SUPPLEMENTARY MATERIAL FOR

Pentafluorosulfanyl-containing triclocarban analogs with potent antimicrobial activity

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[b]*Bacterial Infections and Antimicrobial Therapies, Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology, Baldiri Reixac 15-21, 08028 Barcelona, Spain*

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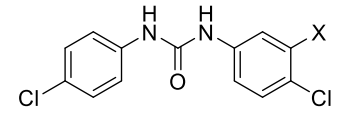
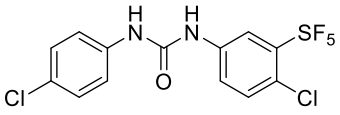
Figure S1. Pentafluorosulfanyl ureas 1-14



TCC, X = Cl
Cloflucarban, X = CF_3



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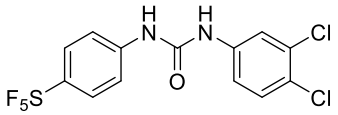

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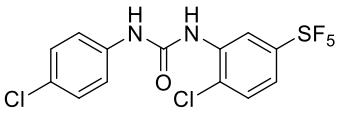

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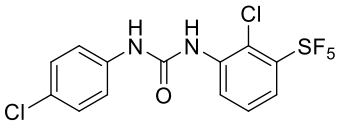

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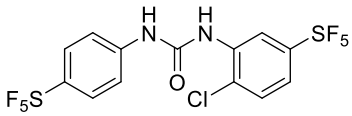

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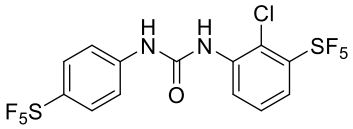

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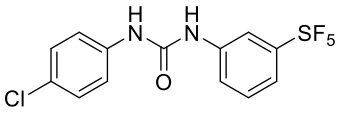

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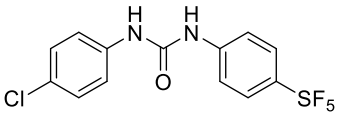

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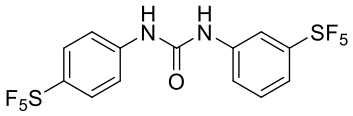

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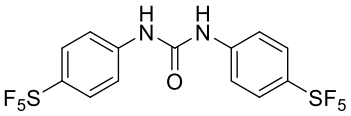

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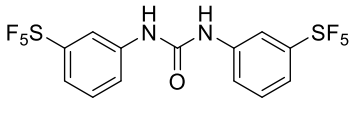

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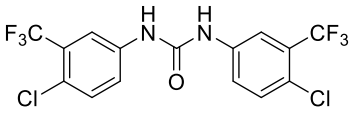

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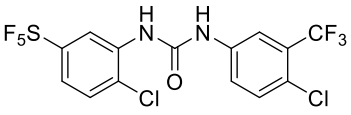

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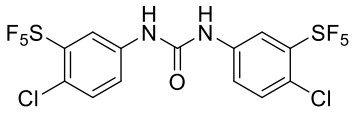
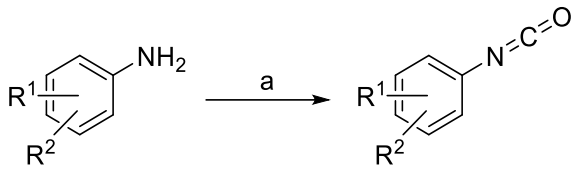


14

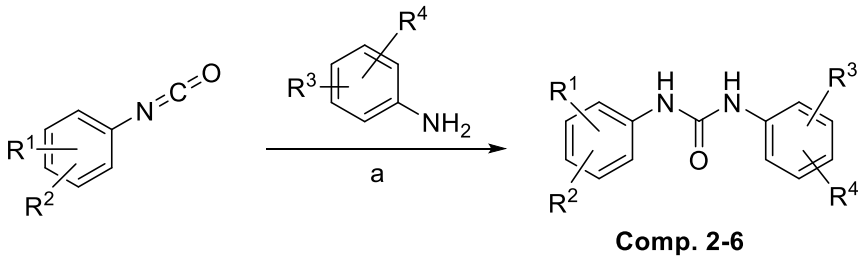
Scheme S1. General procedure for the synthesis of intermediate isocyanates



Reagents and conditions: (a) triphosgene, toluene, Et_3N, 70 ºC, 2 h.

Schemes S2-S4. General synthetic schemes of the final compounds 1-14

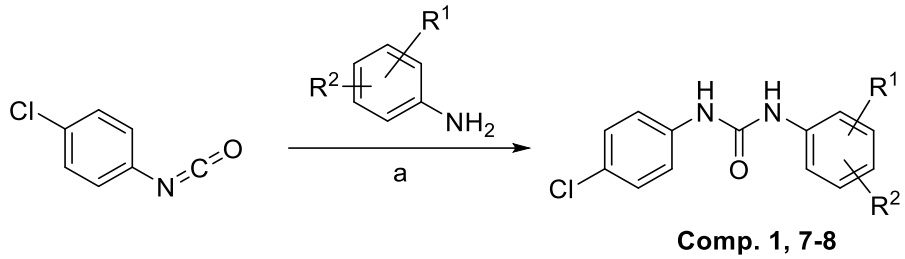
Scheme S2. Synthesis of compounds 2-6



Reagents and conditions: (a) DCM, overnight.

Compound	R^1	R^2	R^3	R^4	Overall yield (%)
2	3-Cl	4-Cl	4-SF_5	H	30
3	5-SF_5	2-Cl	4-Cl	H	47
4	3-SF_5	2-Cl	4-Cl	H	8
5	5-SF_5	2-Cl	4-SF_5	H	6
6	4-SF_5	H	3-SF_5	2-Cl	9

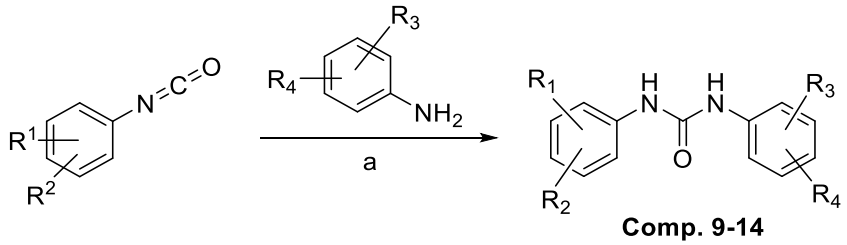
Scheme S3. Synthesis of compounds 1, 7-8



Reagents and conditions: (a) pyridine, 1 h.

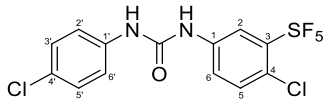
Compound	R^1	R^2	Overall yield (%)
1	3-SF_5	4-Cl	17
7	3-SF_5	H	62
8	4-SF_5	H	80

Scheme S4. Synthesis of compounds 9-14



Reagents and conditions: (a) *n*-BuLi, anh. TFH, overnight.

Compound	R^1	R^2	R^3	R^4	Overall yield (%)
9	3-SF_5	H	4-SF_5	H	20
10	4-SF_5	H	4-SF_5	H	22
11	3-SF_5	H	3-SF_5	H	49
12	3-CF_3	4-Cl	3-CF_3	4-Cl	35
13	5-SF_5	2-Cl	3-CF_3	4-Cl	22
14	3-SF_5	4-Cl	3-SF_5	4-Cl	23



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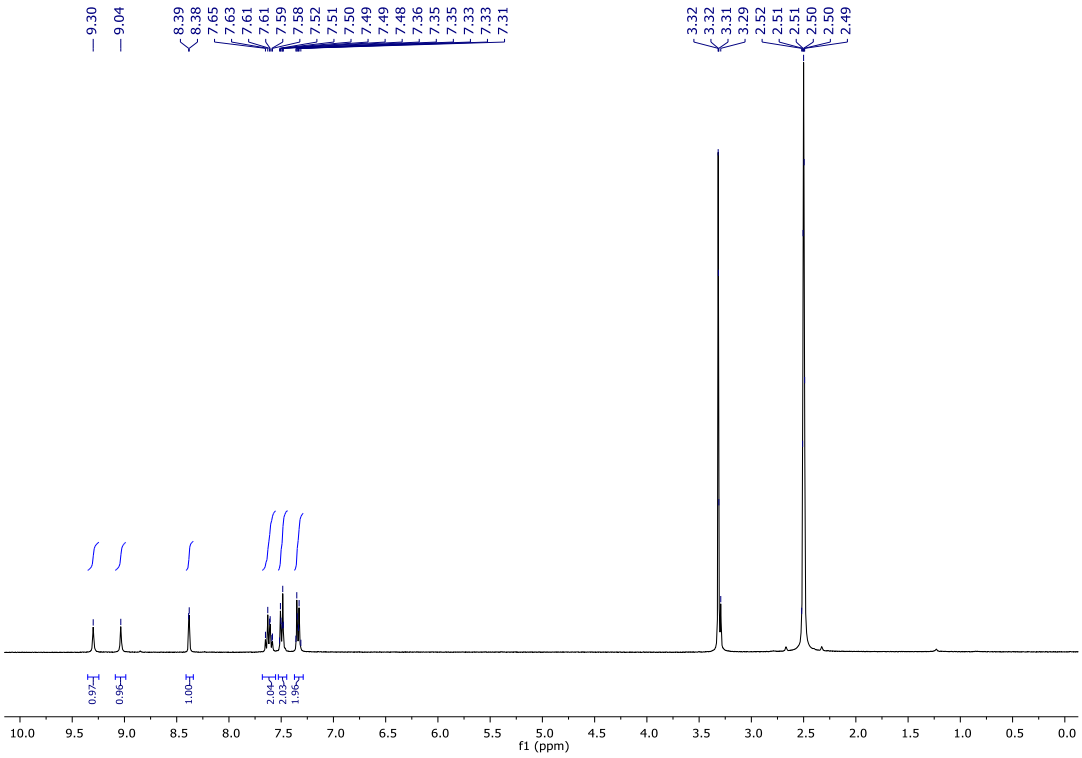
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8.38
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7.63
7.61
7.61
7.59
7.58
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7.49
7.49
7.48
7.36
7.35
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7.33
7.31
3.32
3.32
3.31
3.29
2.52
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2.04
2.03
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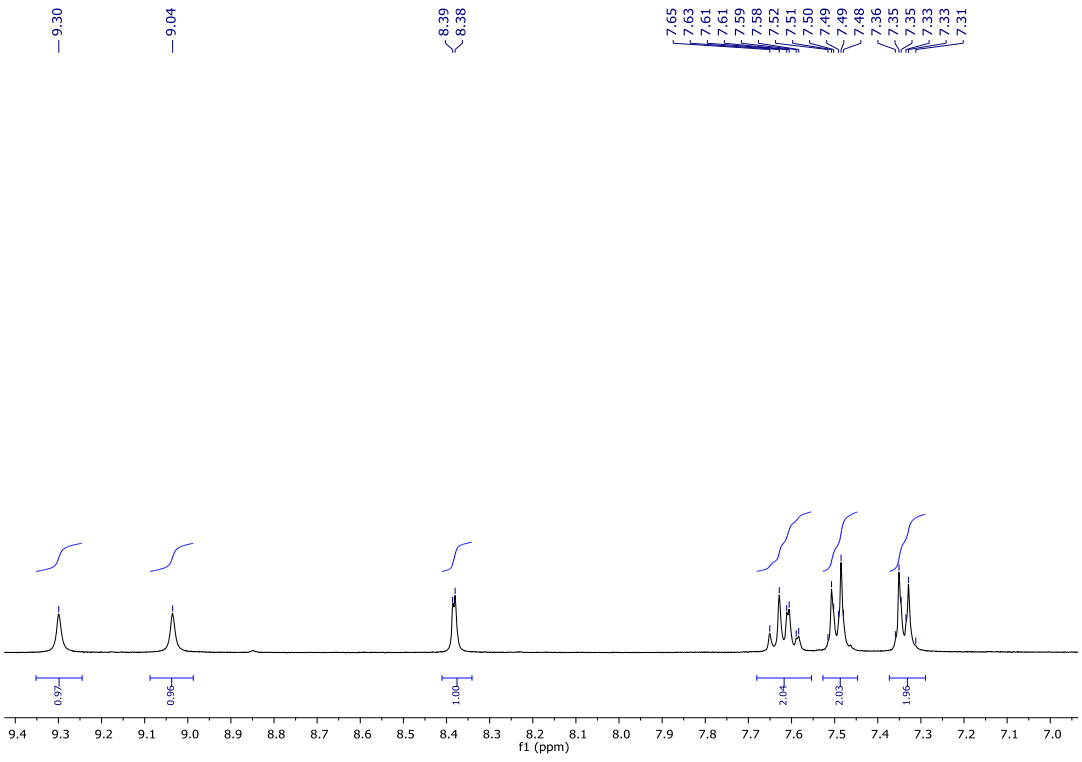
f1 (ppm)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7.65
7.63
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7.58
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7.50
7.49
7.49
7.48
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7.35
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7.33
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0.96
1.00
2.04
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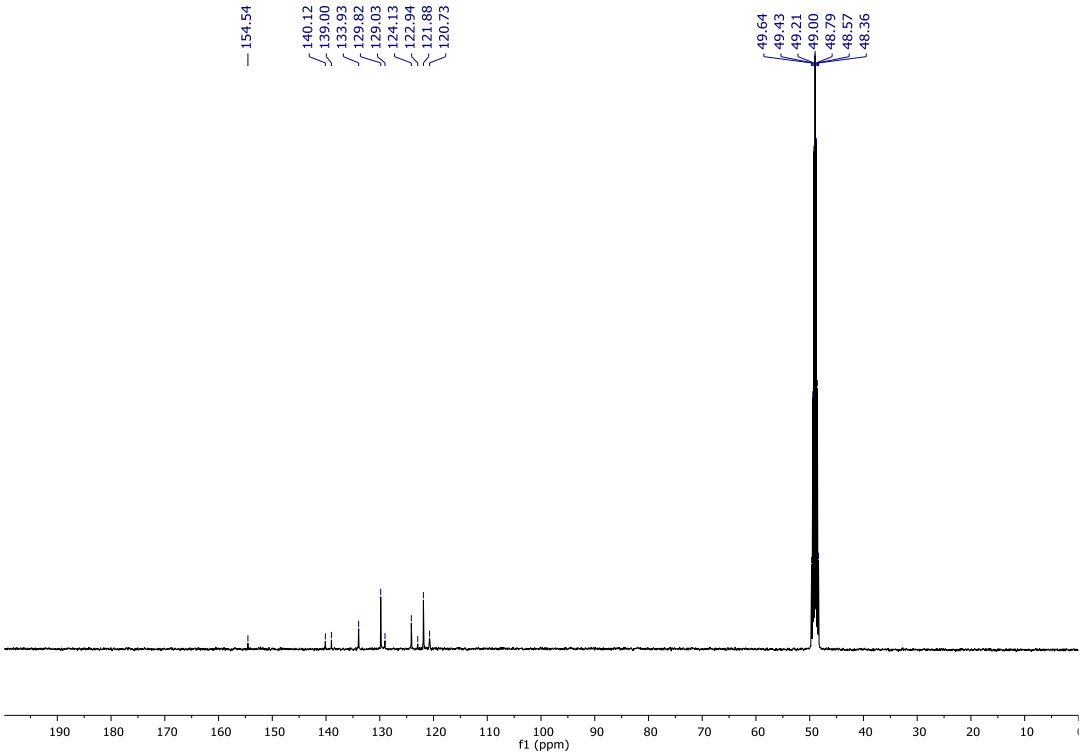
1.96
f1 (ppm)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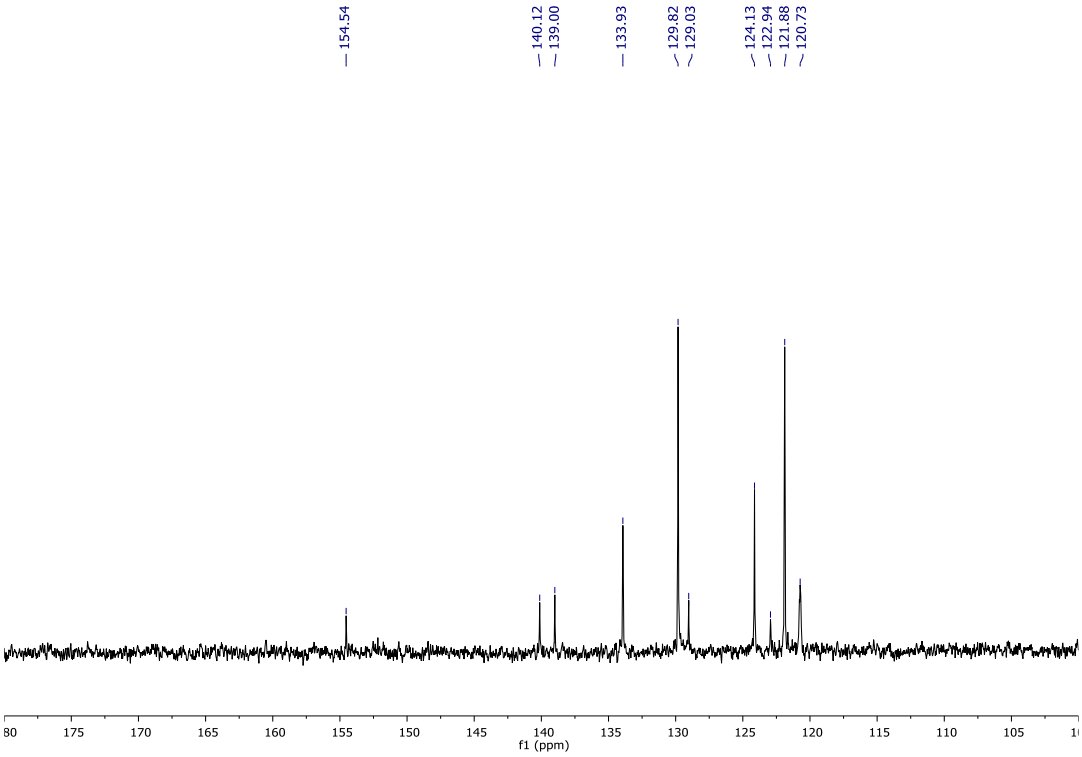
f1 (ppm)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129.03
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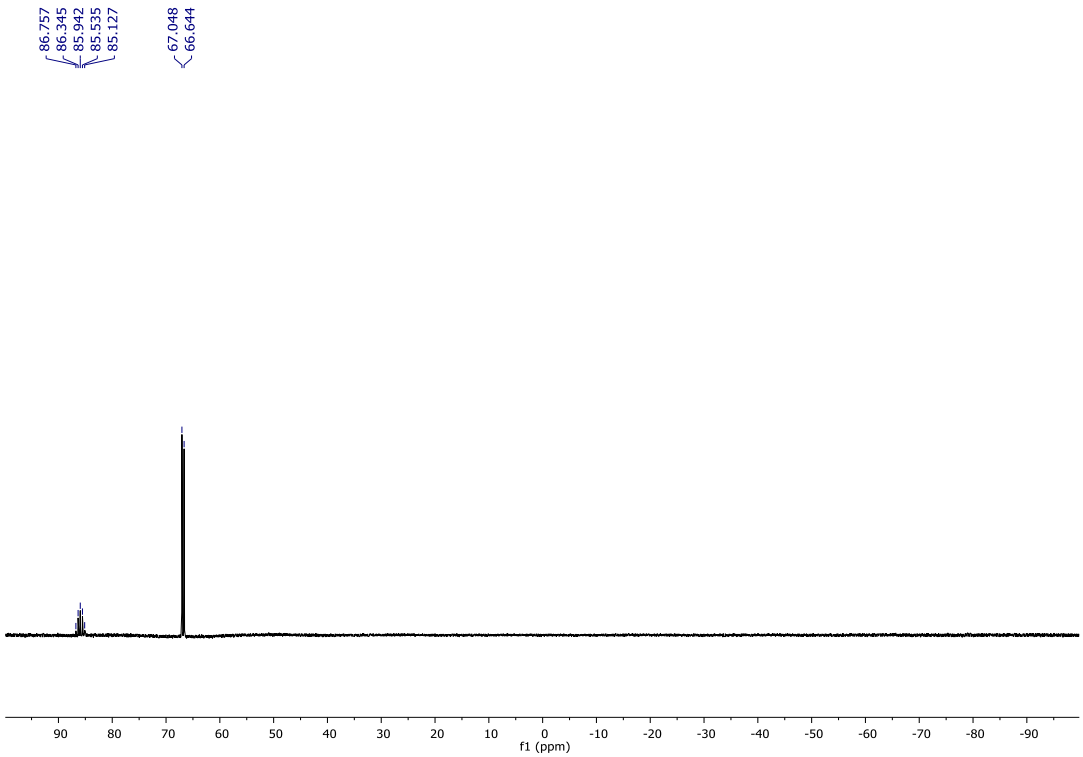
122.94
121.88
120.73
f1 (ppm)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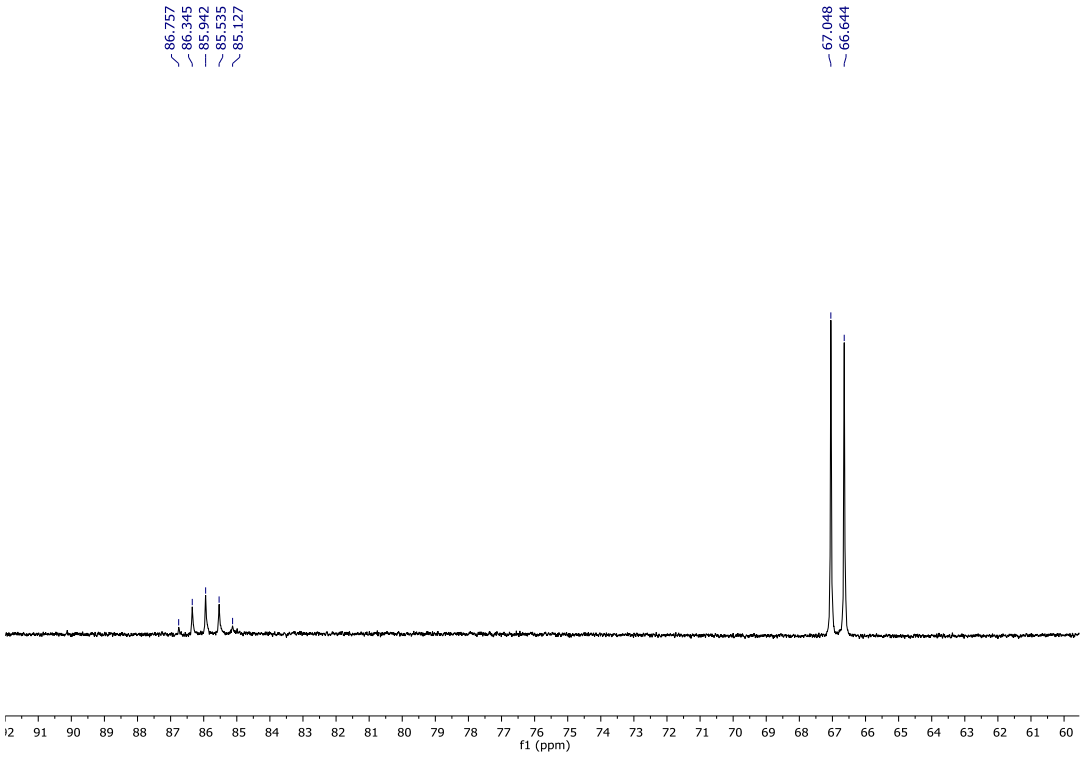
f1 (ppm)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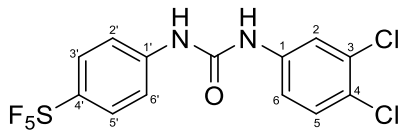
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H
N
O
Cl
Cl
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2'
3'
4'
5'
6'
1
2
3
4
5
6

2


9.33
9.13
7.88
7.87
7.82
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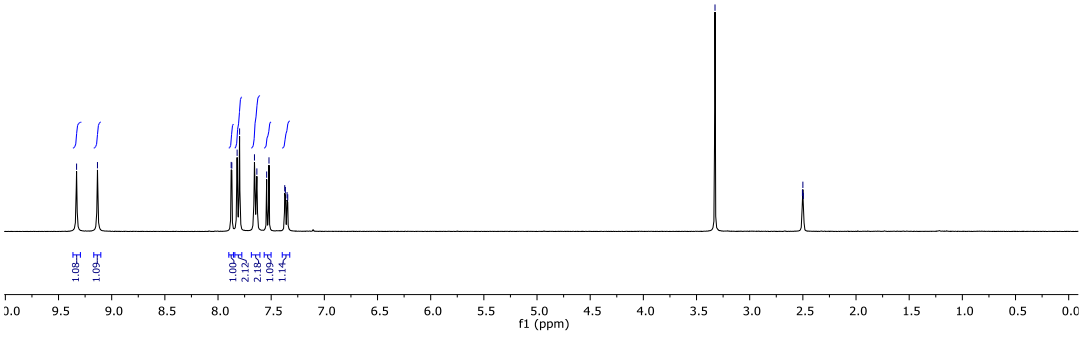
2.50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f1 (ppm)


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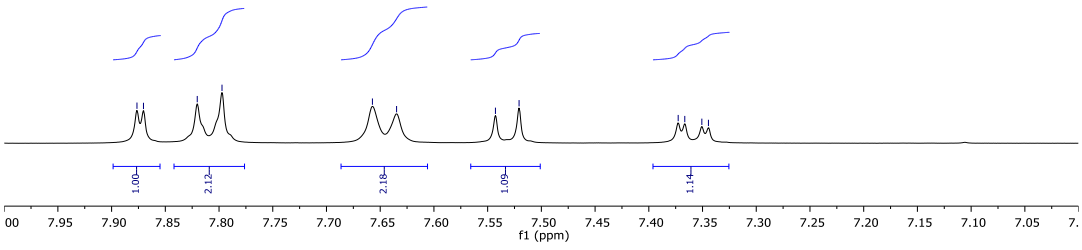
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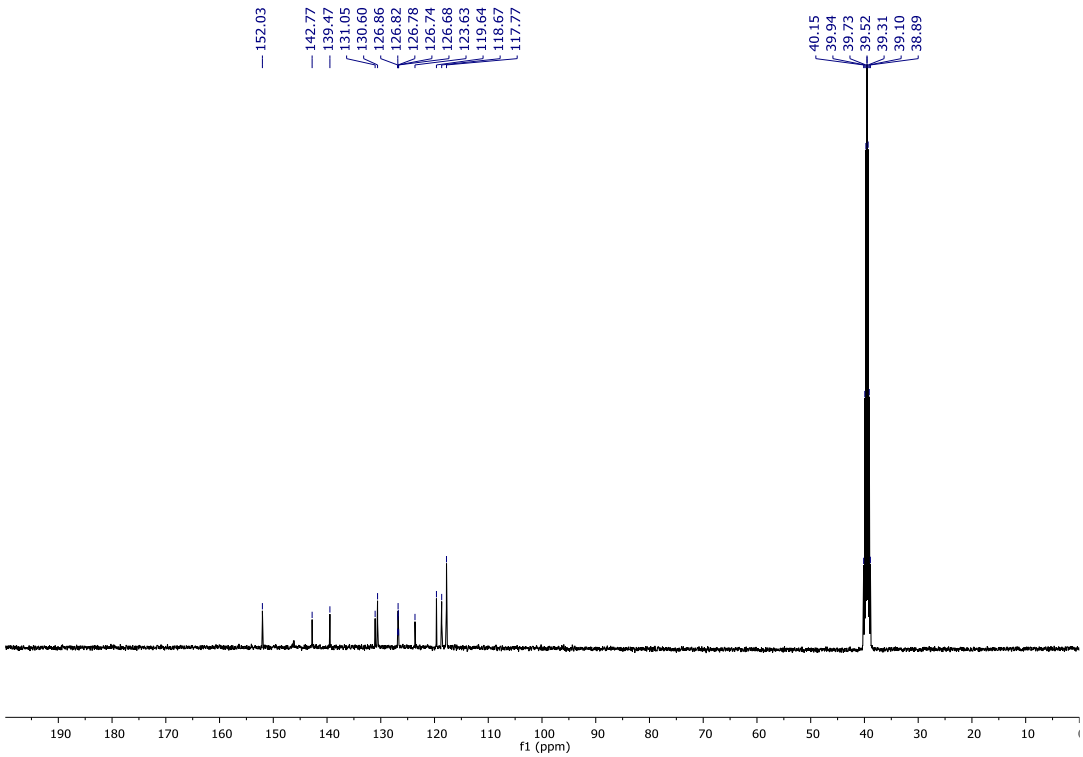
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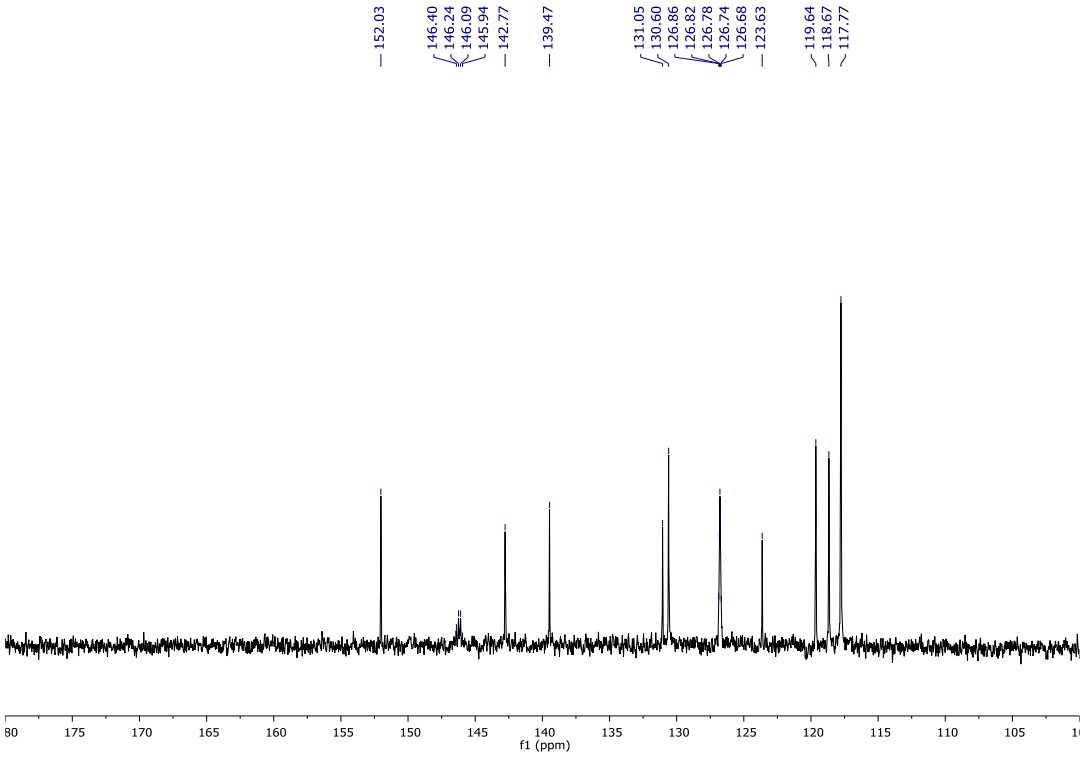
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119.64
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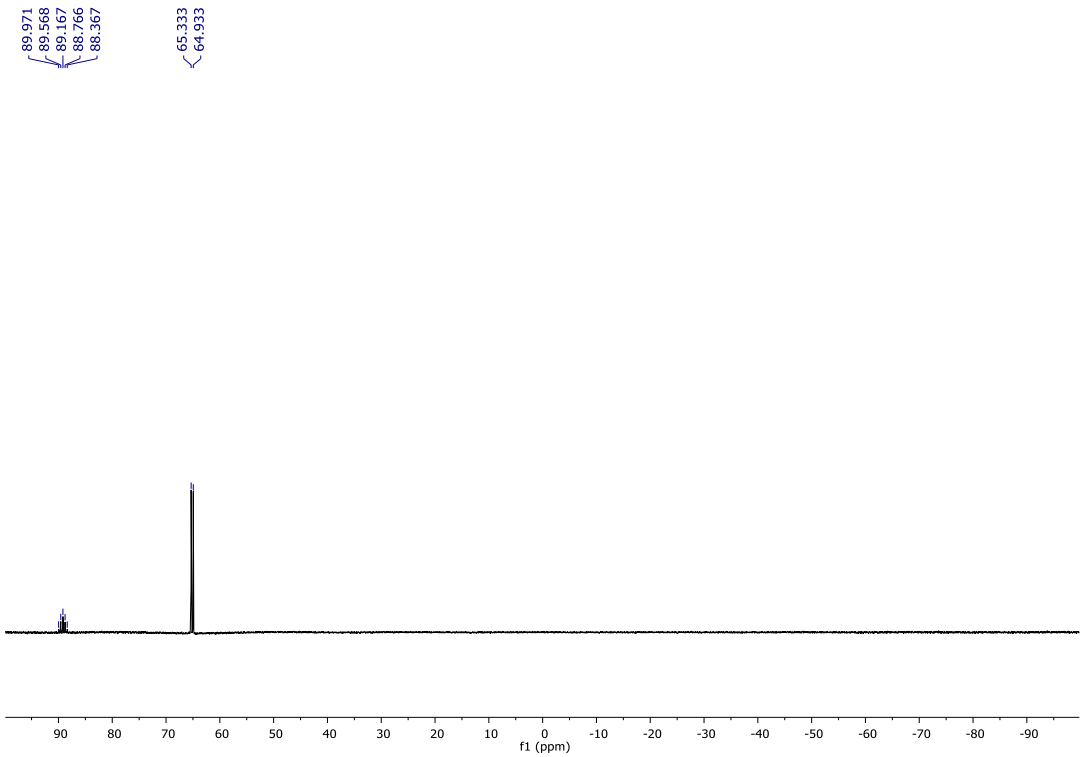
f1 (ppm)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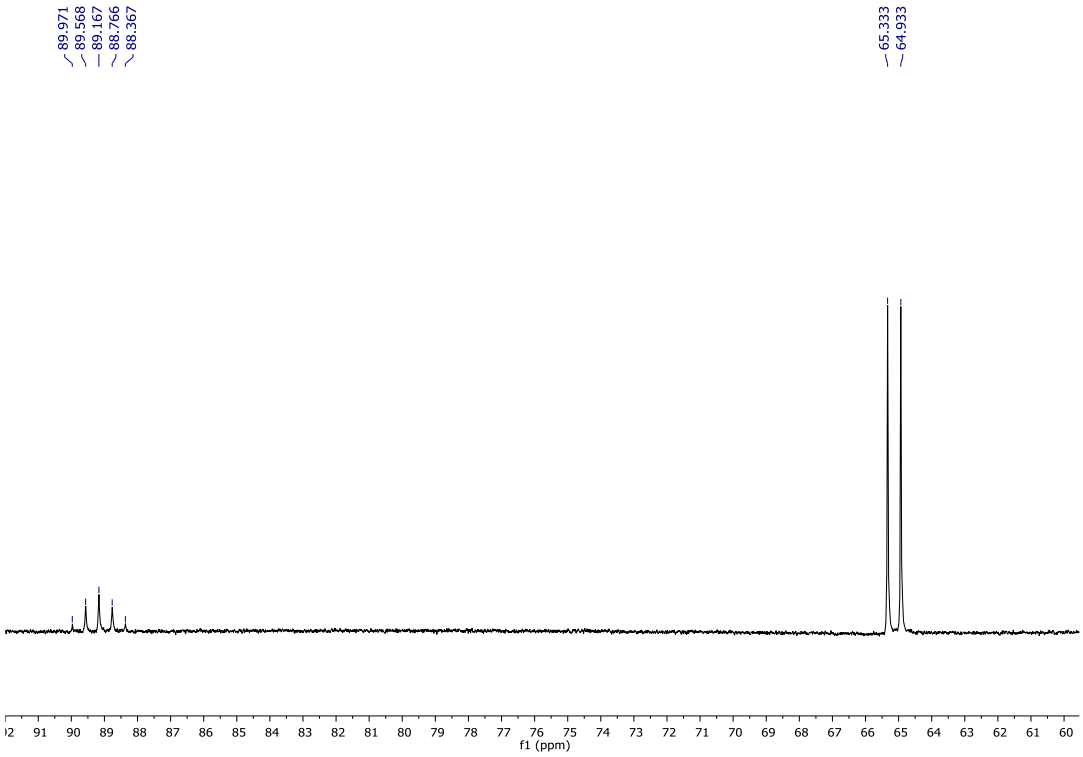
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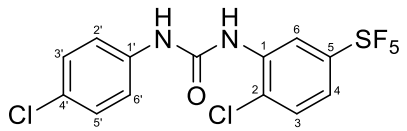
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2
3
4
5
6
1'
2'
3'
4'
5'
6'

3


9.69
8.84
8.83
8.66
7.73
7.71
7.56
7.55
7.54
7.53
7.52
7.52
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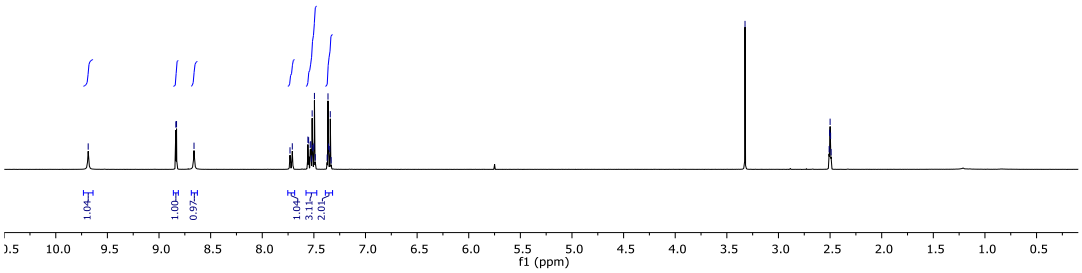
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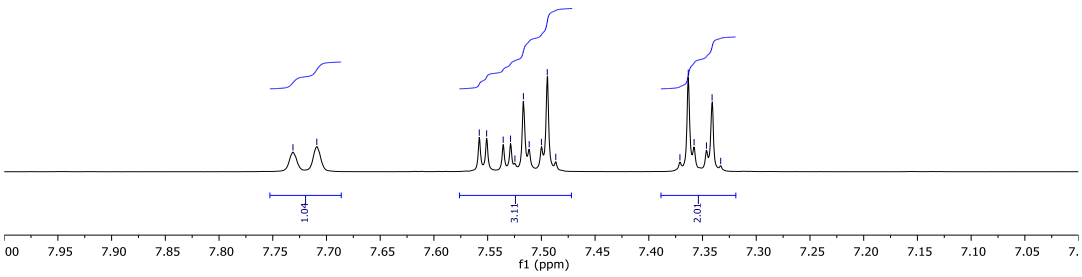
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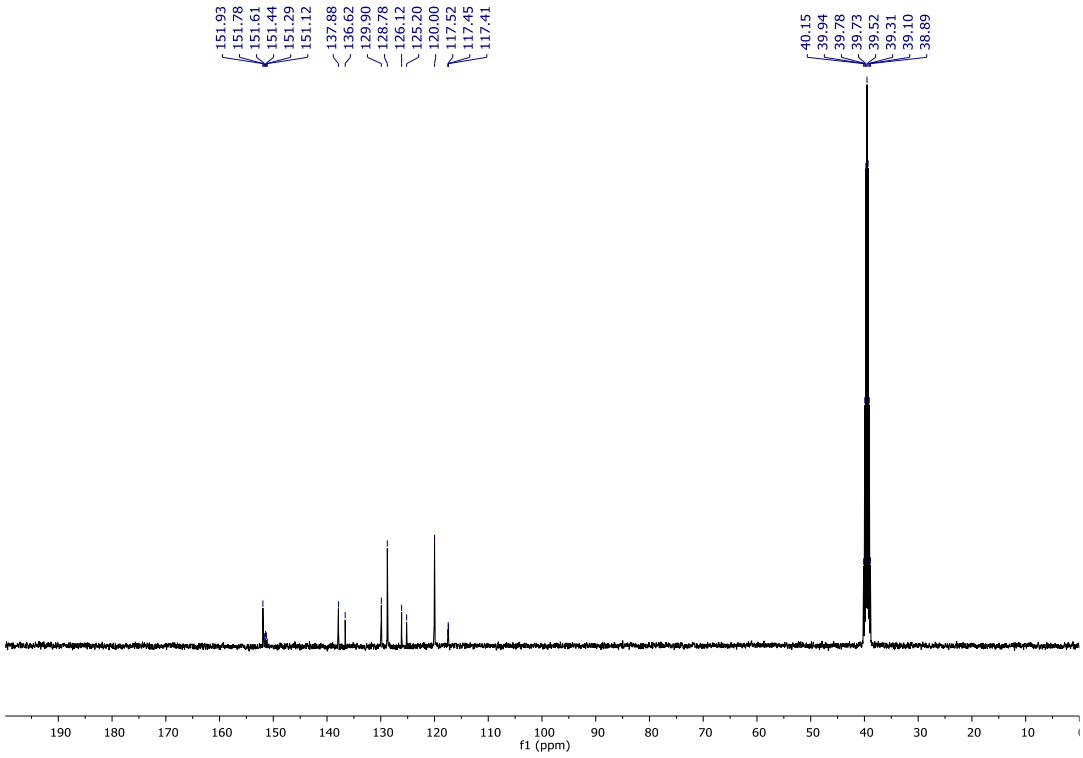
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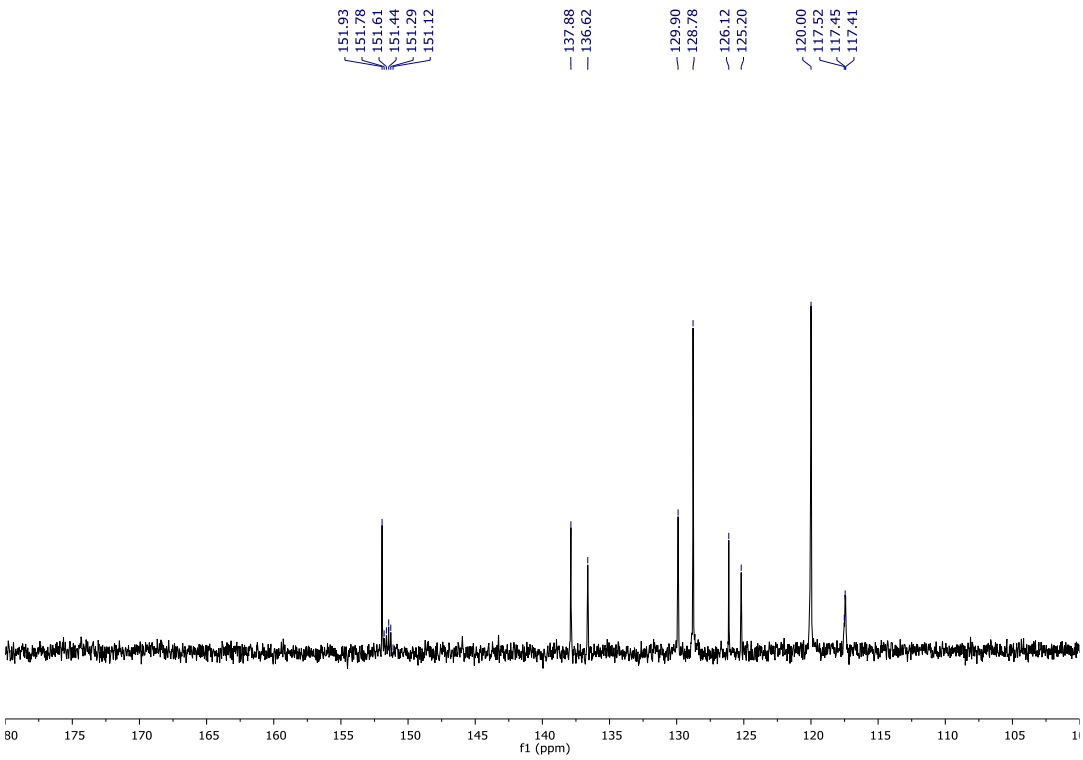
38.89
f1 (ppm)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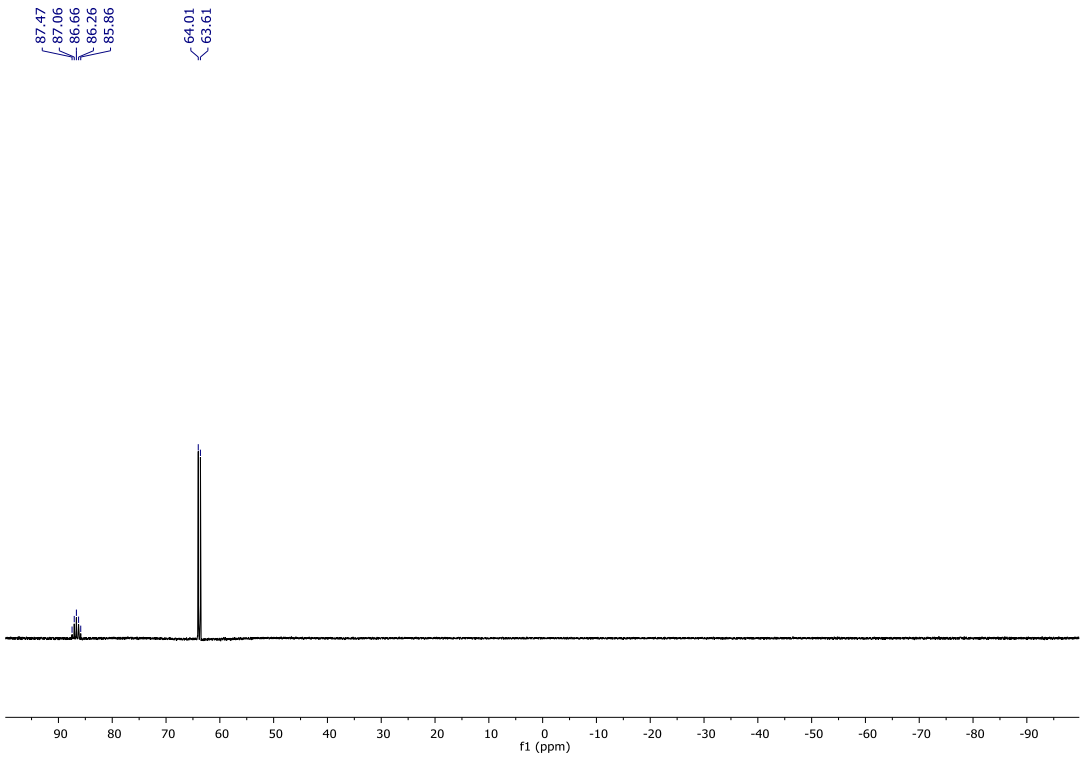
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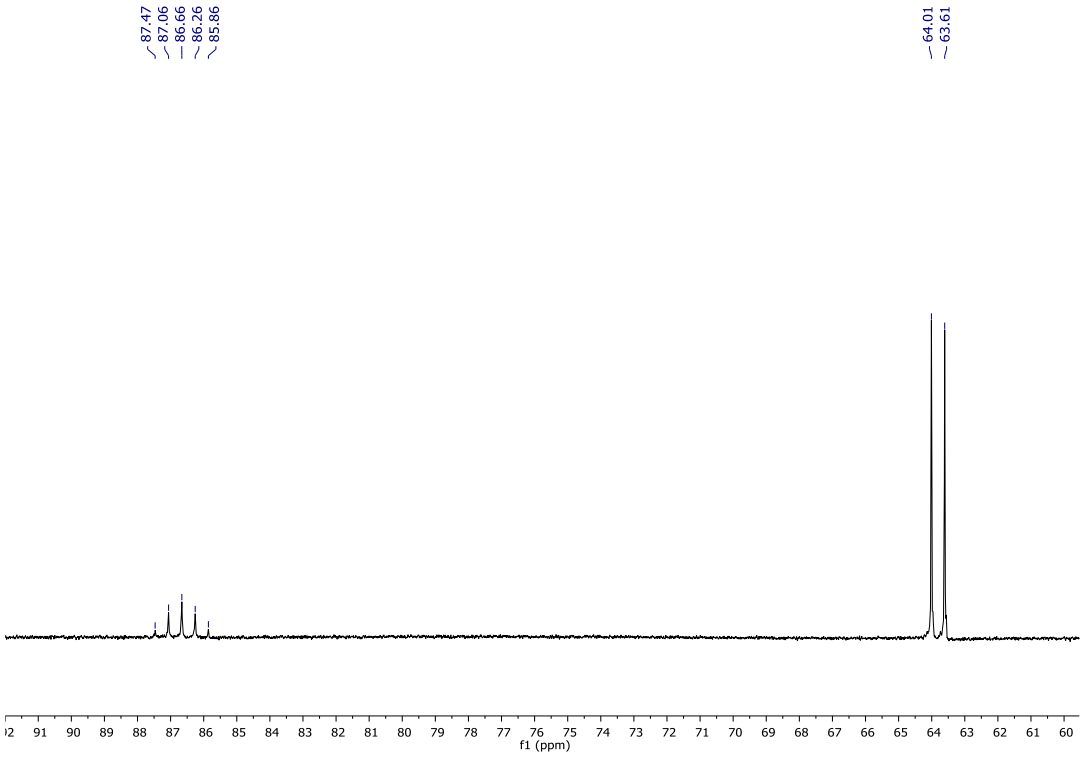
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85.86
64.01
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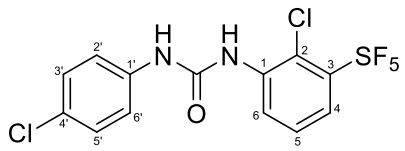
f1 (ppm)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H
N
O
Cl
SF5
Cl
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2
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4
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6
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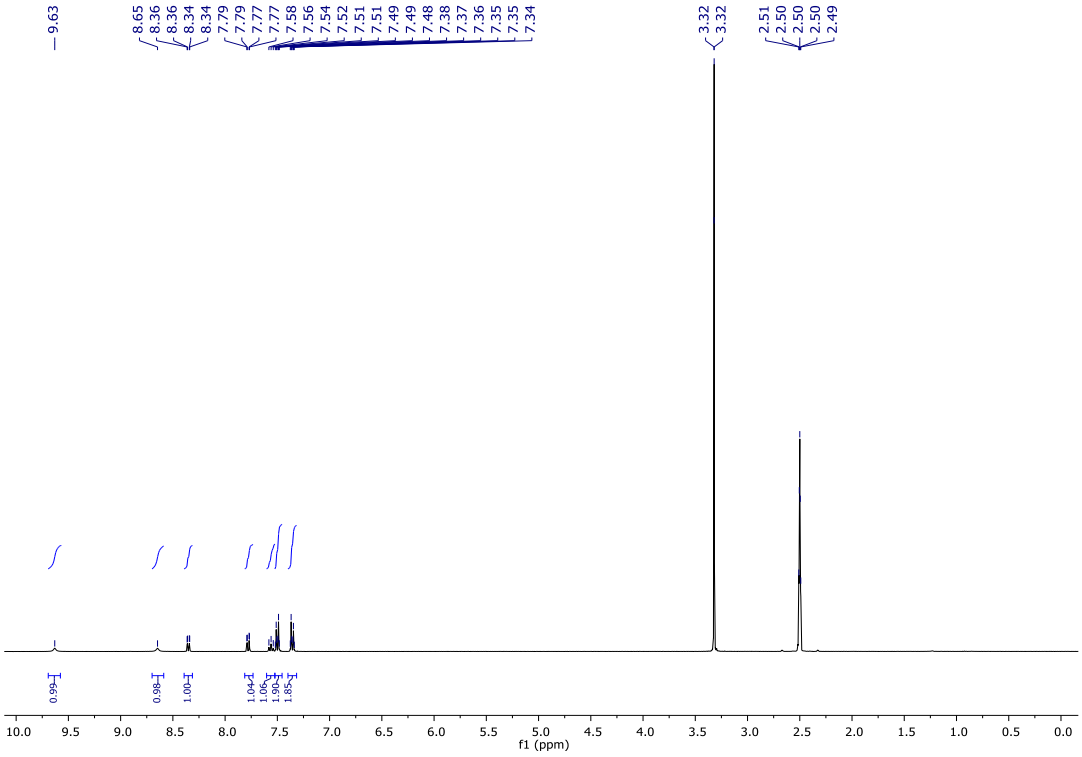
2'
3'
4'
5'
6'

4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7.51
7.51
7.49
7.49
7.48
7.38
7.37
7.36
7.35
7.35
7.34
3.32
3.32
2.51
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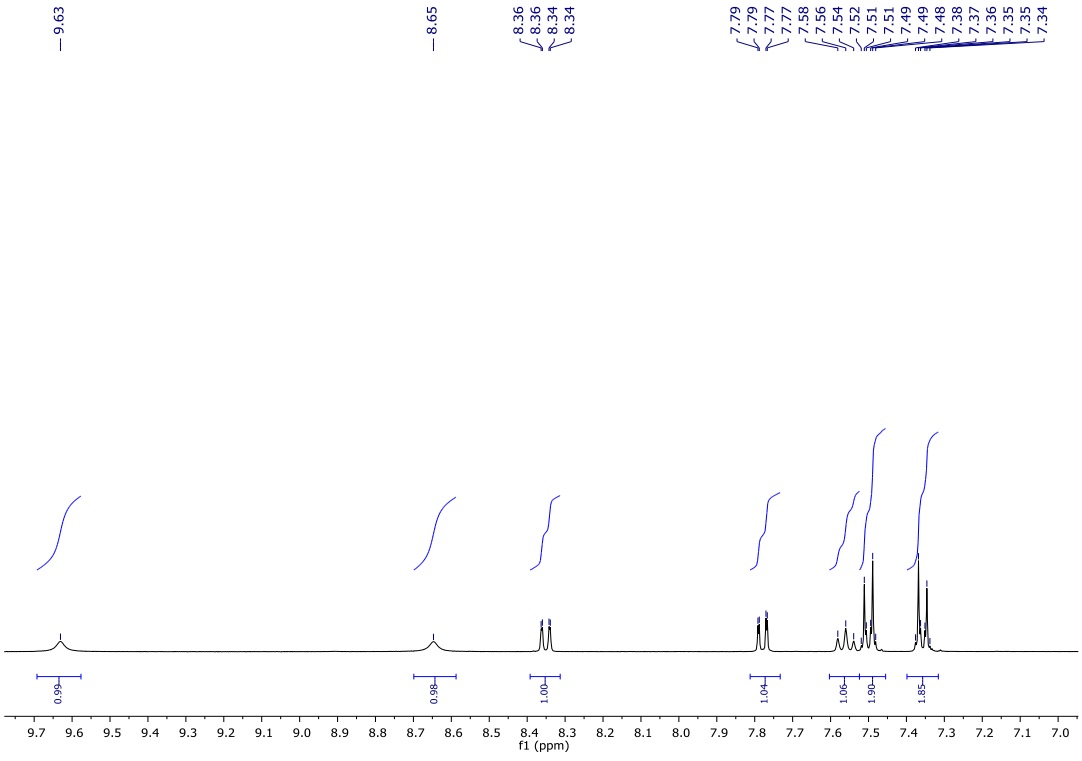
0.98
1.00
1.04
1.06
1.90
1.85
f1 (ppm)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7.79
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7.77
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7.56
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7.51
7.51
7.49
7.49
7.48
7.38
7.37
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7.34
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0.98
1.00
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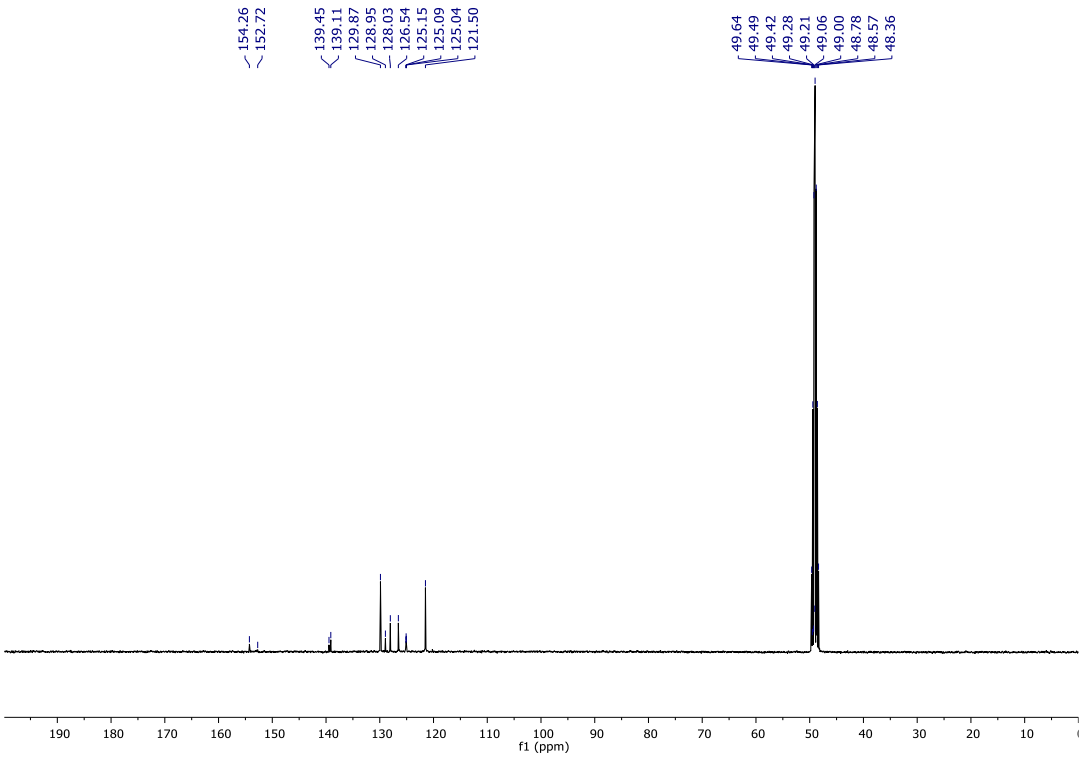
1.06
1.90
1.85
f1 (ppm)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128.03
126.54
125.15
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125.04
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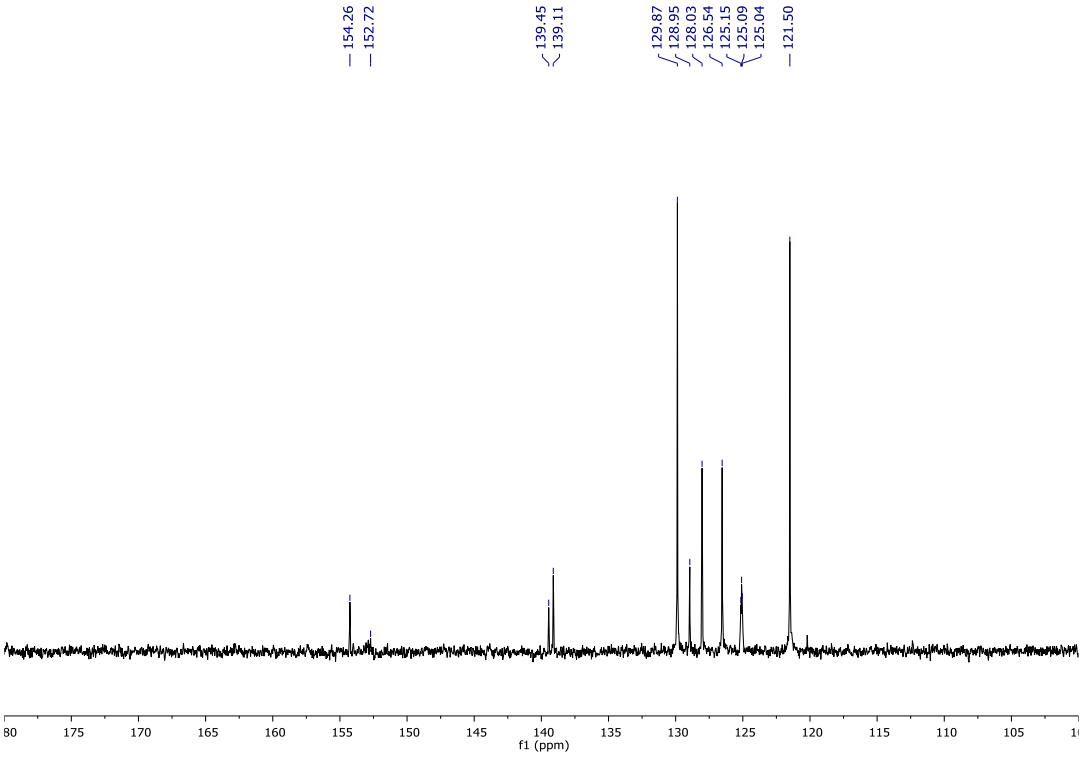
49.00
48.78
48.57
48.36
f1 (ppm)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126.54
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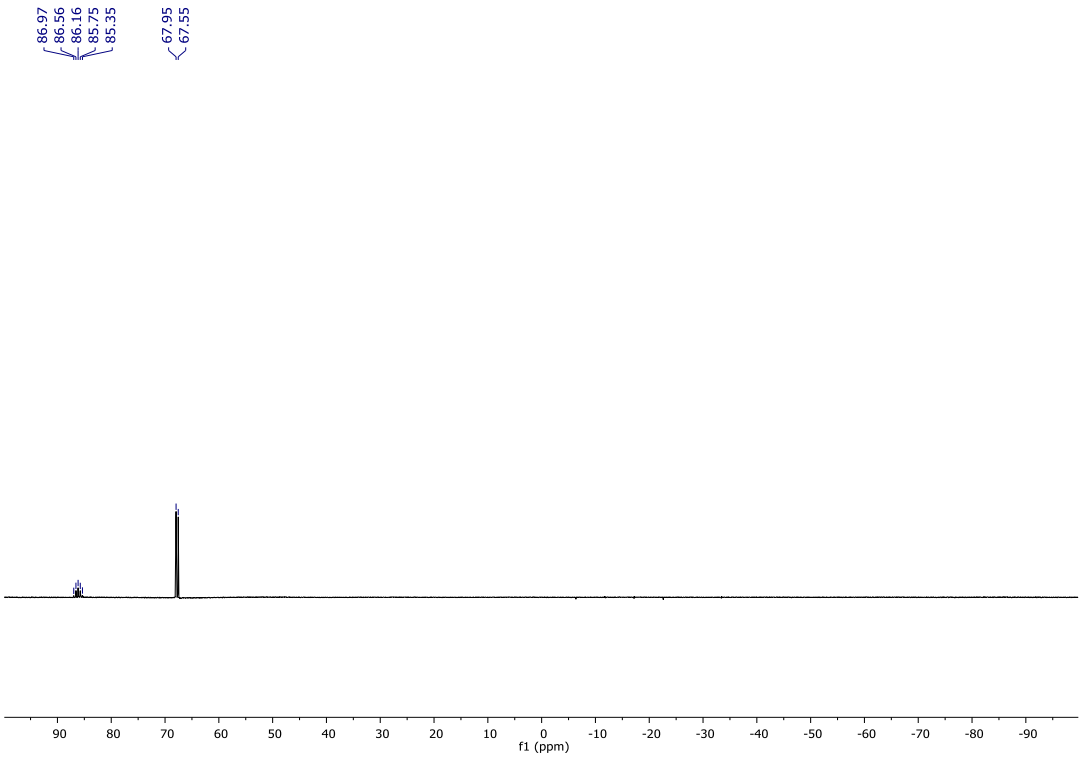
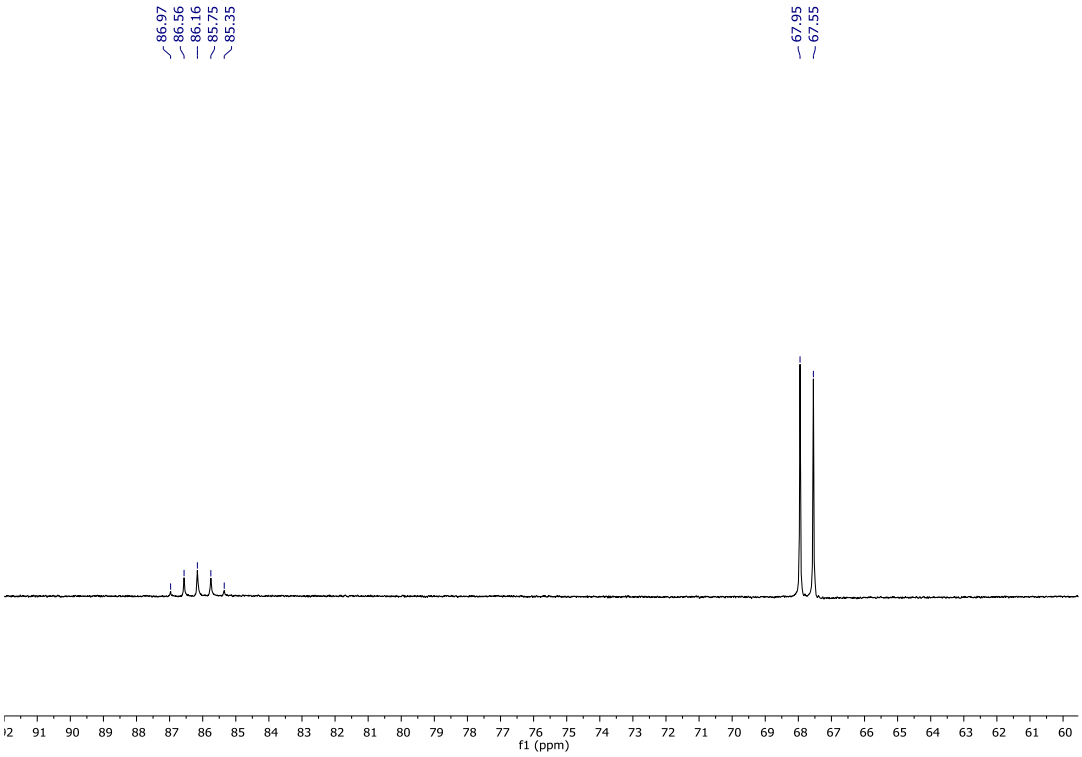
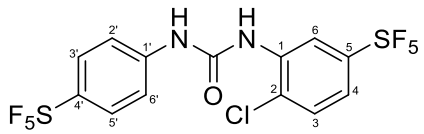
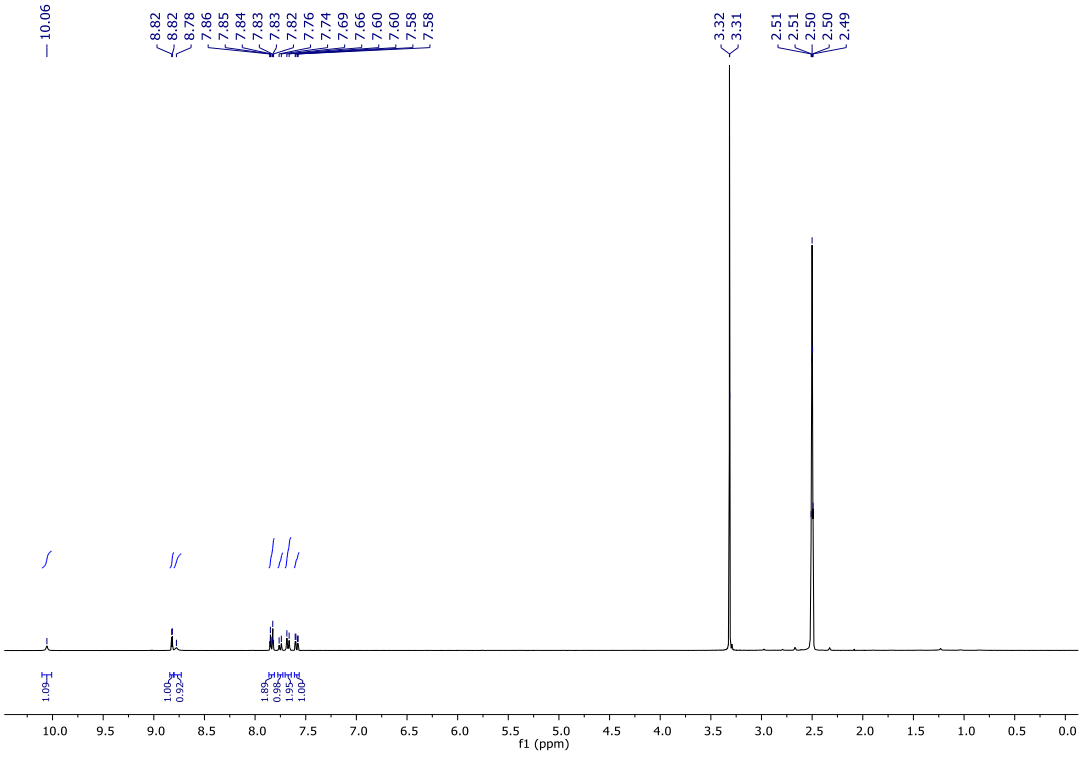
125.09
125.04
121.50
f1 (ppm)


86.97
86.56
86.16
85.75
85.35
67.95
67.55
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)


86.97
86.56
86.16
85.75
85.35
67.95
67.55
92 91 90 89 88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 63 62 61 60
f1 (ppm)


H
N
H
N
O
Cl
SF5
F5S
1
2
3
4
5
6
1'
2'
3'
4'
5'
6'

5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8.82
8.78
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7.84
7.83
7.83
7.82
7.76
7.74
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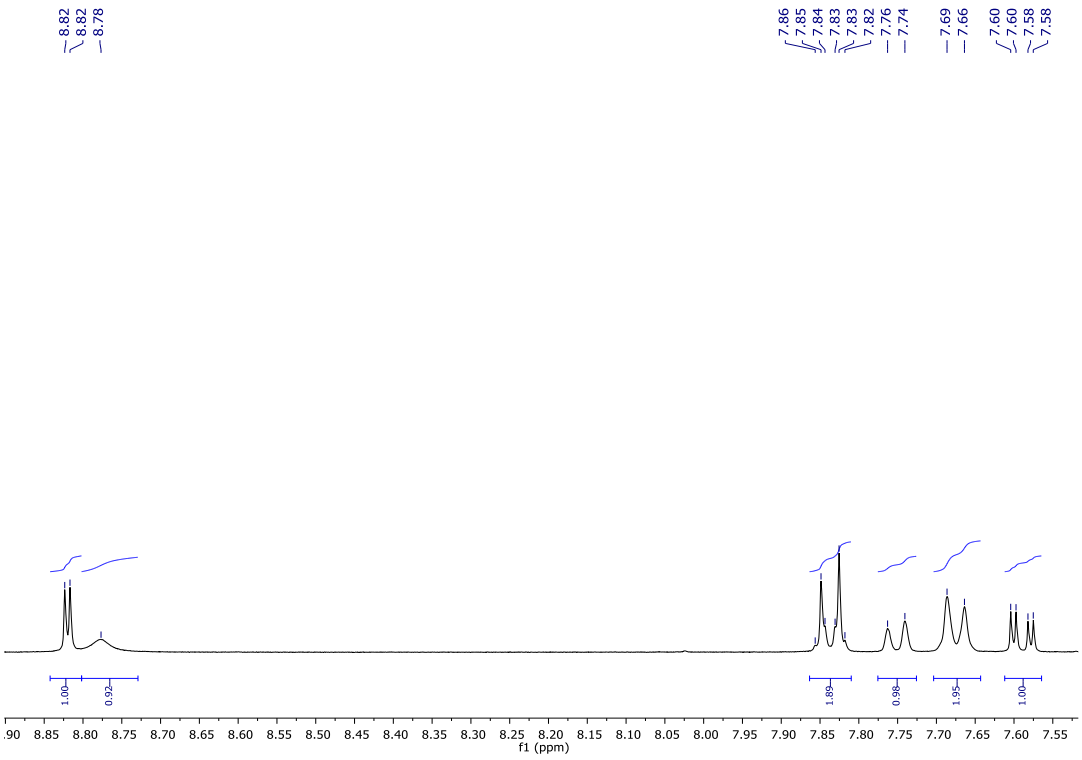
7.66
7.60
7.58
7.58
3.32
3.31
2.51
2.51
2.50
2.50
2.49
1.09
1.05
0.92
1.89
0.98
1.95
1.00
f1 (ppm)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8.82
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7.84
7.83
7.83
7.82
7.76
7.74
7.69
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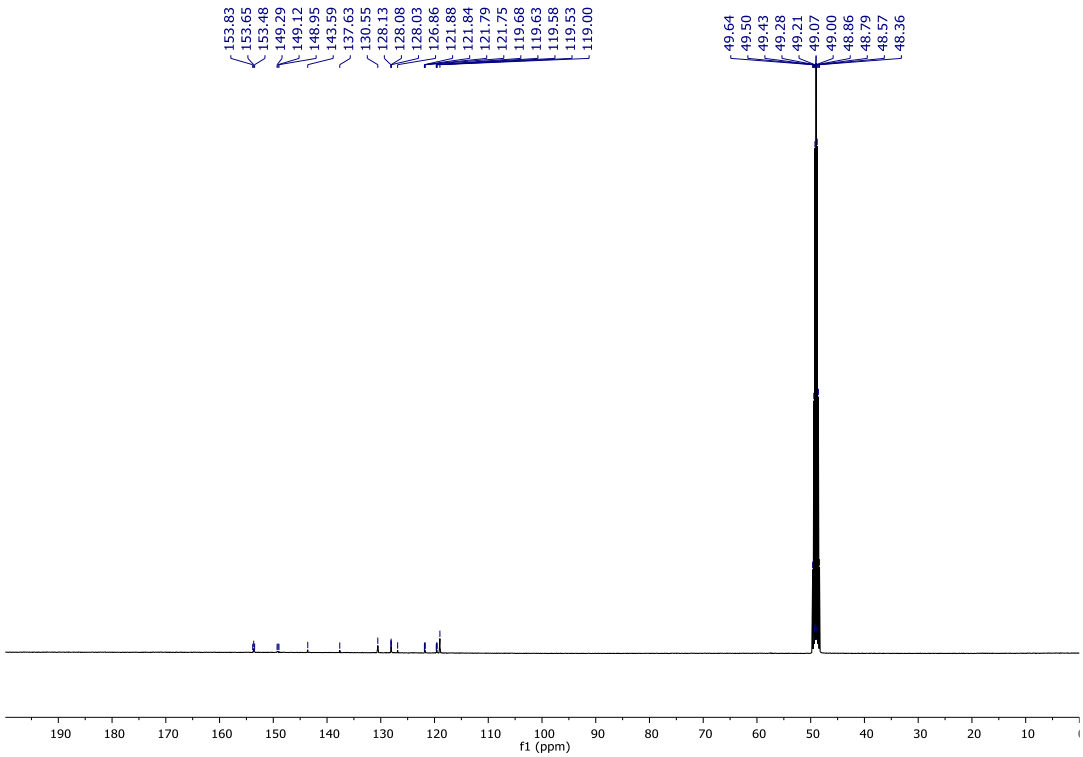
7.60
7.58
7.58
1.00
0.92
1.89
0.98
1.95
1.00
f1 (ppm)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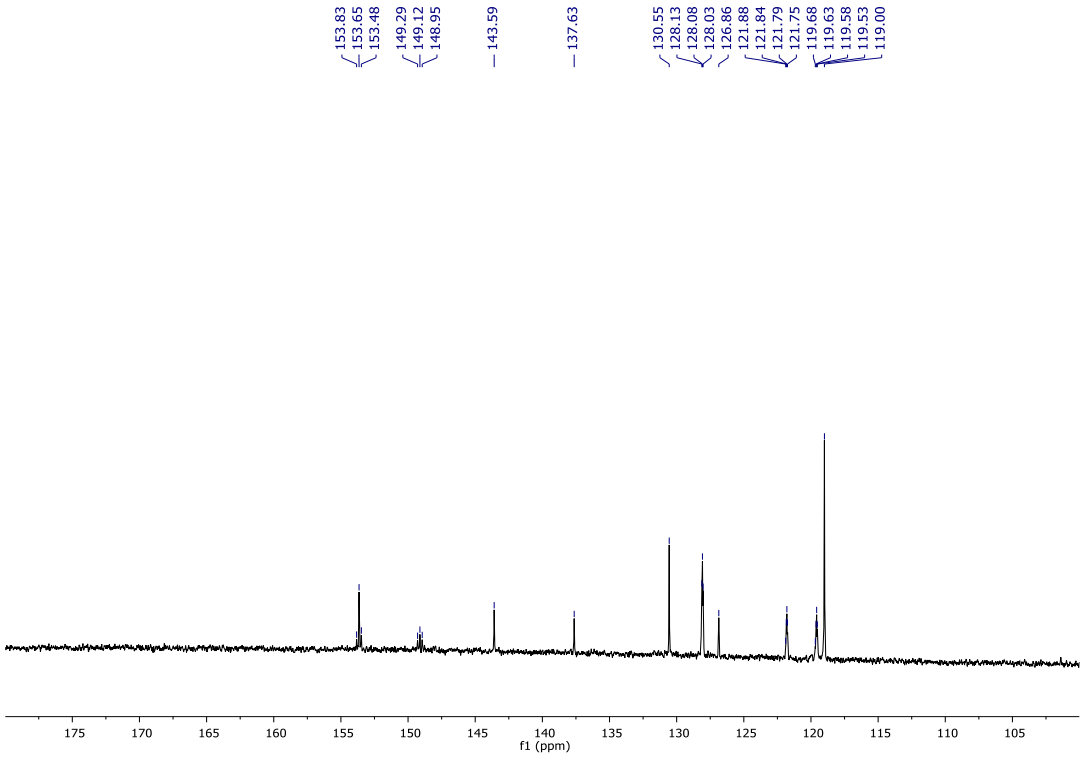
148.95
143.59
137.63
130.55
128.13
128.08
128.03
126.86
121.88
121.84
121.79
121.75
119.68
119.63
119.58
119.53
119.00
49.64
49.50
49.43
49.28
49.21
49.07
49.00
48.86
48.79
48.57
48.36
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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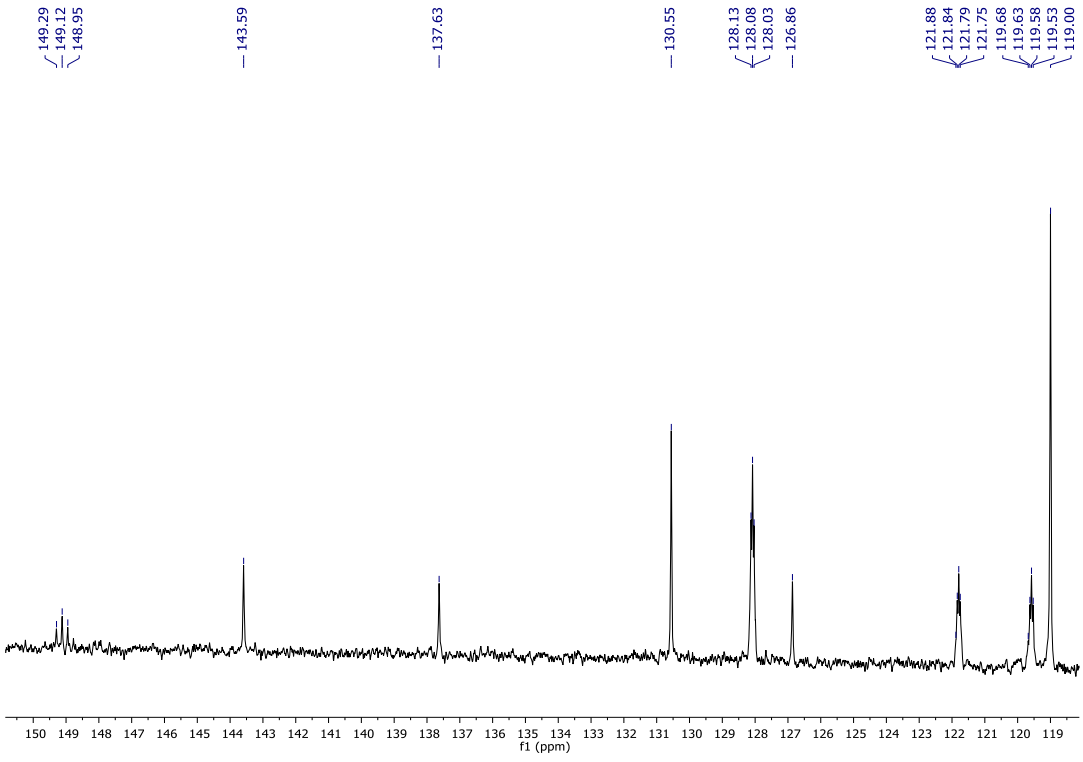
153.65
153.48
149.29
149.12
148.95
143.59
137.63
130.55
128.13
128.08
128.03
126.86
121.88
121.84
121.79
121.75
119.68
119.63
119.58
119.53
119.00
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105
f1 (ppm)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143.59
137.63
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128.13
128.08
128.03
126.86
121.88
121.84
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121.75
119.68
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119.00
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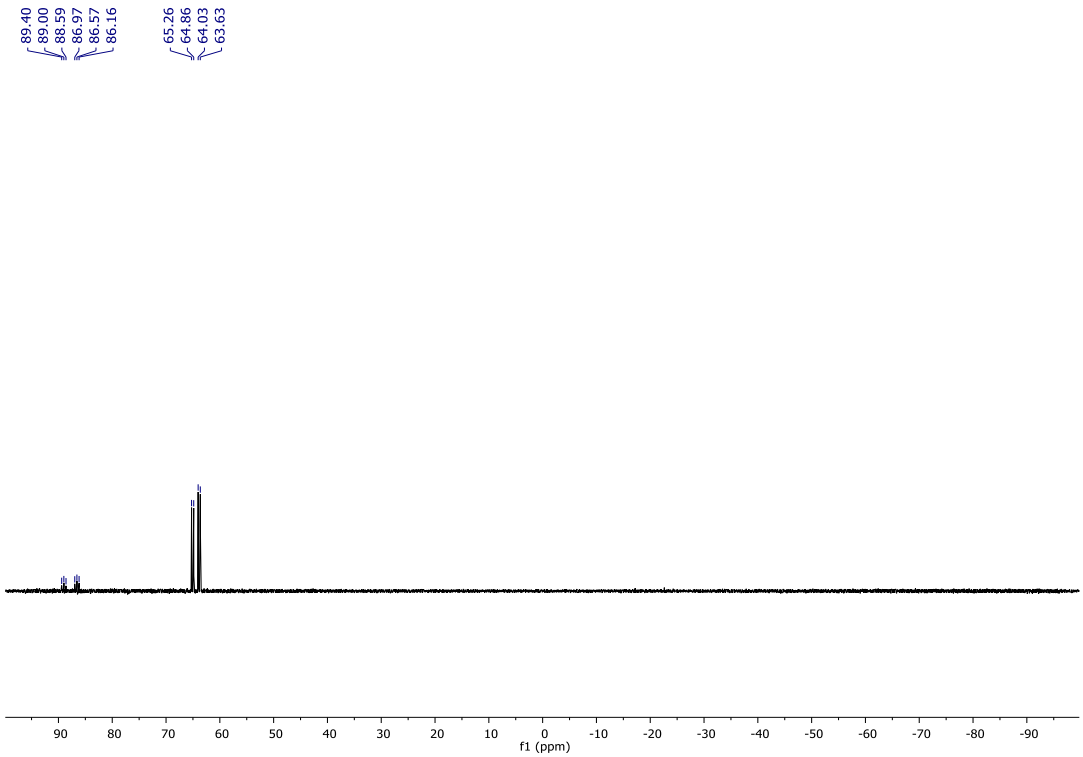
f1 (ppm)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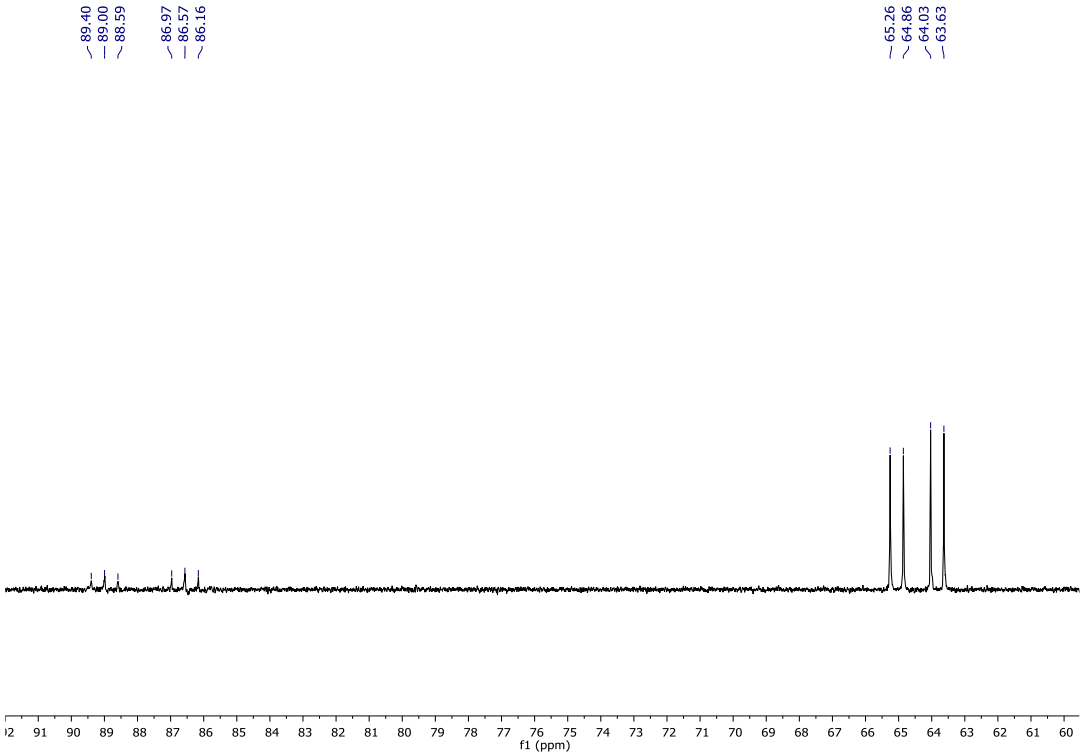
65.26
64.86
64.03
63.63
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)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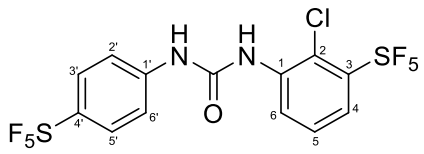
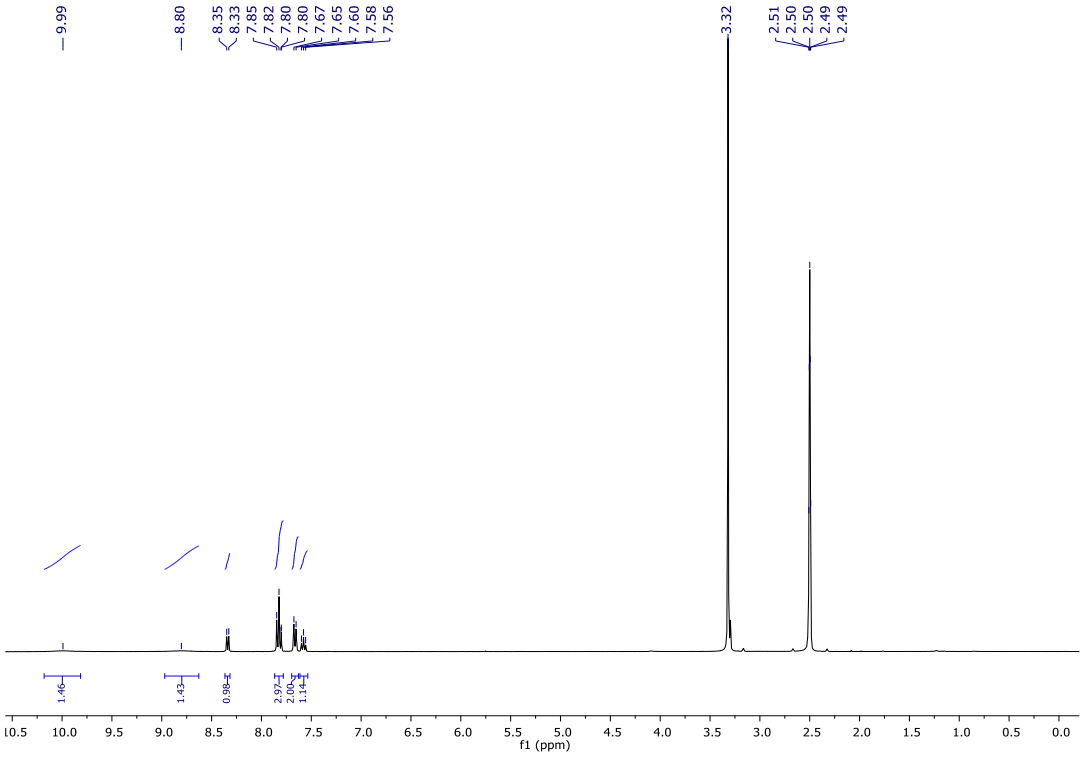
89.00
88.59
86.97
86.57
86.16
65.26
64.86
64.03
63.63
92 91 90 89 88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 63 62 61 60
f1 (ppm)


H
N
H
N
O
Cl
SF5
F5S
1'
2'
3'
4'
5'
6'
1
2
3
4
5
6

6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7.80
7.80
7.67
7.65
7.60
7.58
7.56
3.32
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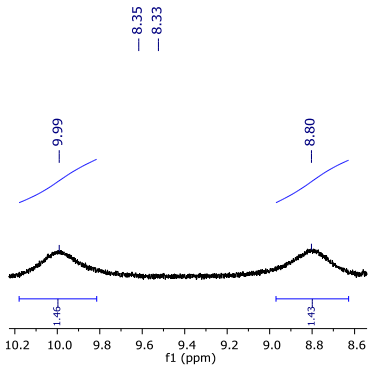
2.50
2.50
2.49
2.49
1.46
1.43
0.98
2.97
2.00
1.14
f1 (ppm)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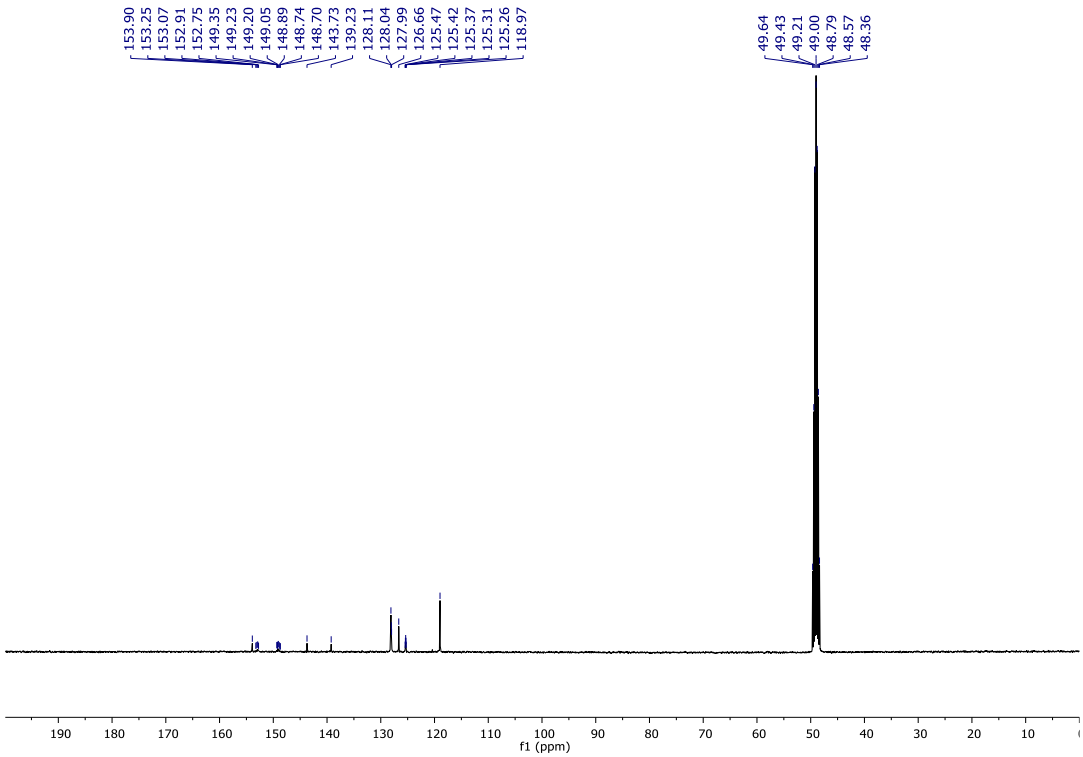
8.33
9.99
8.80
1.46
1.43
f1 (ppm)

8.35
8.33
7.85
7.82
7.80
7.80
7.67
7.65
7.60
7.58
7.56
0.98
2.97
2.00
1.14
f1 (ppm)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143.73
139.23
128.11
128.04
127.99
126.66
125.47
125.42
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49.43
49.21
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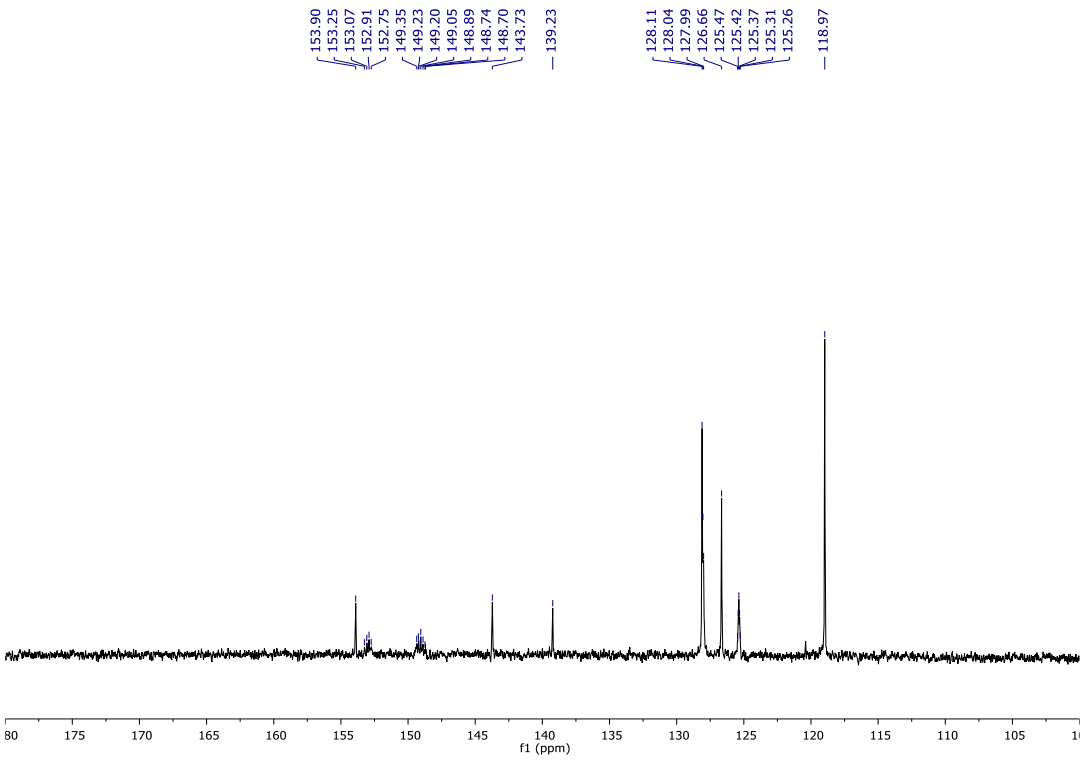
48.79
48.57
48.36
f1 (ppm)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149.20
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148.70
143.73
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128.11
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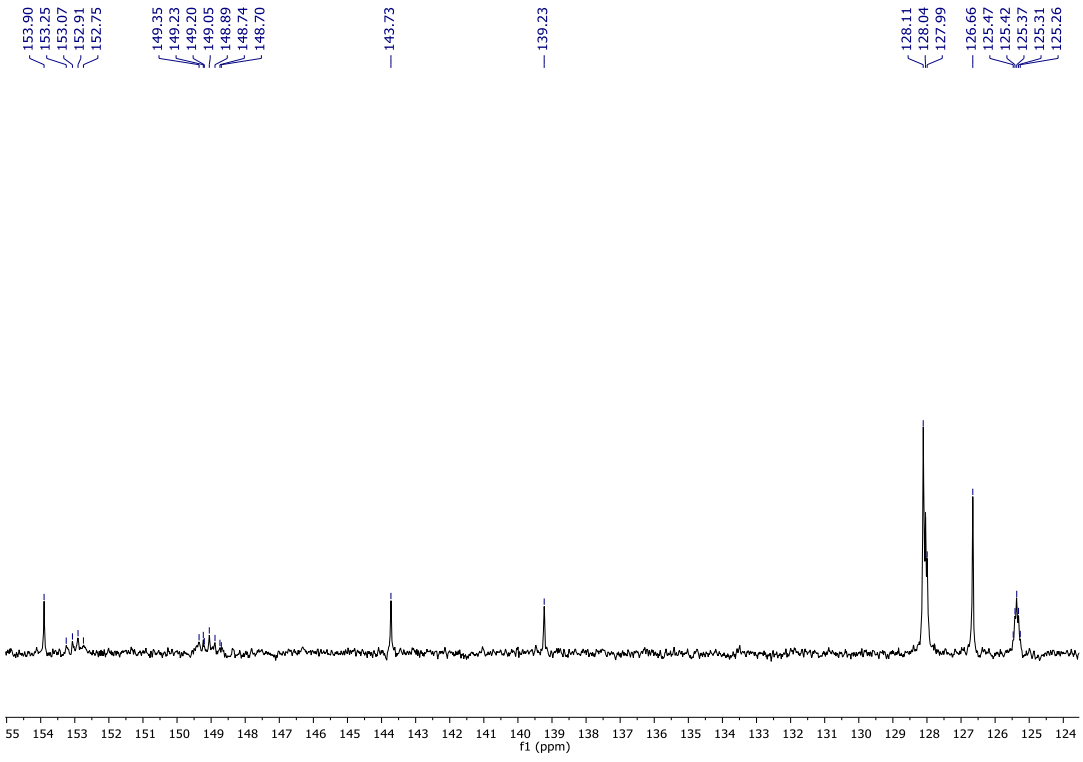
127.99
126.66
125.47
125.42
125.37
125.31
125.26
118.97
f1 (ppm)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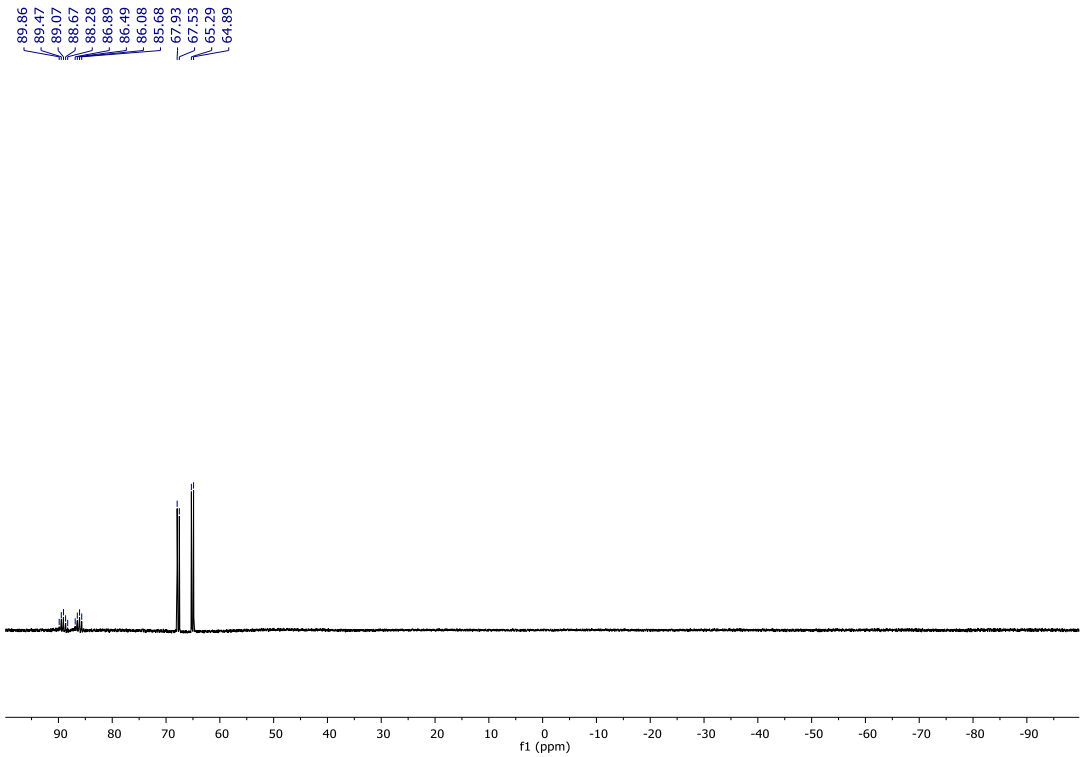
148.70
143.73
139.23
128.11
128.04
127.99
126.66
125.47
125.42
125.37
125.31
125.26
55 154 153 152 151 150 149 148 147 146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124
f1 (ppm)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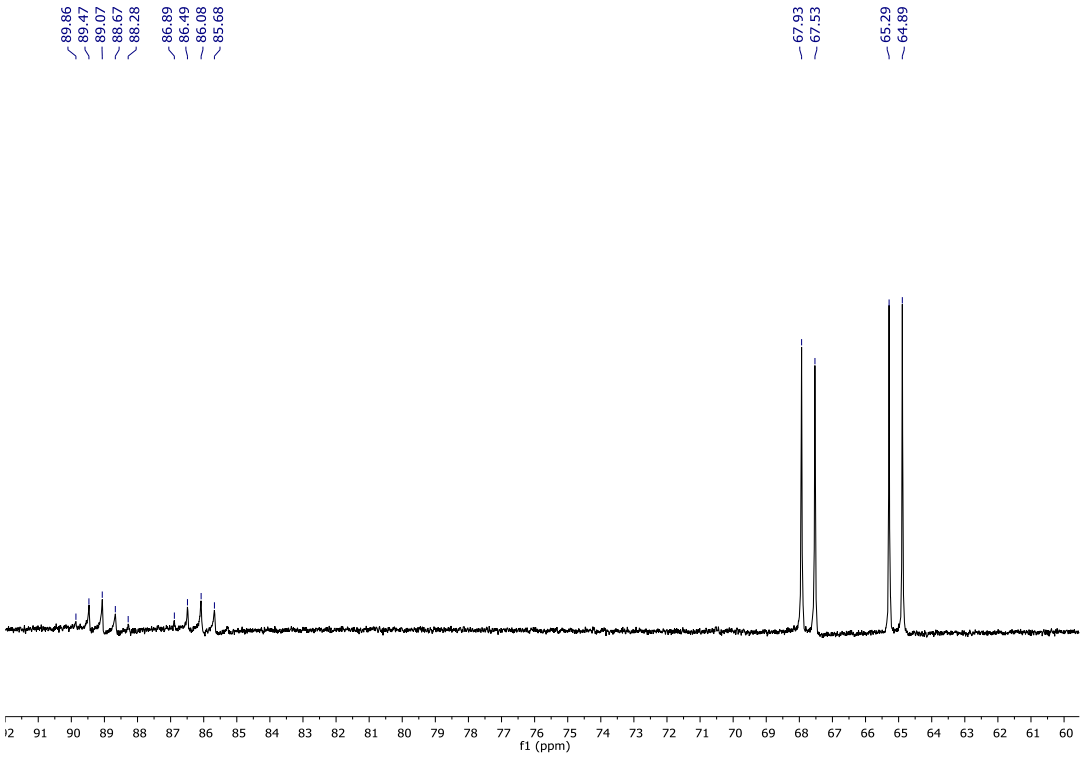
f1 (ppm)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89.47
89.07
88.67
88.28
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86.49
86.08
85.68
67.93
67.53
65.29
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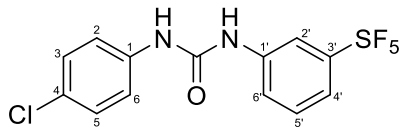
f1 (ppm)


H
N
H
N
O
Cl
SF5
1
2
3
4
5
6
1'
2'
3'
4'
5'
6'

7


9.16
8.95
8.24
8.23
8.23
7.57
7.56
7.56
7.55
7.54
7.54
7.52
7.51
7.51
7.49
7.49
7.48
7.47
7.47
7.46
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7.33
7.32
7.32
3.33
2.51
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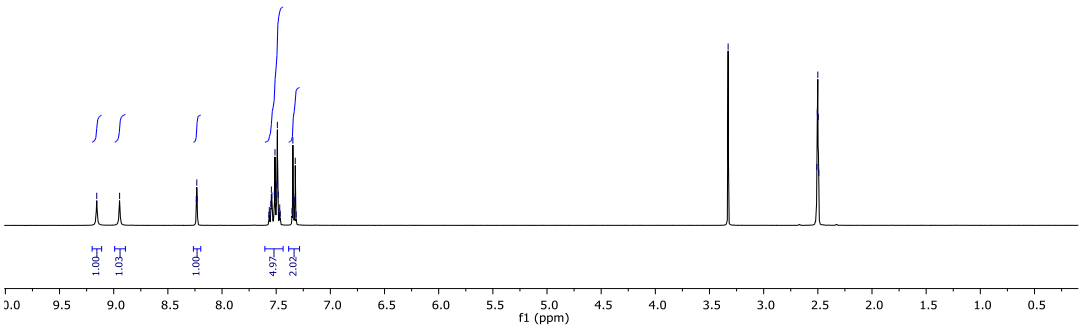
2.50
2.50
2.49


1.00
1.03
1.00
4.97
2.02
f1 (ppm)


8.24
8.23
8.23
7.57
7.56
7.56
7.55
7.54
7.54
7.52
7.51
7.51
7.49
7.49
7.48
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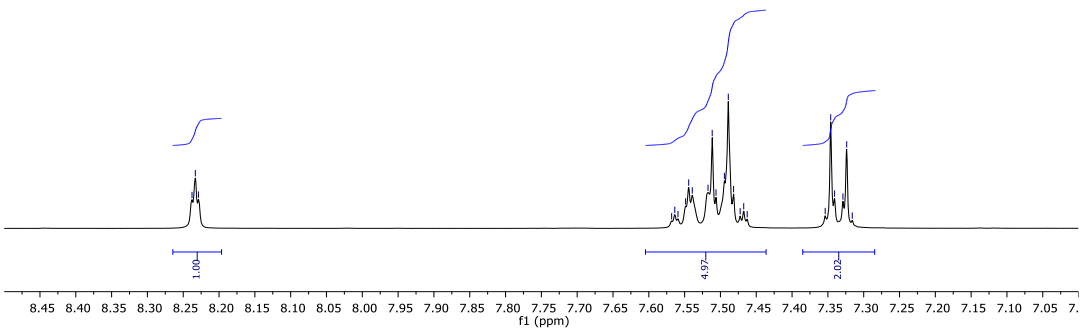
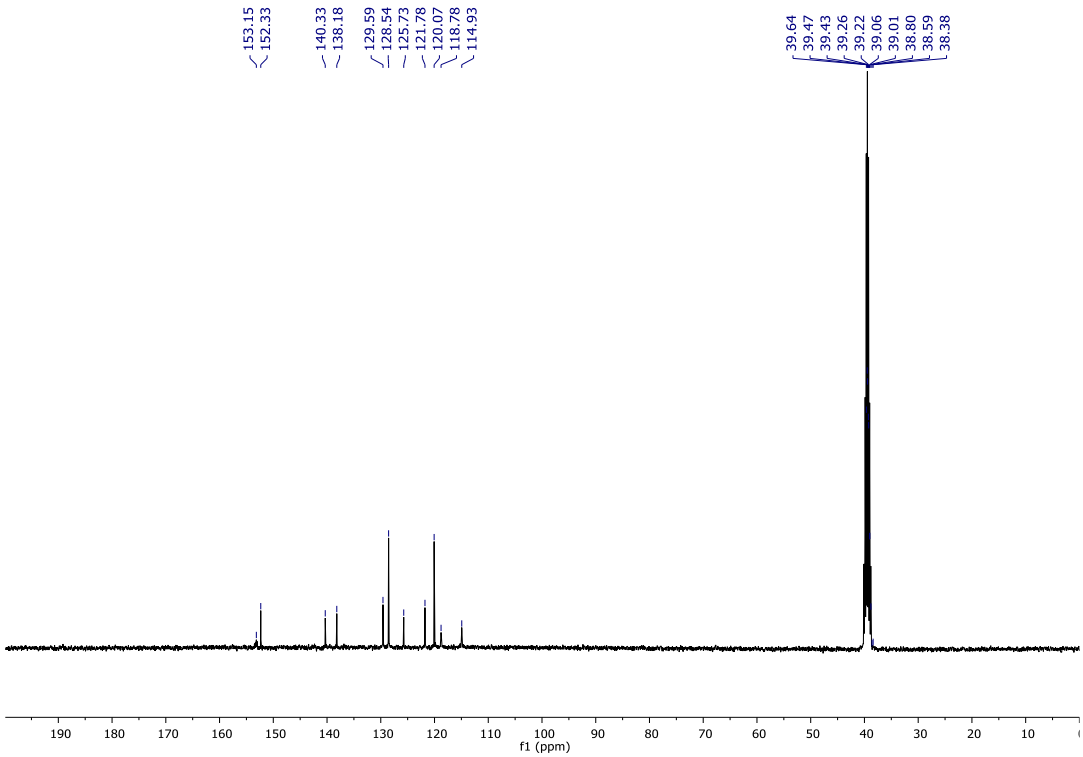
7.35
7.34
7.33
7.32
7.32


1.00
4.97
2.02
f1 (ppm)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152.33
140.33
138.18
129.59
128.54
125.73
121.78
120.07
118.78
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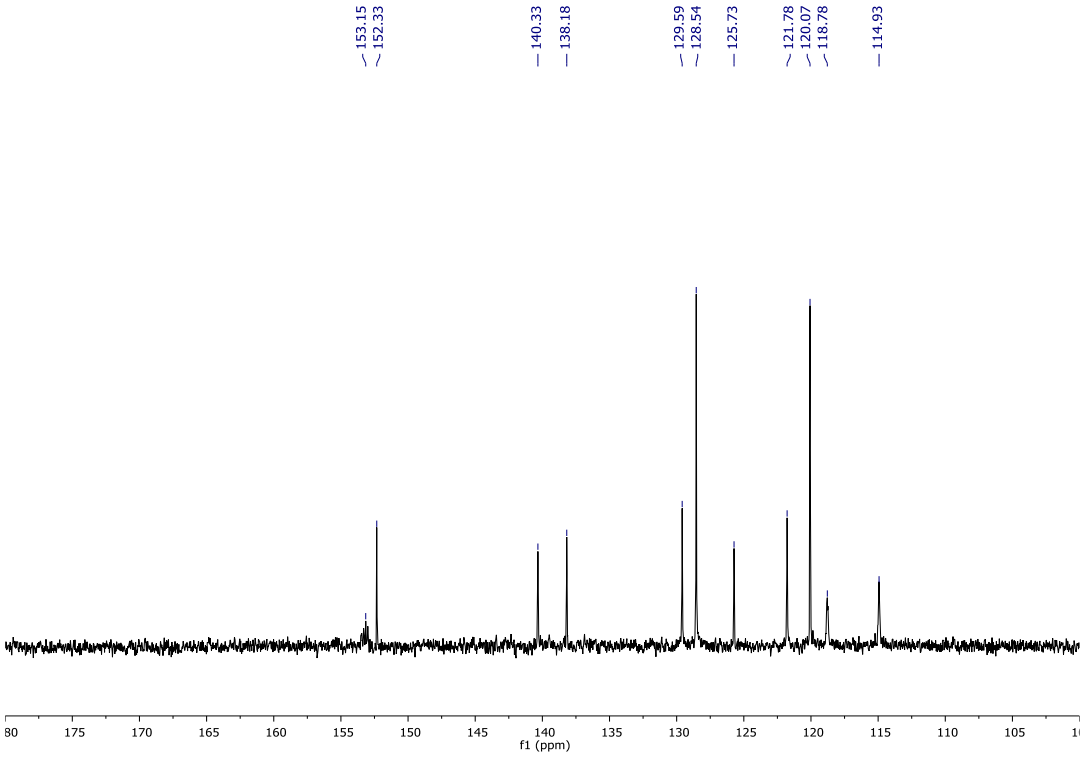
39.47
39.43
39.26
39.22
39.06
39.01
38.80
38.59
38.38
f1 (ppm)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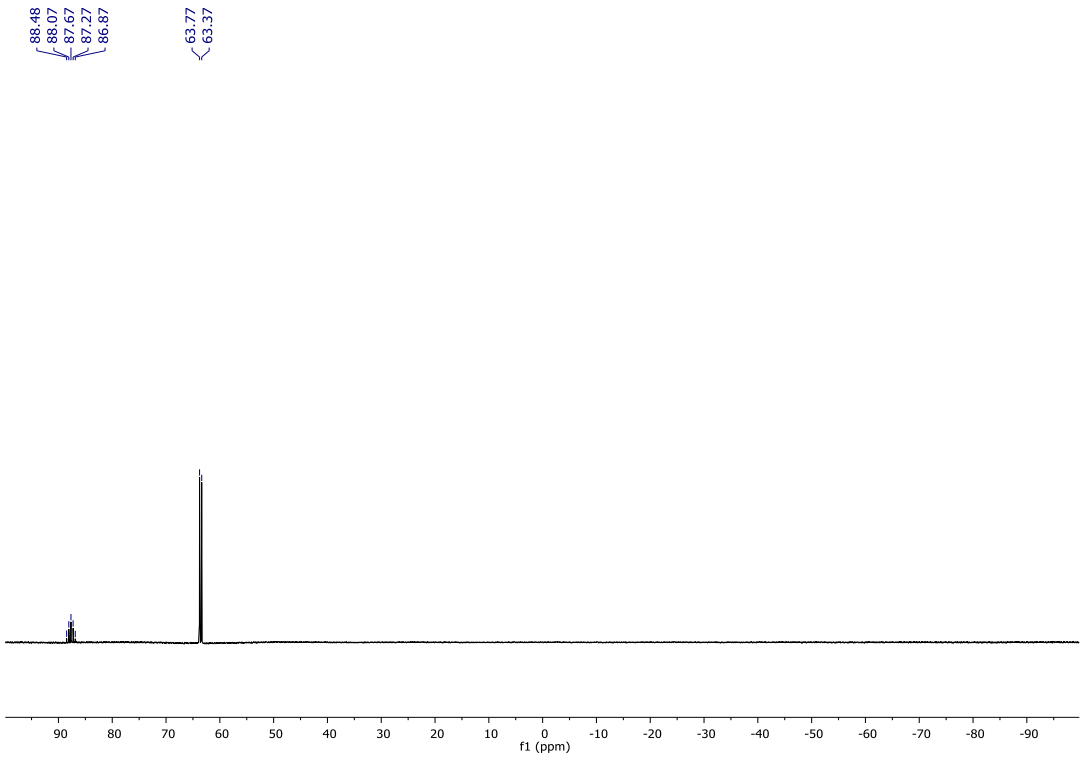
152.33
140.33
138.18
129.59
128.54
125.73
121.78
120.07
118.78
114.93
f1 (ppm)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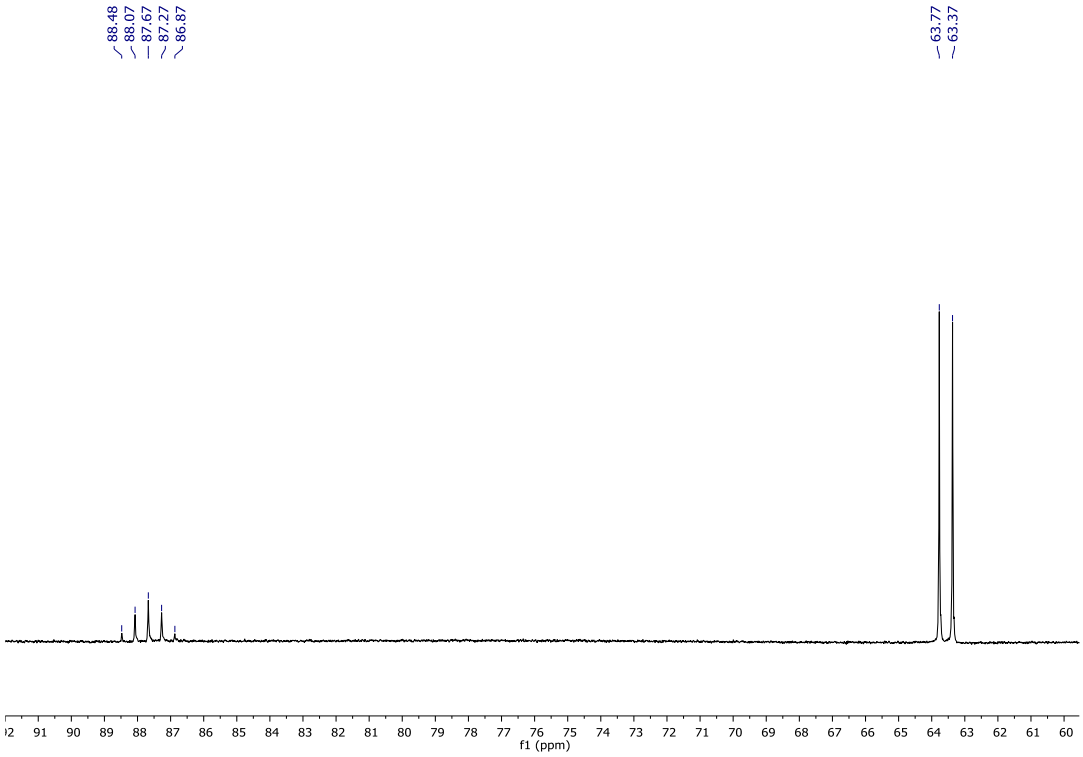
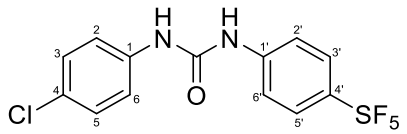
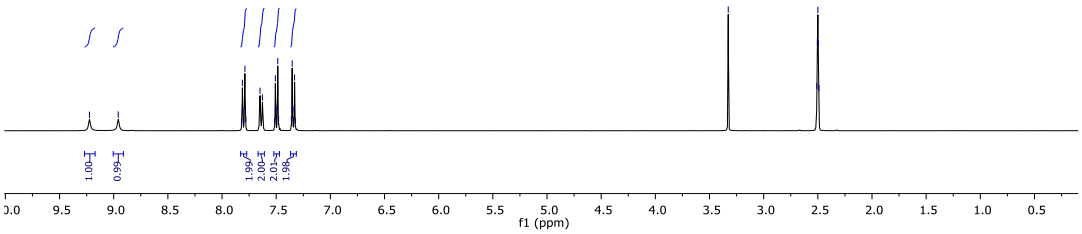
88.07
87.67
87.27
86.87
63.77
63.37
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)


88.48
88.07
87.67
87.27
86.87
63.77
63.37
92 91 90 89 88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 63 62 61 60
f1 (ppm)


H
N
H
N
O
Cl
SF5
1
2
3
4
5
6
1'
2'
3'
4'
5'
6'

8


9.22
8.96
7.82
7.81
7.81
7.79
7.78
7.65
7.63
7.52
7.51
7.50
7.49
7.49
7.48
7.36
7.35
7.35
7.34
7.33
7.32
3.33
2.51
2.50
2.50
2.49
2.49


1.00
0.99
1.99
2.00
1.98
f1 (ppm)


7.82
7.81
7.81
7.79
7.78
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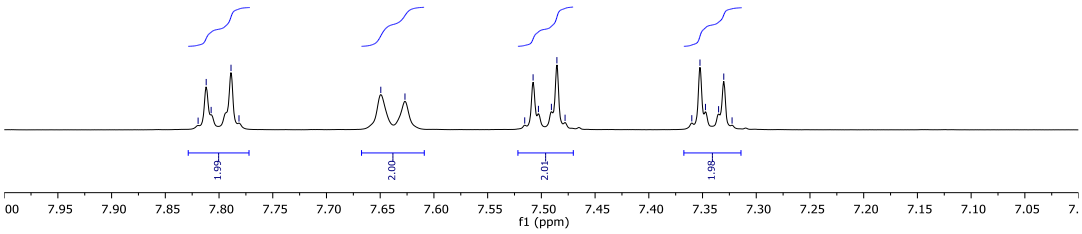
7.63
7.52
7.51
7.50
7.49
7.49
7.48
7.36
7.35
7.35
7.34
7.33
7.32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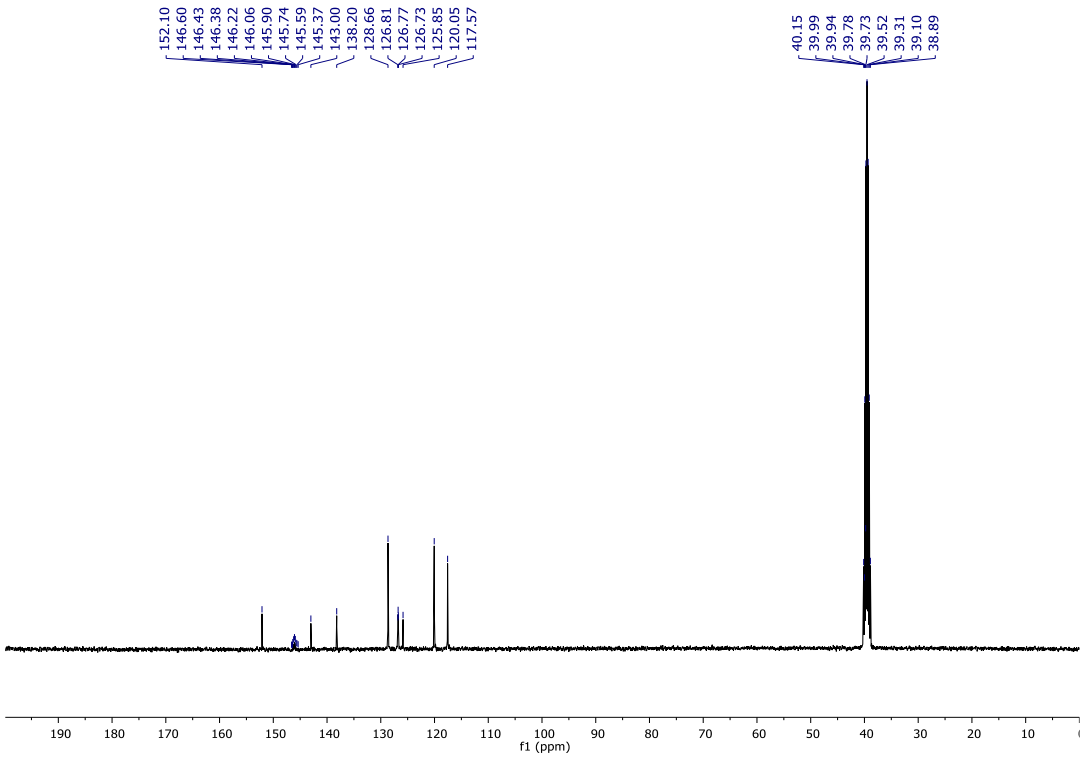
f1 (ppm)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145.74
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143.00
138.20
128.66
126.81
126.77
126.73
125.85
120.05
117.57
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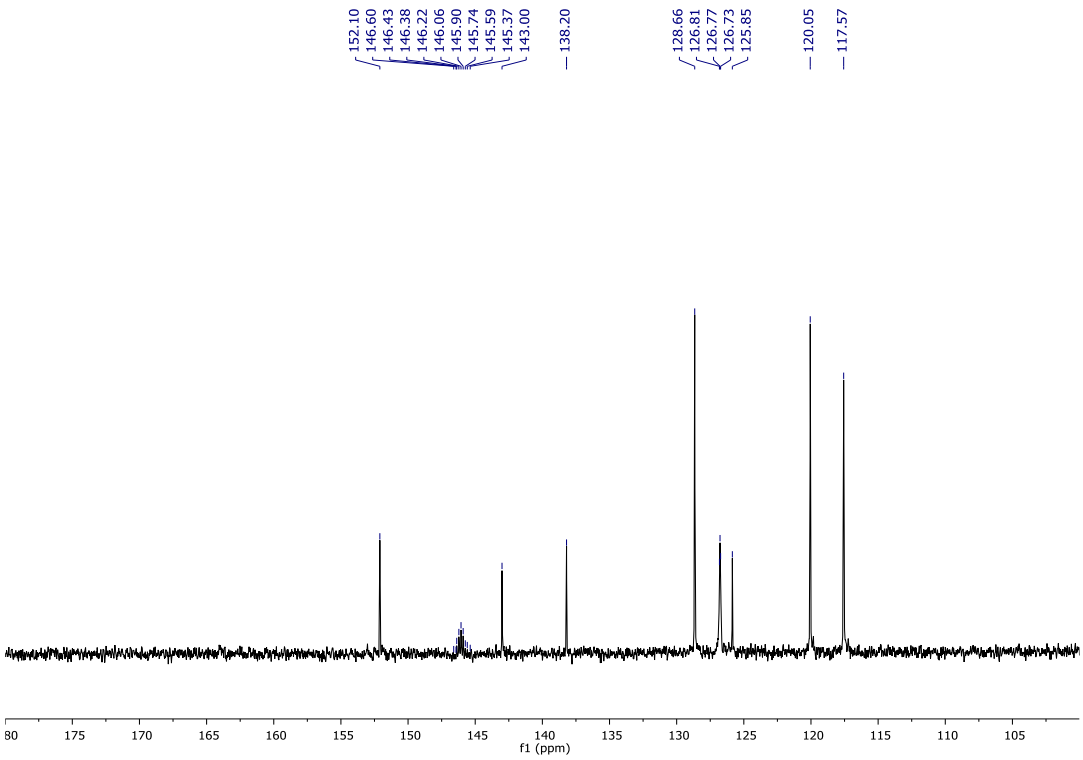
39.78
39.73
39.52
39.31
39.10
38.89
f1 (ppm)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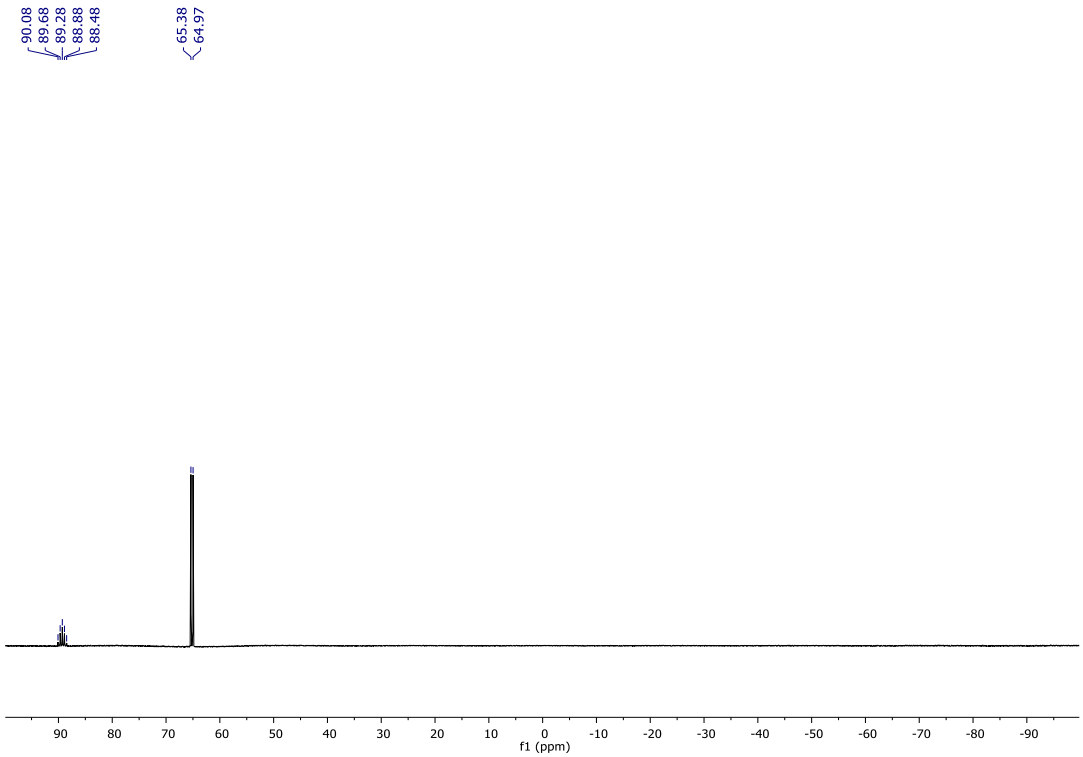
125.85
120.05
117.57
f1 (ppm)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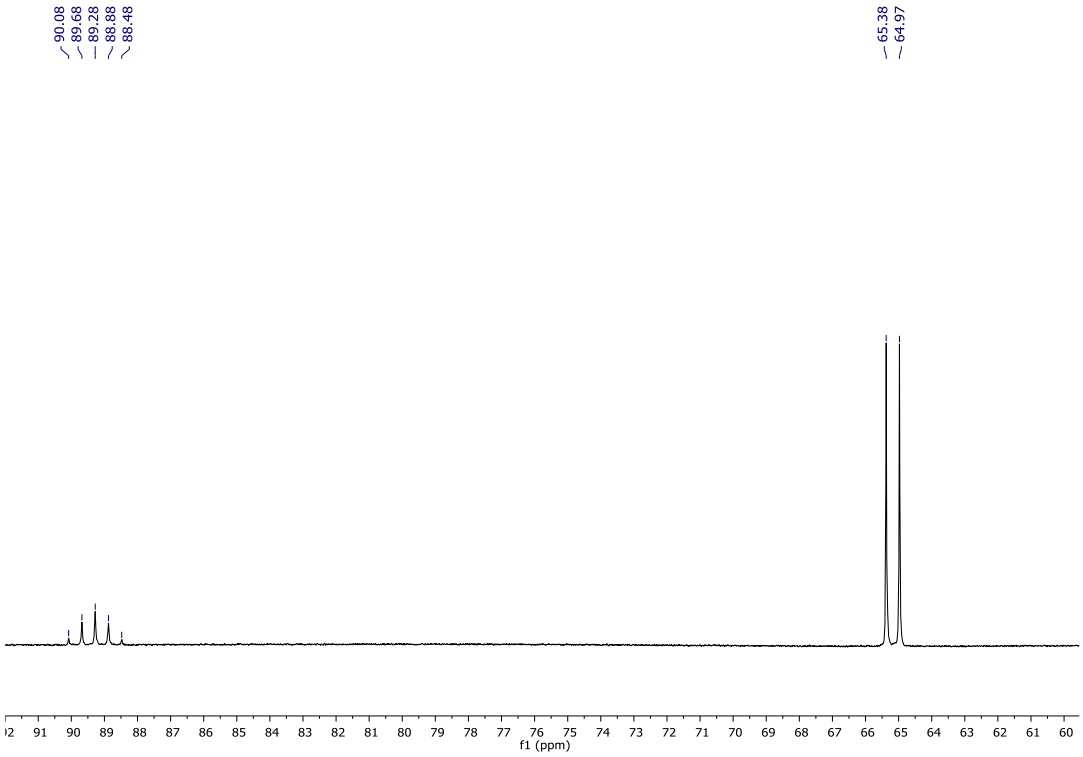
f1 (ppm)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64.97
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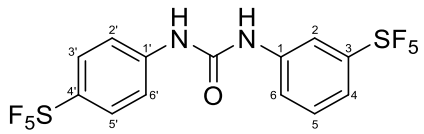
f1 (ppm)



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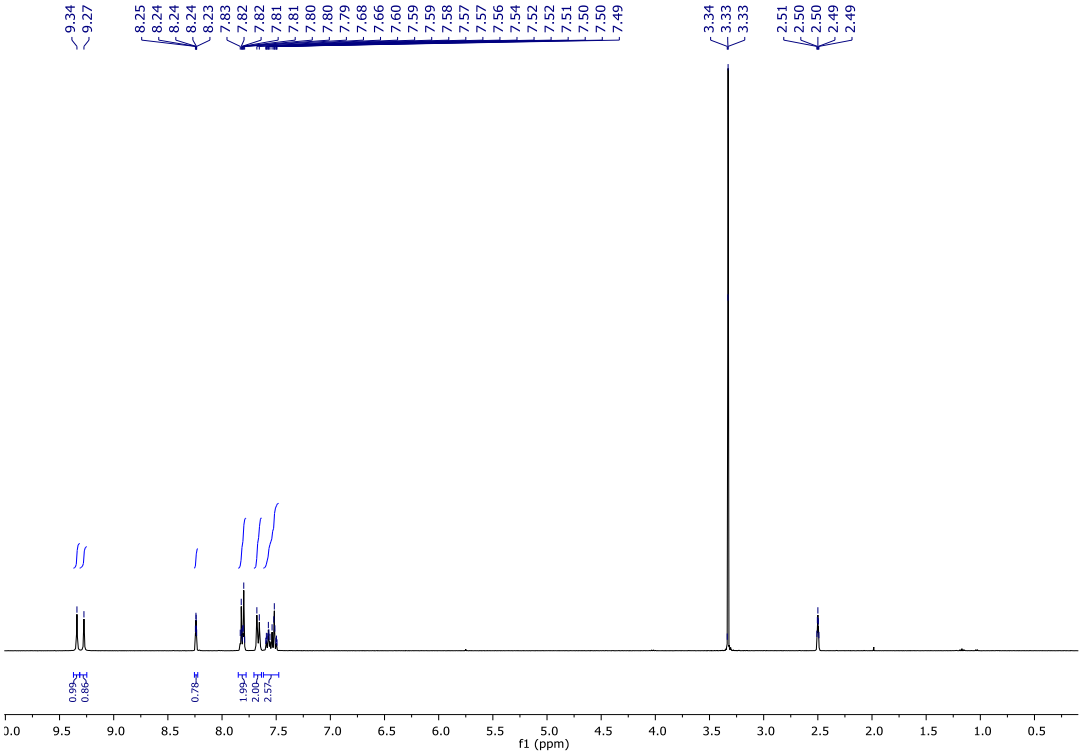
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7.82
7.81
7.81
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7.79
7.68
7.66
7.60
7.59
7.59
7.58
7.57
7.57
7.56
7.54
7.52
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7.51
7.50
7.50
7.49
3.34
3.33
3.33
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2.50
2.50
2.49
2.49
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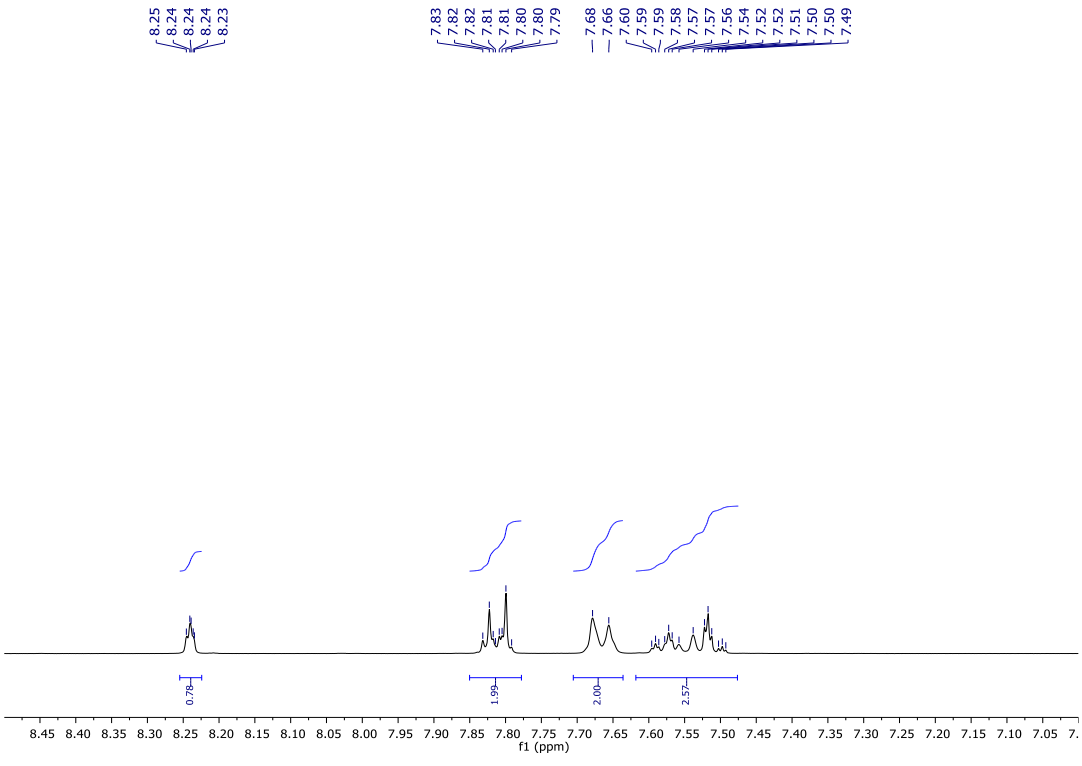
0.86
0.78
1.99
2.00
2.57
f1 (ppm)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7.80
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7.60
7.59
7.59
7.58
7.57
7.57
7.56
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7.50
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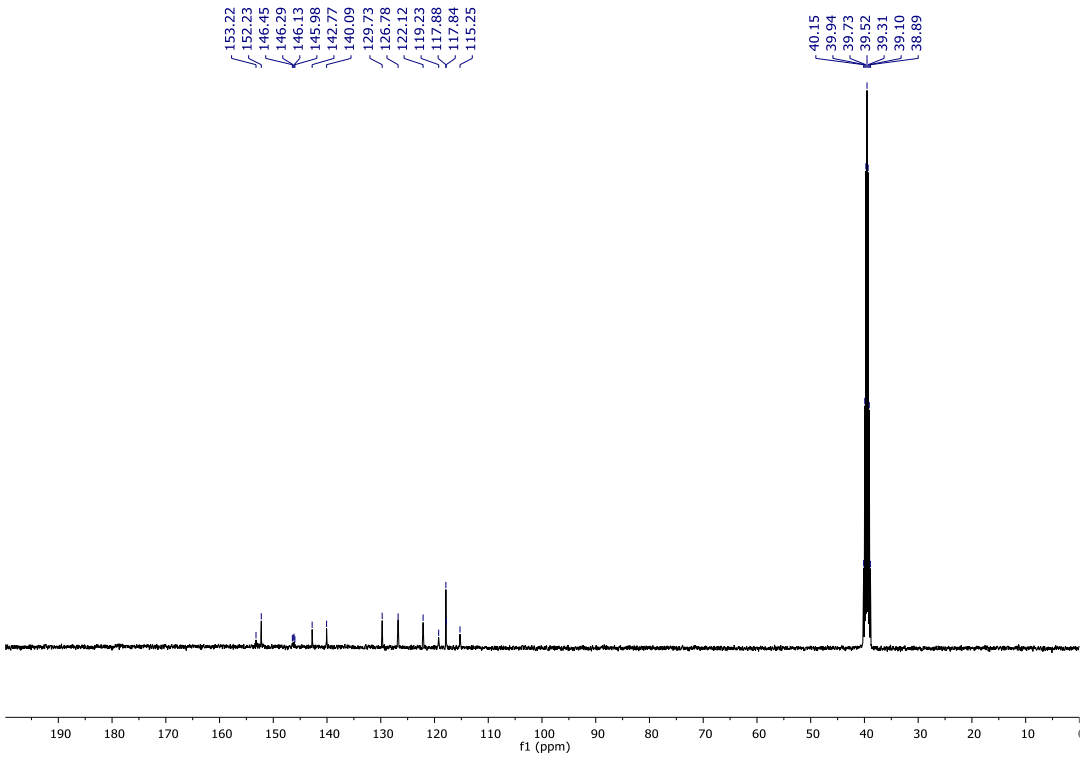
0.78
1.99
2.00
2.57
f1 (ppm)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140.09
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122.12
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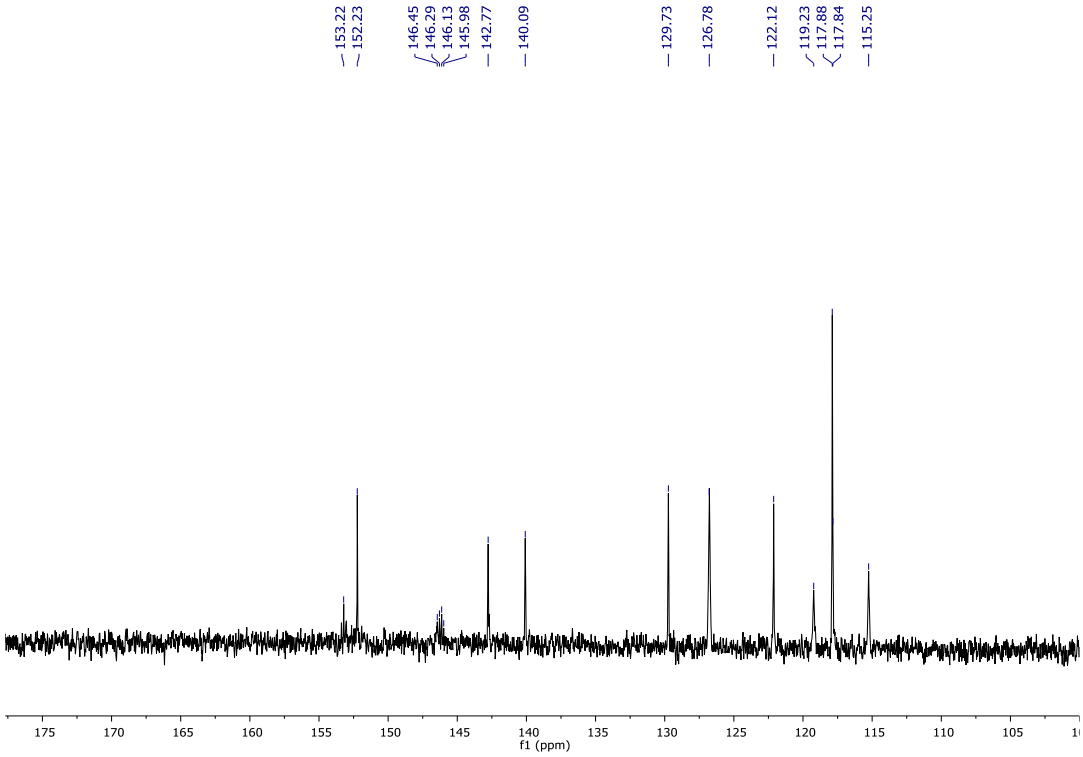
115.25
40.15
39.94
39.73
39.52
39.31
39.10
38.89
f1 (ppm)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152.23
146.45
146.29
146.13
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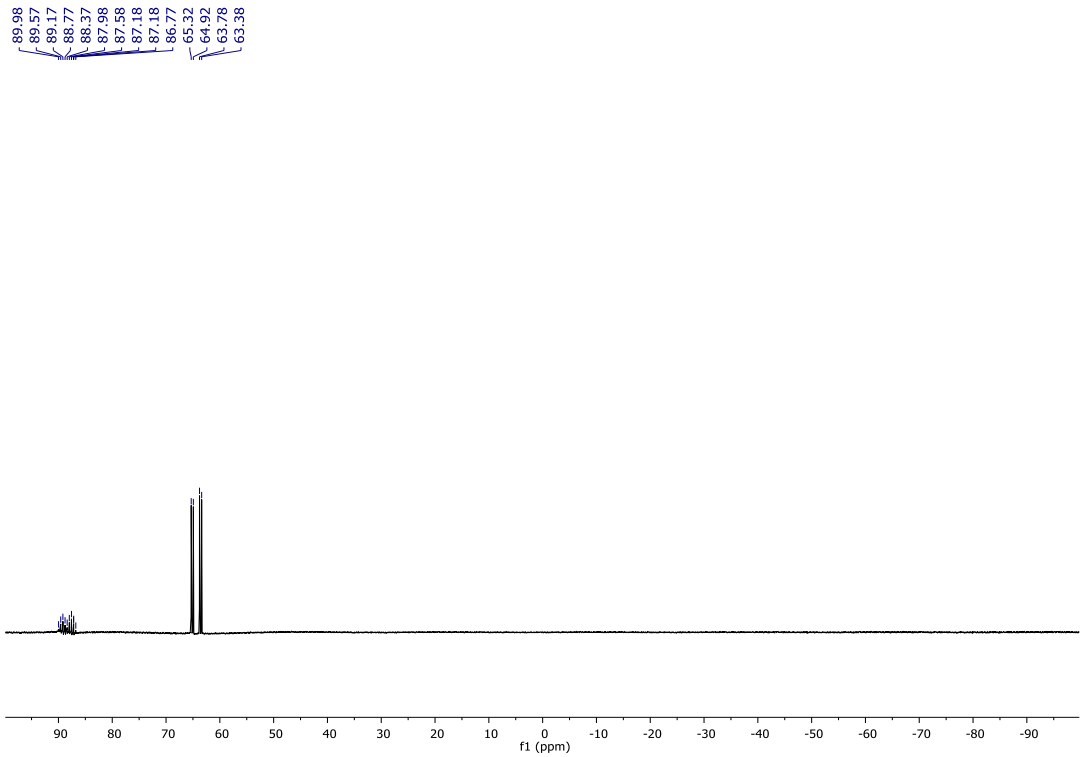
140.09
129.73
126.78
122.12
119.23
117.88
117.84
115.25
f1 (ppm)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87.58
87.18
87.18
86.77
65.32
64.92
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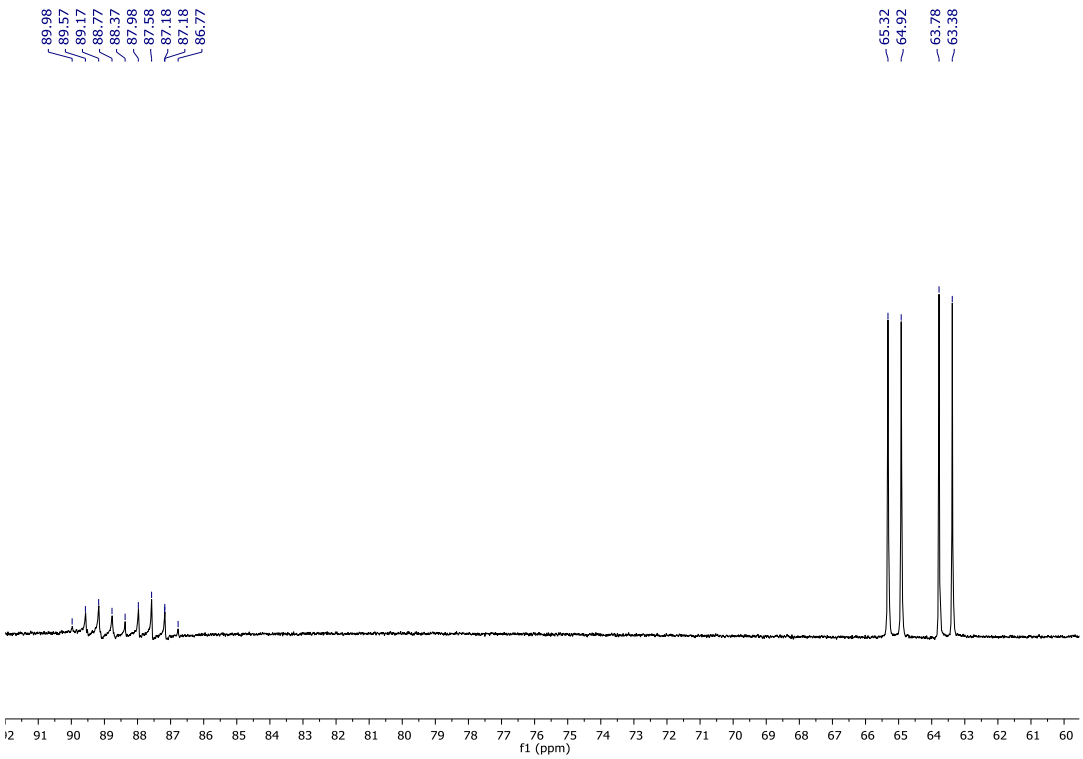
f1 (ppm)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88.77
88.37
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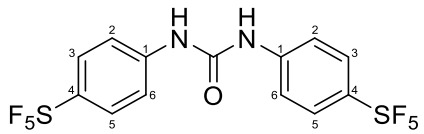
87.58
87.18
87.18
86.77
65.32
64.92
63.78
63.38
92 91 90 89 88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 63 62 61 60
f1 (ppm)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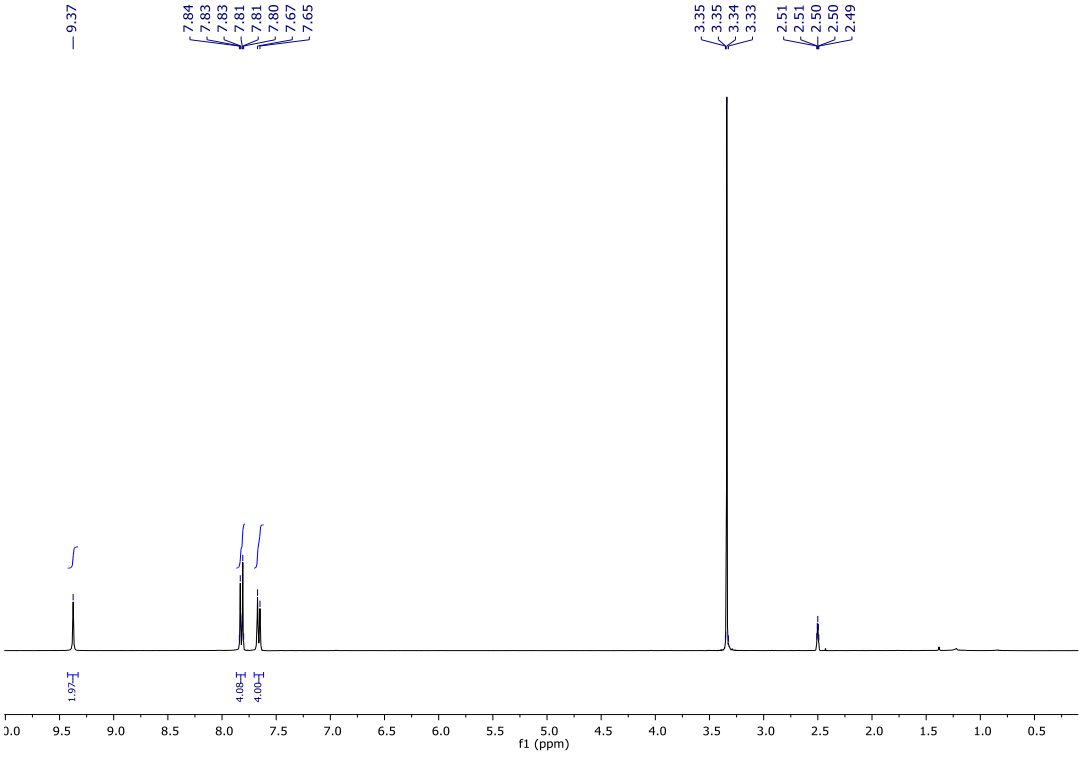
H
N
O
F5S
SF5

10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7.67
7.65
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3.34
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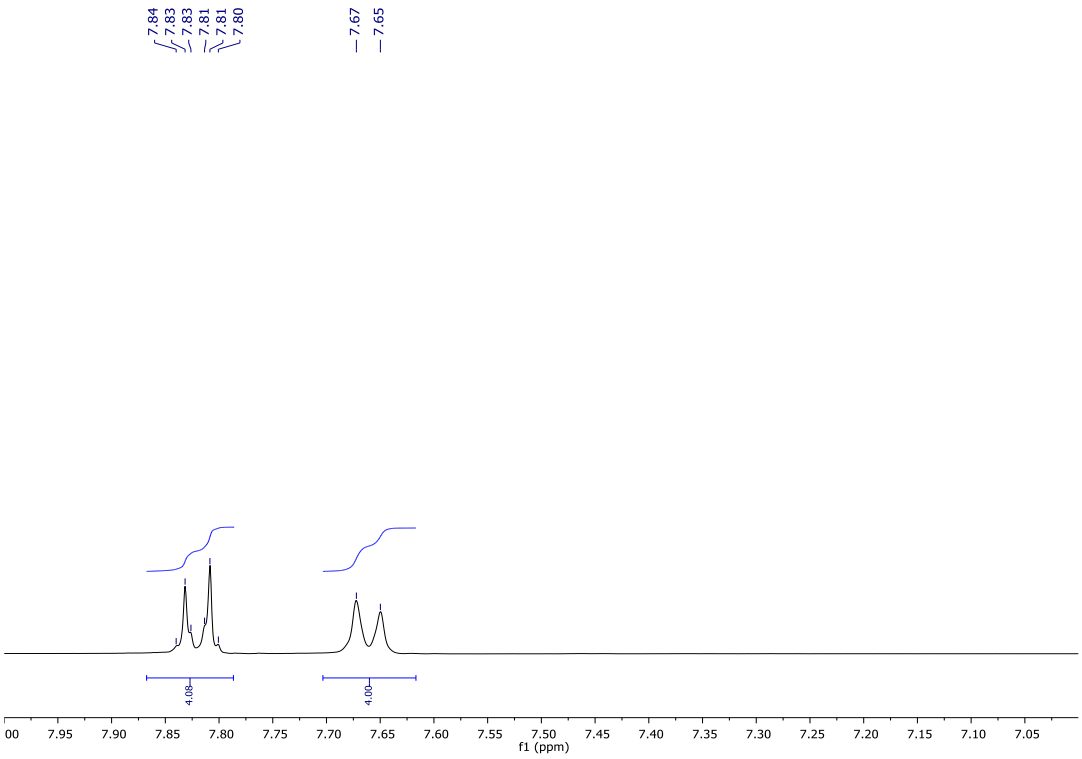
2.49
1.97
4.08
4.00
f1 (ppm)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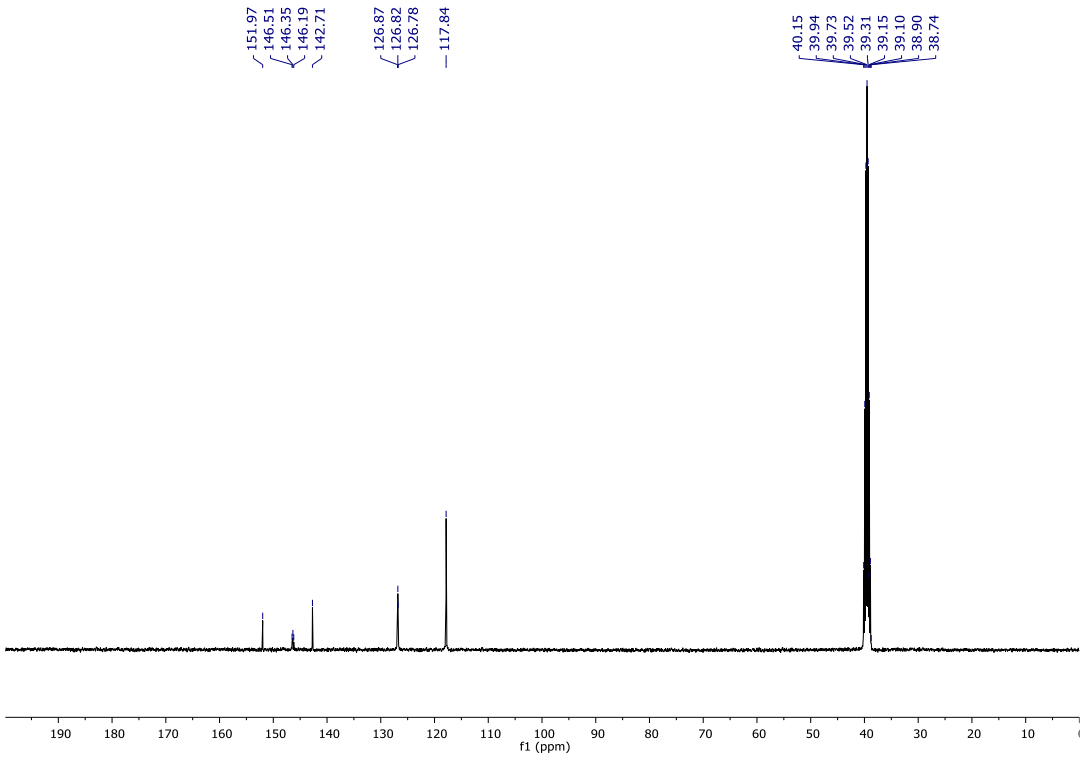
7.81
7.80
7.67
7.65
4.08
4.00
f1 (ppm)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126.78
117.84
40.15
39.94
39.73
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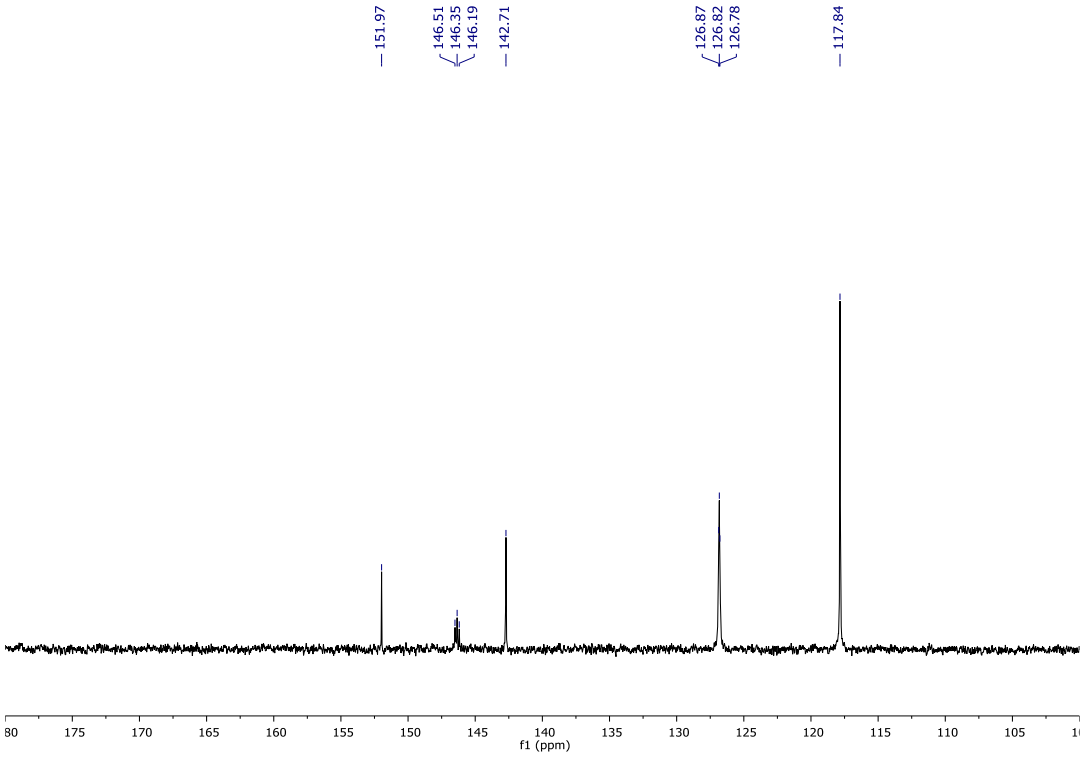
39.15
39.10
38.90
38.74
f1 (ppm)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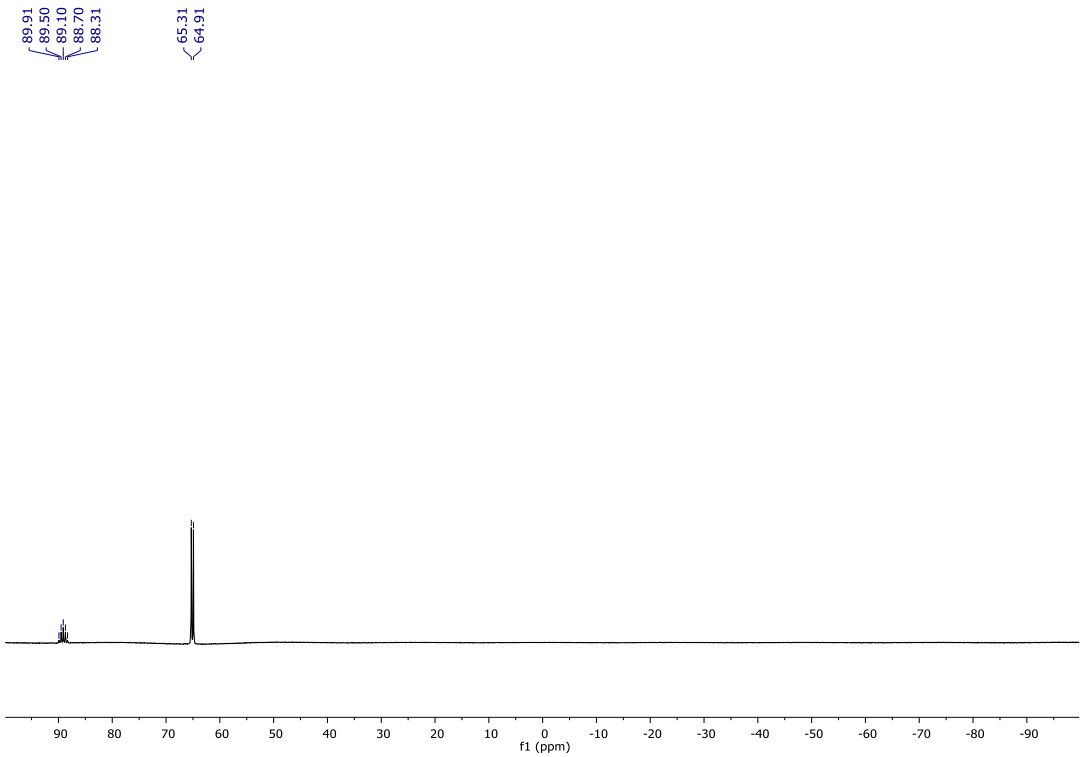
146.51
146.35
146.19
142.71
126.87
126.82
126.78
117.84
f1 (ppm)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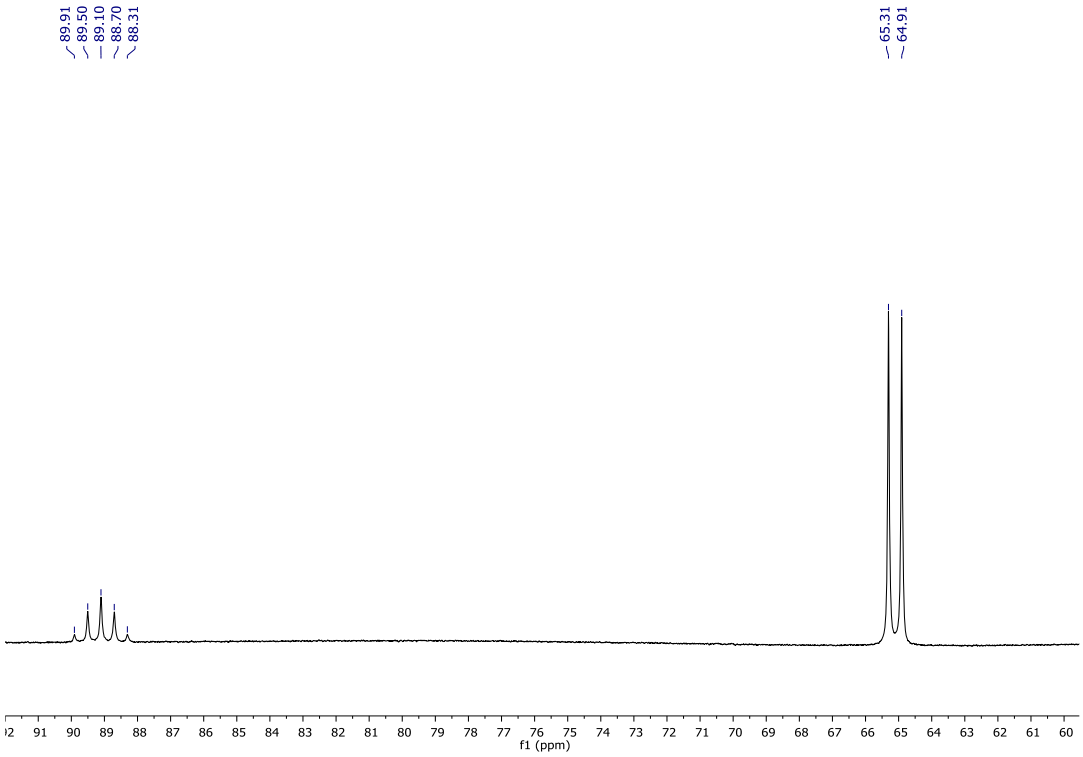
88.31
65.31
64.91
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)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89.10
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64.91
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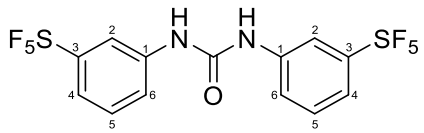
f1 (ppm)



11


9.27
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7.62
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7.60
7.59
7.55
7.53
7.52
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7.50
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7.49
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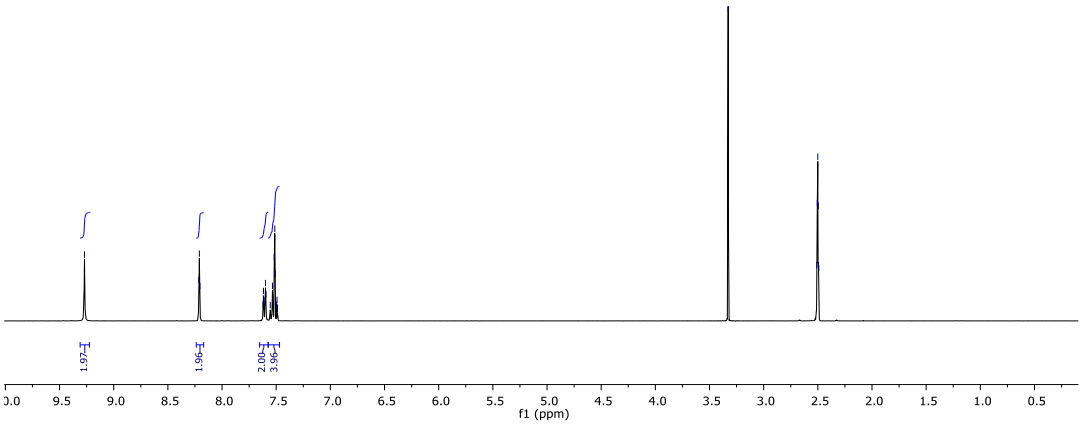
2.51
2.51
2.50
2.50
2.49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1.96
2.00
3.96
f1 (ppm)


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7.51
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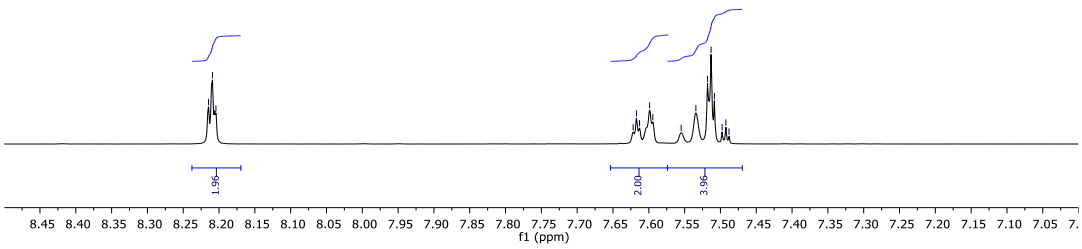
7.49
7.49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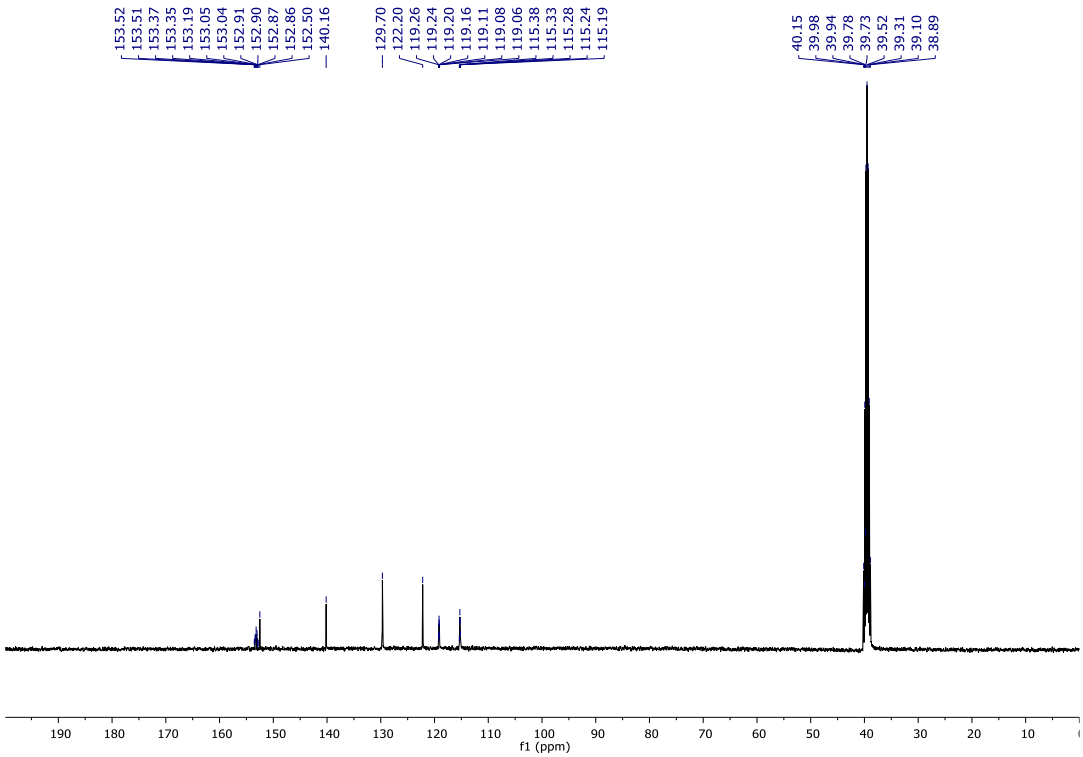
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152.86
152.50
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119.26
119.24
119.20
119.16
119.11
119.08
119.06
115.38
115.33
115.28
115.24
115.19
40.15
39.98
39.94
39.78
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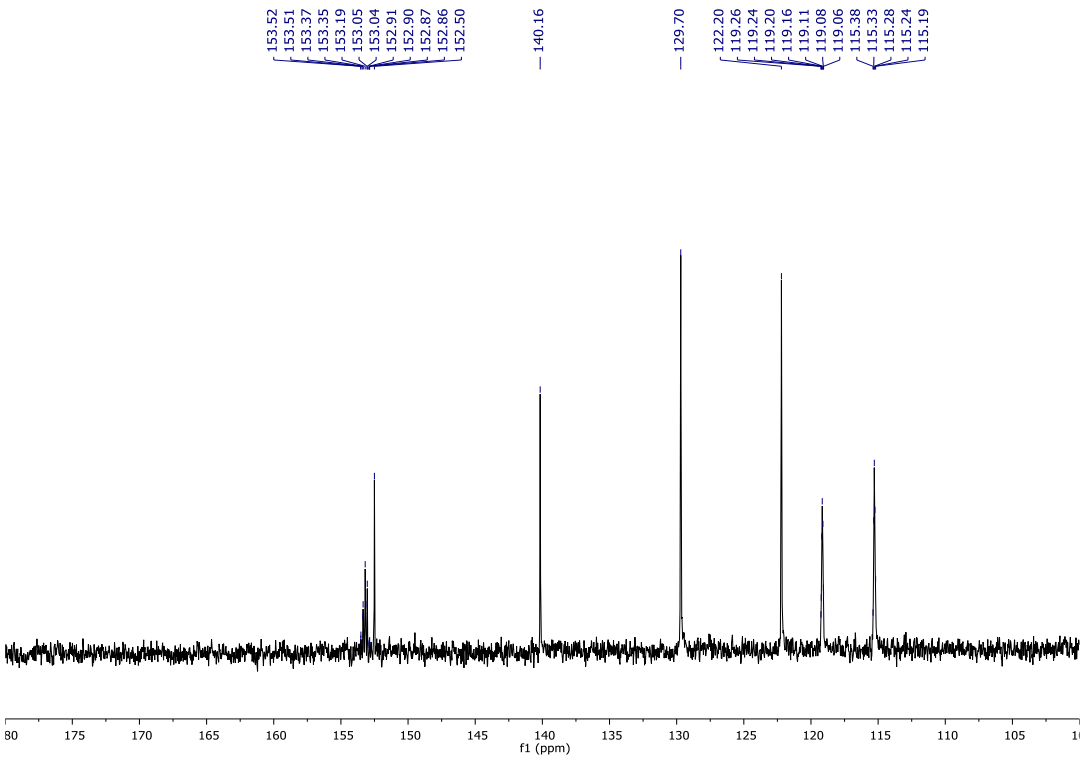
f1 (ppm)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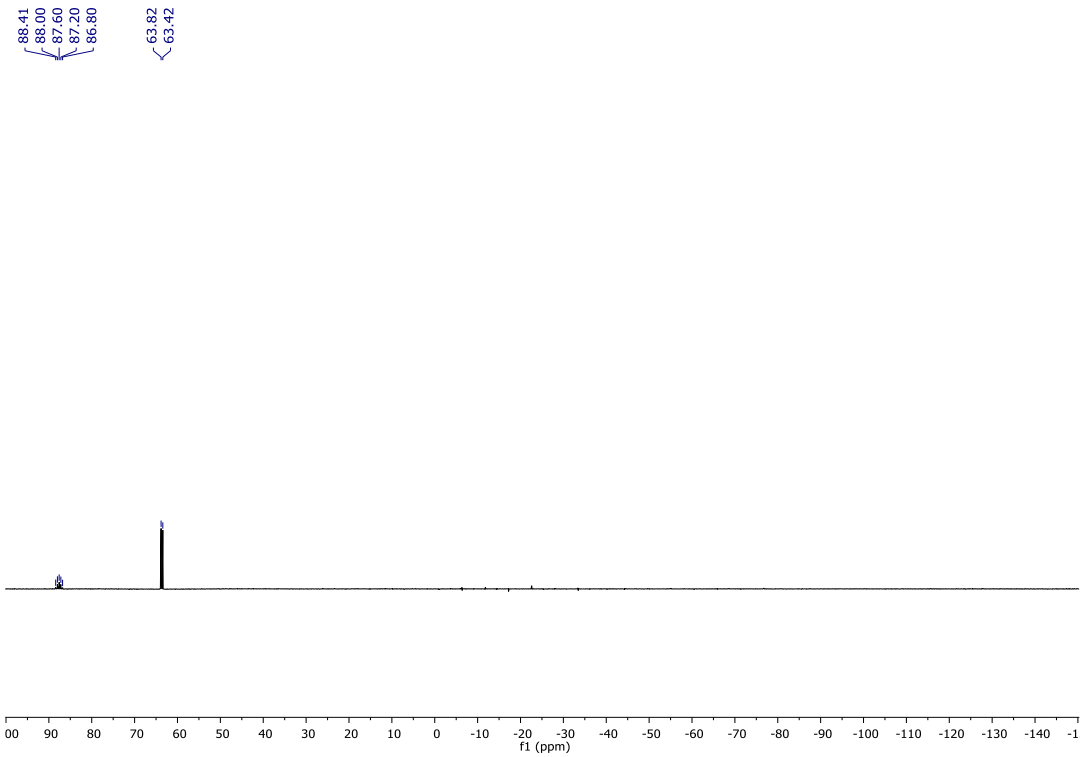
152.86
152.50
140.16
129.70
122.20
119.26
119.24
119.20
119.16
119.11
119.08
119.06
115.38
115.33
115.28
115.24
115.19
80 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105
f1 (ppm)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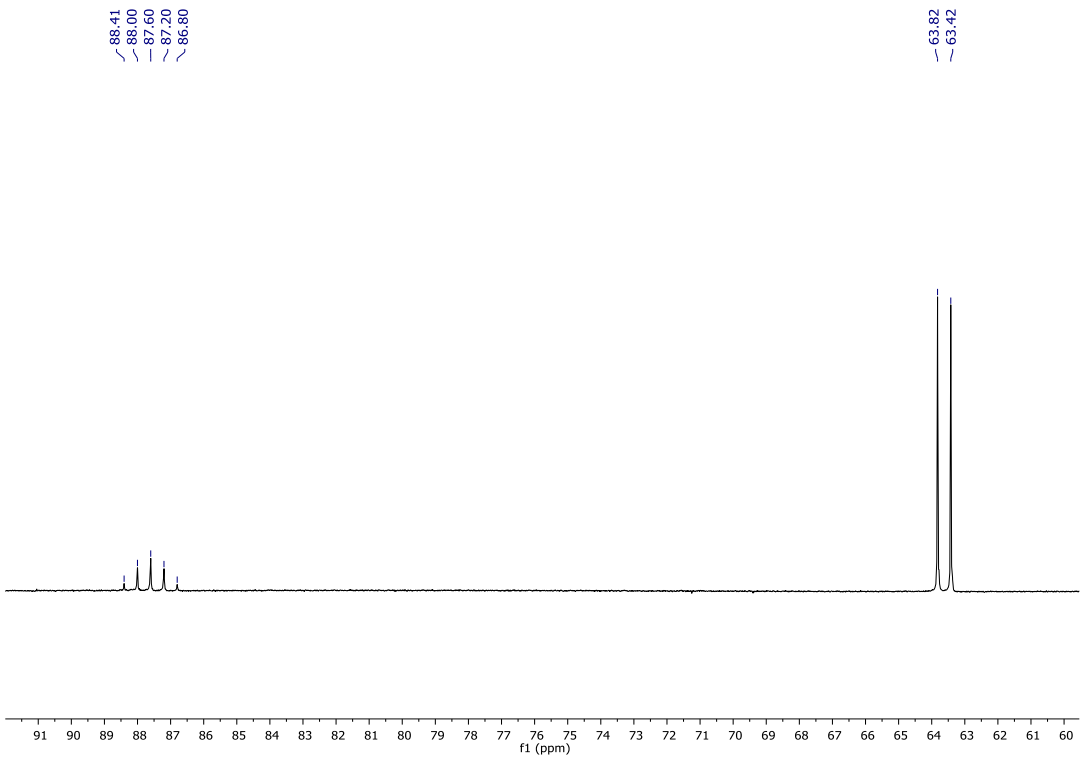
63.42
f1 (ppm)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88.00
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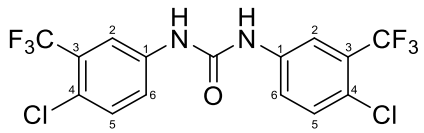
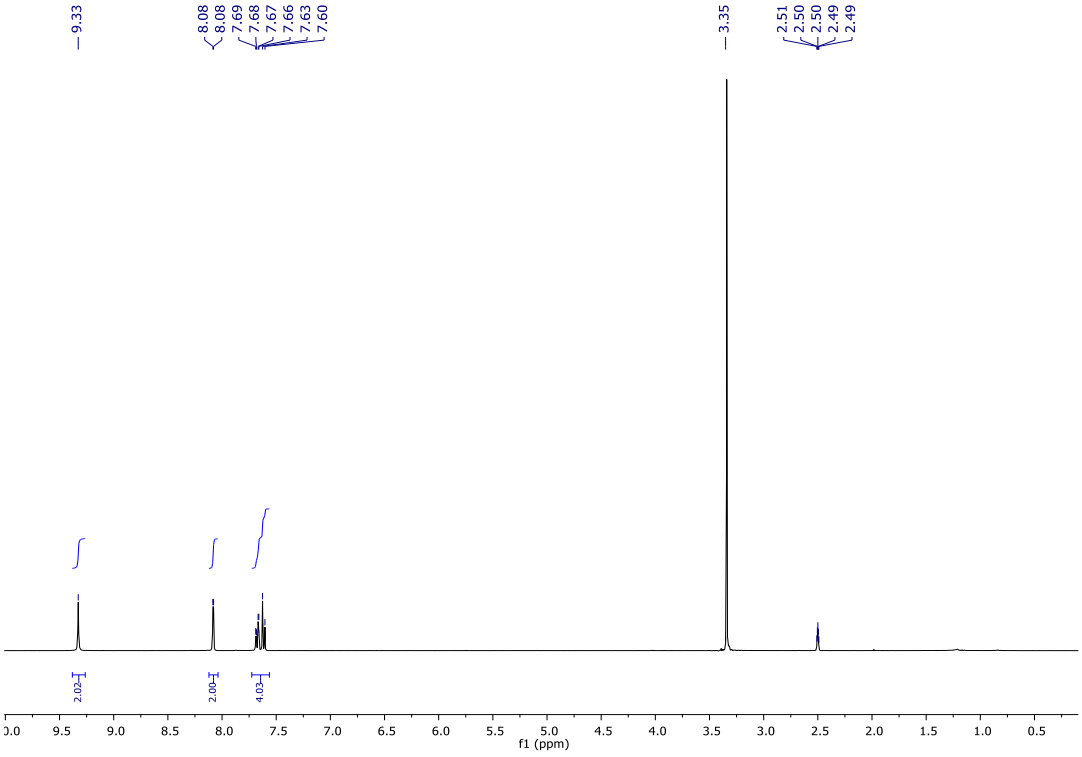
87.20
86.80
63.82
63.42
f1 (ppm)



12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8.08
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7.68
7.67
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7.60
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2.51
2.50
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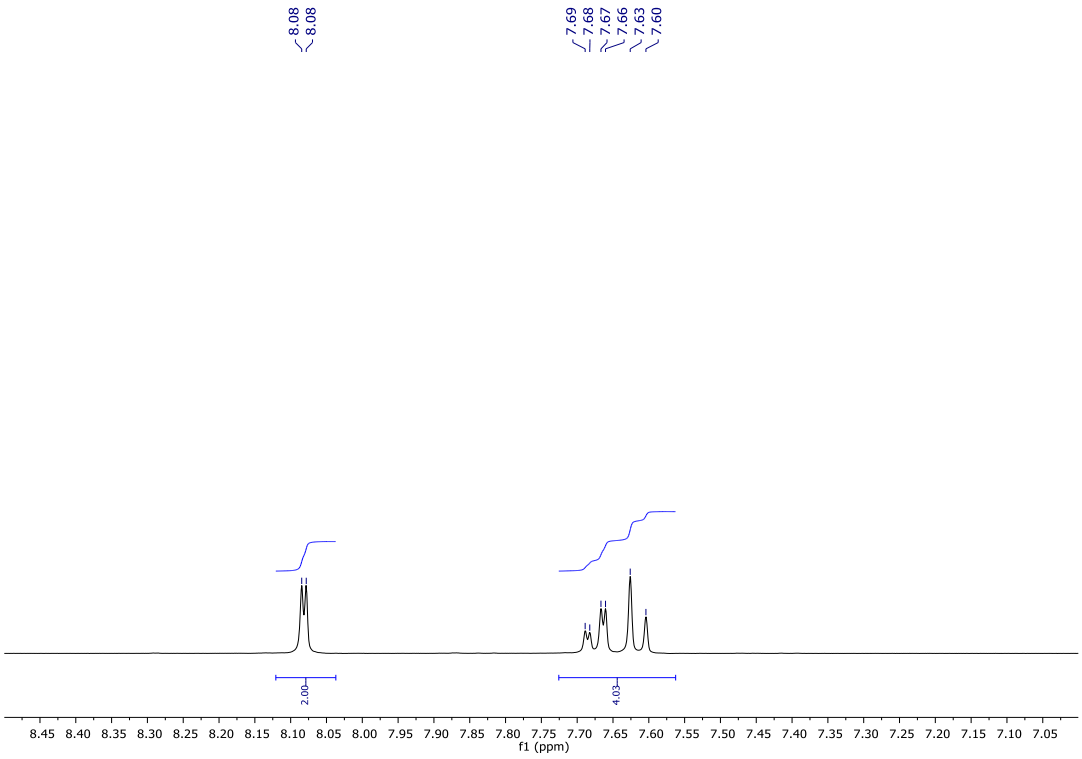
2.49
2.02
2.00
4.03
f1 (ppm)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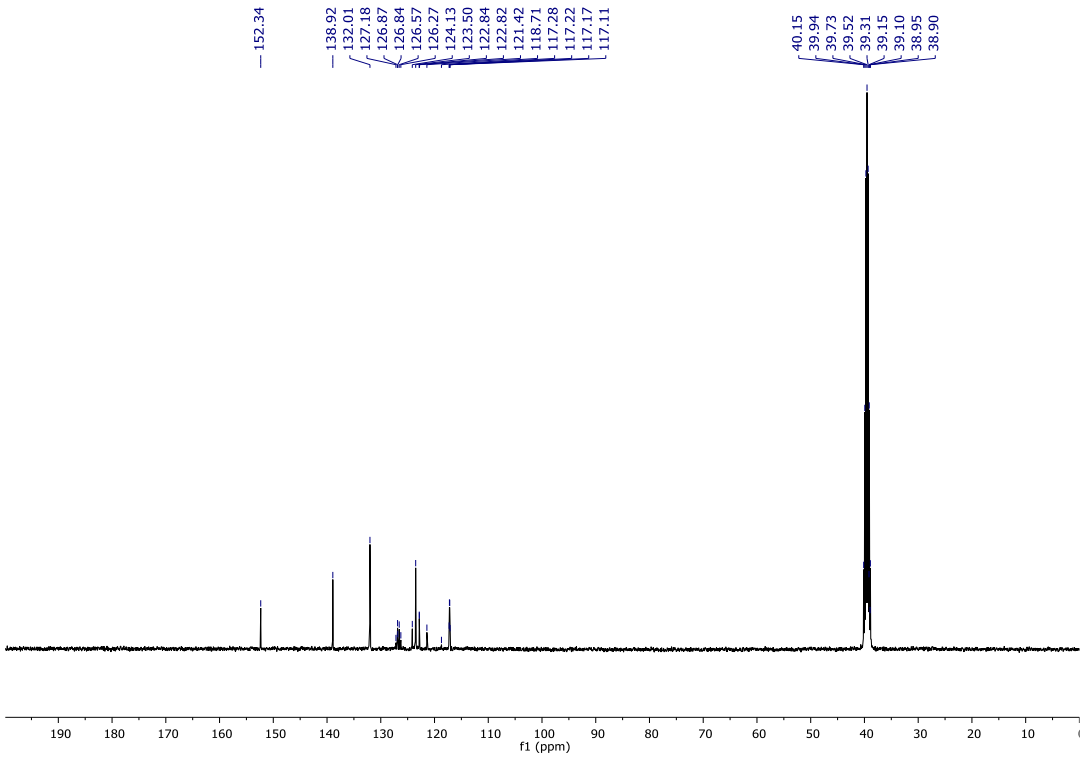
8.08
7.69
7.68
7.67
7.66
7.63
7.60
2.00
4.03
f1 (ppm)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126.87
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126.57
126.27
124.13
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122.84
122.82
121.42
118.71
117.28
117.22
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117.11
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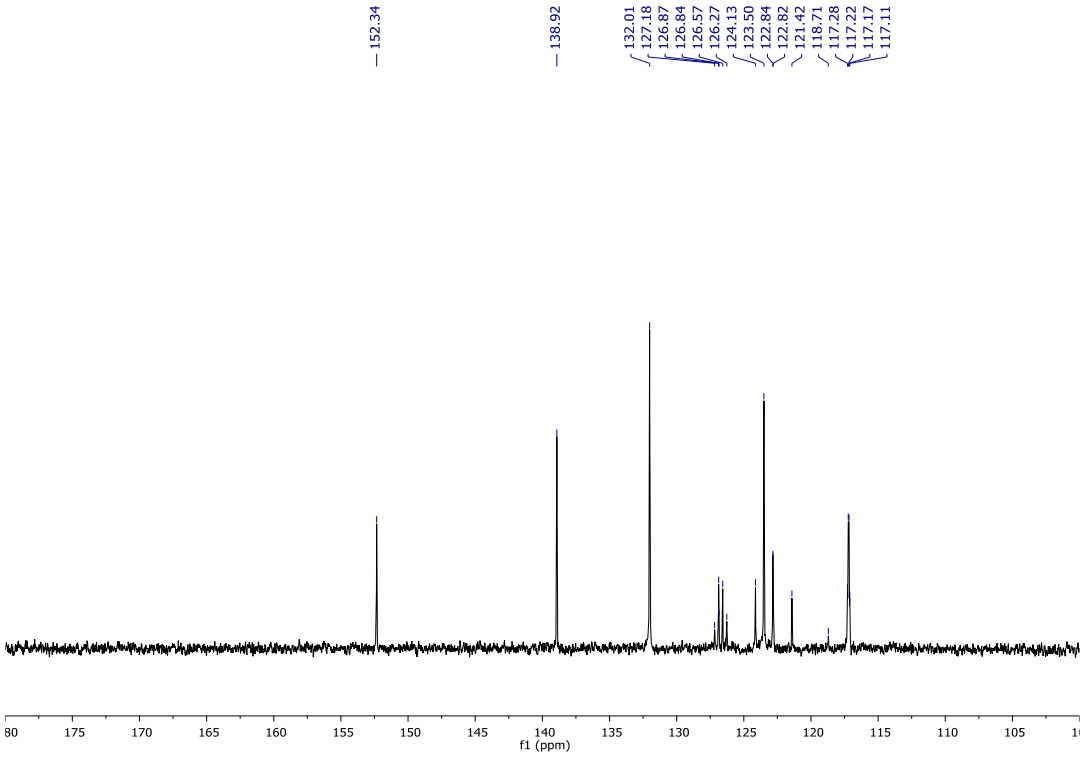
39.94
39.73
39.52
39.31
39.15
39.10
38.95
38.90
f1 (ppm)


152.34
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132.01
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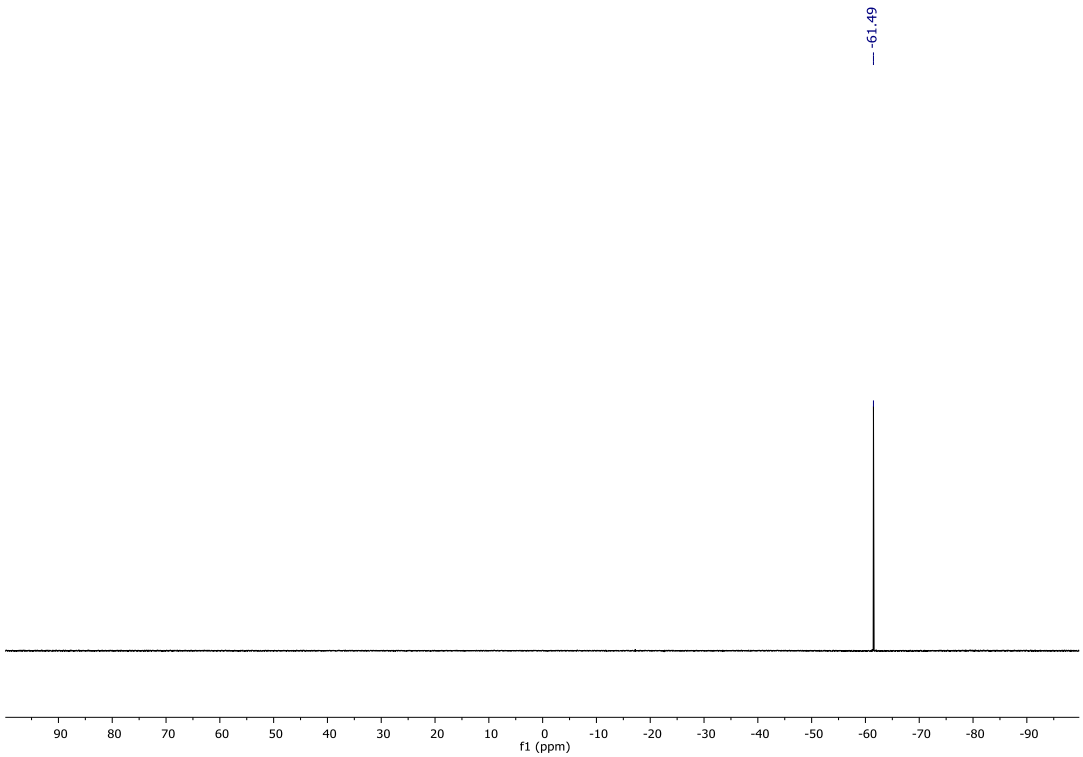
117.28
117.22
117.17
117.11
f1 (ppm)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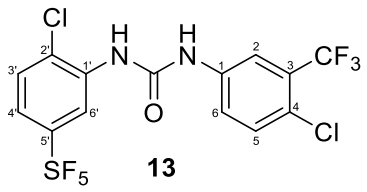
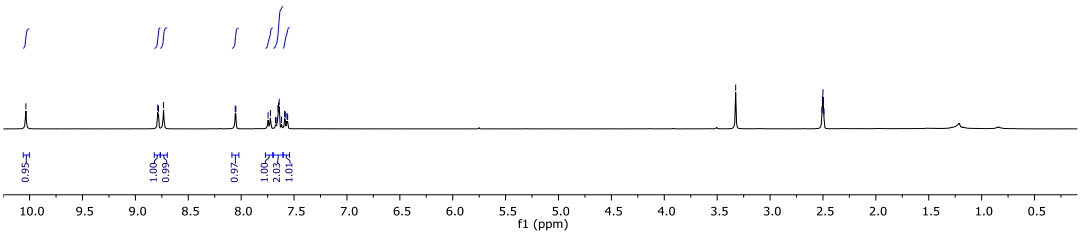
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


Cl
H
N
H
N
O
CF3
Cl
SF5
2'
1'
3'
4'
6'
5'
1
2
3
4
5
6

13


10.04
8.79
8.78
8.73
8.06
8.05
7.75
7.72
7.68
7.67
7.65
7.65
7.64
7.62
7.59
7.58
7.57
7.56
3.33
2.51
2.50
2.50
2.50
2.49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0.99
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1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


8.79
8.78
8.73
8.06
8.05
7.75
7.72
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7.67
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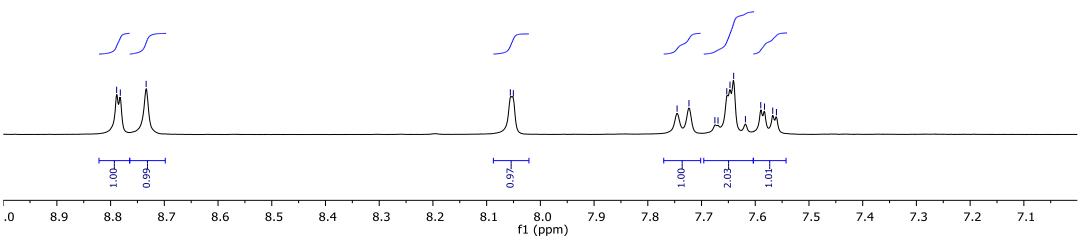
7.65
7.64
7.62
7.59
7.58
7.57
7.56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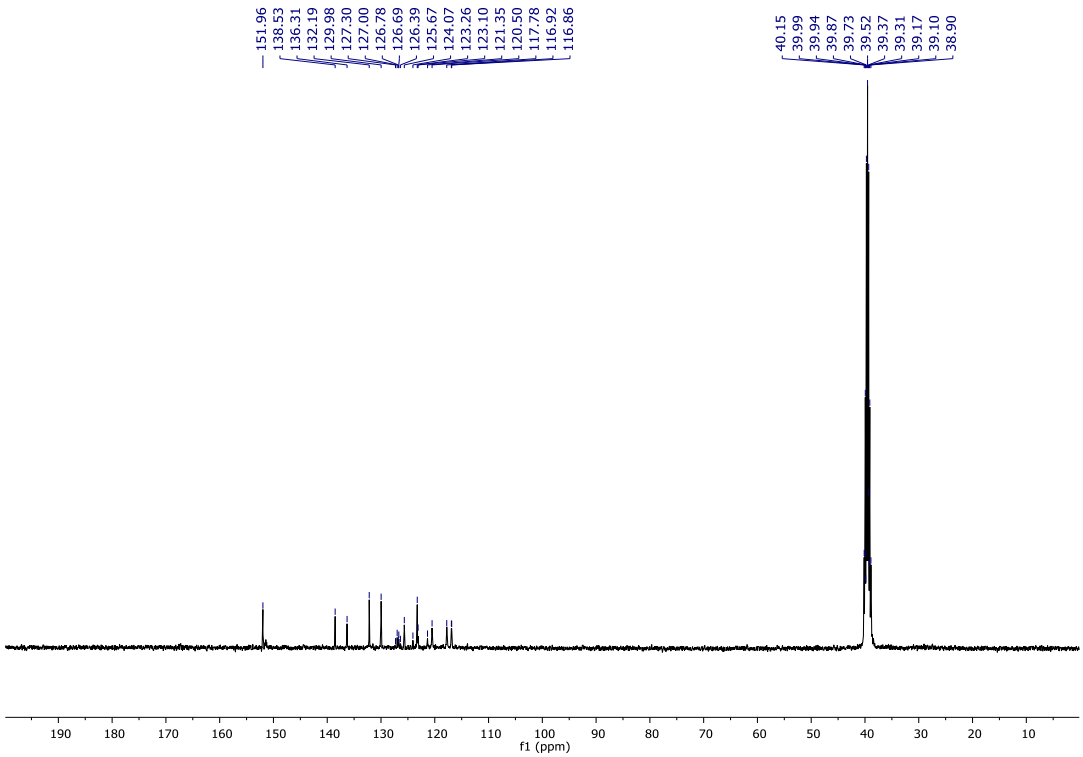
1.01
.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)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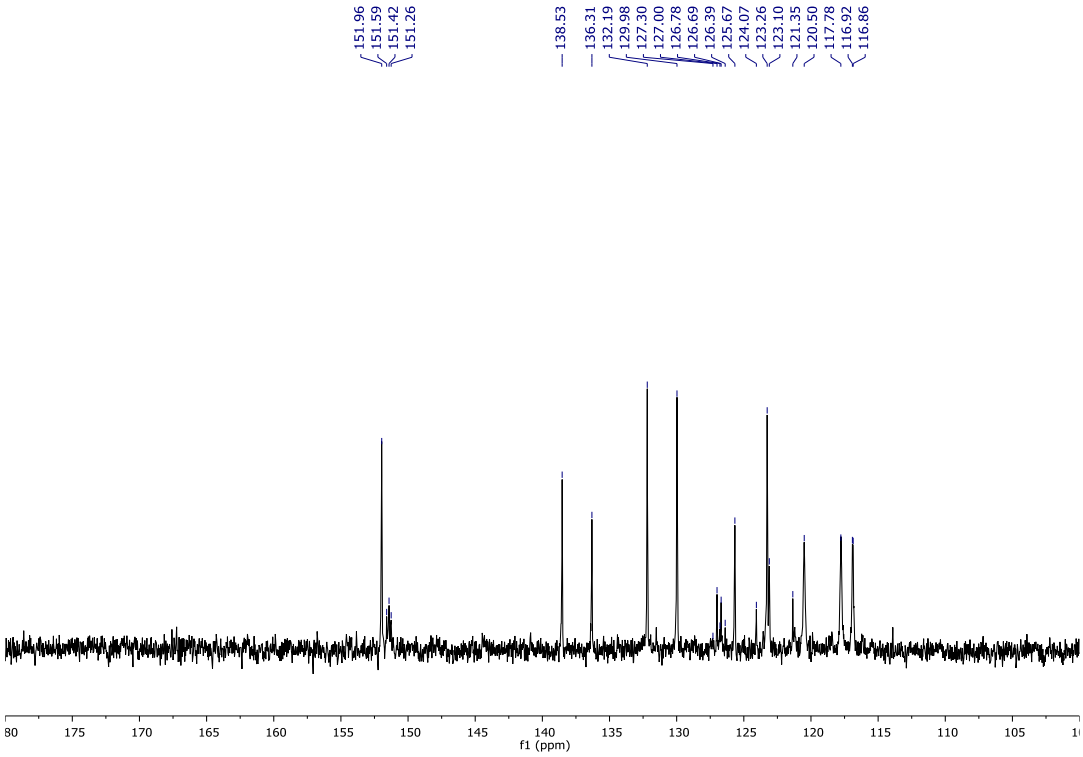
136.31
132.19
129.98
127.30
127.00
126.78
126.69
126.39
125.67
124.07
123.26
123.10
121.35
120.50
117.78
116.92
116.86
40.15
39.99
39.94
39.87
39.73
39.52
39.37
39.31
39.17
39.10
38.90
f1 (ppm)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126.78
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123.10
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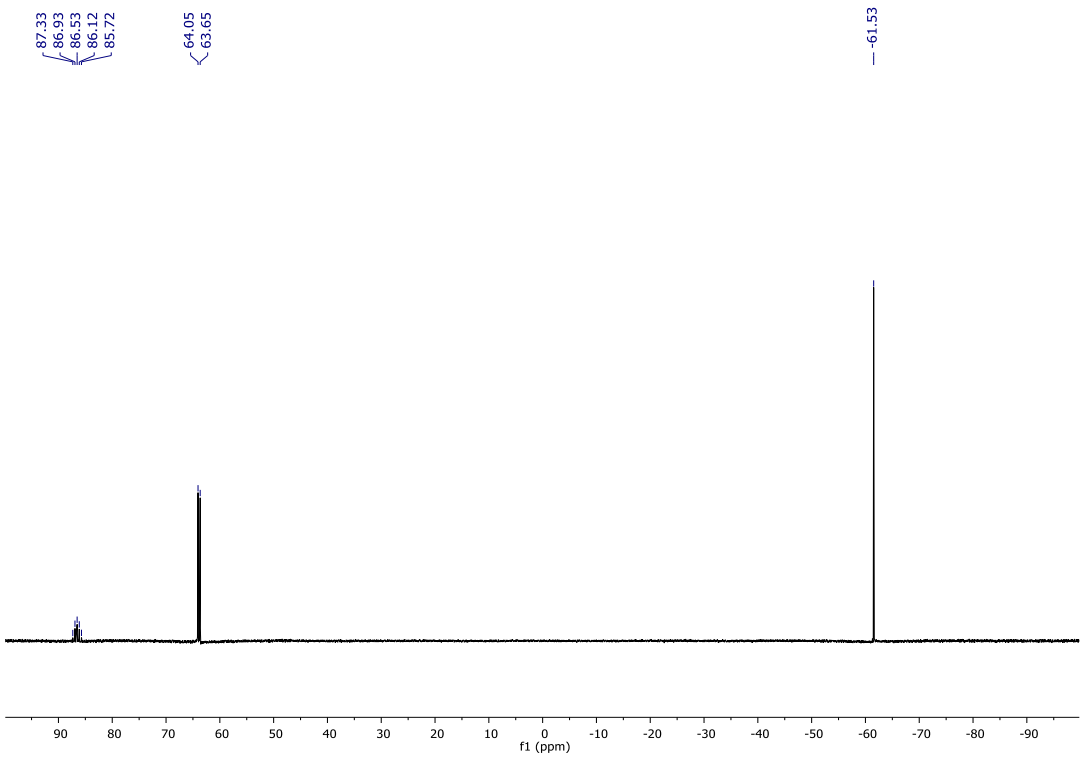
120.50
117.78
116.92
116.86
f1 (ppm)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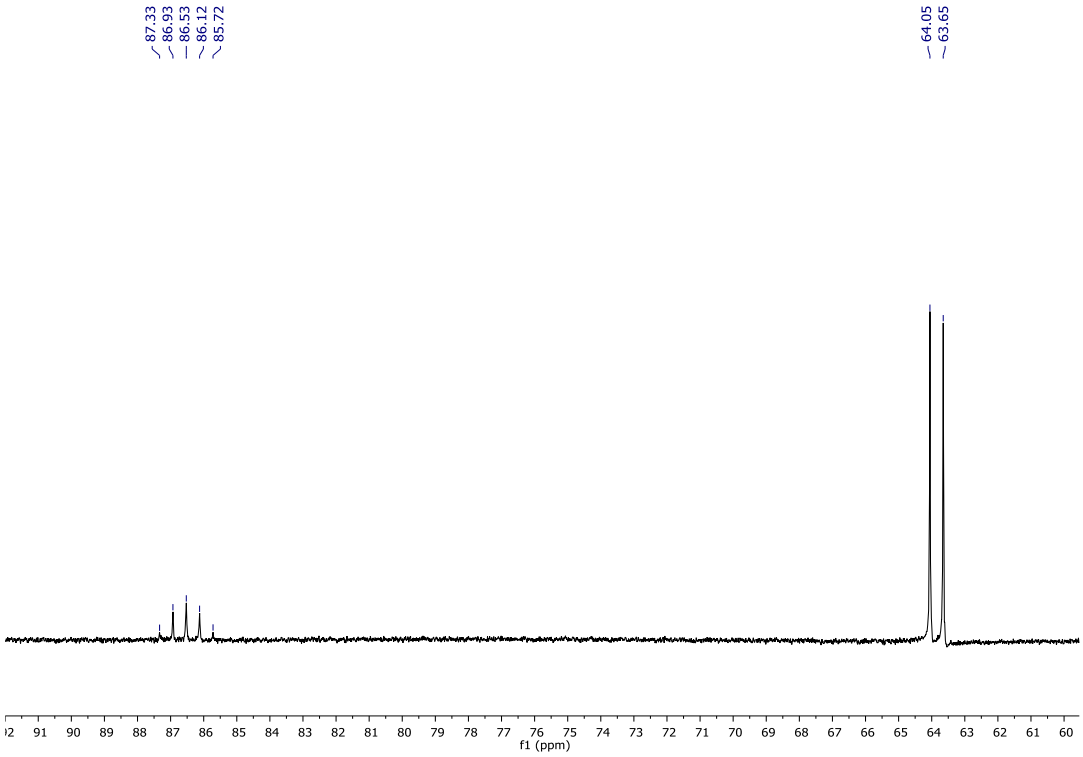
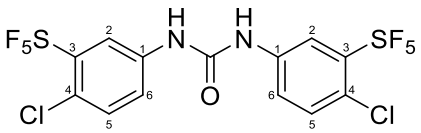
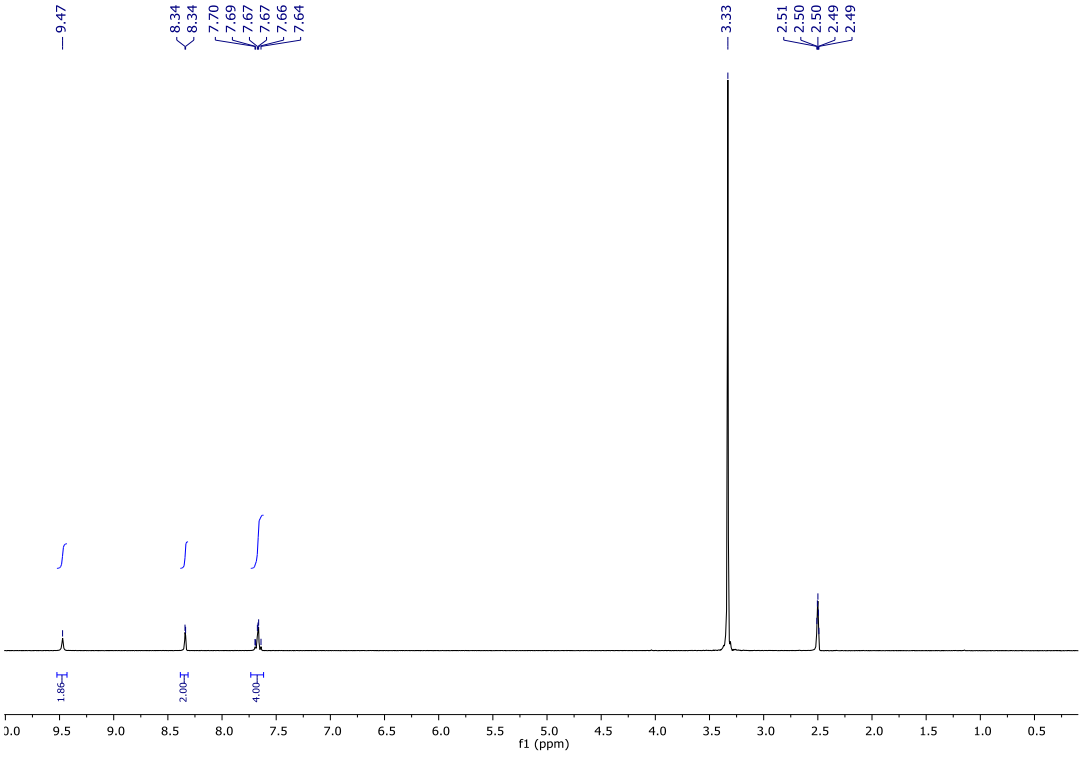
86.53
86.12
85.72
64.05
63.65
-61.53
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)


87.33
86.93
86.53
86.12
85.72
64.05
63.65
92 91 90 89 88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 63 62 61 60
f1 (ppm)


F5S
SF5
Cl
Cl
H
N
H
N
O

14


9.47
8.34
8.34
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7.69
7.67
7.67
7.66
7.64
3.33
2.51
2.50
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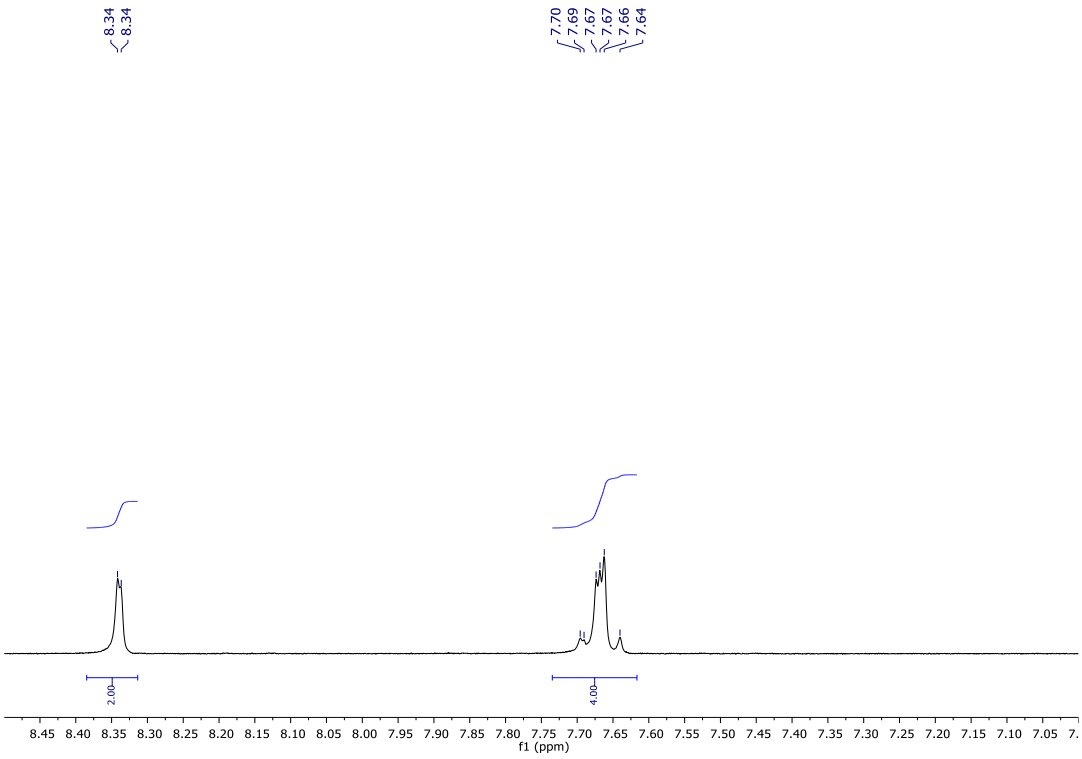
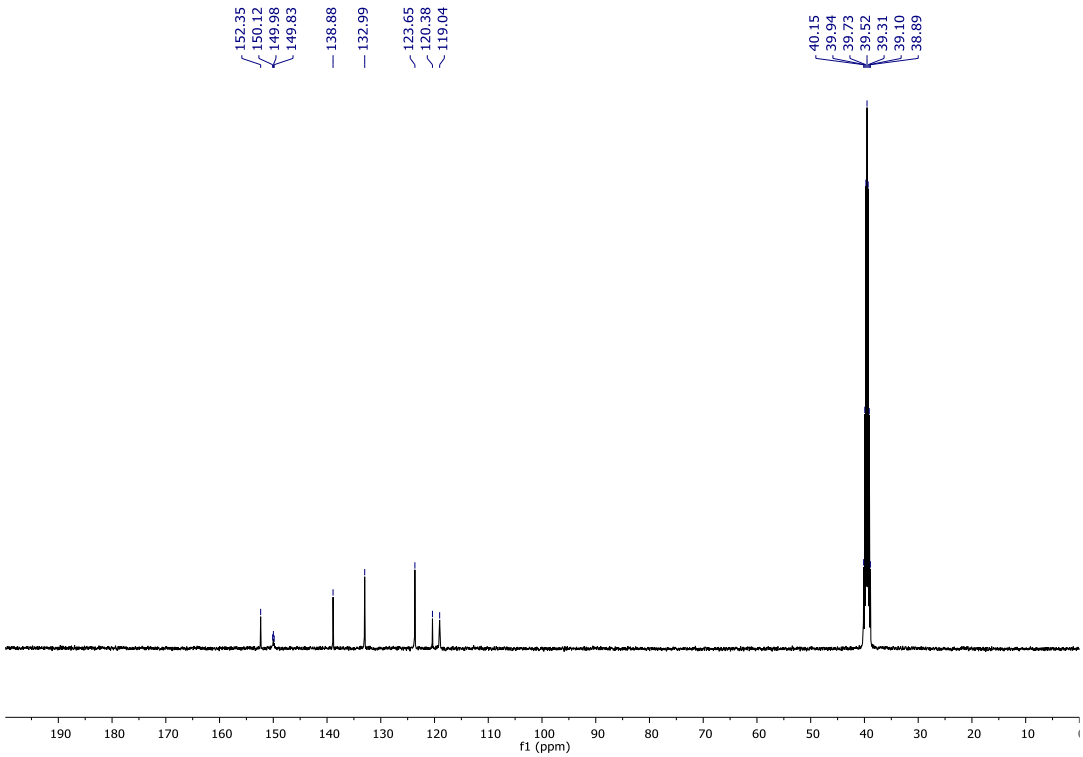
2.49
1.86
2.00
4.00
f1 (ppm)


8.34
8.34
7.70
7.69
7.67
7.67
7.66
7.64
2.00
4.00
f1 (ppm)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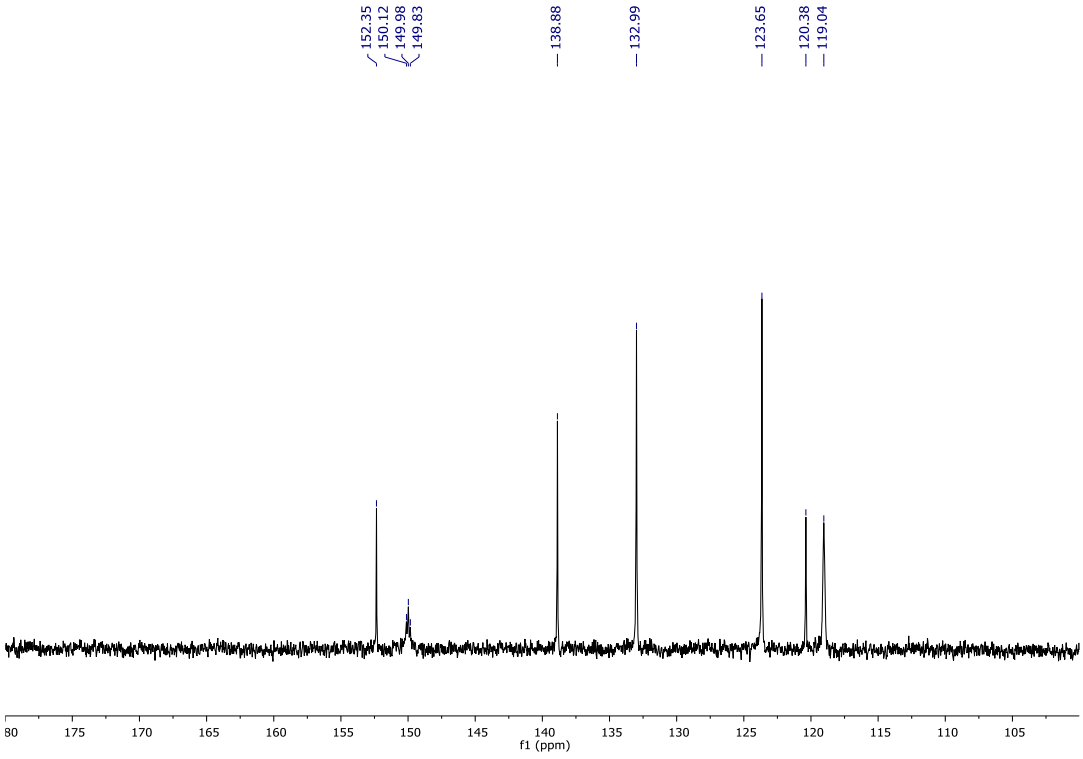
39.73
39.52
39.31
39.10
38.89
f1 (ppm)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150.12
149.98
149.83
138.88
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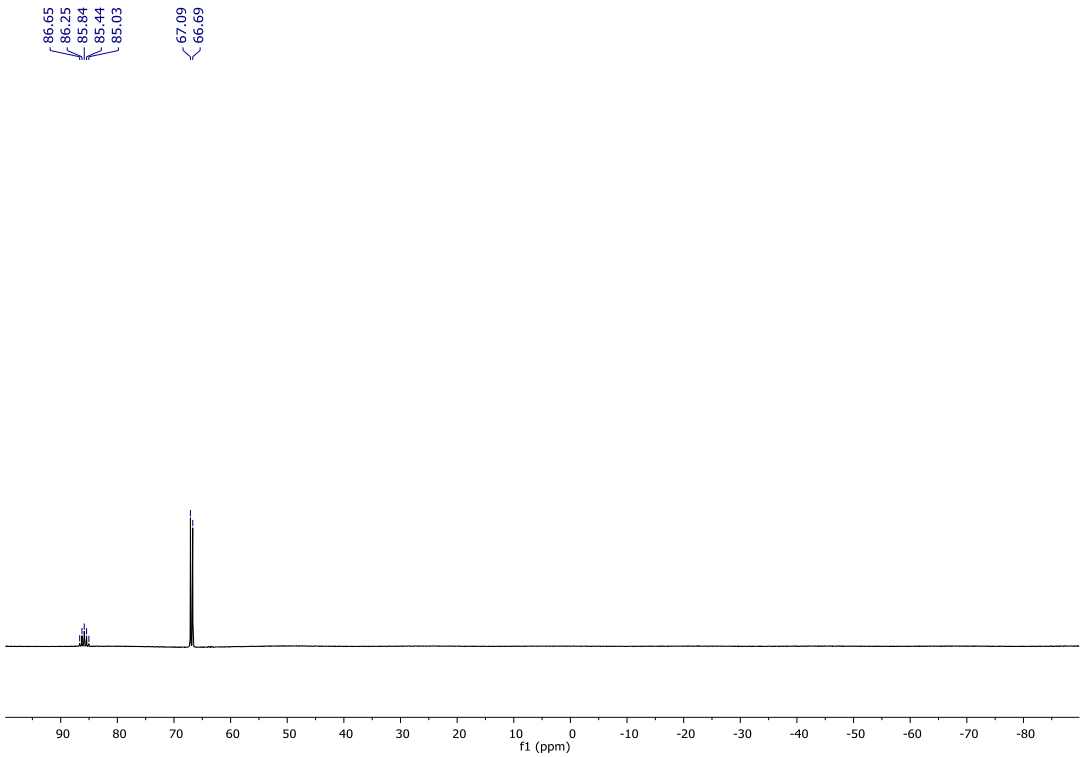
123.65
120.38
119.04
f1 (ppm)


86.65
86.25
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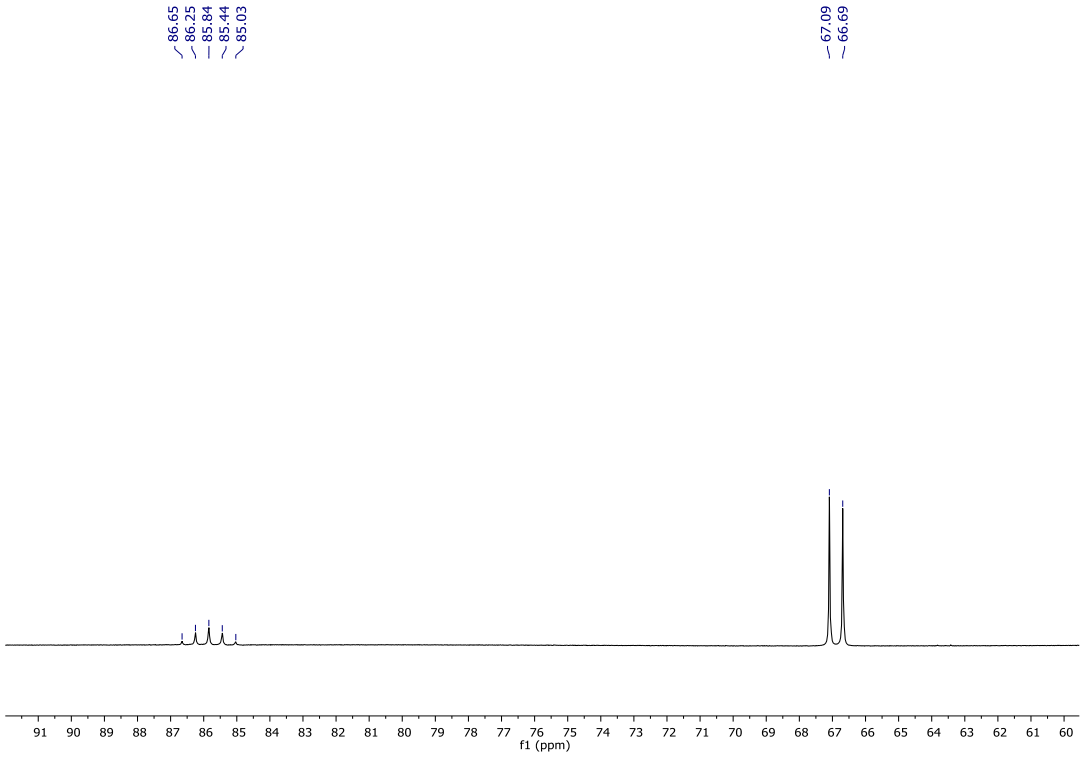
85.44
85.03
67.09
66.69
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80
f1 (ppm)


86.65
86.25
85.84
85.44
85.03
67.09
66.69
91 90 89 88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 63 62 61 60
f1 (ppm)