Supporting Information

Design, Synthesis, and Biological Evaluation of Substituted 4,6-Dihydrospiro[[1,2,3]triazolo[4,5-*b*]pyridine-7,3'-indoline]-2',5(3*H*)-dione Analogues as Potent NS4B Inhibitors for the Treatment of Dengue Virus Infection

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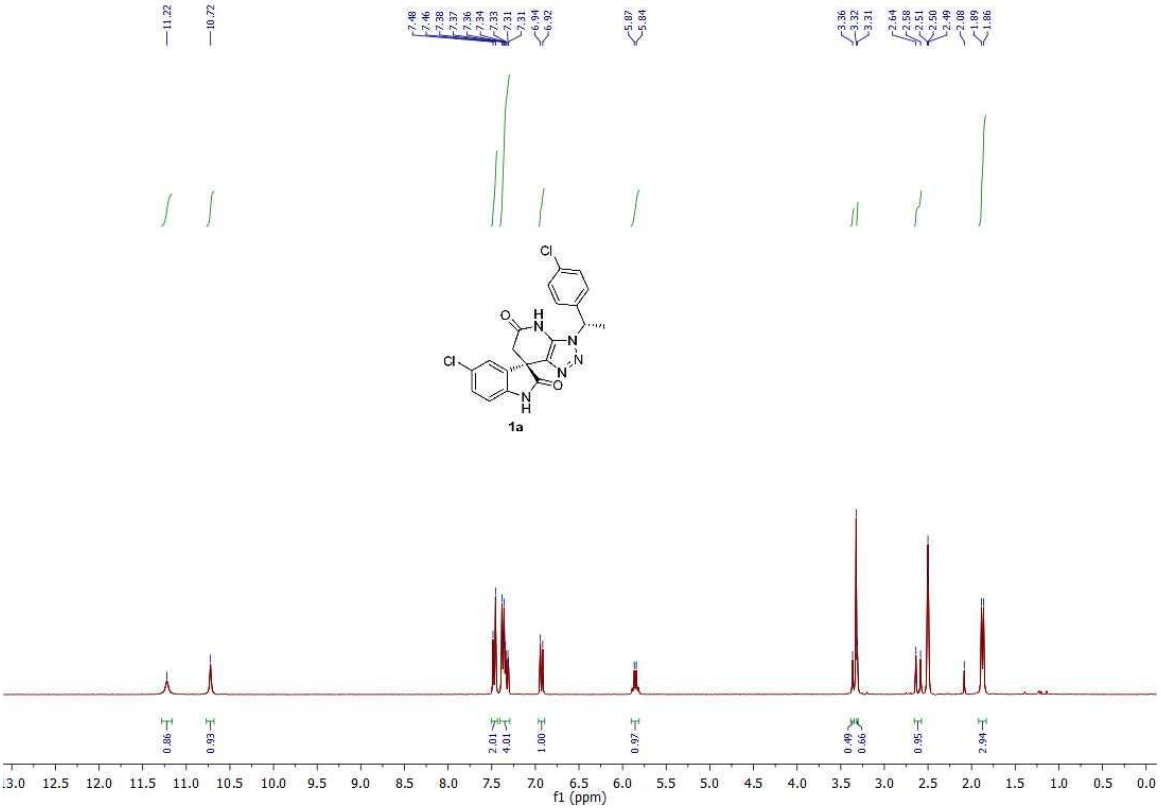
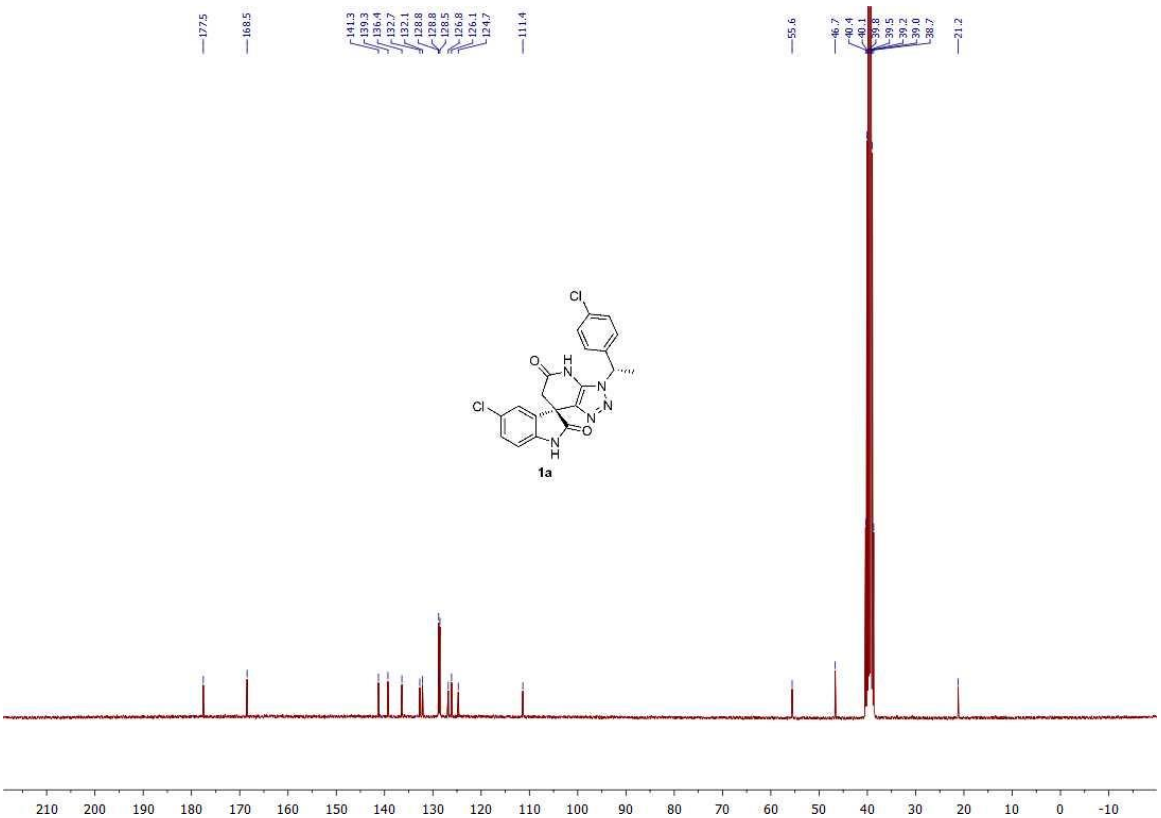
Table of Contents

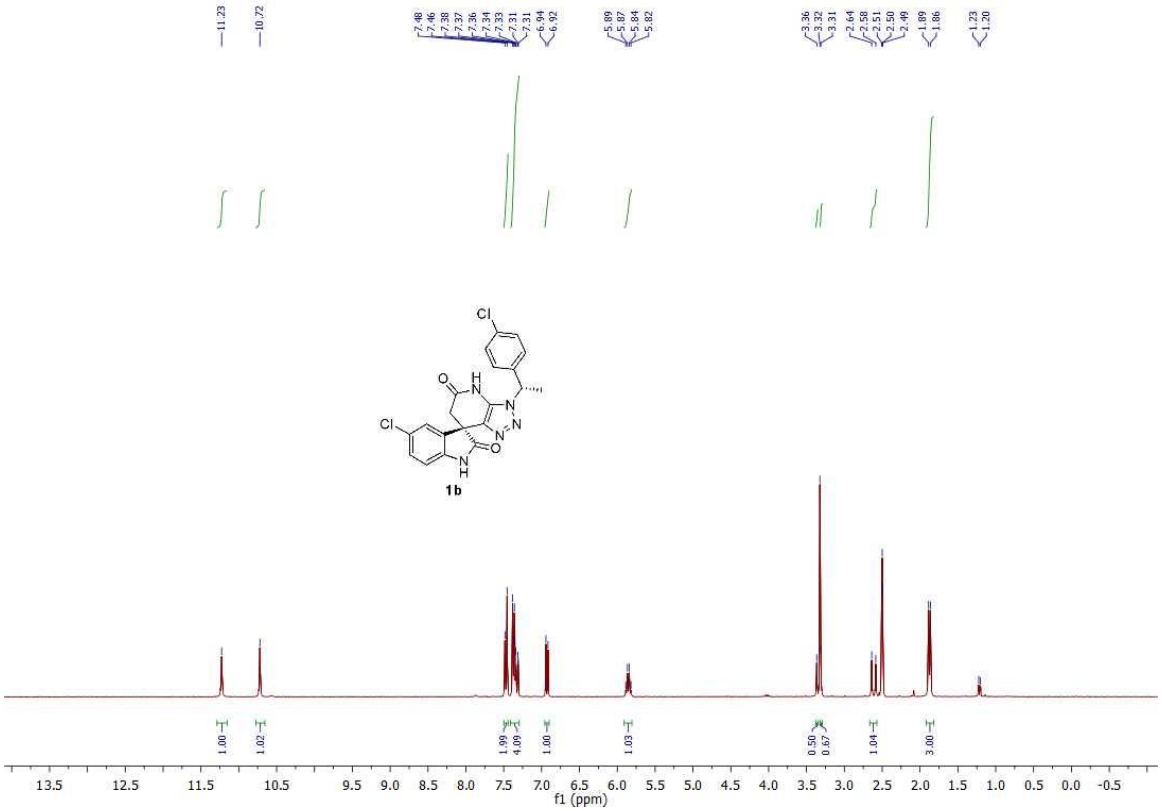
Copies of ^{1}H and ^{13}C NMR spectra……..S2-S65

Table S1. Crystal Data for compound **7**……..……..S66

Copies of ^{1}H and ^{13}C NMR Spectra



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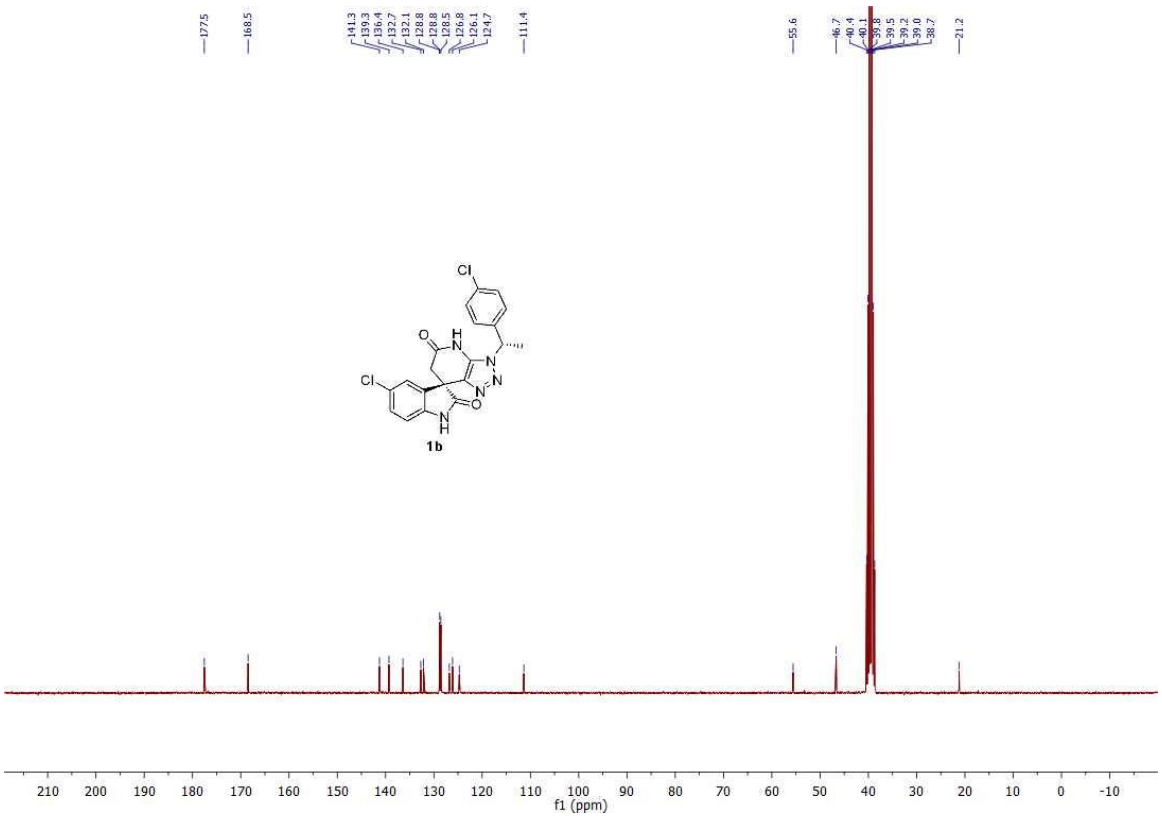
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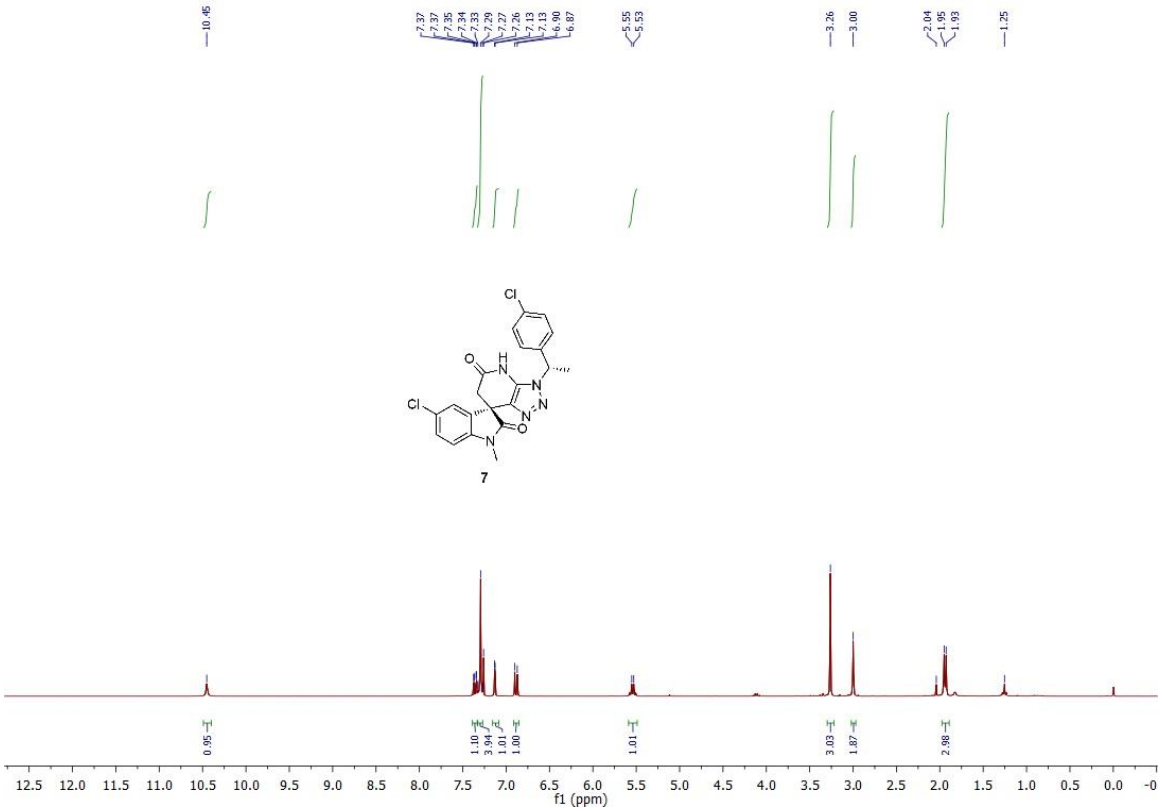
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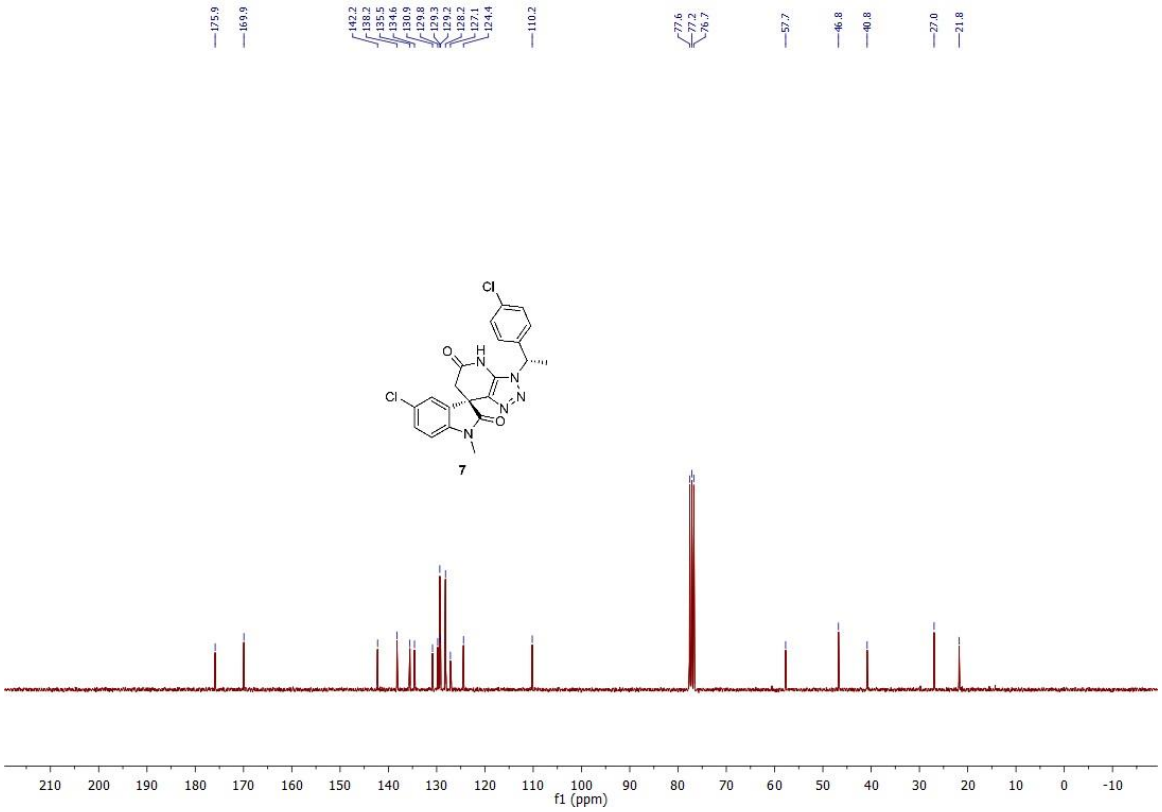
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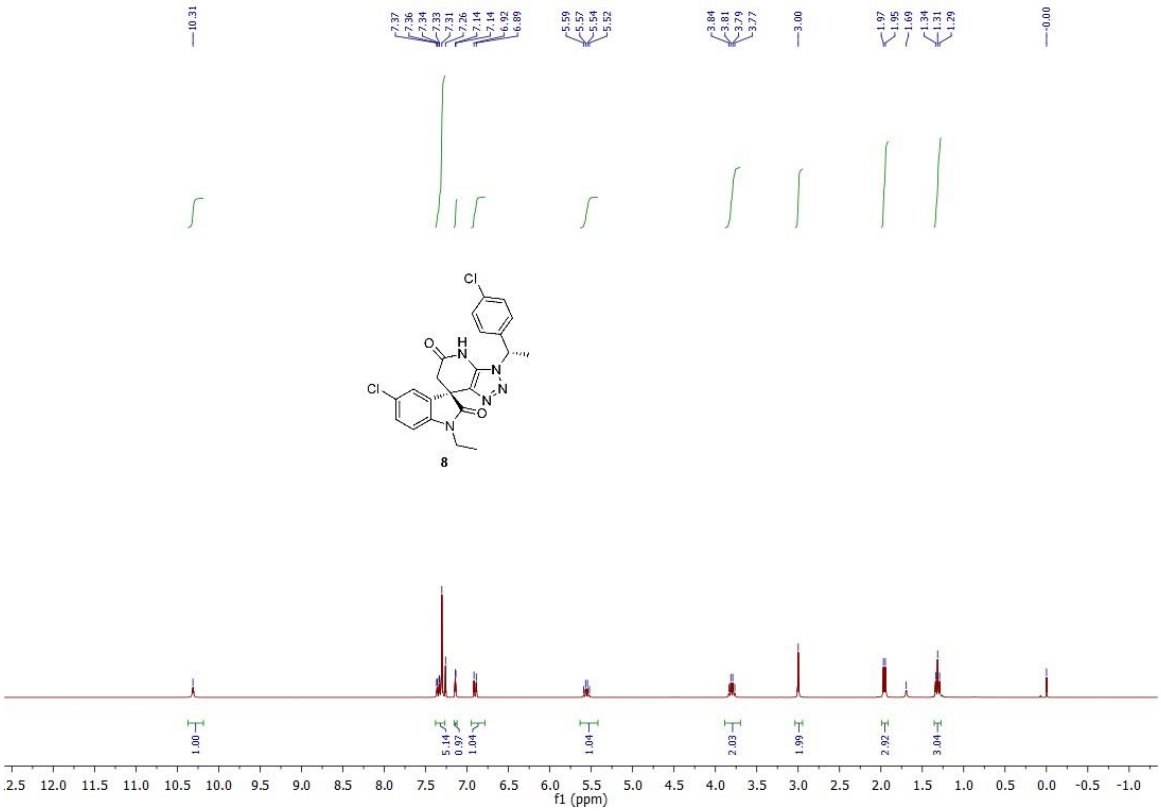
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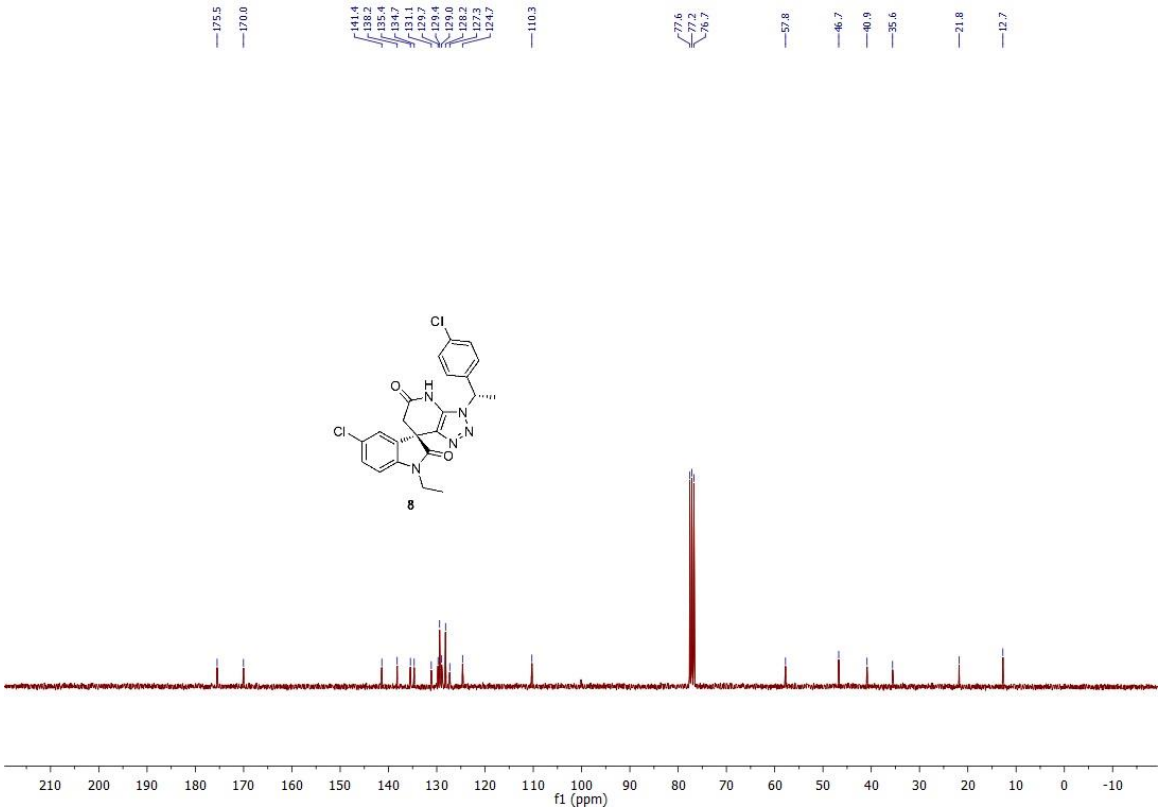
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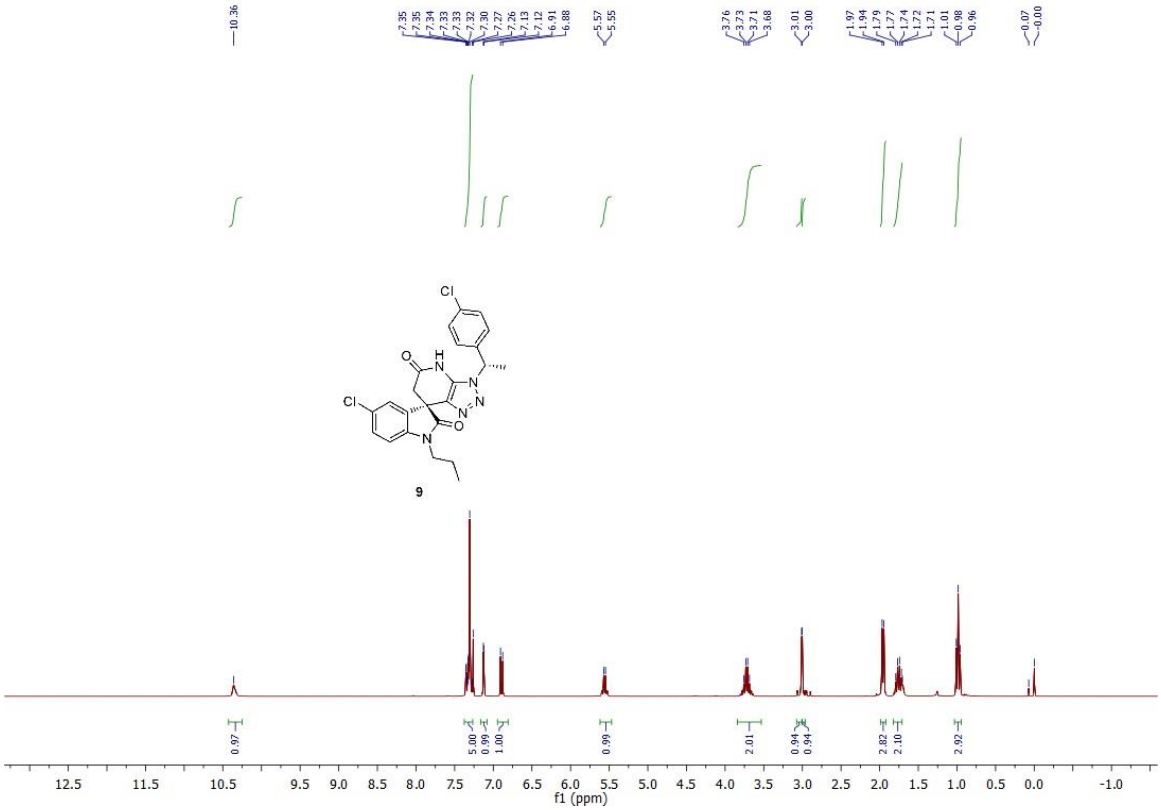
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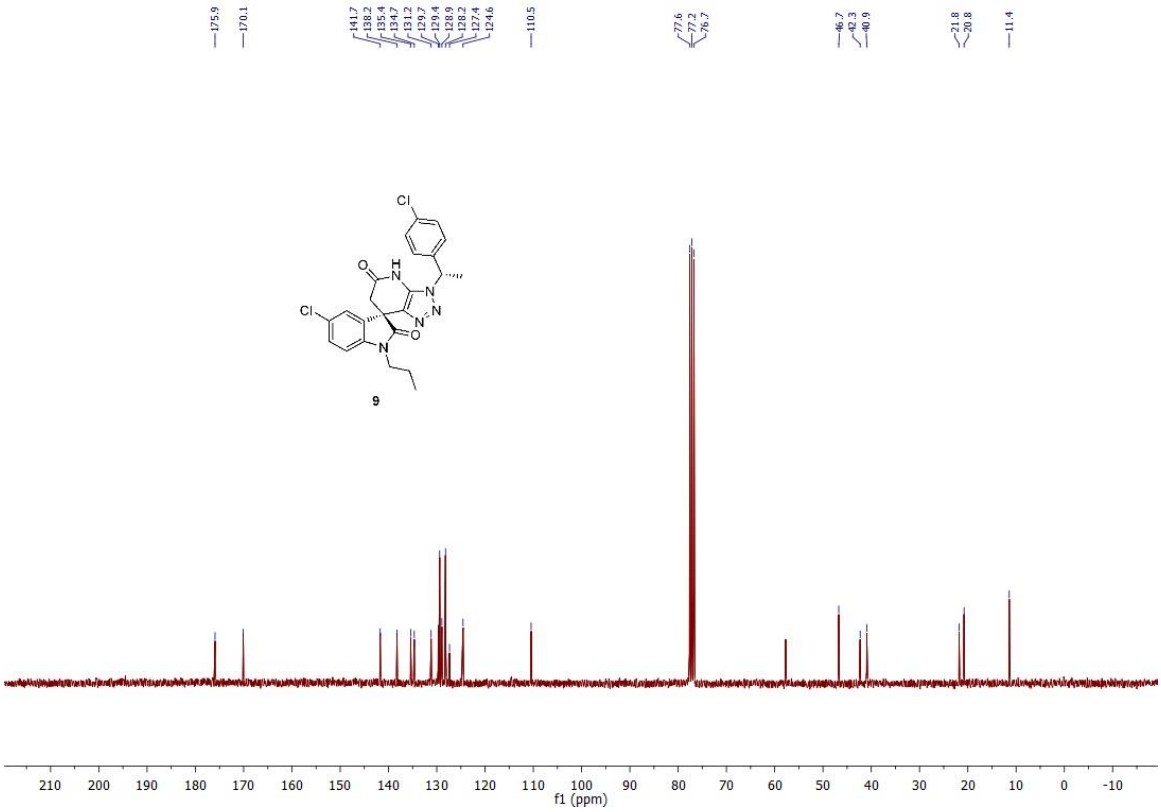
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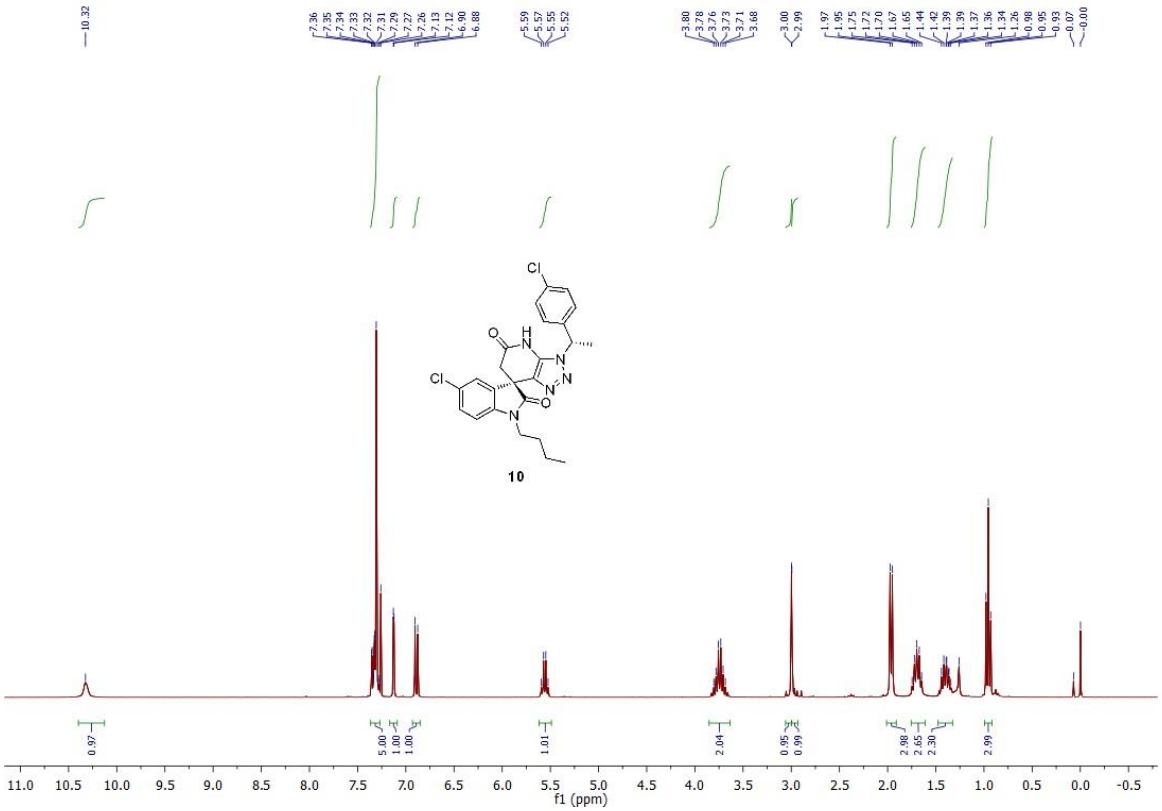
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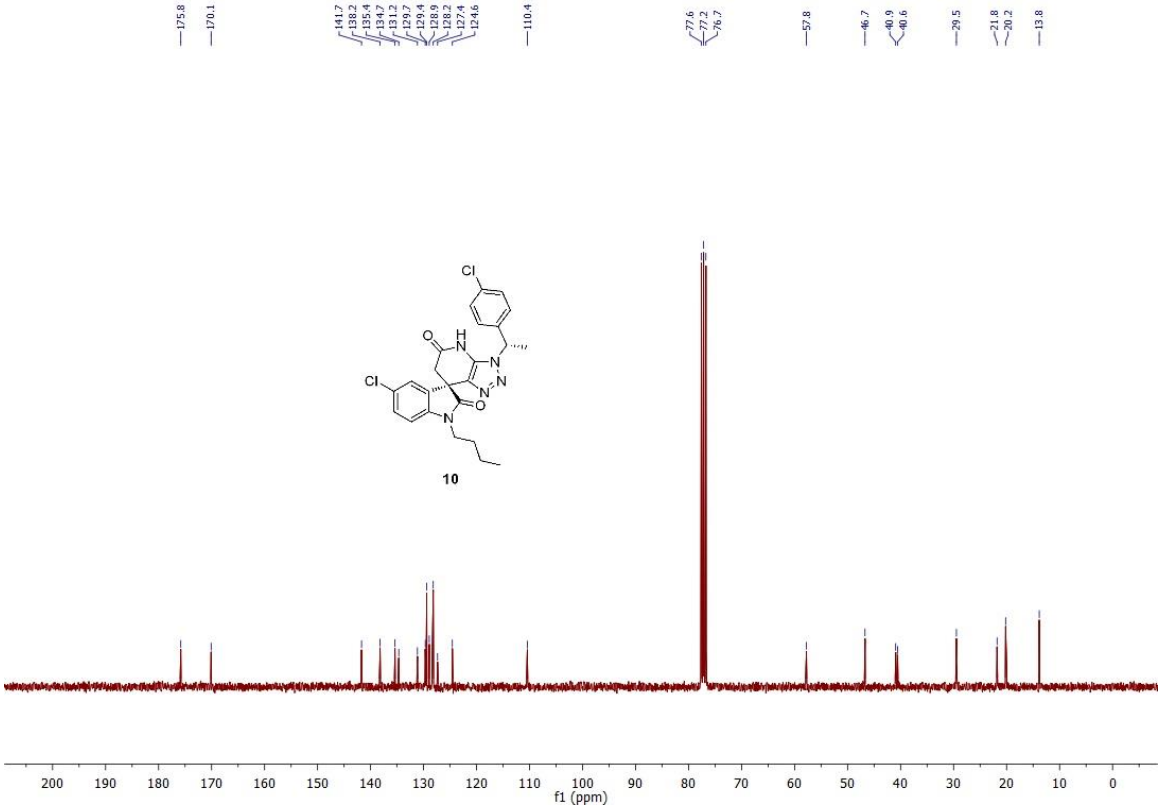
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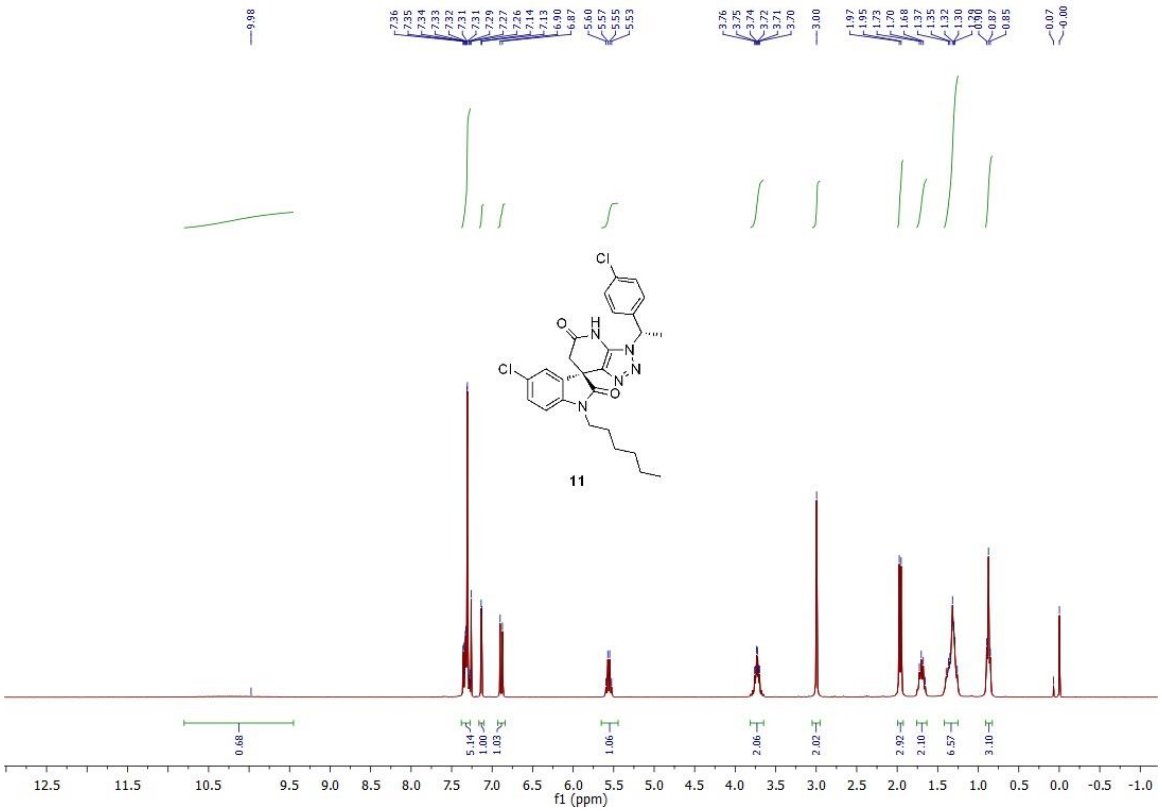
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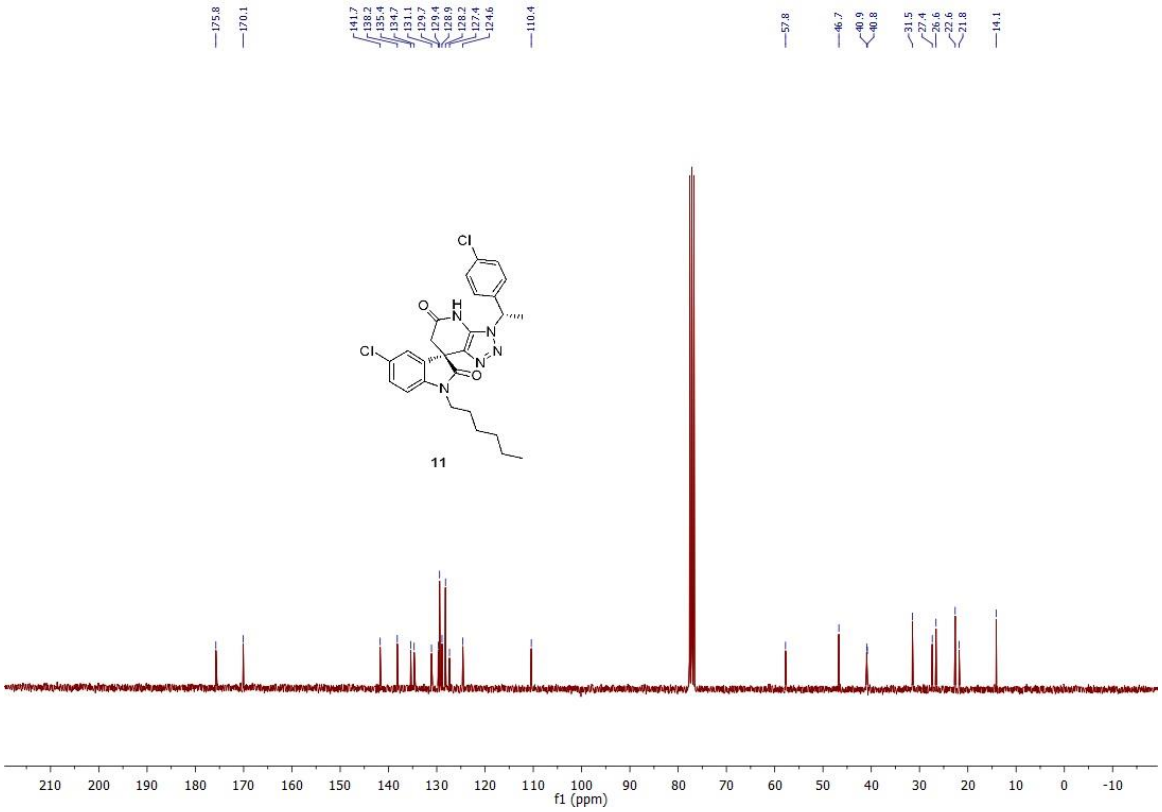
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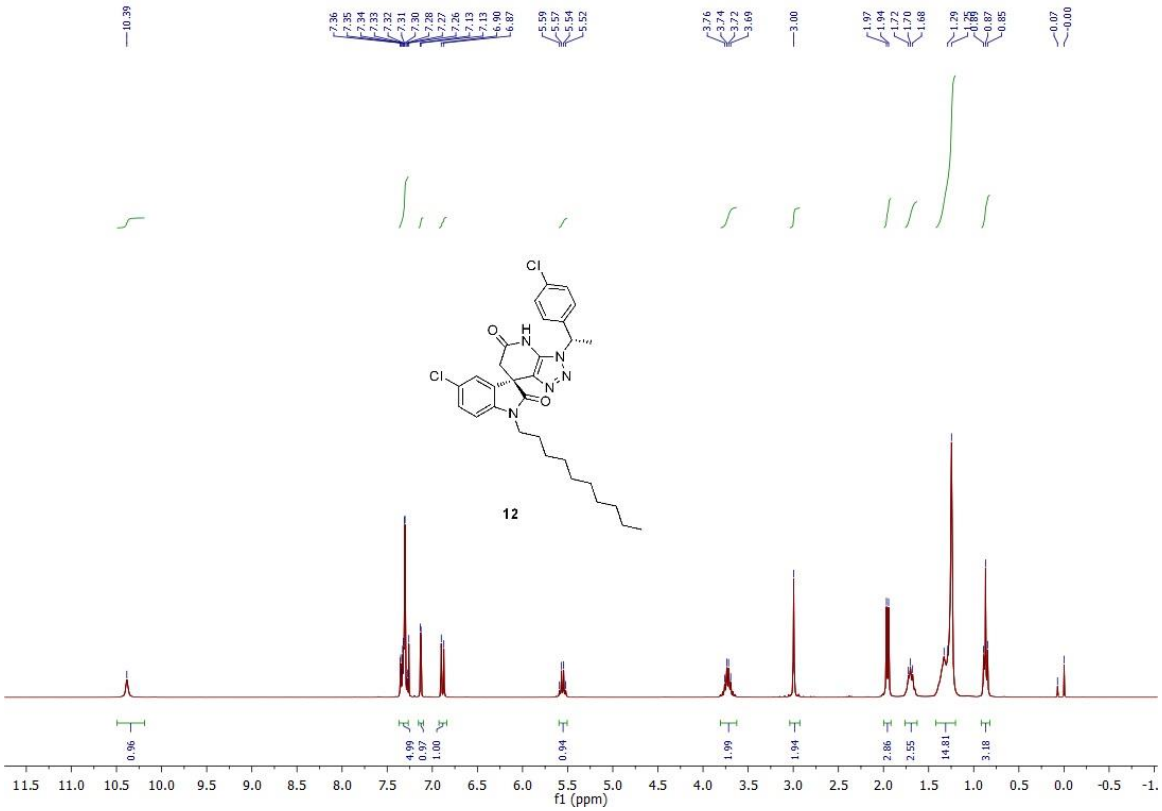
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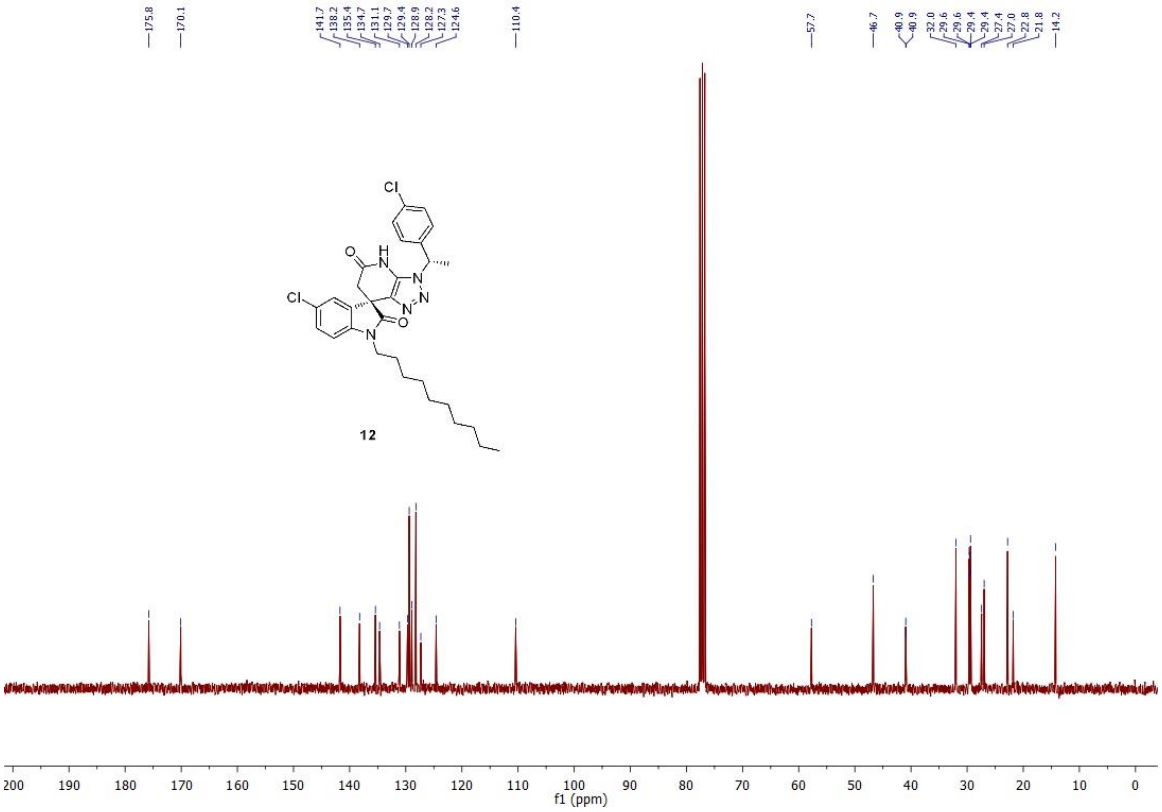
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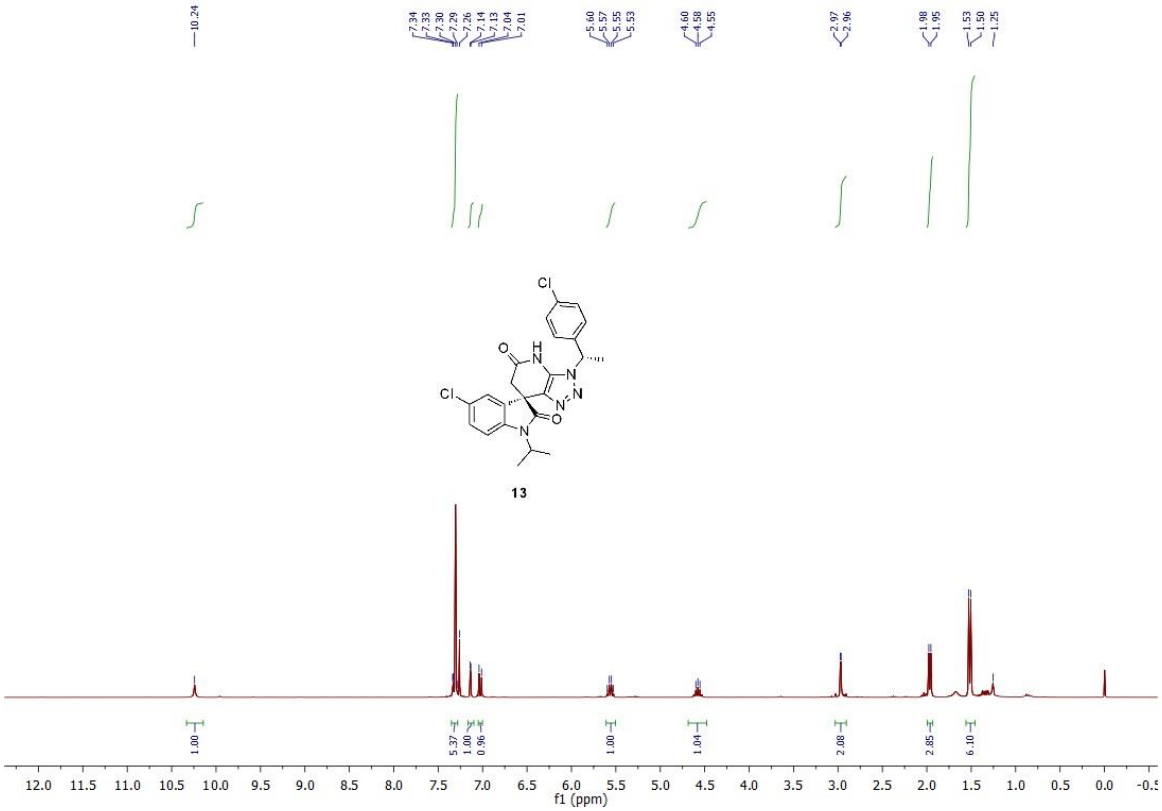
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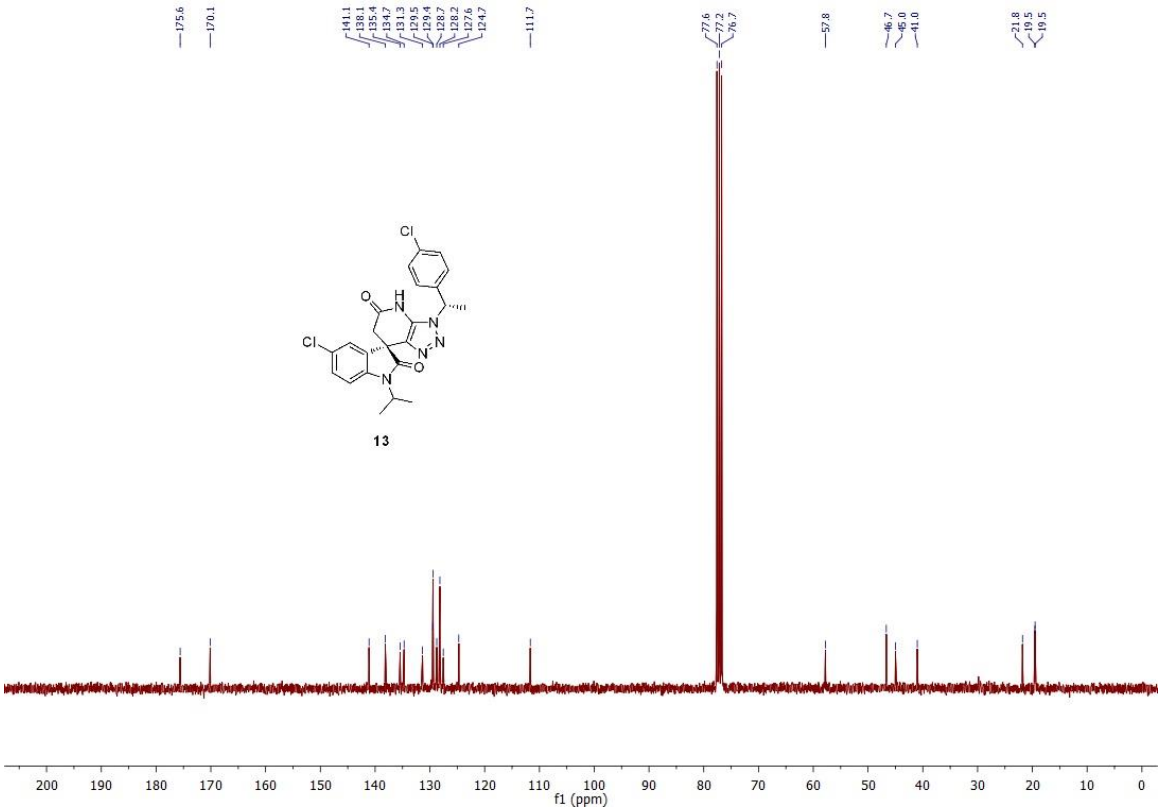
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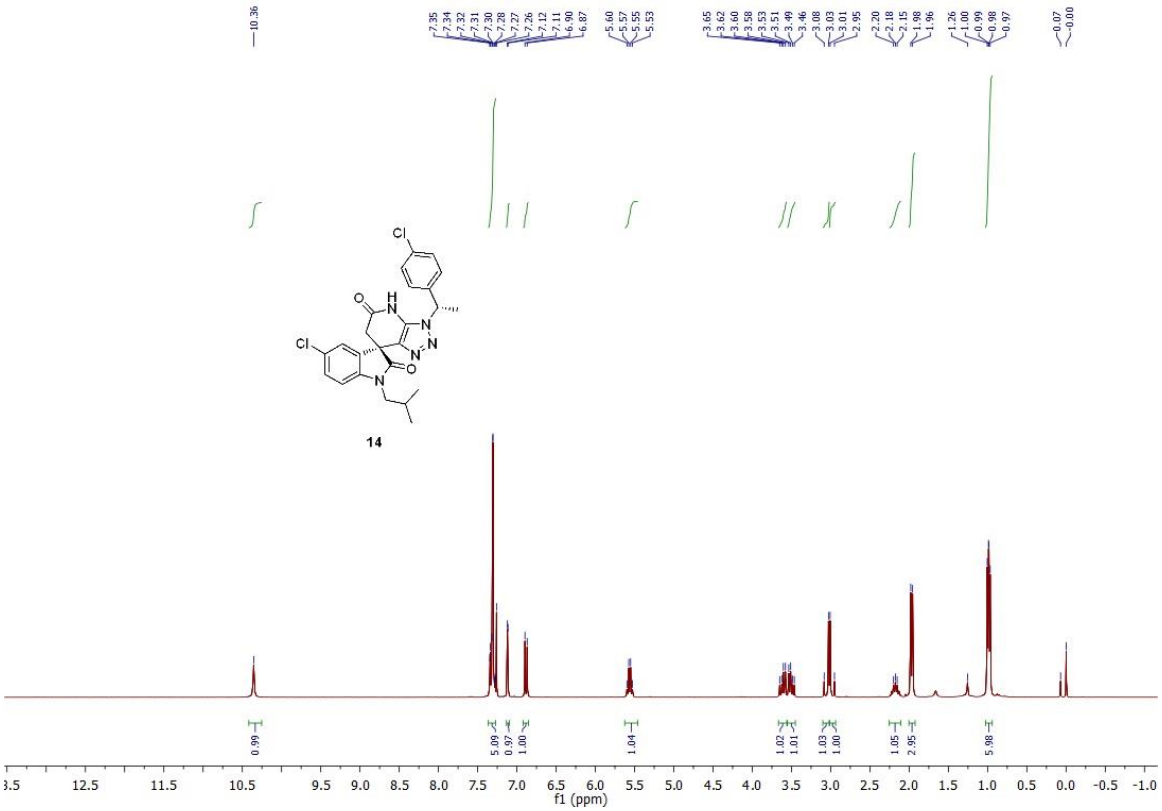
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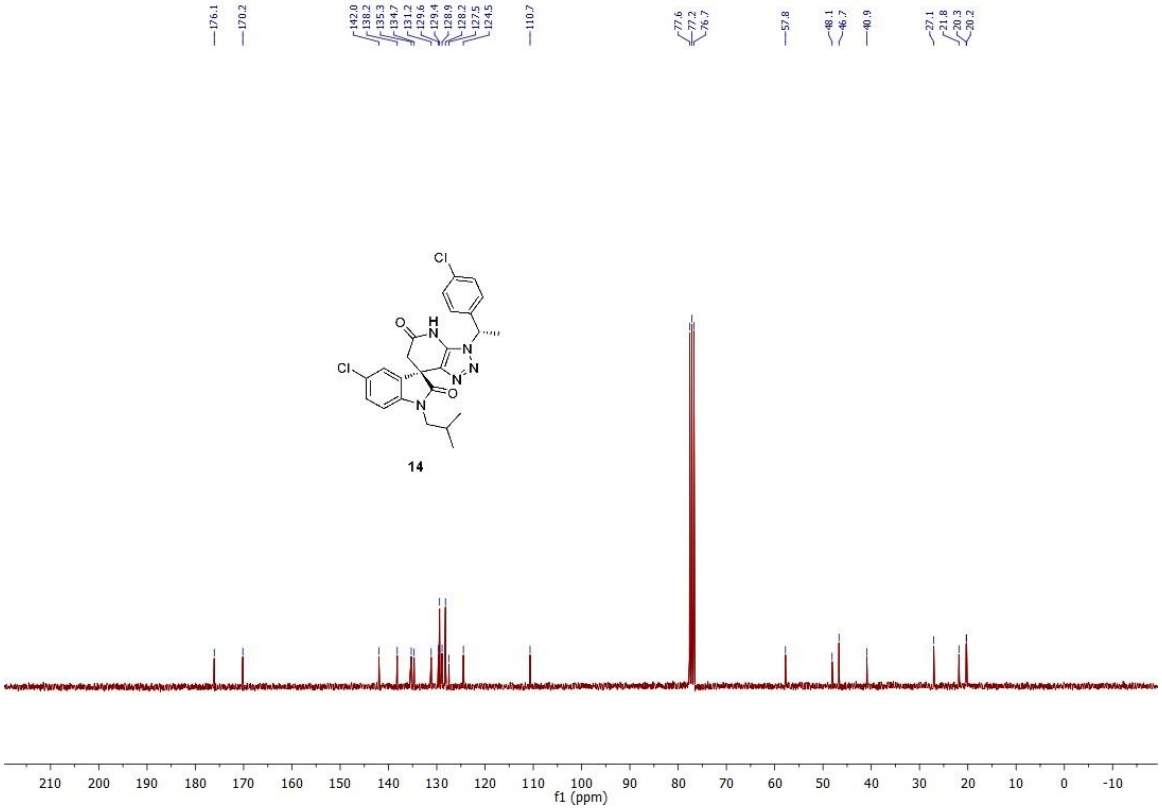
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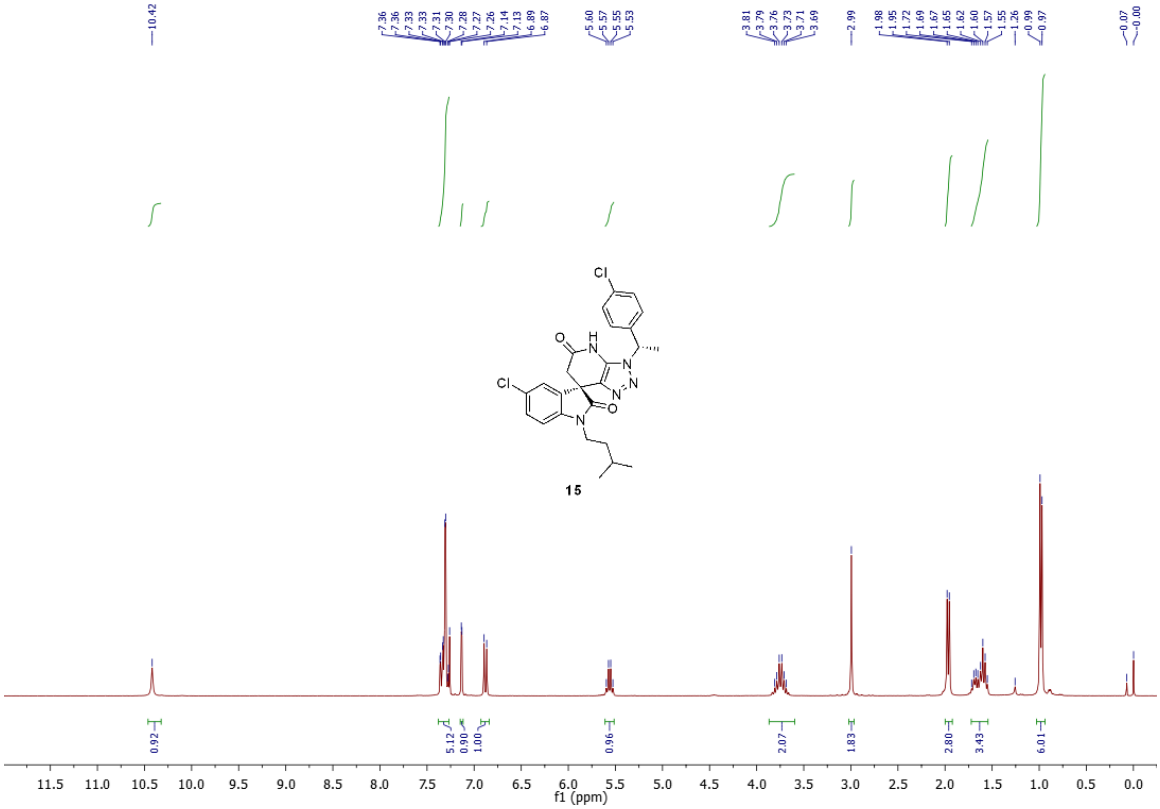
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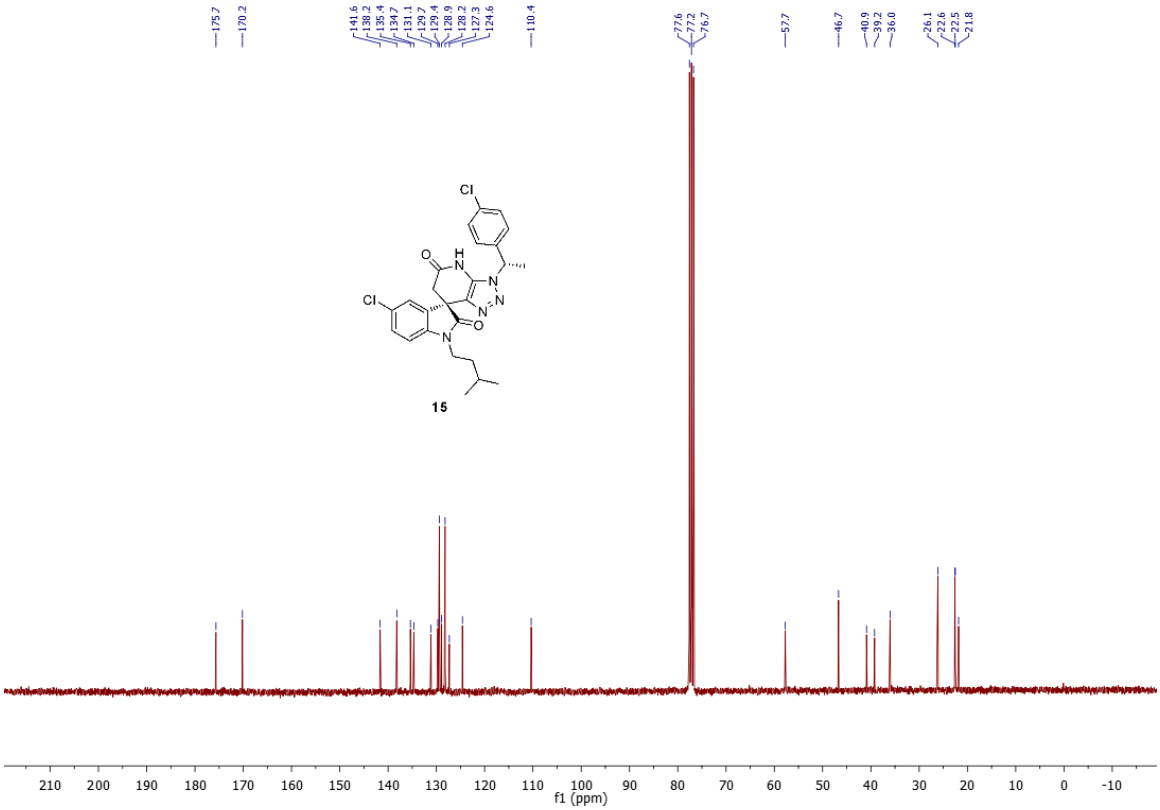
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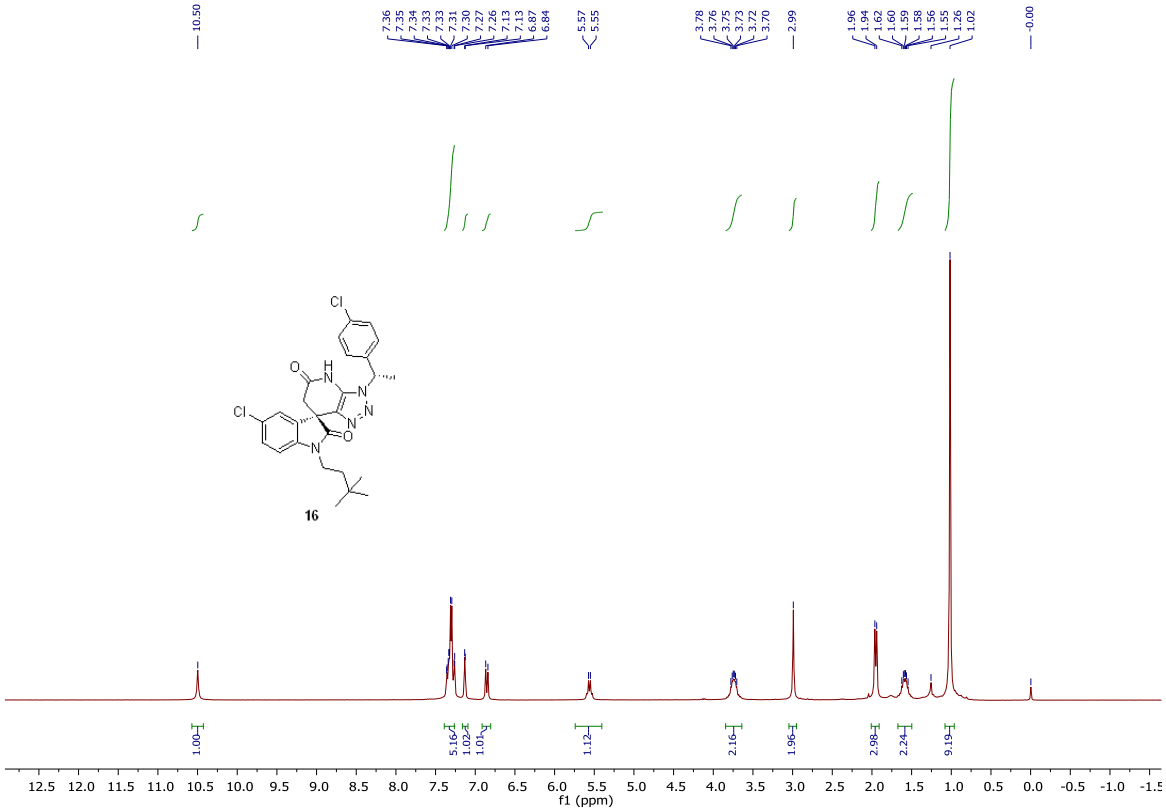
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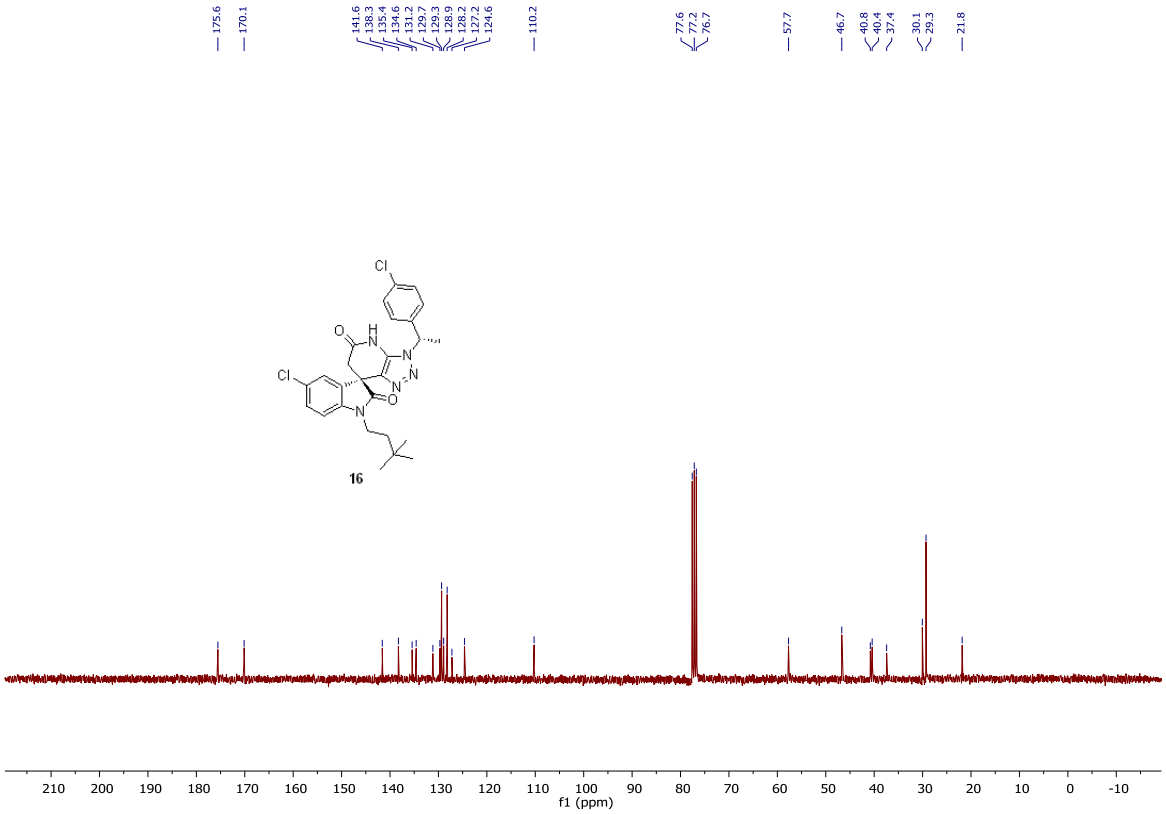
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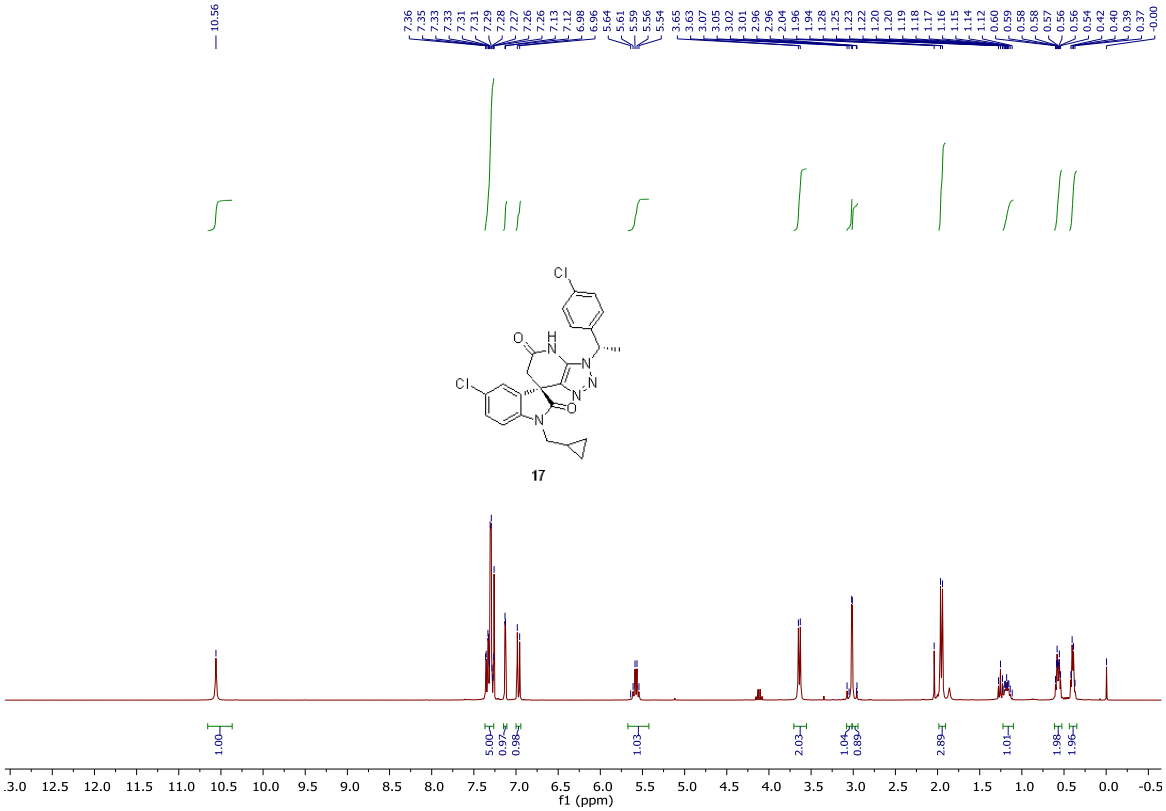
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3.65 3.63 3.07 3.05 3.02 3.01 2.96 2.96 2.04 1.96 1.94 1.28 1.25 1.23 1.22 1.20 1.20 1.19 1.18 1.17 1.16 1.15 1.14 1.12 0.60 0.59 0.58 0.58 0.57 0.56 0.56 0.54 0.42 0.40 0.39 0.37 -0.00
1.00
5.00
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2.03
1.04
0.89
2.89
1.01
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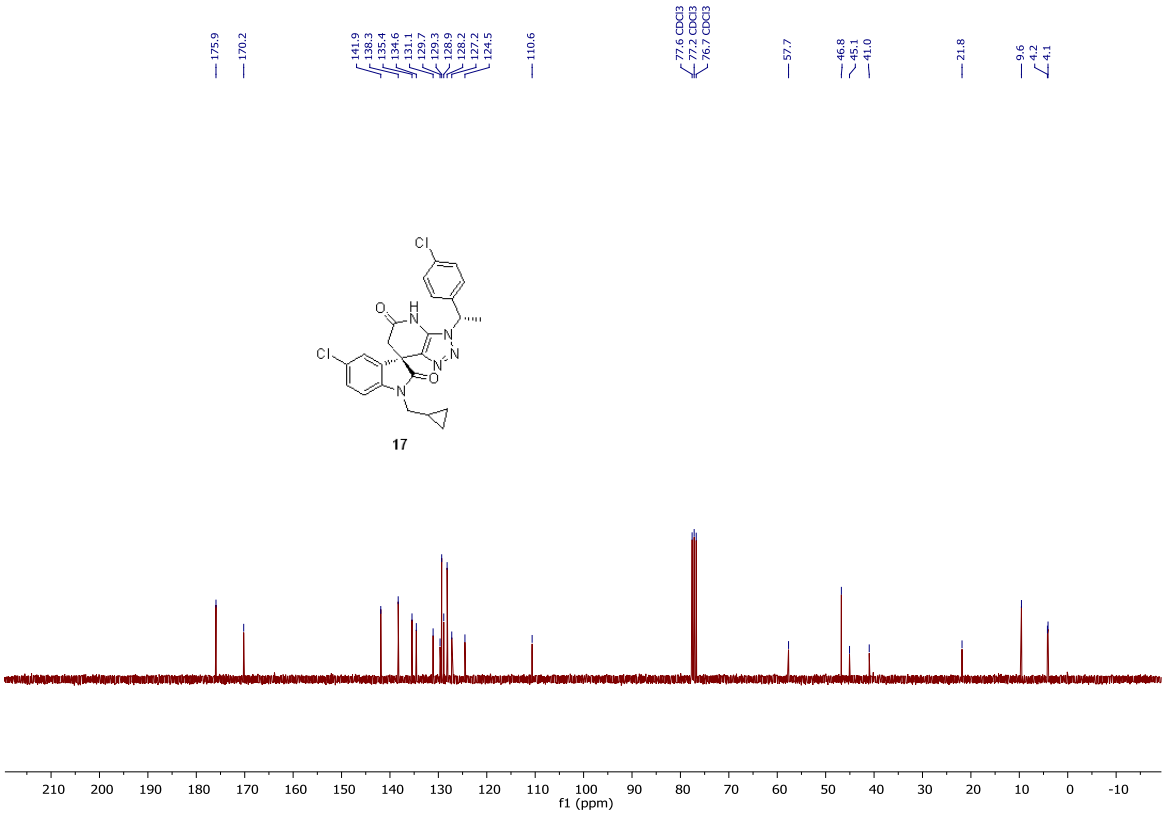
f1 (ppm)

17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128.2
127.2
124.5
110.6
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
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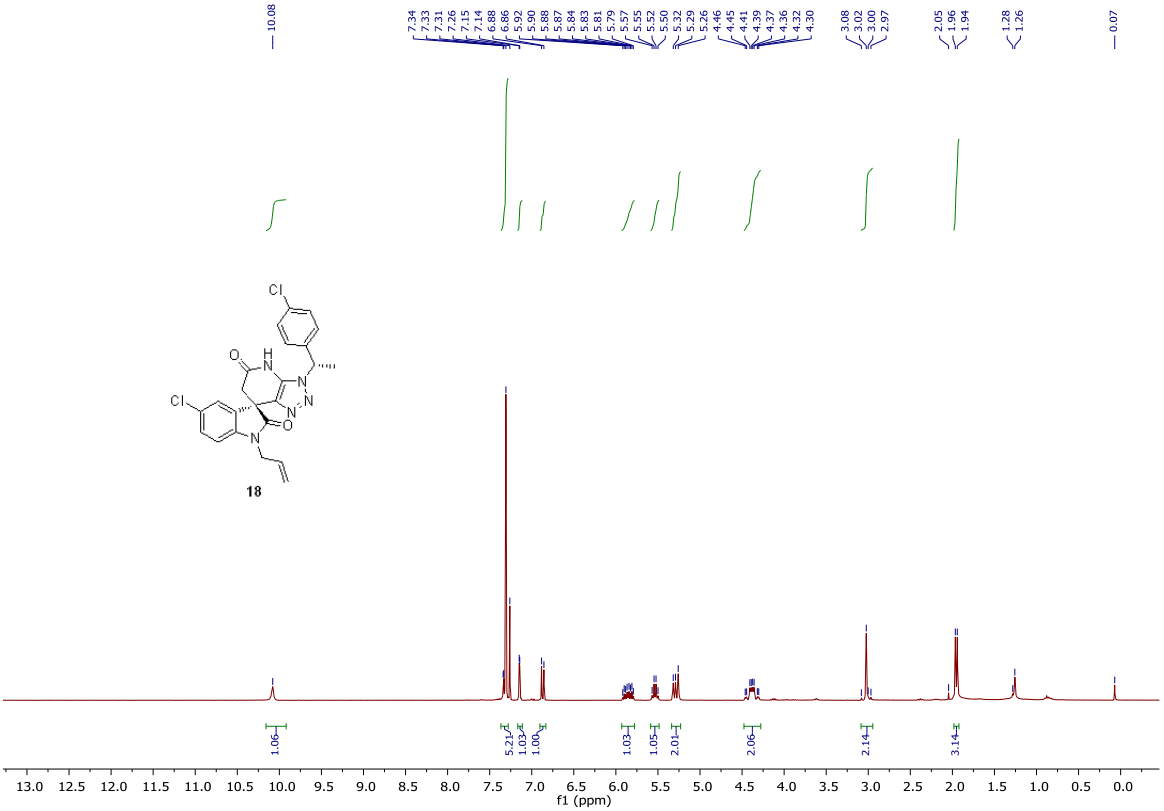
45.1
41.0
21.8
9.6
4.2
4.1
f1 (ppm)

17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5.81
5.79
5.57
5.55
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5.50
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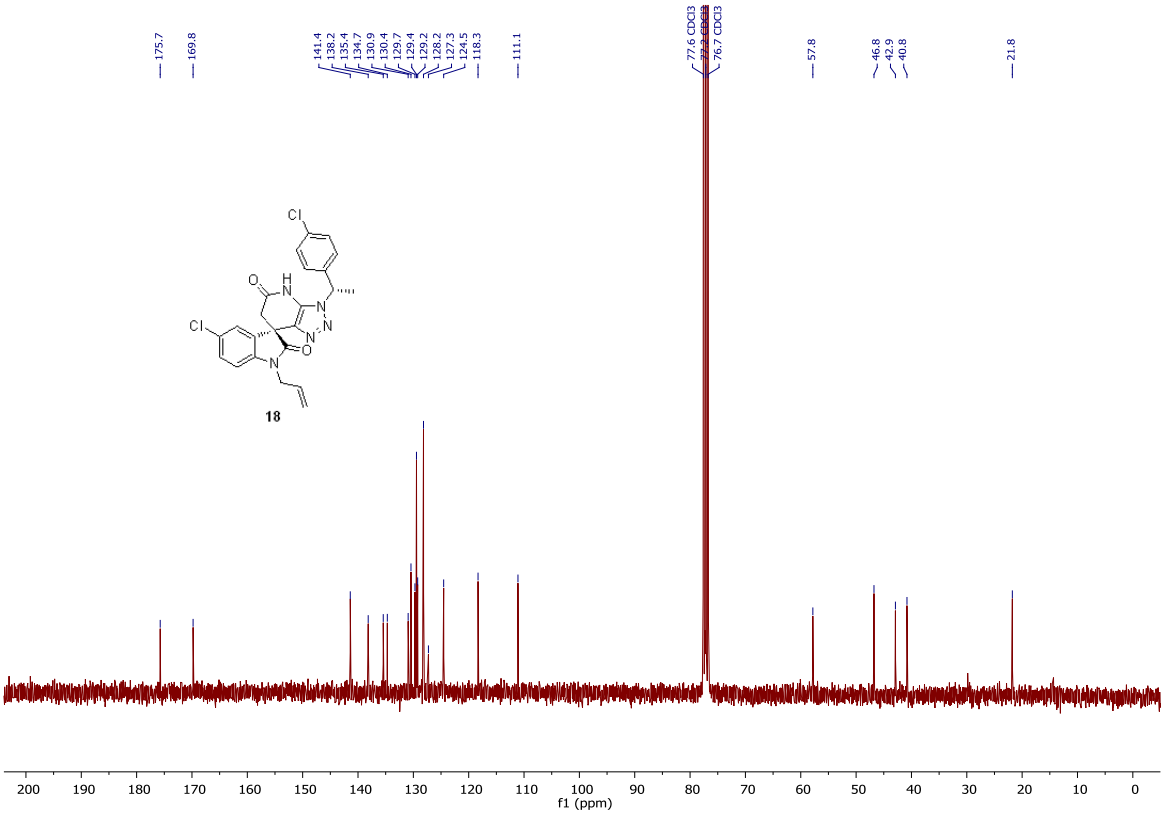
5.29
5.26
4.46
4.45
4.41
4.39
4.37
4.36
4.32
4.30
3.08
3.02
3.00
2.97
2.05
1.96
1.94
1.28
1.26
0.07
Cl
O
H
N
N
N
Cl
O
N
18
1.06
5.21
1.03
1.00
1.03
1.05
2.01
2.06
2.14
3.14
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.2
128.2
127.3
124.5
118.3
111.1
77.6 CDCl3
77.3 CDCl3
76.7 CDCl3
57.8
46.8
42.9
40.8
21.8
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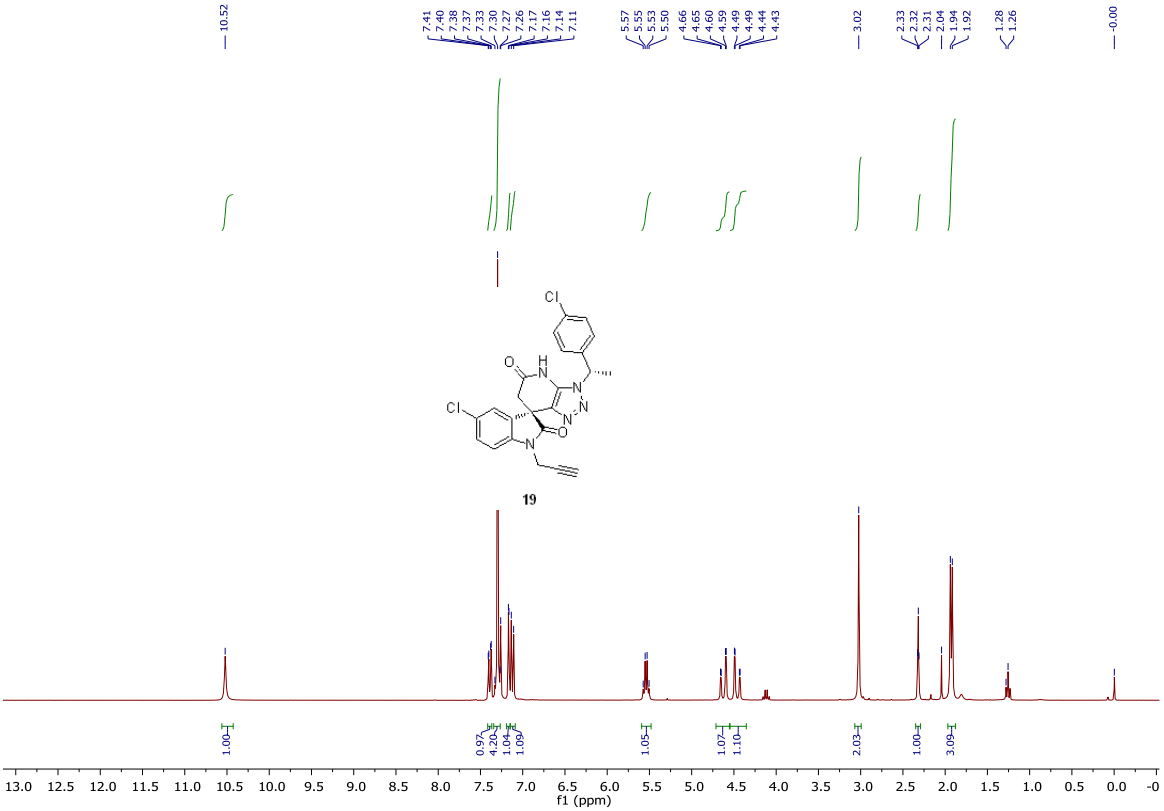
N
N
N
Cl
O
N
18
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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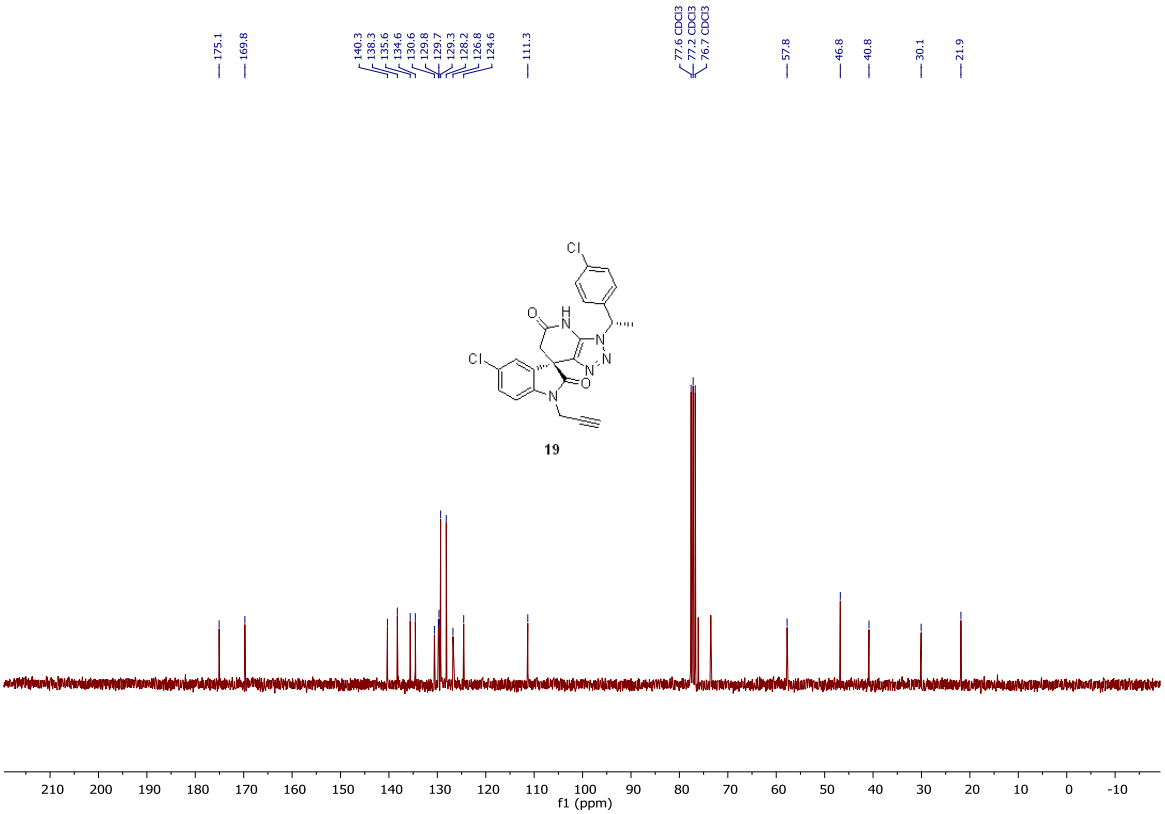
7.14
7.11
5.57
5.55
5.53
5.50
4.66
4.65
4.60
4.59
4.49
4.49
4.44
4.43
3.02
2.33
2.32
2.31
2.04
1.94
1.92
1.28
1.26
-0.00
Cl
O
H
N
N
N
Cl
O
N
19
1.00
0.97
4.20
1.04
1.09
1.05
1.07
1.10
2.03
1.00
3.09
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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129.3
128.2
126.8
124.6
111.3
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.8
40.8
30.1
21.9
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H
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N
Cl
O
N
19
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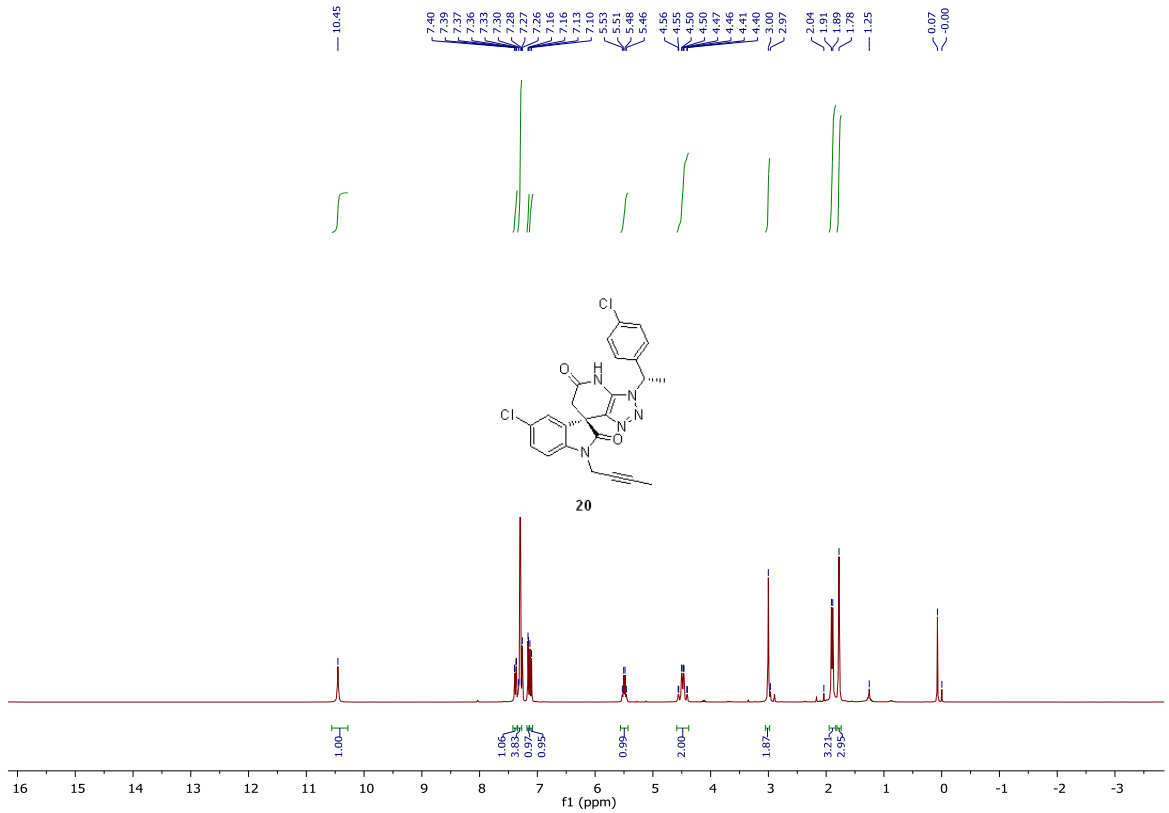
f1 (ppm)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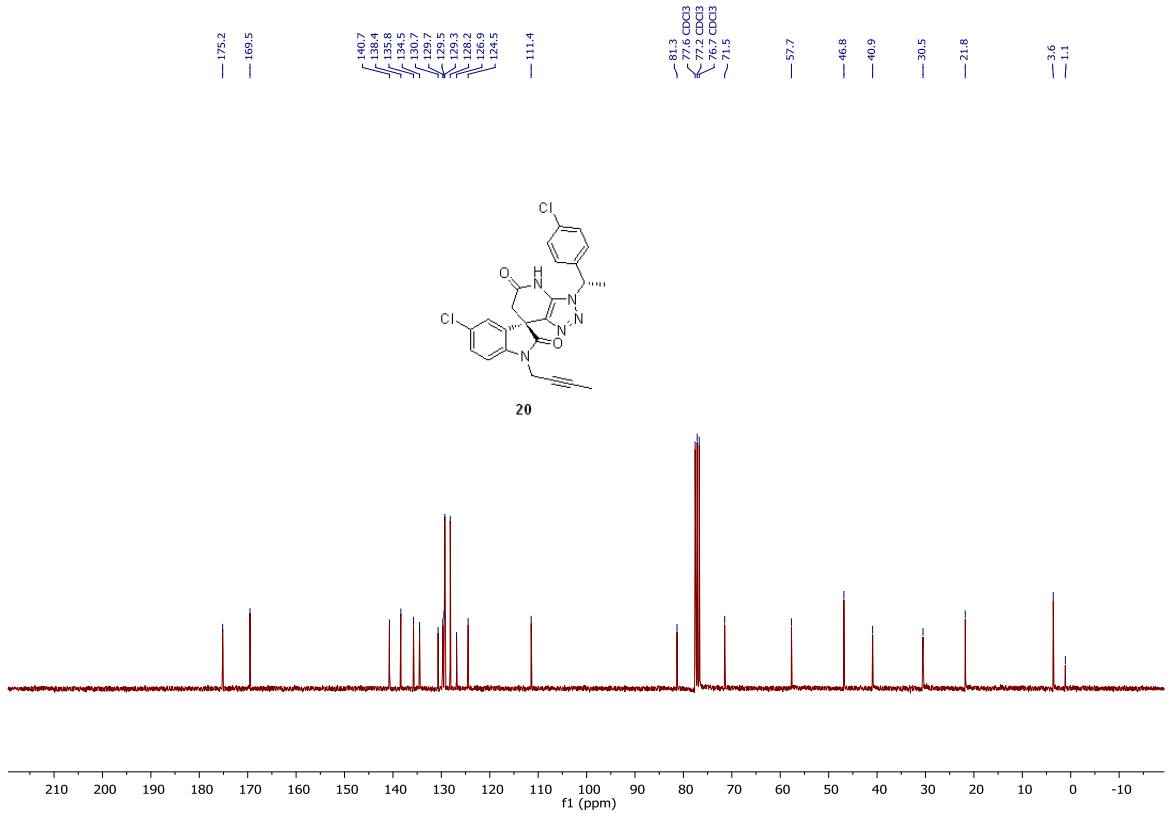
7.30
7.28
7.27
7.26
7.16
7.16
7.13
7.10
5.53
5.51
5.48
5.46
4.56
4.55
4.50
4.50
4.47
4.46
4.41
4.40
3.00
2.97
2.04
1.91
1.89
1.78
1.25
0.07
-0.00
20
1.00
1.06
3.85
0.97
0.95
0.99
2.00
1.87
3.21
2.95
f1 (ppm)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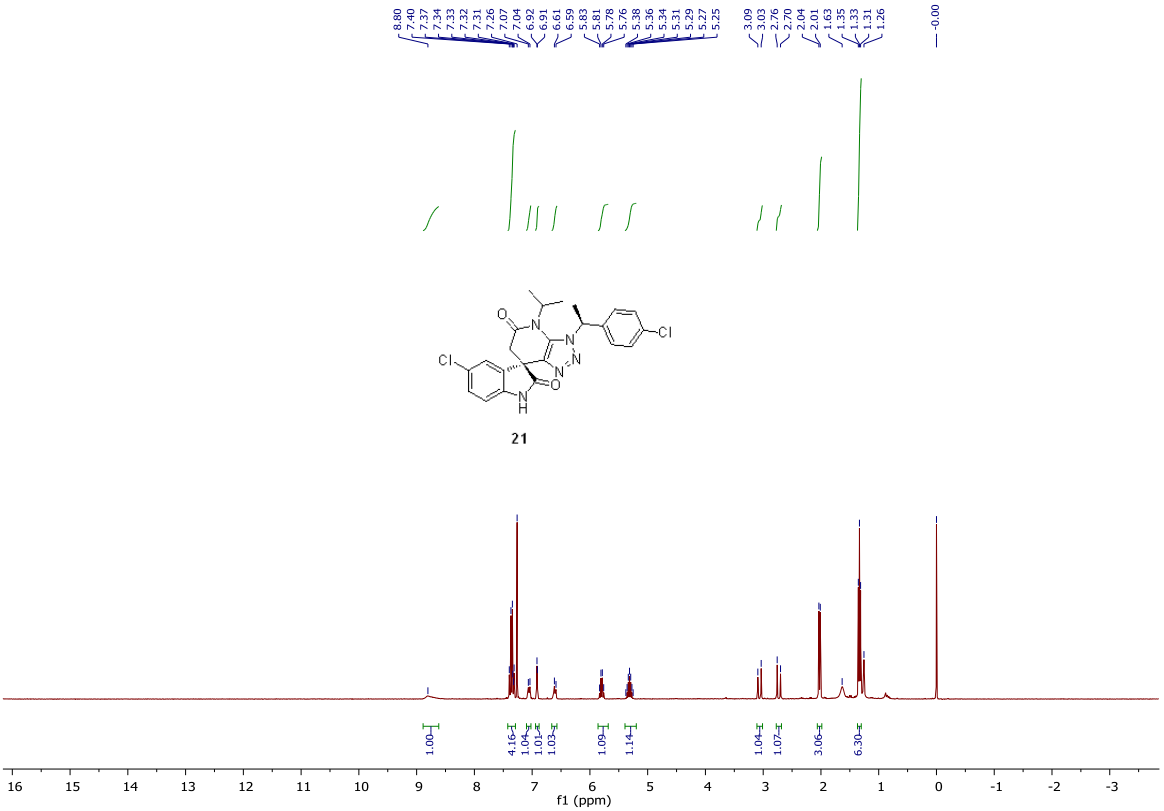
138.4
135.8
134.5
130.7
129.7
129.5
129.3
128.2
126.9
124.5
111.4
81.3
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
71.5
57.7
46.8
40.9
30.5
21.8
3.6
1.1
20
f1 (ppm)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7.26
7.07
7.04
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6.61
6.59
5.83
5.81
5.78
5.76
5.38
5.36
5.34
5.31
5.29
5.27
5.25
3.09
3.03
2.76
2.70
2.04
2.01
1.63
1.35
1.33
1.31
1.26
-0.00
21
1.00
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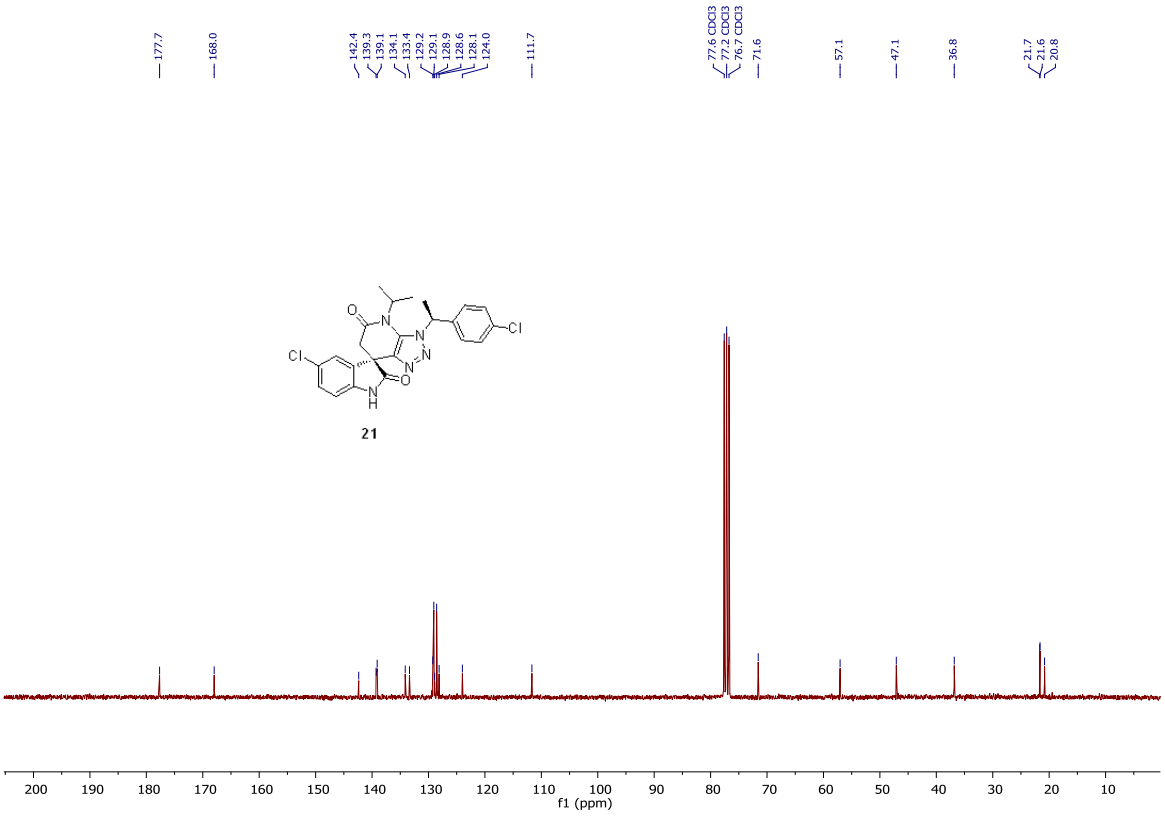
1.04
1.01
1.03
1.09
1.14
1.04
1.07
3.06
6.30
f1 (ppm)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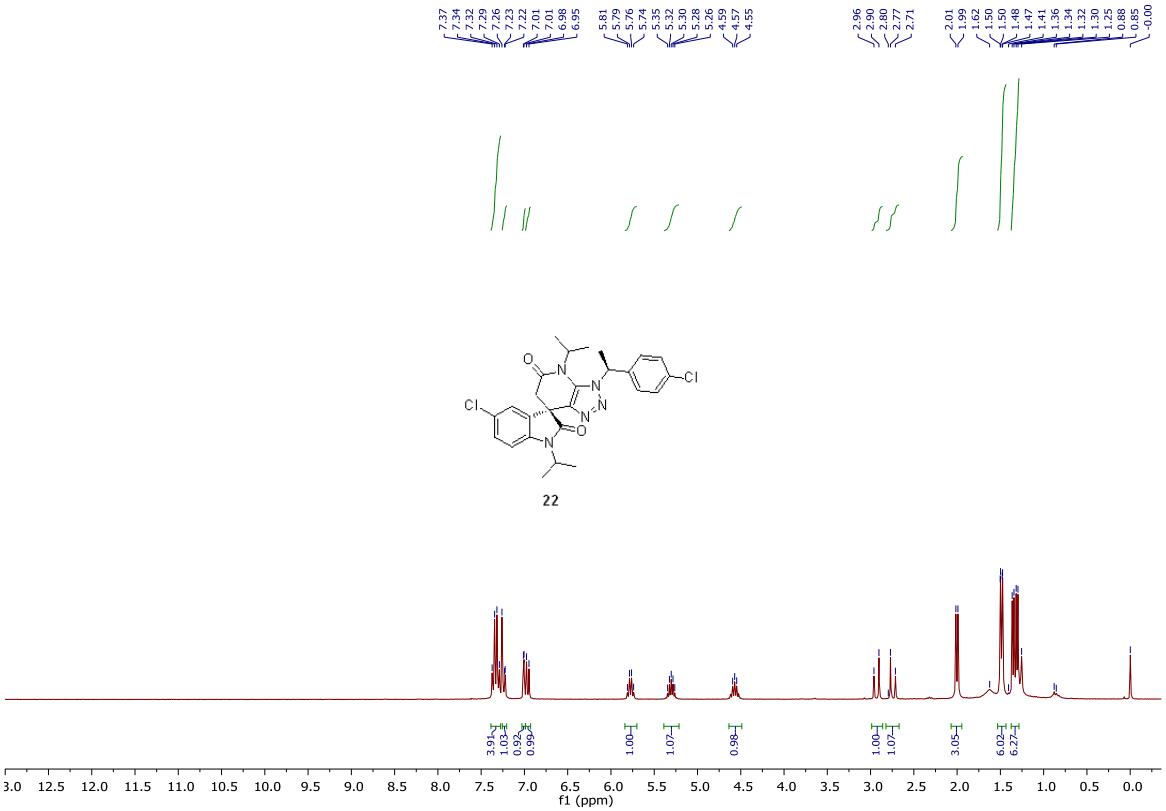
168.0
142.4
139.3
139.1
134.1
133.4
129.2
129.1
128.9
128.6
128.1
124.0
111.7
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
71.6
57.1
47.1
36.8
21.7
21.6
20.8
21
f1 (ppm)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7.23
7.22
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7.01
6.98
6.95
5.81
5.79
5.76
5.74
5.35
5.32
5.30
5.28
5.26
4.59
4.57
4.55
2.96
2.90
2.80
2.77
2.71
2.01
1.99
1.62
1.50
1.50
1.48
1.47
1.41
1.36
1.34
1.32
1.30
1.25
0.88
0.85
-0.00
Cl
Cl
N
N
N
N
O
O
O
22
3.91
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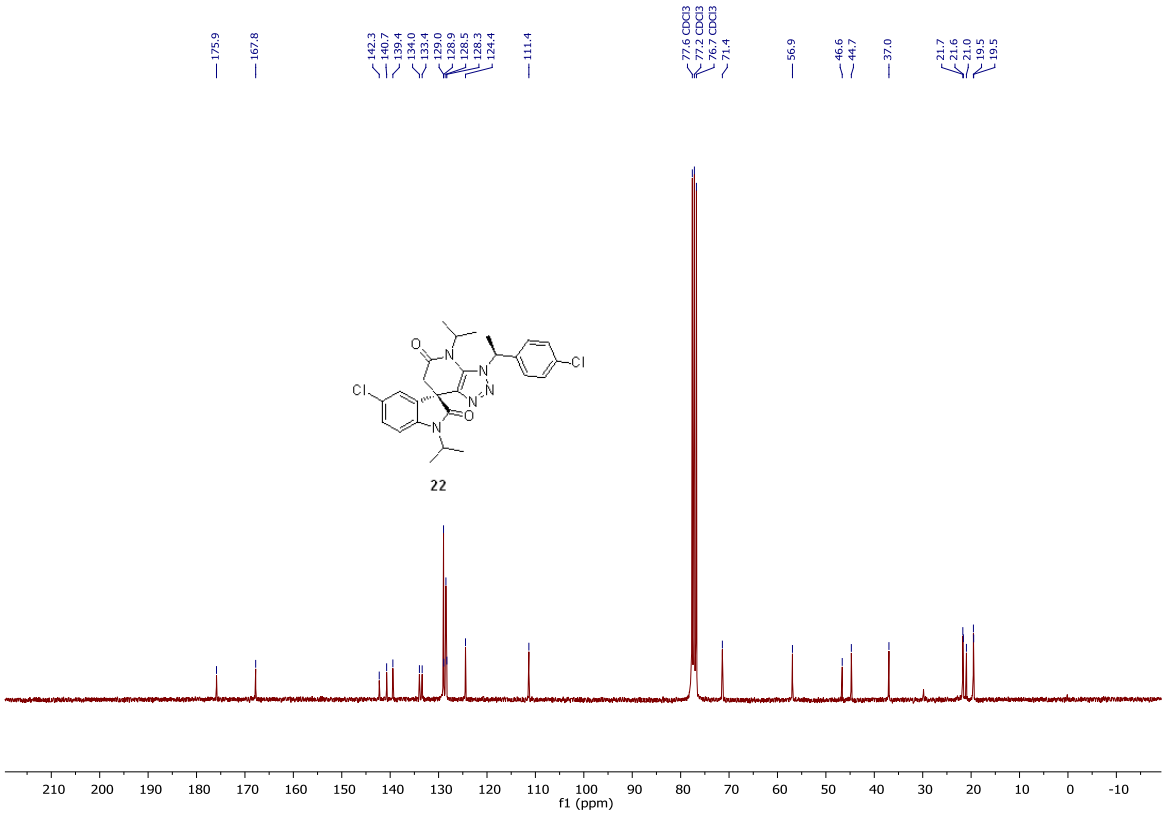
0.99
1.00
1.07
0.98
1.00
1.07
3.05
6.02
6.27
f1 (ppm)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129.0
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128.5
128.3
124.4
111.4
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
71.4
56.9
46.6
44.7
37.0
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21.6
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19.5
19.5
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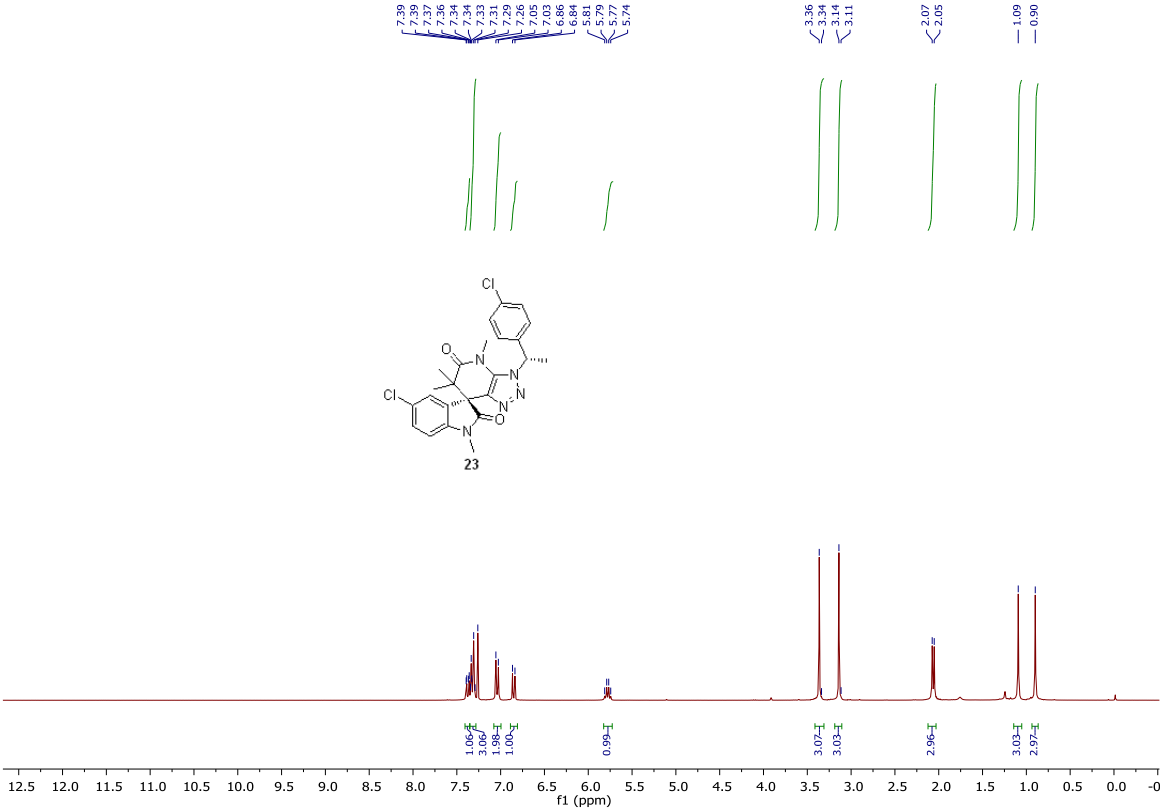
N
N
O
O
O
22
f1 (ppm)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7.03
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6.84
5.81
5.79
5.77
5.74
3.36
3.34
3.14
3.11
2.07
2.05
1.09
0.90
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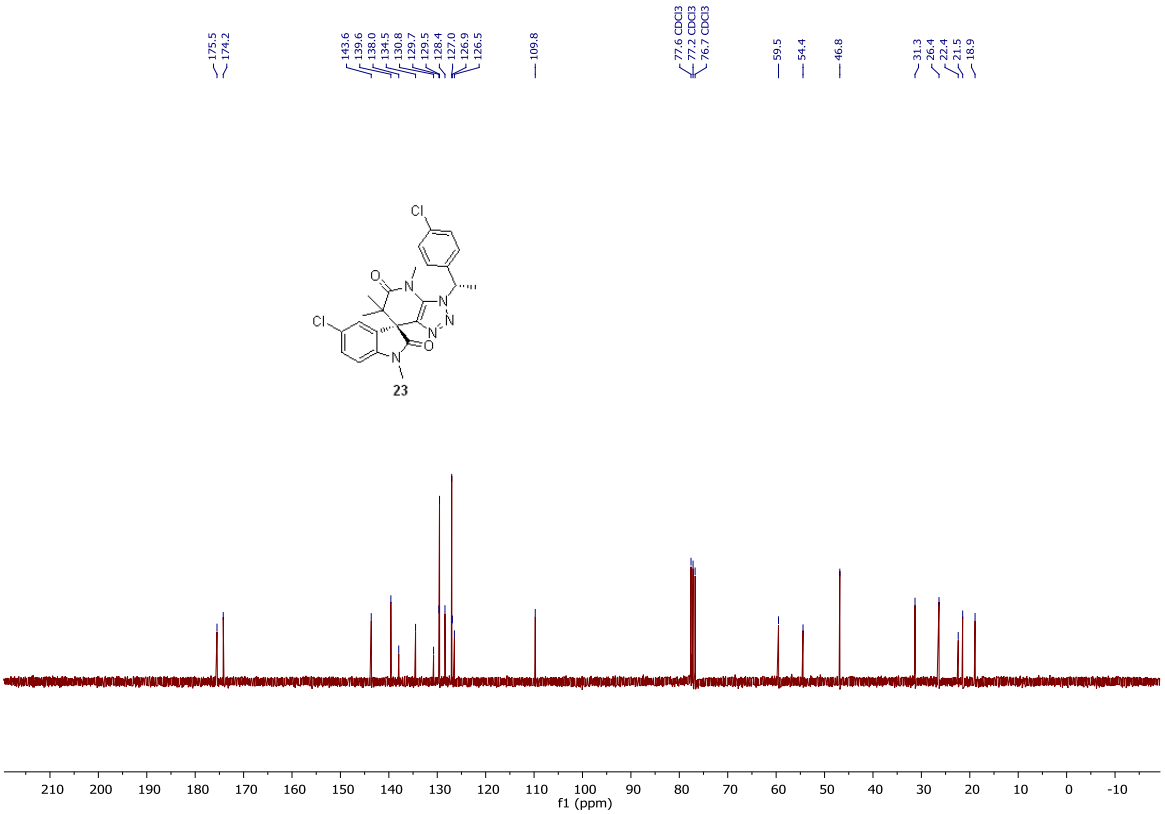
1.98
1.00
0.99
3.07
3.03
2.96
3.03
2.97
f1 (ppm)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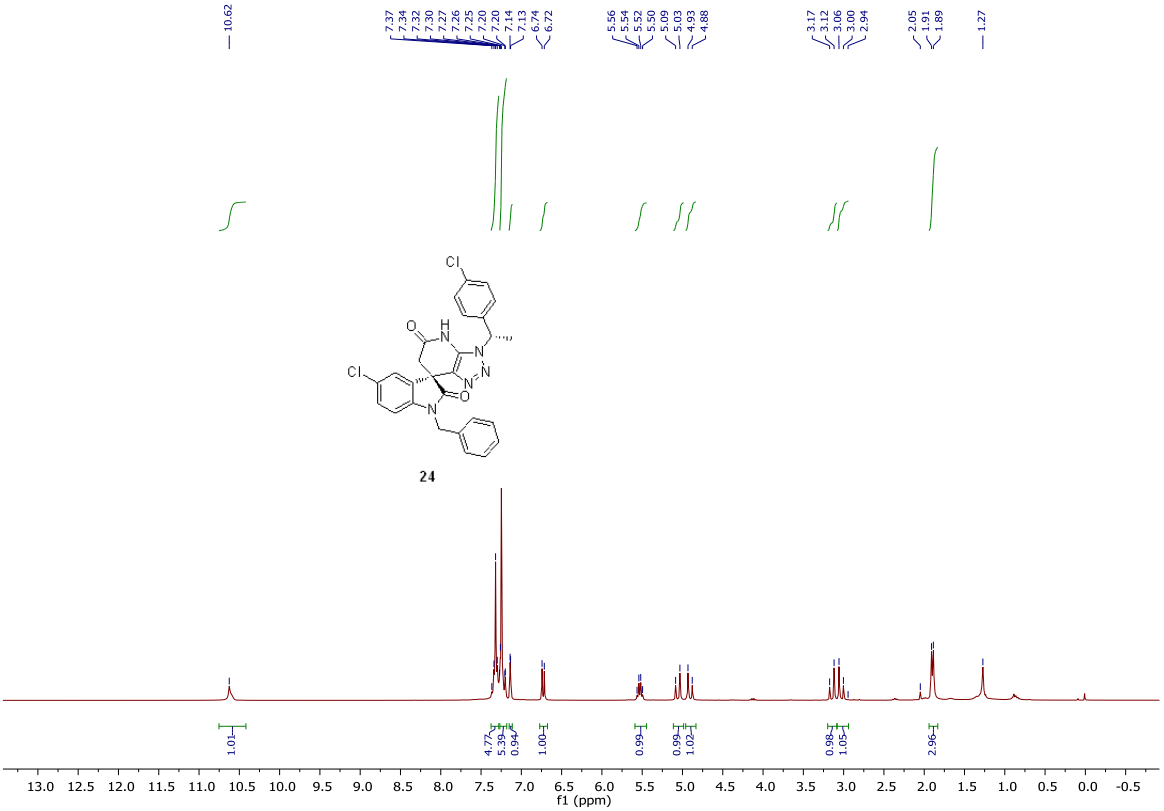
139.6
138.0
134.5
130.8
129.7
129.5
128.4
127.0
126.9
126.5
109.8
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
59.5
54.4
46.8
31.3
26.4
22.4
21.5
18.9
23
f1 (ppm)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6.74
6.72
5.56
5.54
5.52
5.50
5.09
5.03
4.93
4.88
3.17
3.12
3.06
3.00
2.94
2.05
1.91
1.89
1.27
24
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1.00
0.99
0.99
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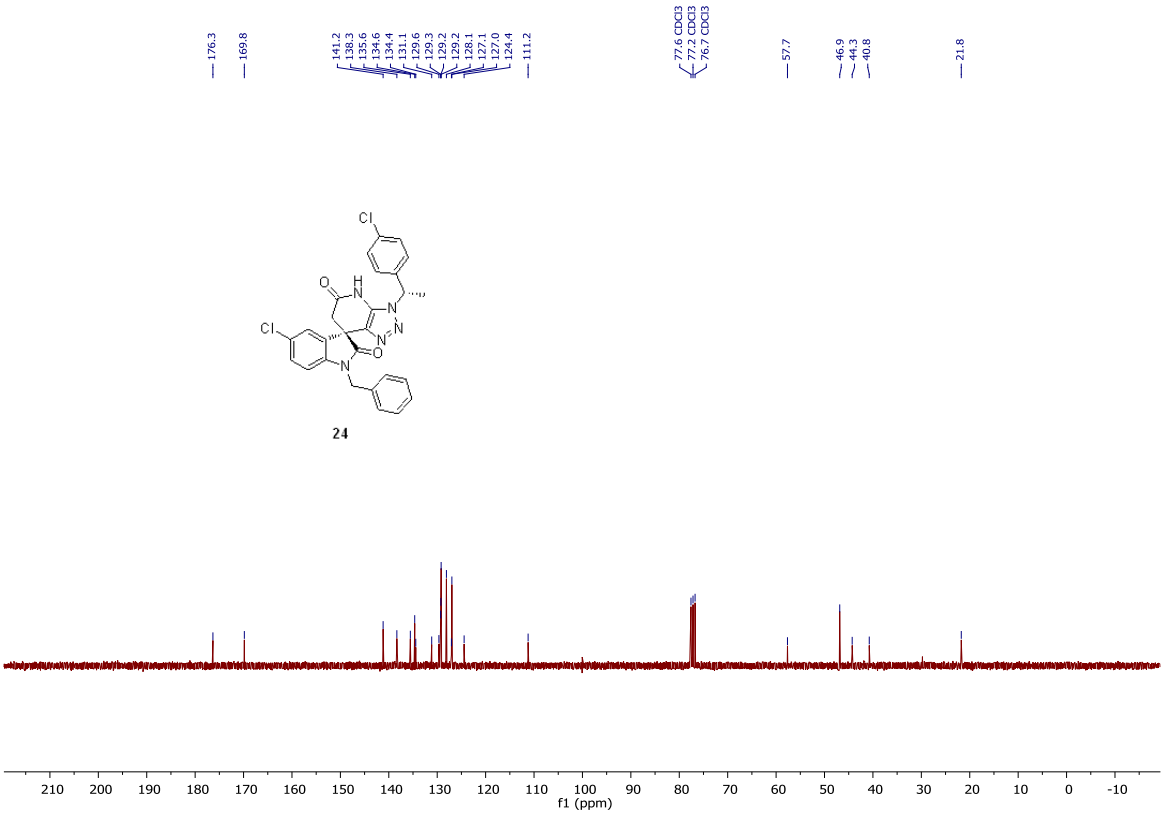
0.98
1.05
2.96
f1 (ppm)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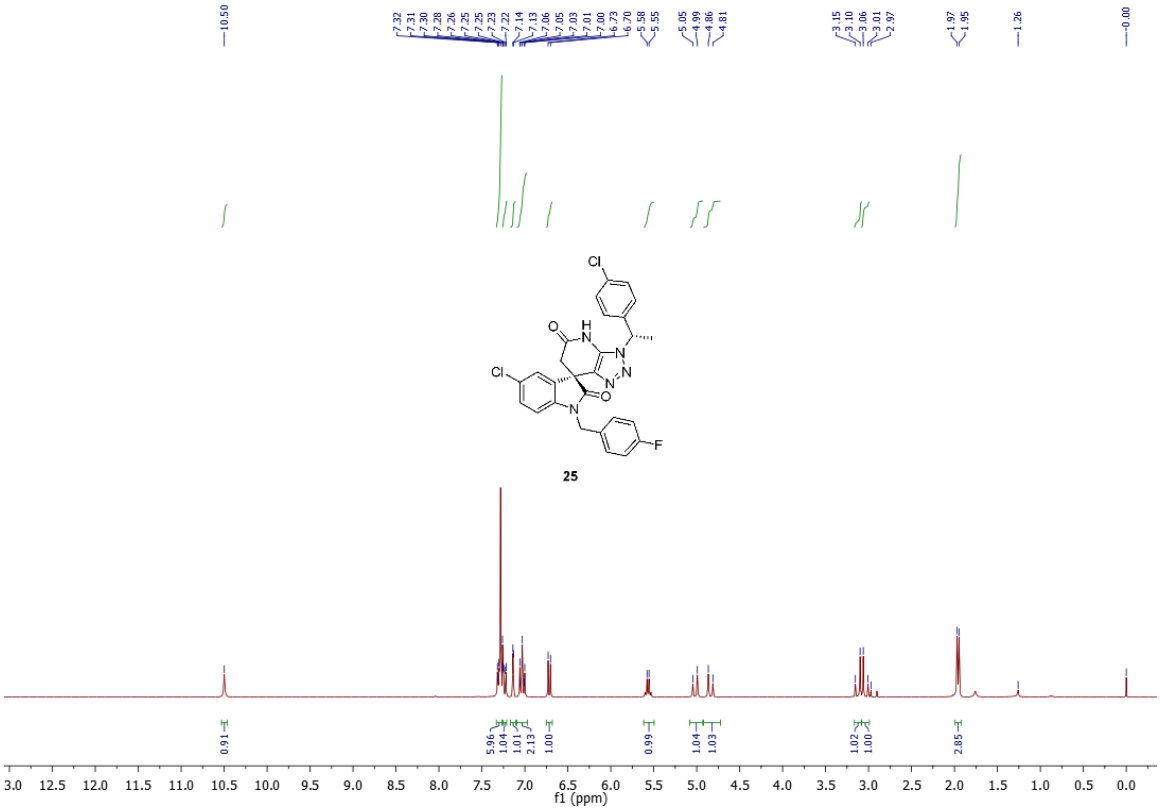
129.3
129.2
129.2
128.1
127.1
127.0
124.4
111.2
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.7
46.9
44.3
40.8
21.8
24
f1 (ppm)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7.22
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7.13
7.06
7.05
7.03
7.01
7.00
6.73
6.70
5.58
5.55
5.05
4.99
4.86
4.81
3.15
3.10
3.06
3.01
2.97
1.97
1.95
1.26
0.00
Cl
O
H
N
N
N
O
Cl
N
F
25
0.91
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2.13
1.00
0.99
1.04
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1.02
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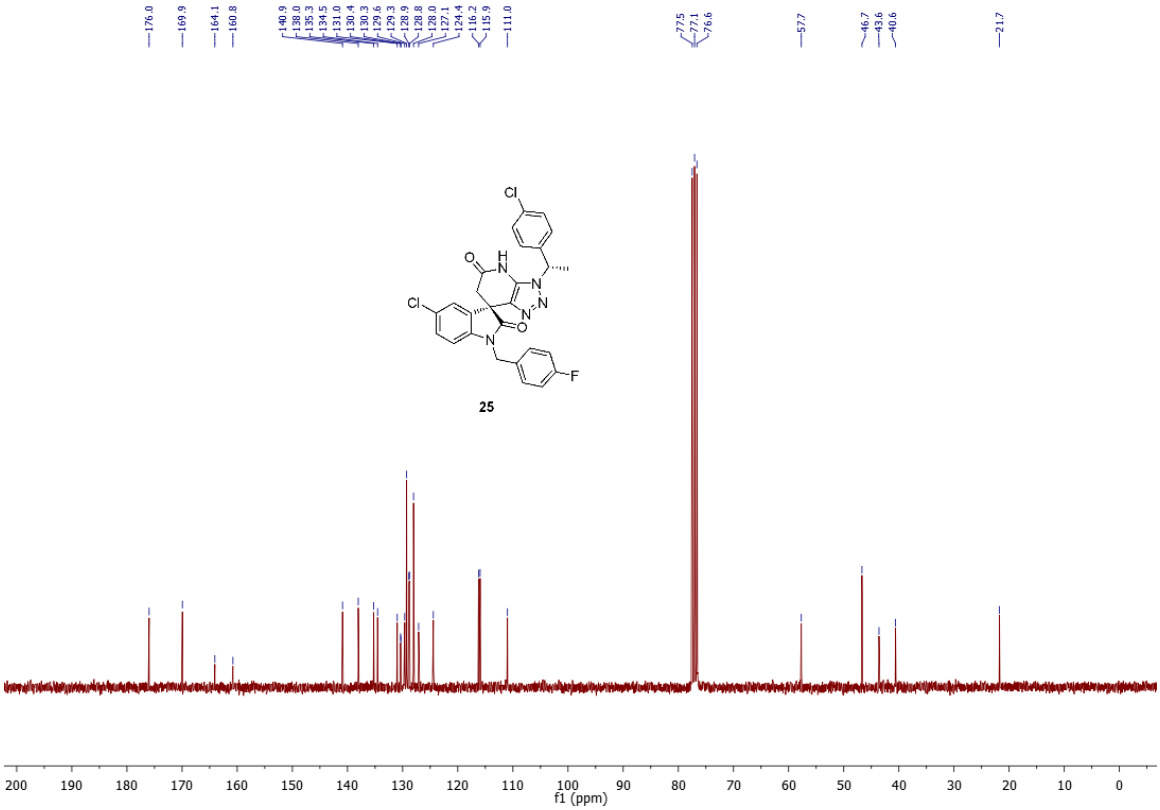
2.85
f1 (ppm)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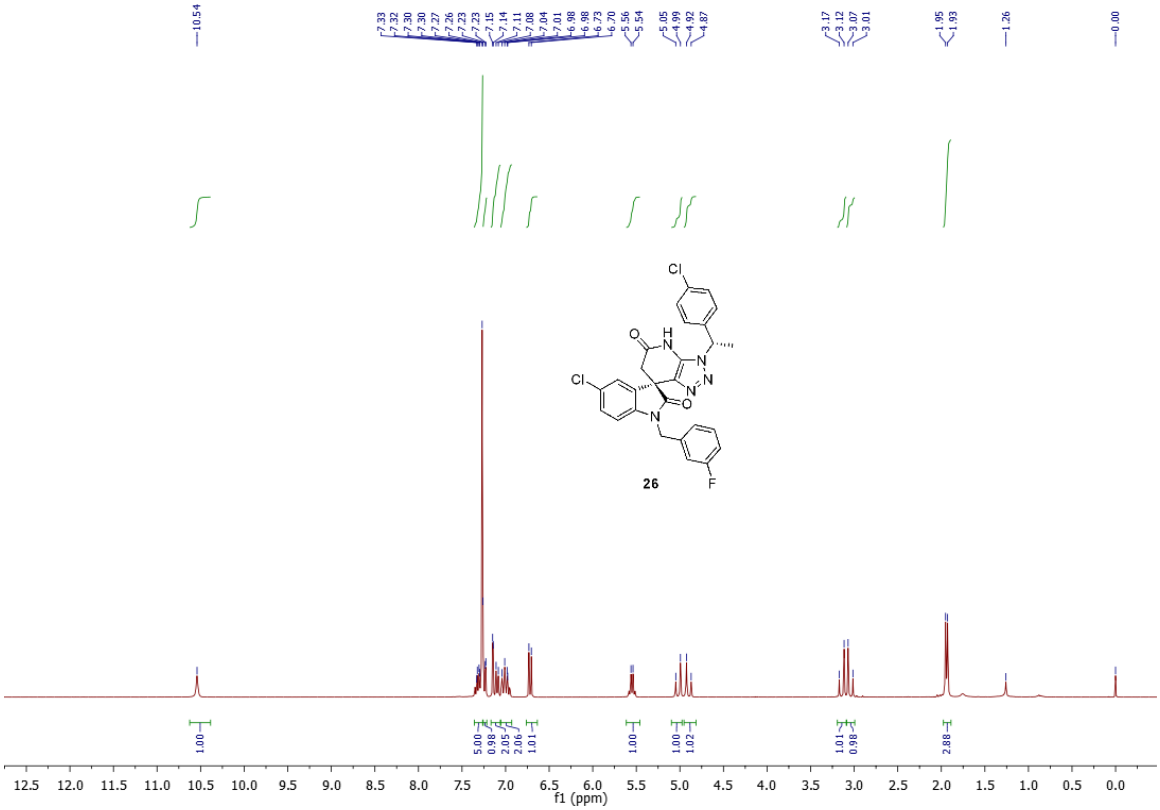
130.4
130.3
129.6
129.3
128.9
128.8
128.0
127.1
124.4
116.2
115.9
111.0
77.5
77.1
76.6
57.7
46.7
43.6
40.6
21.7
Cl
O
H
N
N
N
O
Cl
N
F
25
f1 (ppm)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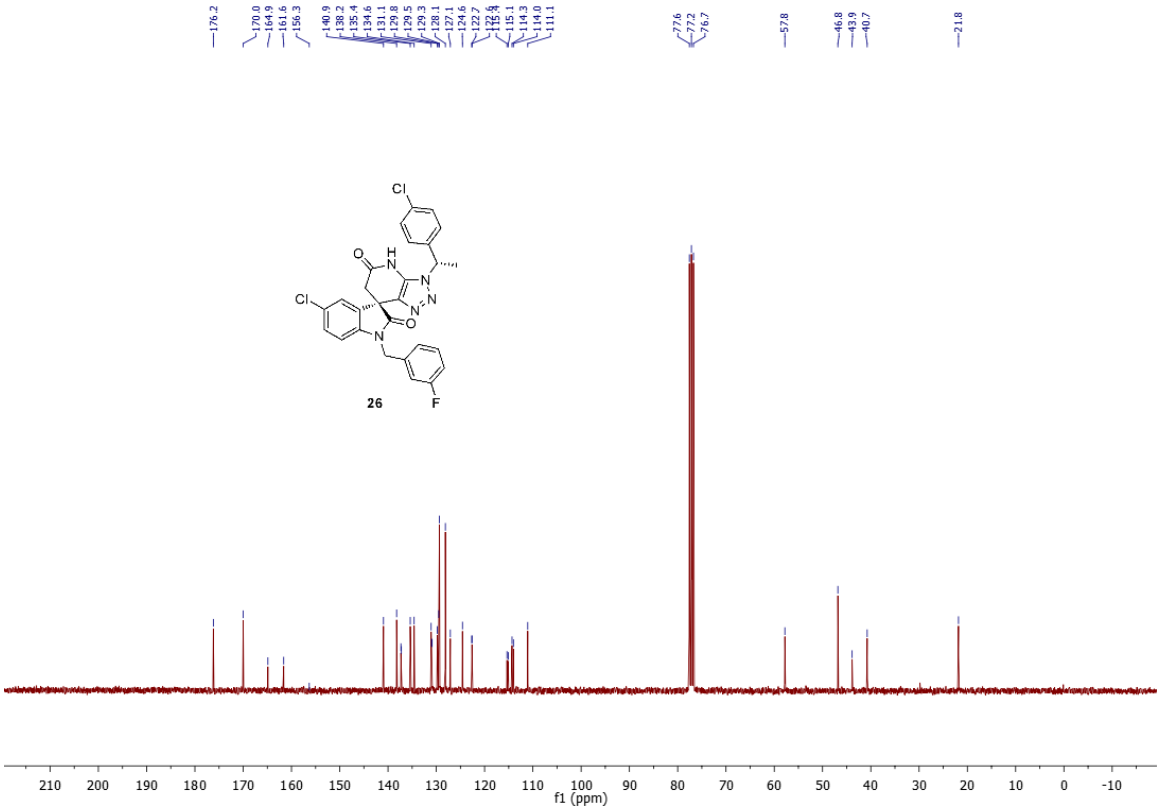
7.04
7.01
6.98
6.98
6.73
6.70
5.56
5.54
5.05
4.99
4.92
4.87
3.17
3.12
3.07
3.01
1.95
1.93
1.26
0.00
Cl
O
H
N
N
N
Cl
O
N
F
26
1.00
5.00
0.98
2.05
2.06
1.01
1.00
1.00
1.02
1.01
0.98
2.88
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.8
129.5
128.1
127.1
124.6
122.7
122.6
115.4
115.1
114.3
114.0
111.1
77.6
77.2
76.7
57.8
46.8
43.9
40.7
21.8
Cl
O
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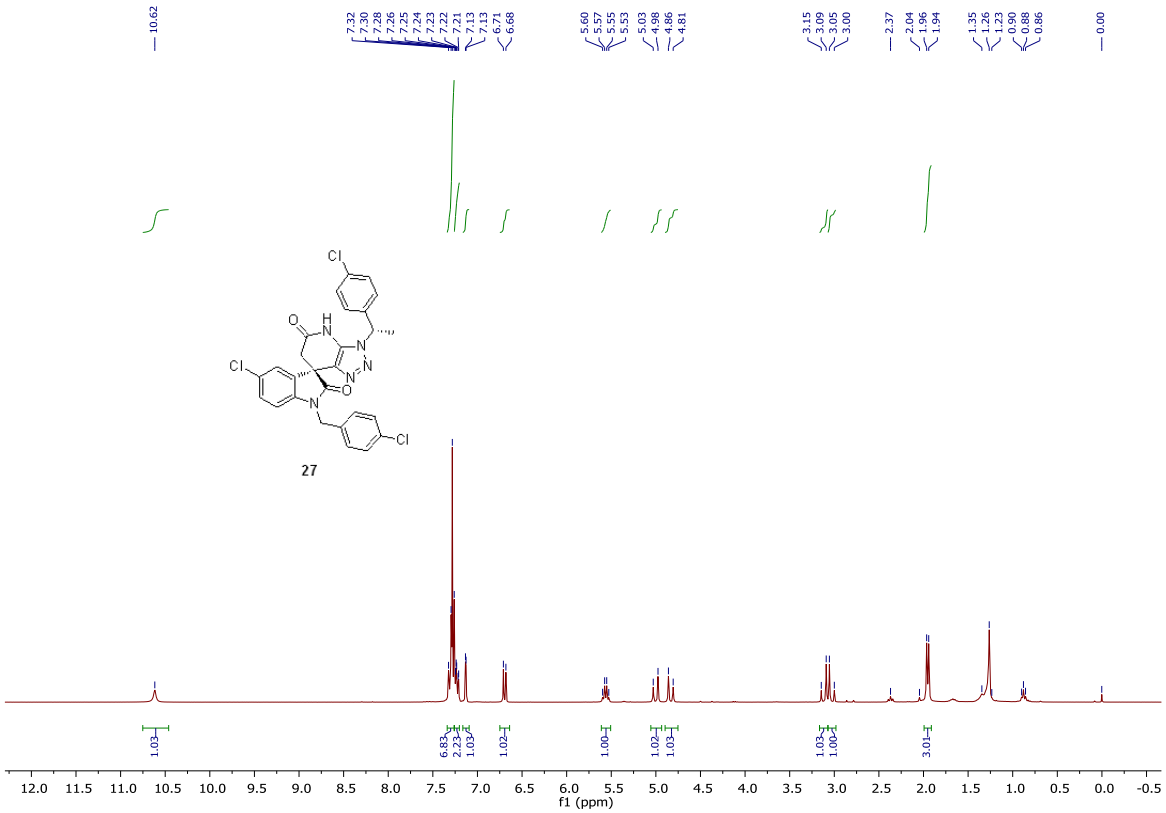
N
N
N
Cl
O
N
F
26
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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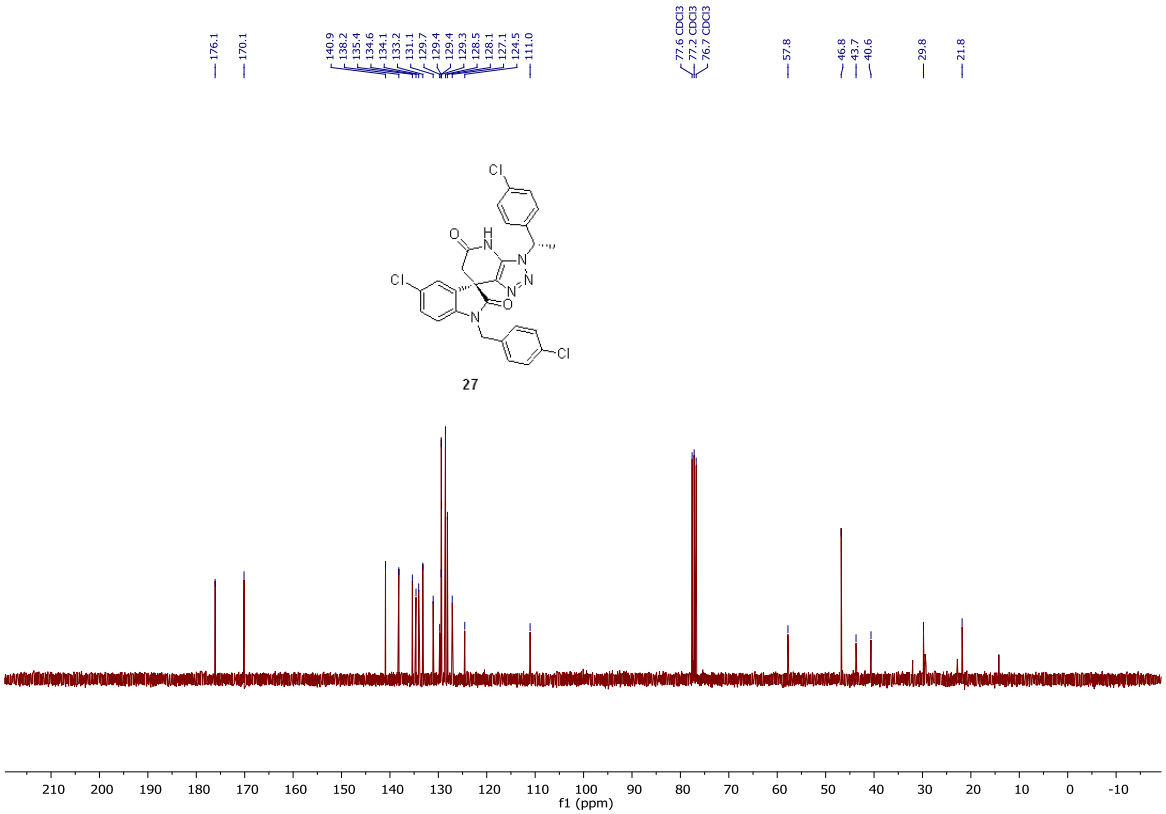
6.71
6.68
5.60
5.57
5.55
5.53
5.03
4.98
4.86
4.81
3.15
3.09
3.05
3.00
2.37
2.04
1.96
1.94
1.35
1.26
1.23
0.90
0.88
0.86
0.00
Cl
O
H
N
N
N
N
O
Cl
N
Cl
27
1.03
6.83
2.23
1.03
1.02
1.00
1.02
1.03
1.03
1.00
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.6
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133.2
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129.7
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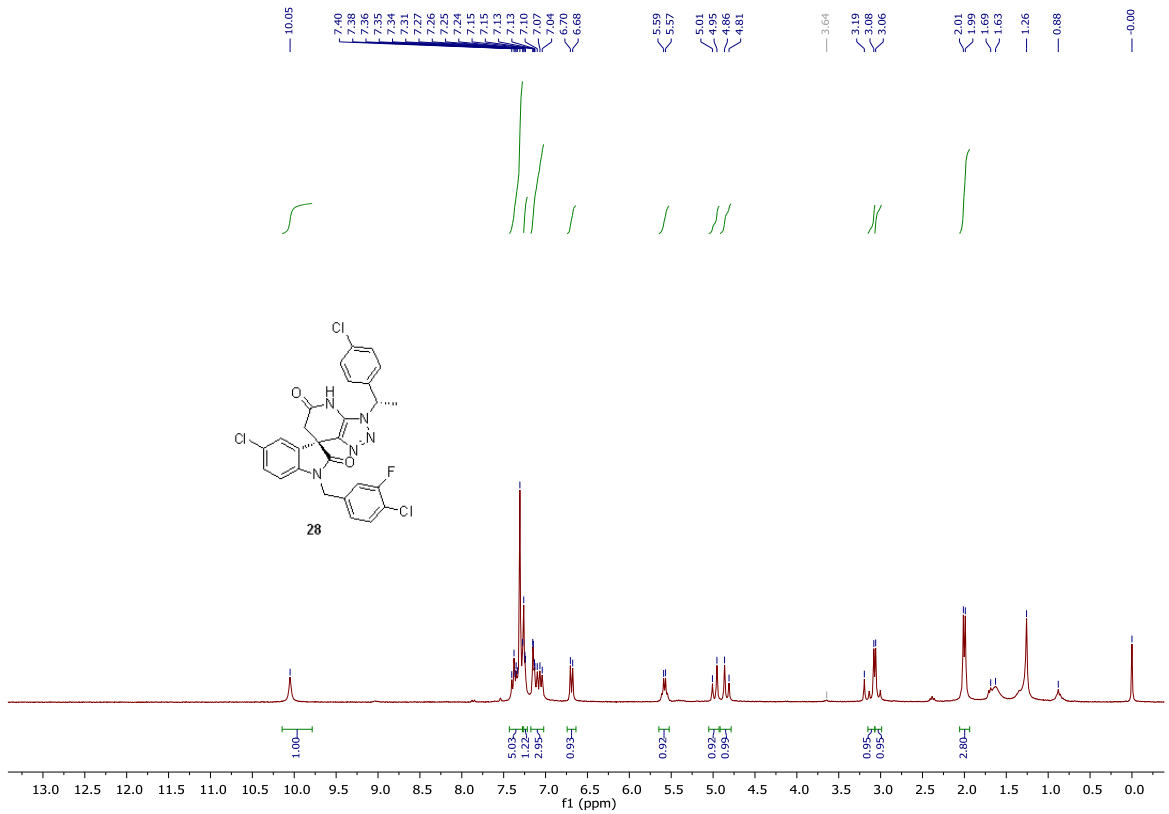
129.4
129.3
128.5
128.1
127.1
124.5
111.0
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.8
43.7
40.6
29.8
21.8
Cl
O
H
N
N
N
N
O
Cl
N
Cl
27
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


10.05
7.40
7.38
7.36
7.35
7.34
7.31
7.27
7.26
7.25
7.24
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7.15
7.13
7.13
7.10
7.07
7.04
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5.57
5.01
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4.81
3.64
3.19
3.08
3.06
2.01
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1.69
1.63
1.26
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-0.00
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0.95
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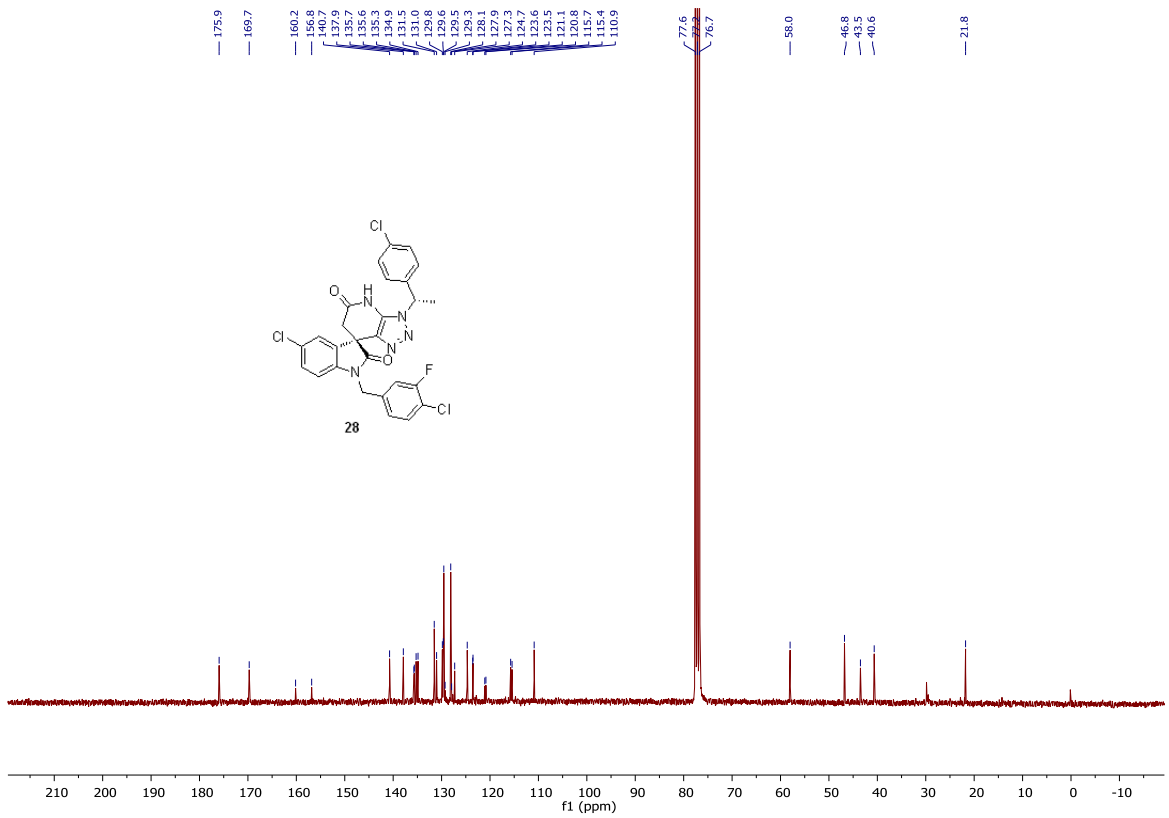
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129.5
129.3
128.1
127.9
127.3
124.7
123.6
123.5
121.1
120.8
115.7
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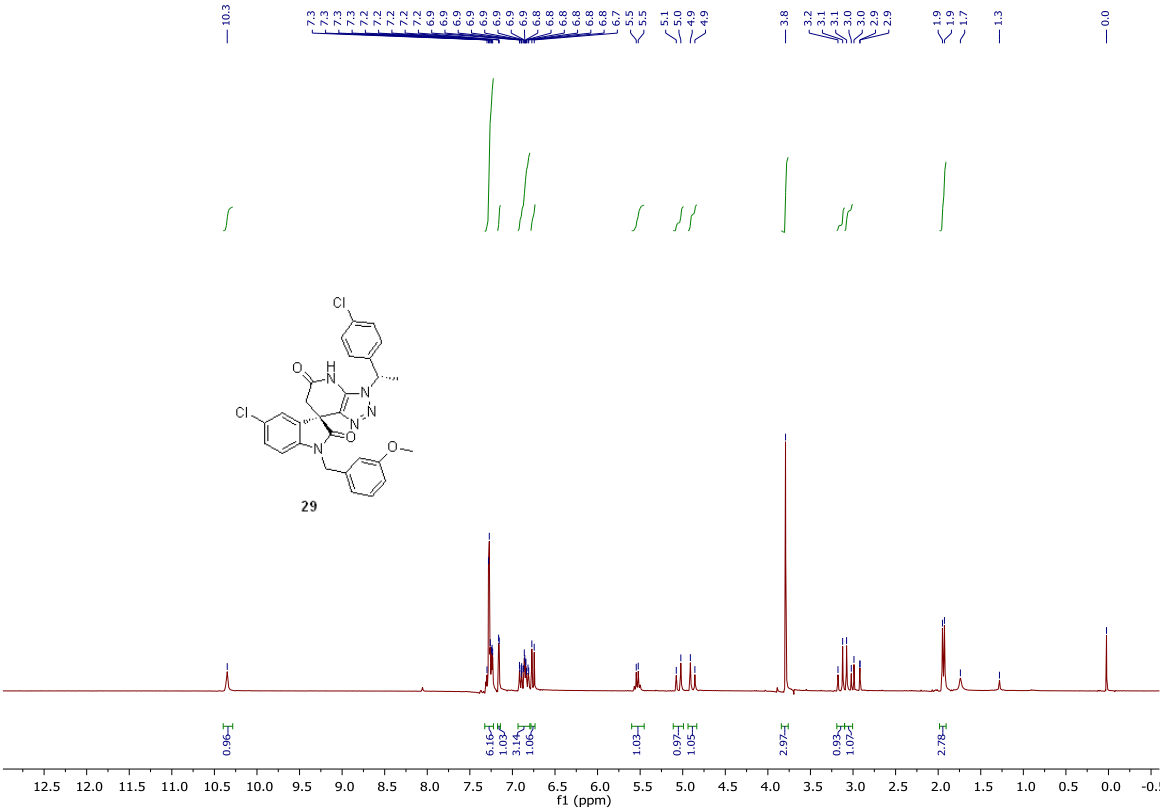
f1 (ppm)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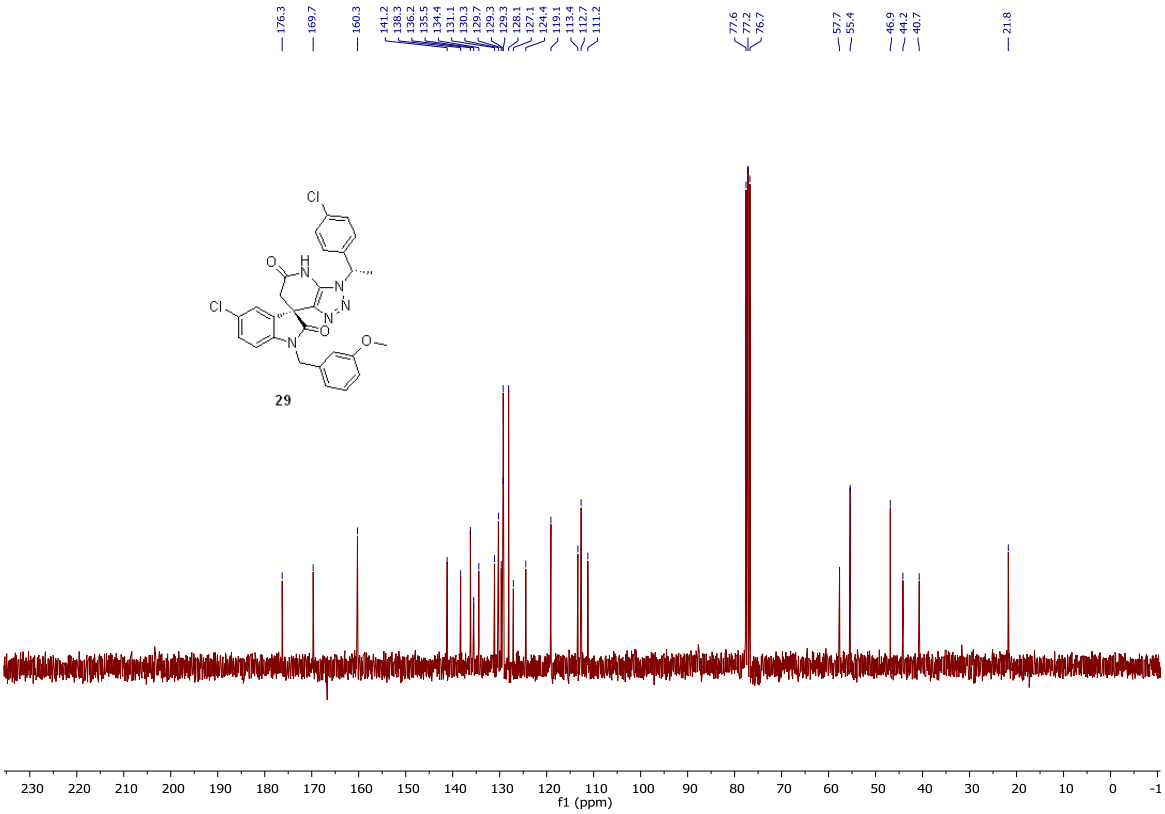
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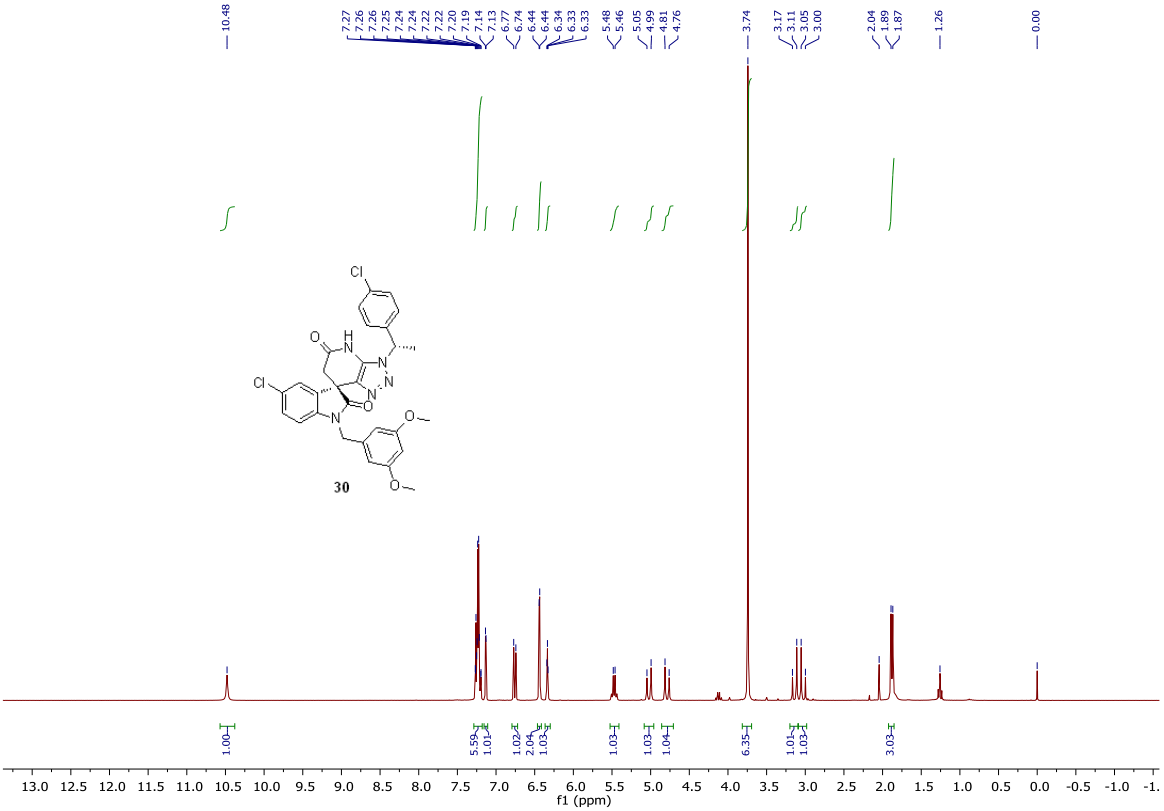
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7.14
7.13
6.77
6.74
6.44
6.44
6.34
6.33
6.33
5.48
5.46
5.05
4.99
4.81
4.76
3.74
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3.11
3.05
3.00
2.04
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1.87
1.26
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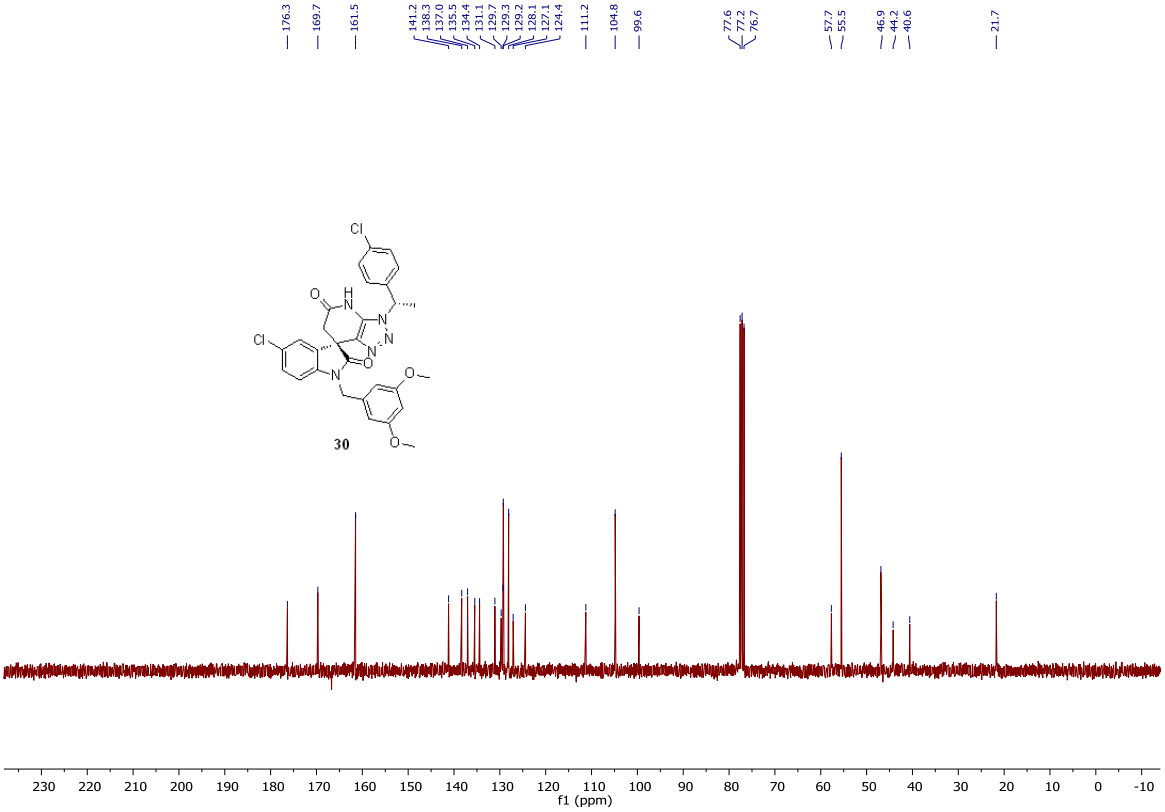
30
f1 (ppm)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128.1
127.1
124.4
111.2
104.8
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77.2
76.7
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55.5
46.9
44.2
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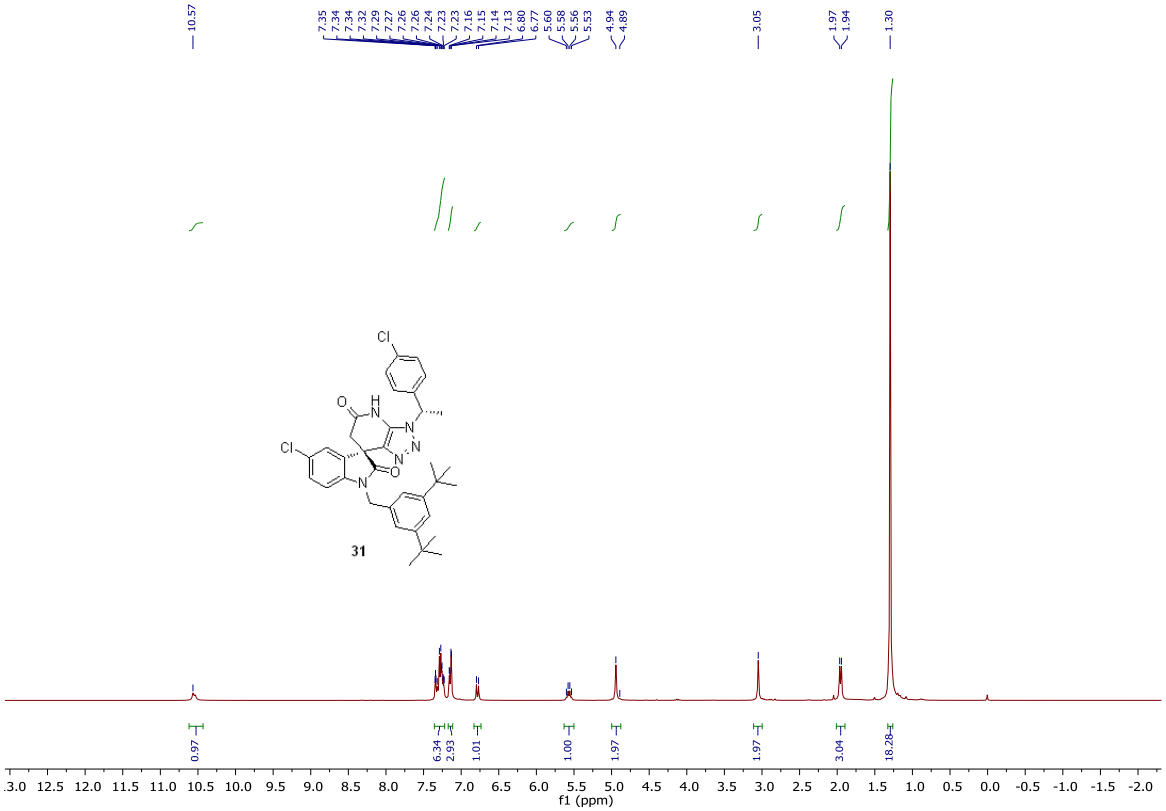
21.7
30
f1 (ppm)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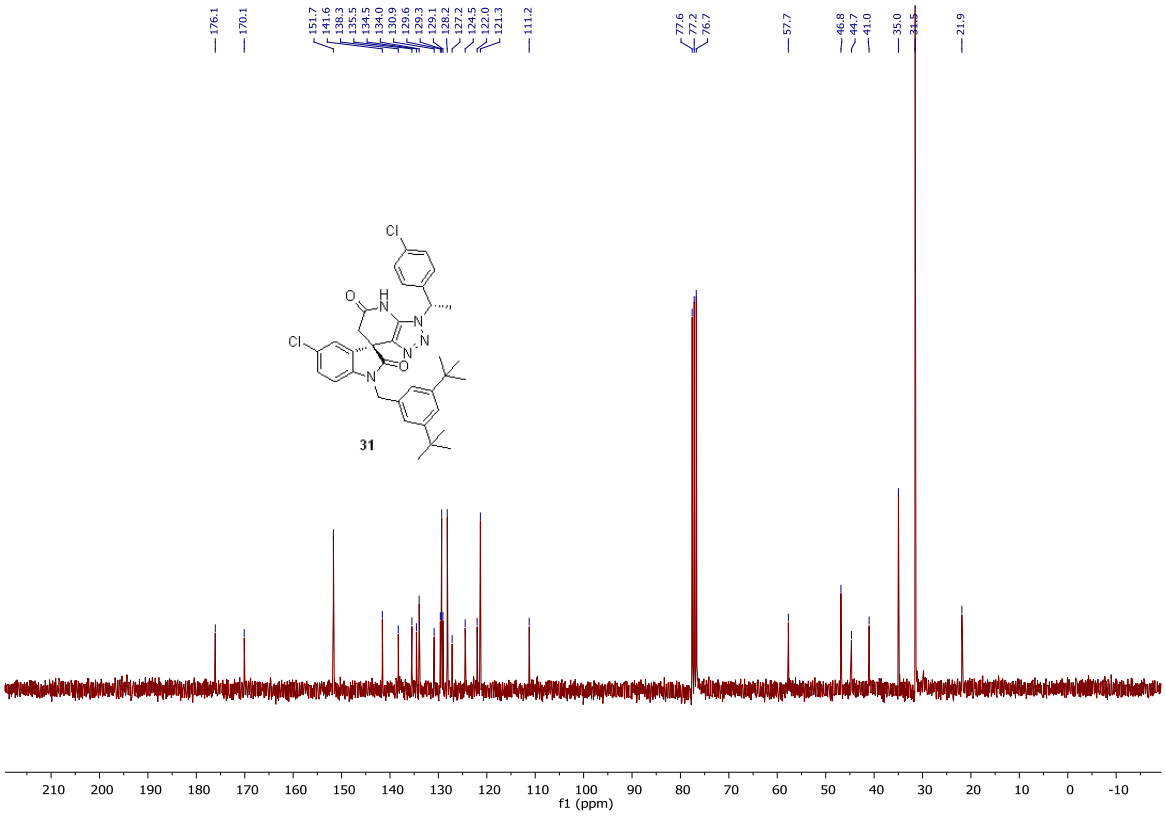
7.23
7.16
7.15
7.14
7.13
6.80
6.77
5.60
5.58
5.56
5.53
4.94
4.89
3.05
1.97
1.94
1.30
0.97
6.34
2.93
1.01
1.00
1.97
1.97
3.04
18.28
f1 (ppm)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134.5
134.0
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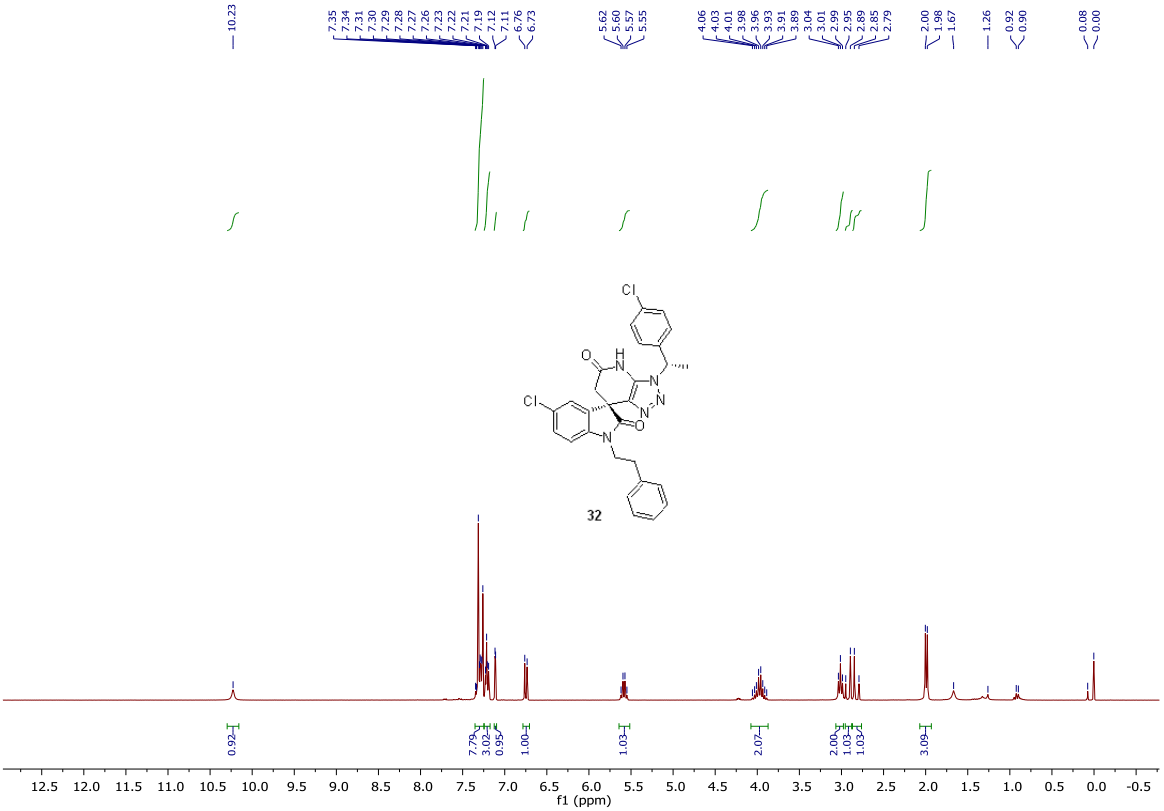
129.1
128.2
127.2
124.5
122.0
121.3
111.2
77.6
77.2
76.7
57.7
46.8
44.7
41.0
35.0
31.5
21.9
f1 (ppm)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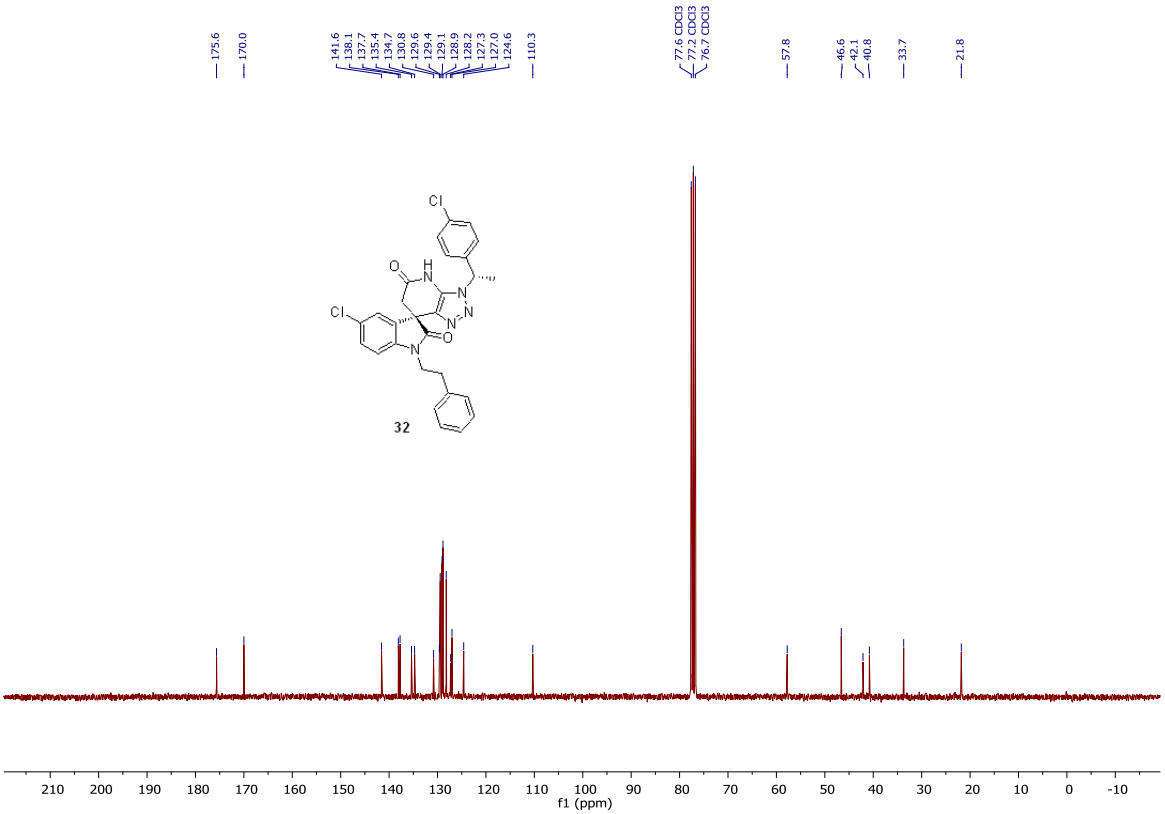
7.35 7.34 7.31 7.30 7.29 7.28 7.27 7.26 7.23 7.22 7.21 7.19 7.12 7.11 6.76 6.73
5.62 5.60 5.57 5.55
4.06 4.03 4.01 3.98 3.96 3.93 3.91 3.89 3.04 3.01 2.99 2.95 2.89 2.85 2.79
2.00 1.98 1.67
1.26
0.92 0.90
0.08 0.00
Cl
O
H
N
N
N
N
O
Cl
N
32
0.92 7.79 3.02 0.95 1.00 1.03 2.07 2.00 1.03 1.03 3.09
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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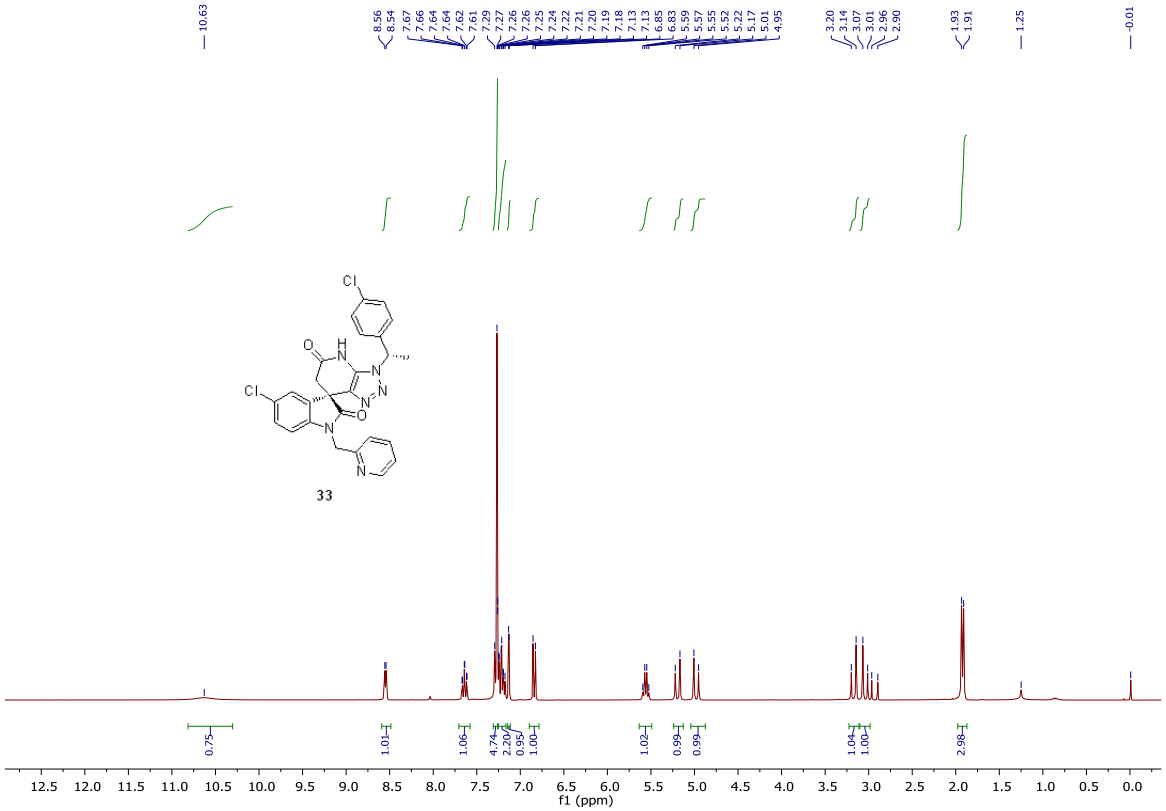
170.0
141.6 138.1 137.7 135.4 134.7 130.8 129.6 129.4 129.1 128.9 128.2 127.3 127.0 124.6
110.3
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.6 42.1 40.8
33.7
21.8
Cl
O
H
N
N
N
N
O
Cl
N
32
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.62
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7.27
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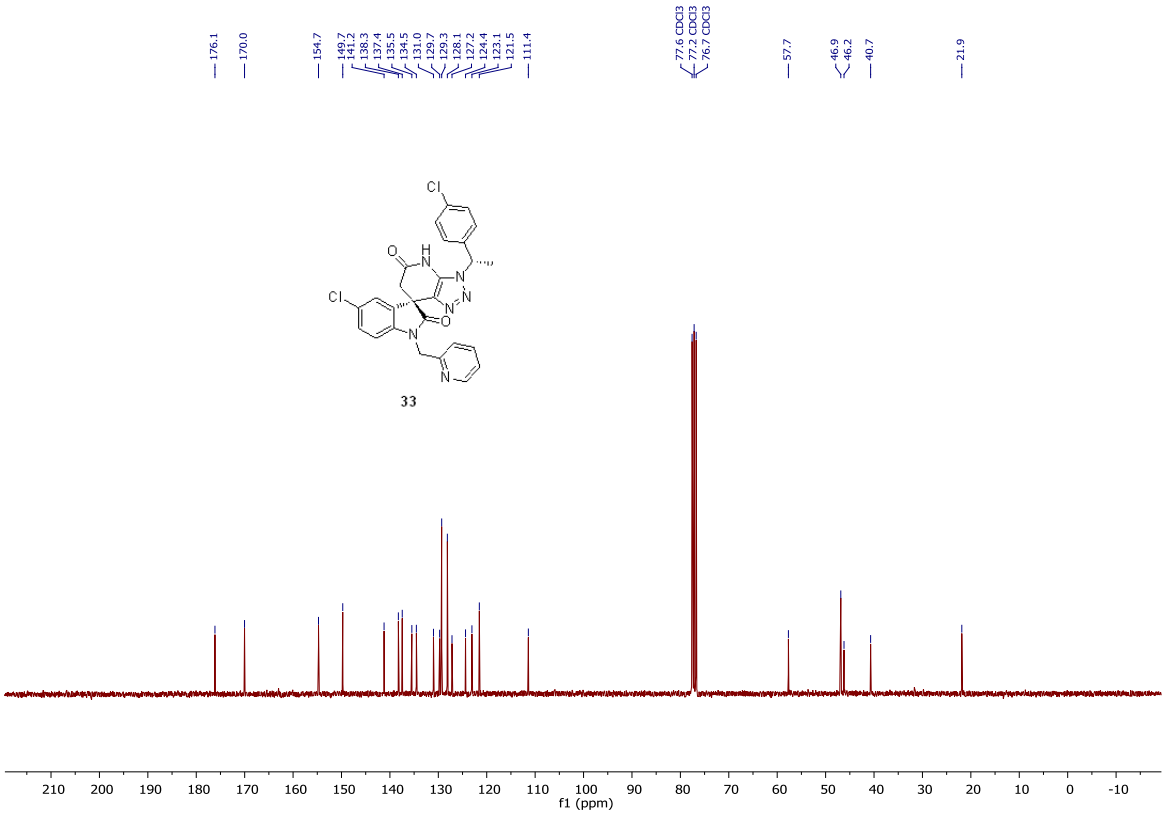
7.26
7.25
7.24
7.22
7.21
7.20
7.19
7.18
7.13
7.13
6.85
6.83
5.59
5.57
5.55
5.52
5.22
5.17
5.01
4.95
3.20
3.14
3.07
3.01
2.96
2.90
1.93
1.91
1.25
-0.01
0.75
1.01
1.06
4.74
2.20
0.95
1.00
1.02
0.99
0.99
1.04
1.00
2.98
f1 (ppm)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170.0
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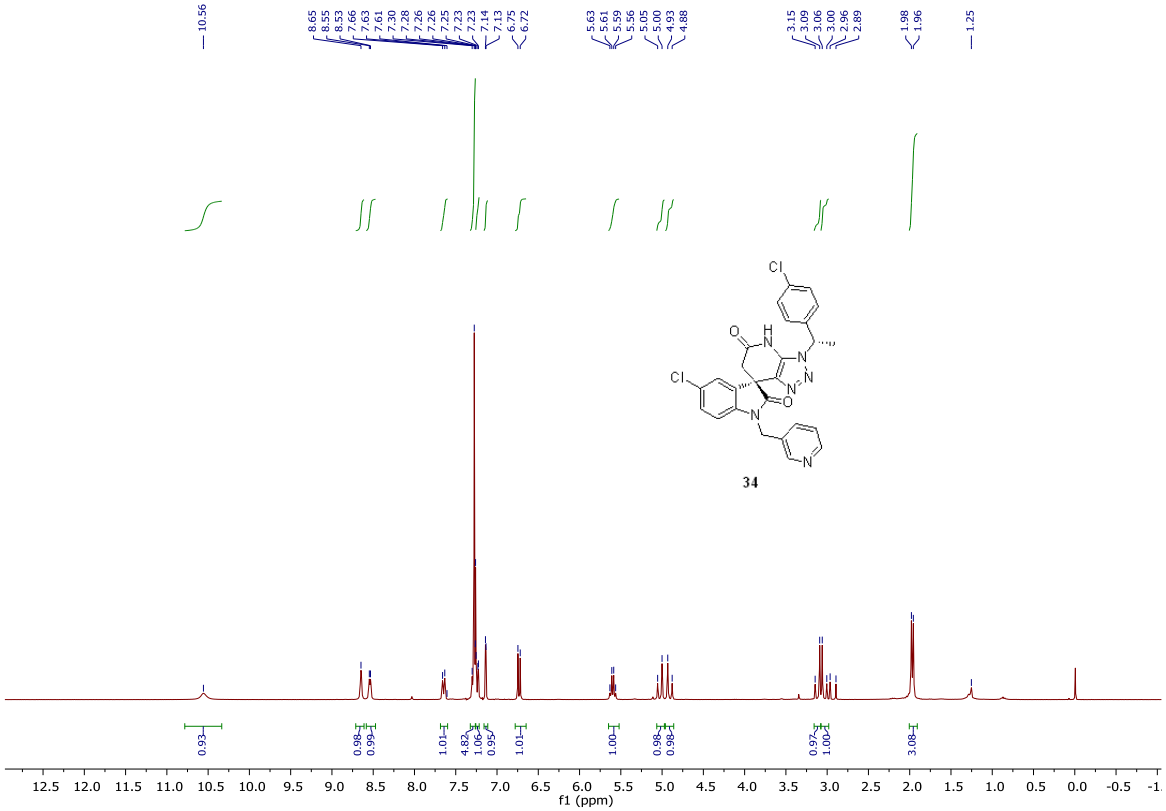
138.3
137.4
135.5
134.5
131.0
129.7
129.3
128.1
127.2
124.4
123.1
121.5
111.4
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.7
46.9
46.2
40.7
21.9
f1 (ppm)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7.26
7.26
7.25
7.23
7.23
7.14
7.13
6.75
6.72
5.63
5.61
5.59
5.56
5.05
5.00
4.93
4.88
3.15
3.09
3.06
3.00
2.96
2.89
1.98
1.96
1.25
0.93
0.98
0.99
1.01
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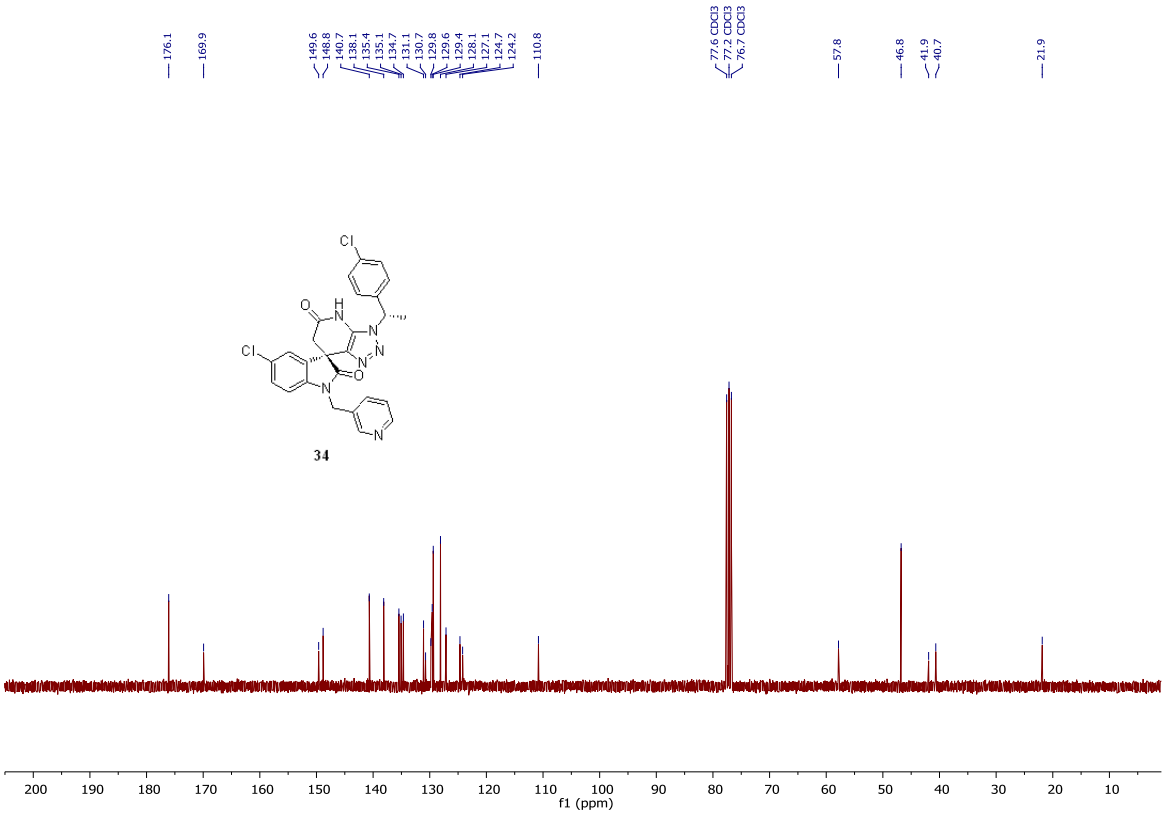
1.06
0.95
1.01
1.00
0.98
0.98
0.97
1.00
3.08
f1 (ppm)

34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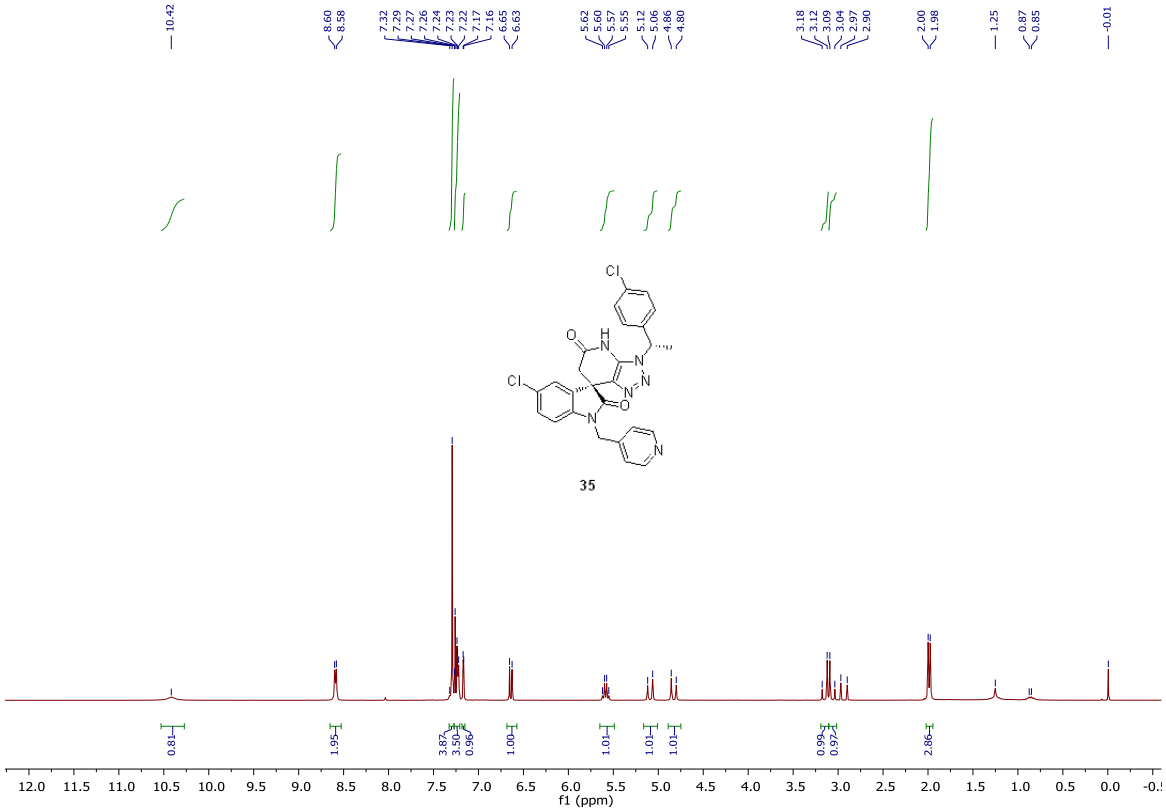
140.7
138.1
135.4
135.1
134.7
131.1
130.7
129.8
129.6
129.4
128.1
127.1
124.7
124.2
110.8
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.8
41.9
40.7
21.9
f1 (ppm)

34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7.22
7.17
7.16
6.65
6.63
5.62
5.60
5.57
5.55
5.12
5.06
4.86
4.80
3.18
3.12
3.09
3.04
2.97
2.90
2.00
1.98
1.25
0.87
0.85
-0.01
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0.81
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3.87
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0.96
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1.01
1.01
1.01
0.99
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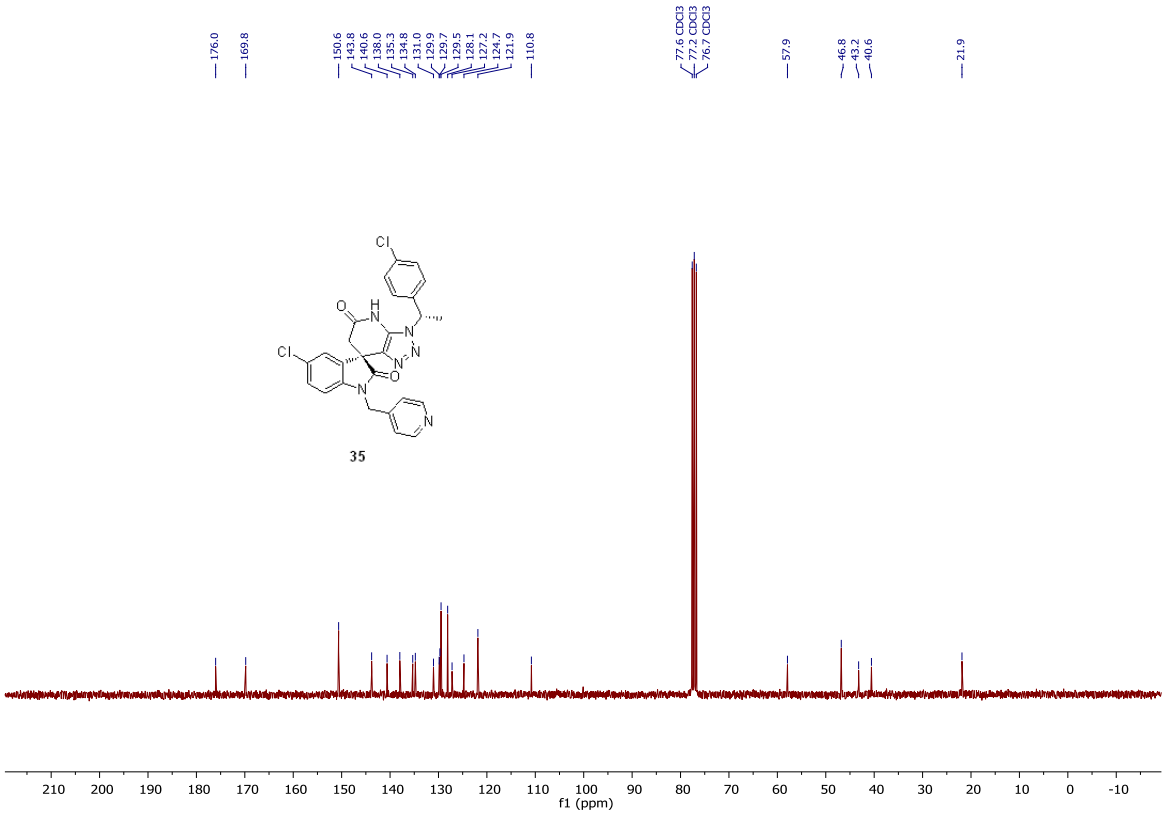
2.86
f1 (ppm)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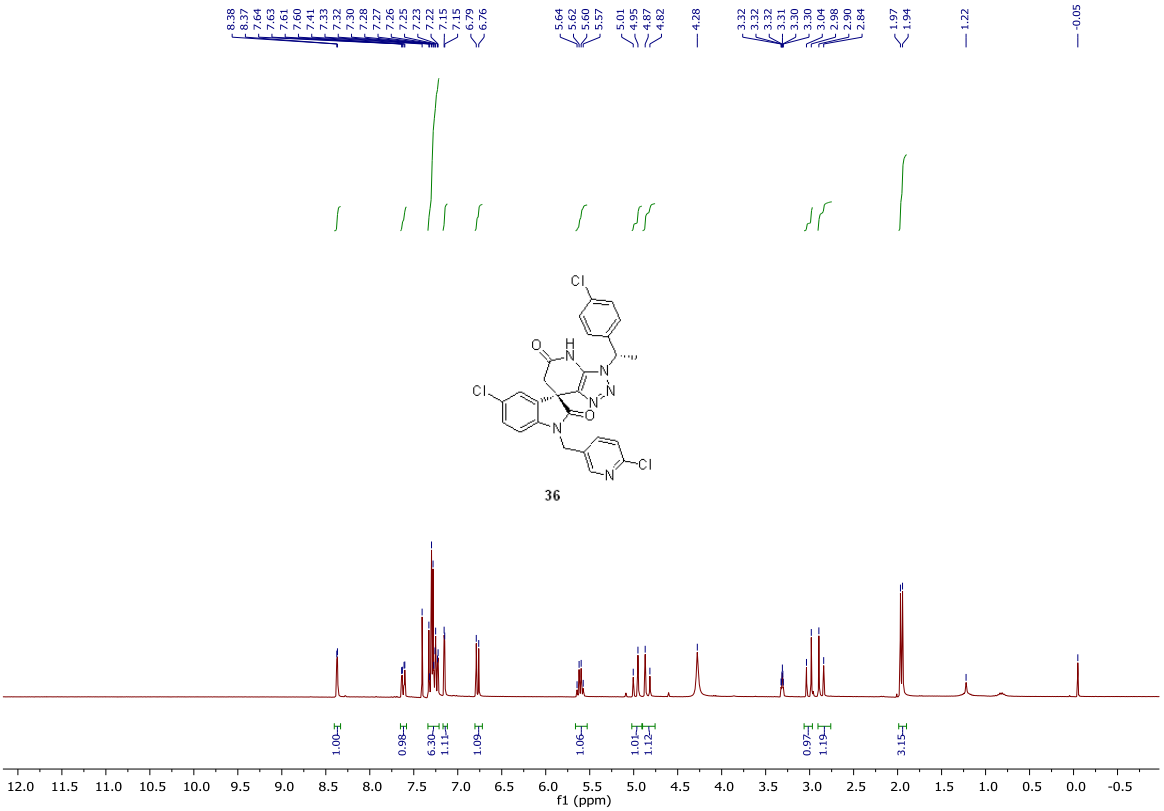
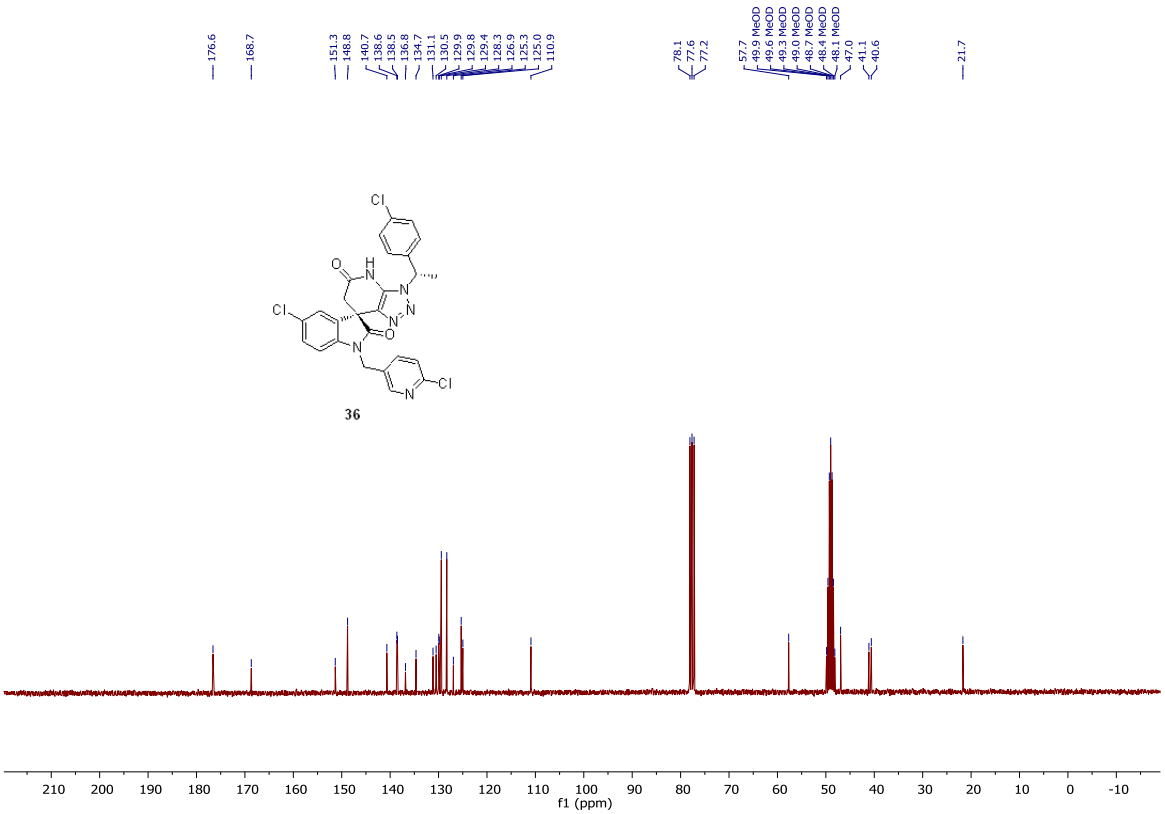
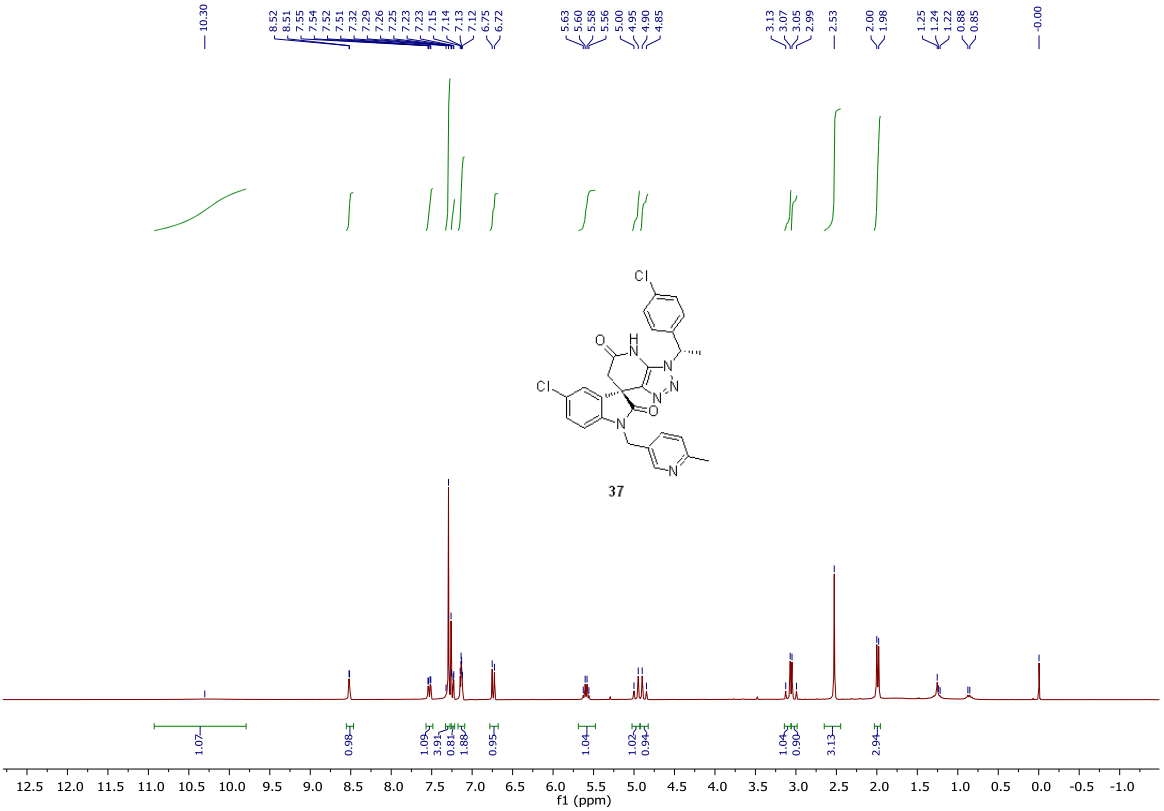
129.7
129.5
128.1
127.2
124.7
121.9
110.8
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.9
46.8
43.2
40.6
21.9
35
f1 (ppm)


36
f1 (ppm)


36
f1 (ppm)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7.14
7.13
7.12
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6.72
5.63
5.60
5.58
5.56
5.00
4.95
4.90
4.85
3.13
3.07
3.05
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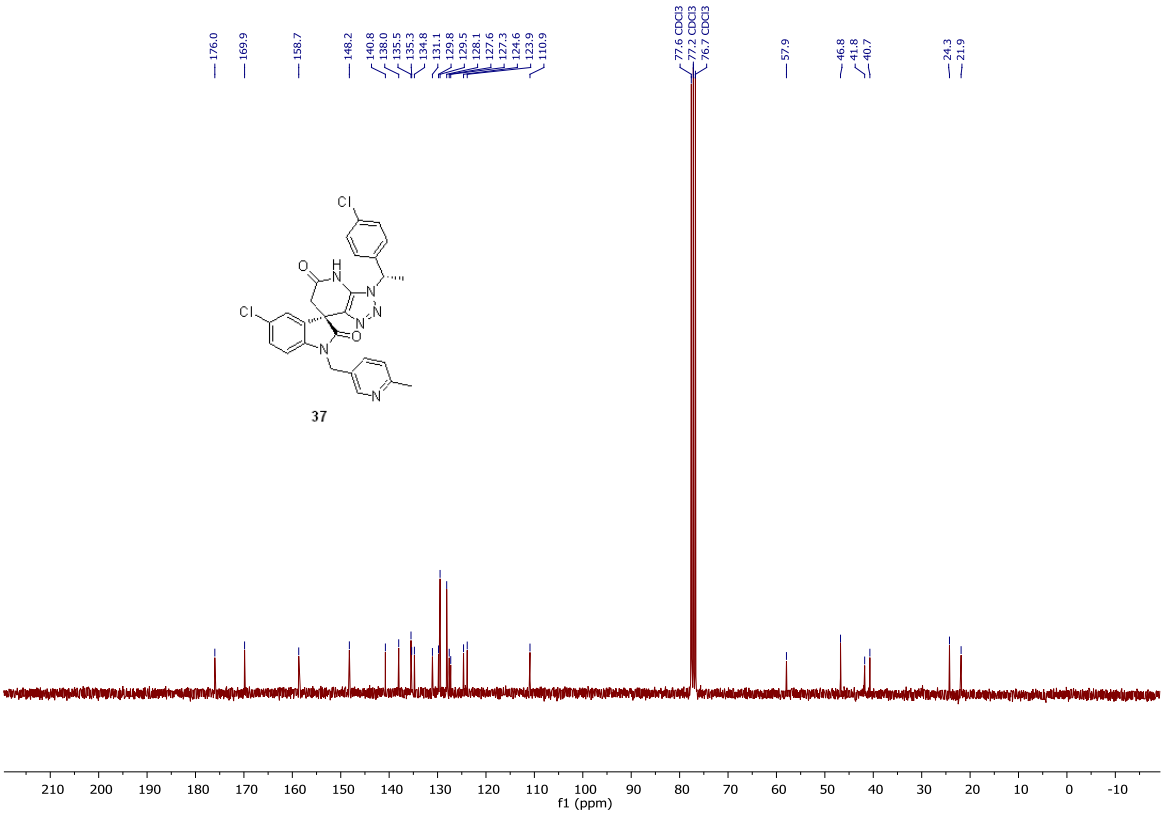
1.24
1.22
0.88
0.85
-0.00
37
f1 (ppm)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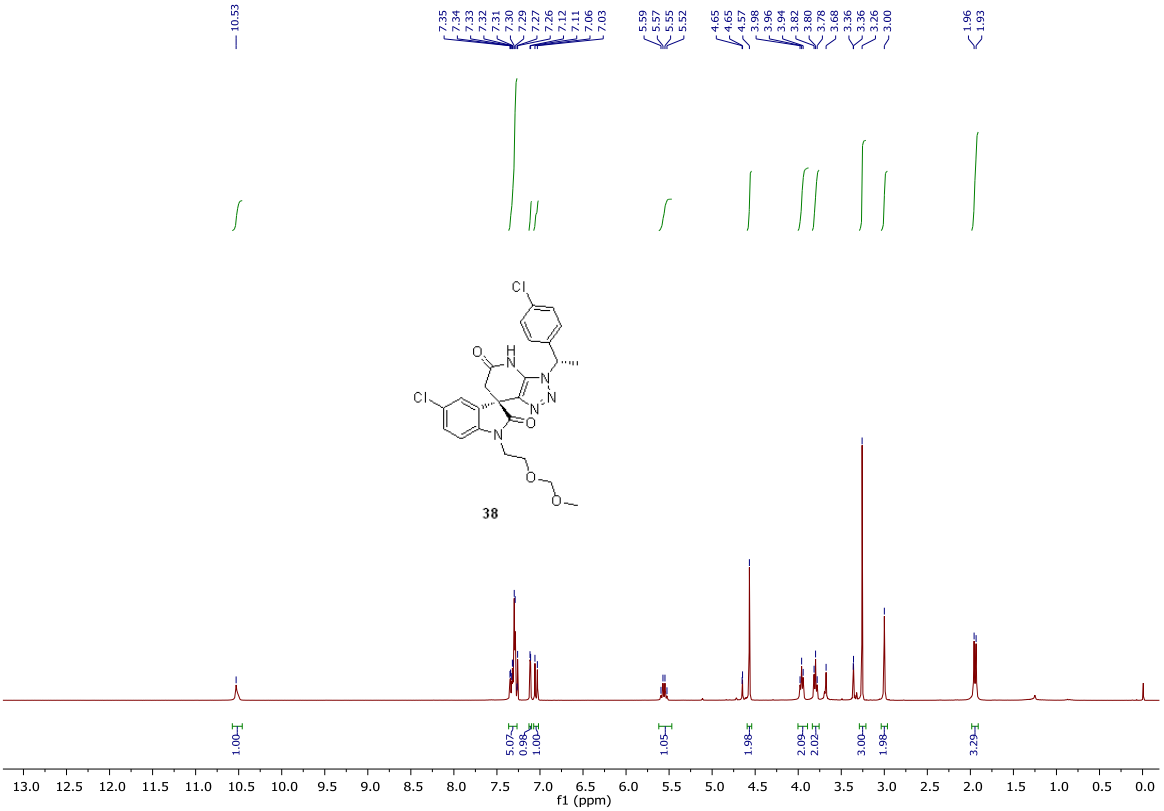
131.1
129.8
129.5
128.1
127.6
127.3
124.6
123.9
110.9
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.9
46.8
41.8
40.7
24.3
21.9
37
f1 (ppm)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7.11
7.06
7.03
5.59
5.57
5.55
5.52
4.65
4.65
4.57
3.98
3.96
3.94
3.82
3.80
3.78
3.68
3.36
3.36
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3.00
1.96
1.93
Cl
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H
N
N
N
Cl
O
N
O
O
38
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5.07
0.98
1.00
1.05
1.98
2.09
2.02
3.00
1.98
3.29
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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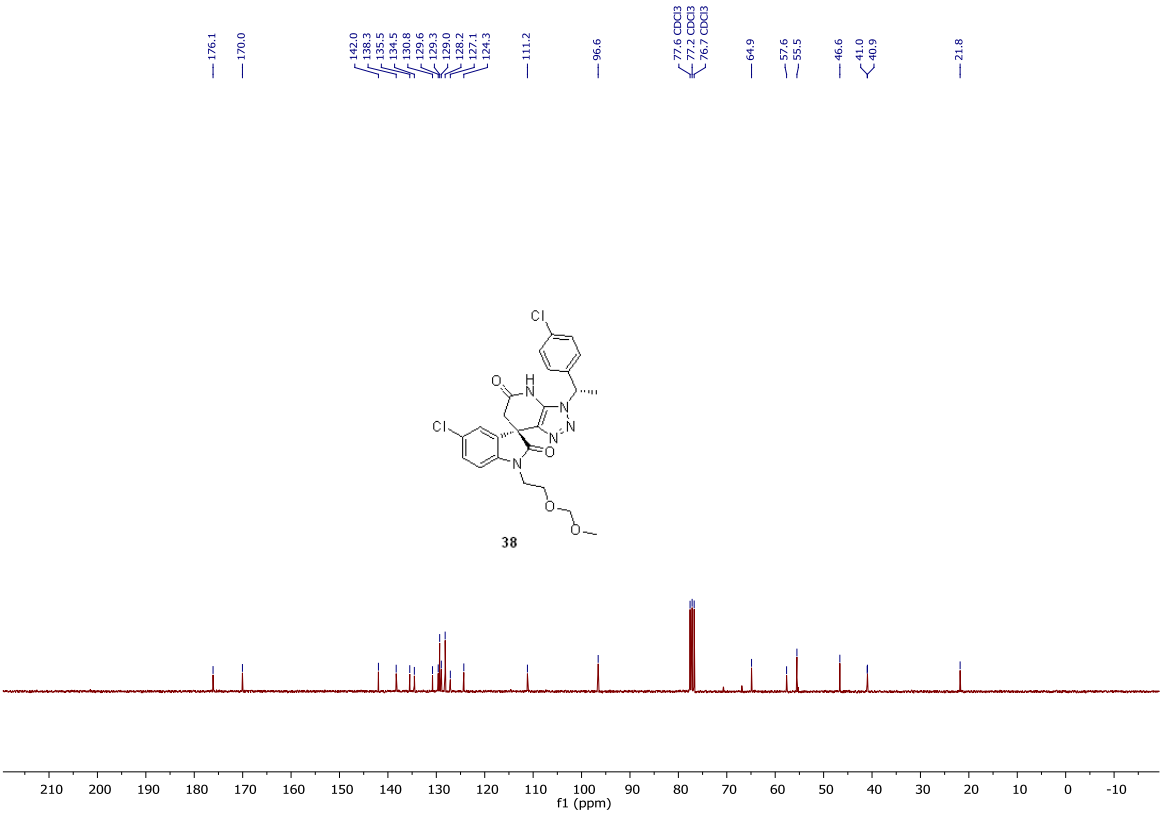
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128.2
127.1
124.3
111.2
96.6
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
64.9
57.6
55.5
46.6
41.0
40.9
21.8
Cl
O
H
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N
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O
N
O
O
38
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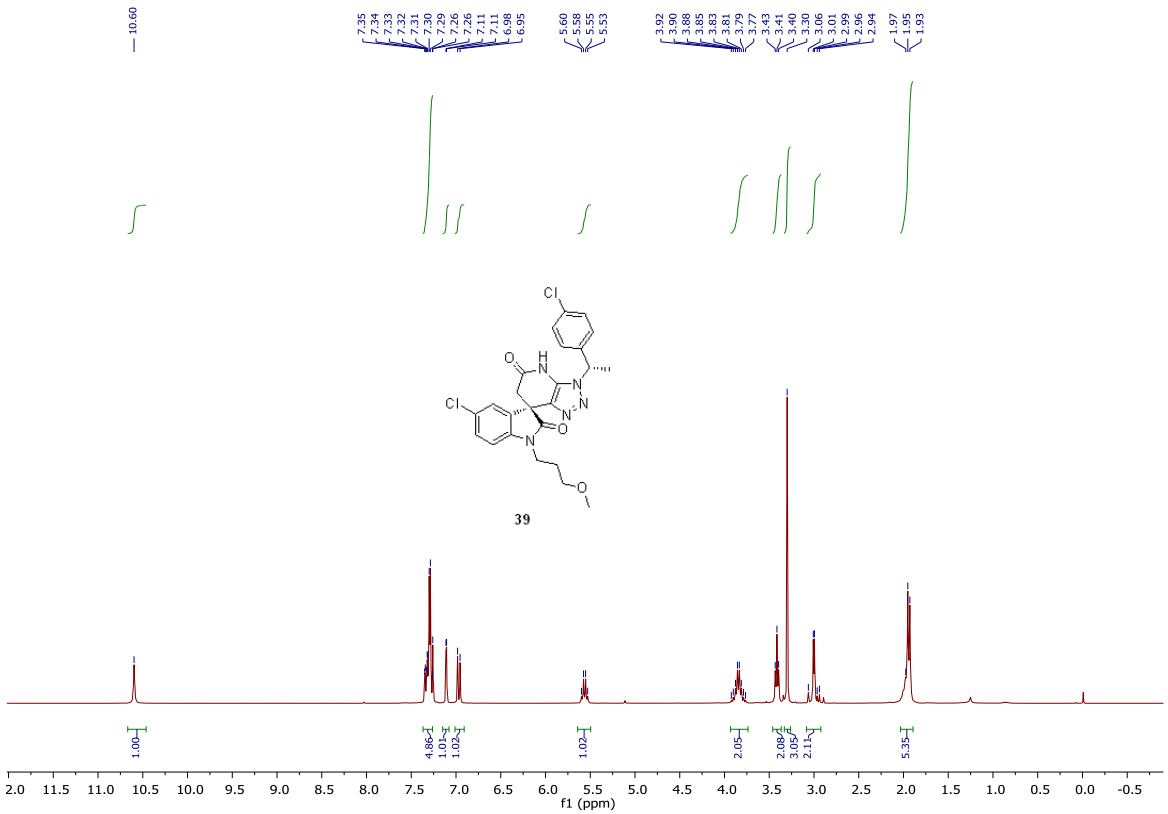
f1 (ppm)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7.11
6.98
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5.60
5.58
5.55
5.53
3.92
3.90
3.88
3.85
3.83
3.81
3.79
3.77
3.43
3.41
3.40
3.30
3.06
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1.97
1.95
1.93
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1.00
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1.02
2.05
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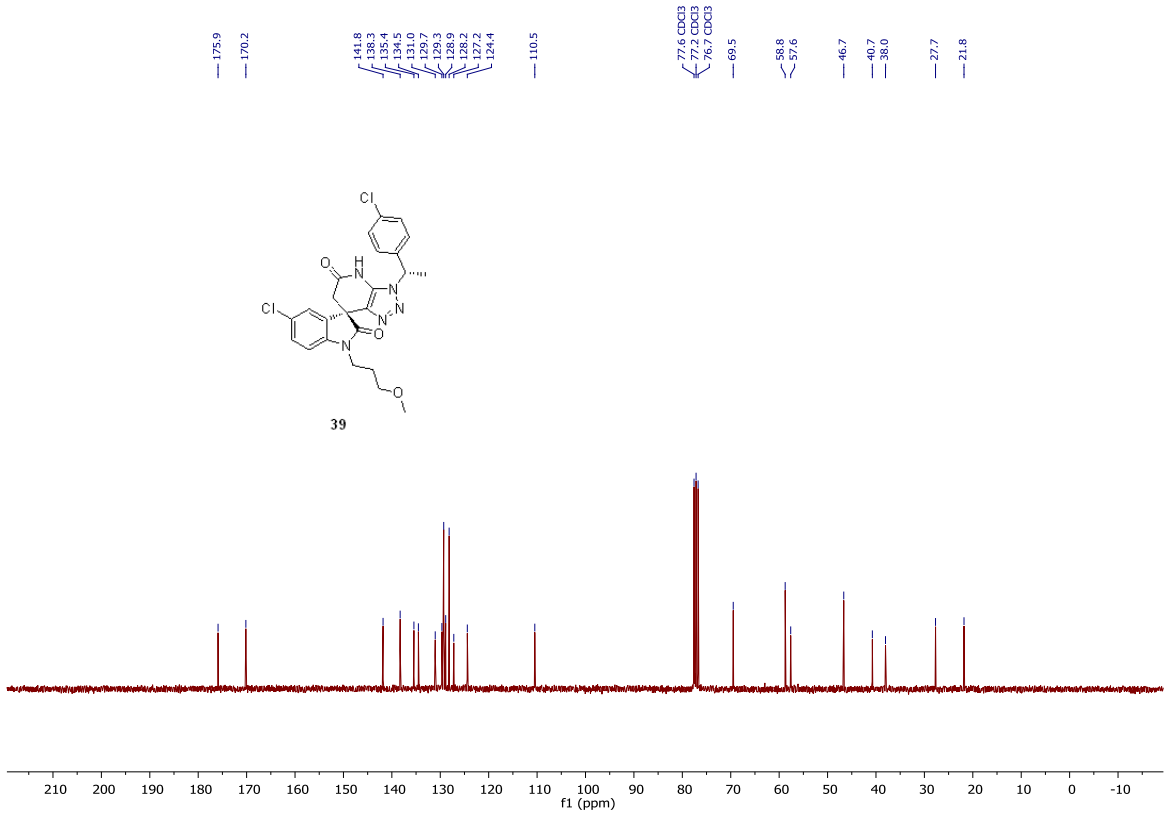
3.05
2.11
5.35
f1 (ppm)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134.5
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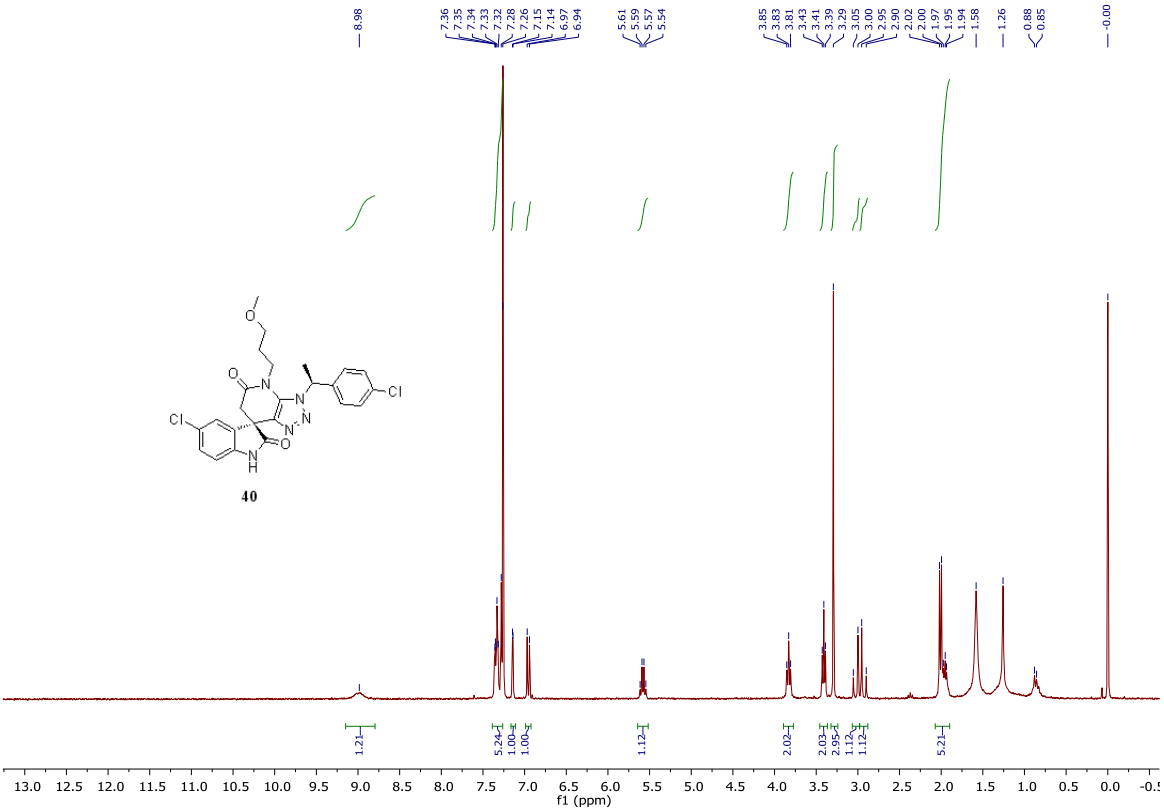
129.7
129.3
128.9
128.2
127.2
124.4
110.5
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
69.5
58.8
57.6
46.7
40.7
38.0
27.7
21.8
39
f1 (ppm)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6.94
5.61
5.59
5.57
5.54
3.85
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3.81
3.43
3.41
3.39
3.29
3.05
3.00
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2.90
2.02
2.00
1.97
1.95
1.94
1.58
1.26
0.88
0.85
-0.00
1.21
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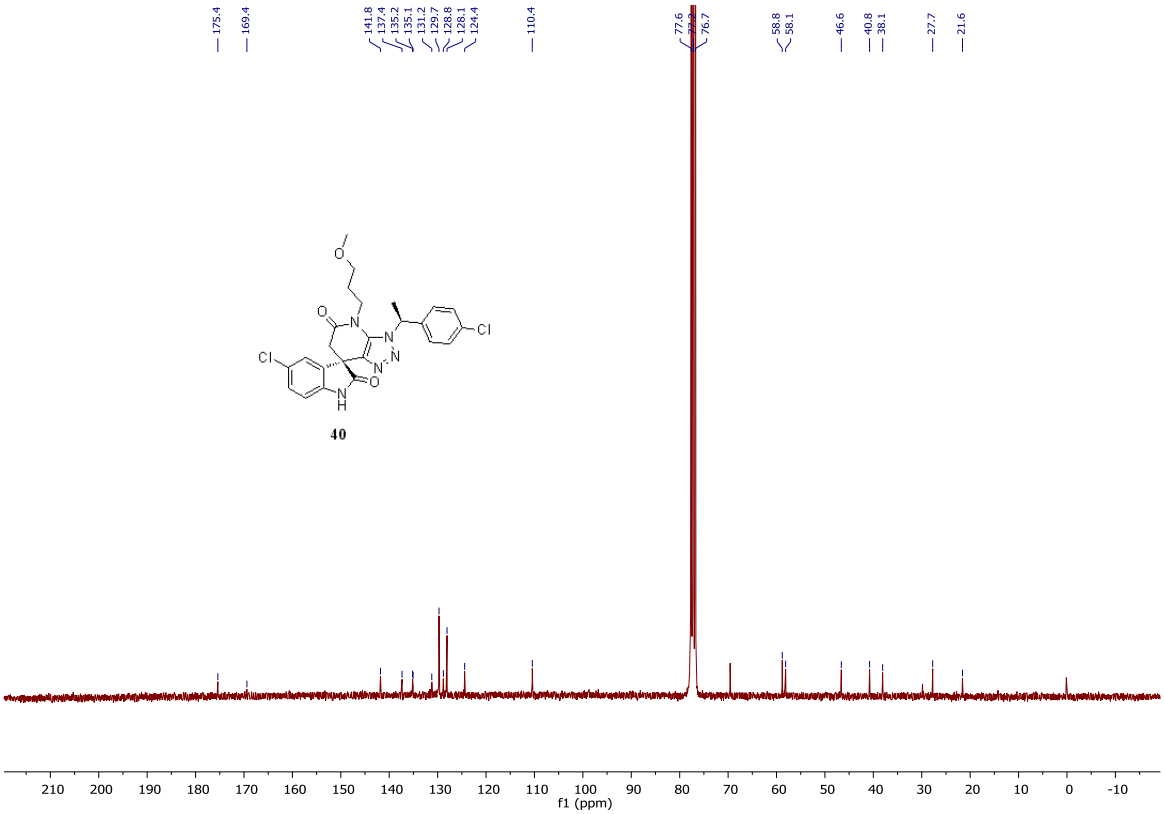
2.03
2.95
1.12
1.12
5.21
f1 (ppm)
40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131.2
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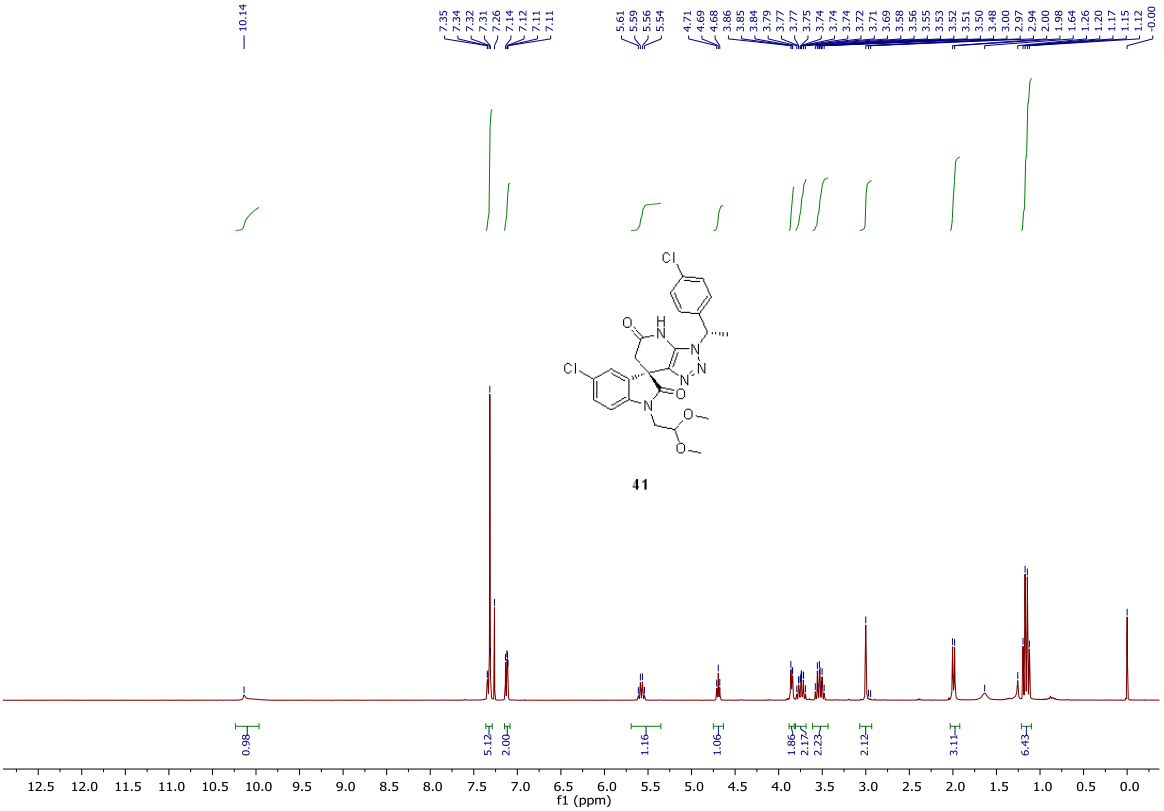
128.1
124.4
110.4
77.6
76.7
58.8
58.1
46.6
40.8
38.1
27.7
21.6
f1 (ppm)
40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5.56
5.54
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4.69
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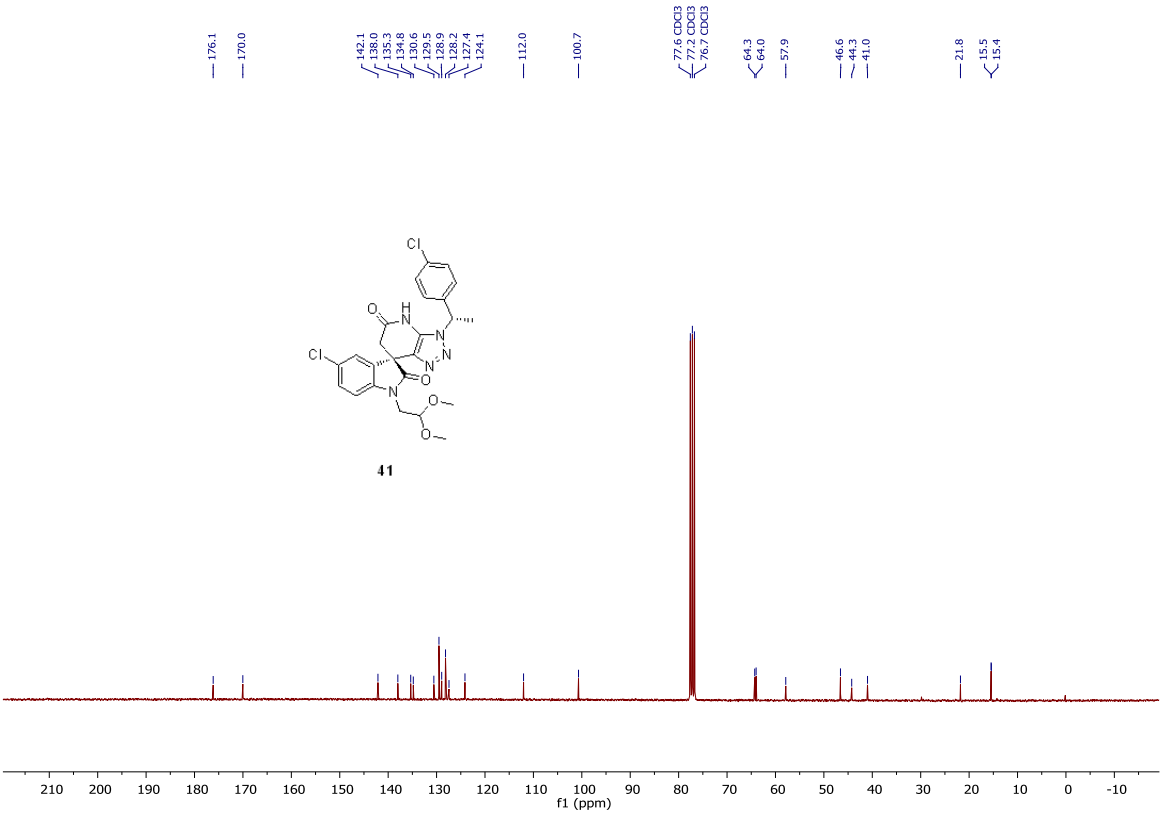
3.86
3.85
3.84
3.79
3.77
3.77
3.75
3.74
3.74
3.74
3.72
3.71
3.69
3.58
3.56
3.55
3.53
3.52
3.51
3.50
3.48
3.00
2.97
2.94
2.00
1.98
1.64
1.26
1.20
1.17
1.15
1.12
-0.00
0.98
5.12
2.00
1.16
1.06
1.86
2.17
2.23
2.12
3.11
6.43
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

41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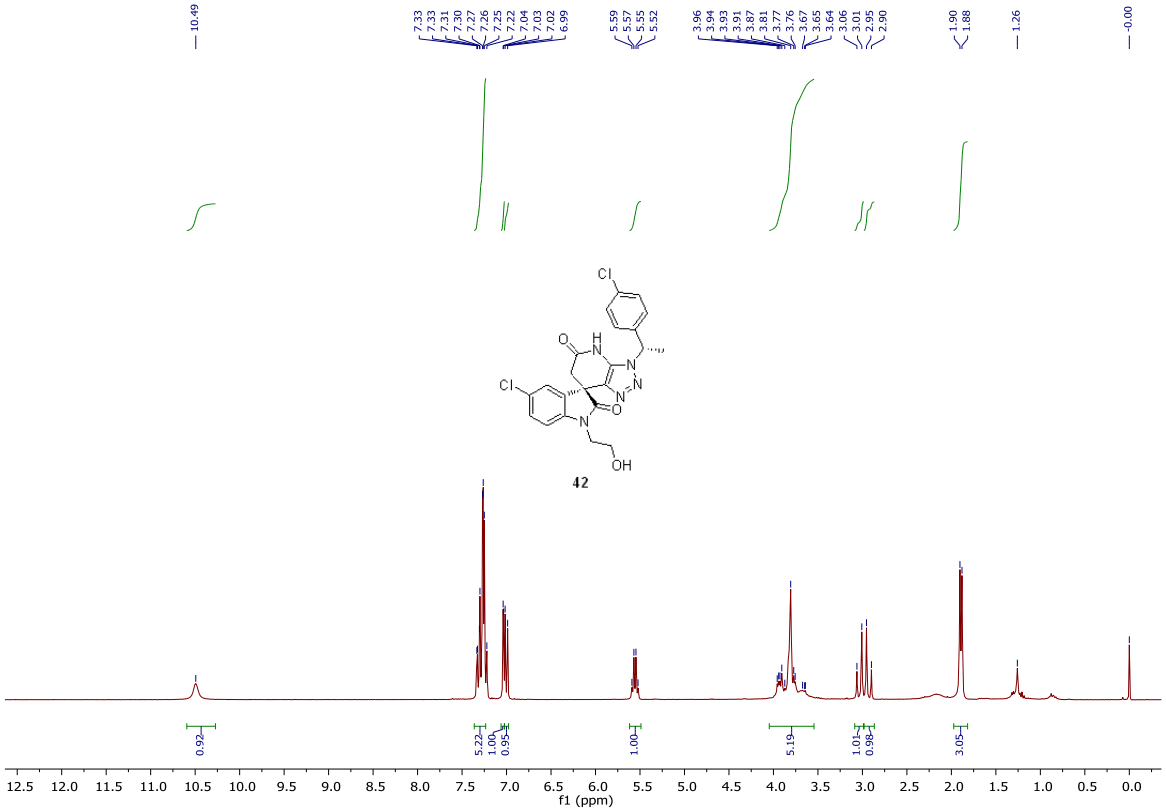
135.3
134.8
130.6
129.5
128.9
128.2
127.4
124.1
112.0
100.7
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
64.3
64.0
57.9
46.6
44.3
41.0
21.8
15.5
15.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

41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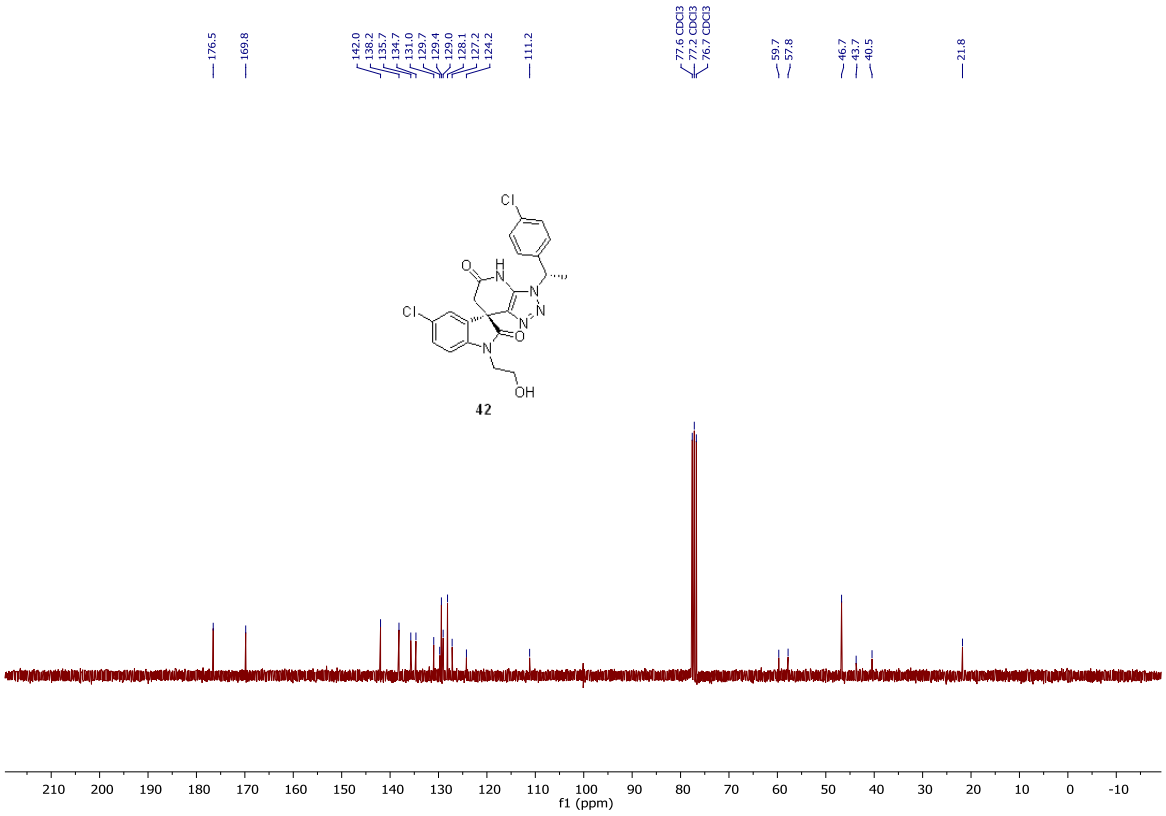
7.04
7.03
7.02
6.99
5.59
5.57
5.55
5.52
3.96
3.94
3.93
3.91
3.87
3.81
3.77
3.76
3.67
3.65
3.64
3.06
3.01
2.95
2.90
1.90
1.88
1.26
-0.00
Cl
O
H
N
N
N
N
O
Cl
N
OH
42
0.92
5.22
1.00
0.95
1.00
5.19
1.01
0.98
3.05
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.7
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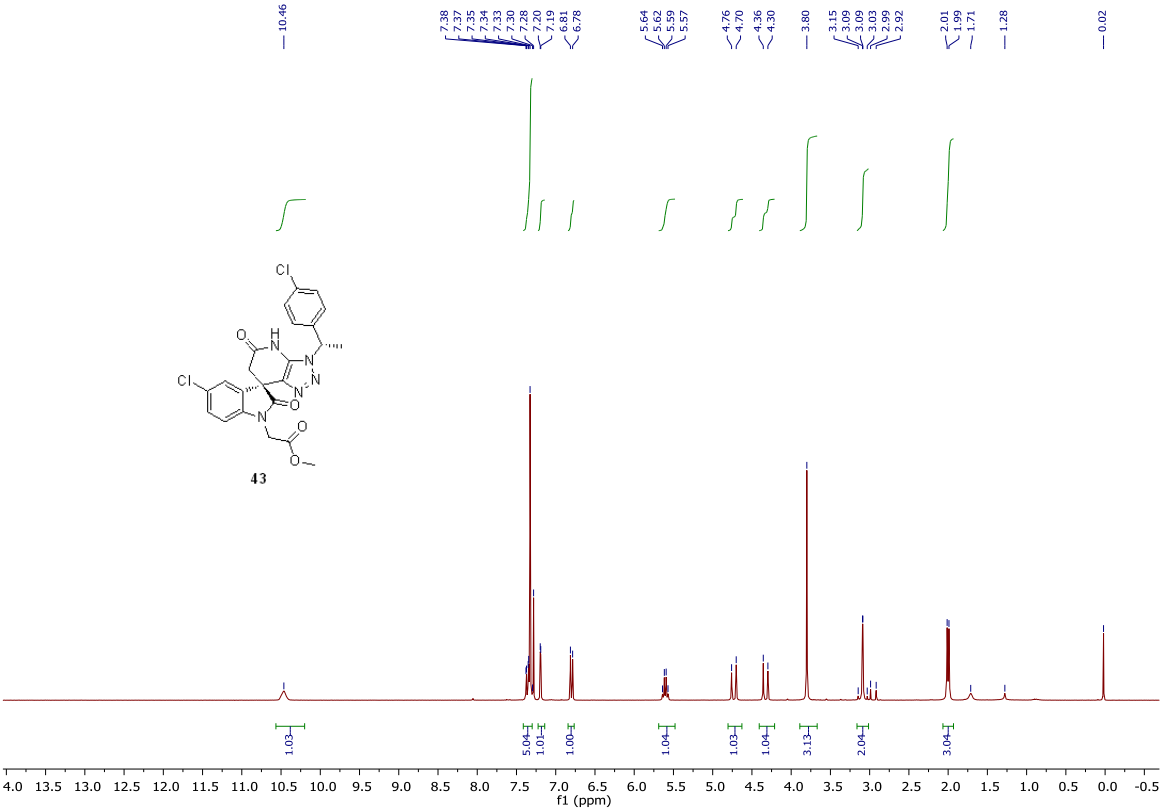
129.0
128.1
127.2
124.2
111.2
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
59.7
57.8
46.7
43.7
40.5
21.8
Cl
O
H
N
N
N
N
O
Cl
N
OH
42
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.19
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6.78
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5.59
5.57
4.76
4.70
4.36
4.30
3.80
3.15
3.09
3.09
3.03
2.99
2.92
2.01
1.99
1.71
1.28
0.02
43
1.03
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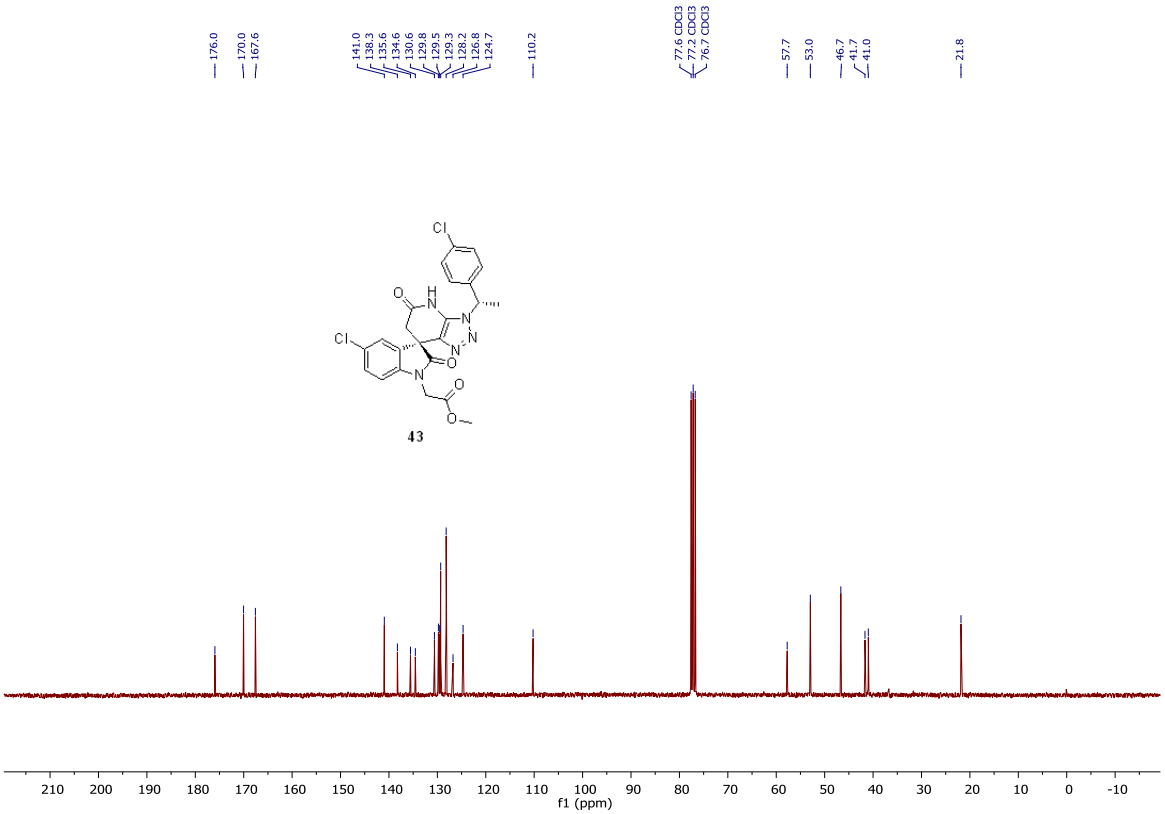
1.01
1.00
1.04
1.03
1.04
3.13
2.04
3.04
f1 (ppm)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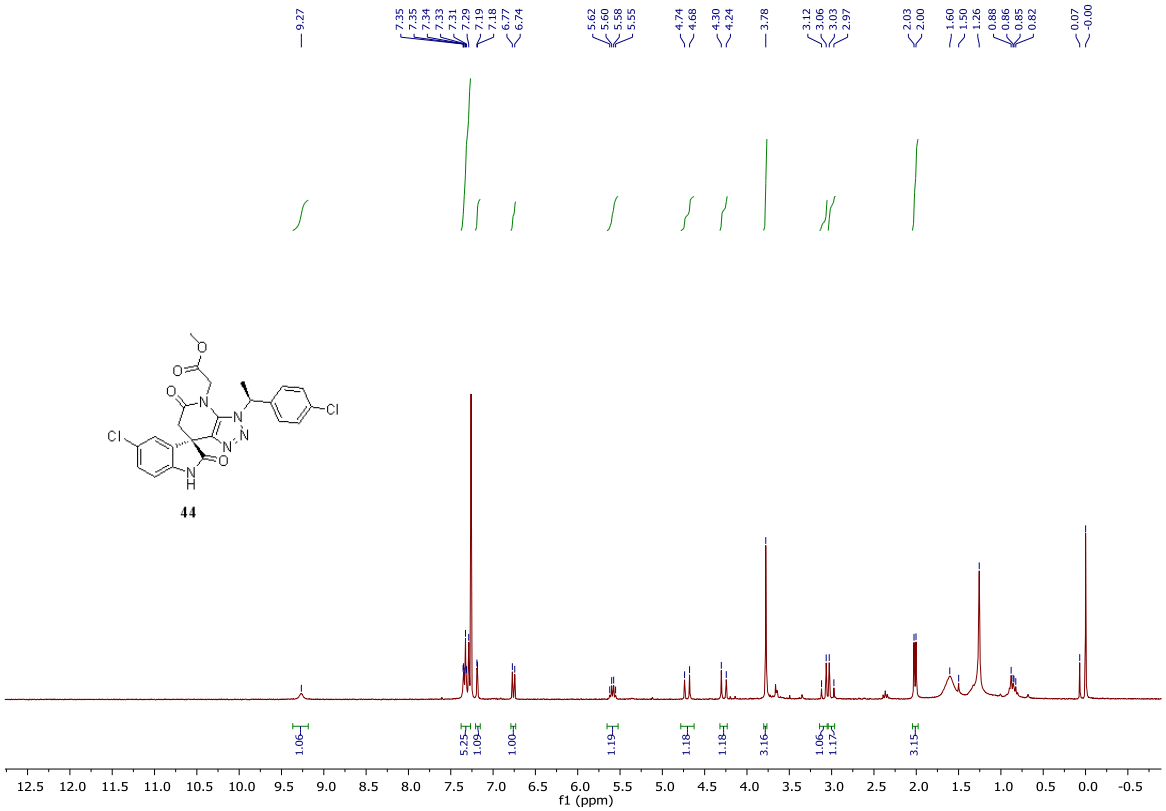
135.6
134.6
130.6
129.8
129.5
129.3
128.2
126.8
124.7
110.2
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.7
53.0
46.7
41.7
41.0
21.8
43
f1 (ppm)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6.77
6.74
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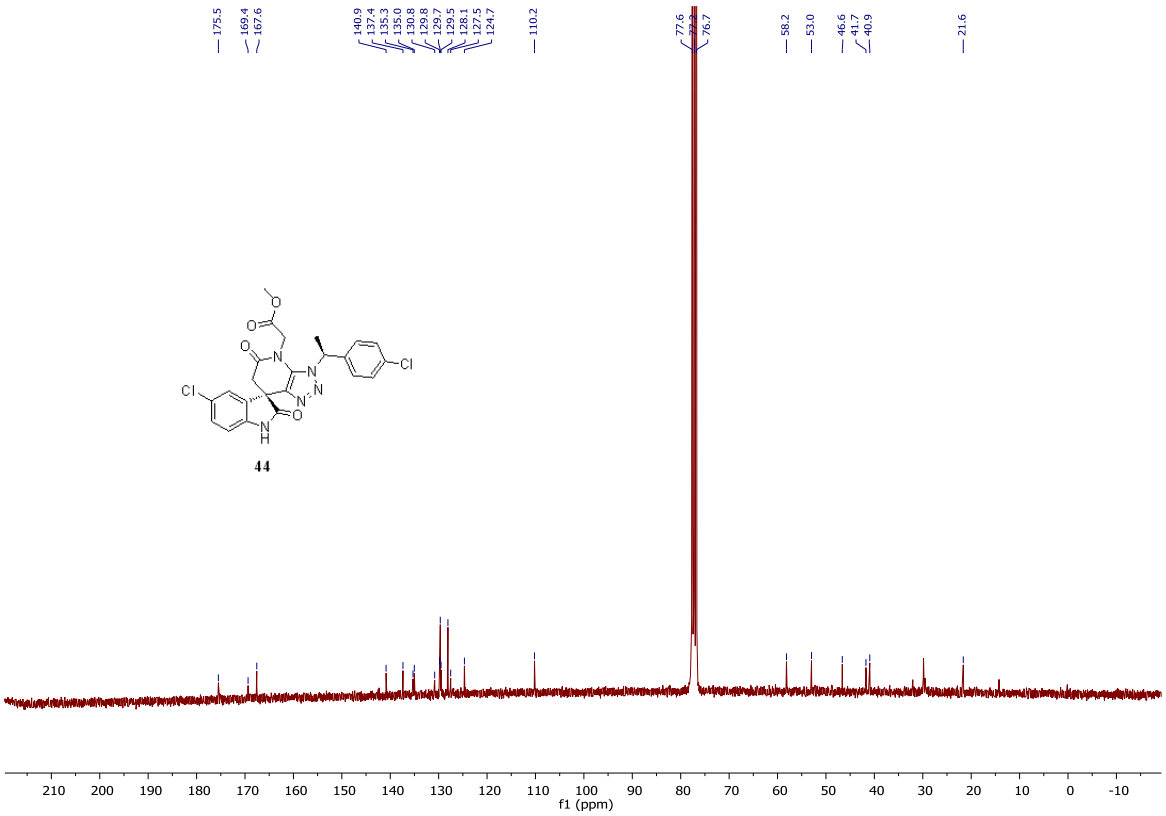
5.60
5.58
5.55
4.74
4.68
4.30
4.24
3.78
3.12
3.06
3.03
2.97
2.03
2.00
1.60
1.50
1.26
0.88
0.86
0.85
0.82
0.07
-0.00
44
1.06
5.25
1.09
1.00
1.19
1.18
1.18
3.16
1.06
1.17
3.15
f1 (ppm)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167.6
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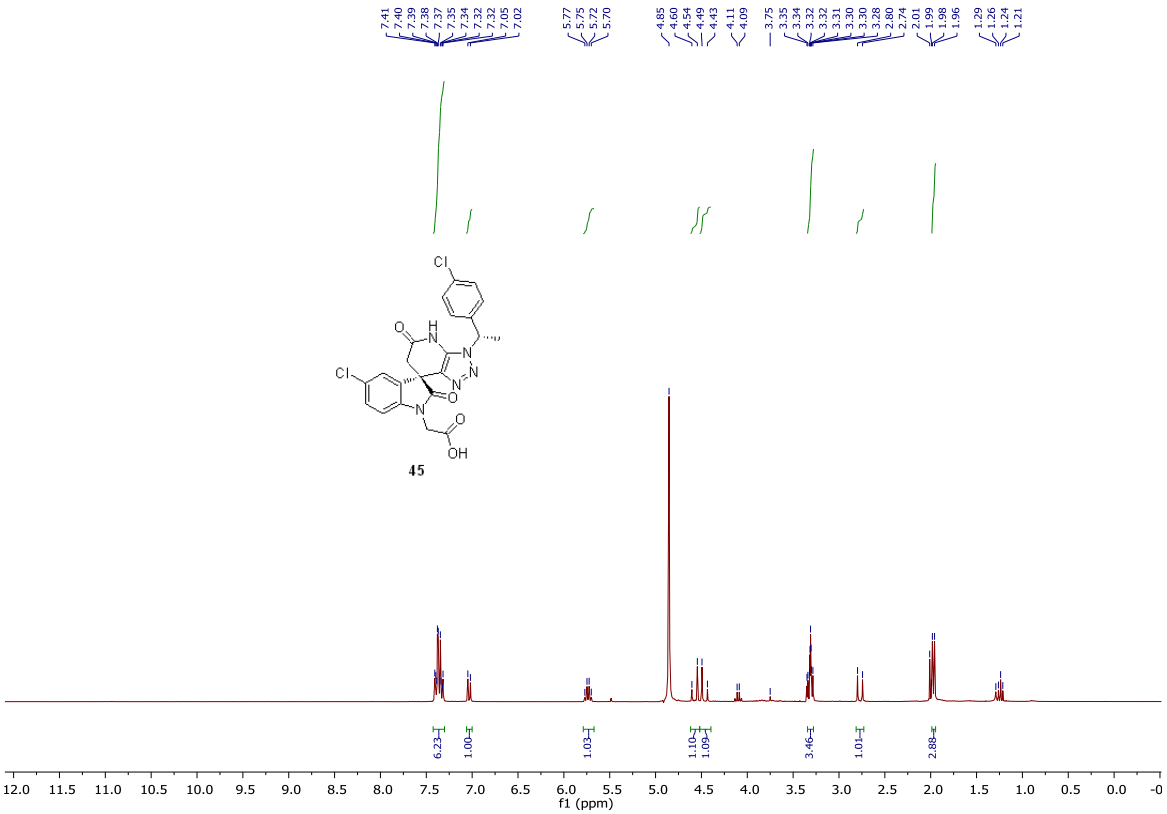
137.4
135.3
135.0
130.8
129.8
129.7
129.5
128.1
127.5
124.7
110.2
77.6
76.7
58.2
53.0
46.6
41.7
40.9
21.6
44
f1 (ppm)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7.32
7.32
7.05
7.02
5.77
5.75
5.72
5.70
4.85
4.60
4.54
4.49
4.43
4.11
4.09
3.75
3.35
3.34
3.32
3.32
3.31
3.30
3.30
3.28
2.80
2.74
2.01
1.99
1.98
1.96
1.29
1.26
1.24
1.21
Cl
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H
N
N
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O
N
O
OH
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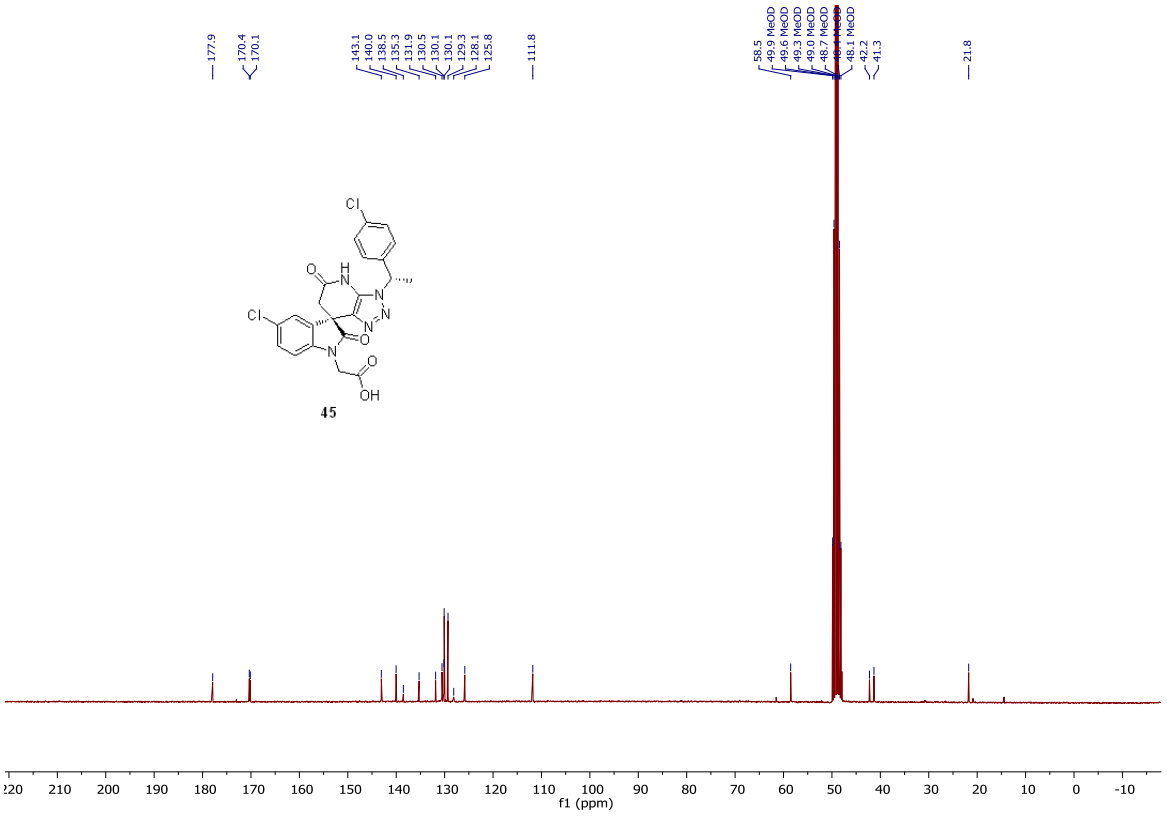
1.03
1.10
1.09
3.46
1.01
2.88
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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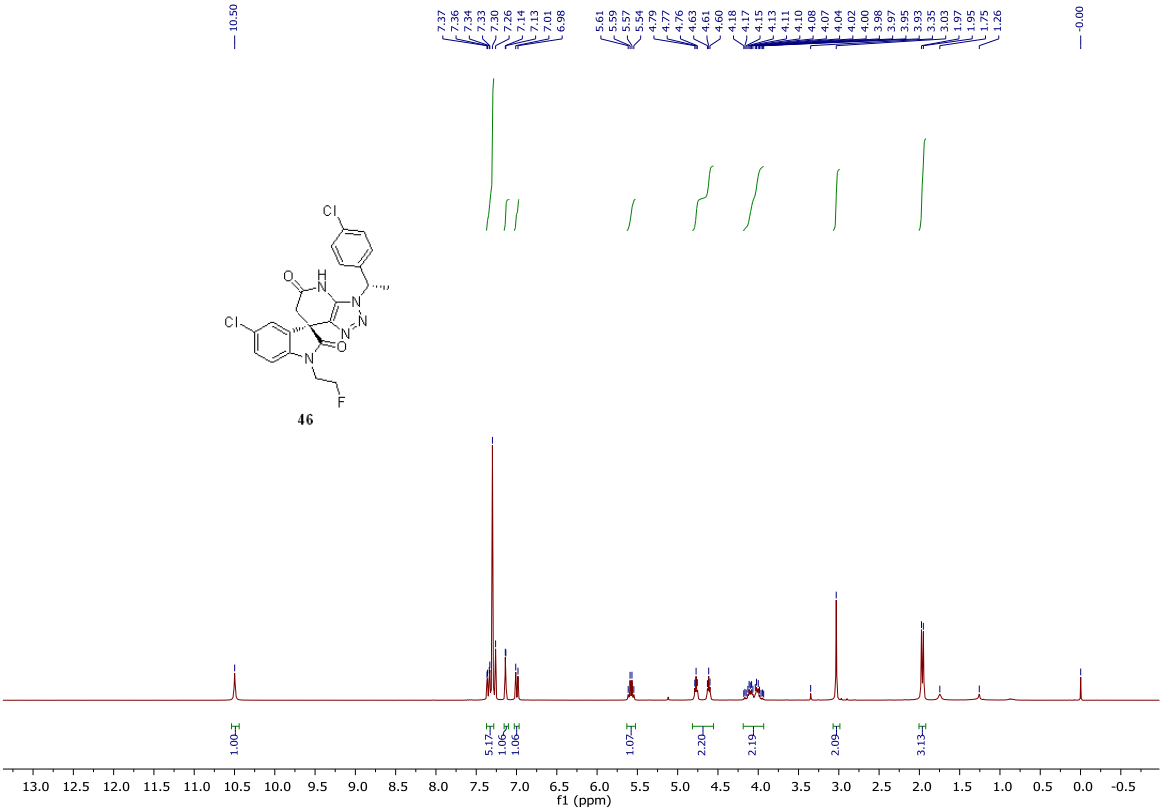
140.0
138.5
135.3
131.9
130.5
130.1
130.1
129.3
128.1
125.8
111.8
58.5
49.9 MeOD
49.6 MeOD
49.3 MeOD
49.0 MeOD
48.7 MeOD
48.1 MeOD
42.2
41.3
21.8
Cl
Cl
O
H
N
N
N
N
O
O
N
O
OH
45
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.13
7.01
6.98
5.61
5.59
5.57
5.54
4.79
4.77
4.76
4.63
4.61
4.60
4.18
4.17
4.17
4.15
4.13
4.11
4.10
4.08
4.07
4.04
4.02
4.00
3.98
3.97
3.95
3.93
3.35
3.03
1.97
1.95
1.75
1.26
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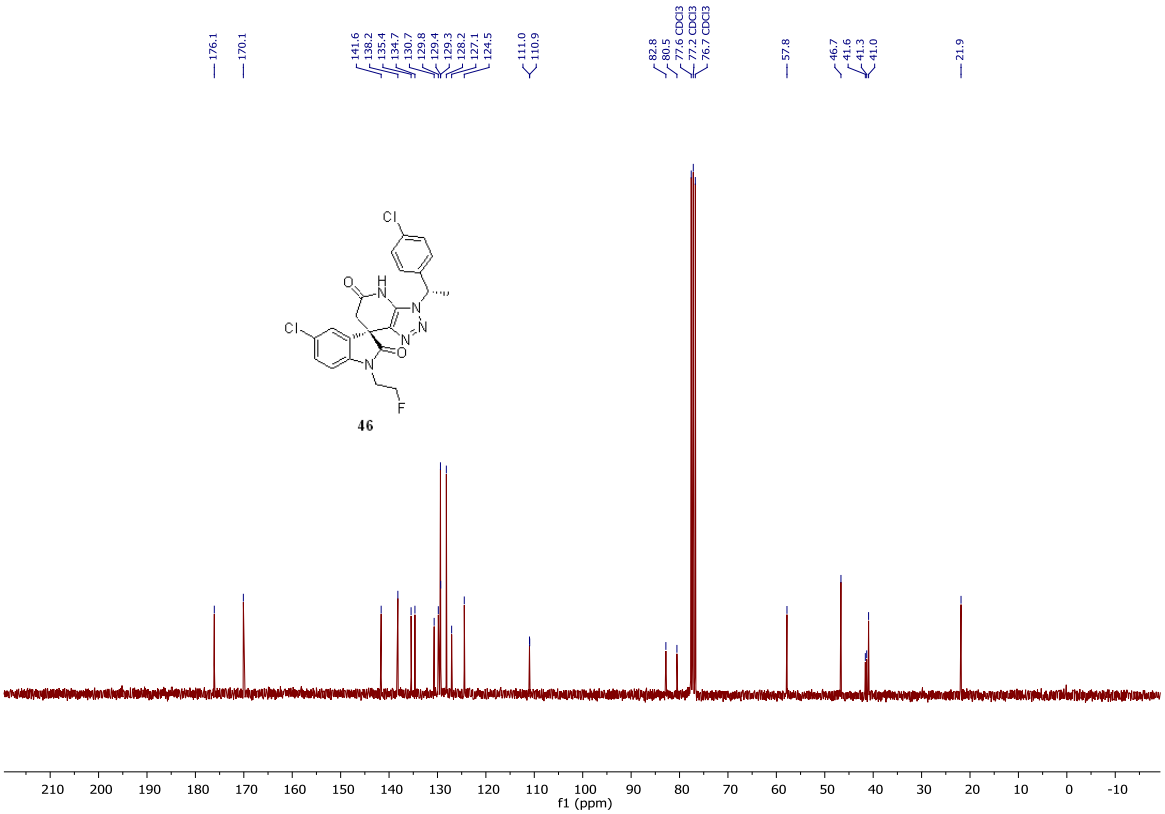
1.06
1.06
1.07
2.20
2.19
2.09
3.13
f1 (ppm)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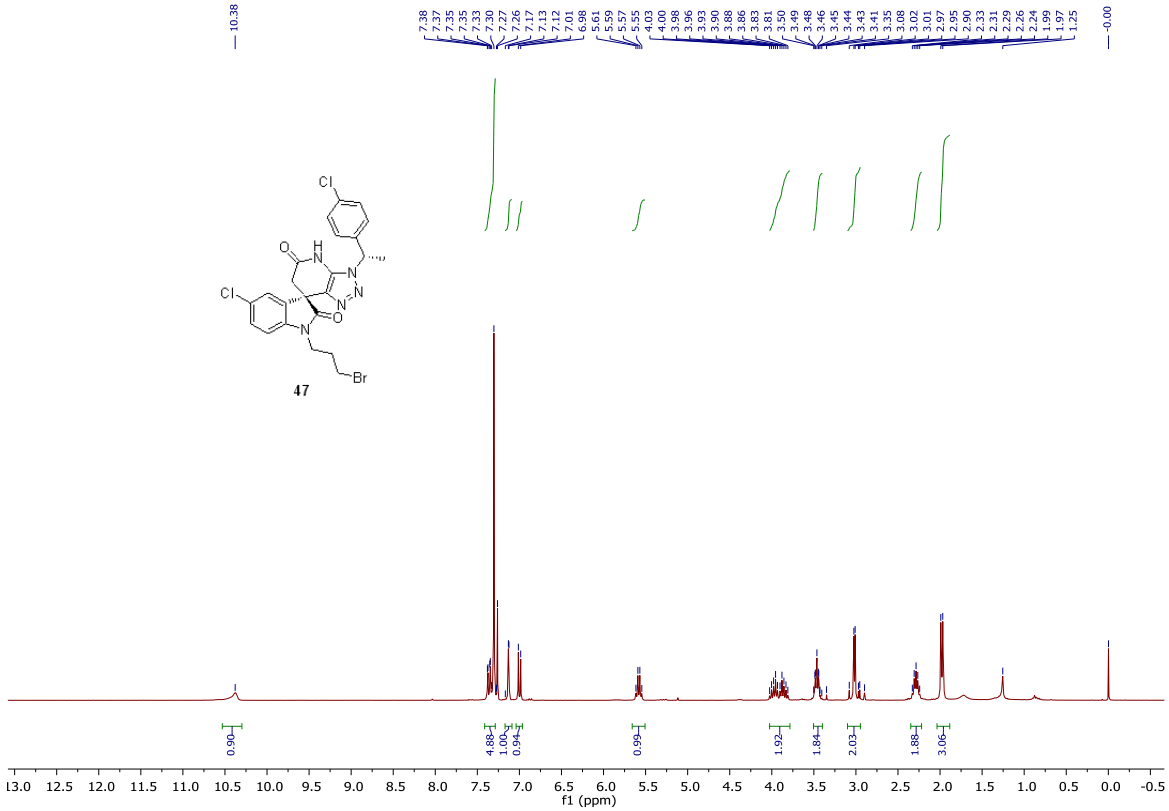
138.2
135.4
134.7
130.7
129.8
129.4
129.3
128.2
127.1
124.5
111.0
110.9
82.8
80.5
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.7
41.6
41.3
41.0
21.9
46
f1 (ppm)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7.01
6.98
5.61
5.59
5.57
5.55
4.03
4.00
3.98
3.96
3.93
3.90
3.88
3.86
3.83
3.81
3.50
3.49
3.48
3.46
3.45
3.44
3.43
3.41
3.35
3.08
3.02
3.01
2.97
2.95
2.90
2.33
2.31
2.29
2.26
2.24
1.99
1.97
1.25
-0.00
Cl
Cl
Br
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2.03
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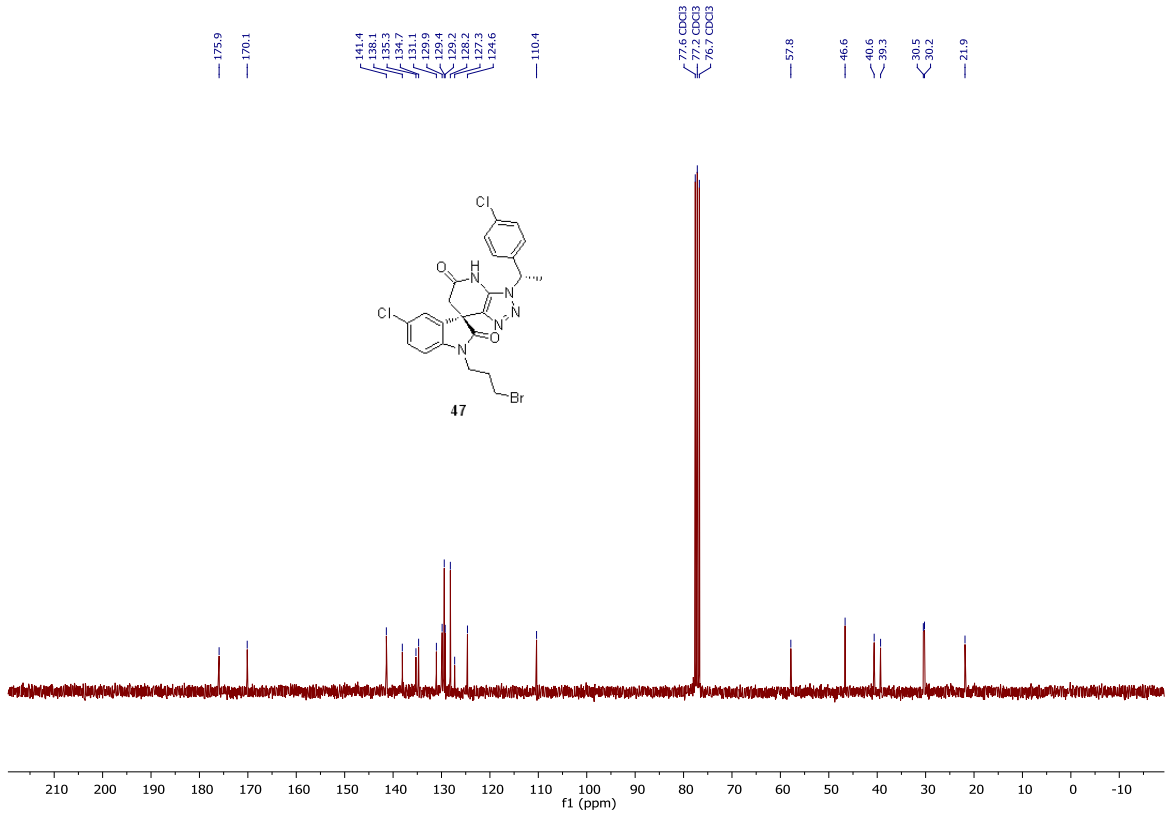
3.06
f1 (ppm)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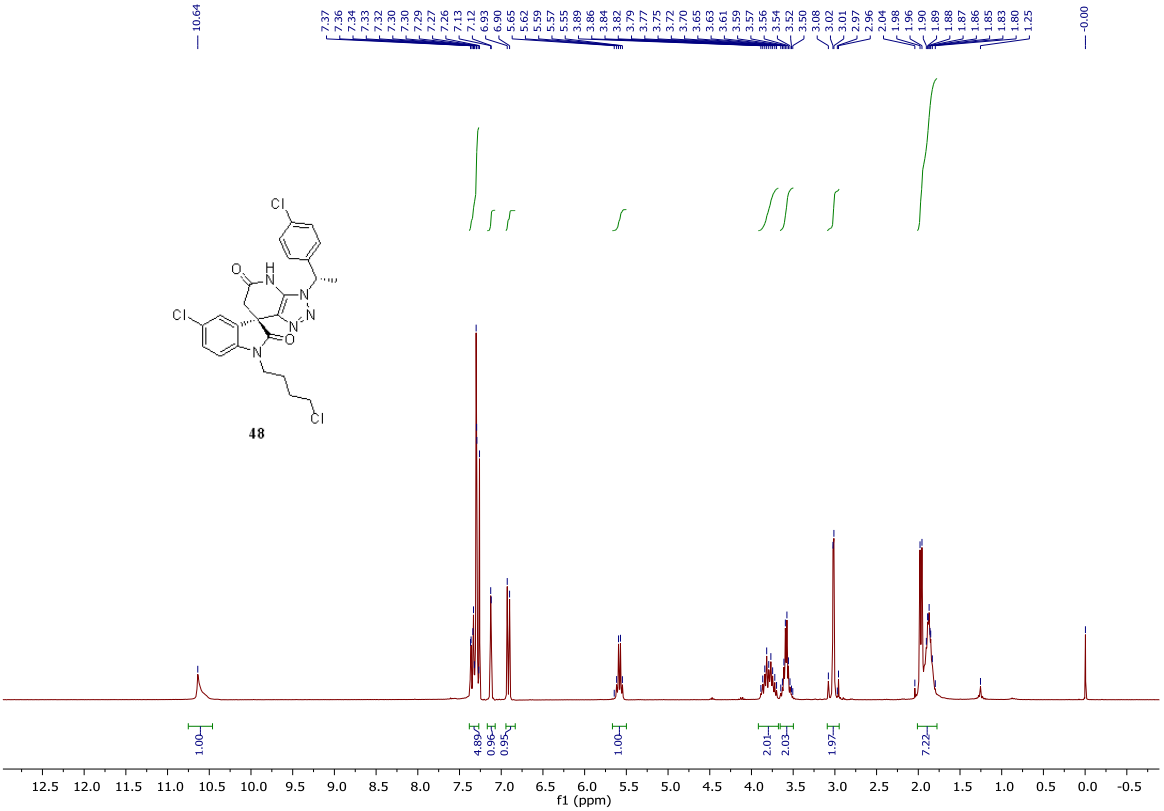
131.1
129.9
129.4
129.2
128.2
127.3
124.6
110.4
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.6
40.6
39.3
30.5
30.2
21.9
Cl
Cl
Br
47
f1 (ppm)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7.26
7.13
7.12
6.93
6.90
5.65
5.62
5.59
5.57
5.55
3.89
3.86
3.84
3.82
3.79
3.77
3.75
3.72
3.70
3.65
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3.61
3.59
3.57
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3.50
3.08
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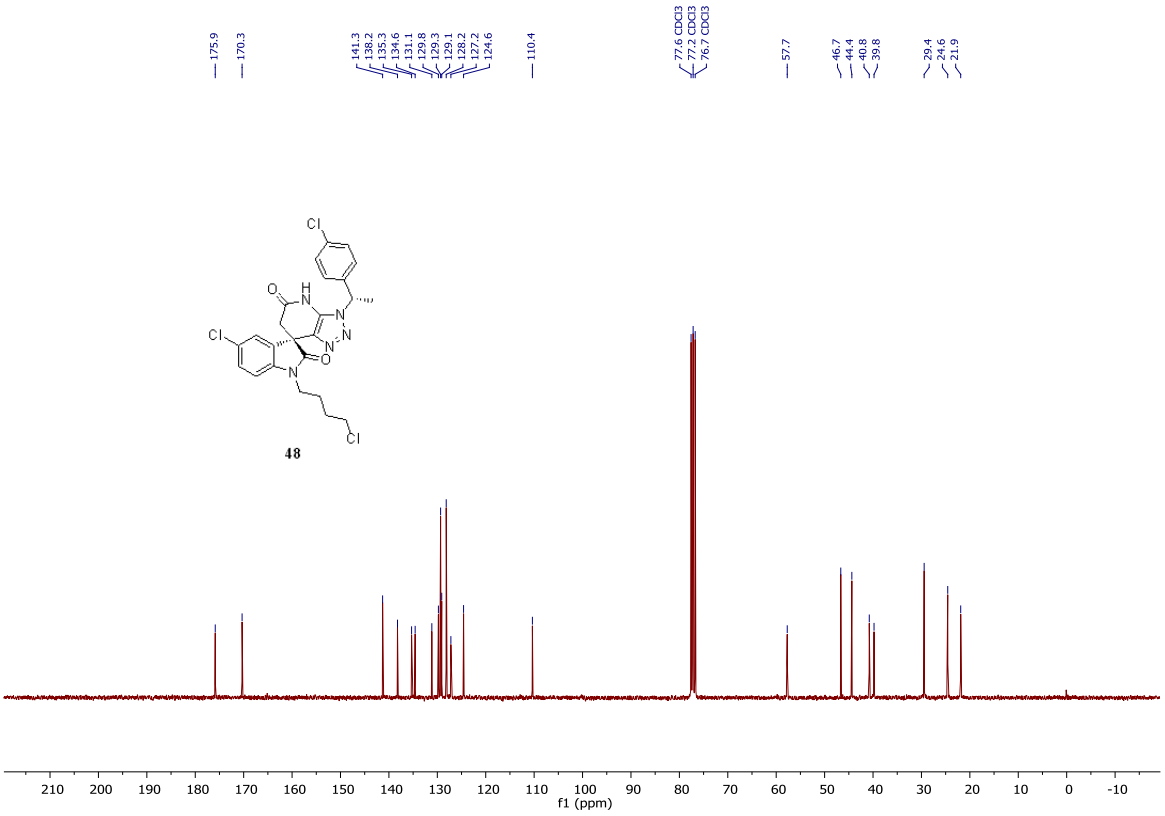
1.80
1.25
-0.00
1.00
4.89
0.96
0.95
1.00
2.01
2.03
1.97
7.22
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

48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135.3
134.6
131.1
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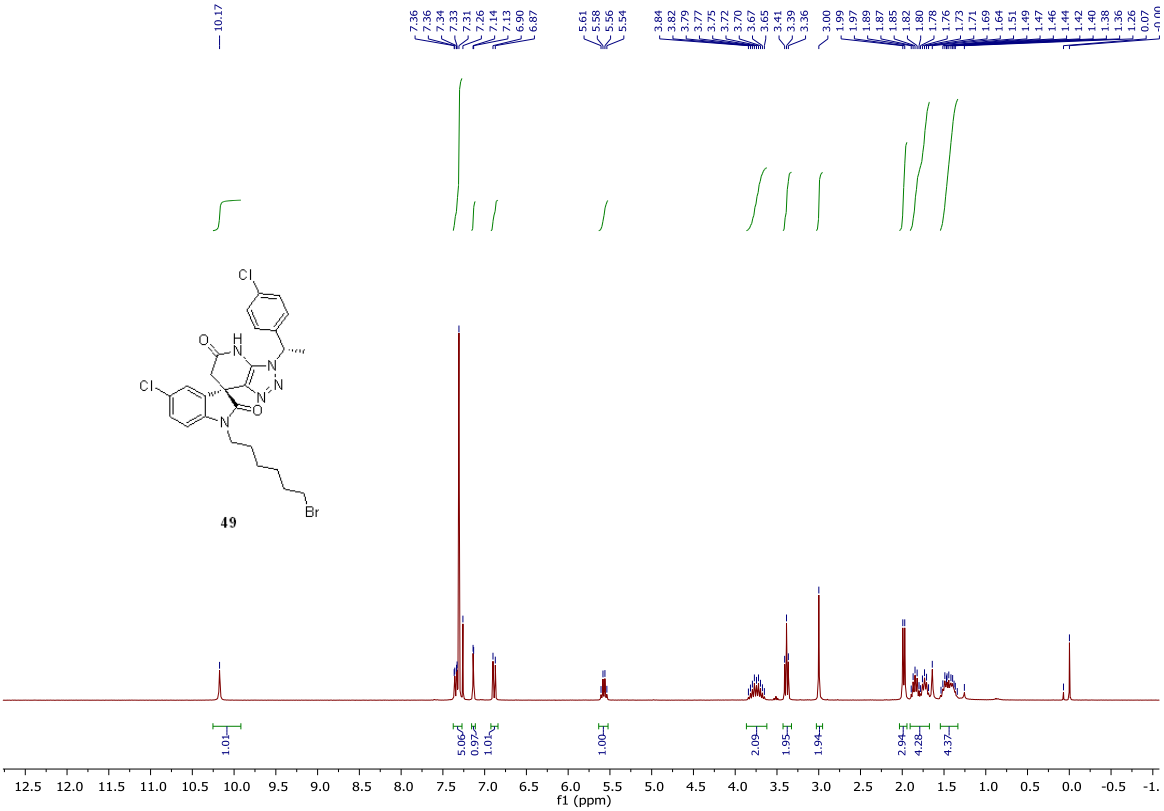
129.1
128.2
127.2
124.6
110.4
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.7
46.7
44.4
40.8
39.8
29.4
24.6
21.9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

48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5.54
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1.76
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1.40
1.38
1.36
1.26
0.07
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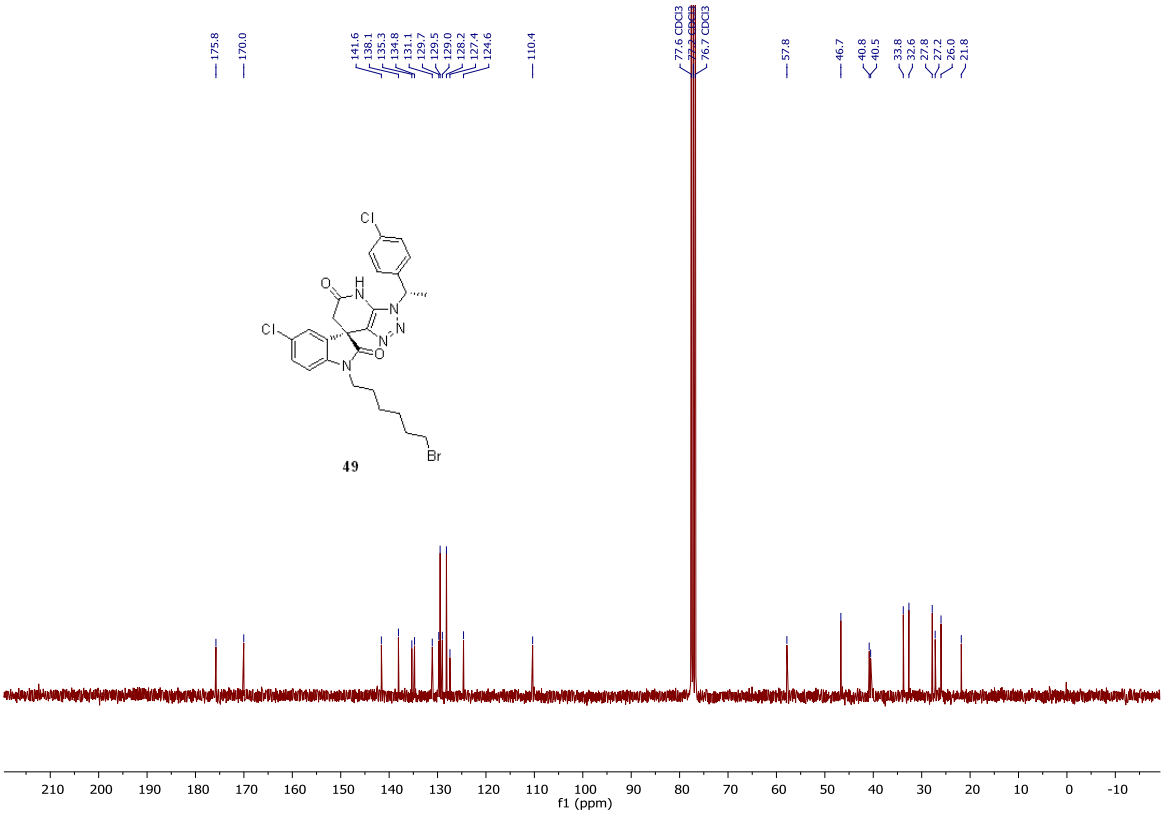
Cl
O
H
N
N
N
Cl
O
N
Br
49
1.01
5.06
0.97
1.01
1.00
2.09
1.95
1.94
2.94
4.28
4.37
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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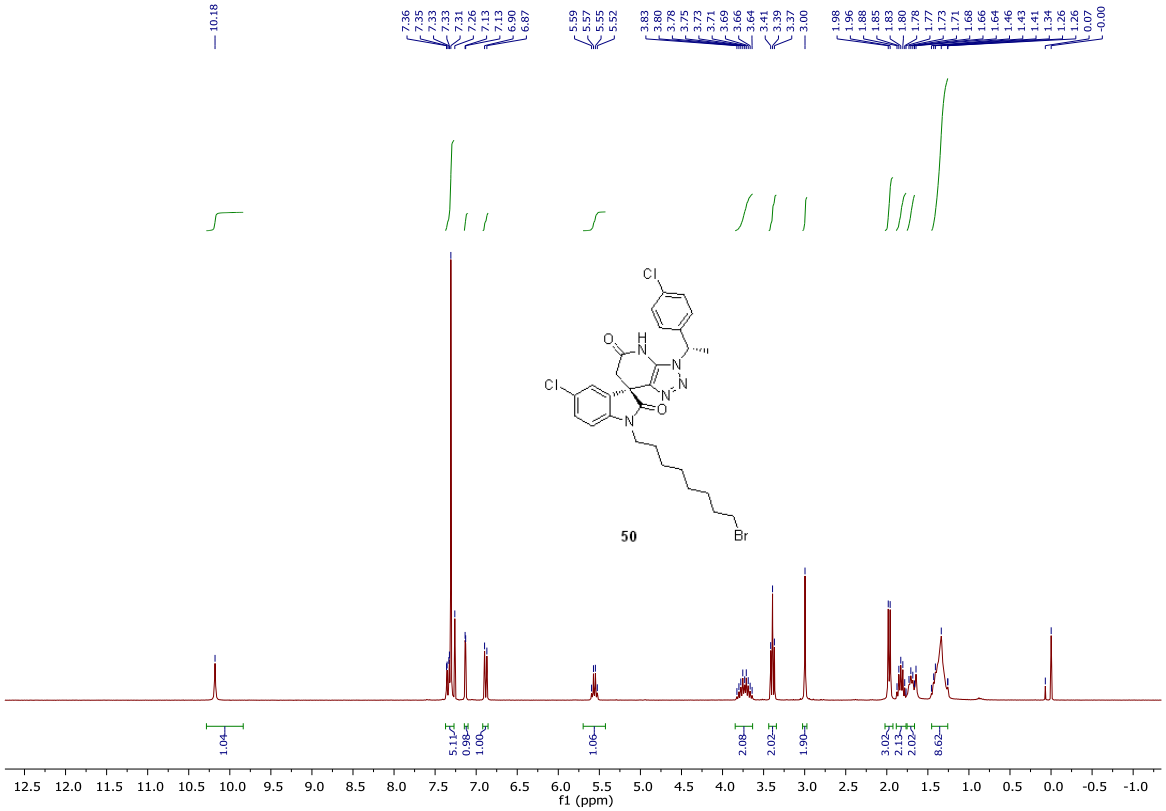
129.7
129.5
129.0
128.2
127.4
124.6
110.4
77.6 CDCl3
77.2 CDCl3
76.7 CDCl3
57.8
46.7
40.8
40.5
33.8
32.6
27.8
27.2
26.0
21.8
Cl
O
H
N
N
N
Cl
O
N
Br
49
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.87
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5.52
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3.80
3.78
3.75
3.73
3.71
3.69
3.66
3.64
3.41
3.39
3.37
3.00
1.98
1.96
1.88
1.85
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1.80
1.78
1.77
1.73
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1.64
1.46
1.43
1.41
1.34
1.26
1.26
0.07
-0.00
50
1.04
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1.06
2.08
2.02
1.90
3.02
2.13
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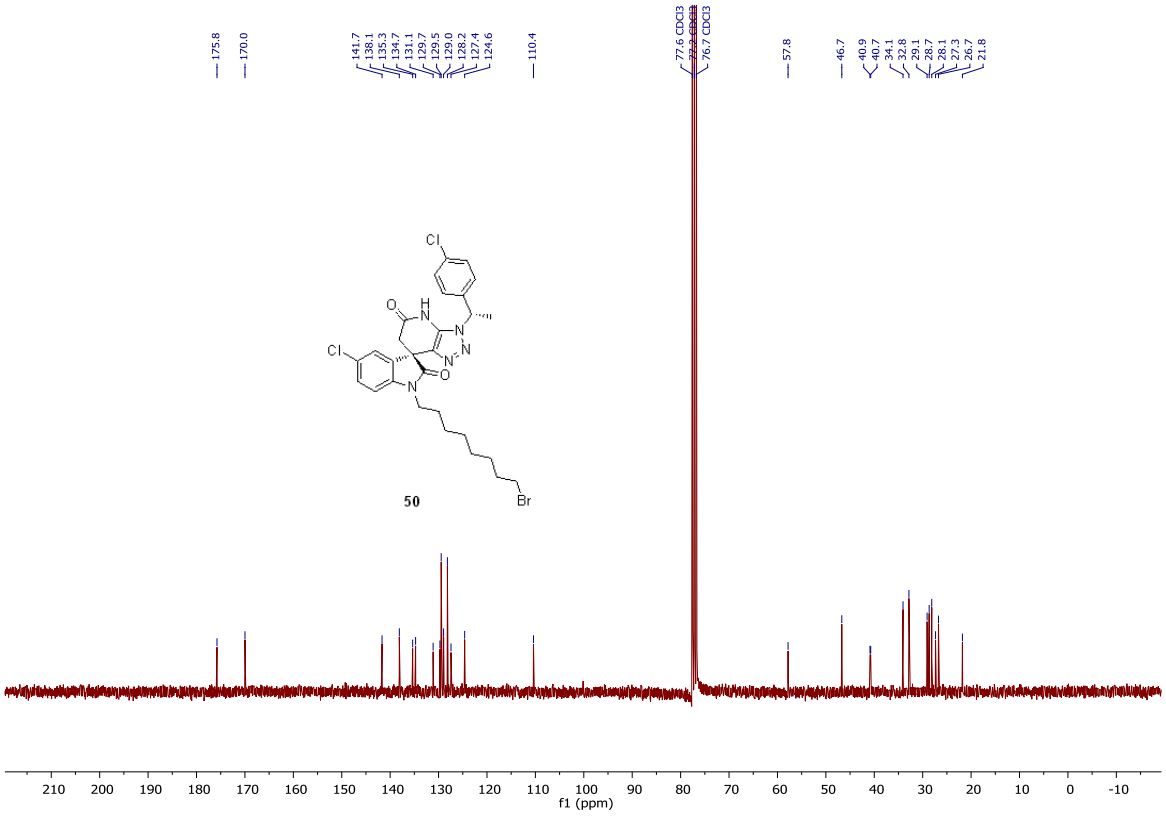
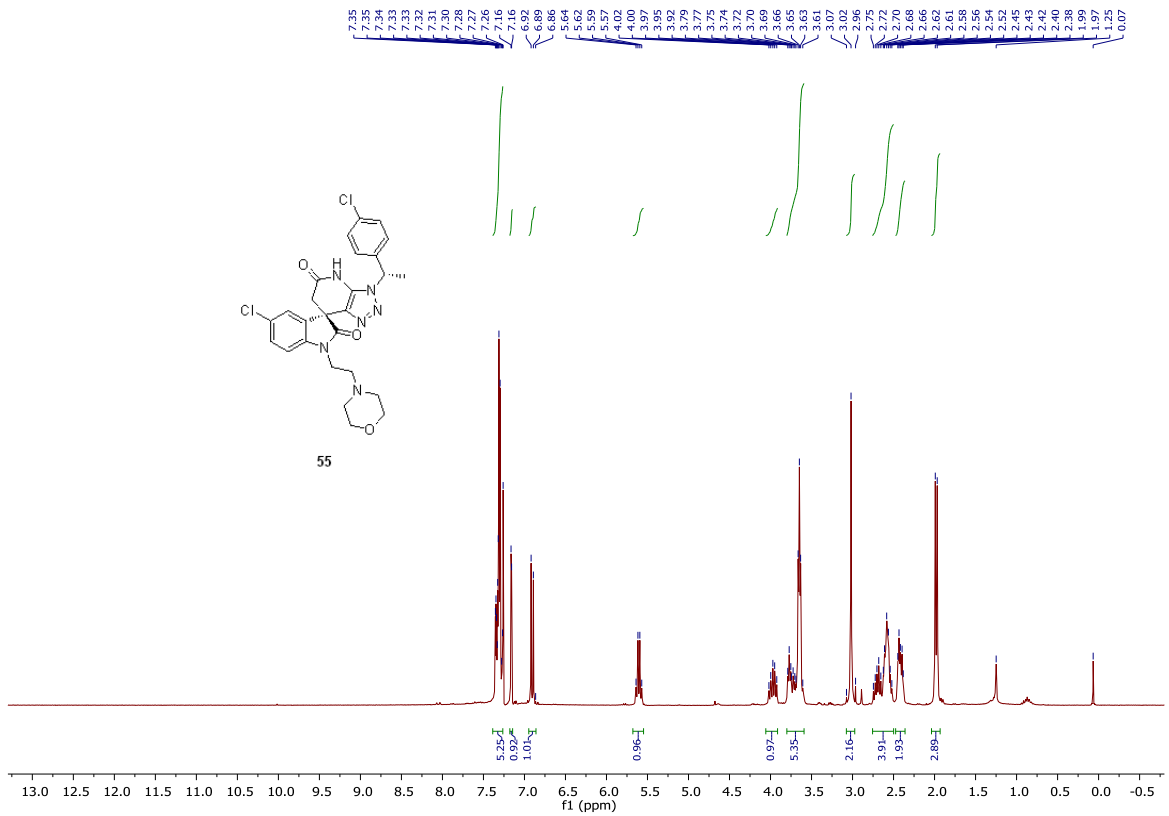
8.62
f1 (ppm)


175.8
170.0
141.7
138.1
135.3
134.7
131.1
129.7
129.5
129.0
128.2
127.4
124.6
110.4
77.6 CDCl3
77.3 CDCl3
76.7 CDCl3
57.8
46.7
40.9
40.7
34.1
32.8
29.1
28.7
28.1
27.3
26.7
21.8
50
f1 (ppm)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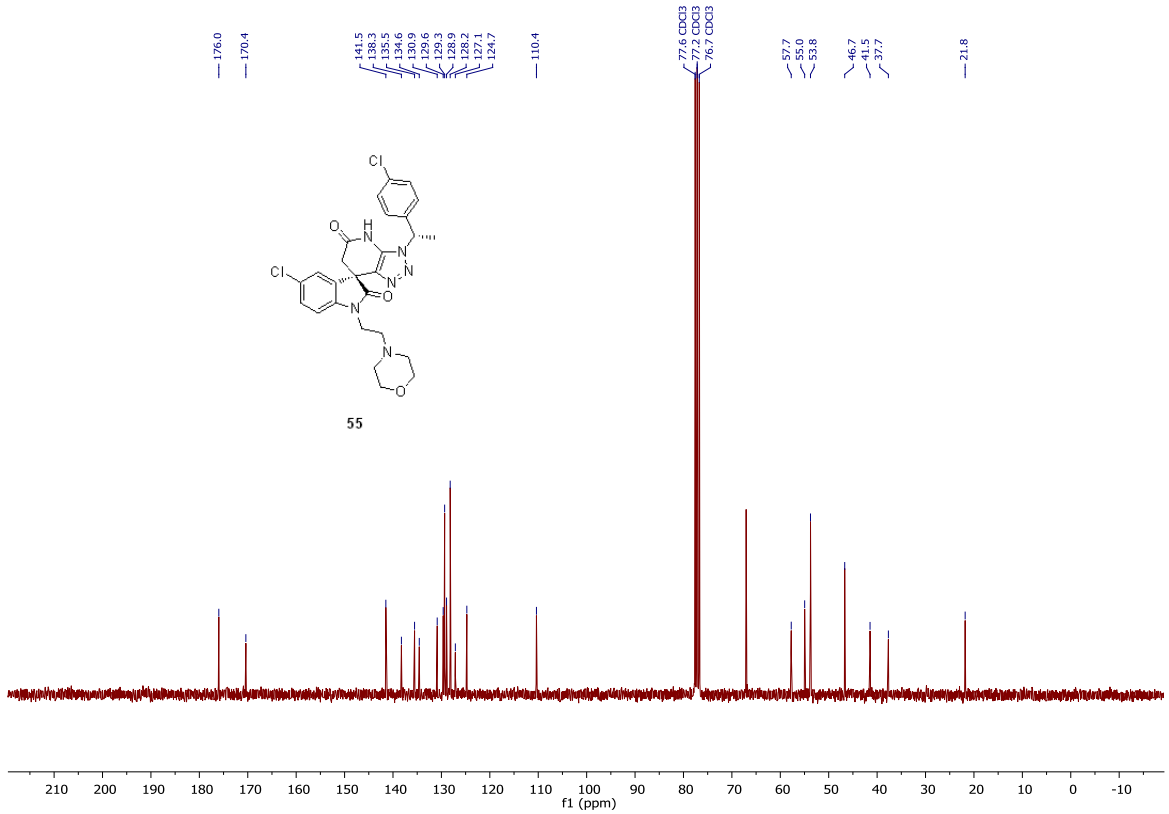
f1 (ppm)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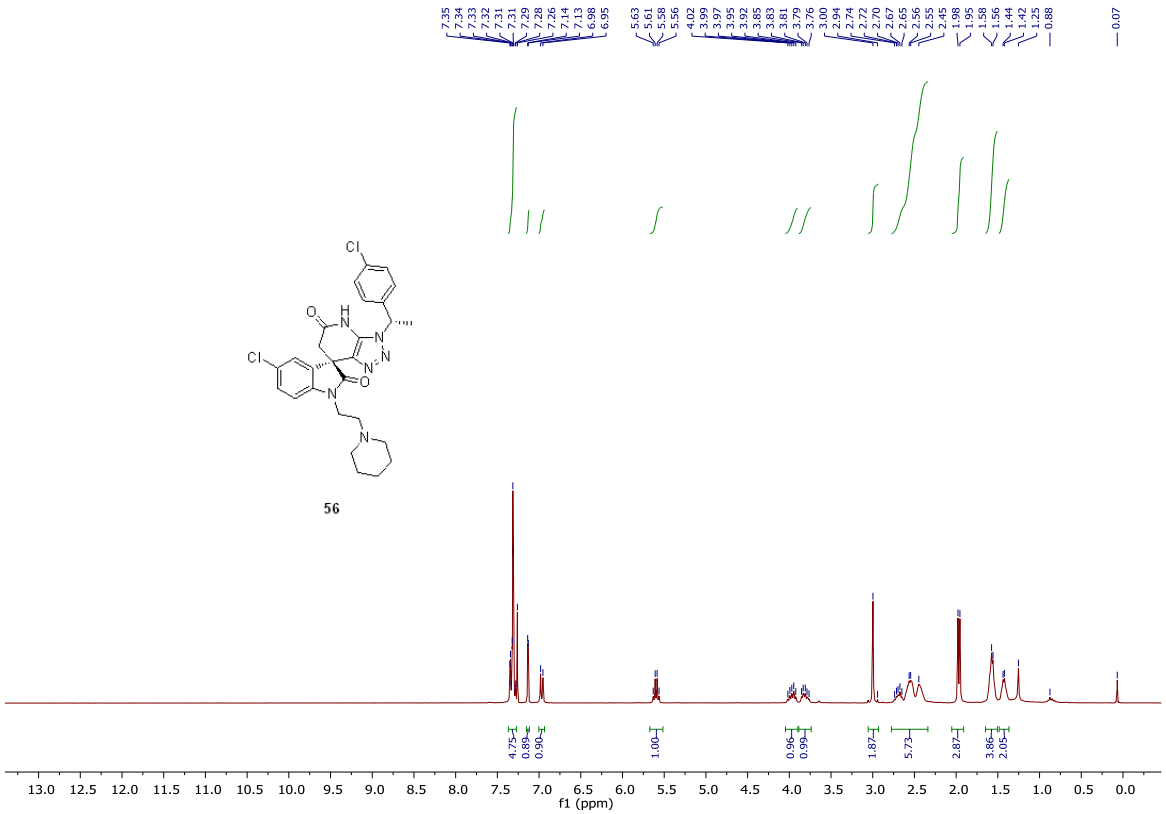
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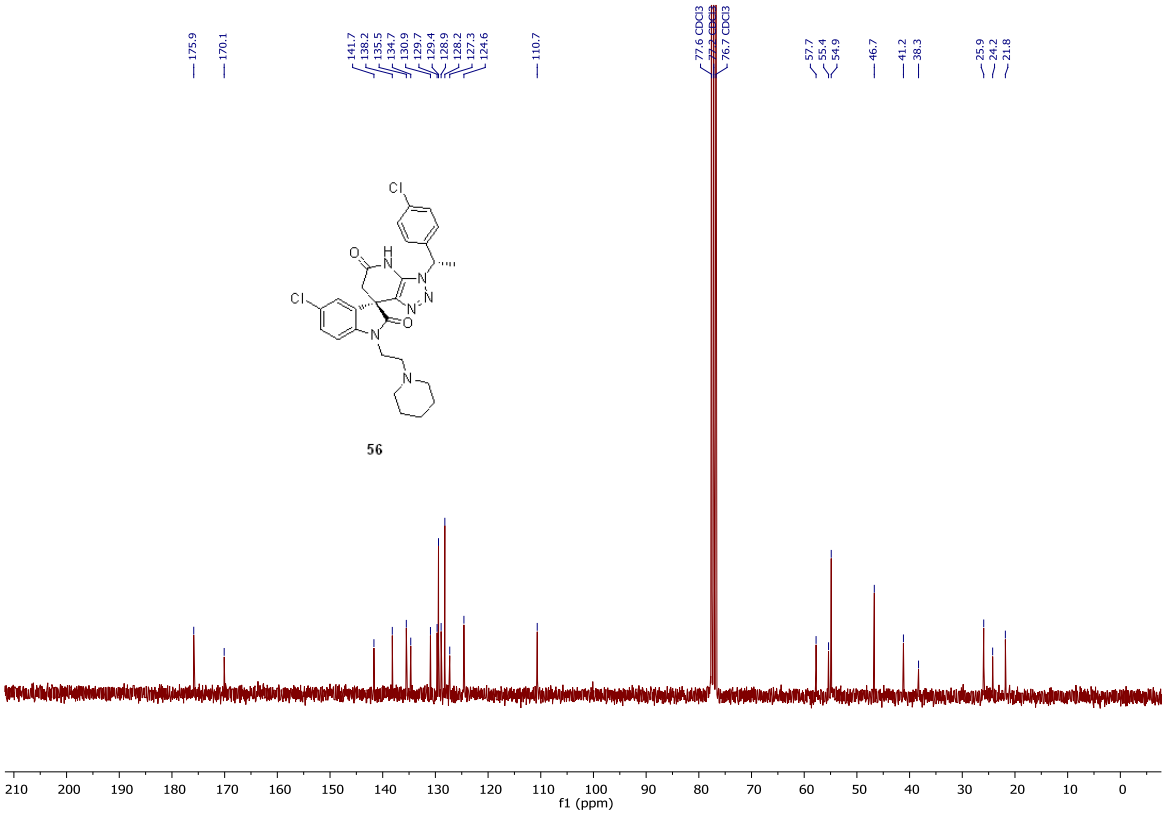
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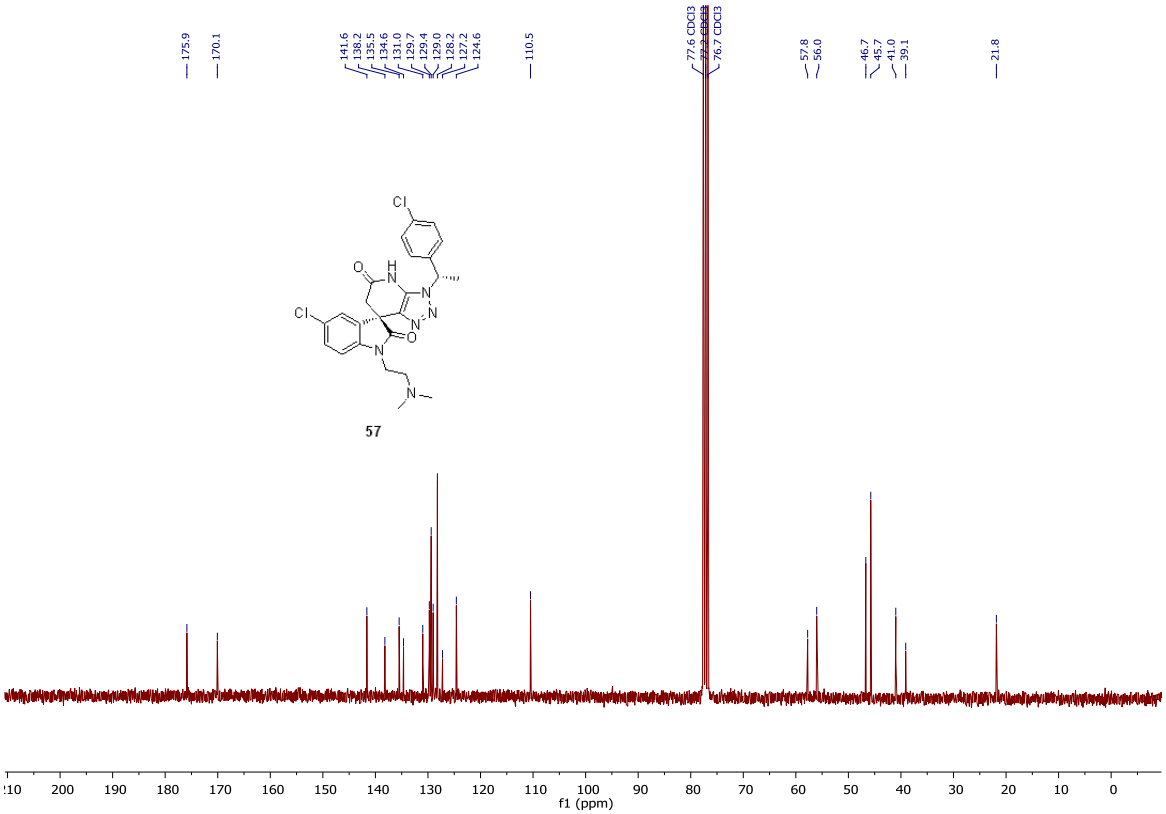
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124.6
110.5
77.6 CDCl3
77.3 CDCl3
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46.7
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39.1
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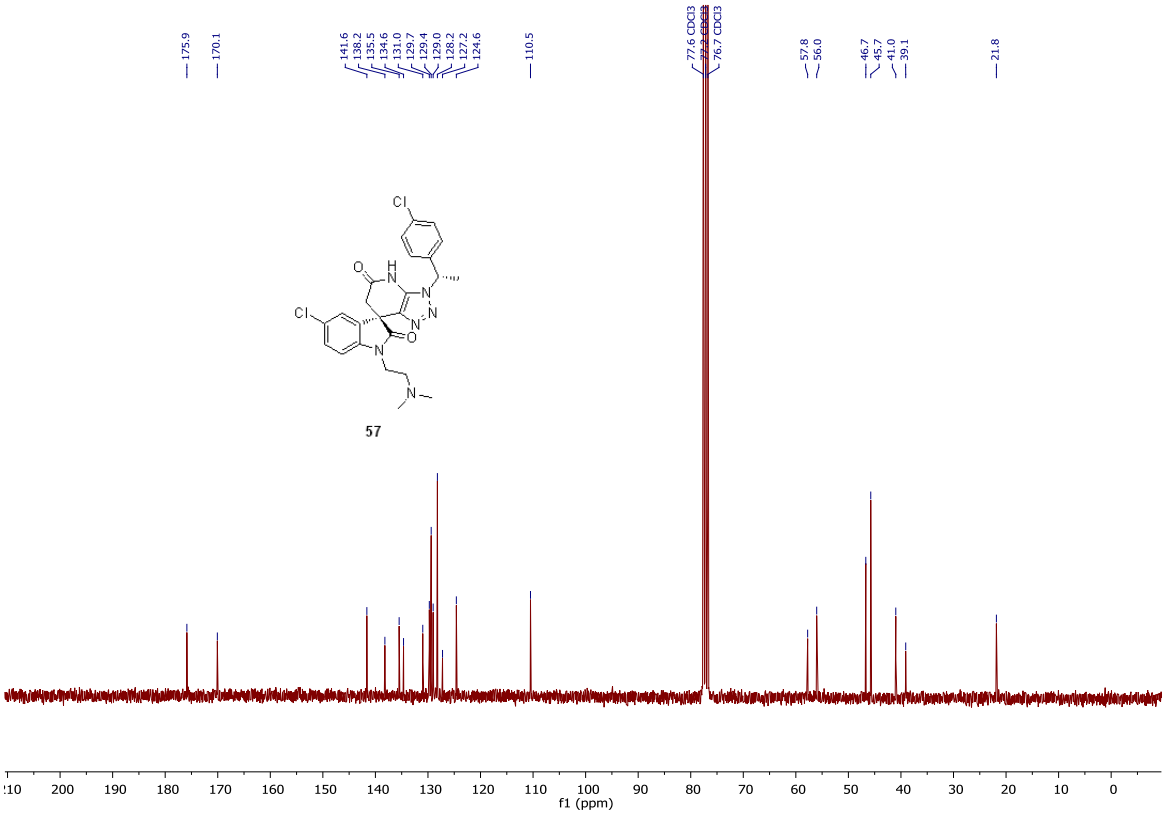
57
f1 (ppm)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110.5
77.6 CDCl3
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46.7
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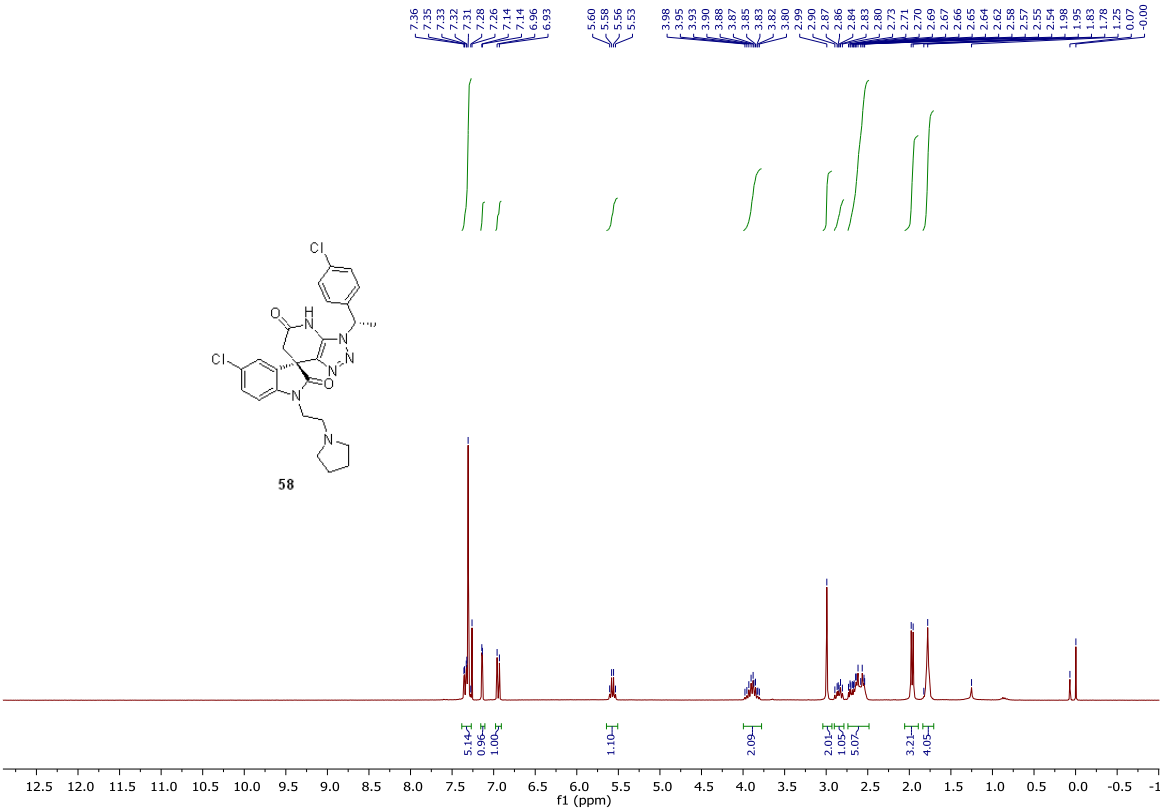
41.0
39.1
21.8
57
f1 (ppm)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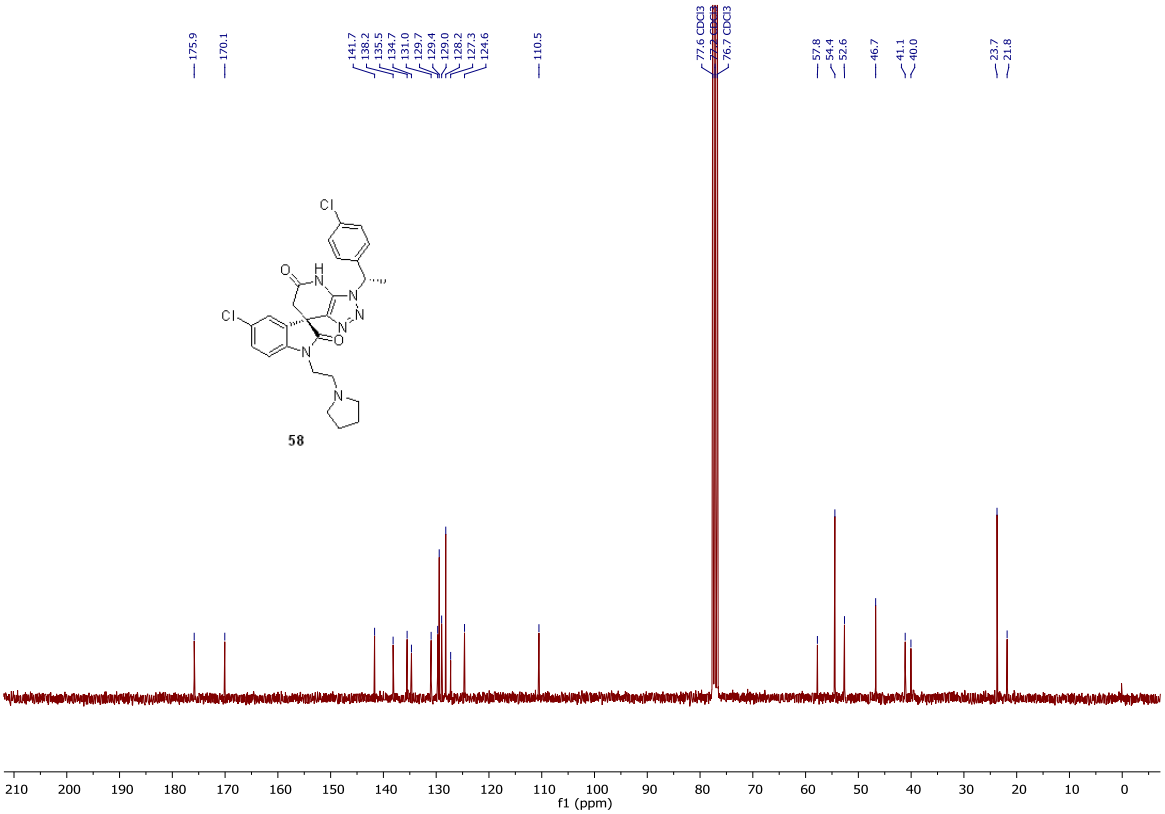
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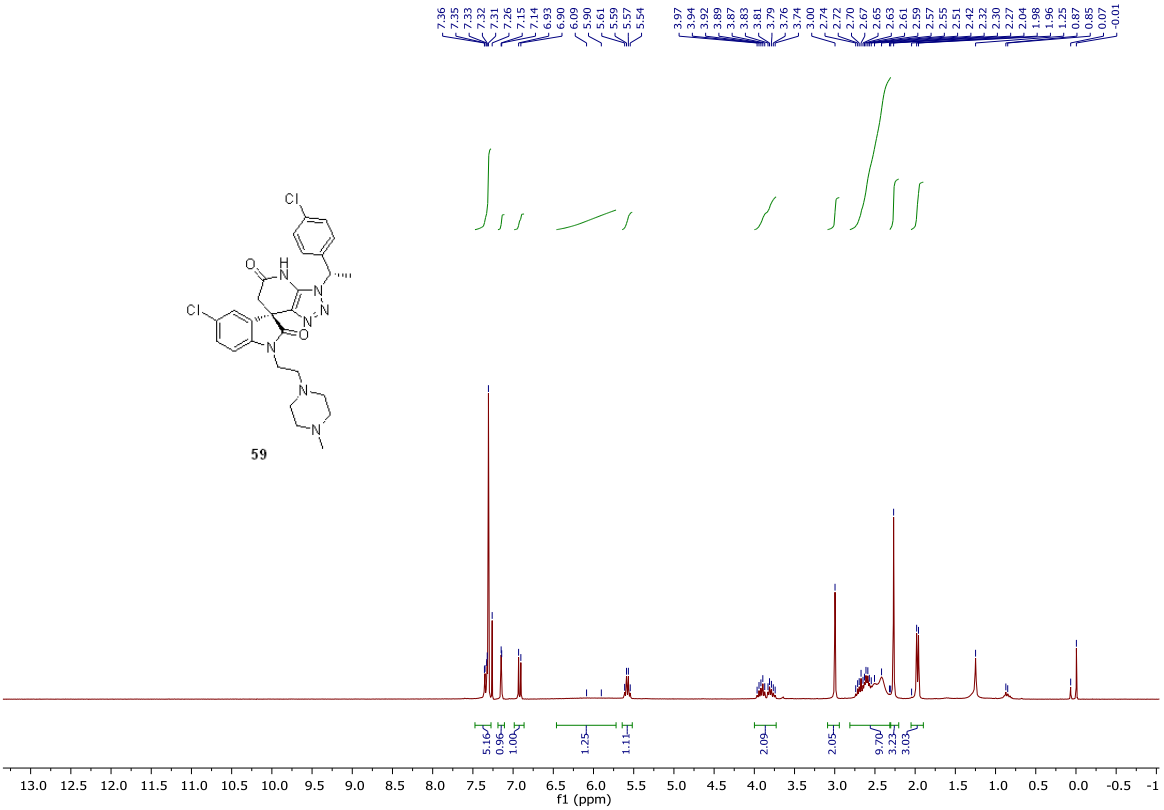
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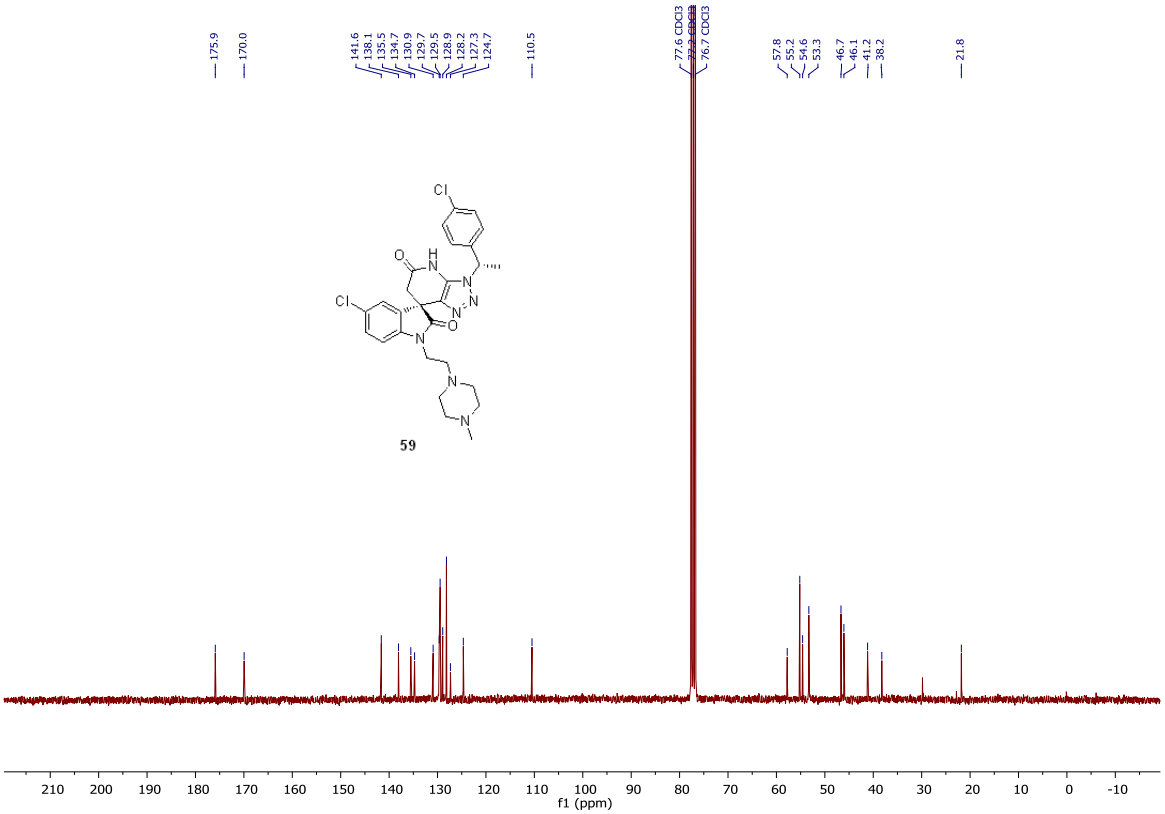
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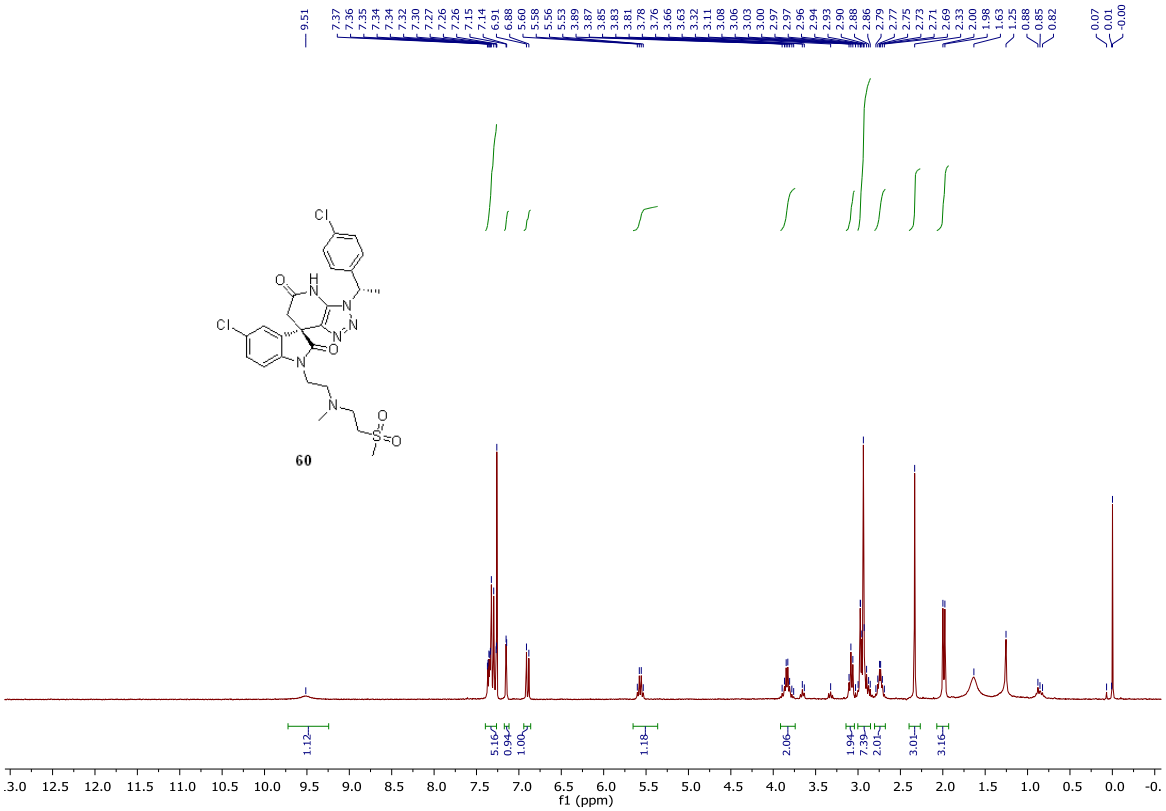
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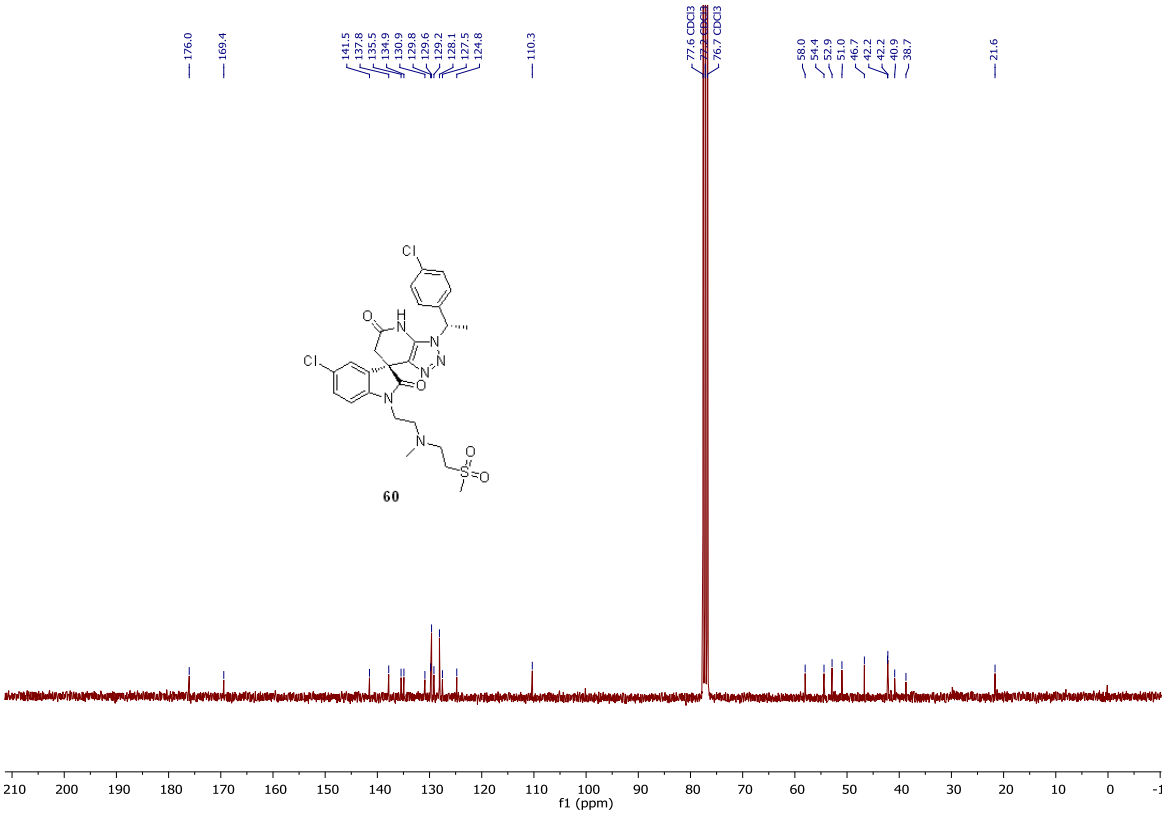
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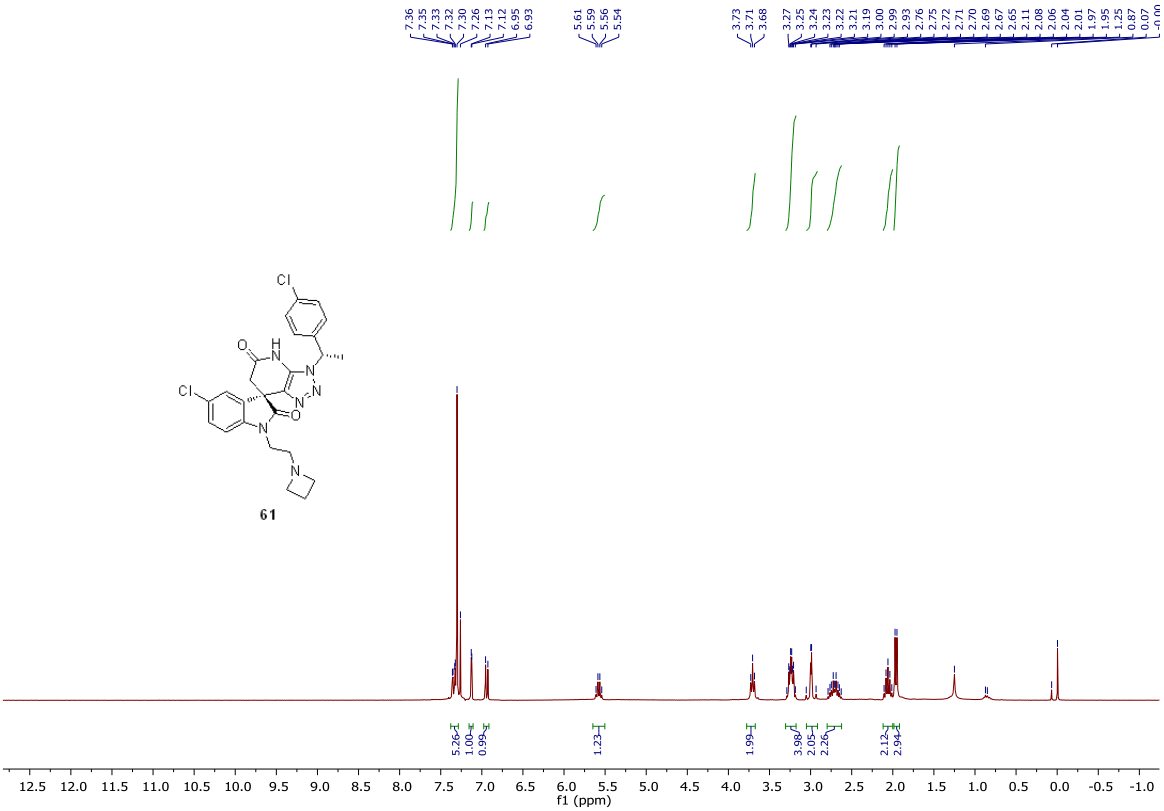
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3.71
3.68
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3.25
3.24
3.23
3.22
3.21
3.19
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2.99
2.93
2.76
2.75
2.72
2.71
2.70
2.69
2.67
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2.11
2.08
2.06
2.04
2.01
1.97
1.95
1.25
0.87
0.07
-0.00
Cl
O
H
N
N
N
N
O
Cl
N
N
61
5.26
1.00
0.99
1.23
1.99
3.98
2.05
2.26
2.12
2.94
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
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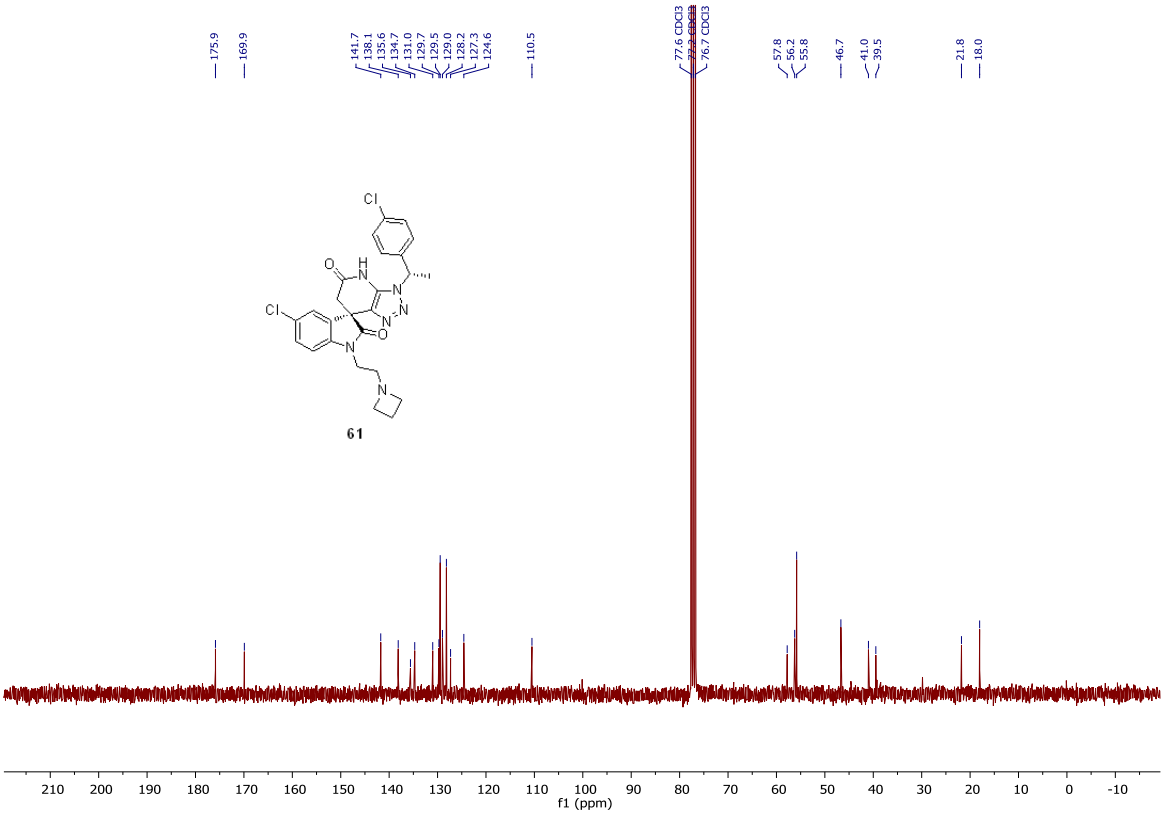
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129.7
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127.3
124.6
110.5
77.6 CDCl3
76.7 CDCl3
57.8
56.2
55.8
46.7
41.0
39.5
21.8
18.0
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O
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N
O
Cl
N
N
61
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
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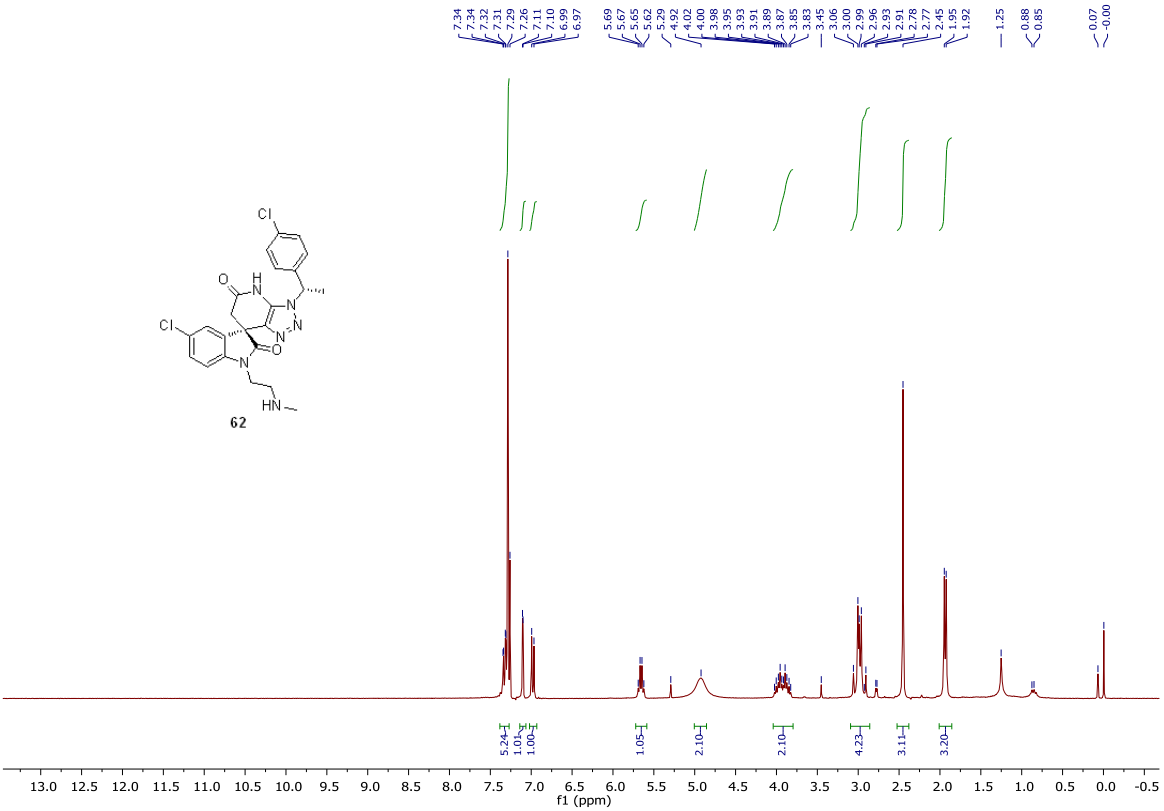
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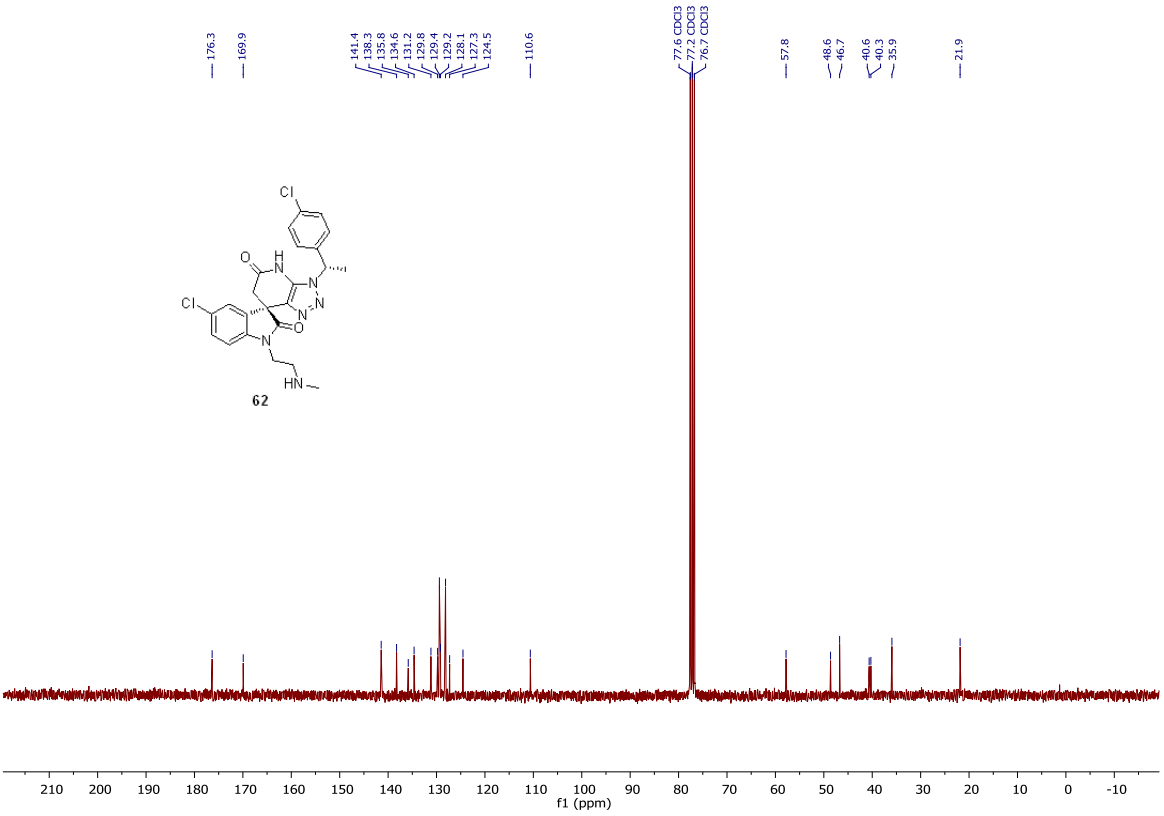
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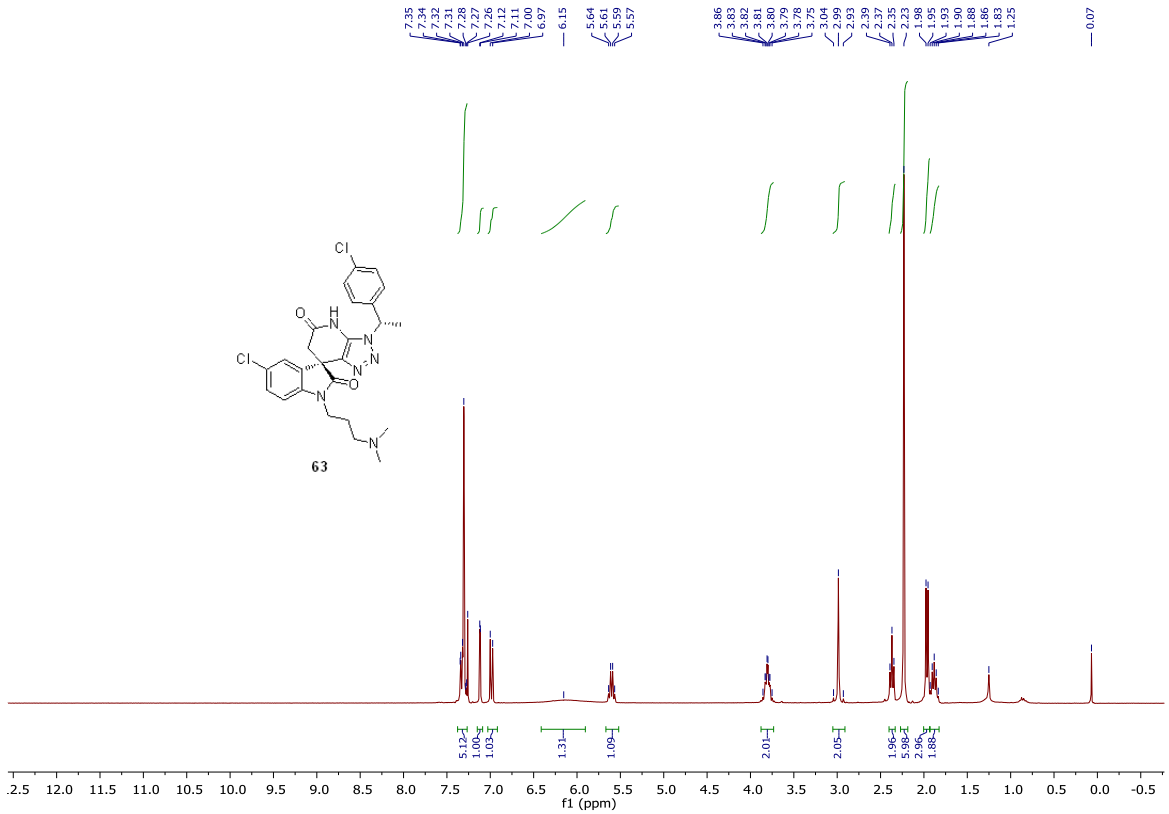
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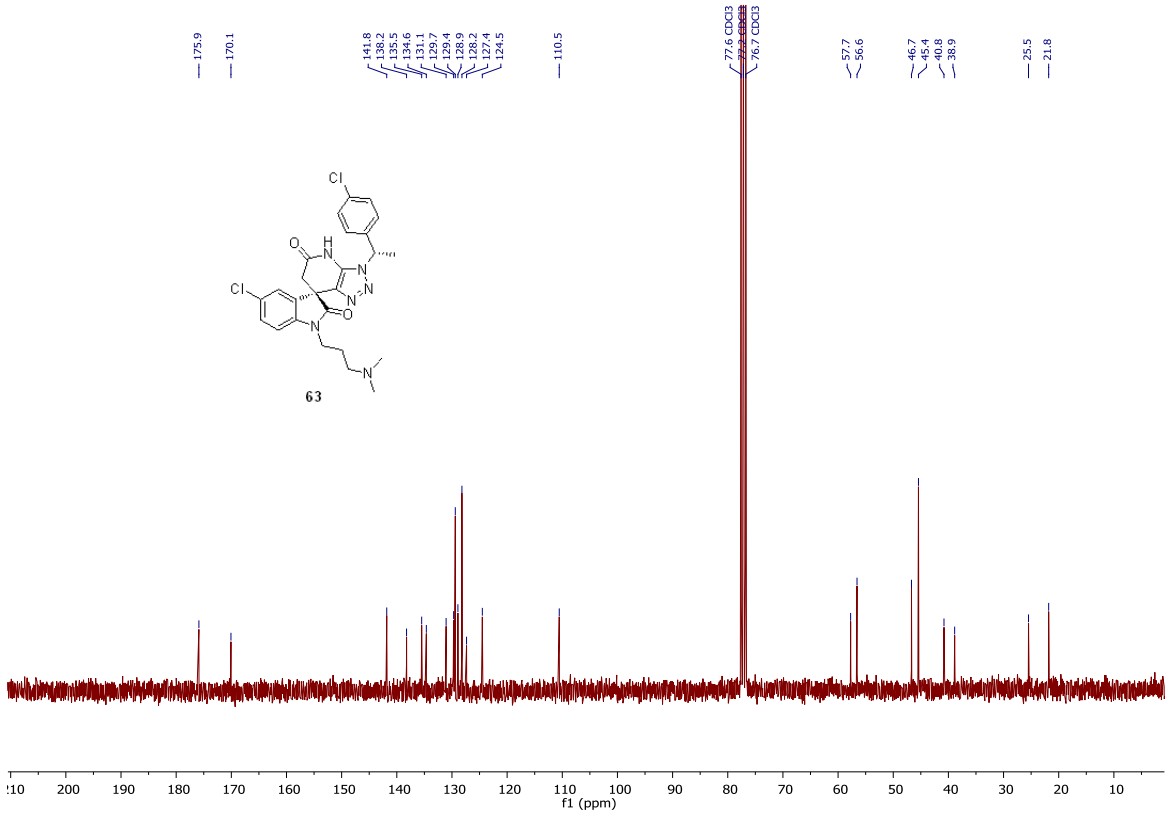
63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124.5
110.5
77.6 CDCl3
76.7 CDCl3
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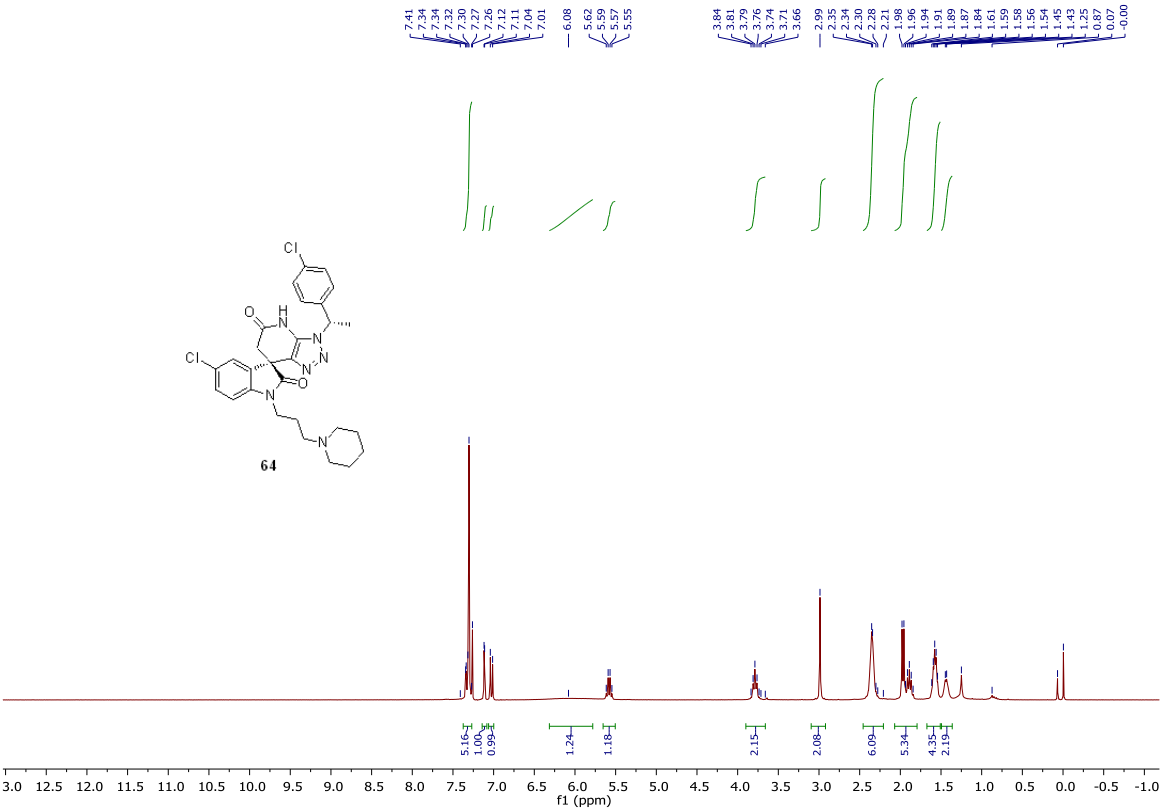
21.8
f1 (ppm)

63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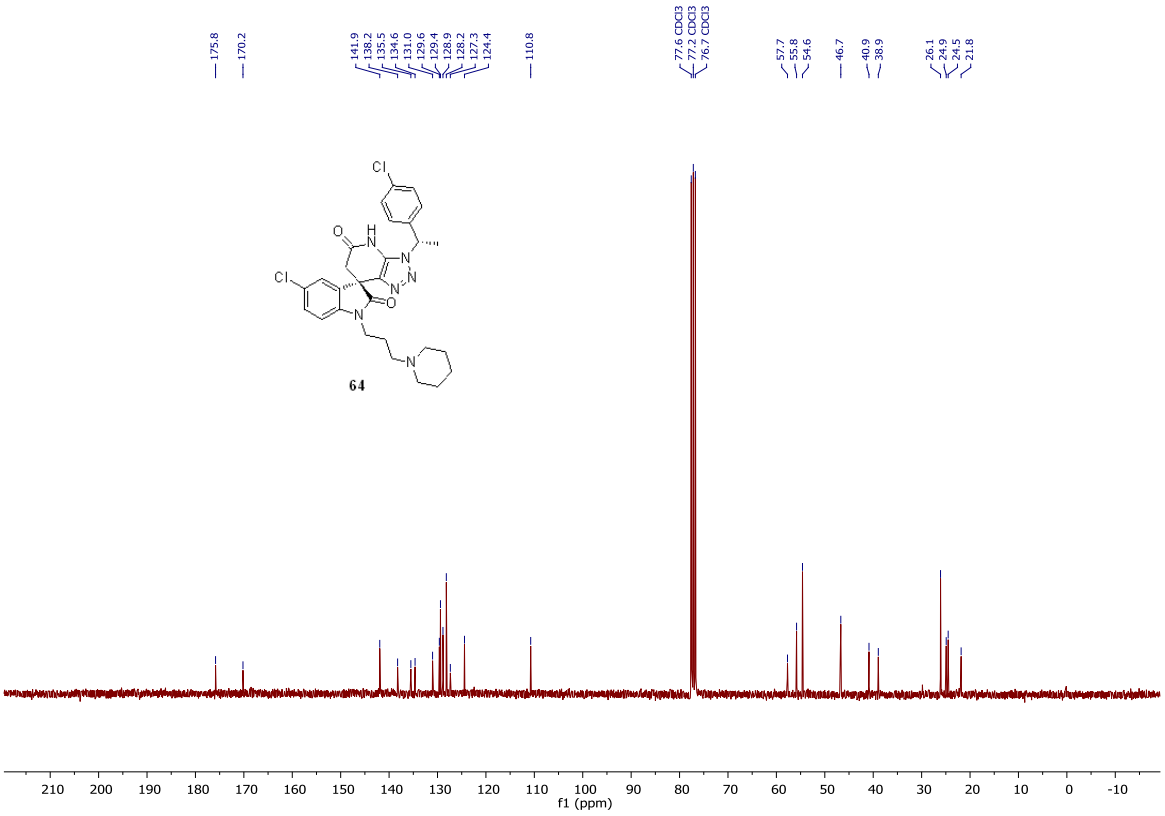
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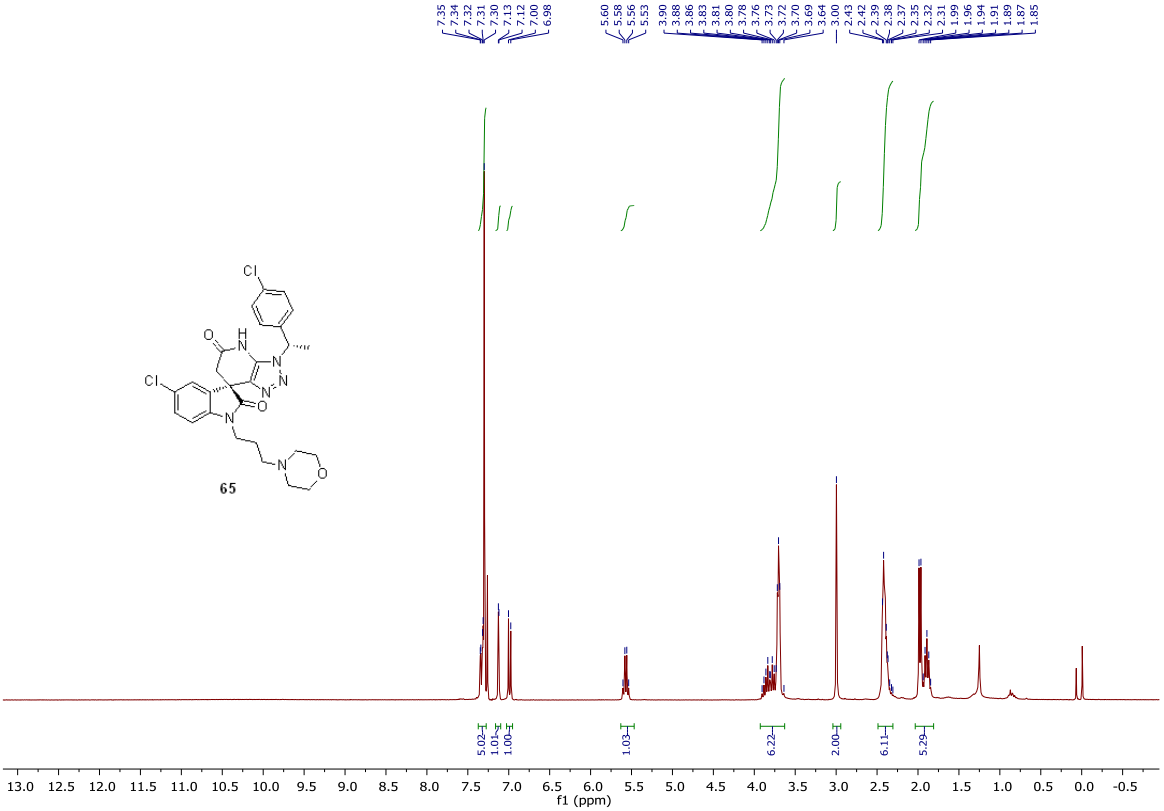
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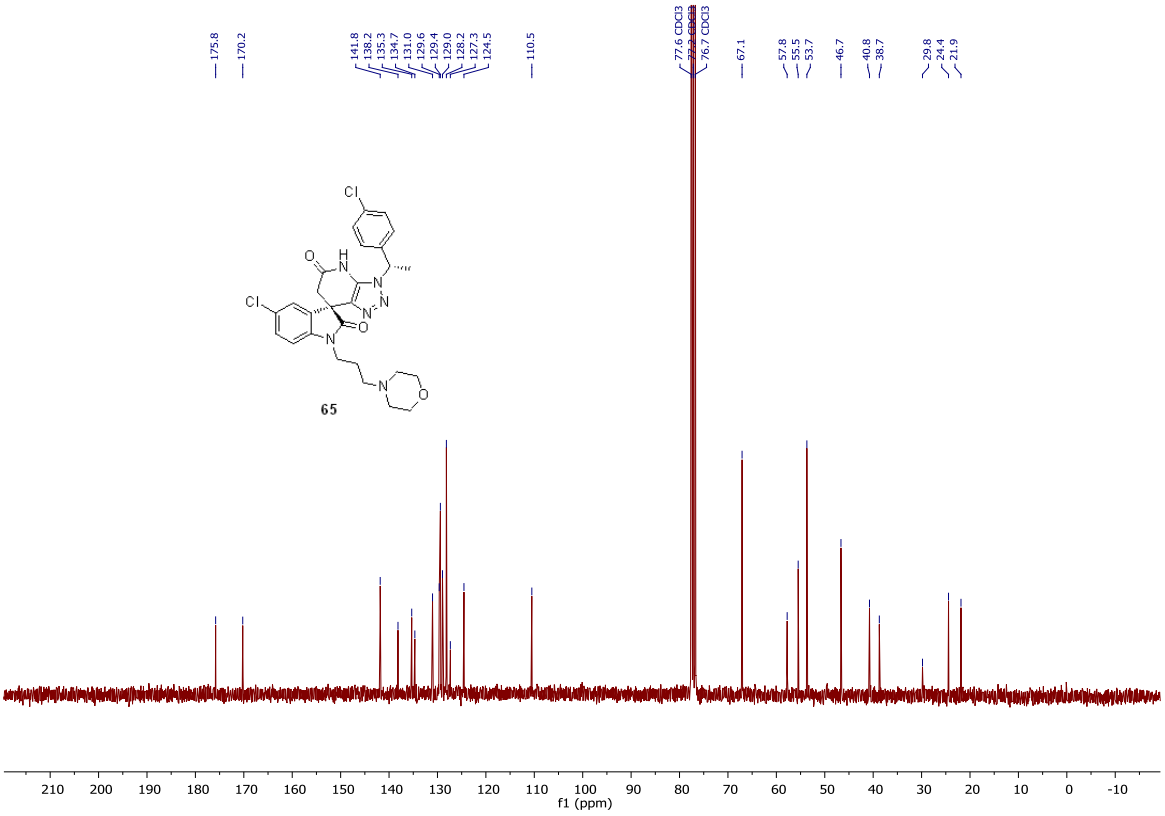
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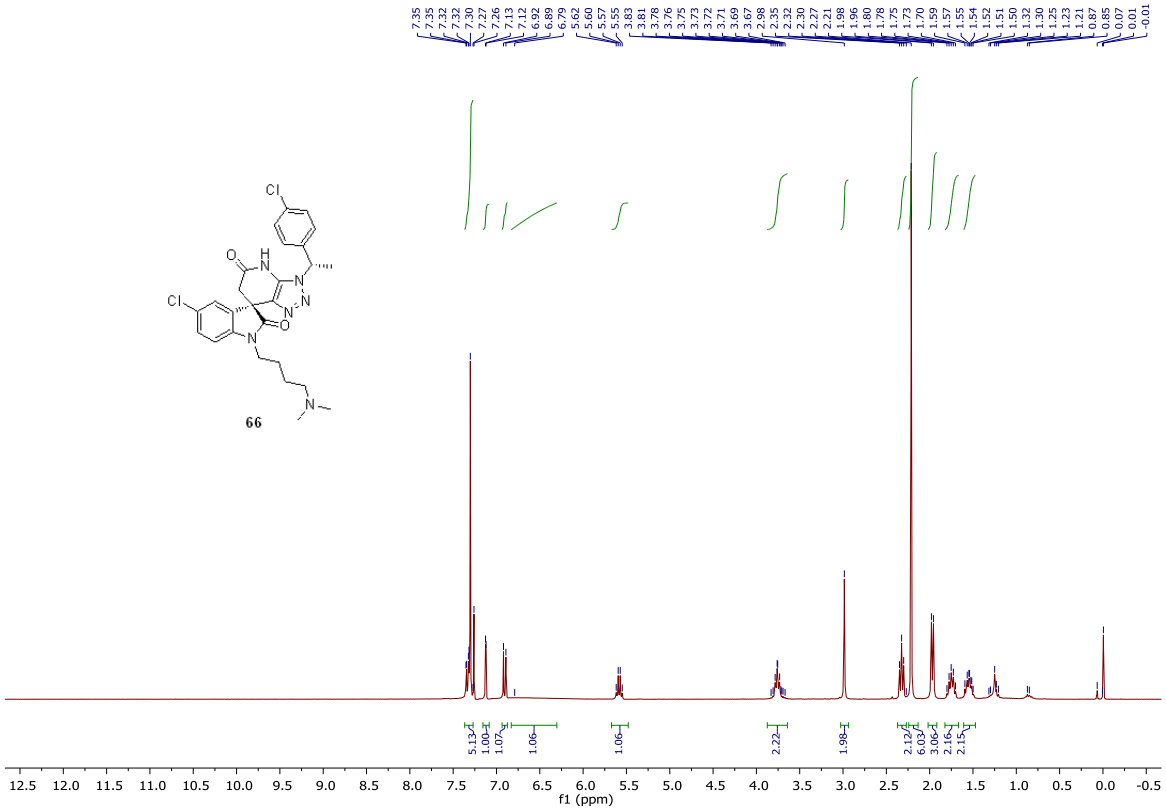
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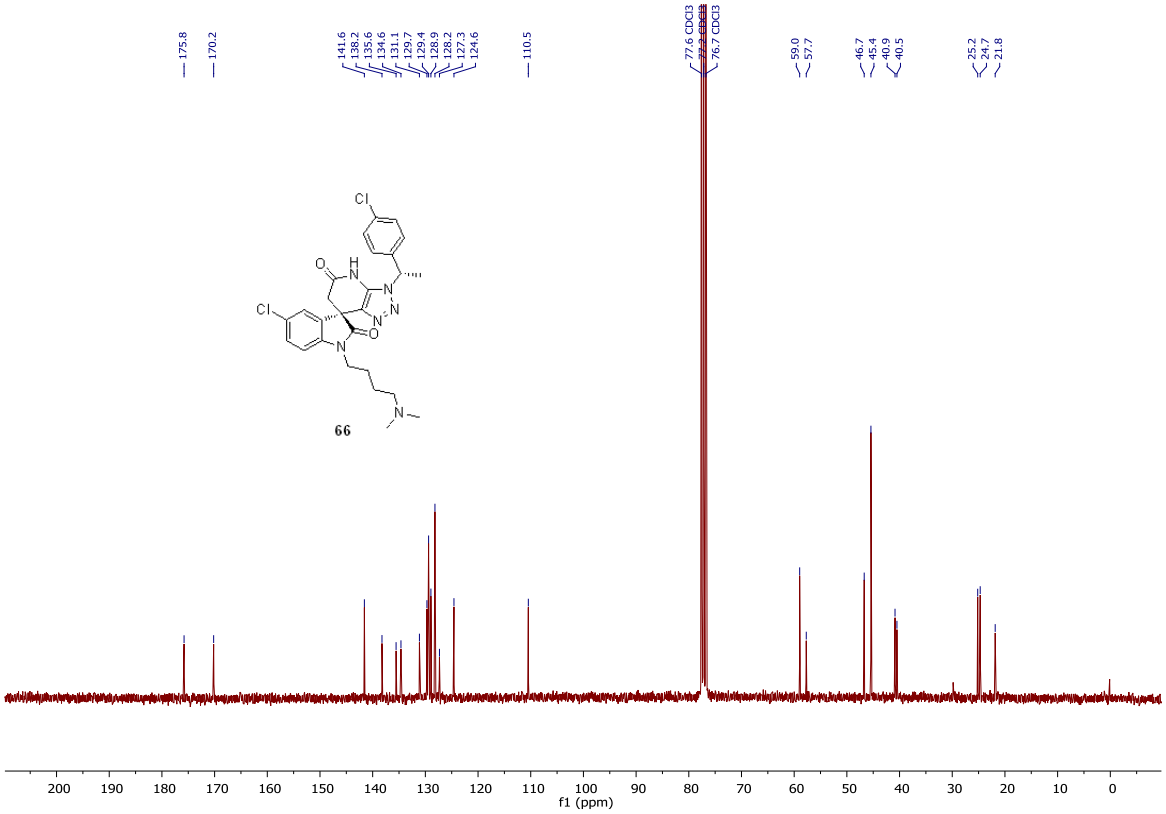
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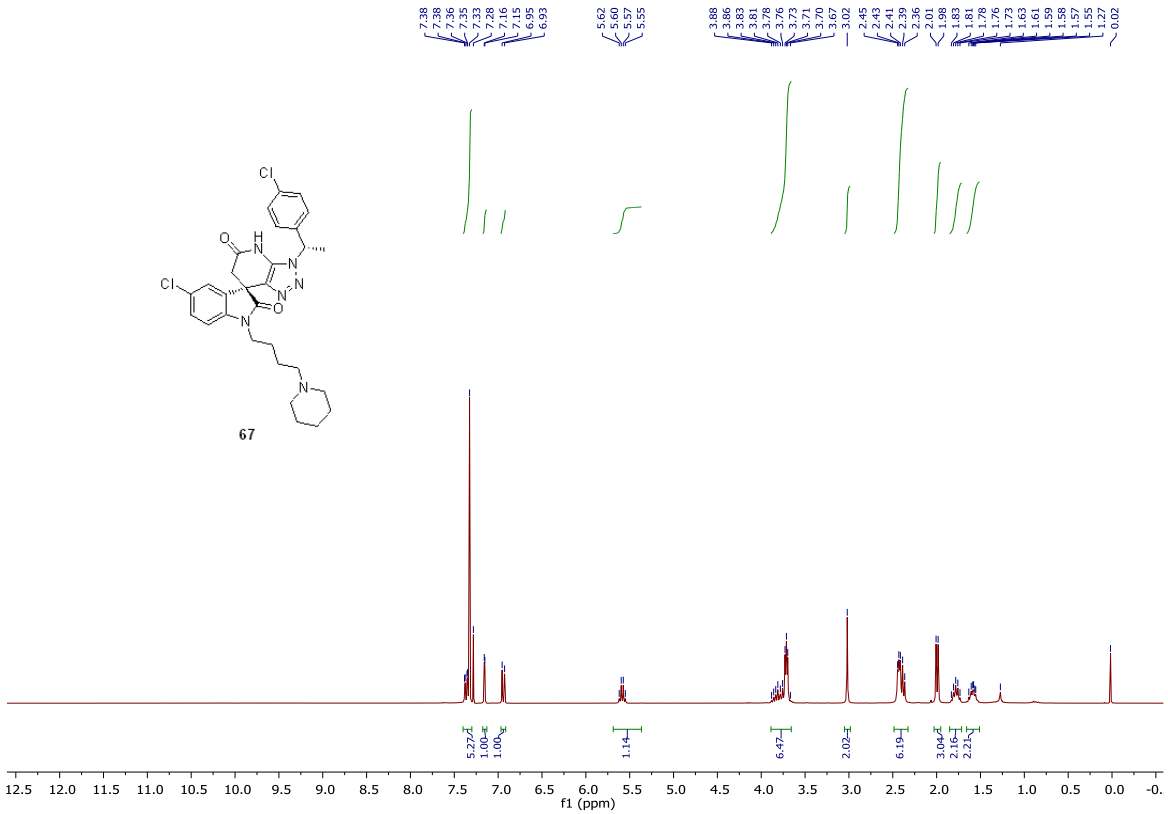
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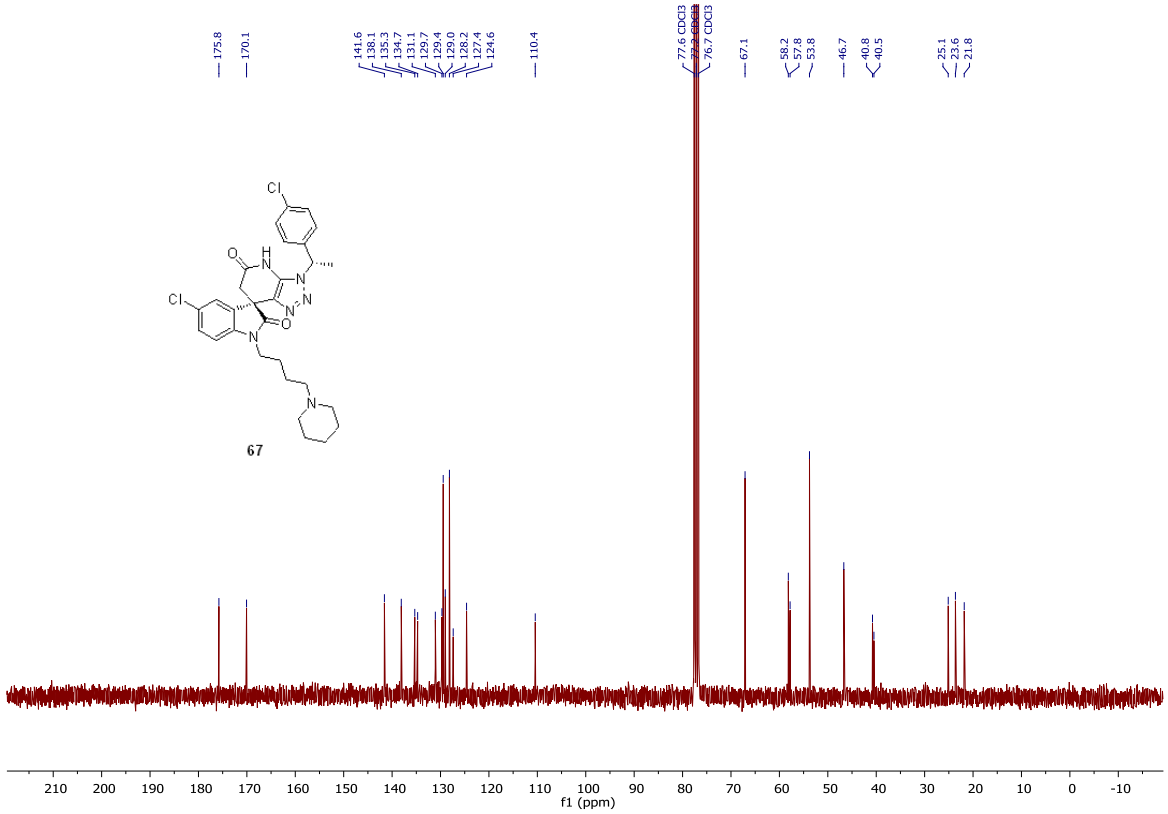
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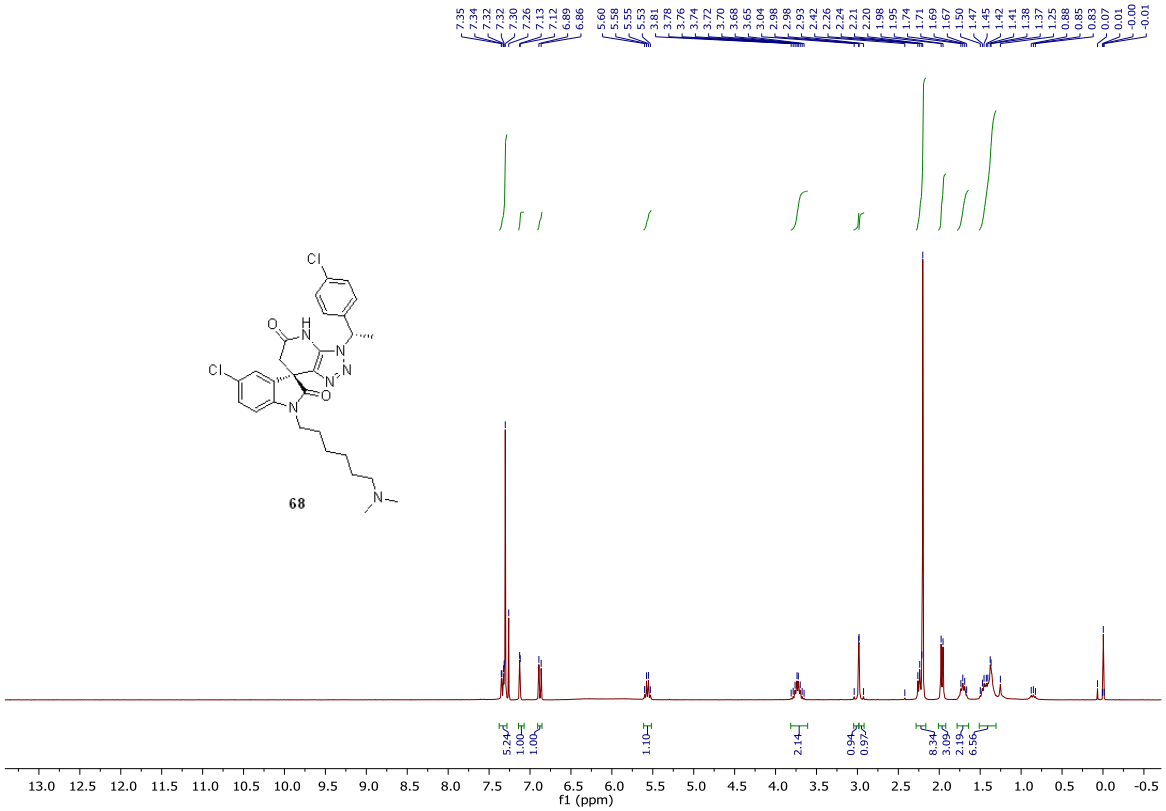
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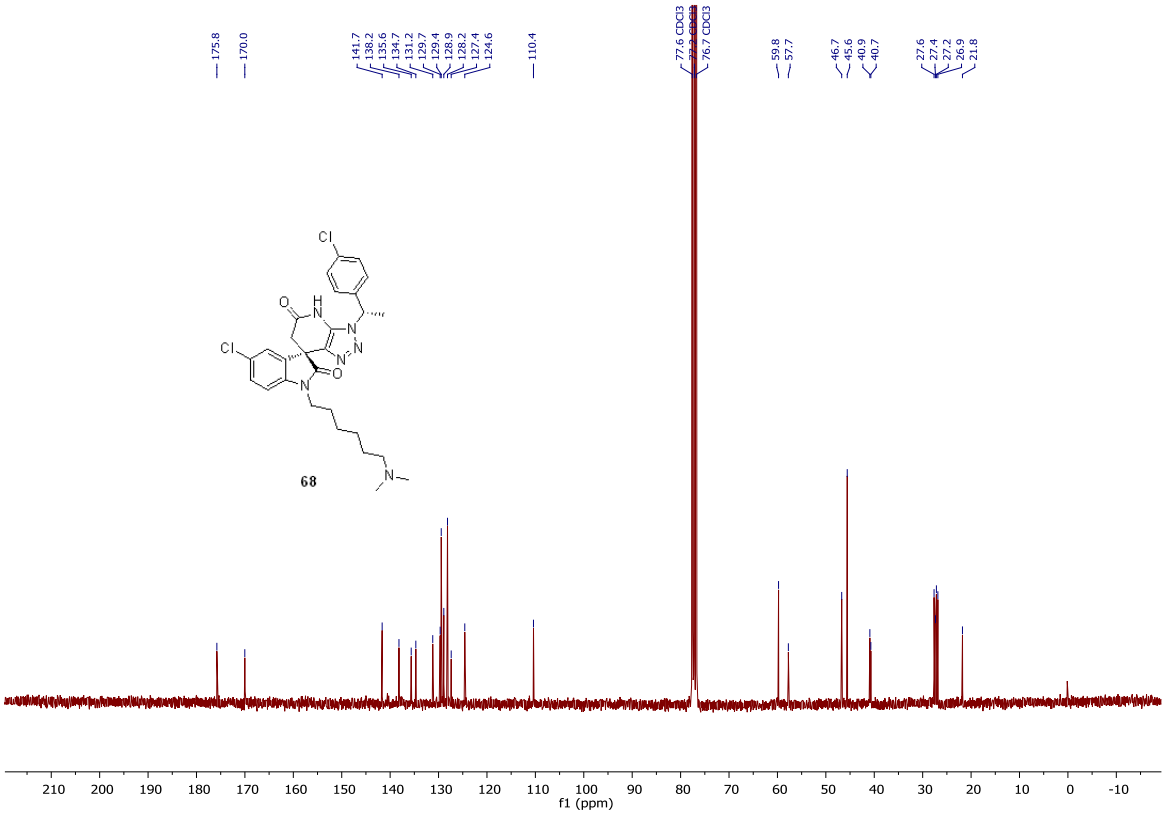
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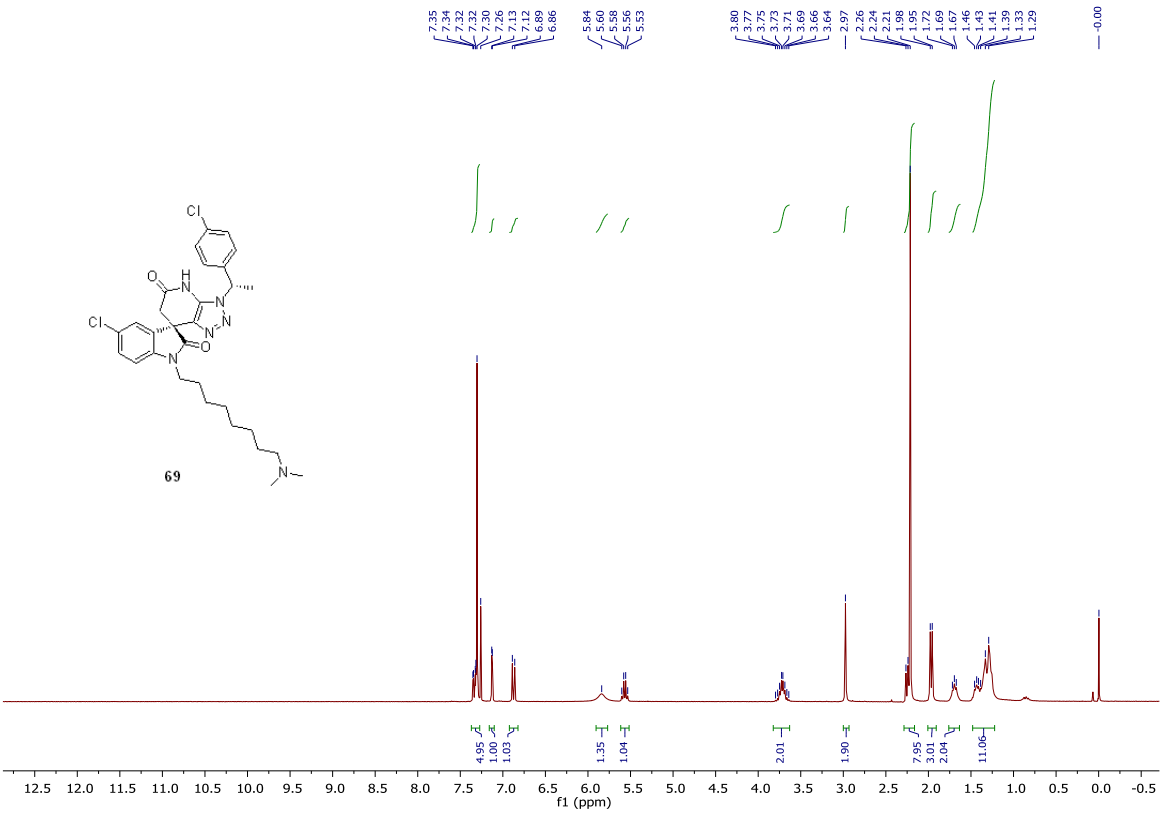
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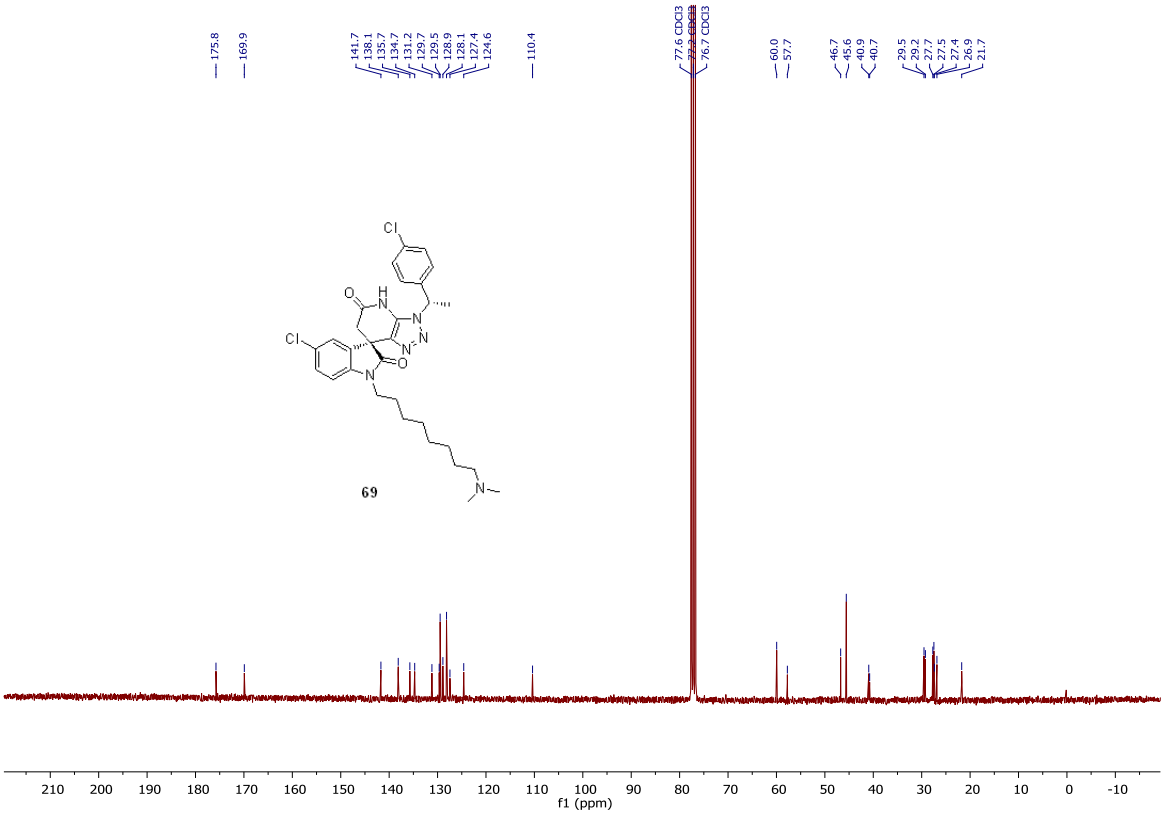
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124.6
110.4
77.6 CDCl3
76.7 CDCl3
60.0
57.7
46.7
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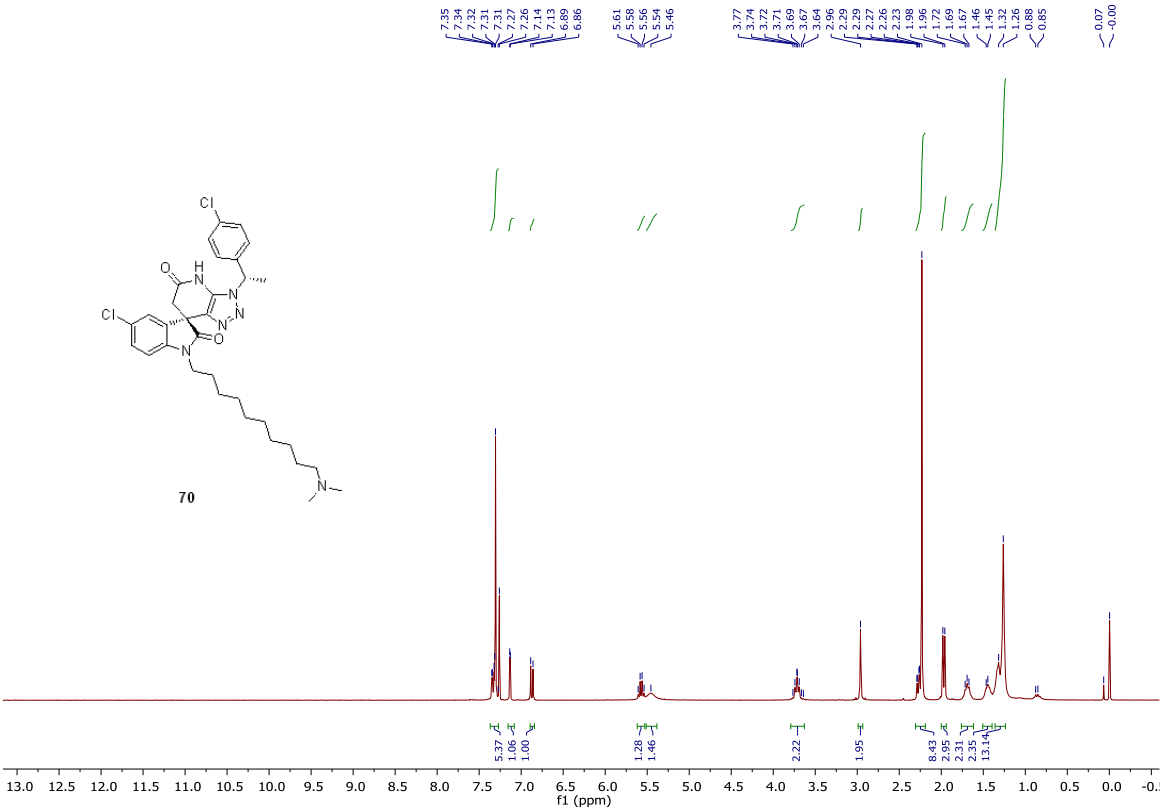
29.5
29.2
27.7
27.5
27.4
26.9
21.7
f1 (ppm)

69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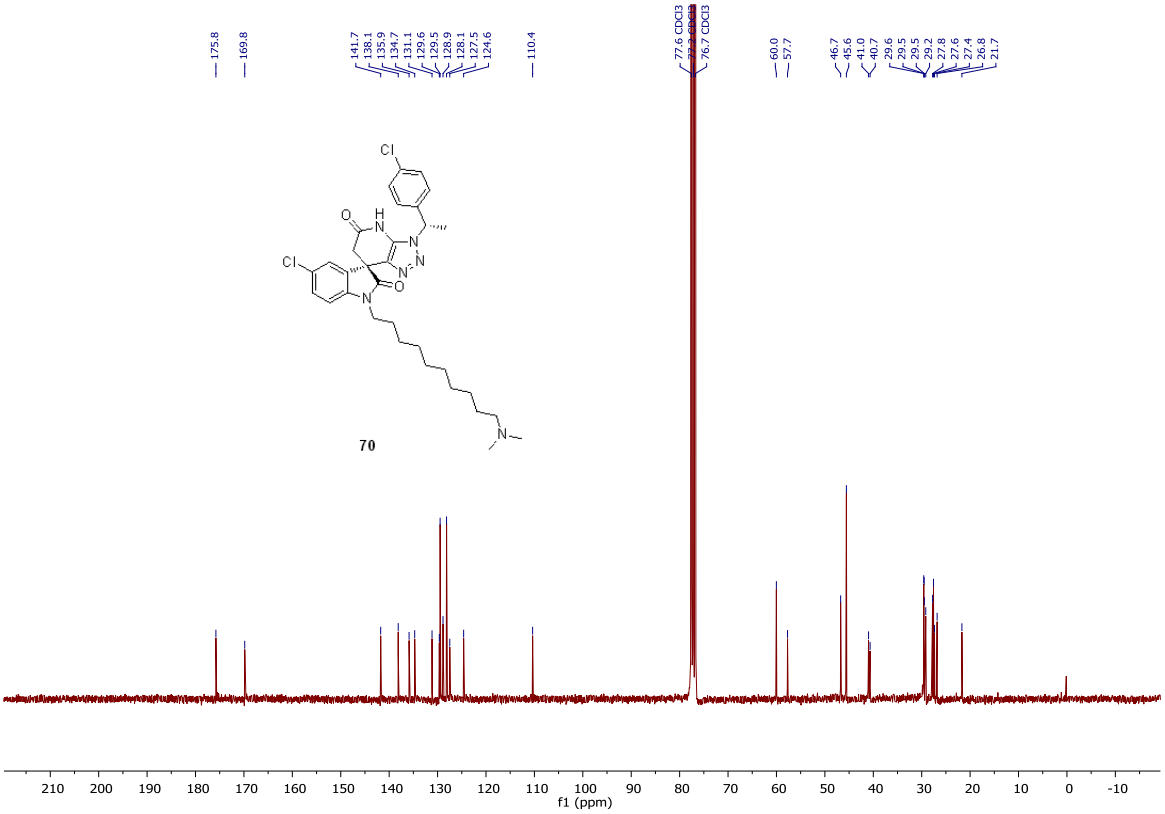
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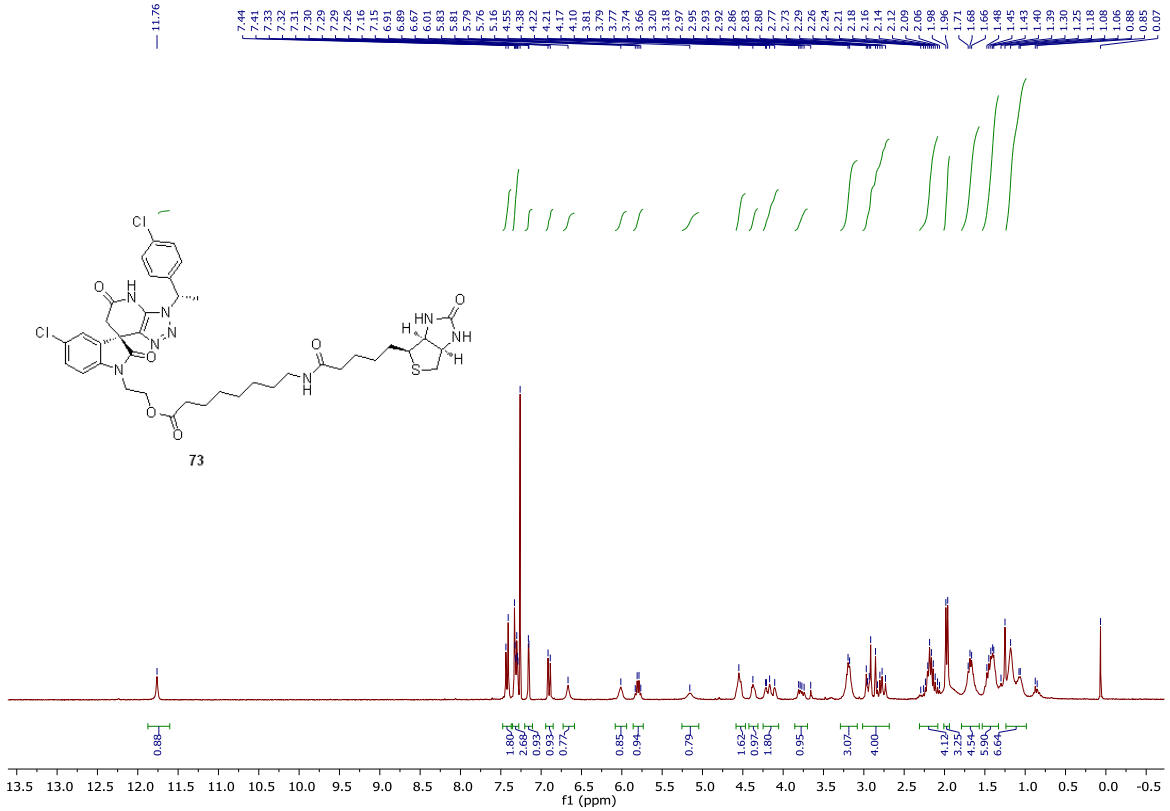
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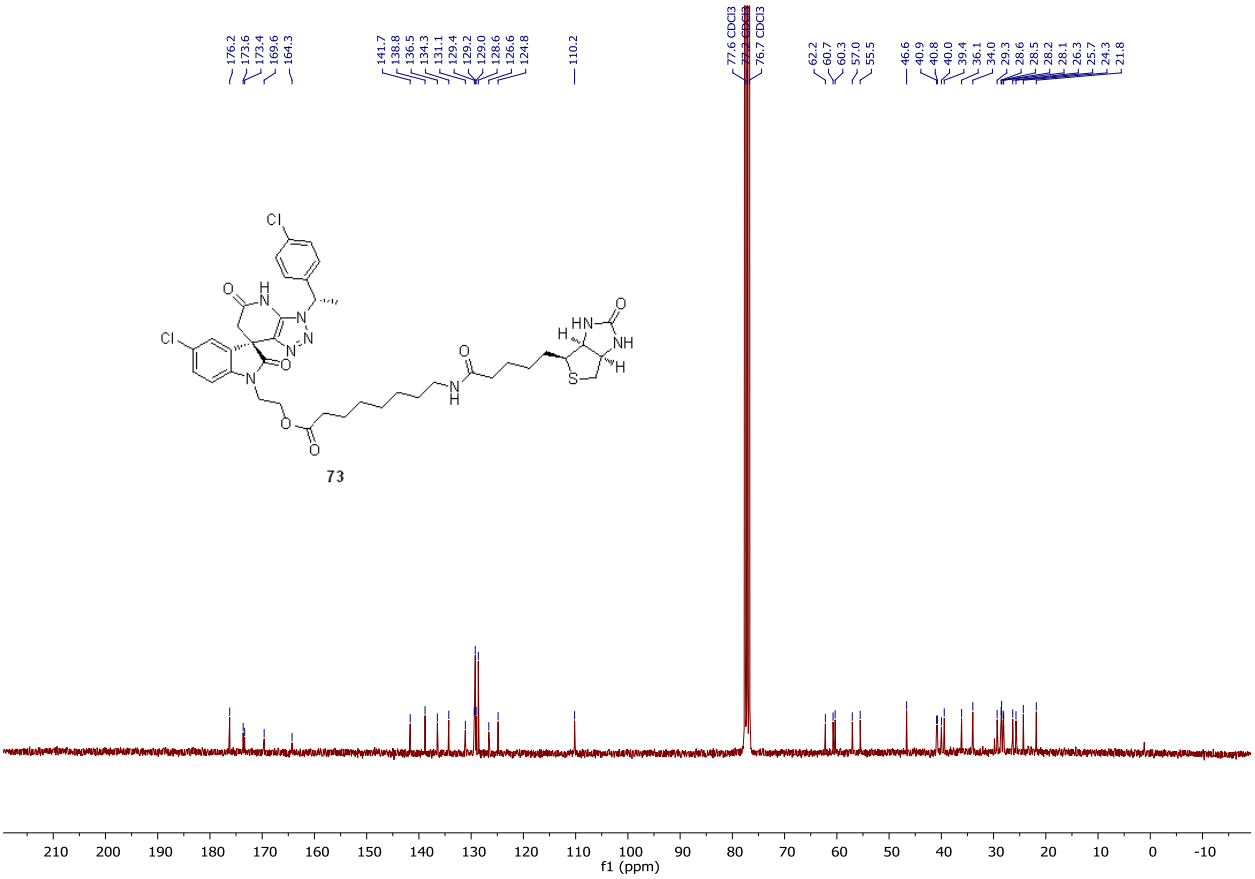
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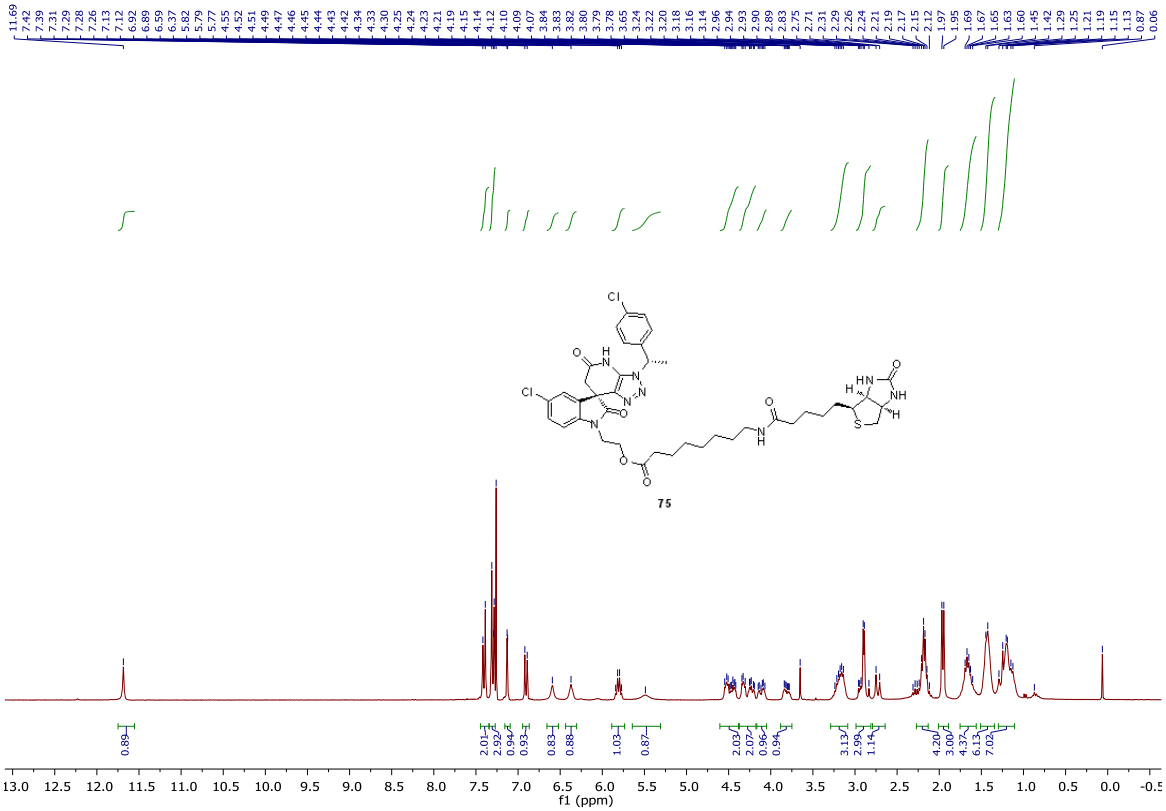
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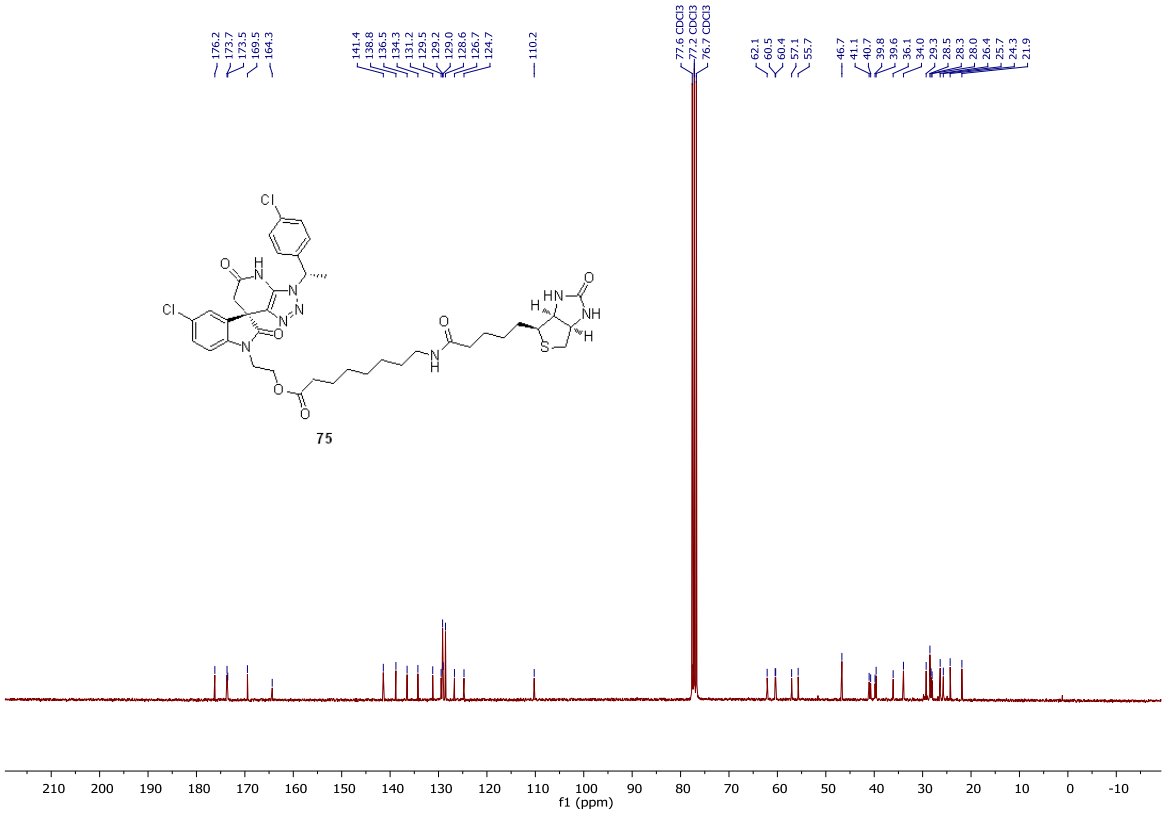
75
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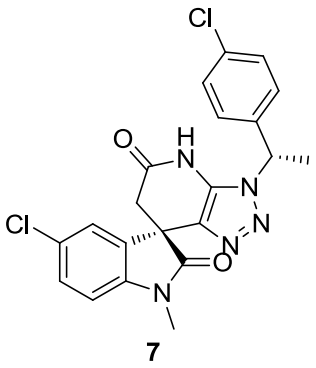
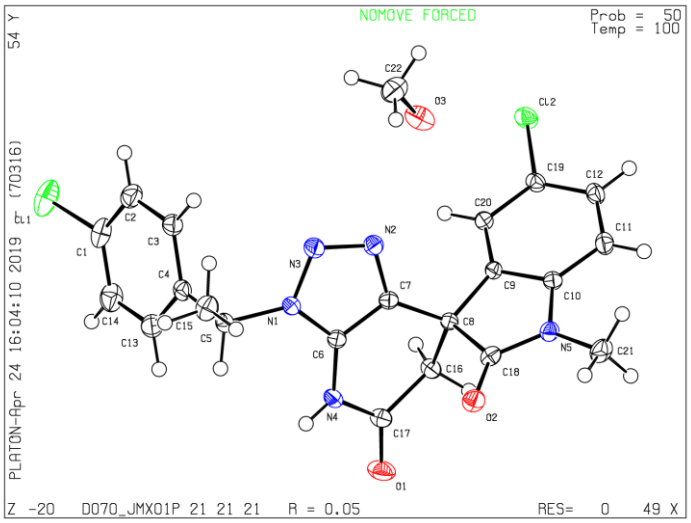
Table S1. Crystal Data for Compound 7[a]





CCDC 1830521	
Compound	**7**
Bond precision	C-C = 0.0049 Å
Wavelength	1.54178
Cell	a = 8.2709 (8); b = 11.8565 (11); c = 22.060 (2) alpha = 90; beta = 90; gamma = 90
Temperature	100 K
Volume	2163.3 (4)
Space group	P 21 21 21
Hall group	P 2ac 2ab
Moiety formula	$C_{21}H_{17}N_5Cl_2O_2$, CH_4O
Sum formula	$C_{22}H_{21}Cl_2N_5O_3$
Mr	473.33
Dx, g cm^{-3}	1.453
Z	4
Mu (mm^{-1})	3.004
F000	980.0
h, k, l_{max}	10, 14, 27
Nref	4081
T_{min}, T_{max}	0.823, 1.000
Data completeness	1.66 / 0.95
Theta (max)	72.545
R (reflections)	0.0483 (4036)
wR2 (reflections)	0.1153 (4081)
S	1.313
Npar	297

[a]The crystal data for compound **7** is based upon the checkCIF/PLATON report (http://checkcif.iucr.org/).