C(22)-H(22)	113.5
C(4)-C(5)-C(16)	118.3(2)	C(24)-C(23)-C(22)	130.9(2)
C(4)-C(5)-C(6)	122.4(2)	C(24)-C(23)-H(23)	114.6
C(16)-C(5)-C(6)	119.3(2)	C(22)-C(23)-H(23)	114.6
C(7)-C(6)-C(5)	121.4(2)	C(23)-C(24)-C(28)	123.6(2)
C(7)-C(6)-H(6)	119.3	C(23)-C(24)-C(25)	120.2(2)
C(5)-C(6)-H(6)	119.3	C(28)-C(24)-C(25)	116.0(2)
C(6)-C(7)-C(8)	121.0(3)	C(24)-C(25)-C(26)	115.2(2)
C(6)-C(7)-H(7)	119.5	C(24)-C(25)-C(27)	109.0(2)
C(8)-C(7)-H(7)	119.5	C(26)-C(25)-C(27)	110.3(2)
C(9)-C(8)-C(17)	119.2(2)	C(24)-C(25)-H(25)	107.4
C(9)-C(8)-C(7)	121.7(3)	C(26)-C(25)-H(25)	107.4
C(17)-C(8)-C(7)	119.1(2)	C(27)-C(25)-H(25)	107.4
C(10)-C(9)-C(8)	120.6(3)	C(25)-C(26)-H(26A)	109.5
C(10)-C(9)-H(9)	119.7	C(25)-C(26)-H(26B)	109.5
C(8)-C(9)-H(9)	119.7	H(26A)-C(26)-H(26B)	109.5
C(9)-C(10)-C(11)	120.6(3)	C(25)-C(26)-H(26C)	109.5
C(9)-C(10)-H(10)	119.7	H(26A)-C(26)-H(26C)	109.5
C(11)-C(10)-H(10)	119.7	H(26B)-C(26)-H(26C)	109.5
C(10)-C(11)-C(12)	120.9(3)	C(25)-C(27)-H(27A)	109.5
C(10)-C(11)-H(11)	119.6	C(25)-C(27)-H(27B)	109.5
C(12)-C(11)-H(11)	119.6	H(27A)-C(27)-H(27B)	109.5
C(11)-C(12)-C(17)	118.8(2)	C(25)-C(27)-H(27C)	109.5
C(11)-C(12)-C(13)	122.7(2)	H(27A)-C(27)-H(27C)	109.5
C(17)-C(12)-C(13)	118.5(2)	H(27B)-C(27)-H(27C)	109.5
C(14)-C(13)-C(12)	121.8(2)	C(29)-C(28)-C(24)	131.4(2)
C(14)-C(13)-H(13)	119.1	C(29)-C(28)-H(28)	114.3
C(12)-C(13)-H(13)	119.1	C(24)-C(28)-H(28)	114.3
C(13)-C(14)-C(15)	121.4(2)	C(28)-C(29)-C(30)	122.4(2)
C(13)-C(14)-H(14)	119.3	C(28)-C(29)-C(19)	130.3(2)
C(15)-C(14)-H(14)	119.3	C(30)-C(29)-C(19)	107.1(2)
C(2)-C(15)-C(16)	119.5(2)	C(32)-C(30)-C(29)	107.5(2)
C(2)-C(15)-C(14)	122.6(2)	C(32)-C(30)-C(31)	126.9(2)
C(16)-C(15)-C(14)	117.9(2)	C(29)-C(30)-C(31)	125.6(2)
C(15)-C(16)-C(5)	120.5(2)	C(30)-C(31)-H(31A)	109.5
C(15)-C(16)-C(17)	120.6(2)	C(30)-C(31)-H(31B)	109.5
C(5)-C(16)-C(17)	118.9(2)	H(31A)-C(31)-H(31B)	109.5
C(8)-C(17)-C(12)	119.9(2)	C(30)-C(31)-H(31C)	109.5
C(8)-C(17)-C(16)	120.3(2)	H(31A)-C(31)-H(31C)	109.5
C(12)-C(17)-C(16)	119.8(2)	H(31B)-C(31)-H(31C)	109.5
C(19)-C(18)-C(32)	107.6(2)	C(30)-C(32)-C(18)	111.6(2)
C(19)-C(18)-C(1)	131.8(2)	C(30)-C(32)-H(32)	124.2
C(32)-C(18)-C(1)	120.5(2)	C(18)-C(32)-H(32)	124.2

Table S33: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **36**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	18(1)	31(1)	-1(1)	7(1)	0(1)
C(2)	18(1)	18(1)	28(1)	-1(1)	6(1)	4(1)
C(3)	18(1)	24(1)	31(1)	-6(1)	4(1)	0(1)
C(4)	23(1)	31(2)	23(1)	-4(1)	4(1)	4(1)
C(5)	21(1)	21(1)	26(1)	0(1)	5(1)	5(1)
C(6)	27(1)	30(2)	24(1)	0(1)	5(1)	4(1)
C(7)	26(1)	28(2)	31(1)	4(1)	9(1)	3(1)
C(8)	18(1)	18(1)	37(2)	0(1)	4(1)	5(1)
C(9)	20(1)	22(1)	46(2)	-2(1)	8(1)	0(1)
C(10)	21(1)	25(2)	50(2)	-8(1)	2(1)	-1(1)
C(11)	24(1)	30(2)	31(1)	-8(1)	-1(1)	4(1)
C(12)	20(1)	21(1)	31(1)	-3(1)	2(1)	5(1)
C(13)	24(1)	26(2)	23(1)	-4(1)	1(1)	7(1)
C(14)	20(1)	21(1)	27(1)	1(1)	6(1)	4(1)
C(15)	16(1)	18(1)	26(1)	-1(1)	2(1)	5(1)
C(16)	17(1)	18(1)	27(1)	-1(1)	2(1)	5(1)
C(17)	18(1)	19(1)	30(1)	-4(1)	3(1)	4(1)
C(18)	17(1)	15(1)	27(1)	-1(1)	3(1)	-2(1)
C(19)	15(1)	13(1)	27(1)	-2(1)	1(1)	-1(1)
C(20)	16(1)	15(1)	27(1)	0(1)	0(1)	-2(1)
C(21)	24(1)	20(1)	28(1)	1(1)	0(1)	2(1)
C(22)	25(1)	23(1)	24(1)	5(1)	-2(1)	1(1)
C(23)	24(1)	26(2)	21(1)	0(1)	4(1)	-2(1)
C(24)	18(1)	23(1)	24(1)	-1(1)	2(1)	-3(1)
C(25)	26(1)	24(2)	25(1)	-2(1)	4(1)	2(1)
C(26)	36(2)	43(2)	26(1)	-5(1)	4(1)	10(1)
C(27)	24(1)	47(2)	38(2)	-8(1)	10(1)	1(1)
C(28)	16(1)	19(1)	26(1)	3(1)	2(1)	0(1)
C(29)	15(1)	17(1)	22(1)	-1(1)	0(1)	-2(1)
C(30)	18(1)	18(1)	24(1)	1(1)	1(1)	0(1)
C(31)	24(1)	23(1)	23(1)	6(1)	4(1)	6(1)
C(32)	21(1)	21(1)	22(1)	0(1)	4(1)	-2(1)

Table S34: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **36**.

	x	y	z	U(eq)
H(1A)	5241	-857	1555	27
H(1B)	6056	-10	2300	27
H(3)	5522	1008	397	29
H(4)	6520	3627	-334	31
H(6)	8009	7093	-451	32
H(7)	9291	10142	92	33
H(9)	10255	12434	1235	35
H(10)	10588	12845	2528	39
H(11)	9616	10174	3274	35
H(13)	8161	6625	3393	29
H(14)	6852	3606	2857	27
H(21A)	5291	-2721	3871	37
H(21B)	6104	-830	3471	37
H(21C)	5129	-2533	2980	37
H(22)	4476	-49	4531	29
H(23)	3355	2894	4926	28
H(25)	1804	8333	4192	30
H(26A)	2209	5195	5519	52
H(26B)	1760	8222	5452	52
H(26C)	3039	7559	5345	52
H(27A)	173	6250	4531	53
H(27B)	757	3374	4493	53
H(27C)	442	5118	3750	53
H(28)	2068	6651	3064	25
H(31A)	2426	8980	1810	35
H(31B)	1464	6736	1796	35
H(31C)	2128	7085	1096	35
H(32)	3974	4247	1125	26

Table S35: Torsion angles [°] for **36**.

C(18)-C(1)-C(2)-C(3)	-101.6(3)	C(11)-C(12)-C(17)-C(16)	-179.6(2)
C(18)-C(1)-C(2)-C(15)	77.9(3)	C(13)-C(12)-C(17)-C(16)	0.1(3)
C(15)-C(2)-C(3)-C(4)	0.3(4)	C(15)-C(16)-C(17)-C(8)	-179.5(2)
C(1)-C(2)-C(3)-C(4)	179.8(2)	C(5)-C(16)-C(17)-C(8)	0.4(3)
C(2)-C(3)-C(4)-C(5)	0.1(4)	C(15)-C(16)-C(17)-C(12)	0.1(4)
C(3)-C(4)-C(5)-C(16)	-0.3(4)	C(5)-C(16)-C(17)-C(12)	180.0(2)
C(3)-C(4)-C(5)-C(6)	178.7(3)	C(2)-C(1)-C(18)-C(19)	-135.7(3)
C(4)-C(5)-C(6)-C(7)	179.3(3)	C(2)-C(1)-C(18)-C(32)	43.5(3)
C(16)-C(5)-C(6)-C(7)	-1.7(4)	C(32)-C(18)-C(19)-C(20)	174.2(2)
C(5)-C(6)-C(7)-C(8)	0.7(4)	C(1)-C(18)-C(19)-C(20)	-6.5(5)
C(6)-C(7)-C(8)-C(9)	-179.0(3)	C(32)-C(18)-C(19)-C(29)	-2.6(3)
C(6)-C(7)-C(8)-C(17)	0.8(4)	C(1)-C(18)-C(19)-C(29)	176.6(3)
C(17)-C(8)-C(9)-C(10)	1.5(4)	C(18)-C(19)-C(20)-C(22)	173.6(3)
C(7)-C(8)-C(9)-C(10)	-178.7(3)	C(29)-C(19)-C(20)-C(22)	-10.1(4)
C(8)-C(9)-C(10)-C(11)	-0.8(4)	C(18)-C(19)-C(20)-C(21)	-7.1(4)
C(9)-C(10)-C(11)-C(12)	-0.4(4)	C(29)-C(19)-C(20)-C(21)	169.2(2)
C(10)-C(11)-C(12)-C(17)	0.8(4)	C(19)-C(20)-C(22)-C(23)	0.8(5)
C(10)-C(11)-C(12)-C(13)	-178.9(3)	C(21)-C(20)-C(22)-C(23)	-178.5(3)
C(11)-C(12)-C(13)-C(14)	179.5(2)	C(20)-C(22)-C(23)-C(24)	5.4(5)
C(17)-C(12)-C(13)-C(14)	-0.2(4)	C(22)-C(23)-C(24)-C(28)	-0.4(5)
C(12)-C(13)-C(14)-C(15)	0.1(4)	C(22)-C(23)-C(24)-C(25)	175.5(3)
C(3)-C(2)-C(15)-C(16)	-0.6(3)	C(23)-C(24)-C(25)-C(26)	28.2(4)
C(1)-C(2)-C(15)-C(16)	179.9(2)	C(28)-C(24)-C(25)-C(26)	-155.6(3)
C(3)-C(2)-C(15)-C(14)	179.9(2)	C(23)-C(24)-C(25)-C(27)	-96.4(3)
C(1)-C(2)-C(15)-C(14)	0.4(4)	C(28)-C(24)-C(25)-C(27)	79.8(3)
C(13)-C(14)-C(15)-C(2)	179.6(2)	C(23)-C(24)-C(28)-C(29)	-4.7(4)
C(13)-C(14)-C(15)-C(16)	0.1(4)	C(25)-C(24)-C(28)-C(29)	179.3(3)
C(2)-C(15)-C(16)-C(5)	0.4(3)	C(24)-C(28)-C(29)-C(30)	-176.4(3)
C(14)-C(15)-C(16)-C(5)	179.9(2)	C(24)-C(28)-C(29)-C(19)	-0.8(5)
C(2)-C(15)-C(16)-C(17)	-179.7(2)	C(18)-C(19)-C(29)-C(28)	-172.5(3)
C(14)-C(15)-C(16)-C(17)	-0.2(3)	C(20)-C(19)-C(29)-C(28)	10.4(4)
C(4)-C(5)-C(16)-C(15)	0.1(3)	C(18)-C(19)-C(29)-C(30)	3.6(3)
C(6)-C(5)-C(16)-C(15)	-179.0(2)	C(20)-C(19)-C(29)-C(30)	-173.4(2)
C(4)-C(5)-C(16)-C(17)	-179.8(2)	C(28)-C(29)-C(30)-C(32)	173.3(2)
C(6)-C(5)-C(16)-C(17)	1.1(4)	C(19)-C(29)-C(30)-C(32)	-3.2(3)
C(9)-C(8)-C(17)-C(12)	-1.1(4)	C(28)-C(29)-C(30)-C(31)	-4.6(4)
C(7)-C(8)-C(17)-C(12)	179.1(2)	C(19)-C(29)-C(30)-C(31)	178.9(2)
C(9)-C(8)-C(17)-C(16)	178.5(2)	C(29)-C(30)-C(32)-C(18)	1.7(3)
C(7)-C(8)-C(17)-C(16)	-1.3(4)	C(31)-C(30)-C(32)-C(18)	179.5(2)
C(11)-C(12)-C(17)-C(8)	0.0(4)	C(19)-C(18)-C(32)-C(30)	0.7(3)
C(13)-C(12)-C(17)-C(8)	179.7(2)	C(1)-C(18)-C(32)-C(30)	-178.7(2)