Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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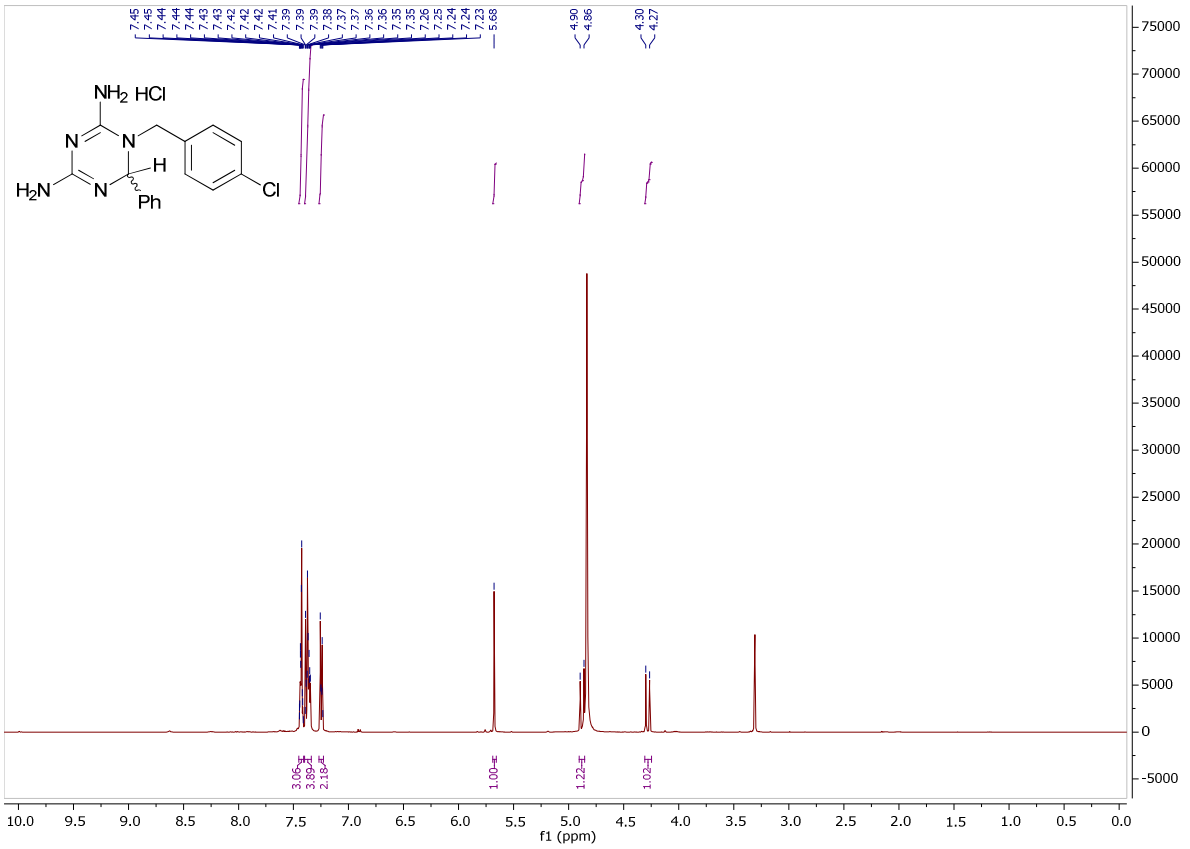
NMR spectra were run on either a Varian 200 MHz Gemini 2000 instrument, or on a 400 MHz Varian INOVA instrument. Chemical shifts (δ scale) are reported in parts per million (ppm) relative to the central peak of methanol, 49.00 ppm for ^{13}C and 3.31 ppm for ^{1}H; chloroform, 77.16 ppm for ^{13}C and 7.26 ppm for ^{1}H. Spectra are reported in the following order: multiplicity, approximate coupling constant (J value) in hertz (Hz), number of protons or carbons; signals were characterized as s (singlet), d (doublet), dd (doublet of doublets), ddd (doublet of doublets of doublets), t (triplet), dt (doublet of triplets), q (quartet), p (pentet), br s (broad signal) and m (multiplet). High resolution mass spectra were generated on a Waters SYNAPT G1 HDMS mass spectrometer operated in electrospray mode. Leucine enkephalin (50 pg/ml) was used as reference calibrant to obtain typical mass accuracies between 1 and 3 mDa. The mass spectrometer was operated in positive mode with a capillary voltage of 2 kV, the sampling cone at 30 V and the extraction cone at 4 V. The source temperature was 120 C and the desolvation temperature was set at 350 °C. Nitrogen gas was used as the nebulisation gas at a flow rate of 450 L/h. Purity of final compounds was determined by UPLC, using a Waters Acquity UPLC coupled in tandem to an UPDA detector (200-500 nm). All chemicals for UPLC-MS work were of ultra-pure LC MS grade and purchased from Fluka (Steinheim, Germany) while ultra-grade solvents were purchased from Honeywell (Burdick & Jackson, Muskegon, USA). The analytical column used was a Waters Acquity HSS C18, 150 x 2.1 mm (1.7 mm) equilibrated at 45 °C in a column heater. The mobile phase consisted of acetonitrile and ultra-pure water containing 0.1% formic acid (v/v). A linear gradient was used to ramp the mobile phase composition from 95% water to 10% water in 6 min. The runtime was 10 min per sample. The software used to control the hyphenated system and do all data manipulation was MassLynx 4.1 (SCN 704).

5a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7.45
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7.44
7.44
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7.42
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7.41
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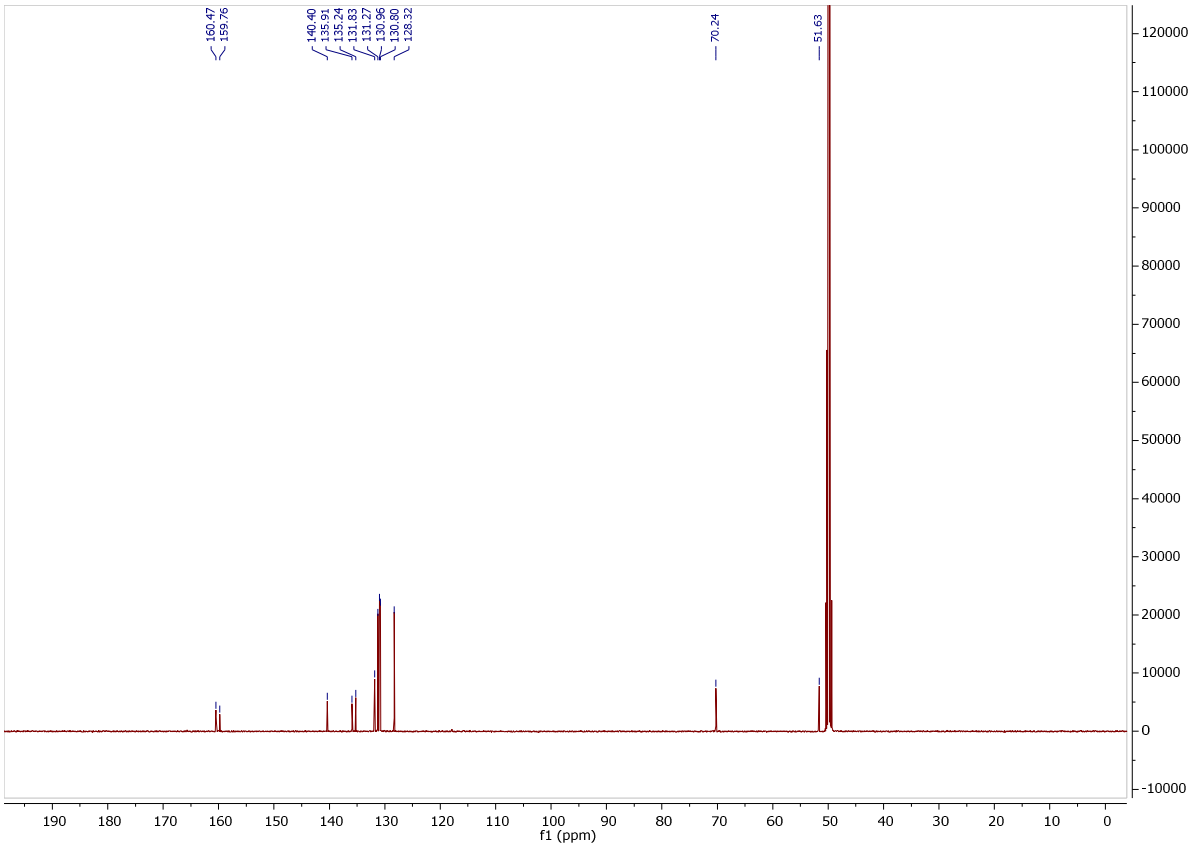
7.39
7.38
7.37
7.37
7.36
7.36
7.35
7.35
7.26
7.25
7.24
7.24
7.23
5.68
4.90
4.86
4.30
4.27
NH2 HCl
N
N
H
H2N
N
Ph
Cl
3.06
3.89
2.18
1.00
1.22
1.02
f1 (ppm)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159.76
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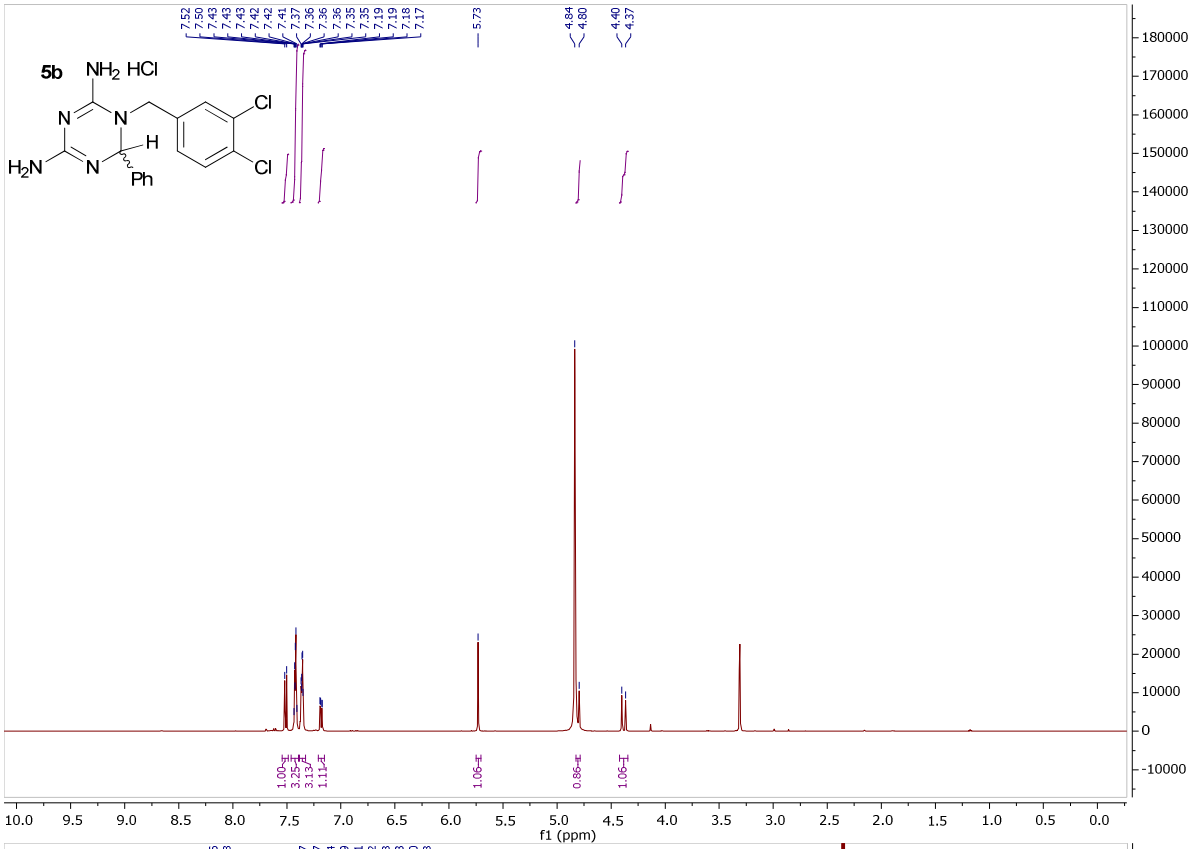
51.63
f1 (ppm)

5b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7.41
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7.36
7.36
7.36
7.35
7.35
7.19
7.19
7.18
7.17
5.73
4.84
4.80
4.40
4.37
5b
NH2 HCl
Cl
Cl
H
Ph
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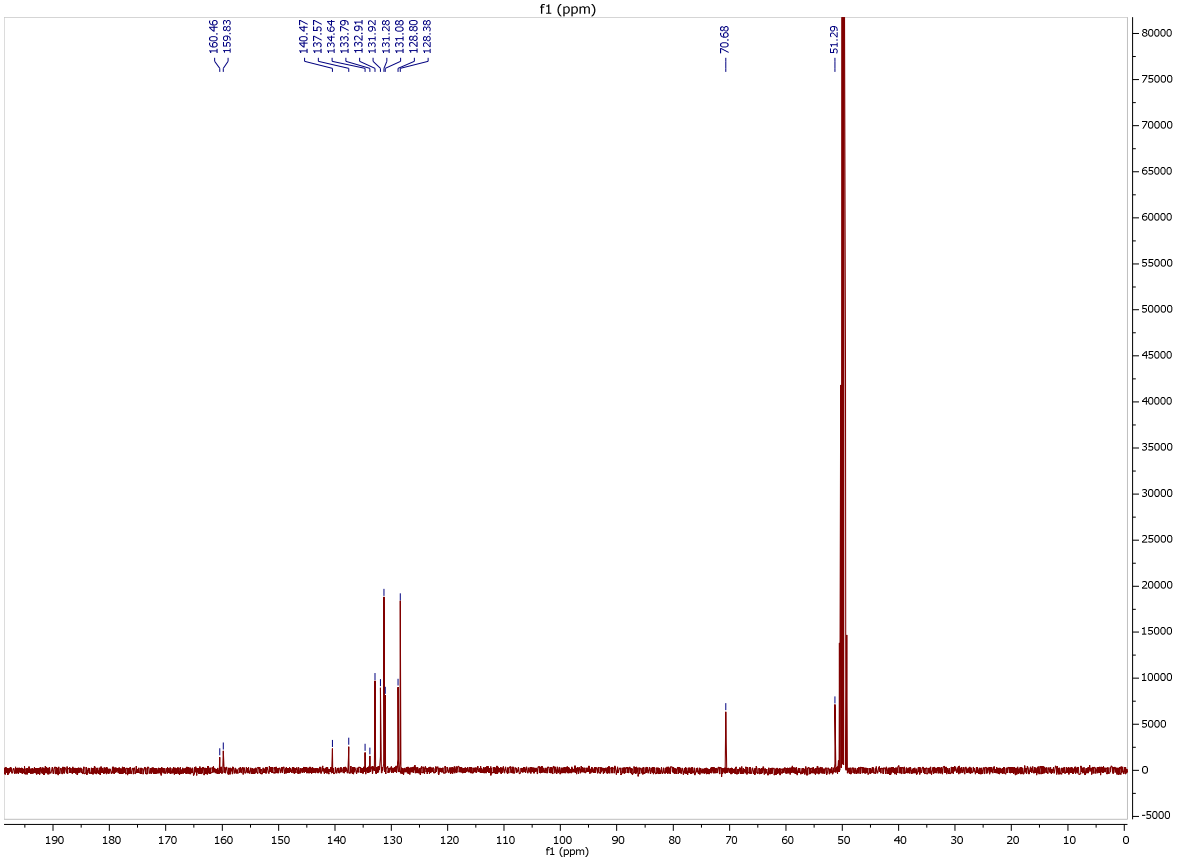
3.25
3.13
1.11
1.06
0.86
1.06
f1 (ppm)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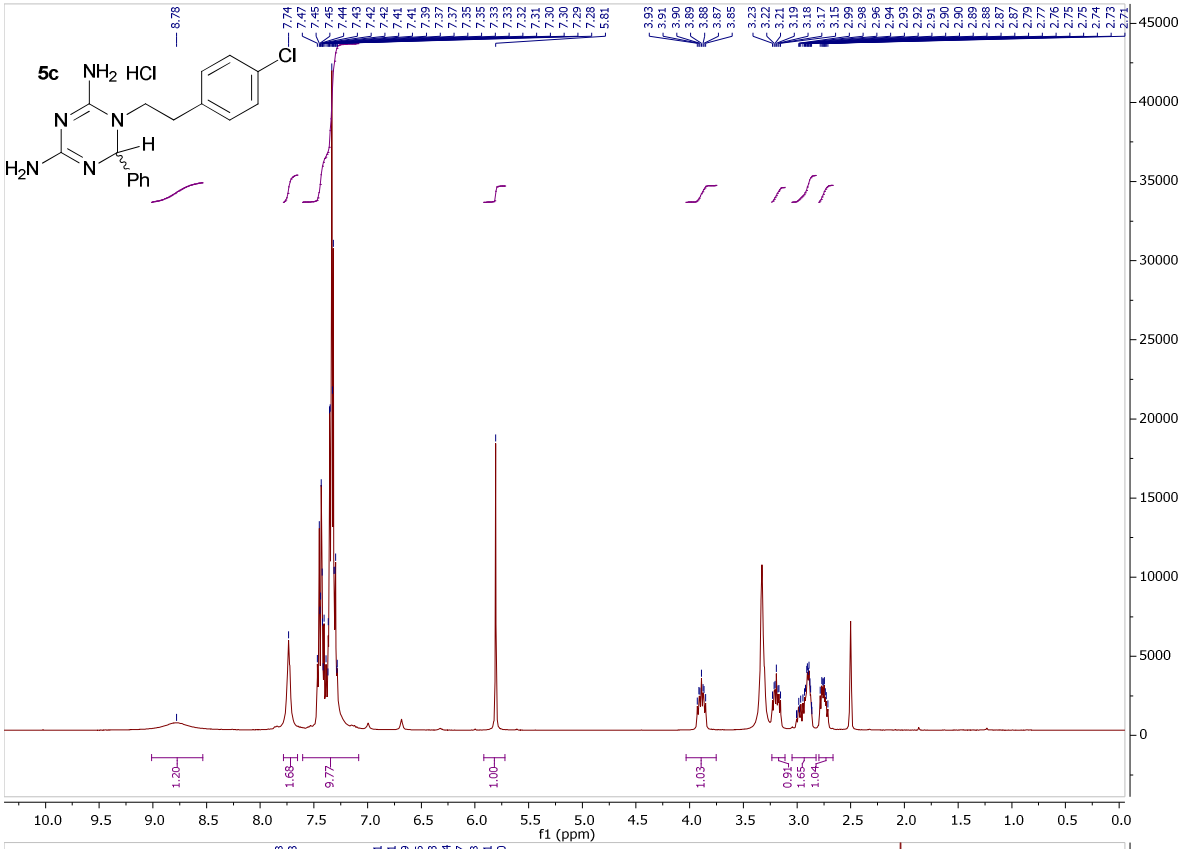
159.83
140.47
137.57
134.64
133.79
132.91
131.92
131.38
131.08
128.80
128.38
70.68
51.29
f1 (ppm)

5c


5c
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Cl
N
N
H
H2N
N
Ph
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7.42
7.42
7.41
7.41
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7.37
7.35
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7.32
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7.30
7.30
7.29
7.28
5.81
3.93
3.91
3.90
3.89
3.88
3.87
3.85
3.23
3.22
3.21
3.19
3.18
3.17
3.15
2.99
2.98
2.96
2.94
2.93
2.92
2.91
2.90
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2.77
2.76
2.75
2.75
2.74
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1.68
9.77
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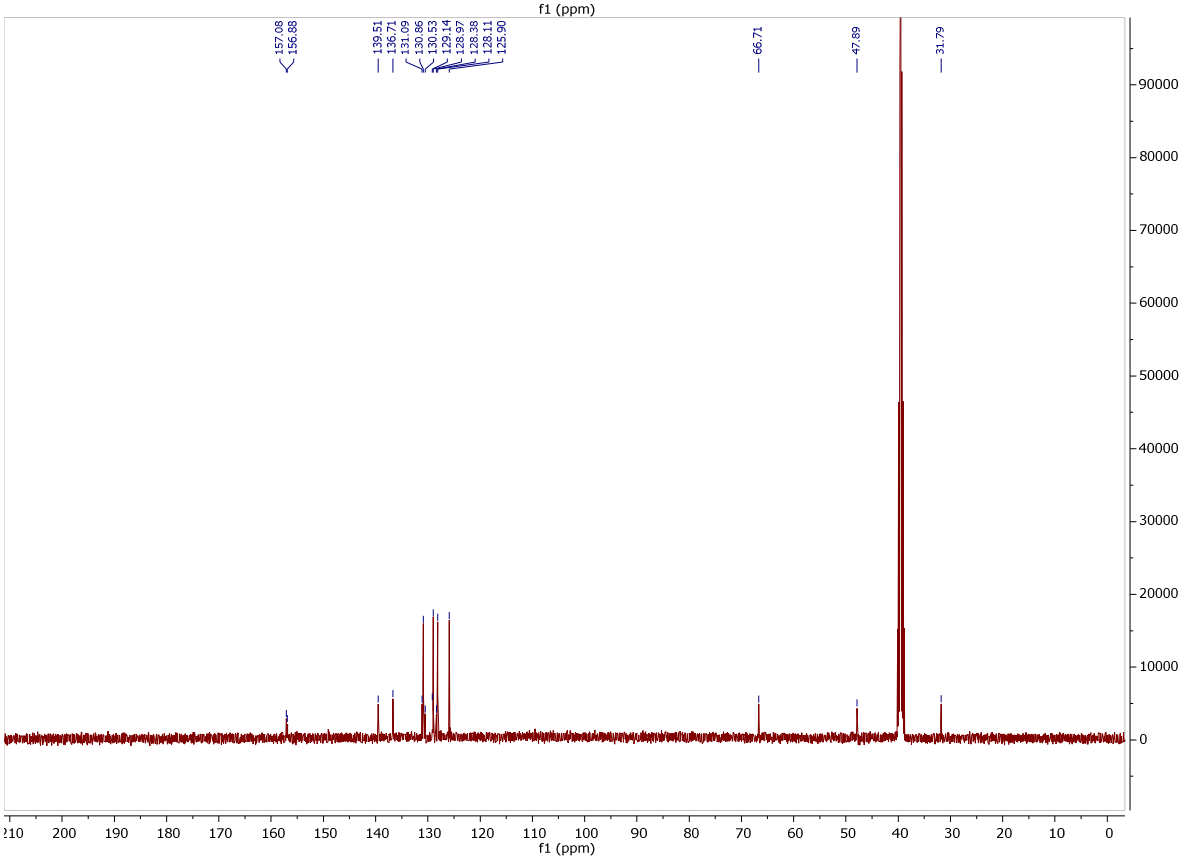
0.91
1.65
1.04
f1 (ppm)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156.88
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128.11
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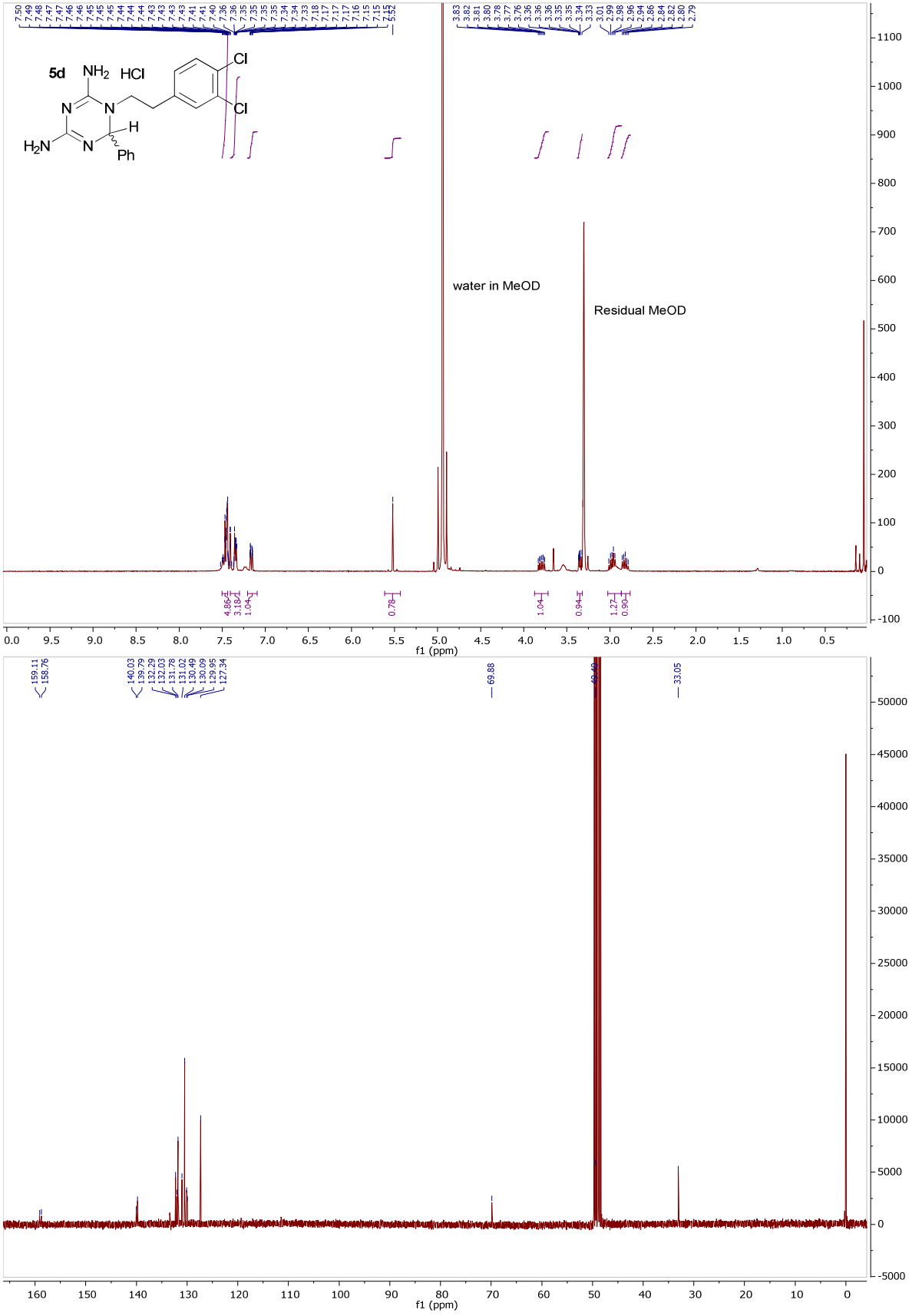
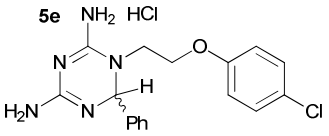
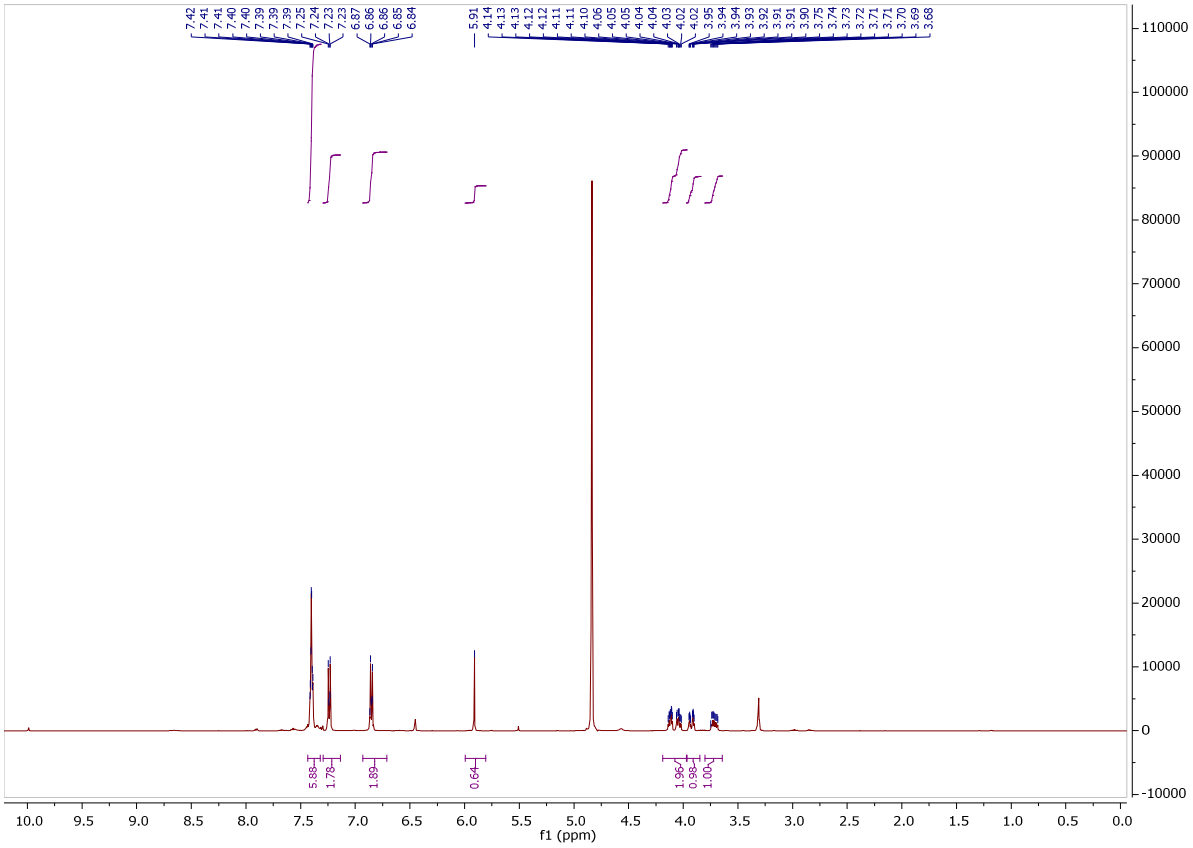
66.71
47.89
31.79
f1 (ppm)

5d


5d
NH2 HCl
Cl
Cl
N
N
H
H2N
N
Ph
water in MeOD
Residual MeOD
f1 (ppm)
f1 (ppm)

5e


NH2 HCl
N
N
O
H
H2N
N
Ph
Cl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5.91
4.14 4.13 4.13 4.12 4.12 4.11 4.11 4.10 4.06 4.05 4.05 4.04 4.04 4.03 4.02 4.02 3.95 3.94 3.94 3.93 3.92 3.91 3.91 3.90 3.75 3.74 3.73 3.72 3.71 3.71 3.70 3.69 3.68
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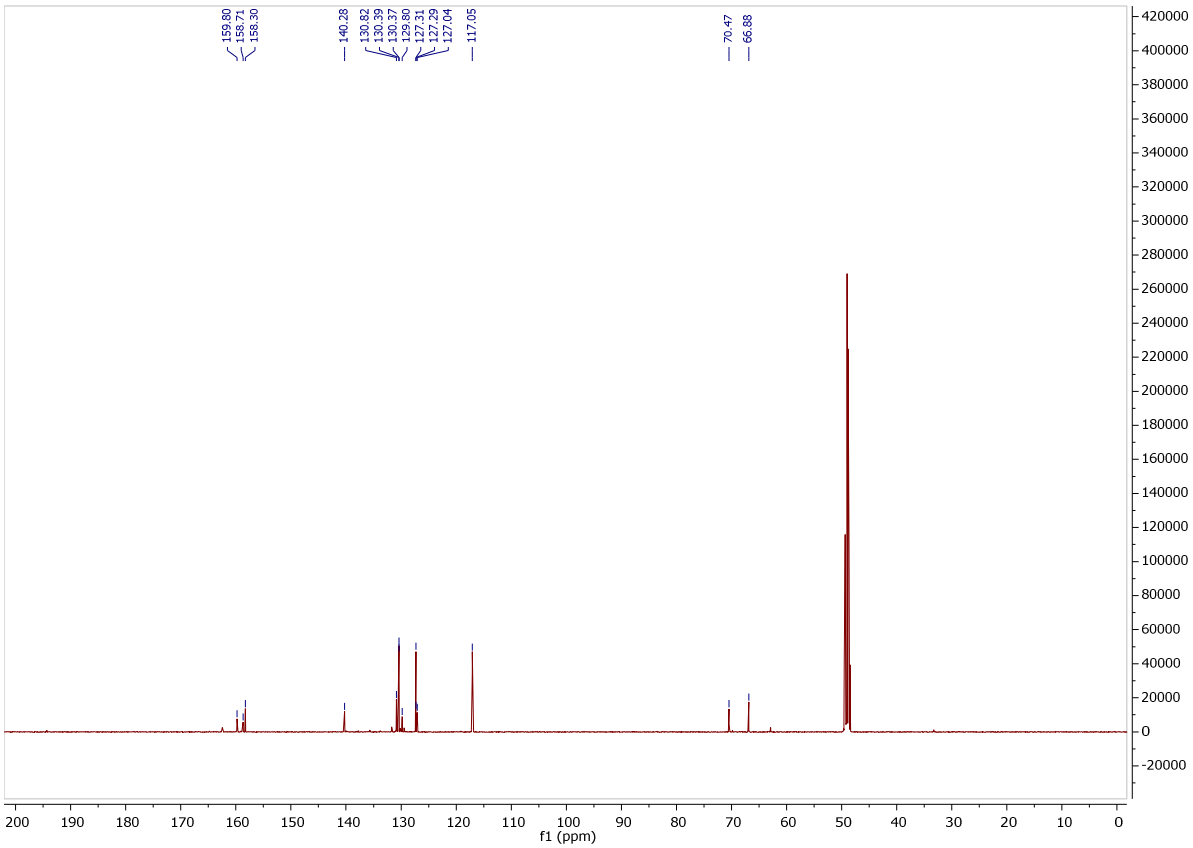
f1 (ppm)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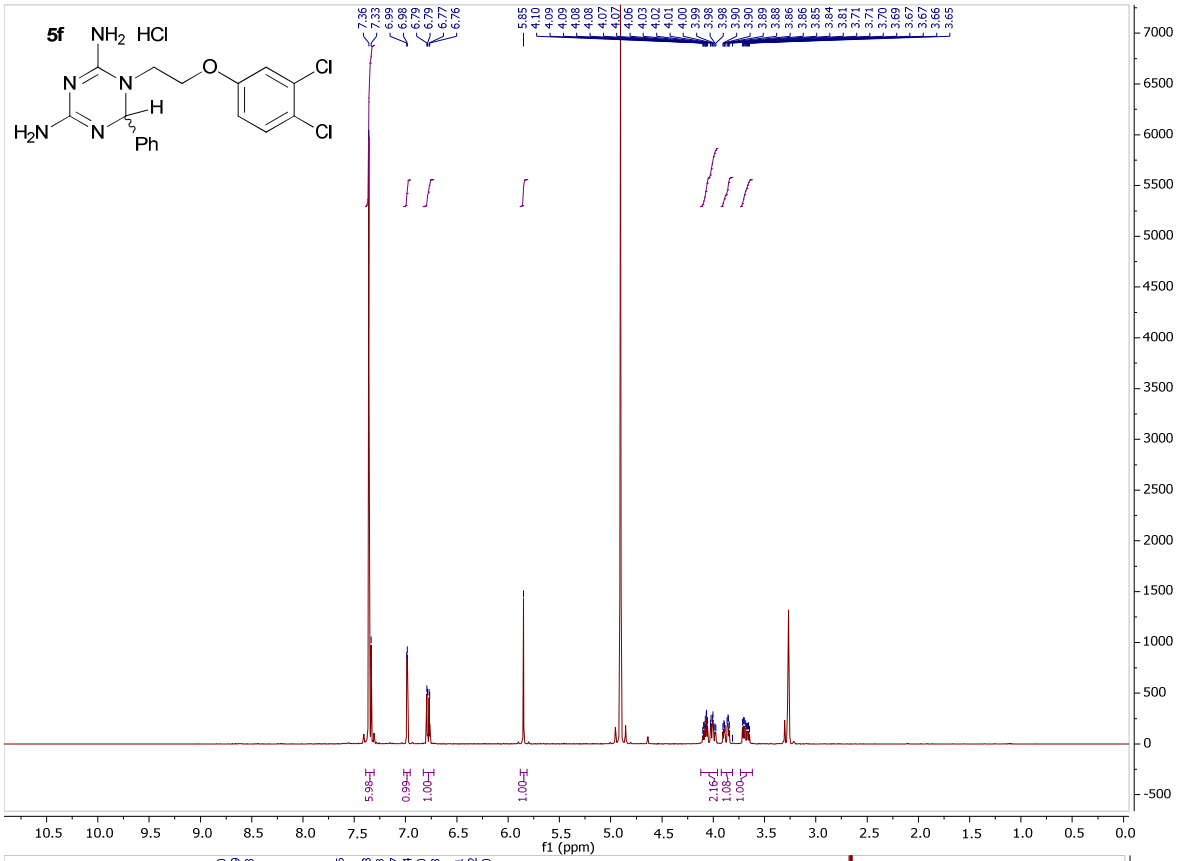
f1 (ppm)

5f


5f
NH2 HCl
N
N
O
Cl
Cl
H
H2N
N
Ph
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6.99
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6.79
6.77
6.76
5.85
4.10
4.09
4.09
4.08
4.08
4.07
4.07
4.06
4.03
4.02
4.01
4.00
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3.85
3.84
3.81
3.71
3.71
3.70
3.69
3.67
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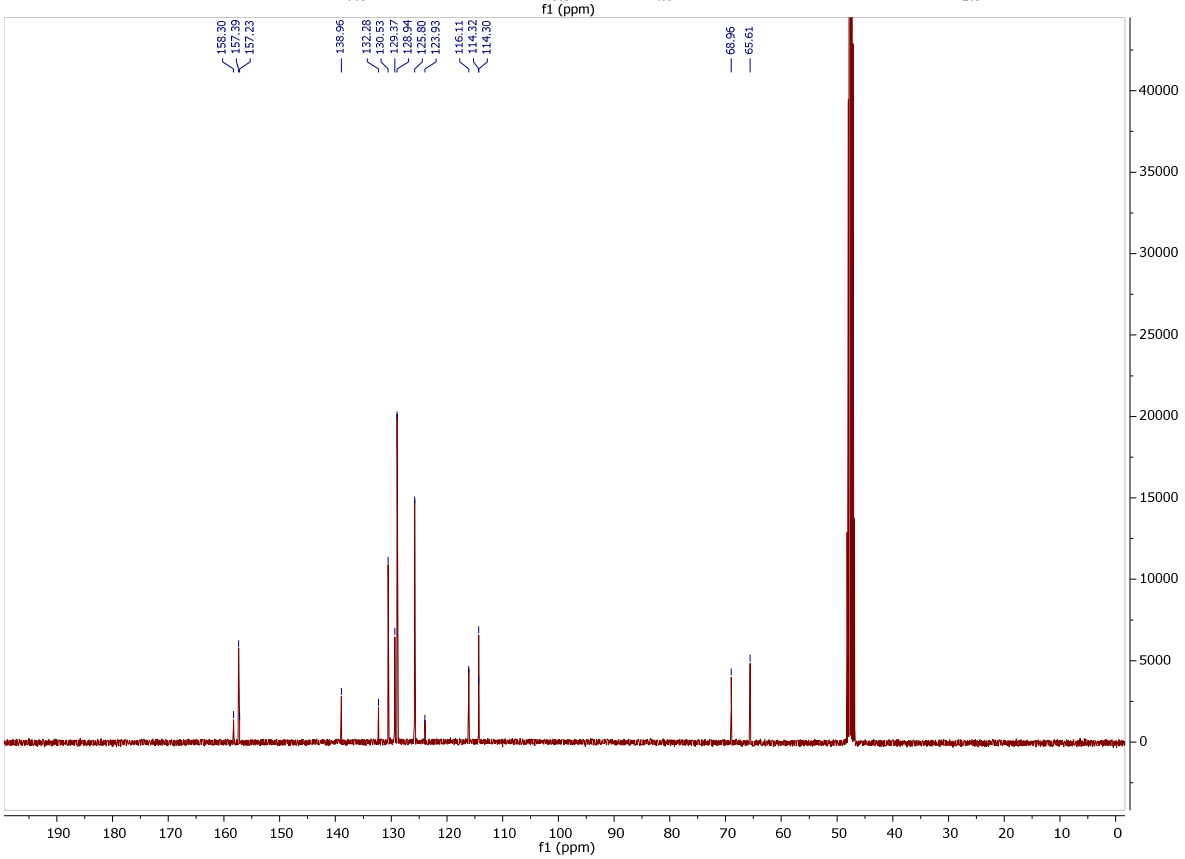
1.00
f1 (ppm)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157.23
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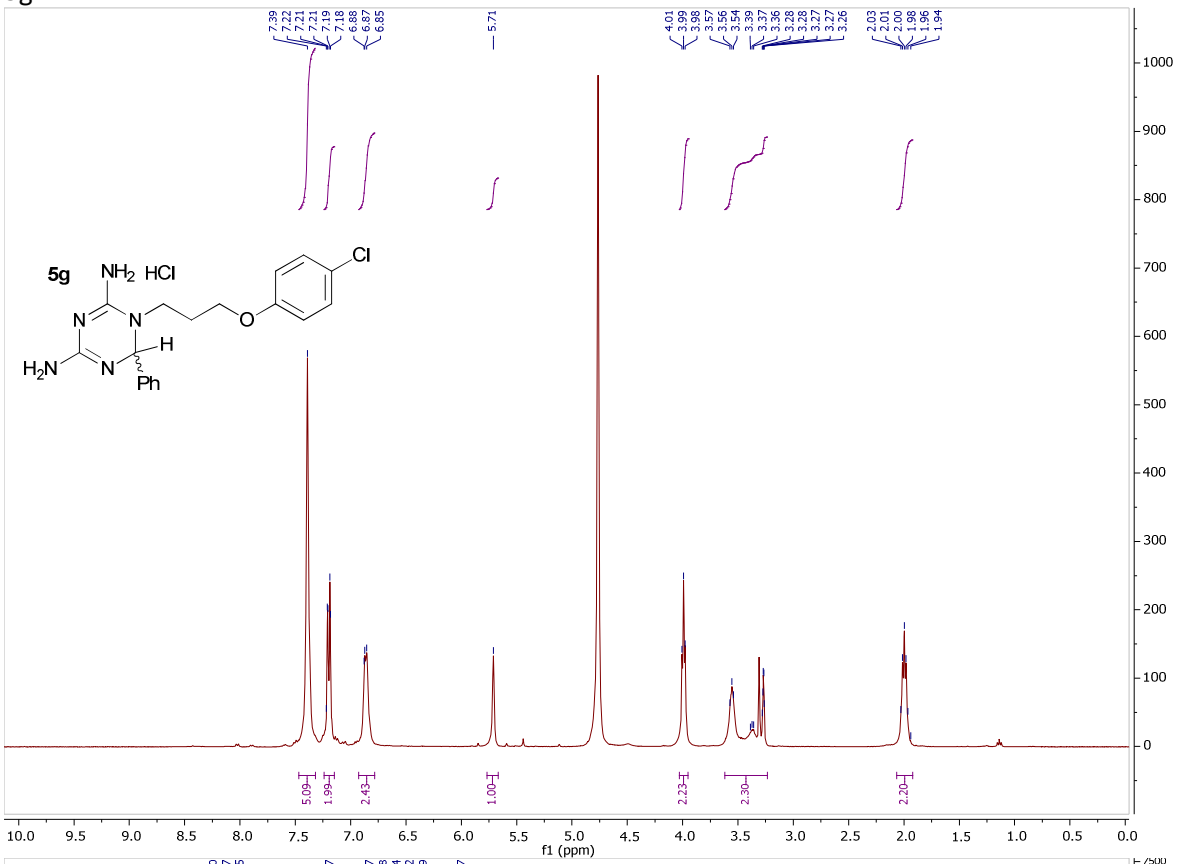
114.30
68.96
65.61
f1 (ppm)

5g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6.85
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4.01
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3.98
3.57
3.56
3.54
3.39
3.37
3.36
3.28
3.28
3.27
3.27
3.26
2.03
2.01
2.00
1.98
1.96
1.94
5g
NH2 HCl
Cl
N
N
O
H
H2N
N
Ph
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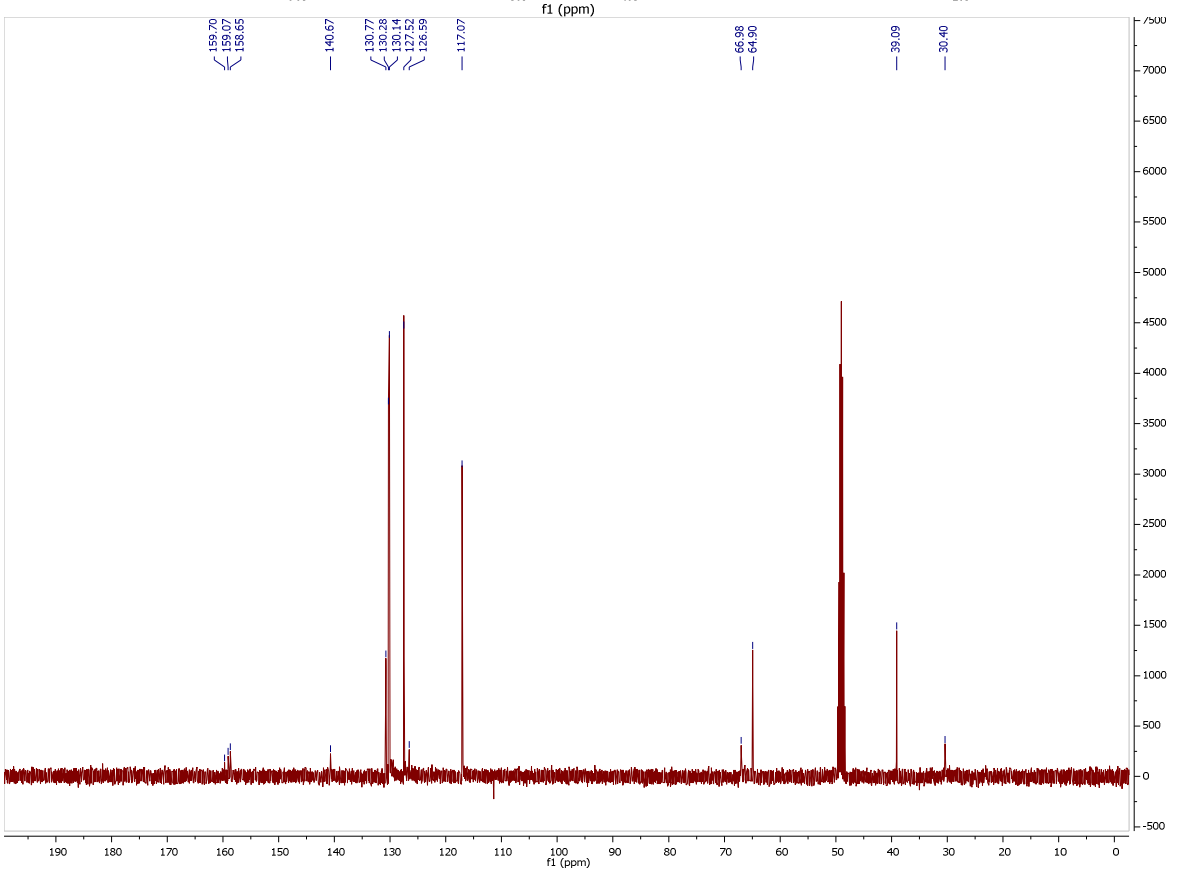
2.43
1.00
2.23
2.30
2.20
f1 (ppm)


159.70
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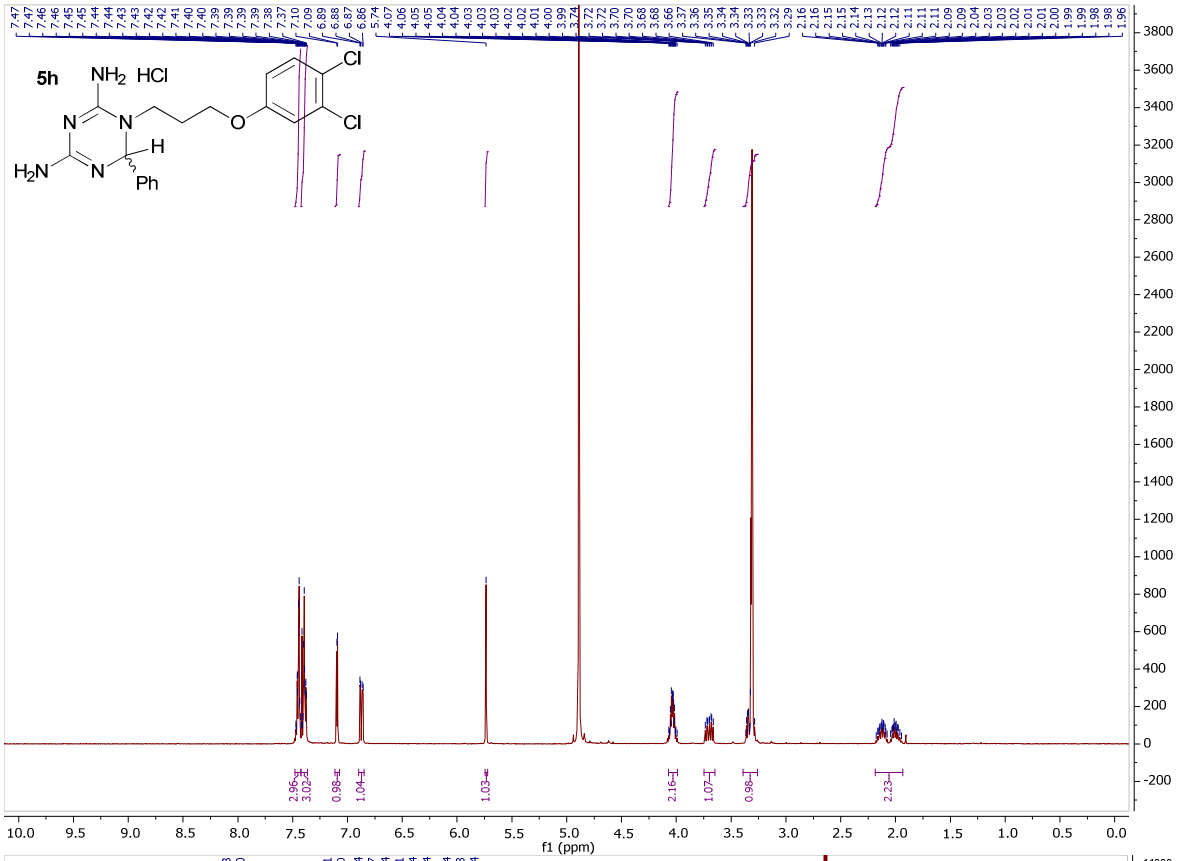
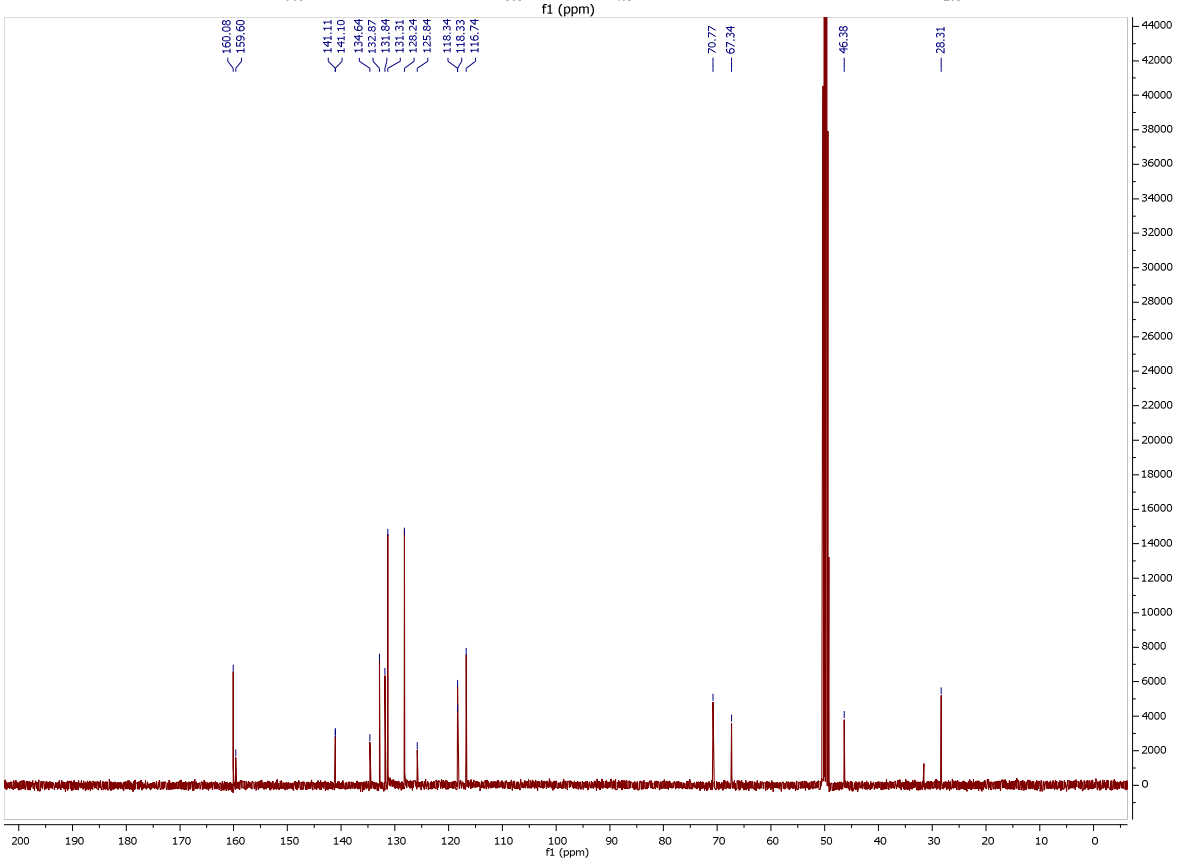
66.98
64.90
39.09
30.40
f1 (ppm)

5h


5h
NH2 HCl
Cl
Cl
N
N
O
H
H2N
N
Ph
f1 (ppm)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159.60
141.11
141.10
134.64
132.87
132.84
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128.24
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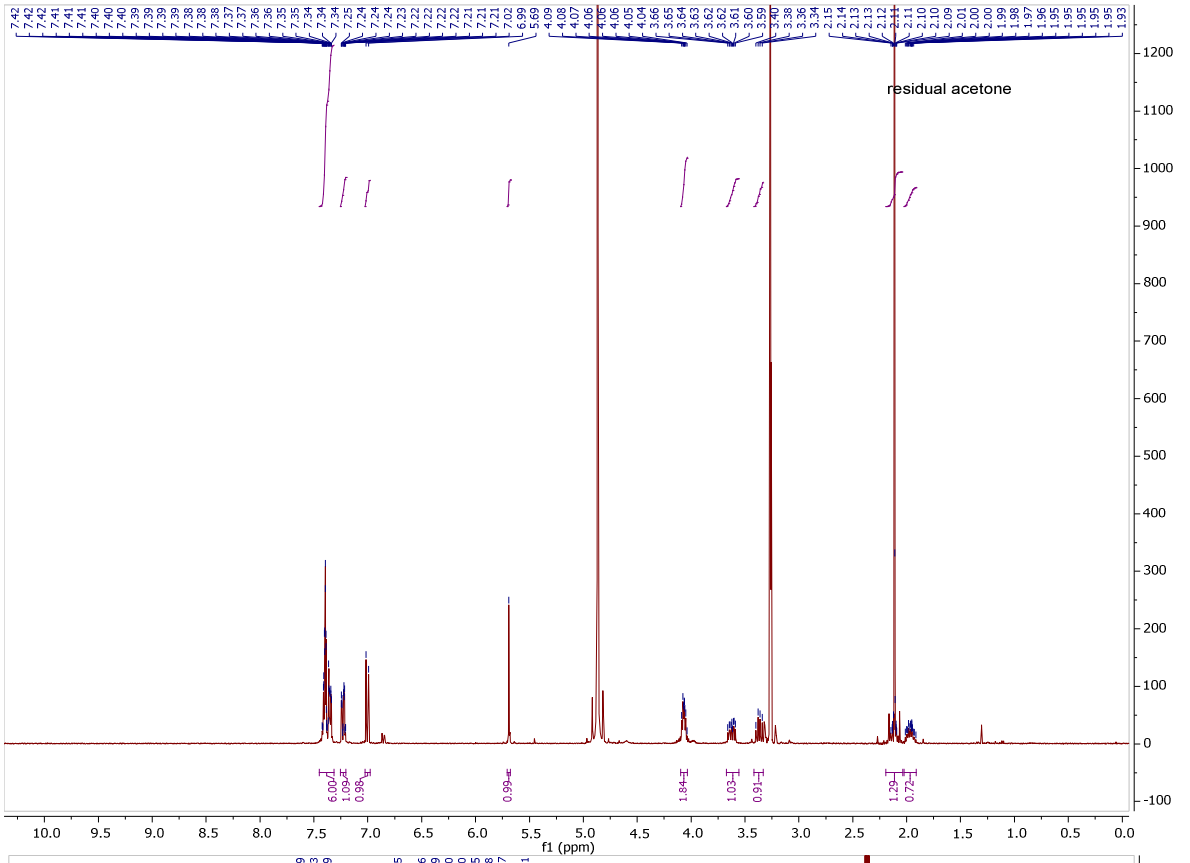
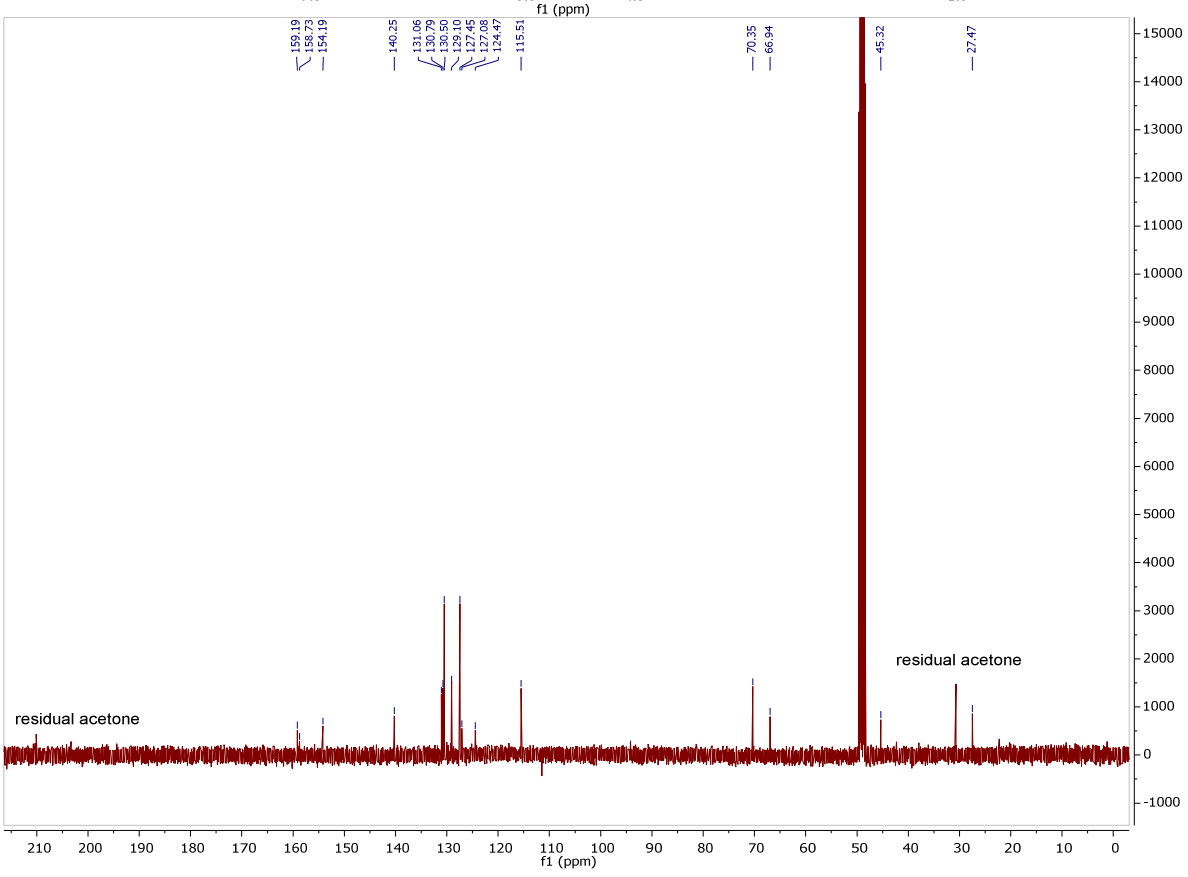
118.34
118.33
116.74
70.77
67.34
46.38
28.31
f1 (ppm)

10a


residual acetone
f1 (ppm)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158.73
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140.25
131.06
130.79
130.50
129.10
127.45
127.08
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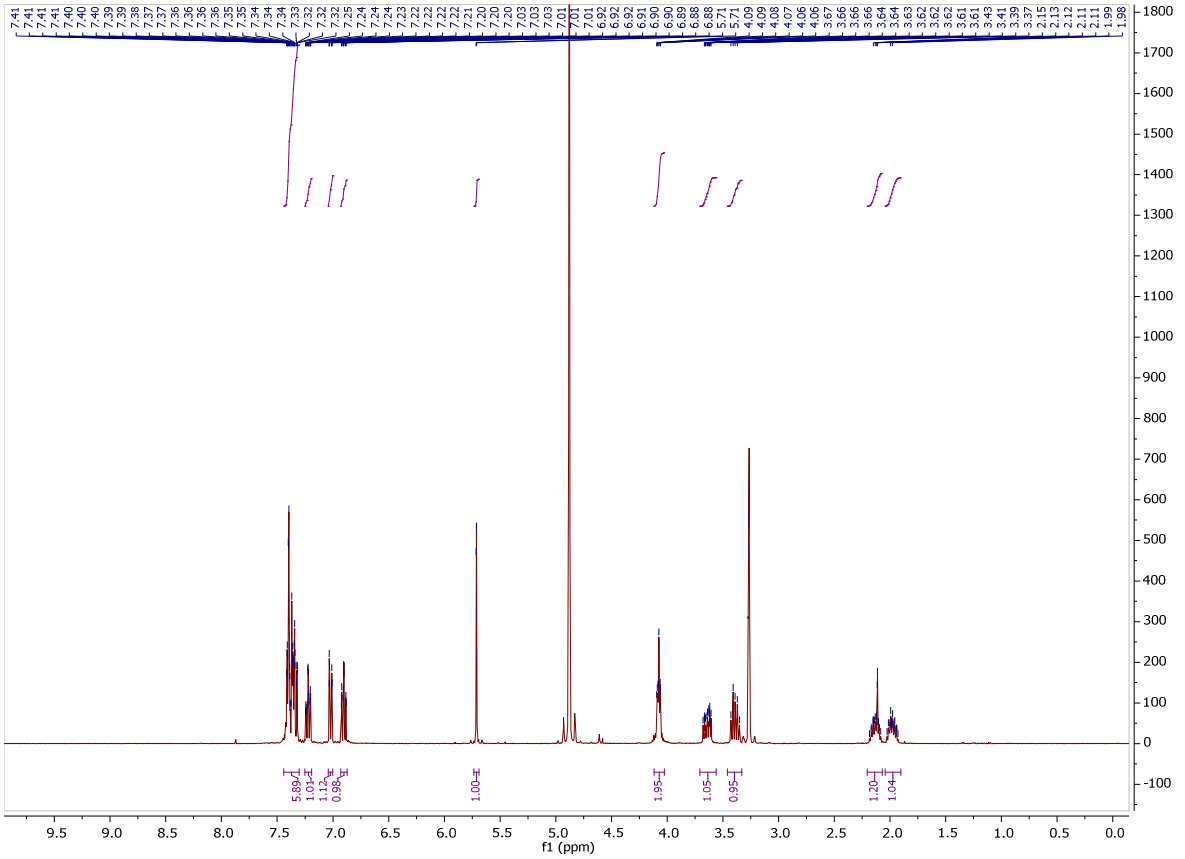
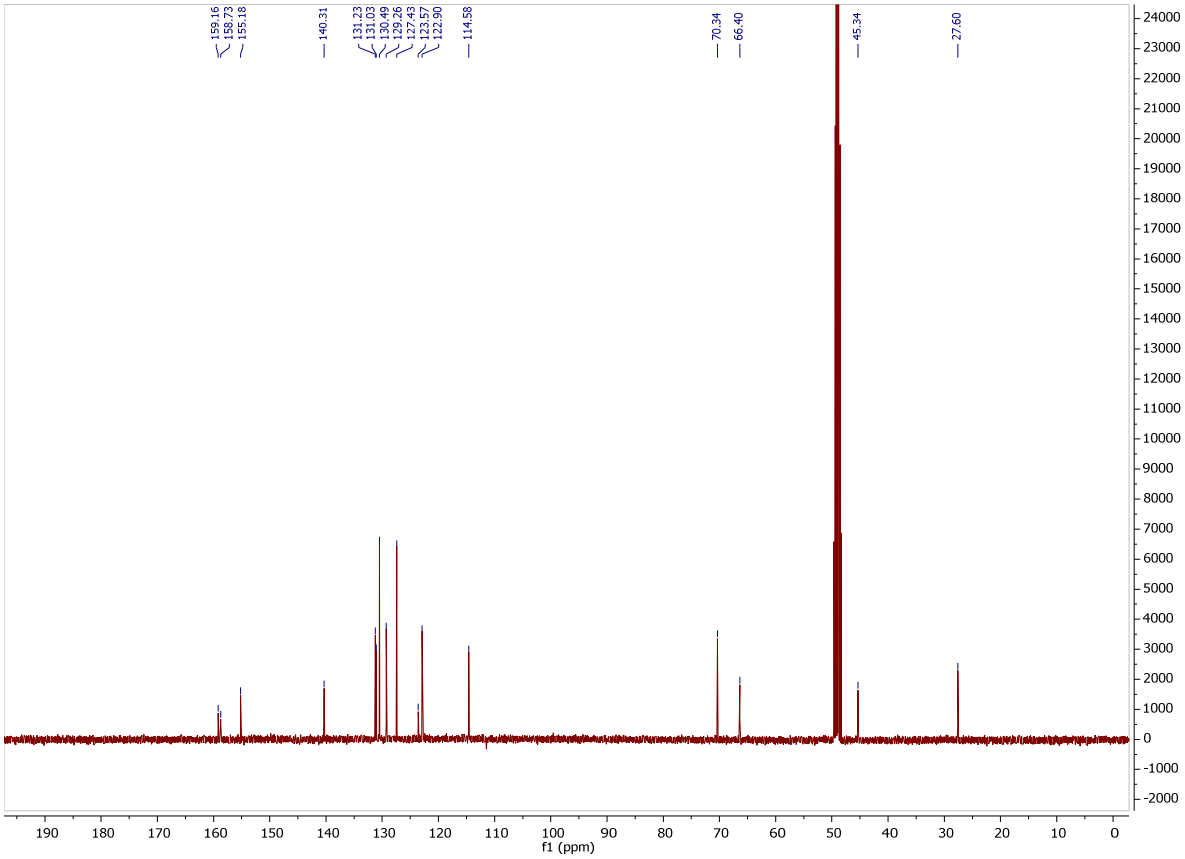
115.51
70.35
66.94
45.32
27.47
residual acetone
residual acetone
f1 (ppm)

10c


f1 (ppm)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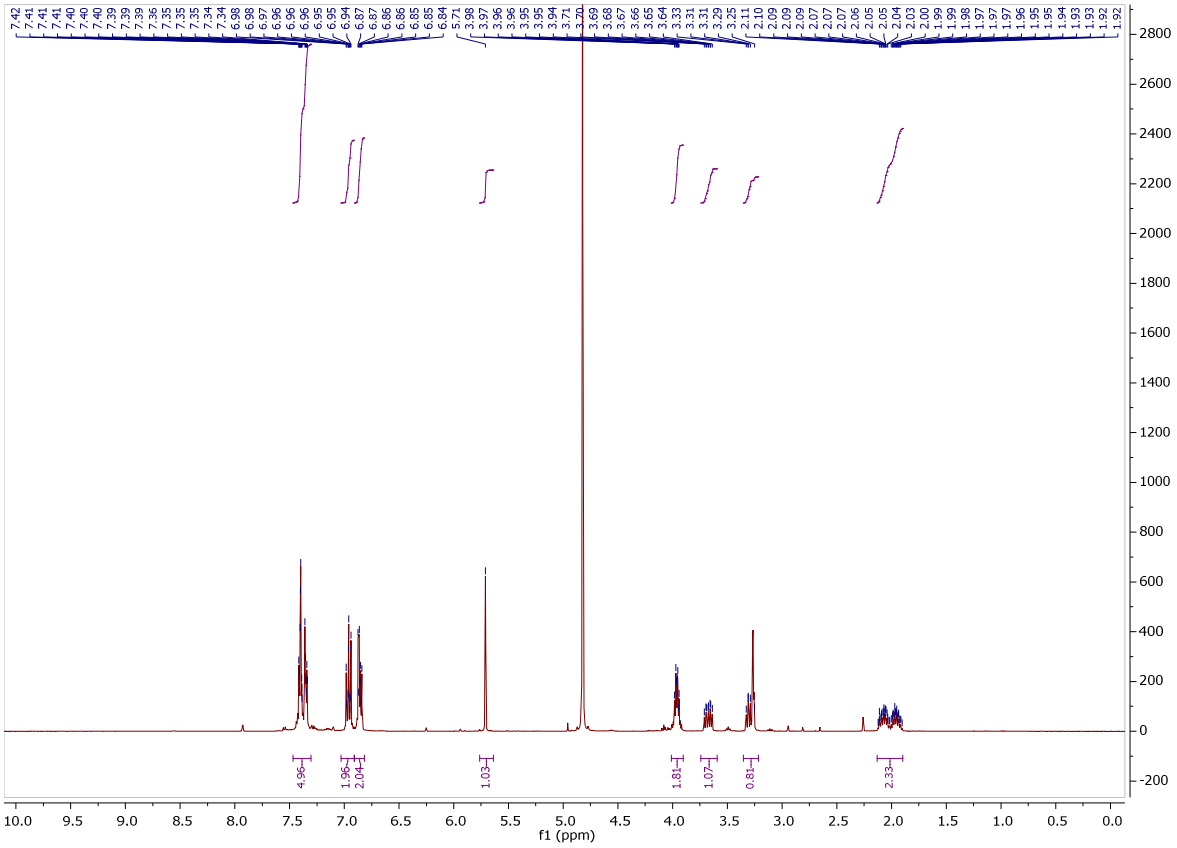
66.40
45.34
27.60
f1 (ppm)

10d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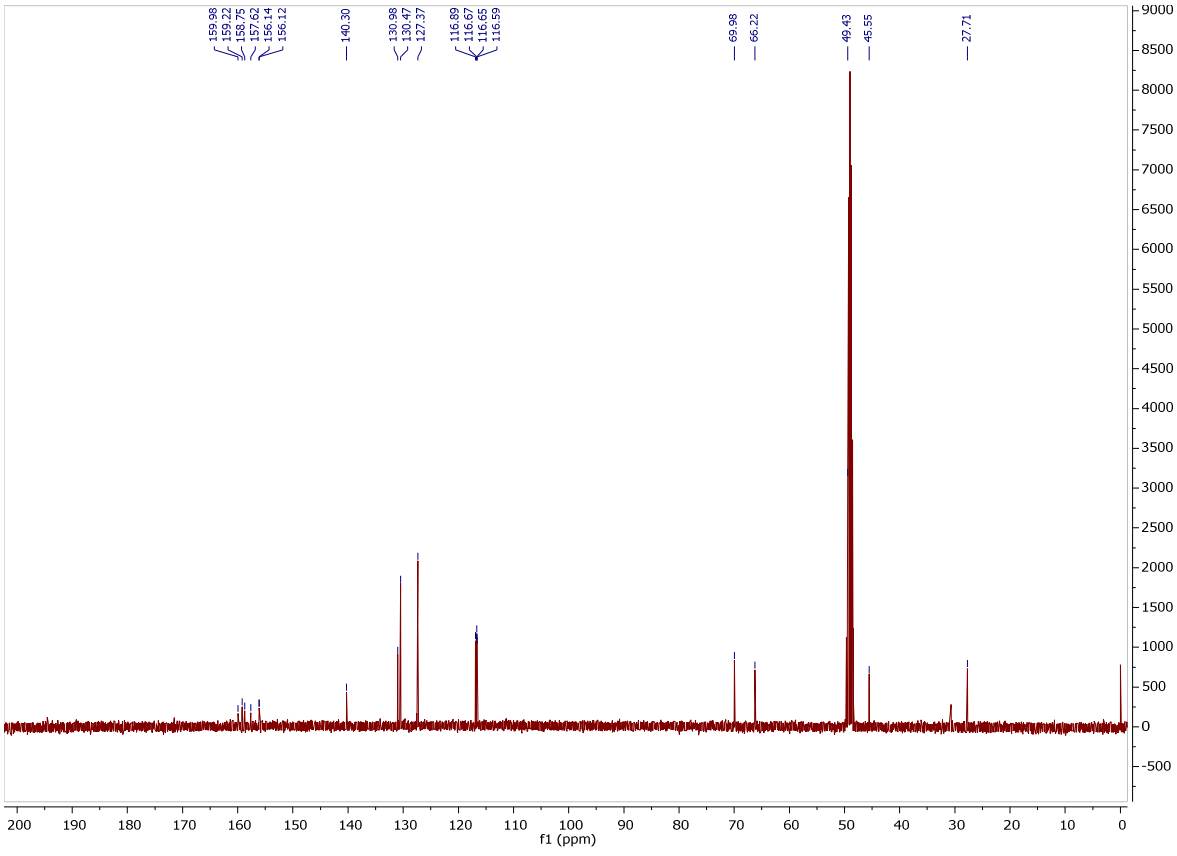
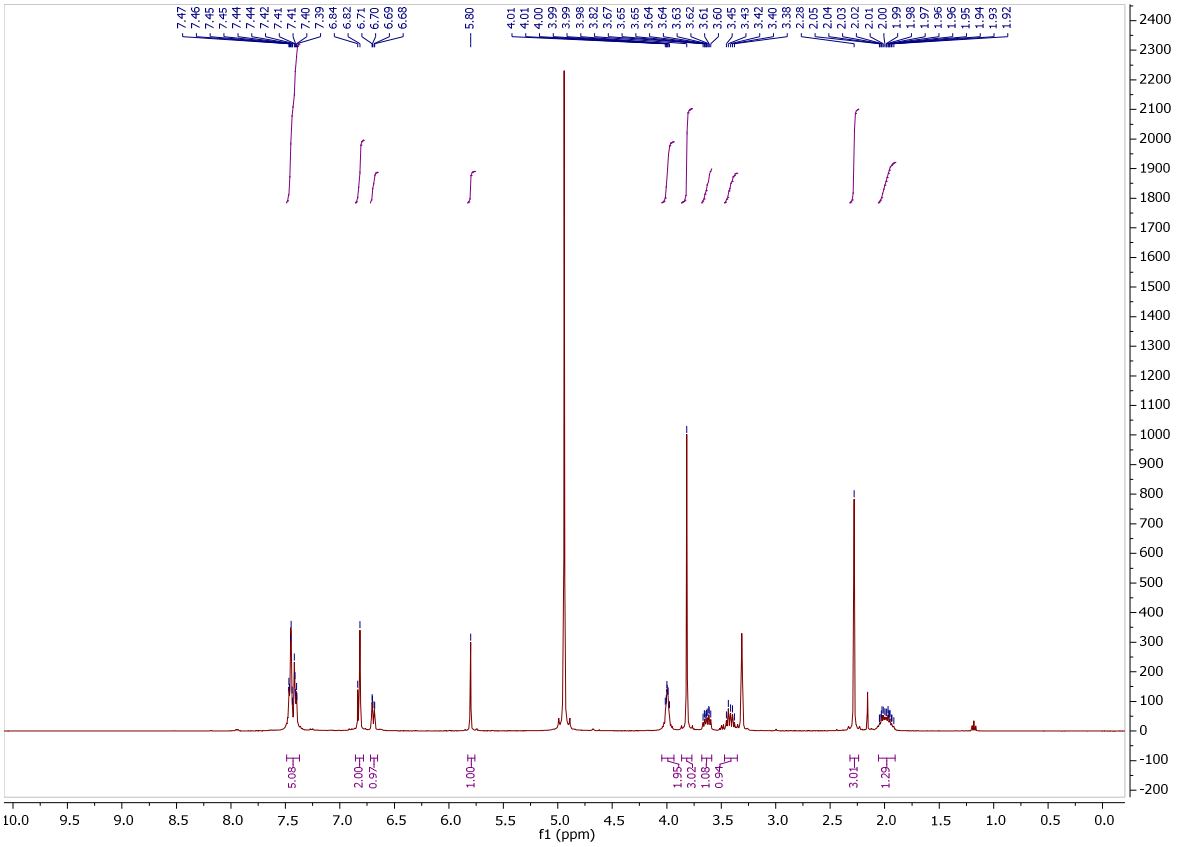
4.96 1.96 2.04 1.03 1.81 1.07 0.81 2.33
f1 (ppm)


159.98 159.22 158.75 157.62 156.14 156.12 140.30 130.98 130.47 127.37 116.89 116.67 116.65 116.59 69.98 66.22 49.43 45.55 27.71
f1 (ppm)

10e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5.80
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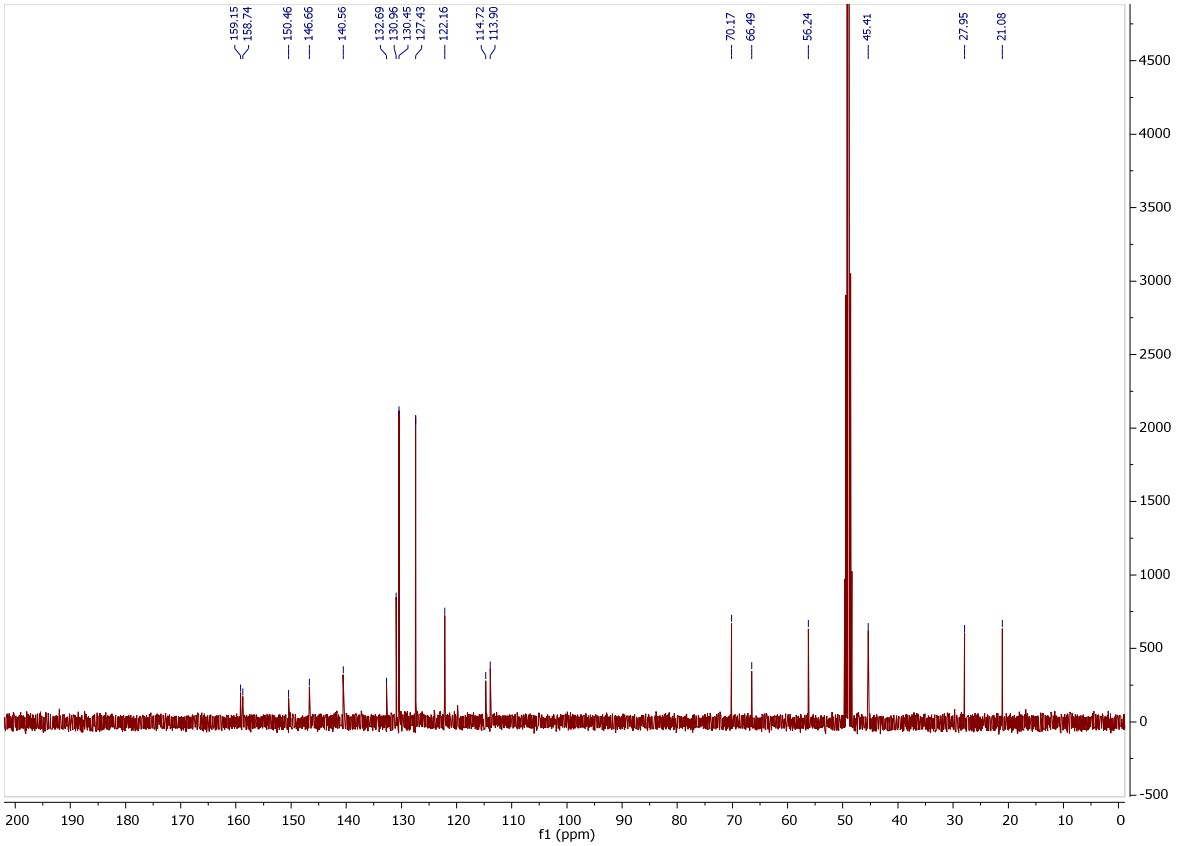
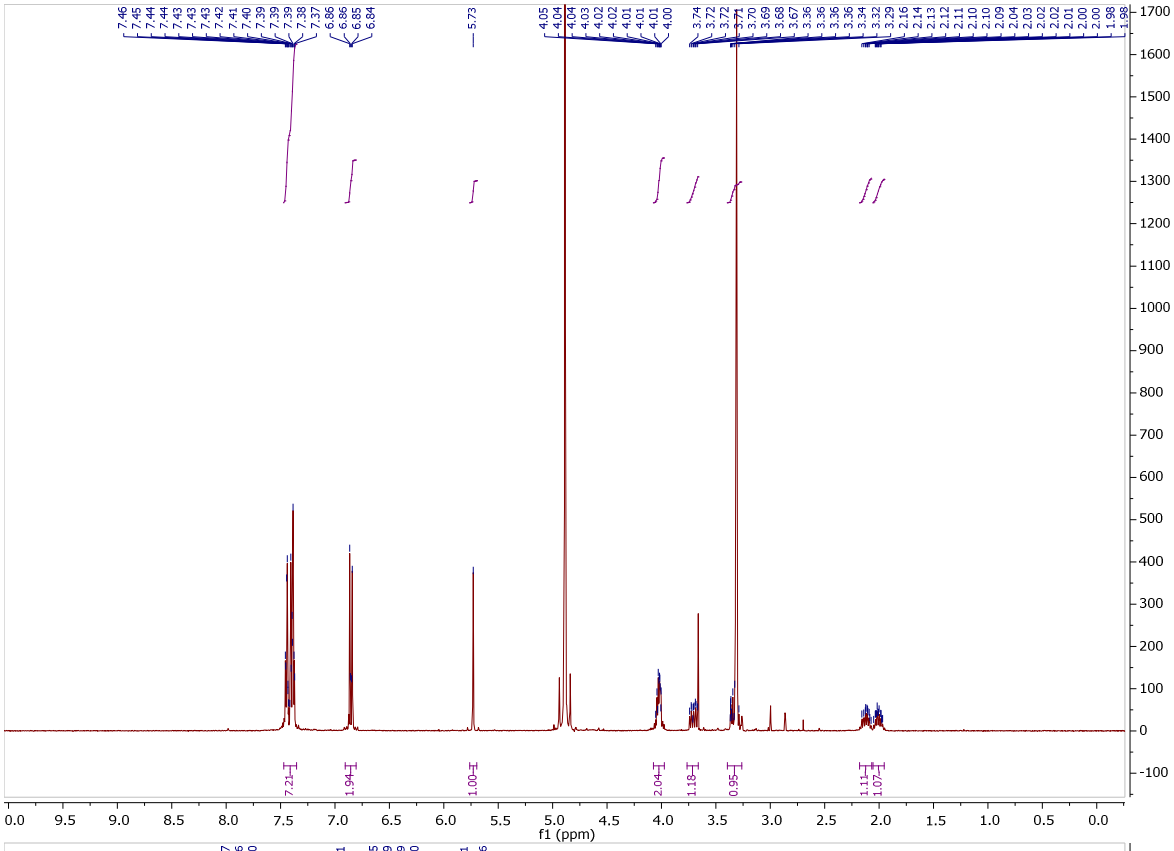
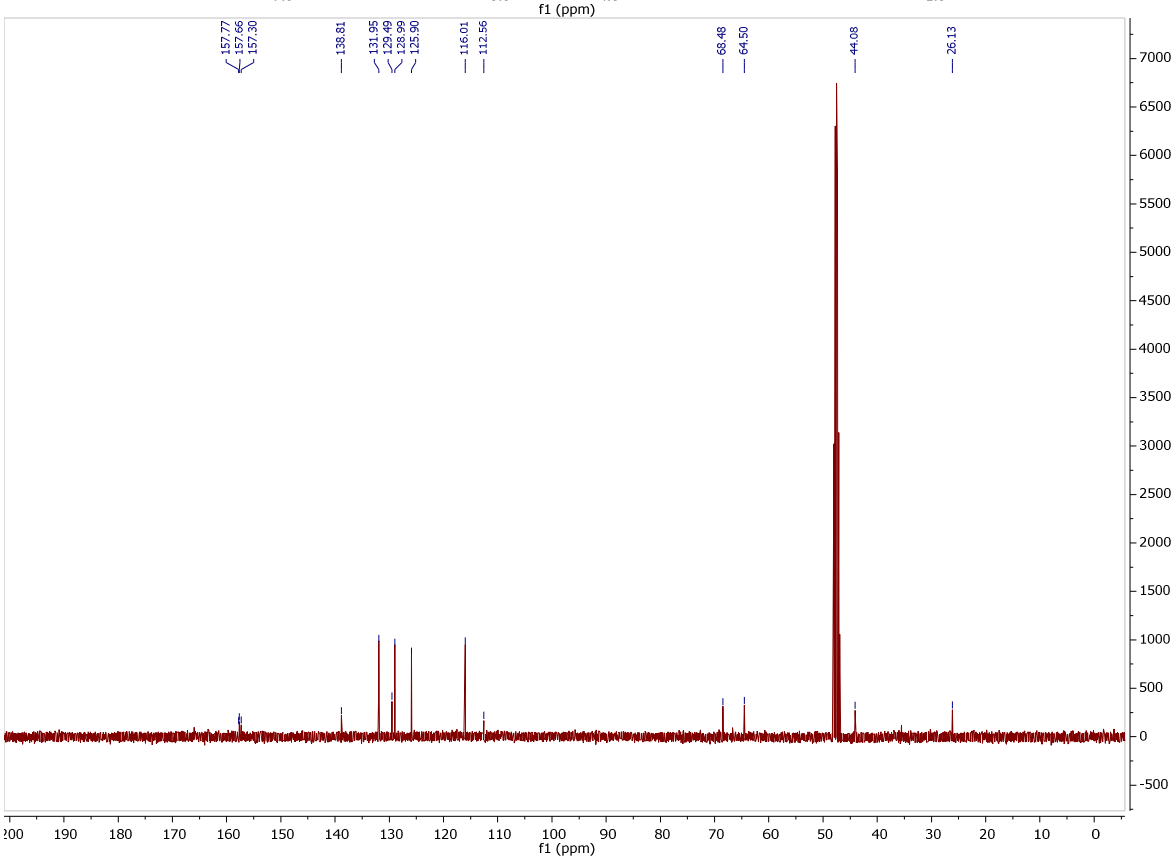
5.08 2.00 0.97 1.00 1.95 3.02 1.08 0.94 3.01 1.29
f1 (ppm)


159.15 158.74 150.46 146.66 140.56 132.69 130.96 130.45 127.43 122.16 114.72 113.90 70.17 66.49 56.24 45.41 27.95 21.08
f1 (ppm)

10f


7.46 7.45 7.44 7.44 7.43 7.43 7.43 7.42 7.41 7.40 7.39 7.39 7.38 7.37 6.86 6.85 6.84
5.73
4.05 4.04 4.04 4.03 4.02 4.02 4.01 4.01 4.01 4.00
3.74 3.72 3.72 3.71 3.70 3.69 3.68 3.67 3.36 3.36 3.36 3.34 3.32 3.29 2.16 2.14 2.13 2.12 2.11 2.10 2.10 2.09 2.04 2.03 2.02 2.02 2.01 2.00 2.00 1.98 1.98
7.21 1.94 1.00 2.04 1.18 0.95 1.11 1.07
f1 (ppm)


157.77 157.66 157.30
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131.95 129.49 128.99 125.90
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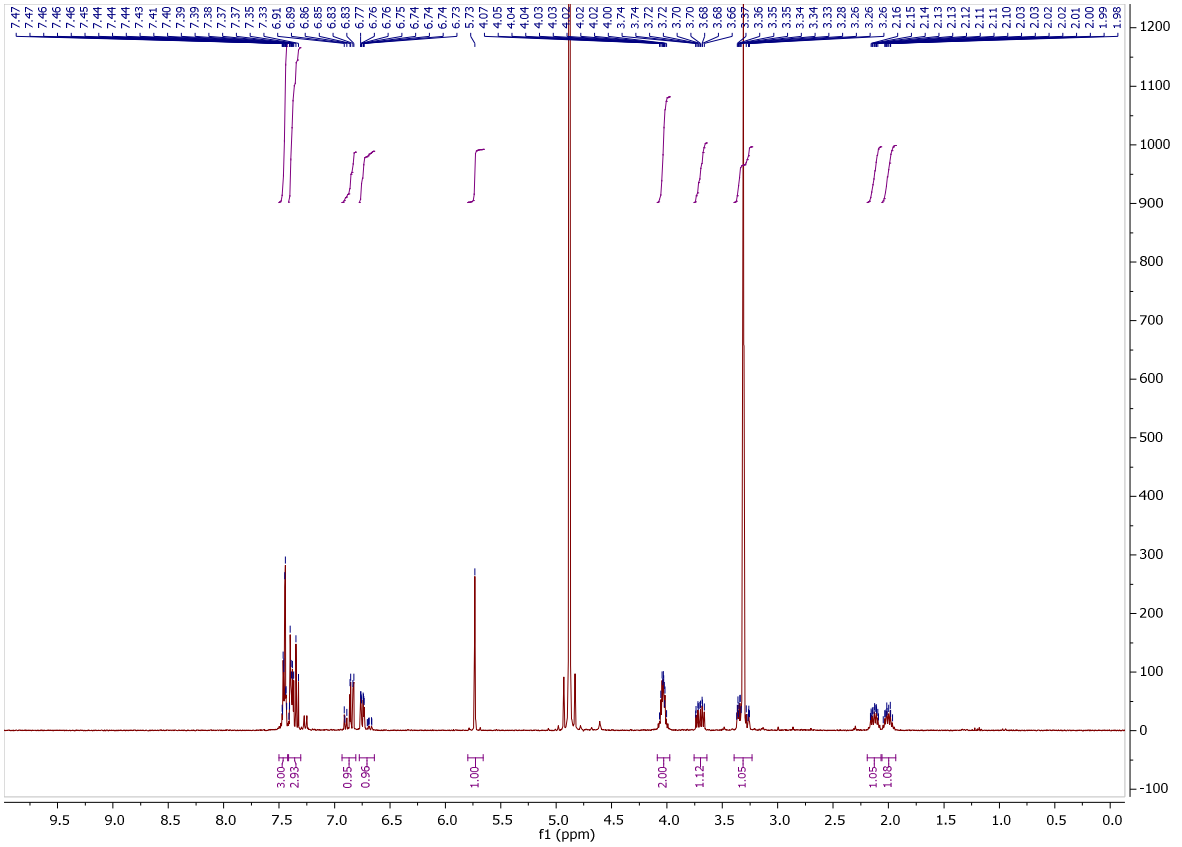
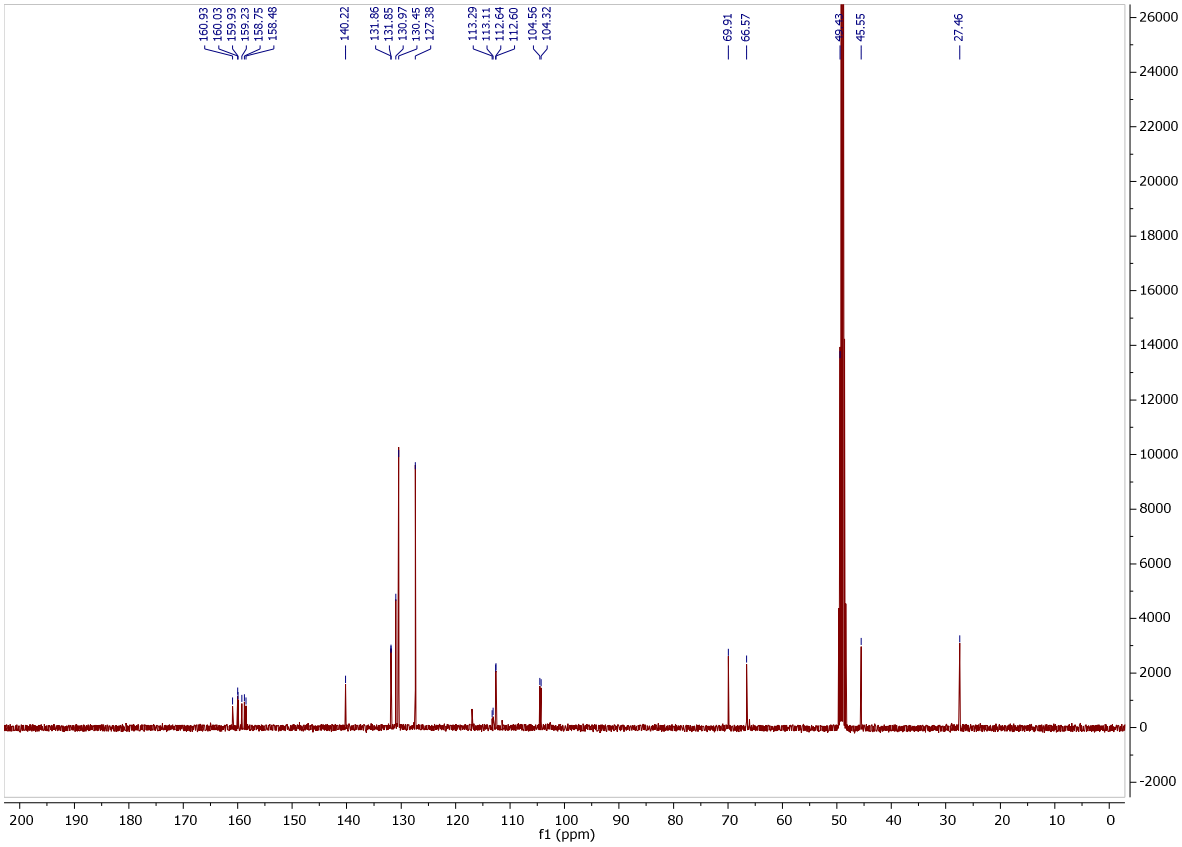
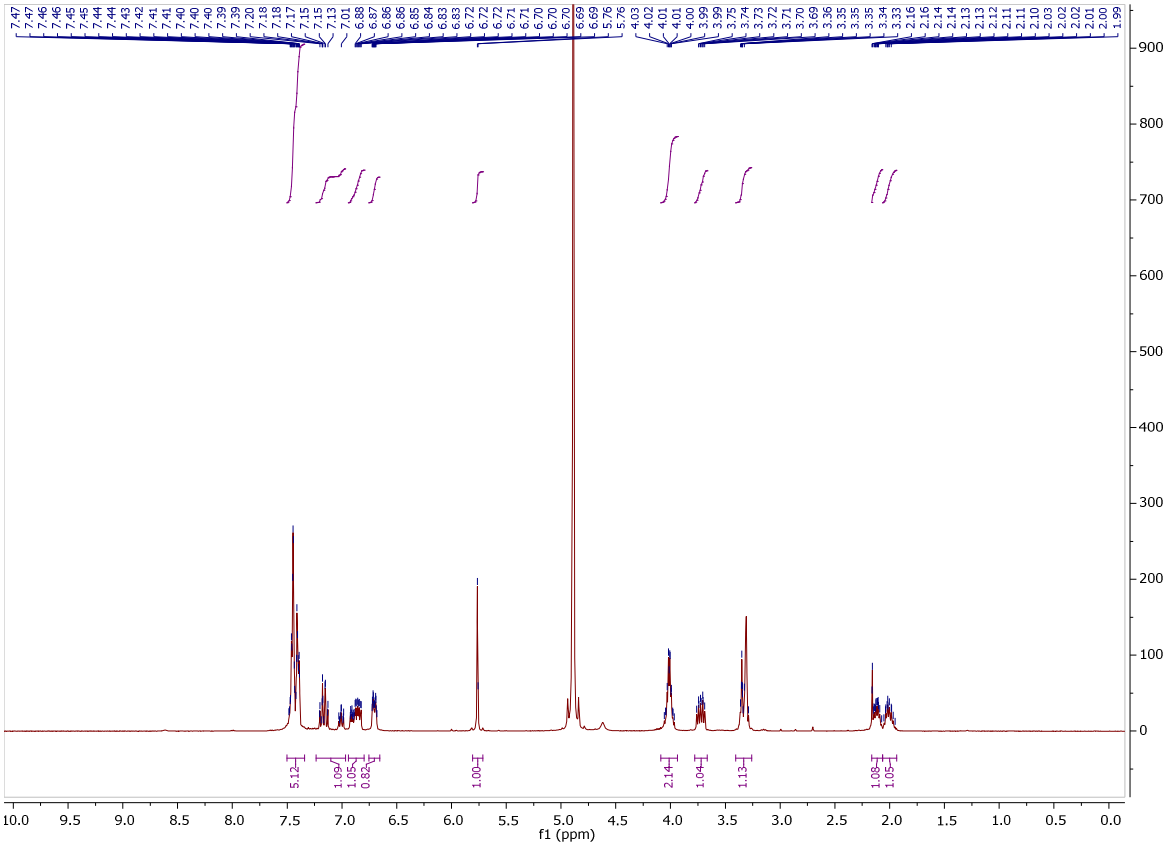
112.56
68.48
64.50
44.08
26.13
f1 (ppm)

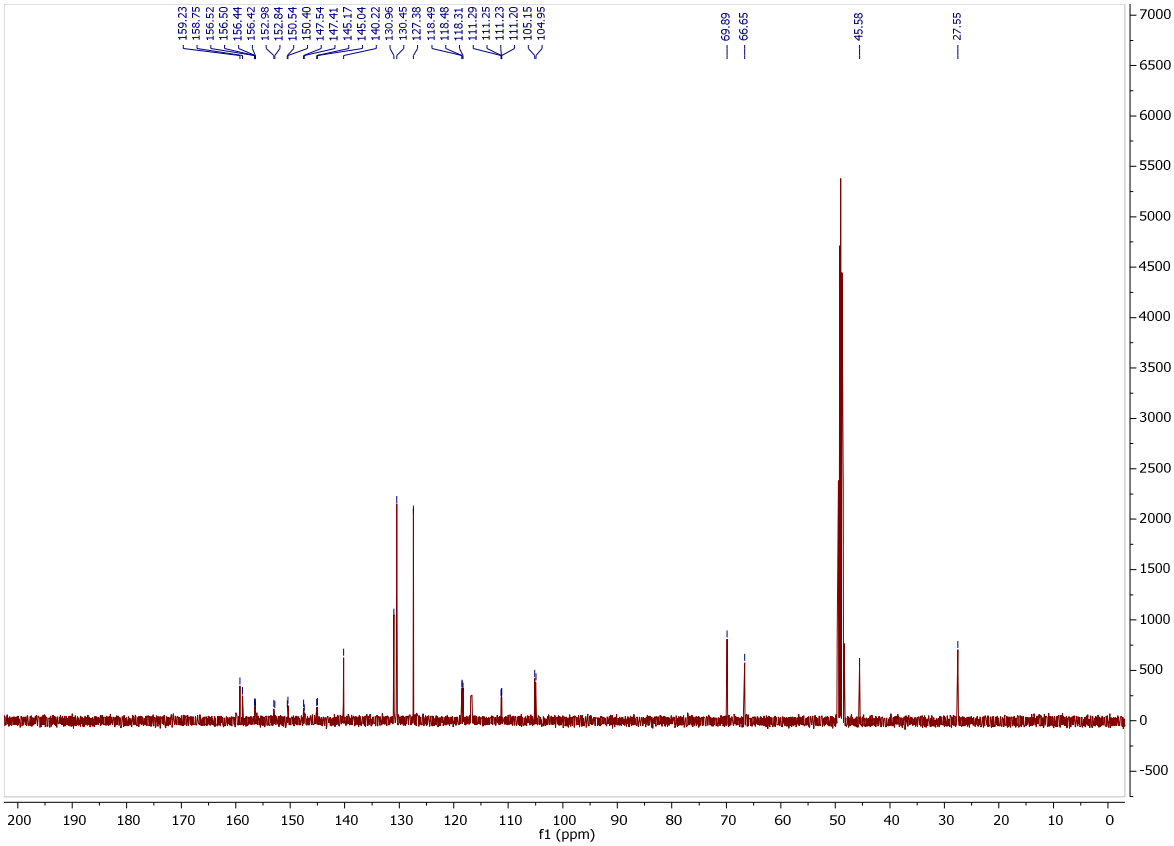
10g


7.47 7.47 7.46 7.46 7.46 7.45 7.44 7.44 7.44 7.43 7.41 7.40 7.39 7.39 7.38 7.37 7.37 7.35 7.33 6.91 6.89 6.86 6.85 6.83 6.83 6.77 6.76 6.76 6.75 6.74 6.74 6.74 6.73 5.73 4.07 4.05 4.04 4.04 4.03 4.03 4.02 4.02 4.02 4.00 3.74 3.72 3.72 3.70 3.70 3.68 3.68 3.66 3.37 3.36 3.35 3.35 3.34 3.34 3.33 3.28 3.26 3.26 3.26 2.16 2.15 2.14 2.13 2.13 2.12 2.11 2.11 2.10 2.03 2.03 2.02 2.02 2.01 2.00 1.99 1.98
3.00 2.93 0.95 0.96 1.00 2.00 1.12 1.05 1.05 1.08
f1 (ppm)

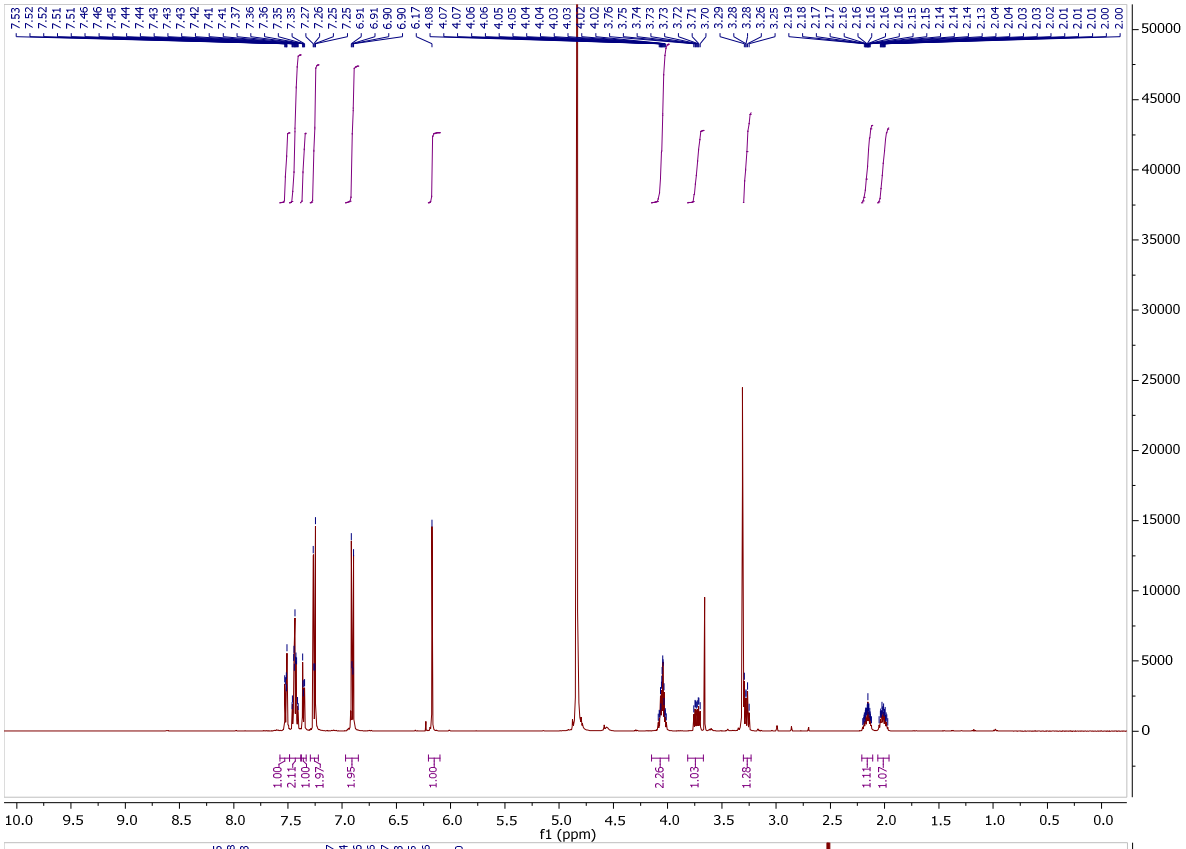

160.93 160.03 159.93 159.23 158.75 158.48 140.22 131.86 131.85 130.97 130.45 127.38 113.29 113.11 112.64 112.60 104.56 104.32 69.91 66.57 49.43 45.55 27.46
f1 (ppm)

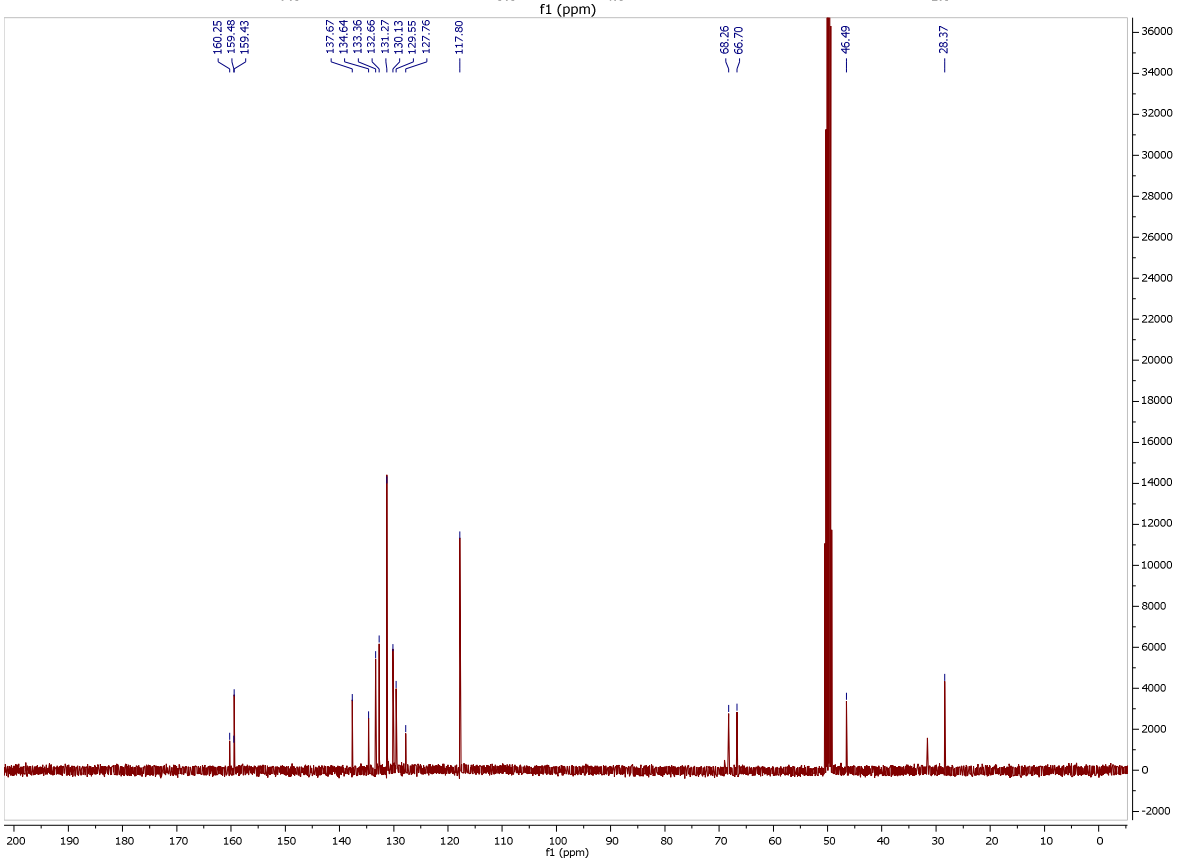
10h


7.47 7.47 7.46 7.46 7.45 7.45 7.44 7.44 7.43 7.42 7.41 7.41 7.40 7.40 7.40 7.39 7.39 7.20 7.18 7.18 7.17 7.15 7.15 7.13 7.01 6.88 6.87 6.86 6.86 6.85 6.84 6.83 6.83 6.72 6.72 6.71 6.71 6.70 6.70 6.70 6.69 6.69 6.69 5.76 5.76 4.03 4.02 4.01 4.01 4.00 3.99 3.99 3.75 3.74 3.73 3.72 3.71 3.70 3.69 3.36 3.35 3.35 3.35 3.34 3.33 2.16 2.16 2.14 2.14 2.13 2.13 2.12 2.11 2.11 2.10 2.03 2.02 2.02 2.01 2.00 1.99
5.12 1.09 1.05 0.82 1.00 2.14 1.04 1.13 1.08 1.05
f1 (ppm)

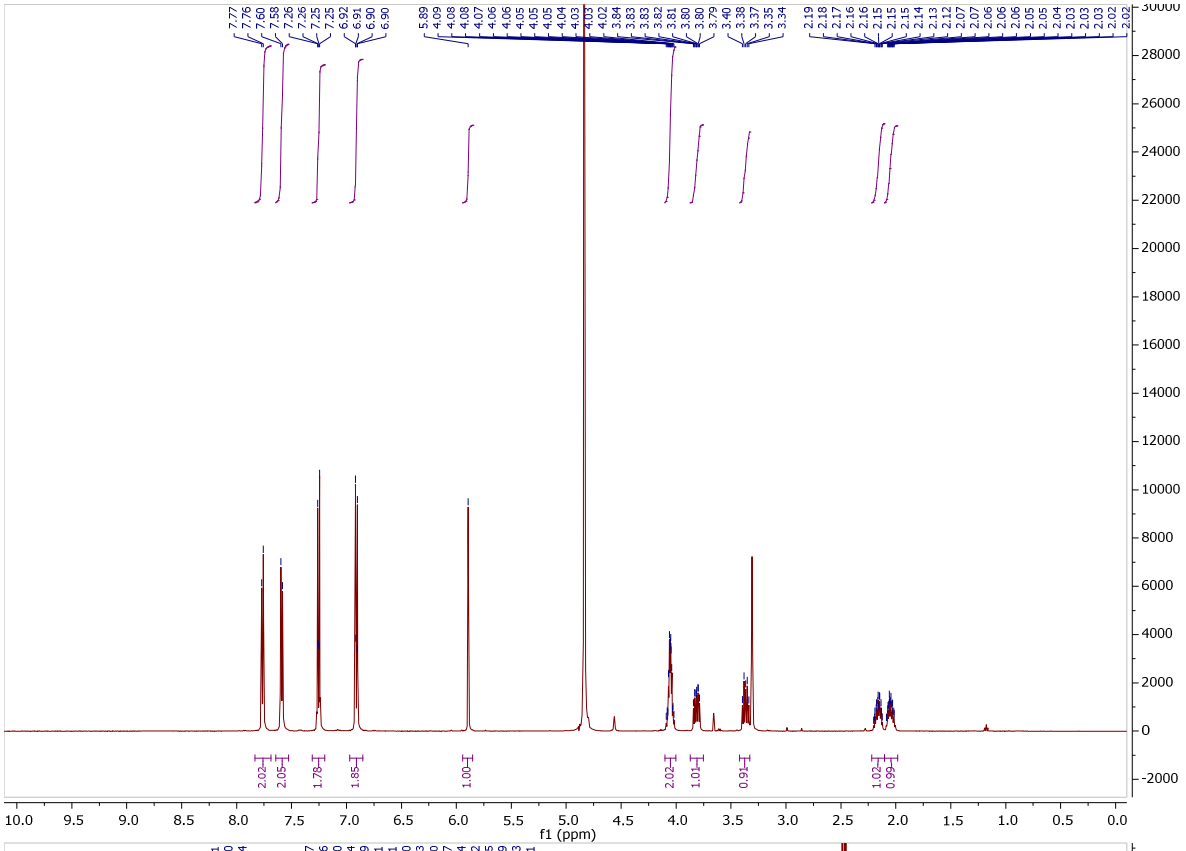

159.23 158.75 156.52 156.50 156.44 156.42 152.98 152.84 150.54 150.40 147.54 147.41 145.17 145.04 140.22 130.96 130.45 127.38 118.49 118.48 118.31 111.29 111.25 111.23 111.20 105.15 104.95
69.89 66.65 45.58 27.55
f1 (ppm)

11a


7.53 7.52 7.52 7.51 7.51 7.46 7.46 7.45 7.44 7.44 7.43 7.43 7.42 7.41 7.41 7.37 7.36 7.36 7.35 7.35 7.27 7.26 7.25 7.25 6.91 6.91 6.90 6.90 6.17 4.08 4.07 4.07 4.06 4.06 4.05 4.05 4.04 4.04 4.03 4.03 4.02 4.02 3.76 3.75 3.74 3.73 3.73 3.72 3.71 3.70 3.29 3.28 3.28 3.26 3.25 2.19 2.18 2.17 2.17 2.16 2.16 2.16 2.16 2.15 2.15 2.14 2.14 2.13 2.04 2.04 2.03 2.03 2.02 2.01 2.01 2.01 2.00 2.00
1.00 2.11 1.00 1.97 1.95 1.00 2.26 1.03 1.28 1.11 1.07
50000 45000 40000 35000 30000 25000 20000 15000 10000 5000 0
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 0.0
f1 (ppm)


160.25 159.48 159.43 137.67 134.64 133.36 132.66 131.27 130.13 129.55 127.76 117.80 68.26 66.70 46.49 28.37
36000 34000 32000 30000 28000 26000 24000 22000 20000 18000 16000 14000 12000 10000 8000 6000 4000 2000 0 -2000
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

11b


7.77
7.76
7.60
7.58
7.26
7.25
7.25
6.92
6.91
6.90
6.90
5.89
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4.08
4.08
4.07
4.06
4.06
4.05
4.05
4.05
4.04
4.03
4.03
4.02
3.84
3.83
3.83
3.82
3.81
3.80
3.80
3.79
3.40
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3.34
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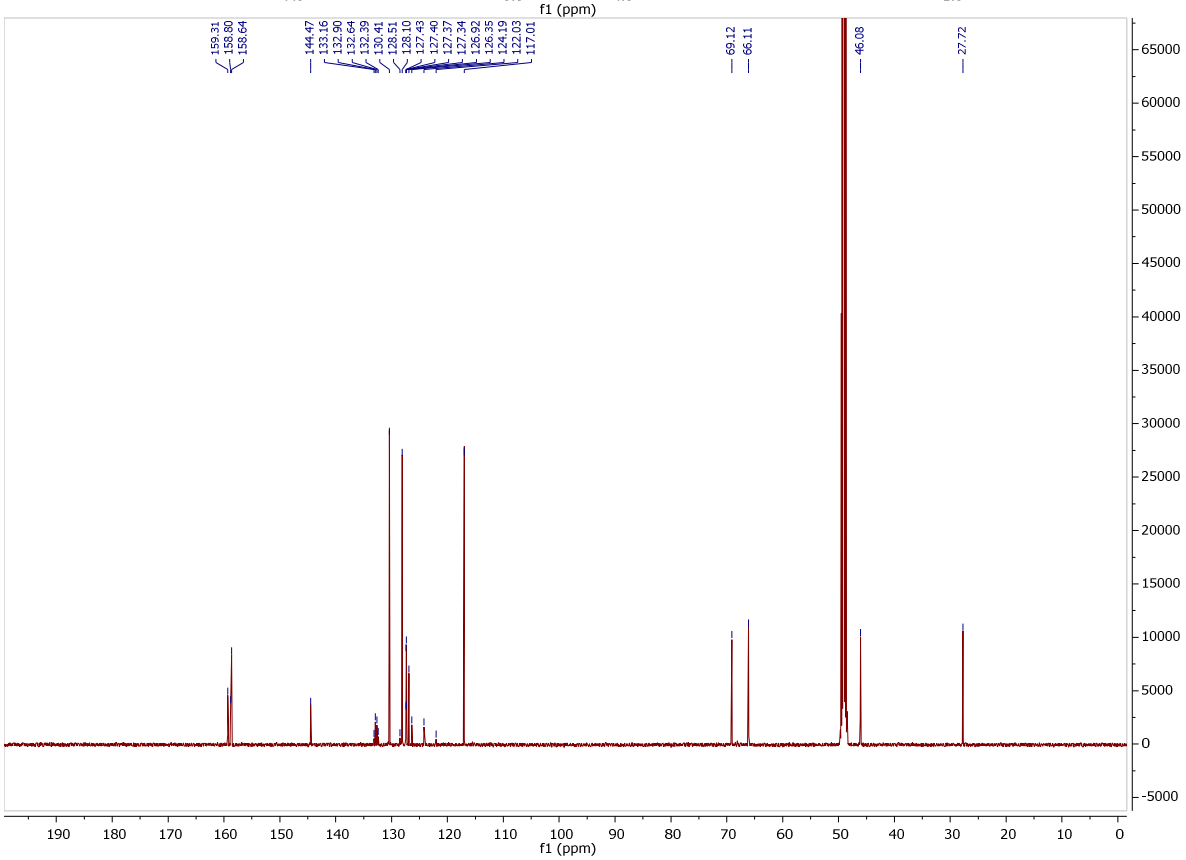
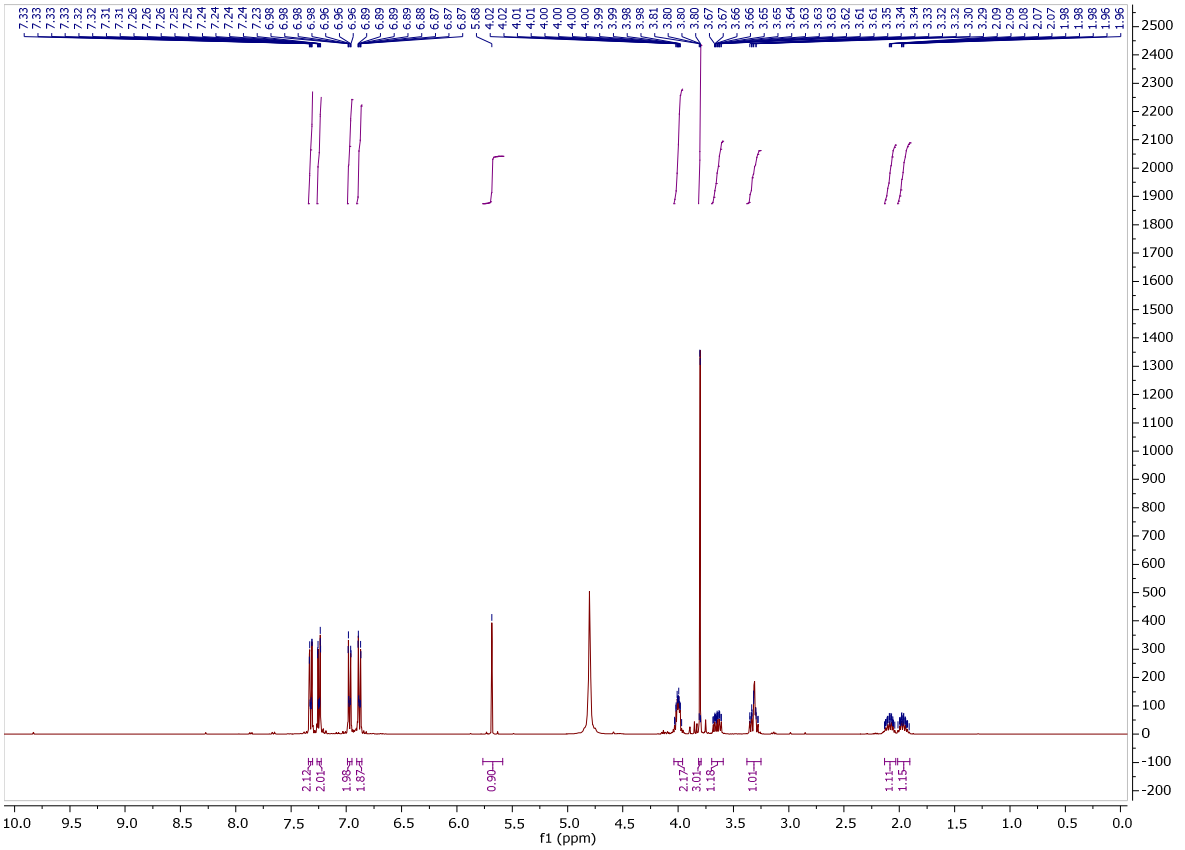
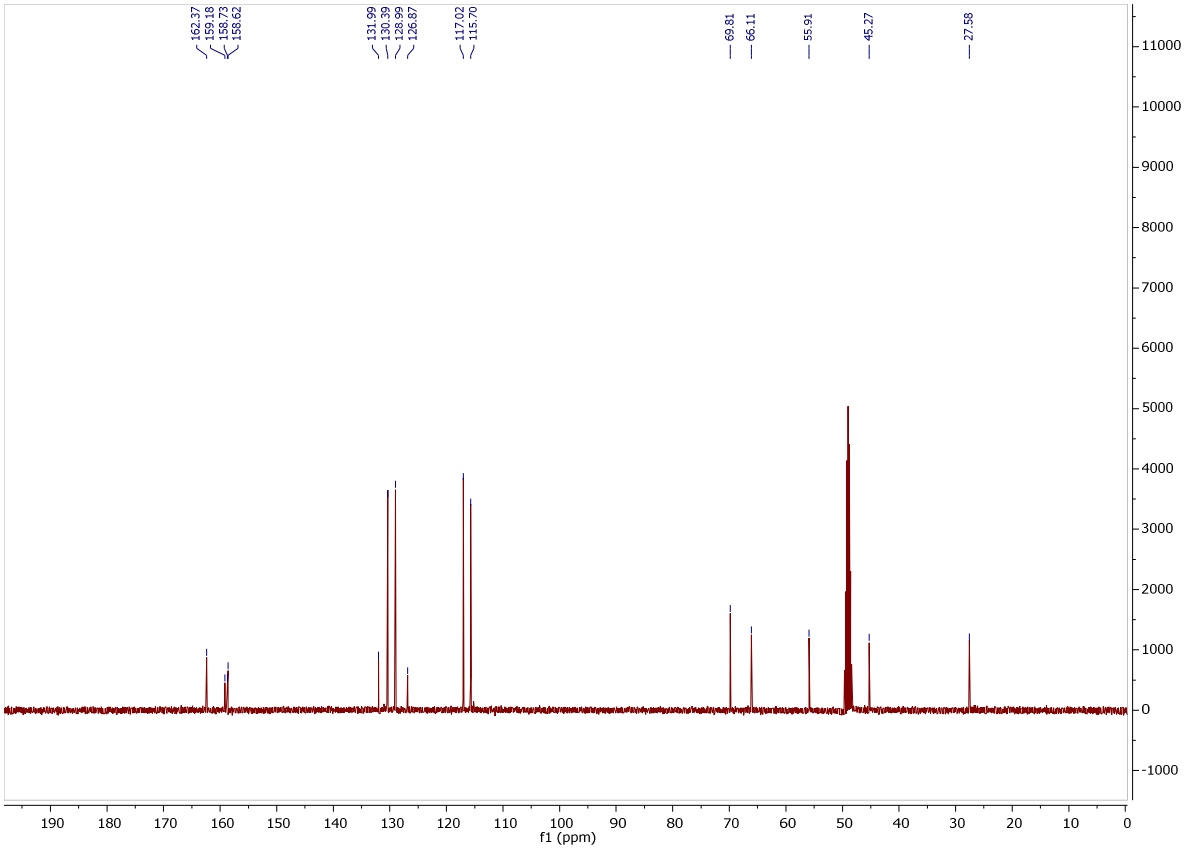
2.18
2.17
2.16
2.16
2.15
2.15
2.14
2.13
2.12
2.07
2.07
2.06
2.06
2.06
2.05
2.05
2.04
2.03
2.03
2.03
2.02
2.02
2.02
2.05
1.78
1.85
1.00
2.02
1.01
0.91
1.02
0.99
f1 (ppm)

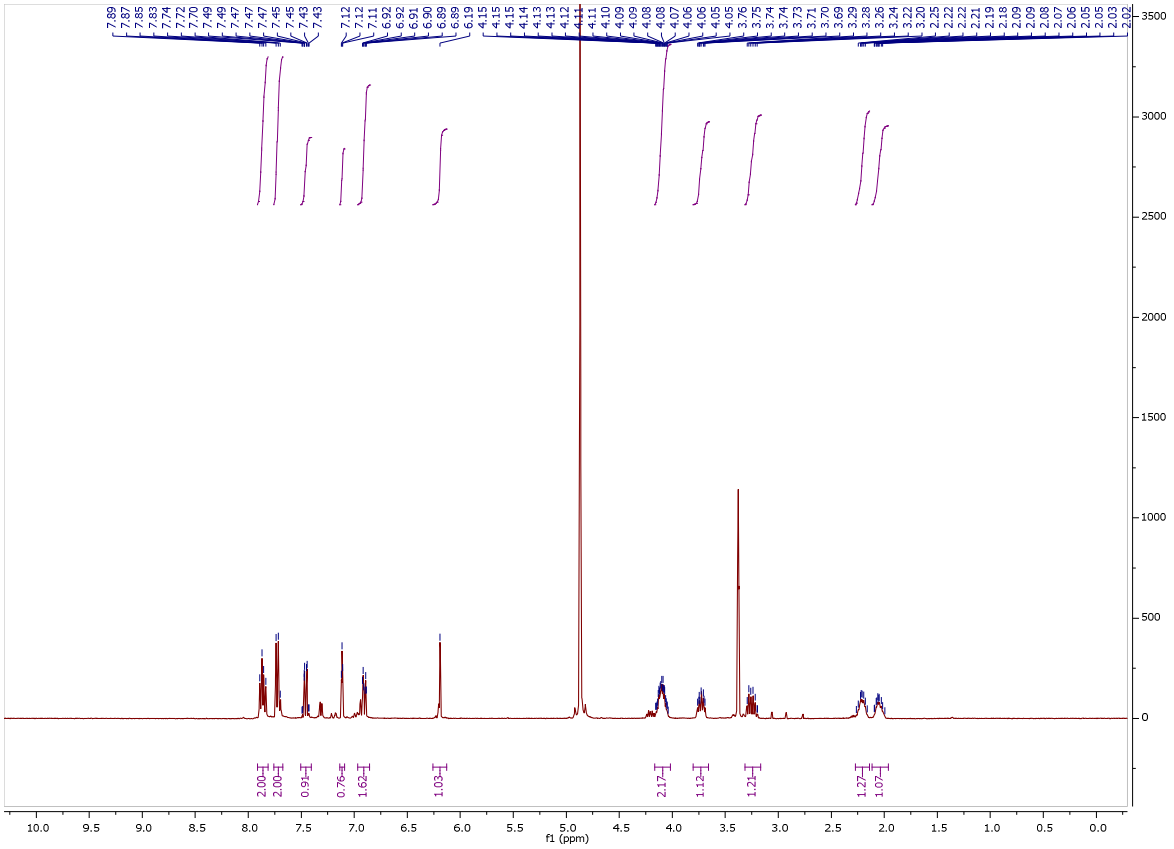

159.31
158.80
158.64
144.47
133.16
132.90
132.64
132.39
130.41
128.51
128.10
127.43
127.40
127.37
127.34
126.92
126.35
124.19
122.03
117.01
69.12
66.11
46.08
27.72
f1 (ppm)

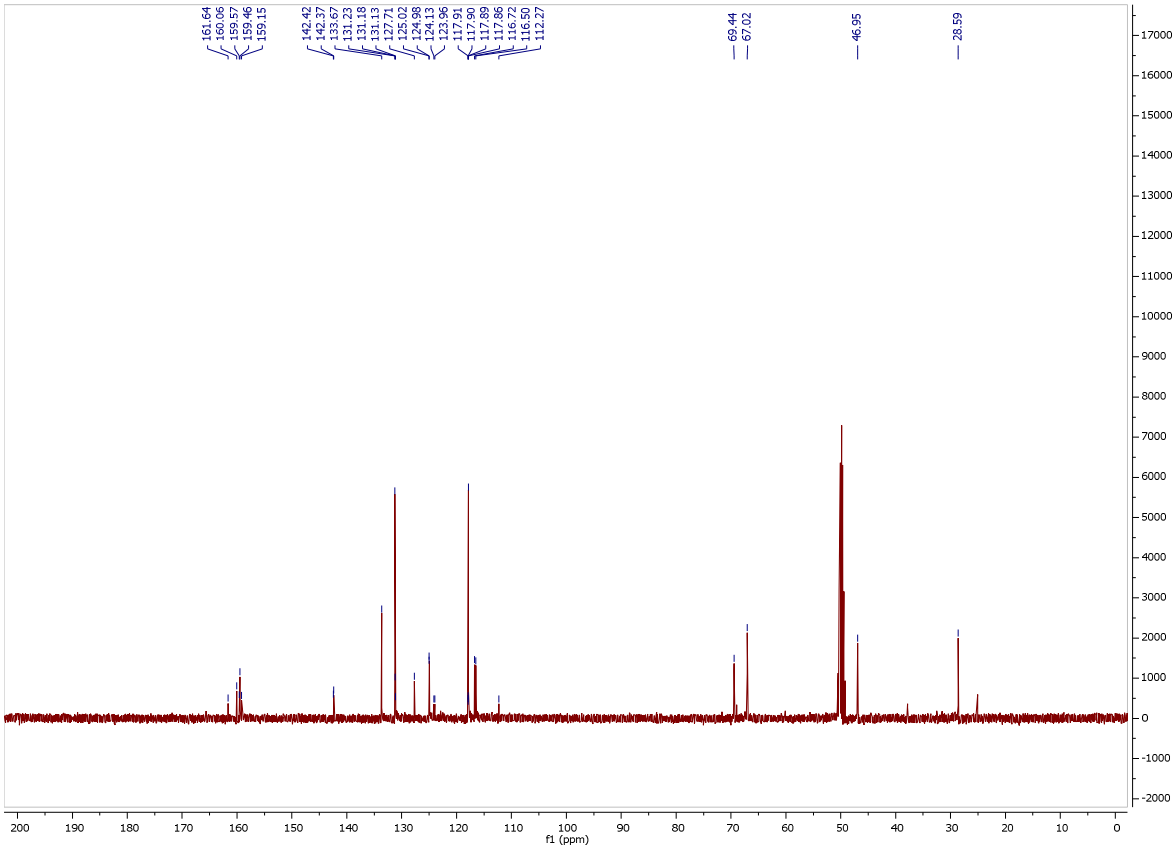
11c


f1 (ppm)

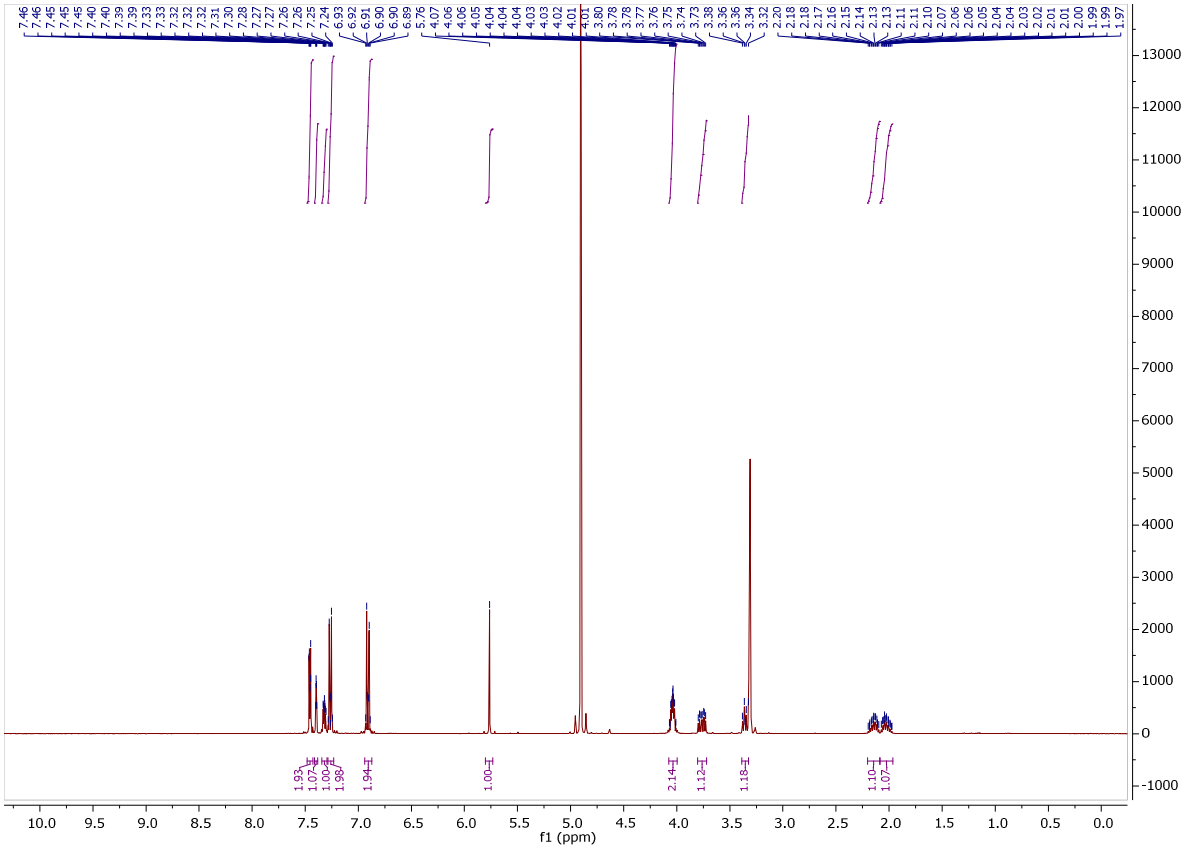

162.37
159.18
158.73
158.62
131.99
130.39
128.99
126.87
117.02
115.70
69.81
66.11
55.91
45.27
27.58
f1 (ppm)

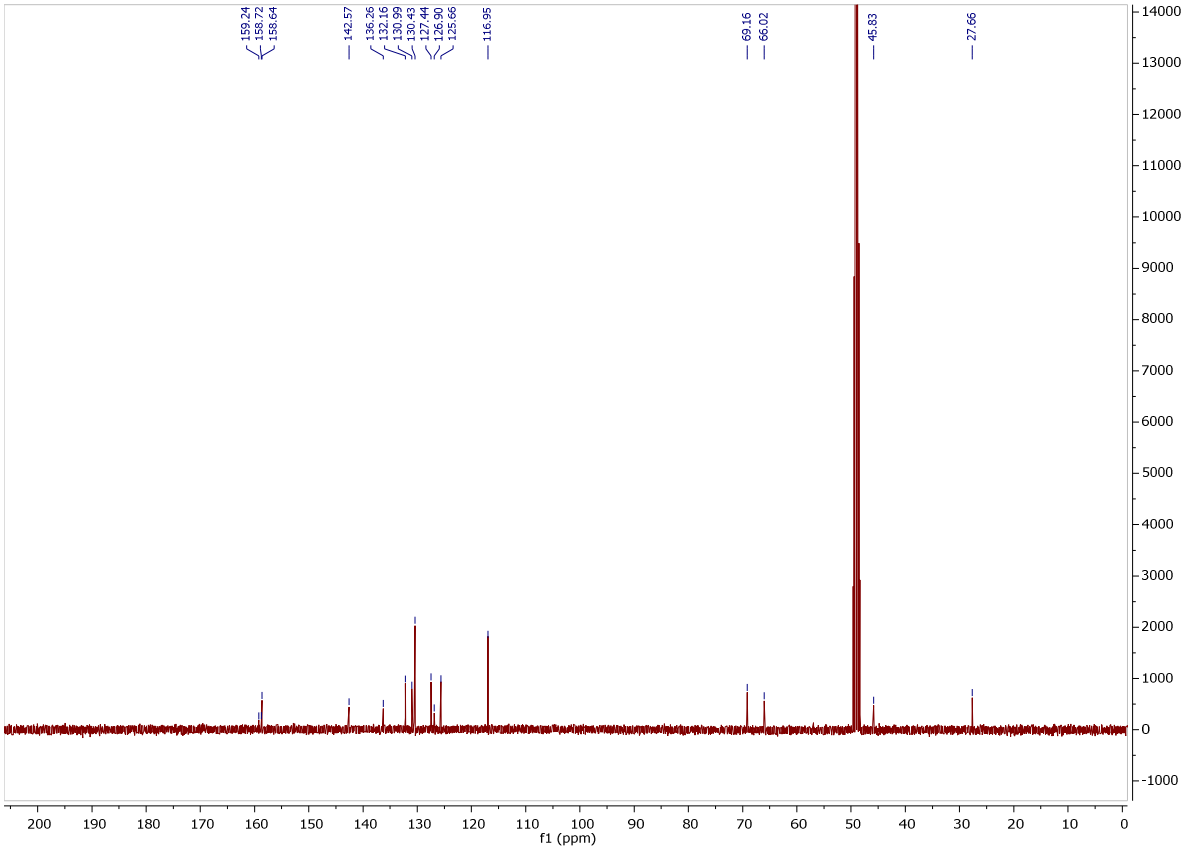
11d


7.89 7.87 7.85 7.83 7.74 7.72 7.70 7.49 7.49 7.47 7.47 7.47 7.45 7.45 7.43 7.43
7.12 7.12 7.11 6.92 6.92 6.91 6.90 6.89 6.89 6.19
4.15 4.15 4.15 4.14 4.13 4.12 4.11 4.11 4.10 4.09 4.09 4.08 4.08 4.07 4.06 4.06 4.05 4.05 3.76 3.75 3.74 3.74 3.73 3.71 3.70 3.69 3.29 3.28 3.26 3.24 3.22 3.20 2.25 2.22 2.22 2.21 2.19 2.18 2.09 2.09 2.08 2.07 2.06 2.05 2.05 2.03 2.02
2.00 2.00 0.91 0.76 1.62 1.03 2.17 1.13 1.21 1.22 1.07
f1 (ppm)

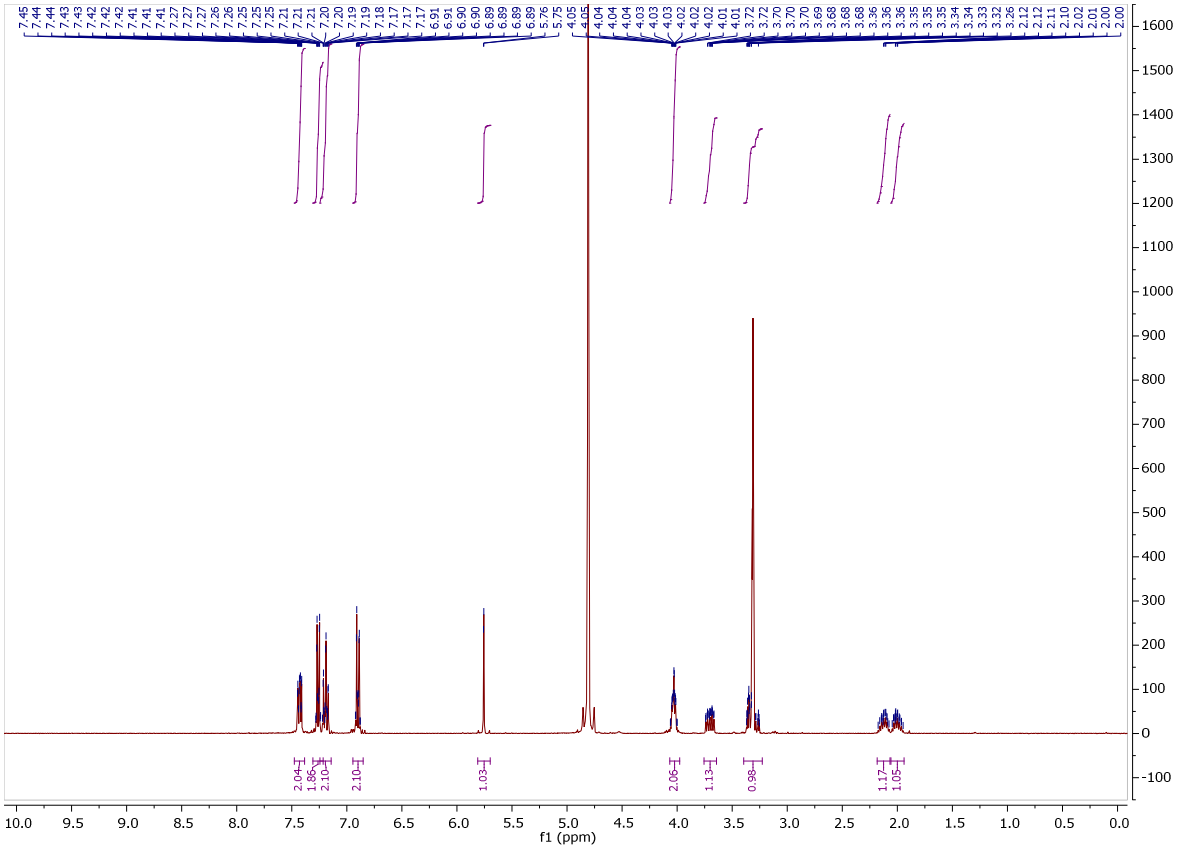

161.64 160.06 159.57 159.46 159.15
142.42 142.37 133.67 131.23 131.18 131.13 127.71 125.02 124.98 124.13 123.96 117.91 117.90 117.89 117.86 116.72 116.59 112.27
69.44 67.02
46.95
28.59
f1 (ppm)

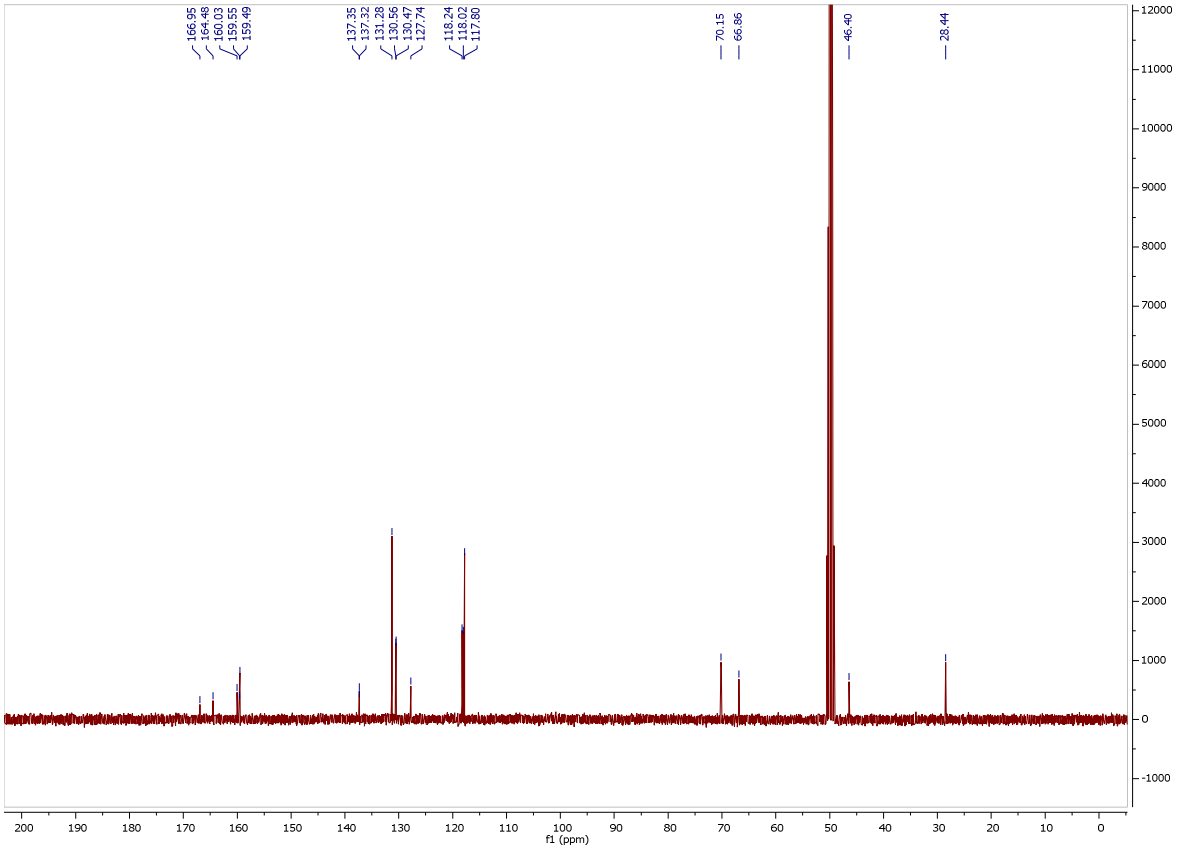
11e


7.46 7.46 7.45 7.45 7.45 7.40 7.40 7.39 7.39 7.33 7.33 7.32 7.32 7.31 7.30 7.28 7.27 7.27 7.26 7.26 7.25 7.24 6.93 6.92 6.91 6.90 6.90 6.89 5.76 4.07 4.06 4.06 4.05 4.04 4.04 4.03 4.03 4.02 4.01 4.01 3.80 3.78 3.78 3.77 3.76 3.75 3.74 3.73 3.38 3.36 3.35 3.34 3.32 3.20 2.18 2.18 2.17 2.16 2.15 2.14 2.13 2.13 2.11 2.10 2.07 2.06 2.06 2.05 2.04 2.04 2.03 2.02 2.01 2.01 2.00 1.99 1.99 1.97
1.93 1.07 1.00 1.98 1.94 1.00 2.14 1.12 1.18 1.10 1.07
f1 (ppm)

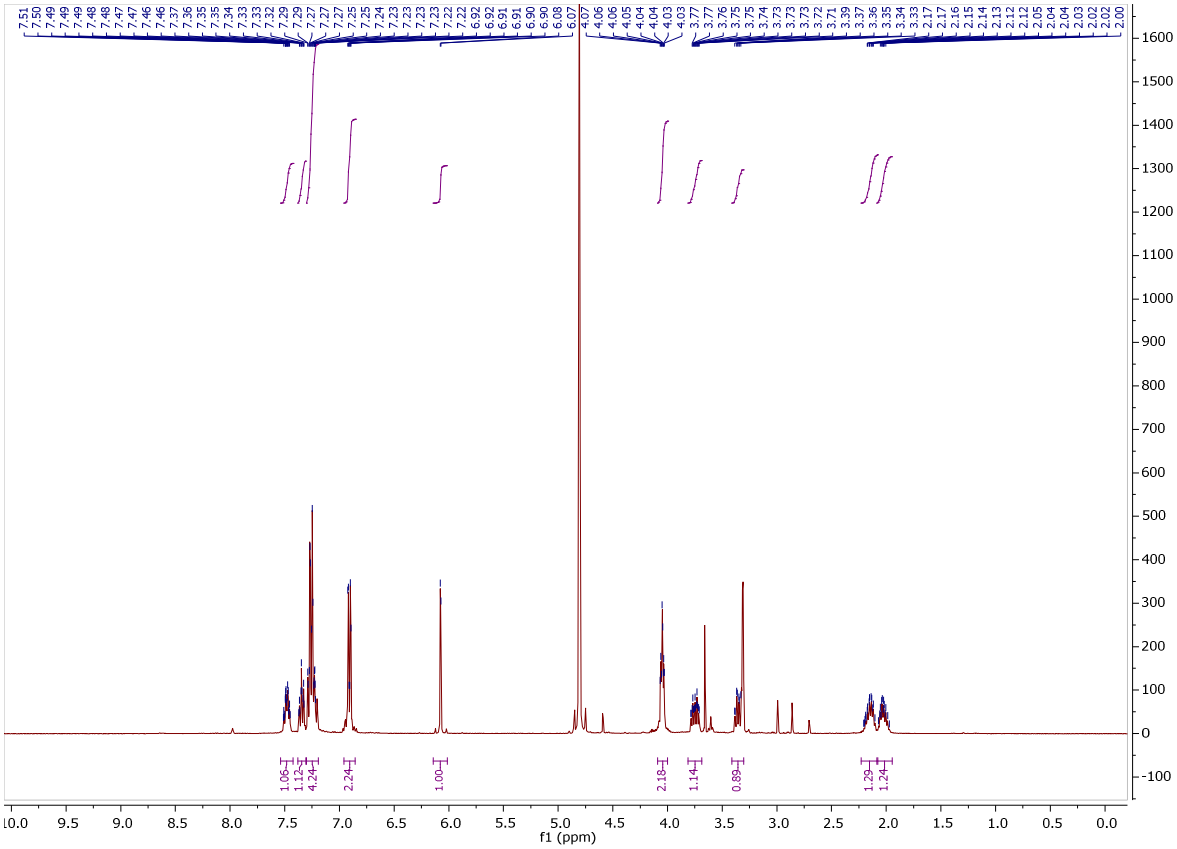

159.24 158.72 158.64 142.57 136.26 132.16 130.99 130.43 127.44 126.90 125.66 116.95 69.16 66.02 45.83 27.66
f1 (ppm)

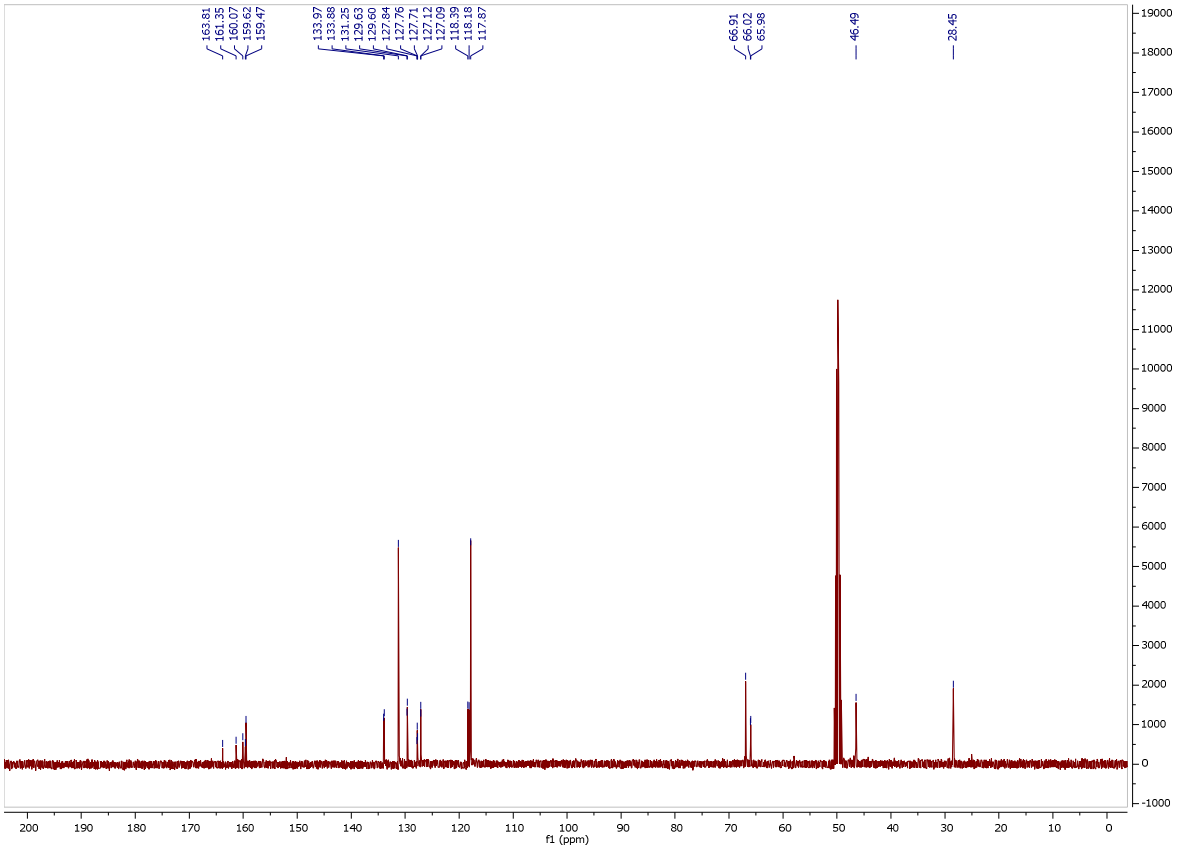
11f


f1 (ppm)

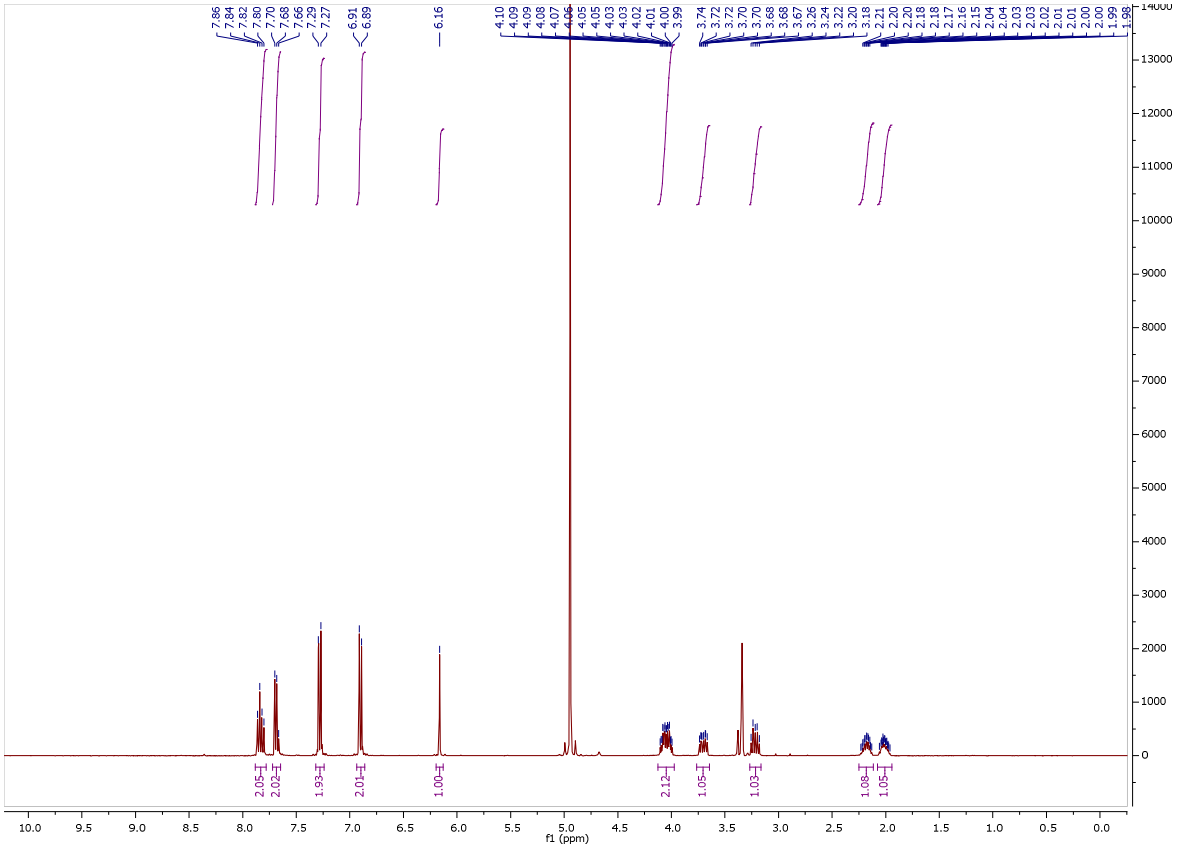

166.95
164.48
160.03
159.55
159.49
137.35
137.32
131.28
130.56
130.47
127.74
118.24
118.02
117.80
70.15
66.86
46.40
28.44
f1 (ppm)

11g


7.51 7.50 7.49 7.49 7.49 7.48 7.48 7.47 7.47 7.46 7.46 7.37 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.29 7.29 7.27 7.27 7.27 7.25 7.25 7.24 7.23 7.23 7.23 7.22 7.22 6.92 6.92 6.91 6.91 6.90 6.90 6.08 6.07
4.07 4.06 4.06 4.05 4.04 4.04 4.03 4.03 3.77 3.77 3.76 3.75 3.74 3.73 3.73 3.73 3.72 3.71 3.39 3.37 3.36 3.35 3.34 3.33 2.17 2.16 2.15 2.14 2.13 2.12 2.12 2.05 2.04 2.04 2.03 2.02 2.02 2.00
1.06 1.12 4.24 2.24 1.00 2.18 1.14 0.89 1.29 1.24
f1 (ppm)


163.81 161.35 160.07 159.62 159.47
133.97 133.88 131.25 129.63 129.60 129.04 127.76 127.71 127.12 127.09 118.39 118.18 117.87
66.91 66.02 65.98
46.49
28.45
f1 (ppm)

11h


7.86
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7.27
6.91
6.89
6.16
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4.09
4.09
4.08
4.08
4.07
4.06
4.05
4.05
4.03
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4.02
4.01
4.00
3.99
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3.72
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3.70
3.70
3.68
3.68
3.67
3.26
3.24
3.22
3.20
3.18
2.21
2.20
2.20
2.18
2.18
2.17
2.16
2.15
2.04
2.04
2.03
2.03
2.02
2.01
2.01
2.00
2.00
1.99
1.98
2.05
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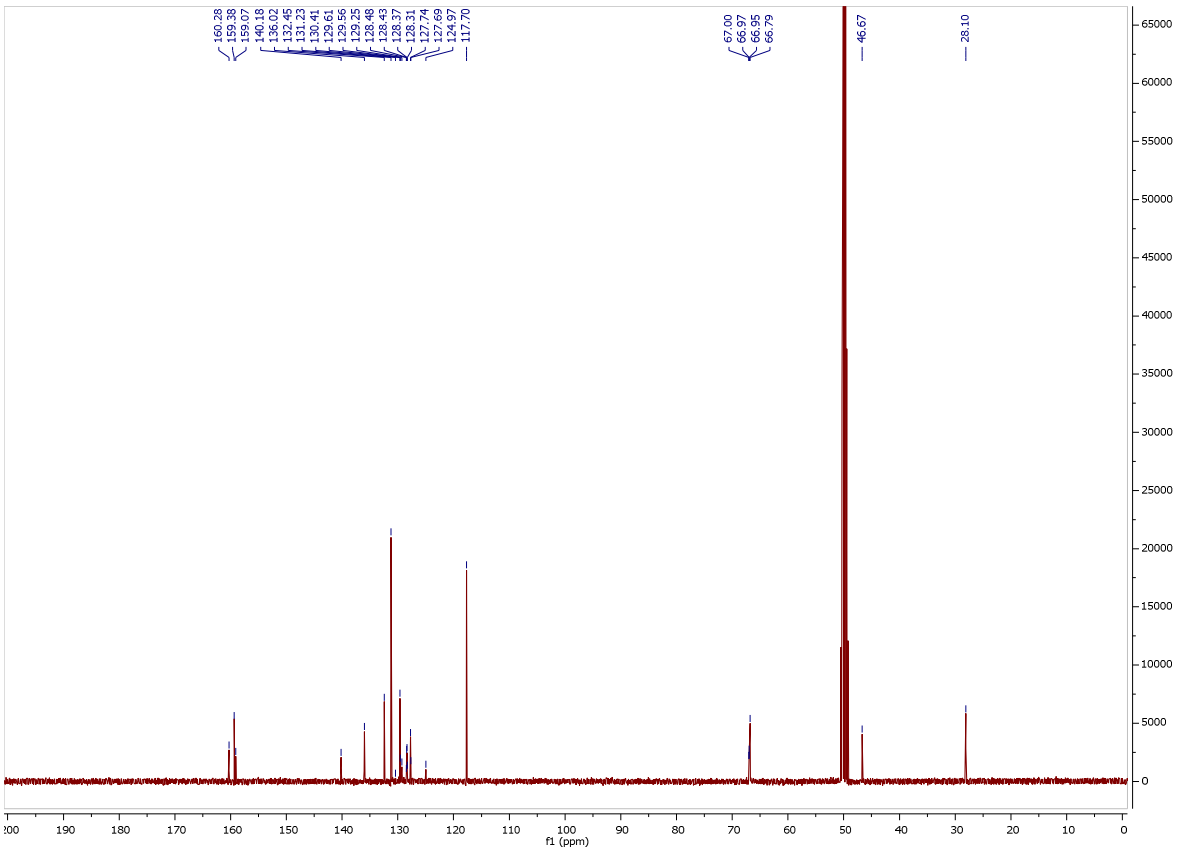
1.93
2.01
1.00
2.12
1.05
1.03
1.08
1.05
f1 (ppm)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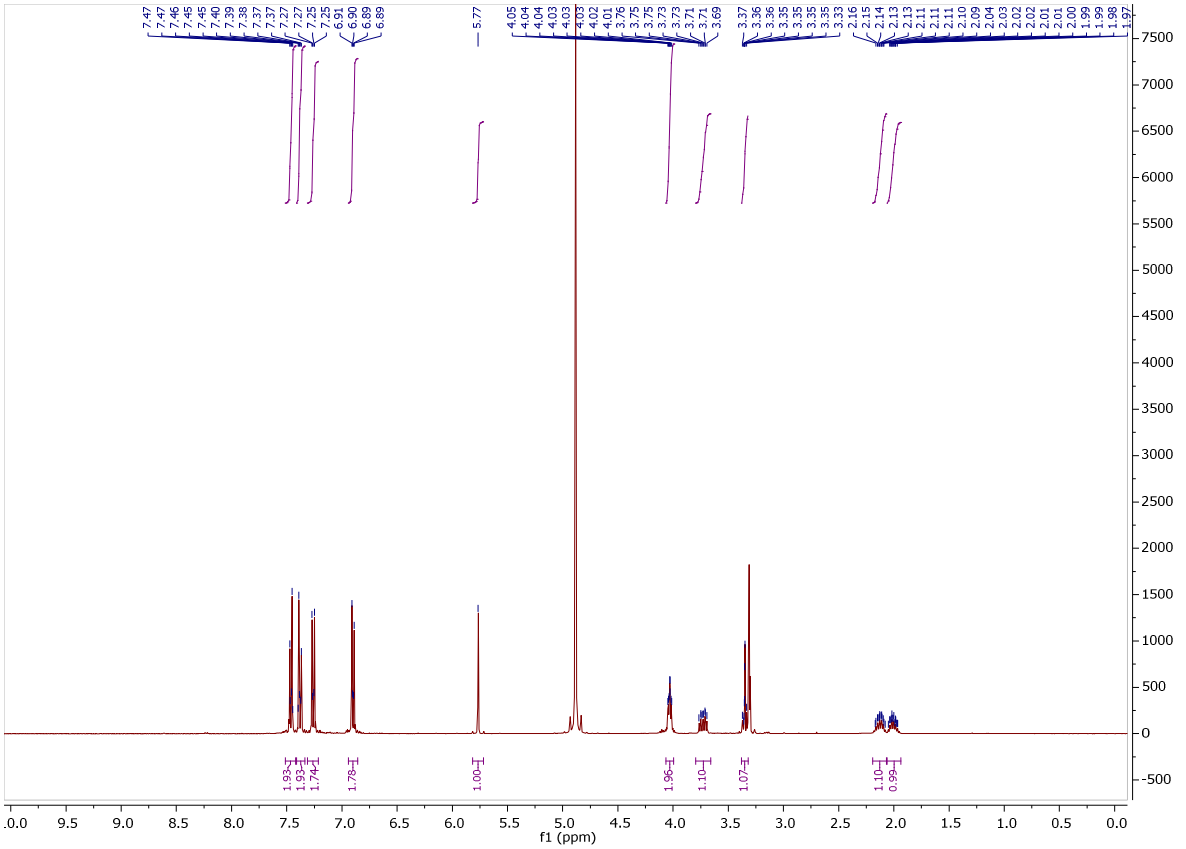
132.45
131.23
130.41
129.61
129.56
129.25
128.48
128.43
128.37
128.31
127.74
127.69
124.97
117.70
67.00
66.97
66.95
66.79
46.67
28.10
f1 (ppm)

11i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7.37
7.37
7.27
7.27
7.25
7.25
6.91
6.90
6.89
6.89
5.77
4.05
4.04
4.04
4.03
4.03
4.02
4.01
3.76
3.75
3.75
3.73
3.73
3.71
3.71
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1.99
1.98
1.97
1.93
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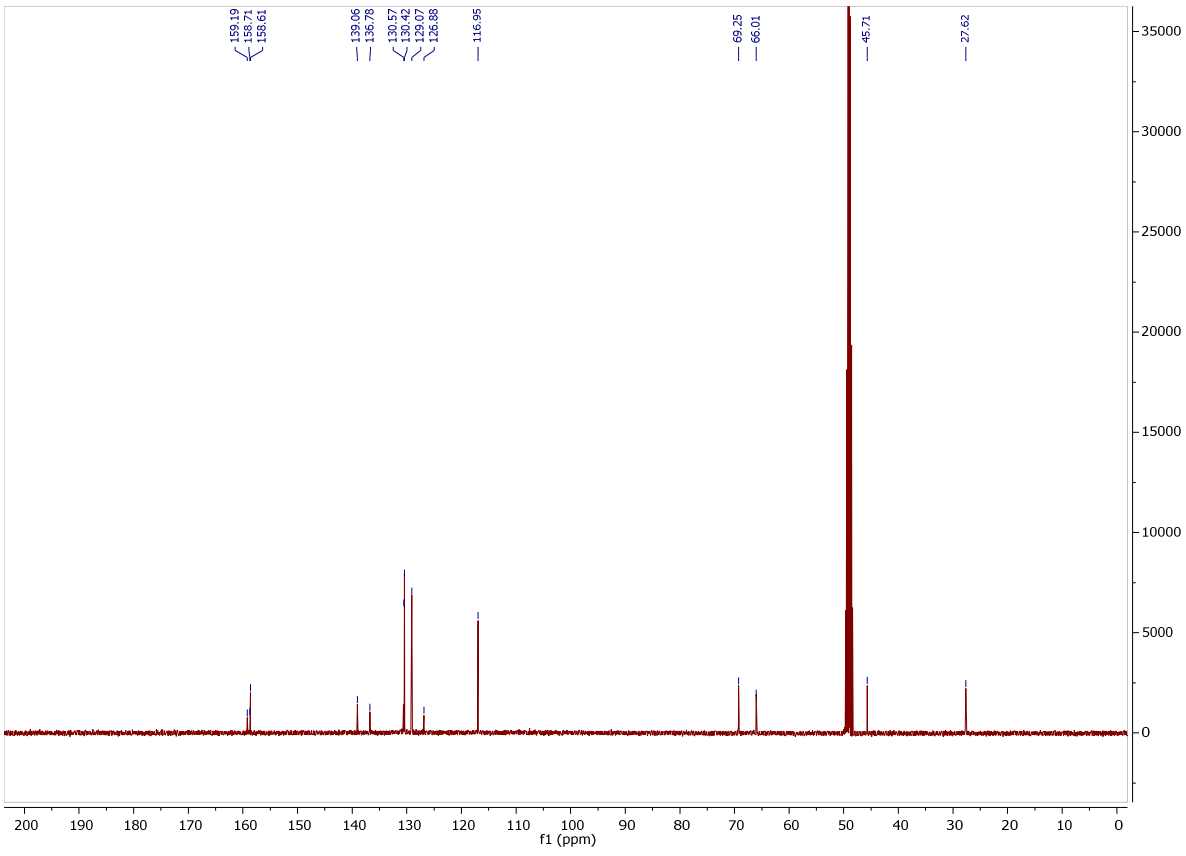
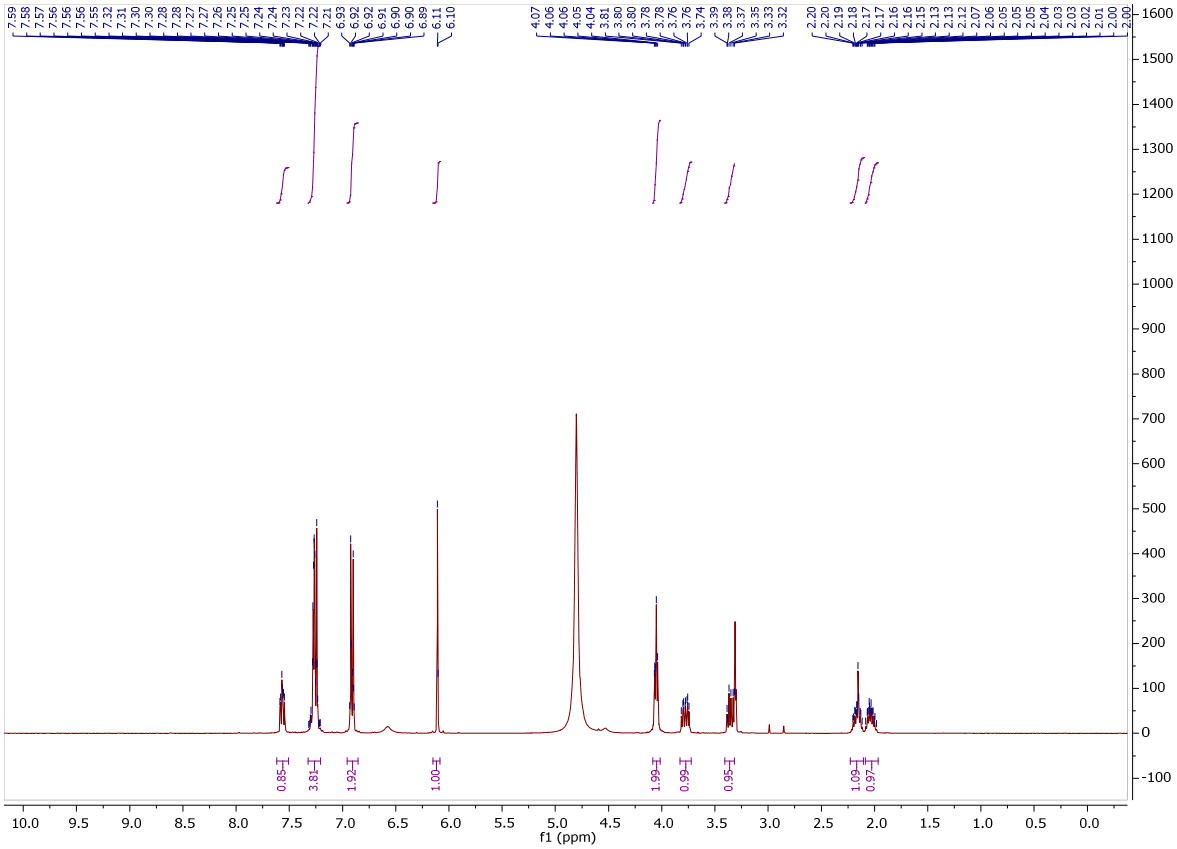
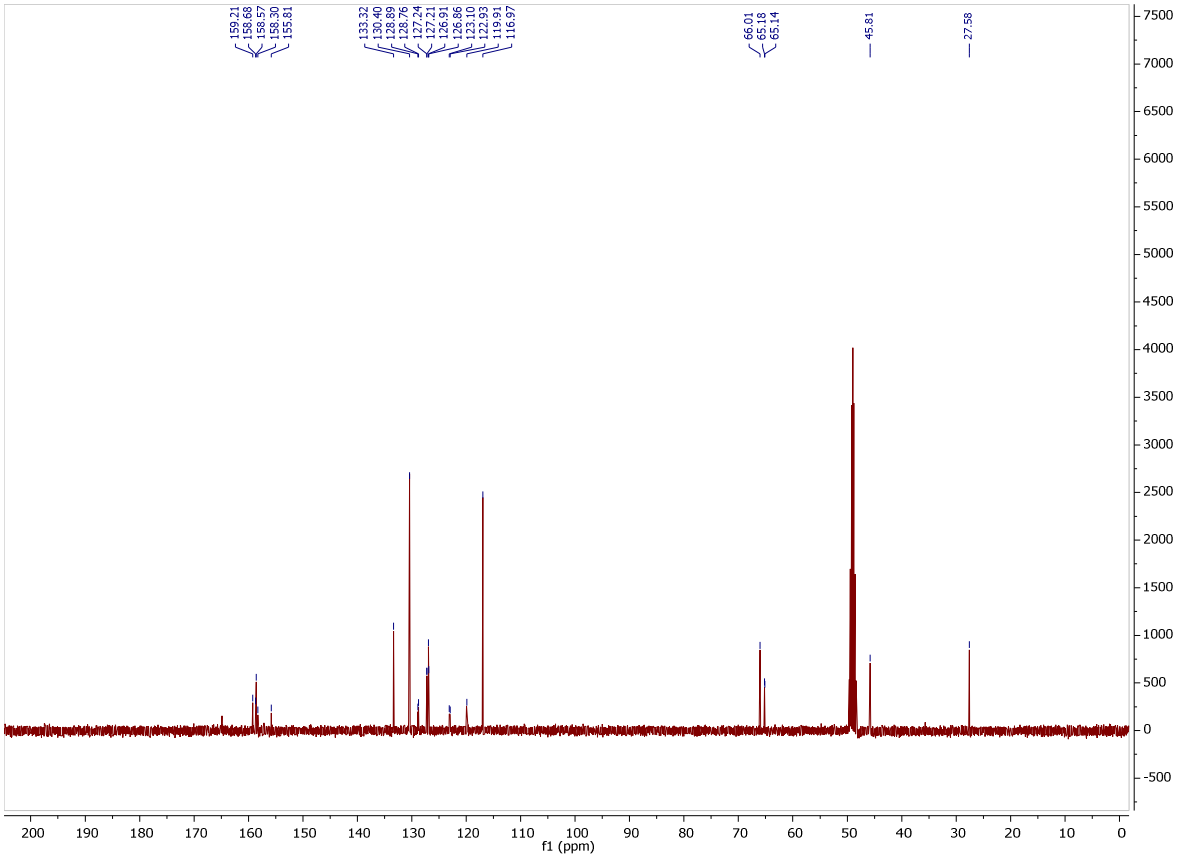
1.74
1.78
1.00
1.96
1.10
1.07
1.10
0.99
f1 (ppm)

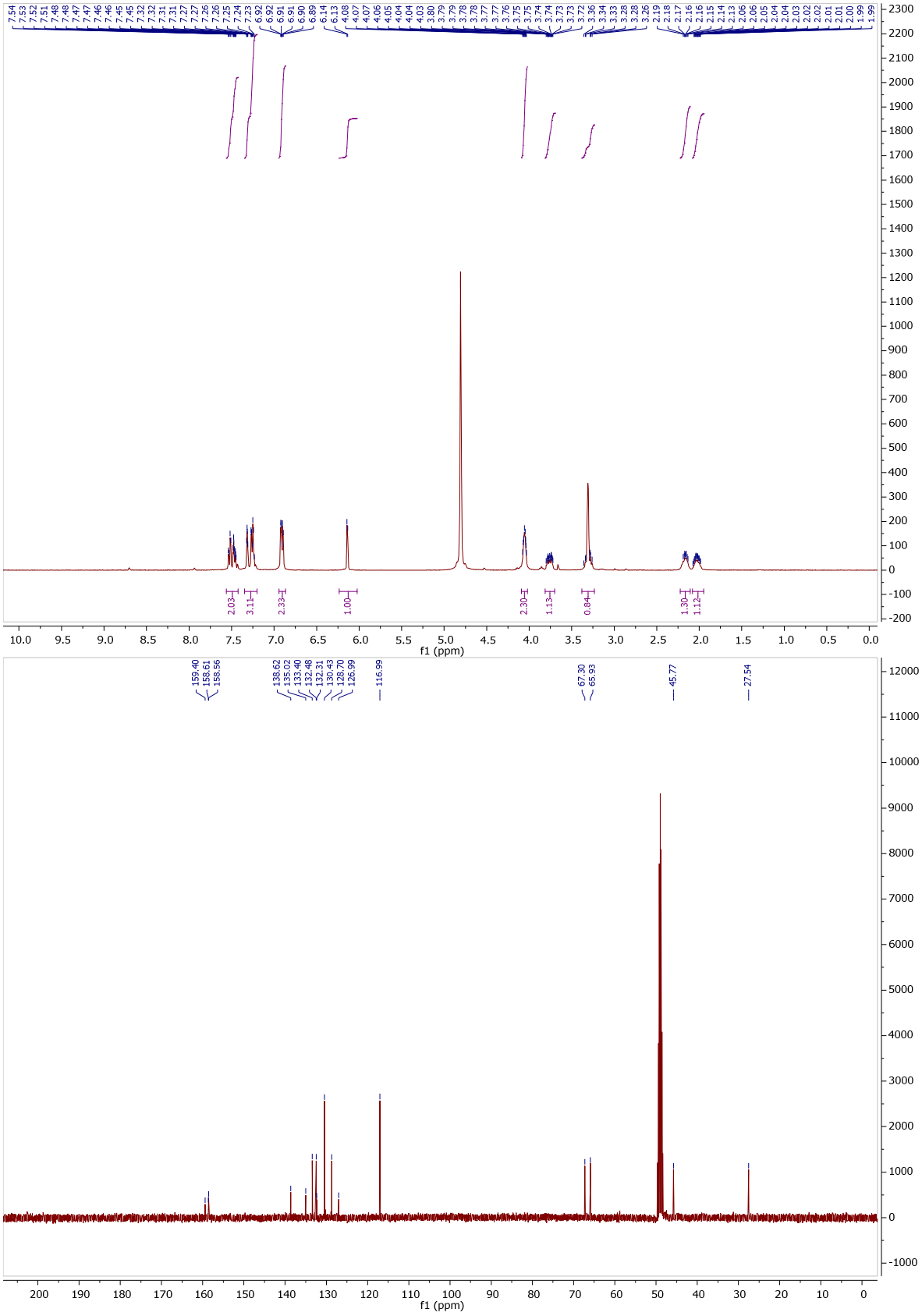

159.19
158.71
158.61
139.06
136.78
130.57
130.42
129.07
126.88
116.95
69.25
66.01
45.71
27.62
f1 (ppm)

11j

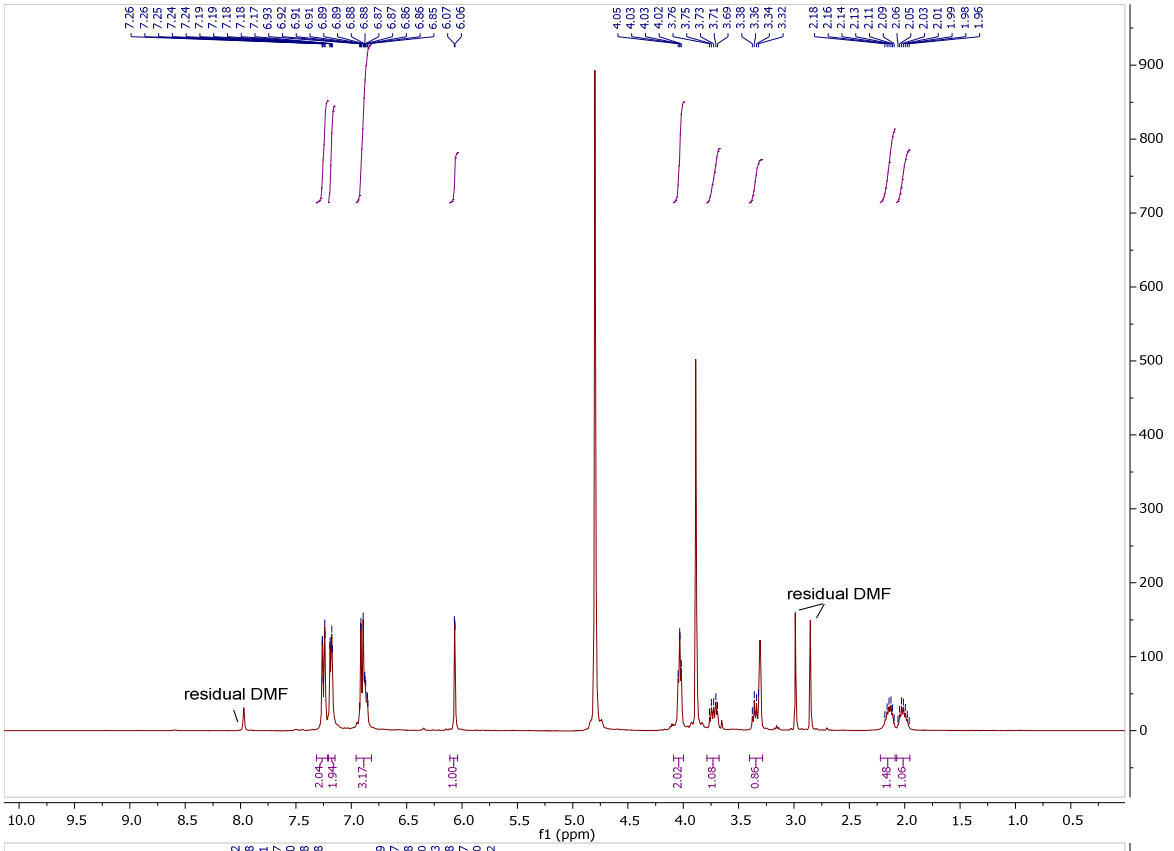

7.59 7.58 7.57 7.56 7.56 7.56 7.55 7.32 7.31 7.30 7.30 7.28 7.28 7.27 7.27 7.26 7.25 7.24 7.24 7.23 7.22 7.22 7.21 6.93 6.92 6.92 6.91 6.90 6.90 6.89 6.11 6.10
4.07 4.06 4.06 4.05 4.04 3.81 3.80 3.80 3.78 3.78 3.76 3.76 3.74 3.39 3.38 3.37 3.35 3.33 3.32
2.20 2.20 2.19 2.18 2.17 2.17 2.16 2.16 2.15 2.13 2.13 2.12 2.07 2.06 2.05 2.05 2.05 2.04 2.03 2.03 2.02 2.01 2.00 2.00
0.85 3.81 1.92 1.00 1.99 0.99 0.95 1.09 0.97
f1 (ppm)

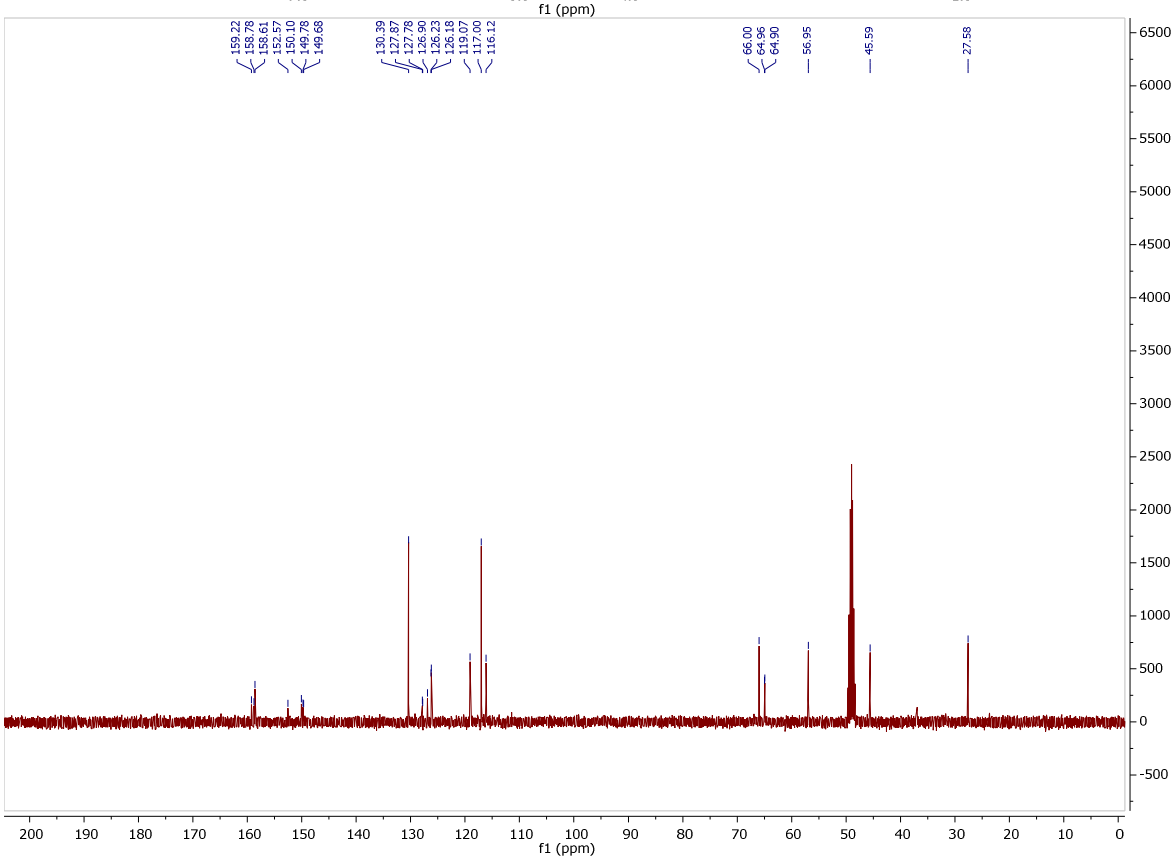

159.21 158.68 158.57 158.30 155.81
133.32 130.40 128.89 128.76 127.24 127.21 126.91 126.86 123.10 123.03 119.91 116.97
66.01 65.18 65.14
45.81
27.58
f1 (ppm)

11k

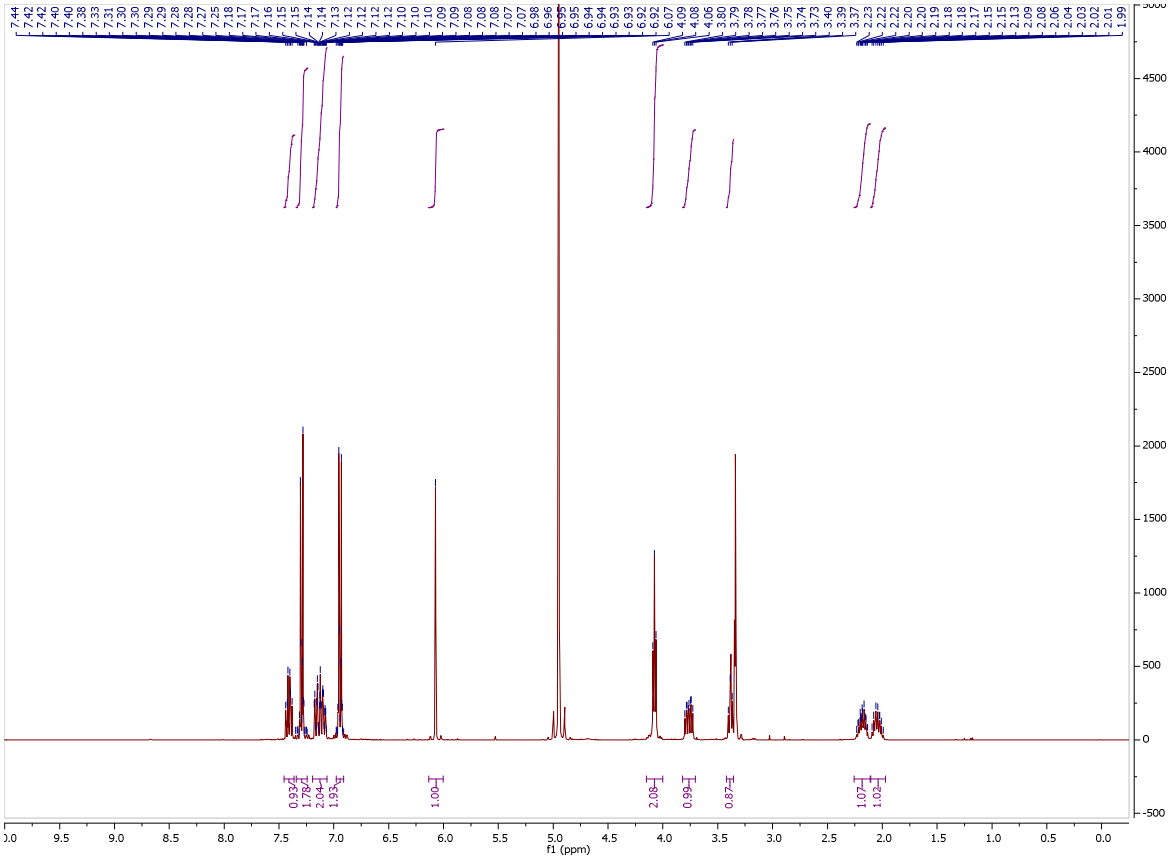

7.54 7.53 7.52 7.51 7.48 7.48 7.47 7.47 7.46 7.46 7.45 7.45 7.32 7.32 7.31 7.31 7.27 7.27 7.26 7.26 7.25 7.24 7.23 6.92 6.92 6.91 6.91 6.90 6.89 6.14 6.13 4.08 4.07 4.07 4.06 4.05 4.04 4.04 4.03 3.80 3.79 3.79 3.78 3.78 3.77 3.77 3.76 3.75 3.75 3.74 3.74 3.73 3.73 3.72 3.36 3.34 3.33 3.28 3.28 3.26 2.19 2.18 2.17 2.16 2.16 2.15 2.14 2.13 2.06 2.06 2.05 2.04 2.04 2.03 2.02 2.01 2.01 2.00 1.99 1.99 1.99
2.03 3.11 2.33 1.00 2.30 1.13 0.84 1.30 1.12
f1 (ppm)
159.40 158.61 158.56 138.62 135.02 133.40 132.48 132.31 130.43 128.70 126.99 116.99 67.30 65.93 45.77 27.54
f1 (ppm)

11l





11m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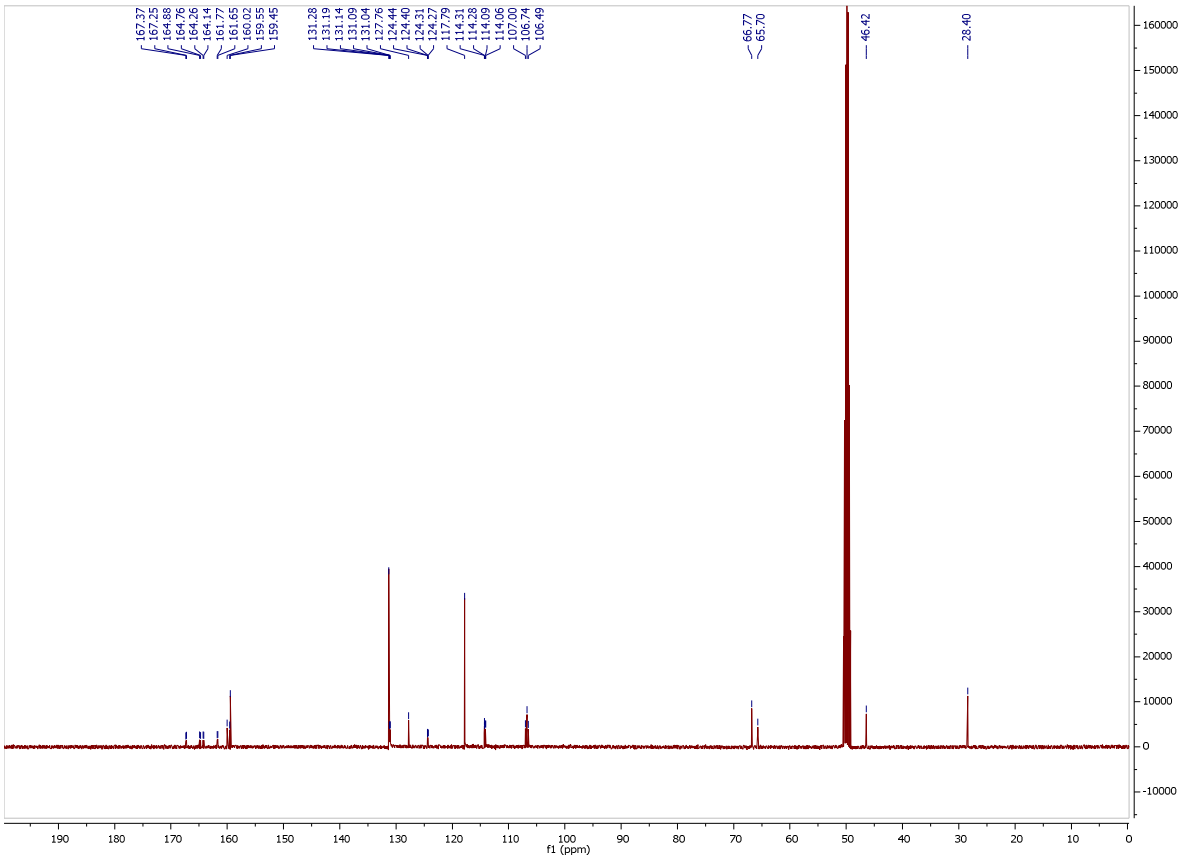
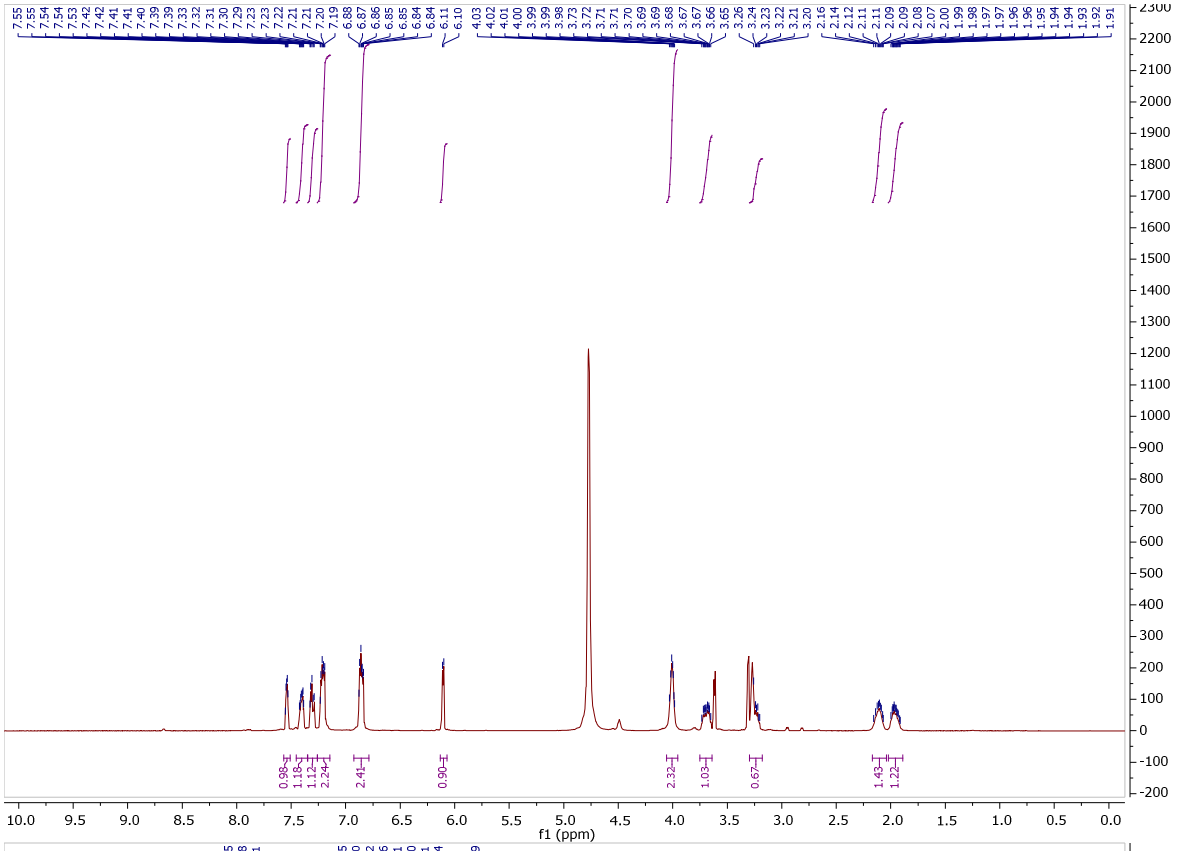
0.93 1.78 2.04 1.93 1.00 2.08 0.99 0.87 1.07 1.03
f1 (ppm)


167.37 167.25 164.88 164.76 164.26 164.14 161.77 161.65 160.02 159.55 159.45 131.28 131.19 131.14 131.09 131.04 127.76 124.44 124.40 124.31 124.27 117.79 114.31 114.28 114.09 114.06 107.00 106.74 106.49 66.77 65.70 46.42 28.40
f1 (ppm)

11n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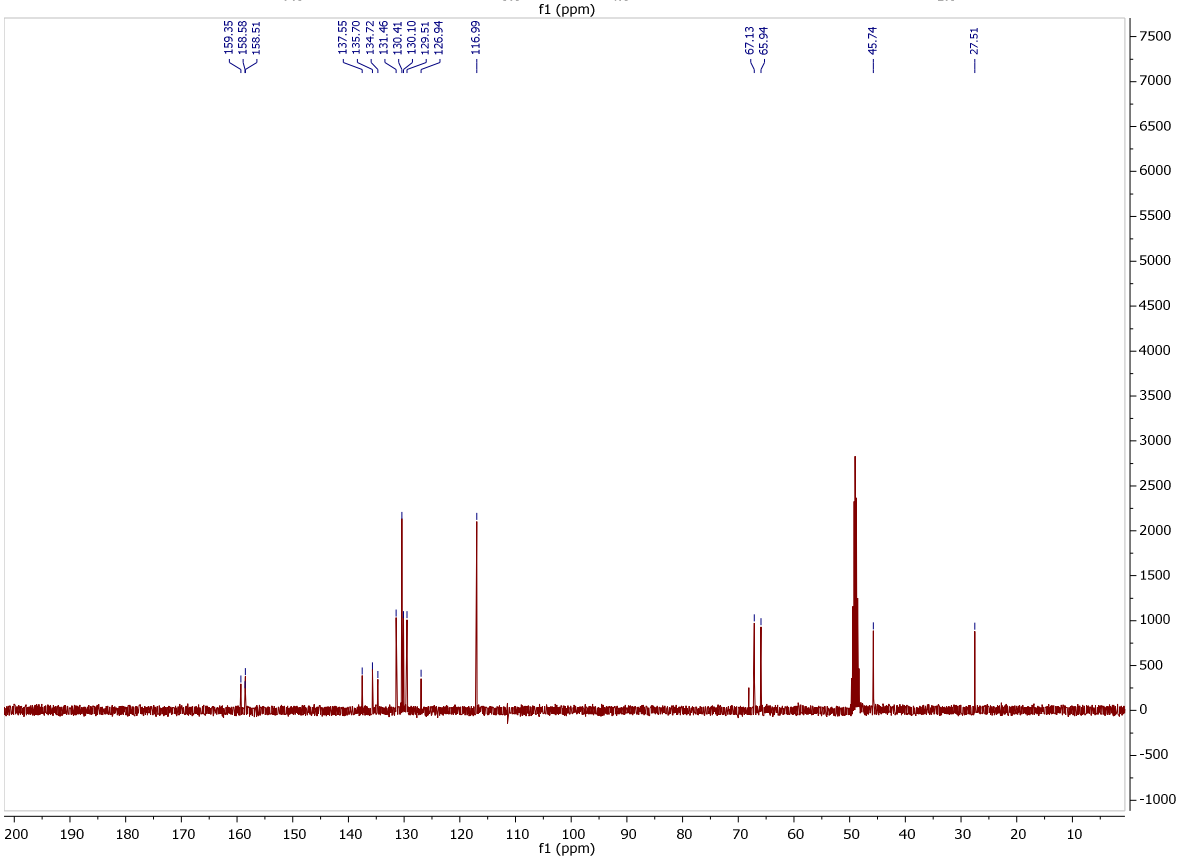
0.98 1.18 1.12 2.24 2.41 0.90 2.32 1.03 0.67 1.43 1.22
f1 (ppm)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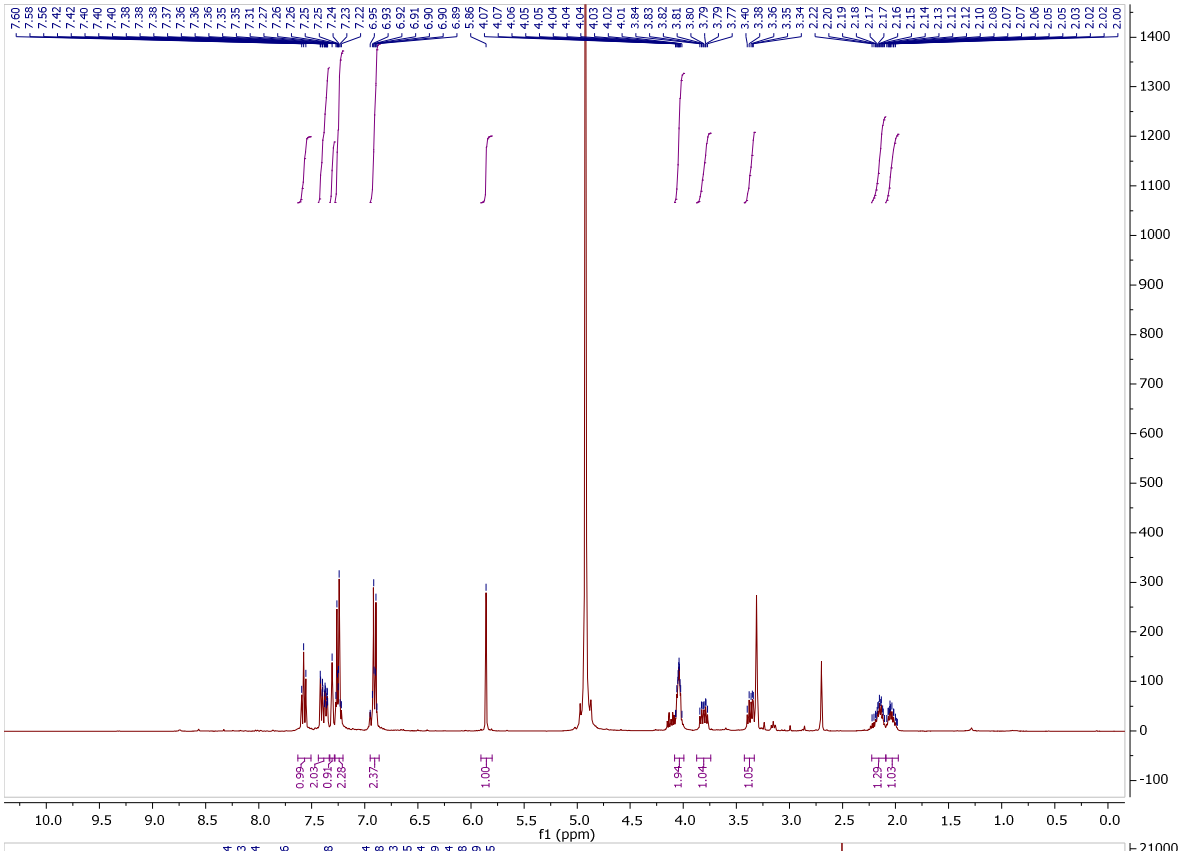
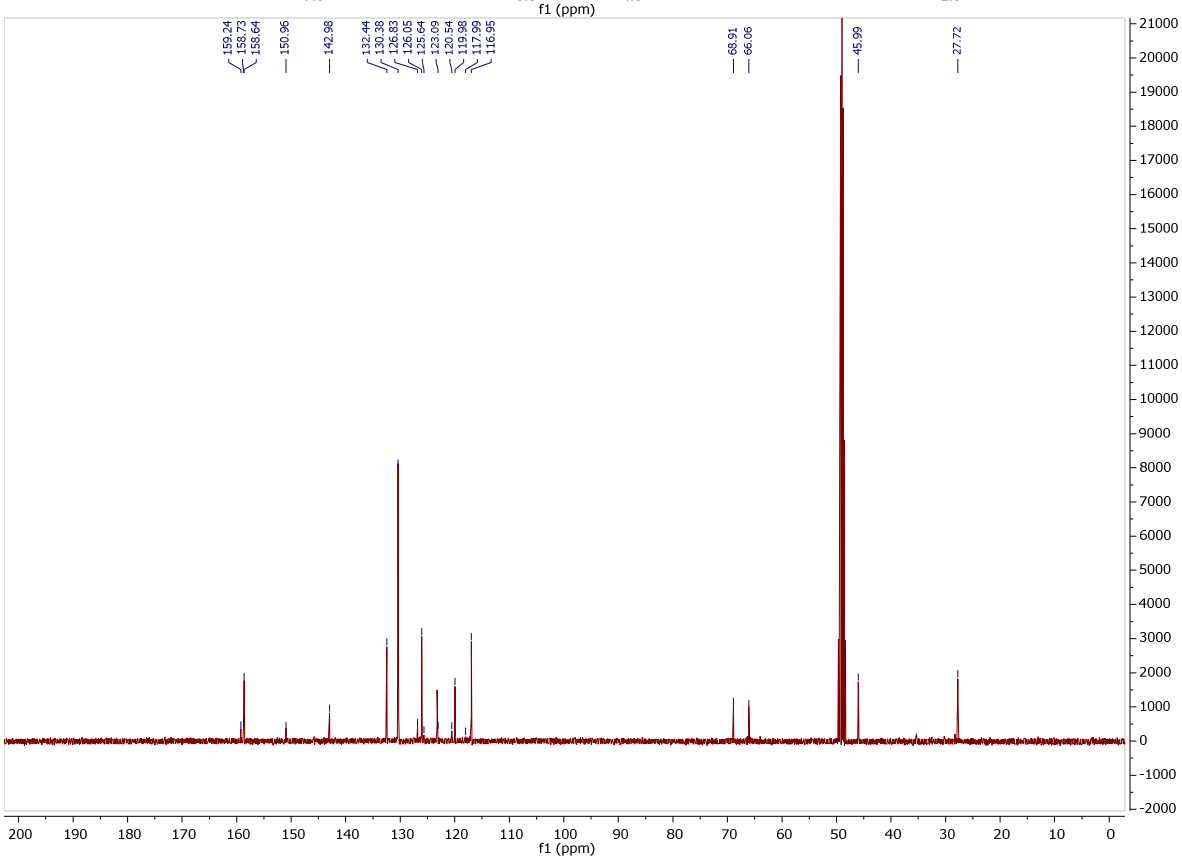
f1 (ppm)

11o


7.60 7.58 7.56 7.42 7.42 7.40 7.40 7.40 7.38 7.38 7.37 7.36 7.36 7.35 7.35 7.31 7.27 7.26 7.26 7.25 7.25 7.24 7.23 7.22 6.95 6.93 6.92 6.91 6.90 6.90 6.89 5.86 4.07 4.06 4.05 4.05 4.04 4.04 4.04 4.03 4.02 4.01 3.84 3.83 3.82 3.81 3.80 3.79 3.79 3.77 3.40 3.38 3.36 3.35 3.34 2.22 2.20 2.19 2.18 2.17 2.17 2.16 2.15 2.14 2.13 2.12 2.12 2.10 2.08 2.07 2.07 2.06 2.05 2.05 2.03 2.02 2.02 2.00
0.99 2.03 0.91 2.28 2.37 1.00 1.94 1.04 1.05 1.29 1.03
f1 (ppm)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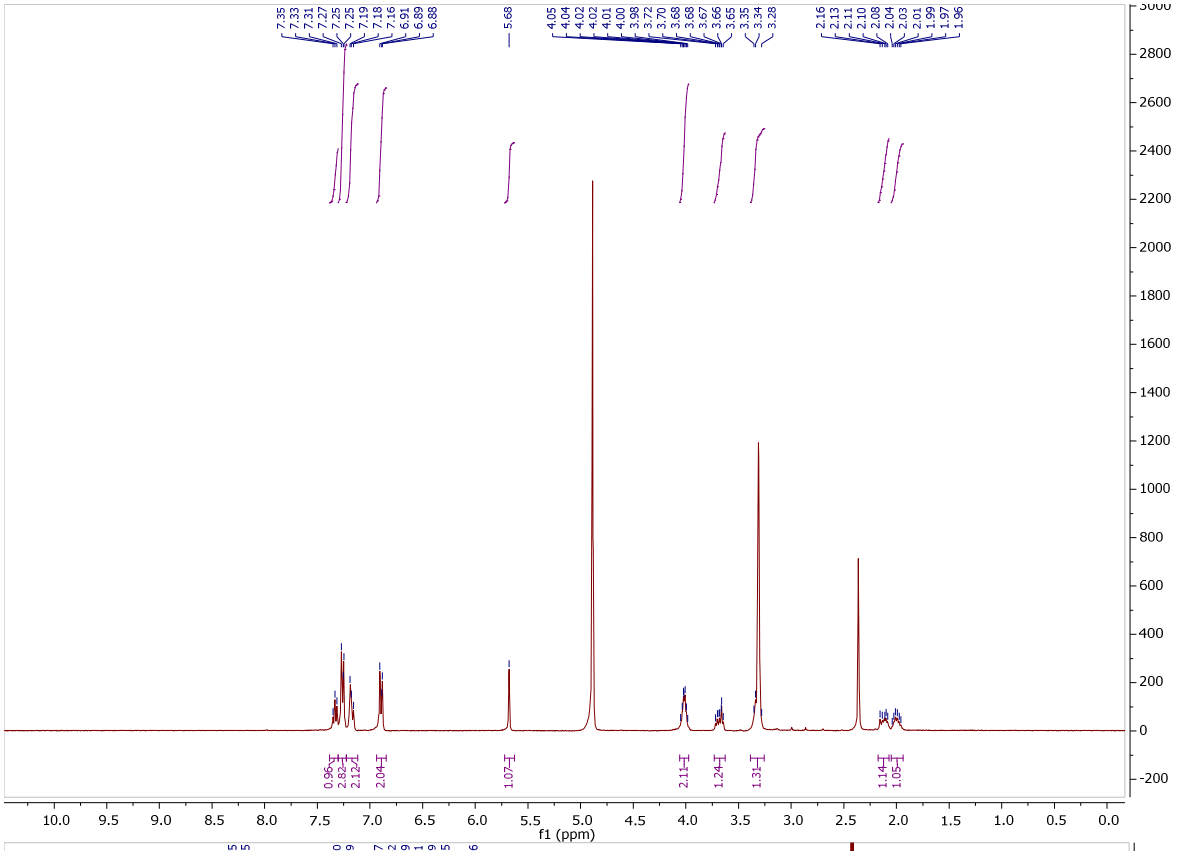
f1 (ppm)

11p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7.27
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7.25
7.19
7.18
7.16
6.91
6.89
6.88
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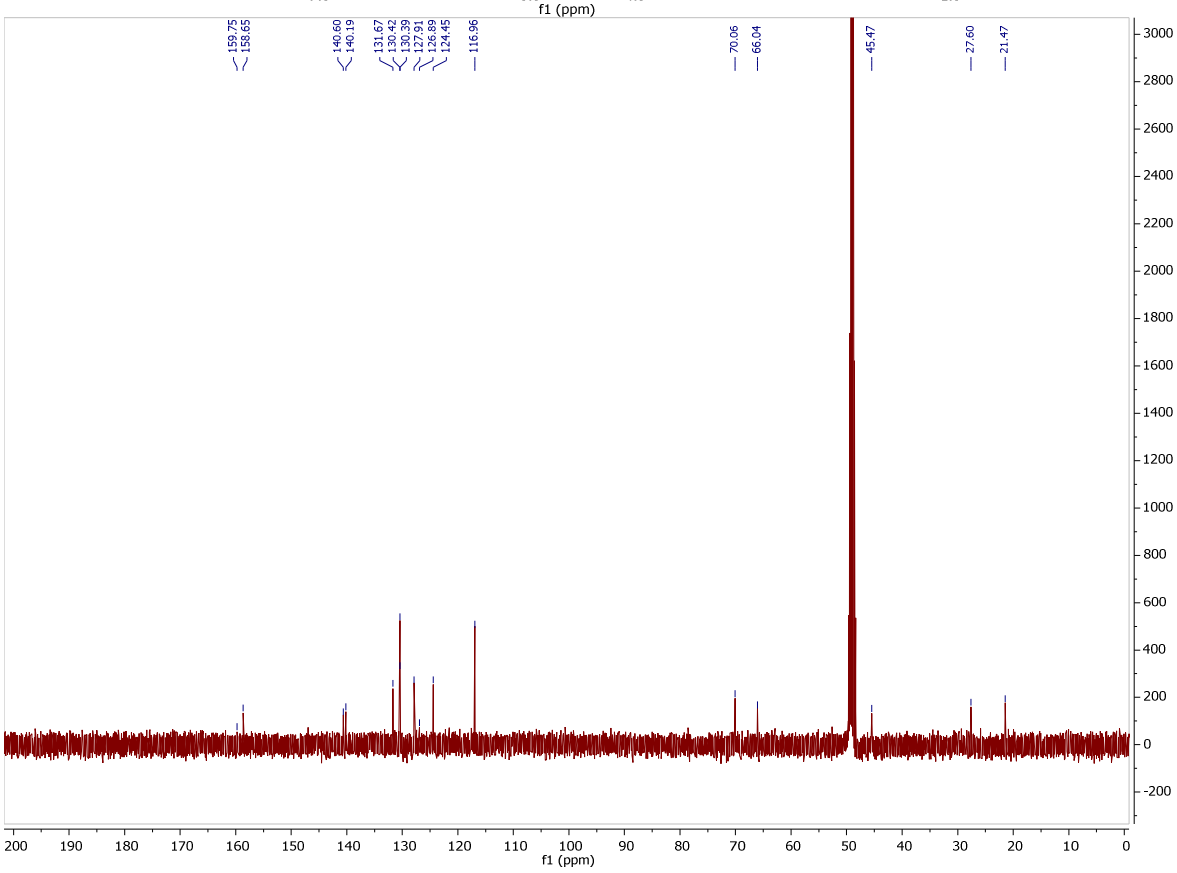
4.05
4.04
4.02
4.02
4.01
4.00
3.98
3.72
3.70
3.68
3.68
3.67
3.66
3.65
3.35
3.34
3.28
2.16
2.13
2.11
2.10
2.08
2.04
2.03
2.01
1.99
1.97
1.96
0.96
2.83
2.12
2.04
1.07
2.11
1.24
1.31
1.14
1.05
f1 (ppm)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140.60
140.19
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130.39
127.91
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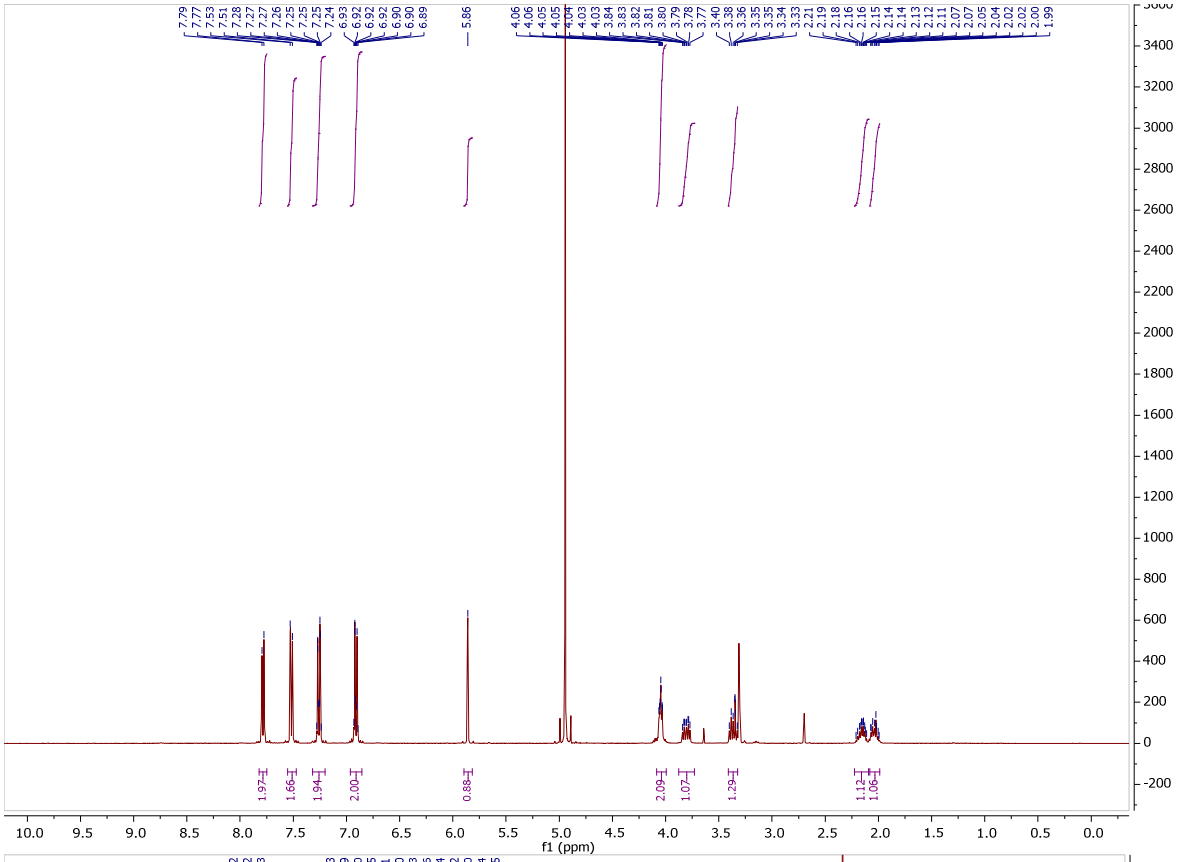
124.45
116.96
70.06
66.04
45.47
27.60
21.47
f1 (ppm)

11q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7.51
7.28
7.27
7.27
7.26
7.25
7.25
7.24
6.93
6.92
6.92
6.90
6.90
6.89
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4.06
4.05
4.05
4.04
4.03
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3.84
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2.19
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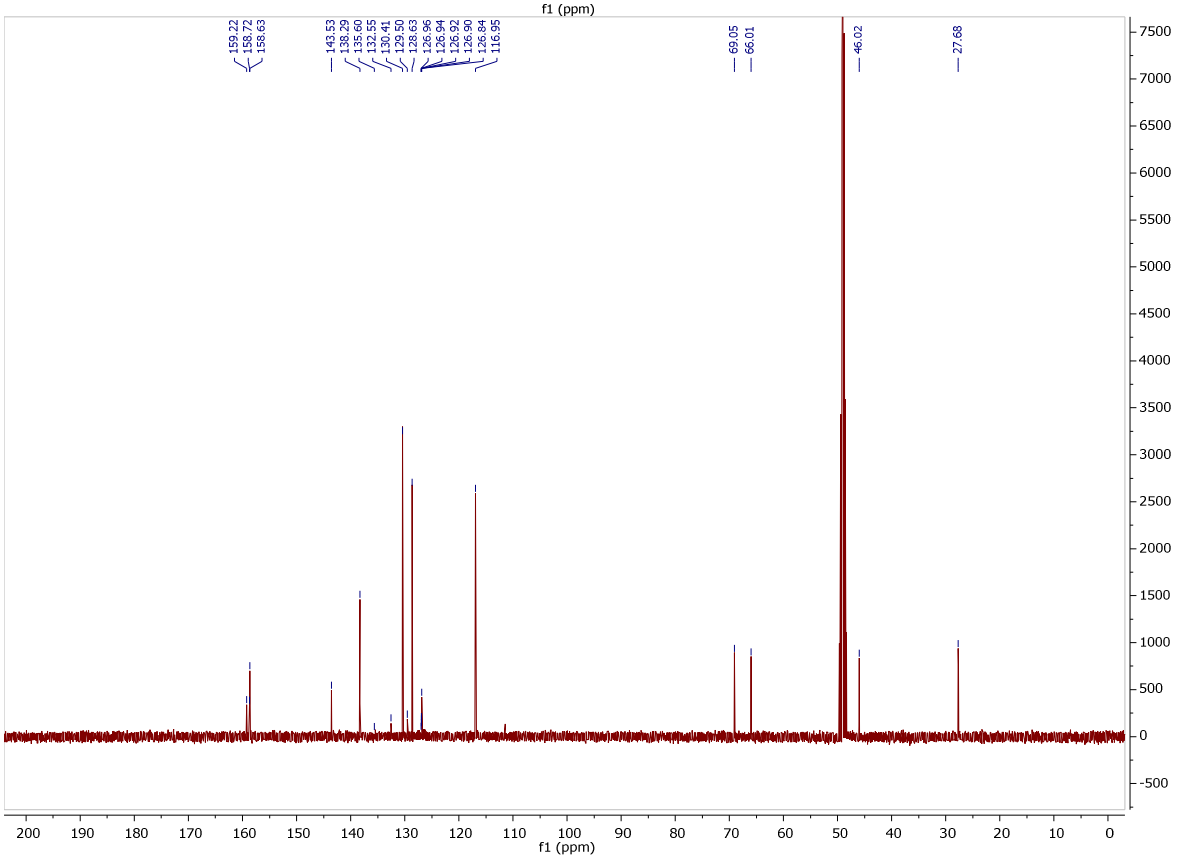
2.16
2.15
2.14
2.14
2.13
2.12
2.11
2.07
2.07
2.05
2.04
2.02
2.02
2.00
1.99
1.97
1.66
1.94
2.00
0.88
2.09
1.07
1.29
1.12
1.06
f1 (ppm)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158.72
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143.53
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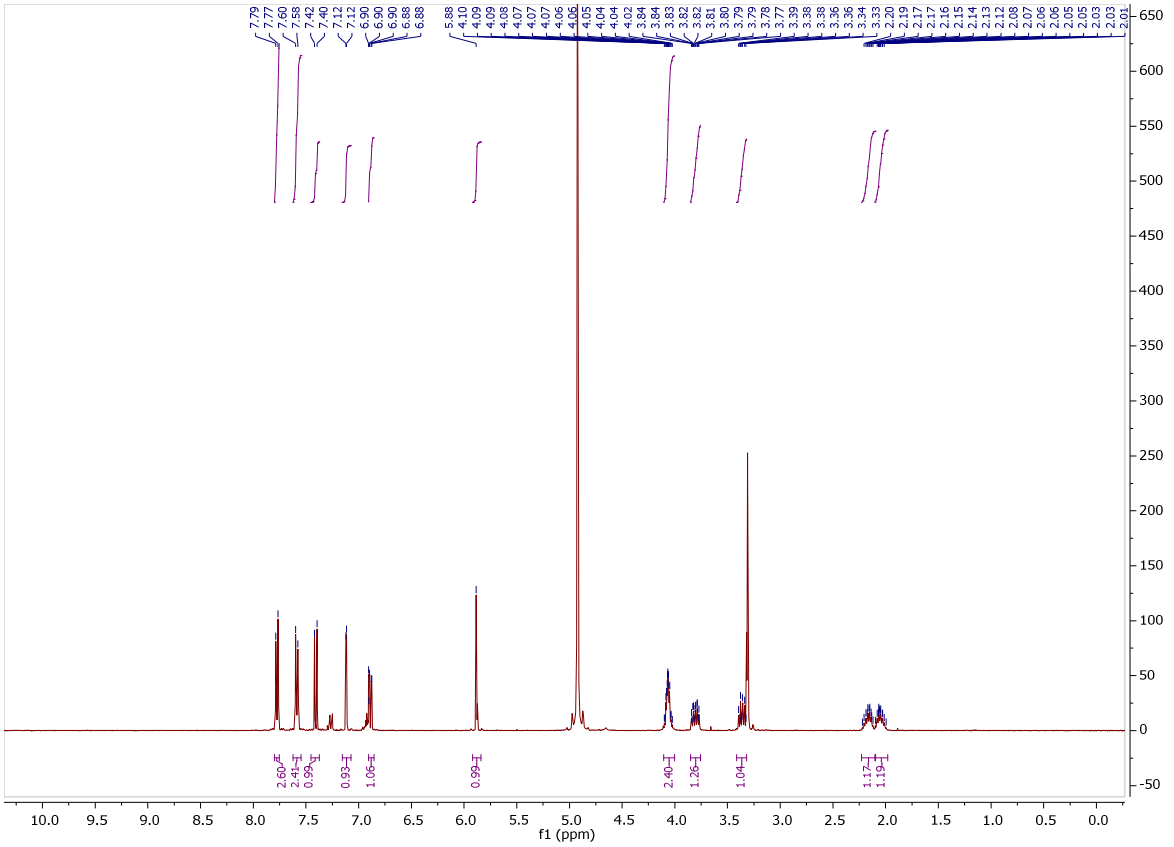
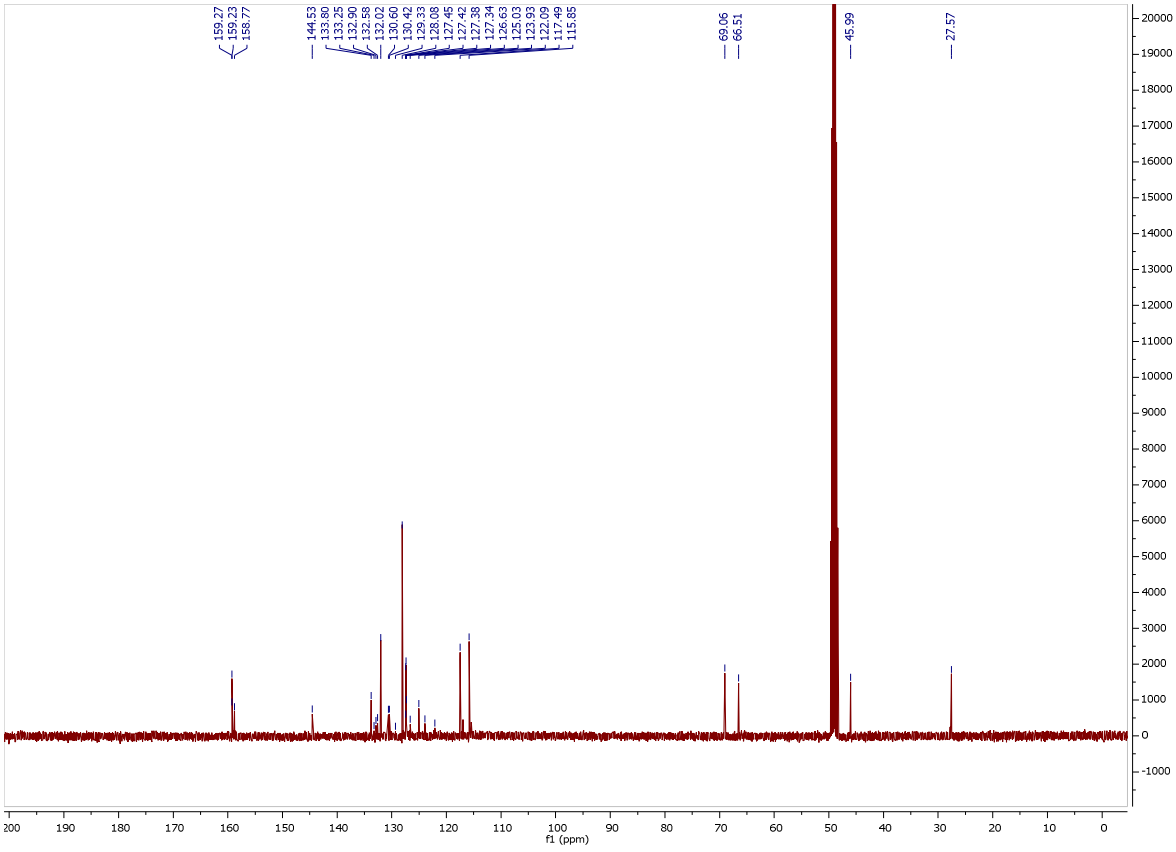
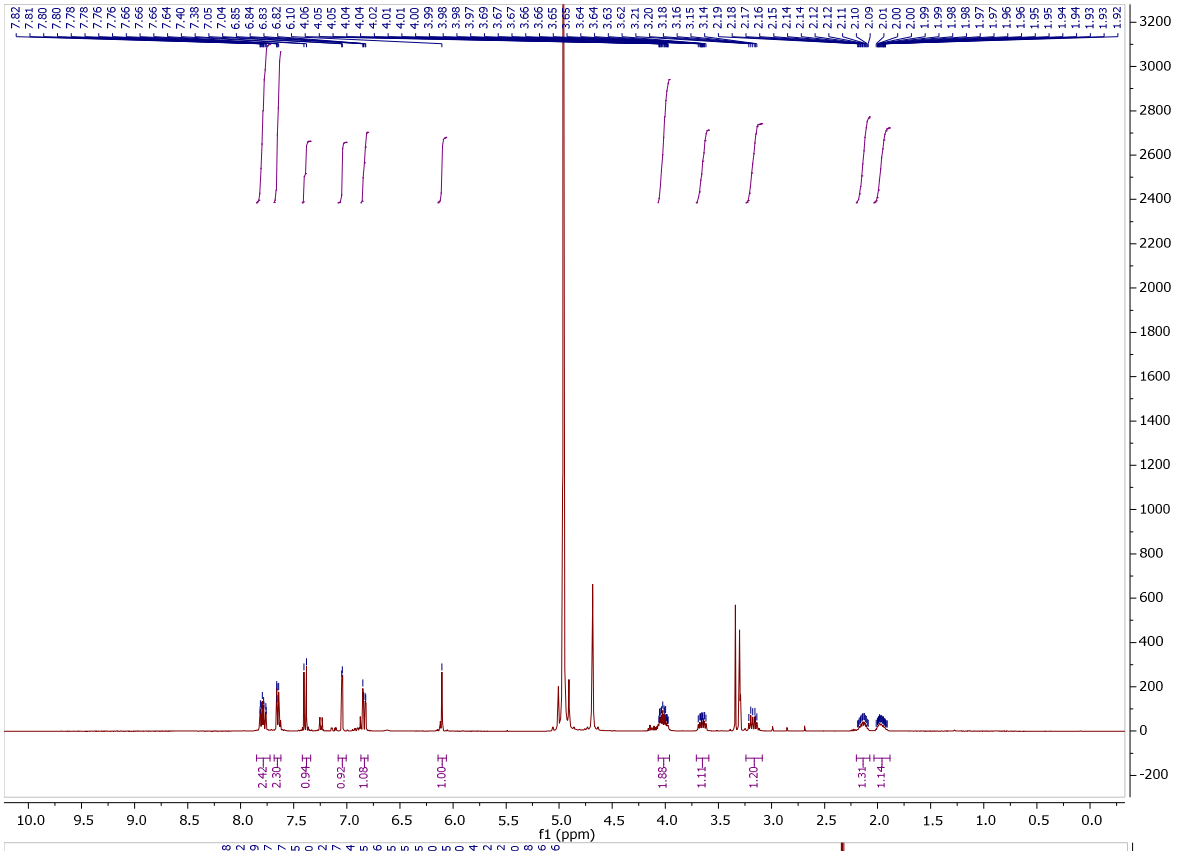
135.60
132.55
130.41
129.50
128.65
126.96
126.94
126.92
126.90
126.84
116.95
69.05
66.01
46.02
27.68
f1 (ppm)

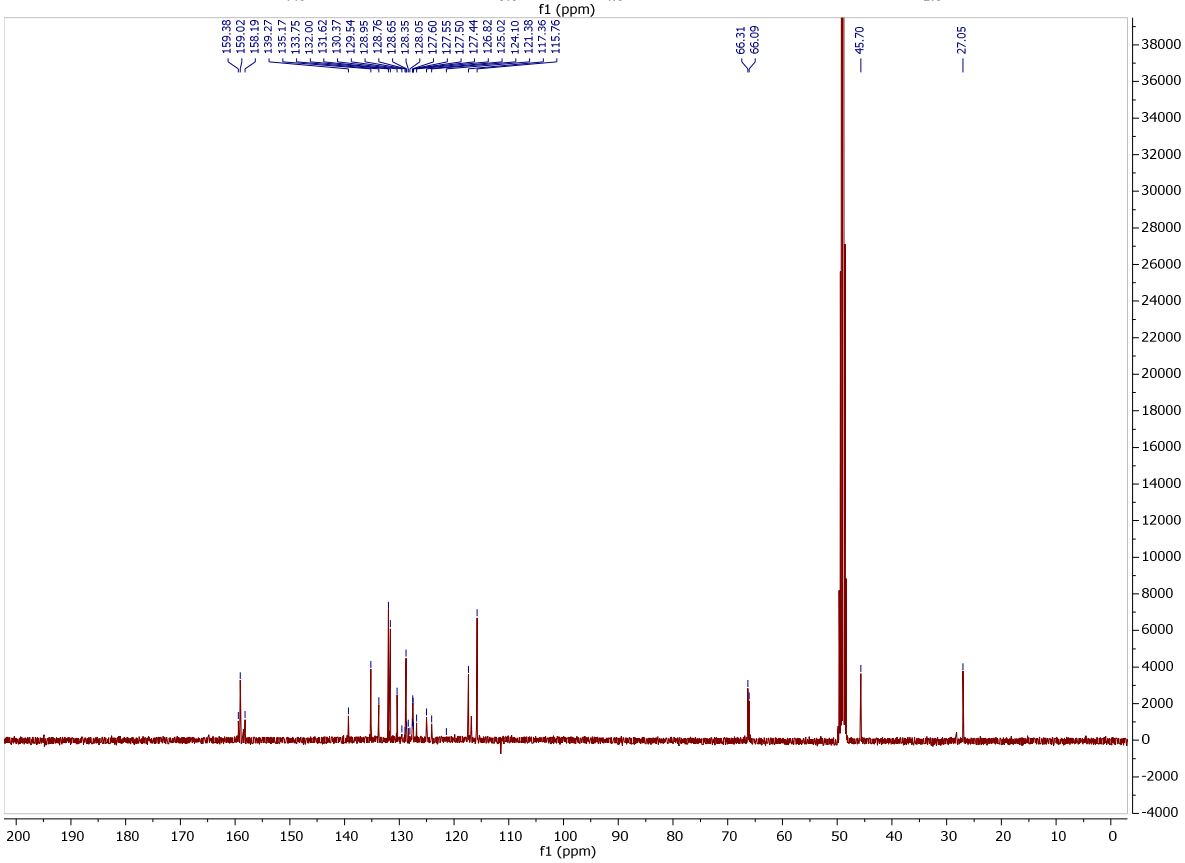
11r


7.79 7.77 7.60 7.58 7.42 7.40 7.12 7.12 6.90 6.90 6.88 6.88
5.88 4.10 4.09 4.09 4.08 4.07 4.07 4.07 4.06 4.06 4.05 4.04 4.04 4.02 3.84 3.84 3.83 3.82 3.82 3.81 3.80 3.79 3.79 3.78 3.77 3.39 3.38 3.38 3.36 3.36 3.34 3.33 2.20 2.19 2.17 2.17 2.16 2.15 2.14 2.13 2.12 2.08 2.07 2.06 2.06 2.05 2.05 2.03 2.03 2.01
2.60 2.41 0.99 0.93 1.06 0.99 2.40 1.26 1.04 1.17 1.19
f1 (ppm)

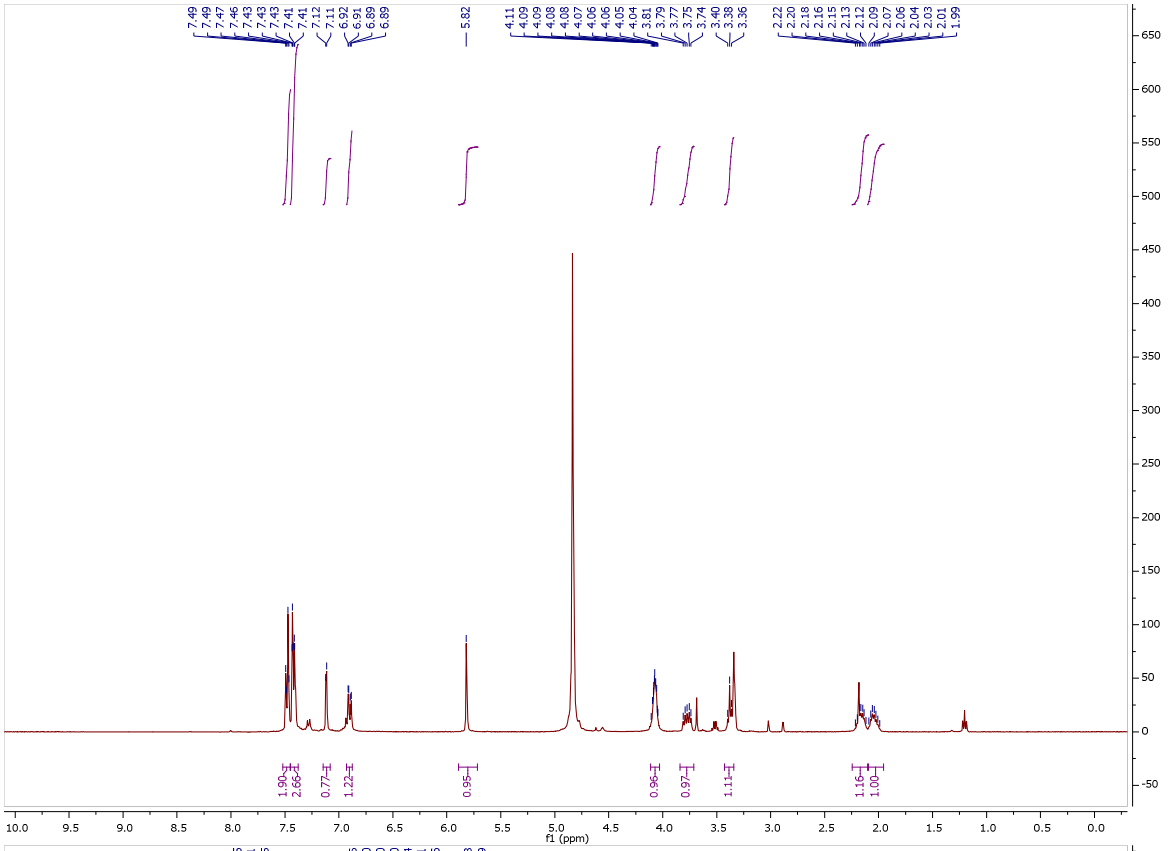

159.27 159.23 158.77
144.53 133.80 133.25 132.90 132.58 132.02 130.60 130.42 129.33 128.08 127.46 127.42 127.38 127.34 126.63 125.03 123.93 122.09 117.49 115.85
69.06 66.51
45.99
27.57
f1 (ppm)

11s





11t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4.09
4.09
4.08
4.08
4.07
4.06
4.06
4.05
4.04
3.81
3.79
3.77
3.75
3.74
3.40
3.38
3.36
2.22
2.20
2.18
2.16
2.15
2.13
2.12
2.09
2.07
2.06
2.04
2.03
2.01
1.99
1.90
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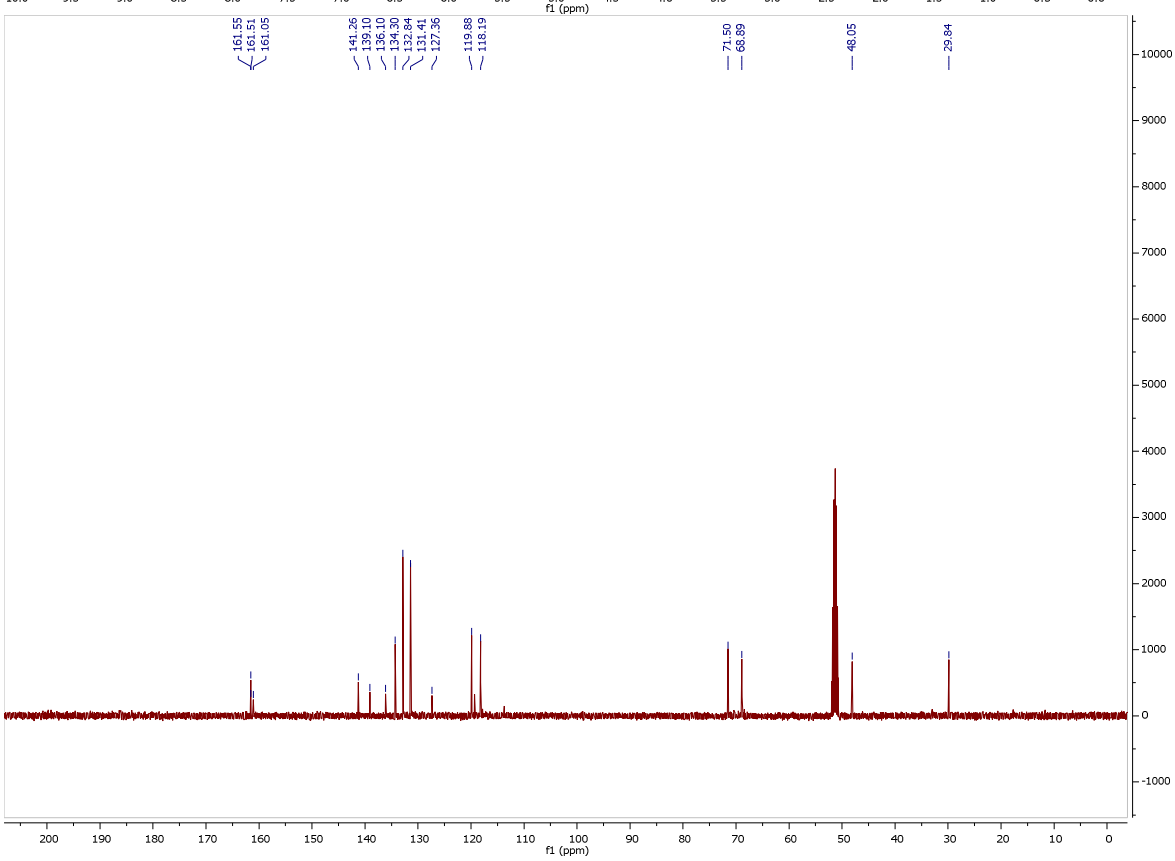
0.77
1.22
0.95
0.96
0.97
1.11
1.16
1.00
f1 (ppm)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161.05
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139.10
136.10
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132.84
131.41
127.36
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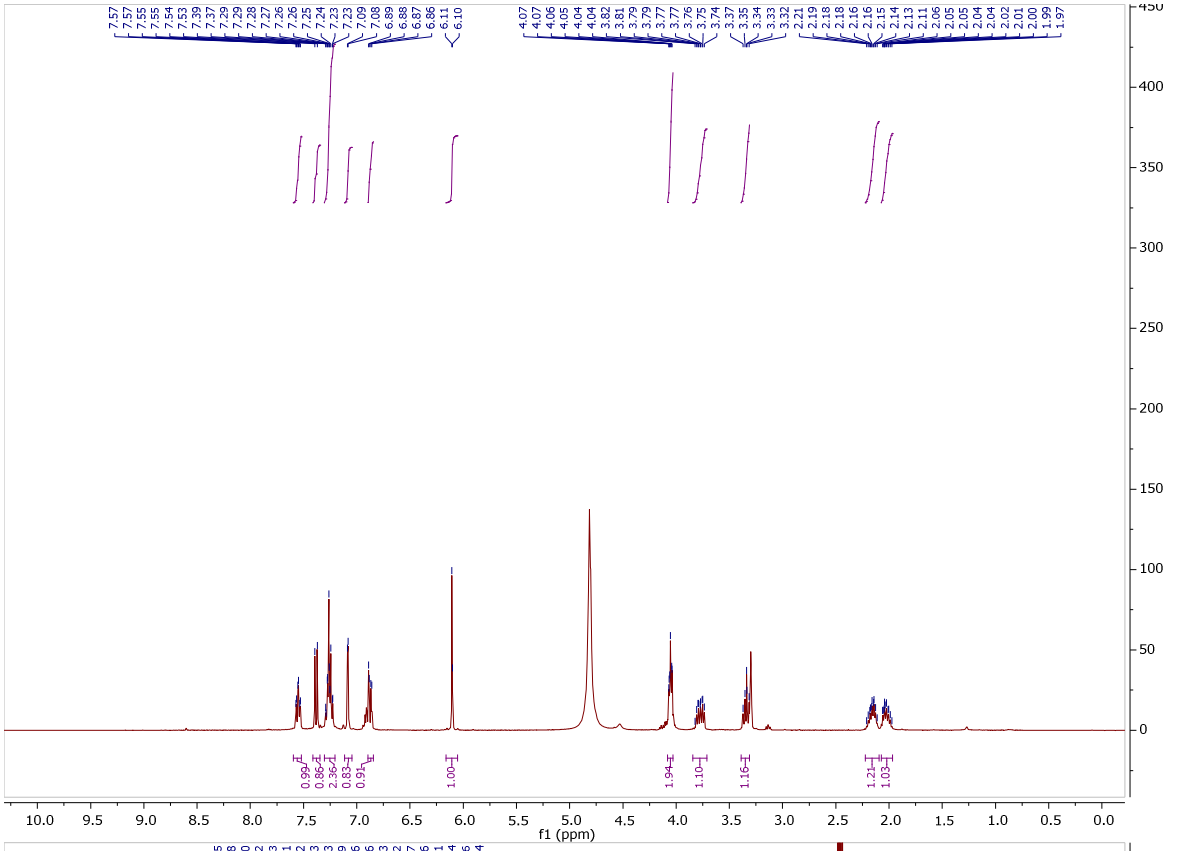
118.19
71.50
68.89
48.05
29.84
f1 (ppm)

11u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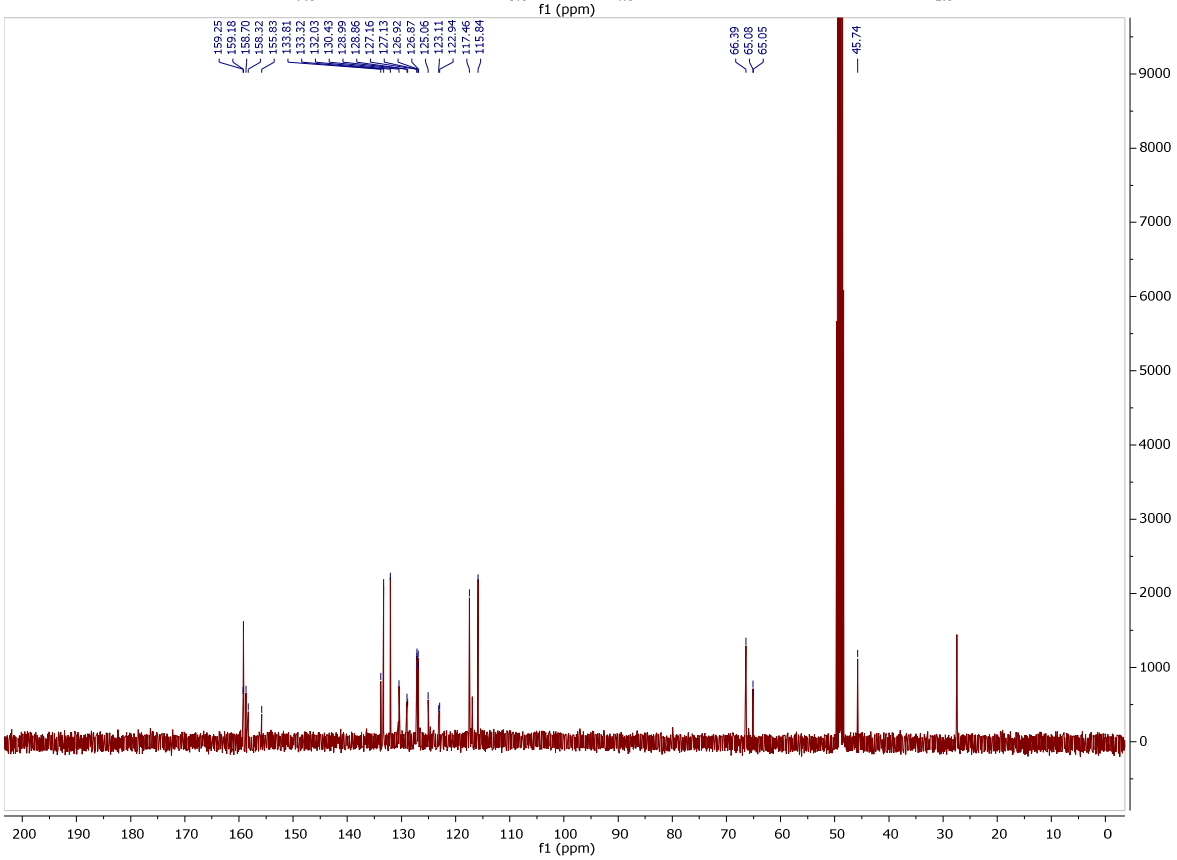
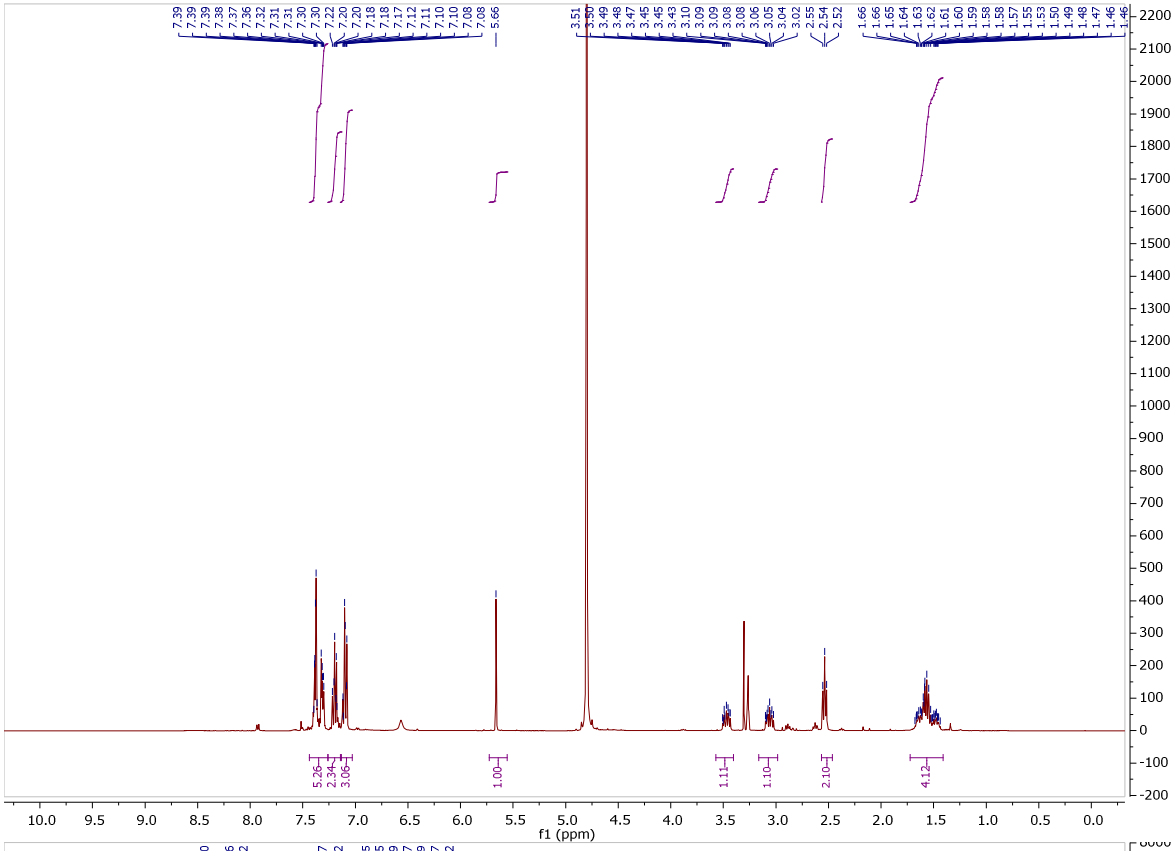
4.07 4.07 4.06 4.05 4.04 4.04 3.82 3.81 3.79 3.79 3.77 3.77 3.76 3.75 3.74 3.37 3.35 3.34 3.33 3.32 2.21 2.19 2.18 2.18 2.16 2.16 2.15 2.14 2.13 2.11 2.06 2.05 2.05 2.04 2.04 2.02 2.01 2.00 1.99 1.97
0.99 0.86 2.36 0.83 0.91 1.00 1.94 1.10 1.16 1.21 1.03
f1 (ppm)


159.25 159.18 158.70 158.32 155.83 133.81 133.32 132.03 130.43 128.99 128.86 127.16 127.13 126.92 126.87 125.06 123.11 122.94 117.46 115.84
66.39 65.08 65.05
45.74
f1 (ppm)

11v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7.31
7.30
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7.22
7.20
7.18
7.18
7.17
7.12
7.11
7.10
7.10
7.08
7.08
5.66
3.51
3.50
3.49
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1.53
1.50
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1.48
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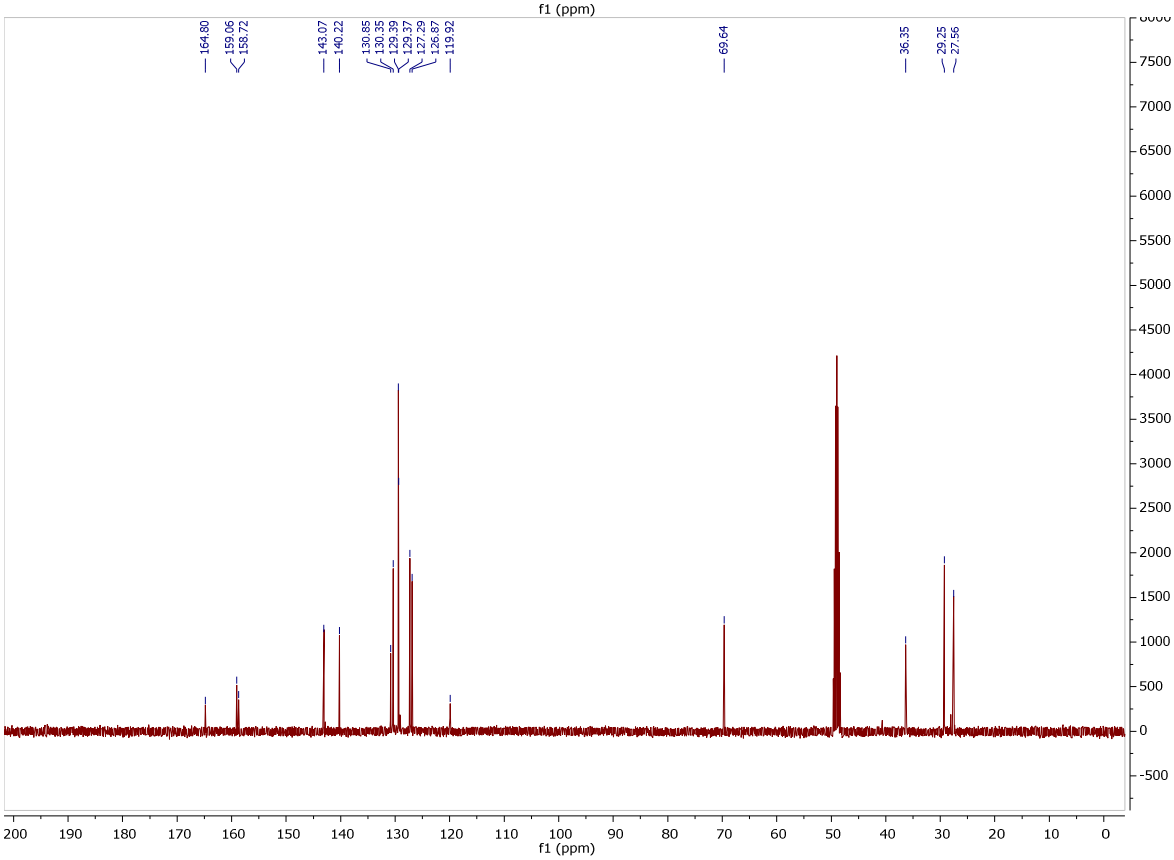
4.12
f1 (ppm)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130.85
130.35
129.39
129.37
127.29
126.87
119.92
69.64
36.35
29.25
27.56
f1 (ppm)