Supplementary Materials

Identification of Substituted Amino Acid Hydrazides as Novel Anti-Tubercular Agents, Using a Scaffold Hopping Approach

Alistair K. Brown [1], Ahmed K.B. Aljohani [1], Fatimah M.A. Alsalem [1], Joseph L. Broadhead [2], Jason H. Gill [3,4], Yucheng Lu [1] and Jonathan D. Sellars [1,4,*]

[1] Biosciences Institute, Faculty of Medical Sciences, Newcastle University, Newcastle upon Tyne NE2 4HH, UK; alistair.brown2@newcastle.ac.uk (A.K.B.); a.aljohani2@newcastle.ac.uk (A.K.B.A.); f.m.a.alsalem2@newcastle.ac.uk (F.M.A.A.); y.lu48@newcastle.ac.uk (Y.L.)

[2] Arcinova, Taylor Drive, Alnwick NE66 2DH, UK; joseph190597@googlemail.com

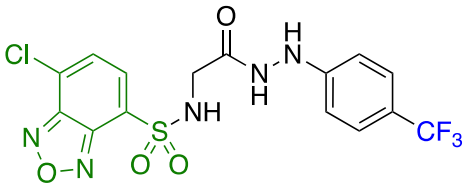
[3] Translational and Clinical Research Institute, Faculty of Medical Sciences, Newcastle University, Newcastle upon Tyne NE2 4HH, UK; jason.gill@newcastle.ac.uk

[4] School of Pharmacy, Faculty of Medical Sciences, King George VI Building, Newcastle upon Tyne NE1 7RU, UK

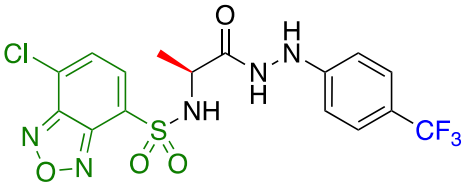
* Correspondence: jon.sellars@newcastle.ac.uk; Tel.: +44-191-2082357

Figure S1: Representative comparison data between our current compounds (this study) and our lead benzoxa-[2,1,3]-diazoles compounds from our previous study.

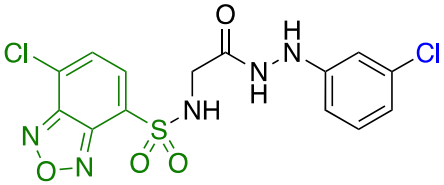
Previous work



MIC *Mtb* WT = 31 μM

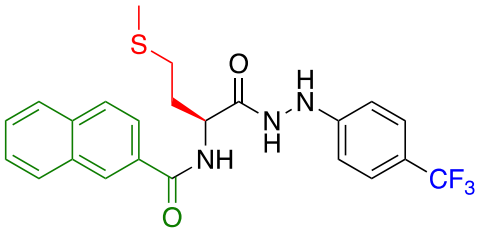


MIC *Mtb* WT = 17 μM

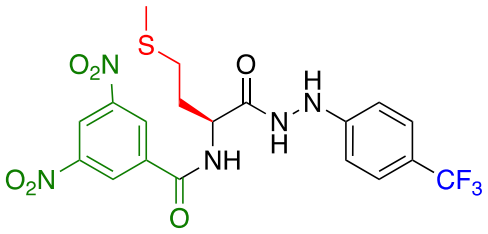


MIC *Mtb* WT = 19 μM

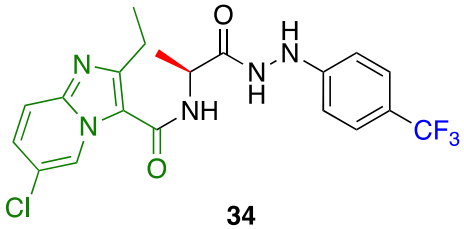
This work



19
MIC *Mtb* WT= 35 μM

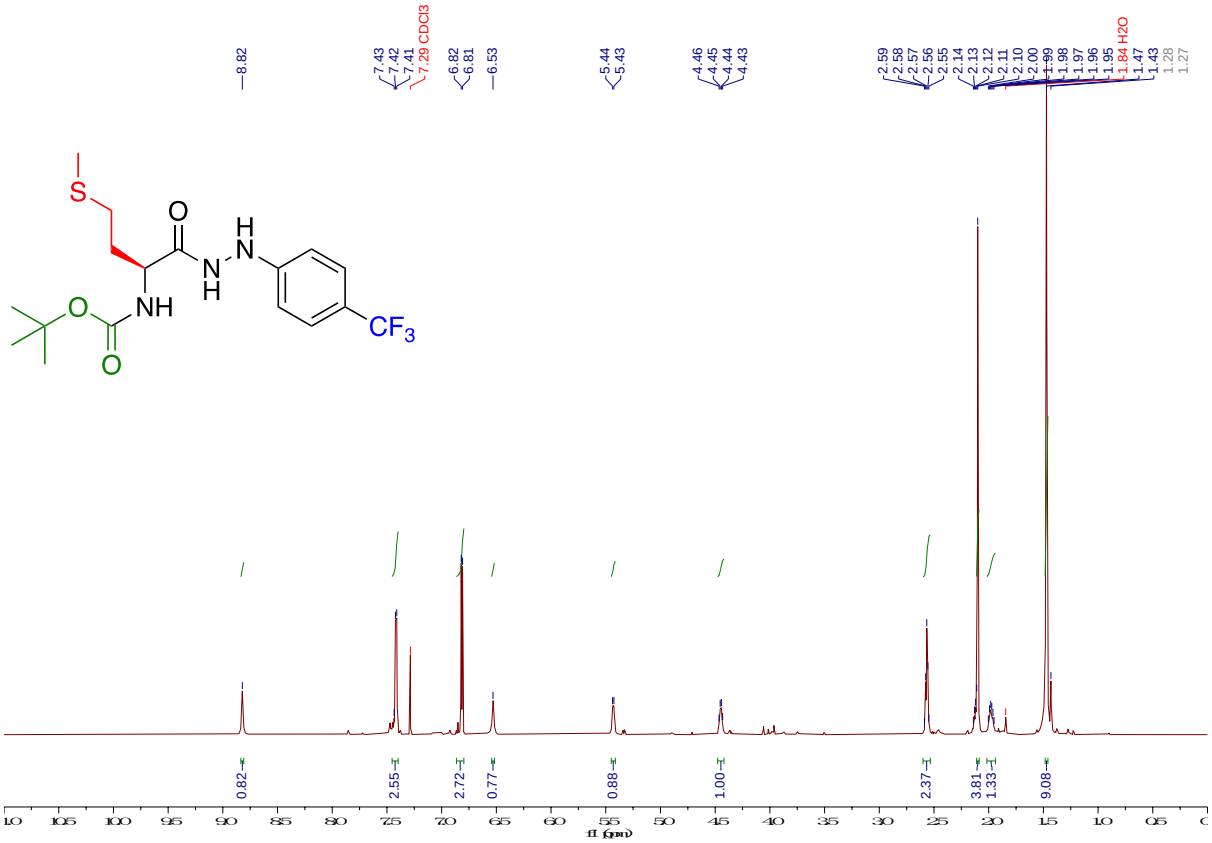


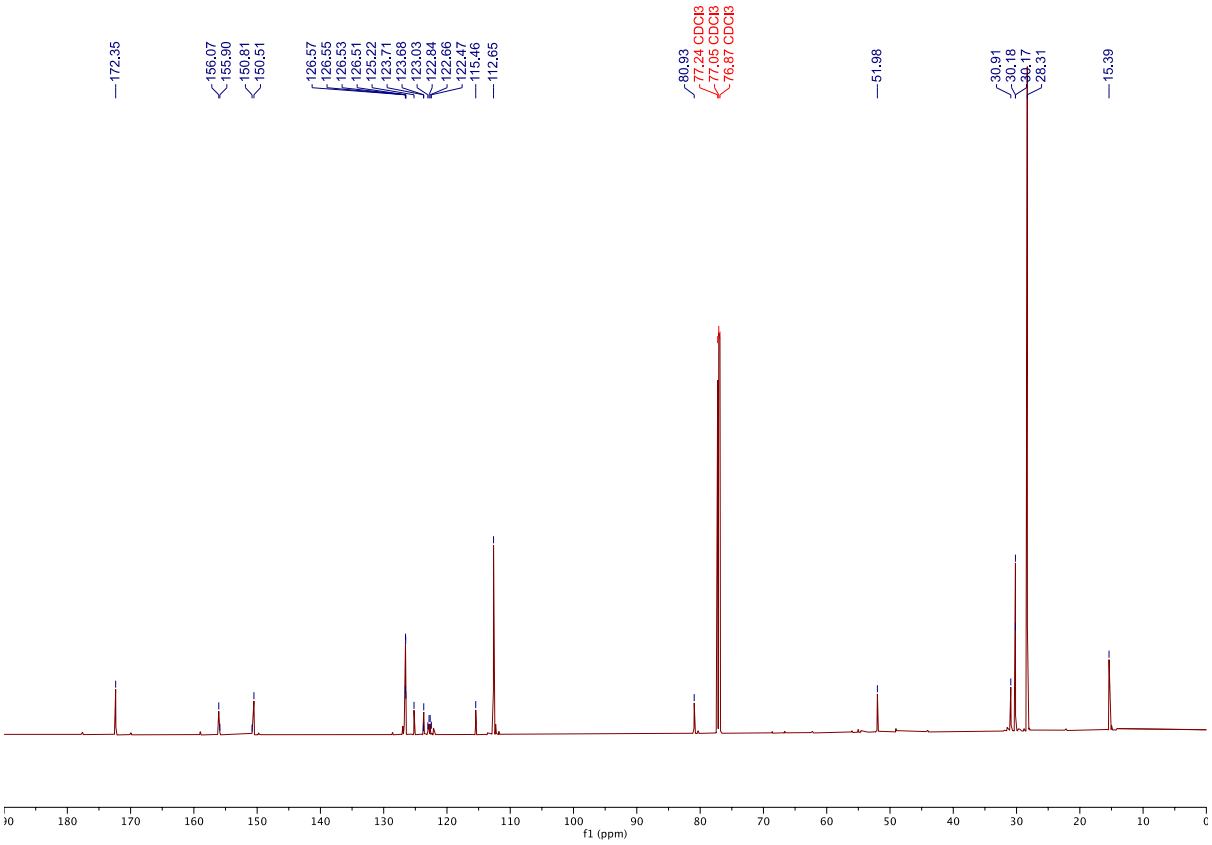
31
MIC *Mtb* WT= 8 μM



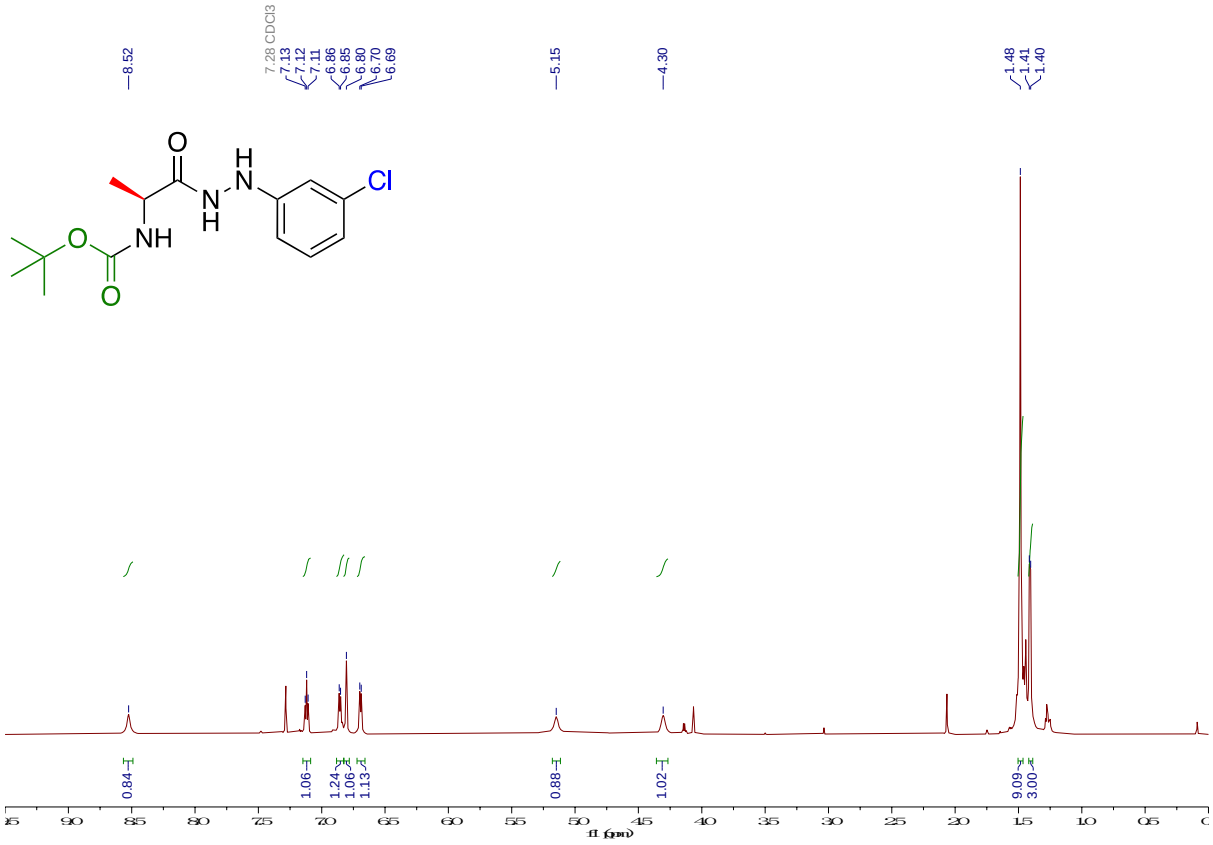
34
MIC *Mtb* WT= 35 μM

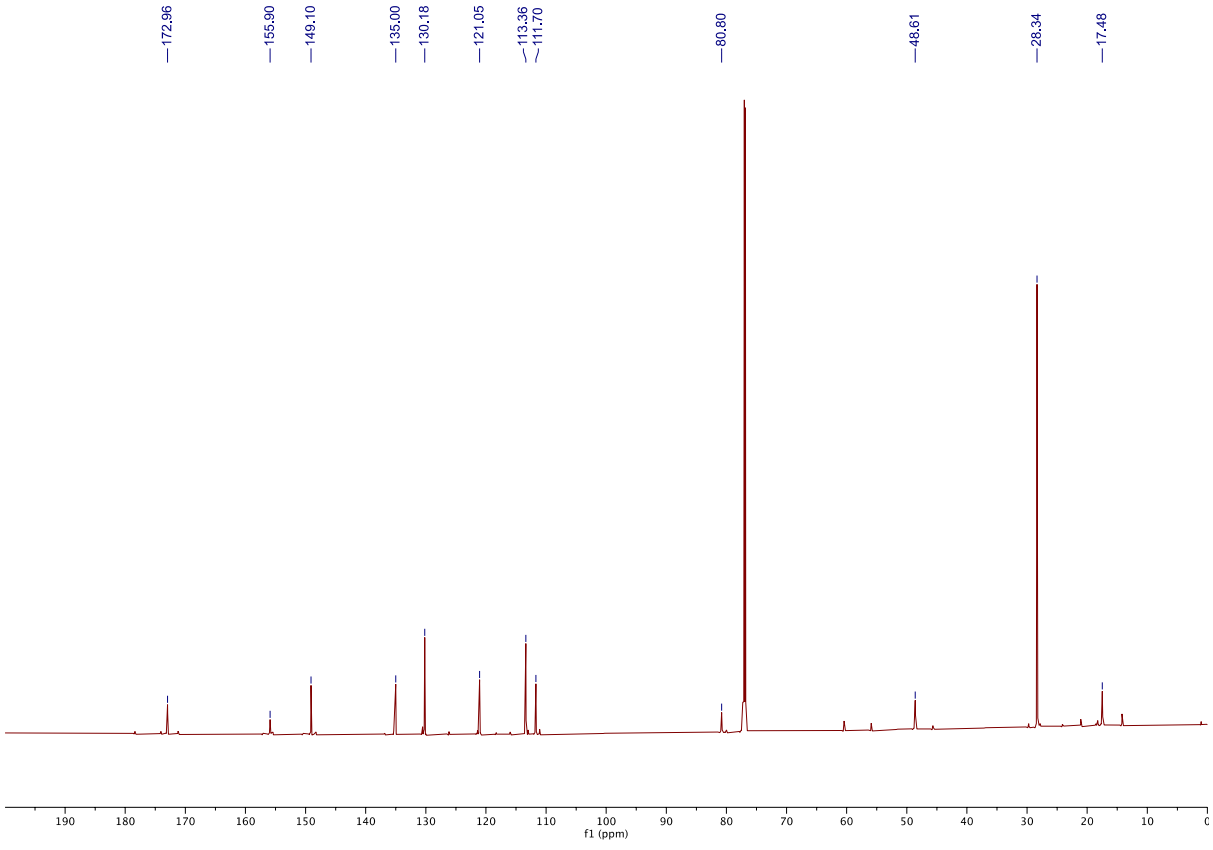
Figure S2: ^{1}H and ^{13}C NMR for all new compounds produced in this study.
Compound 7



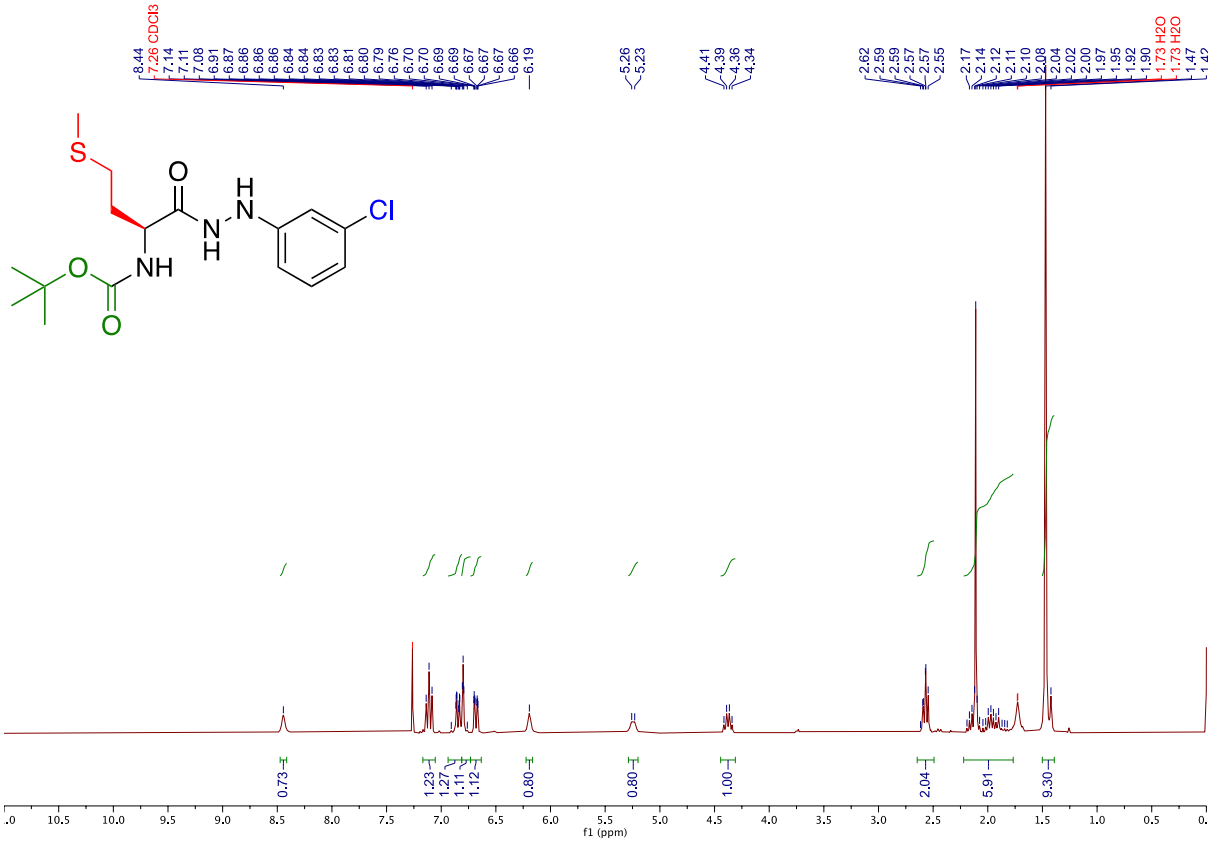


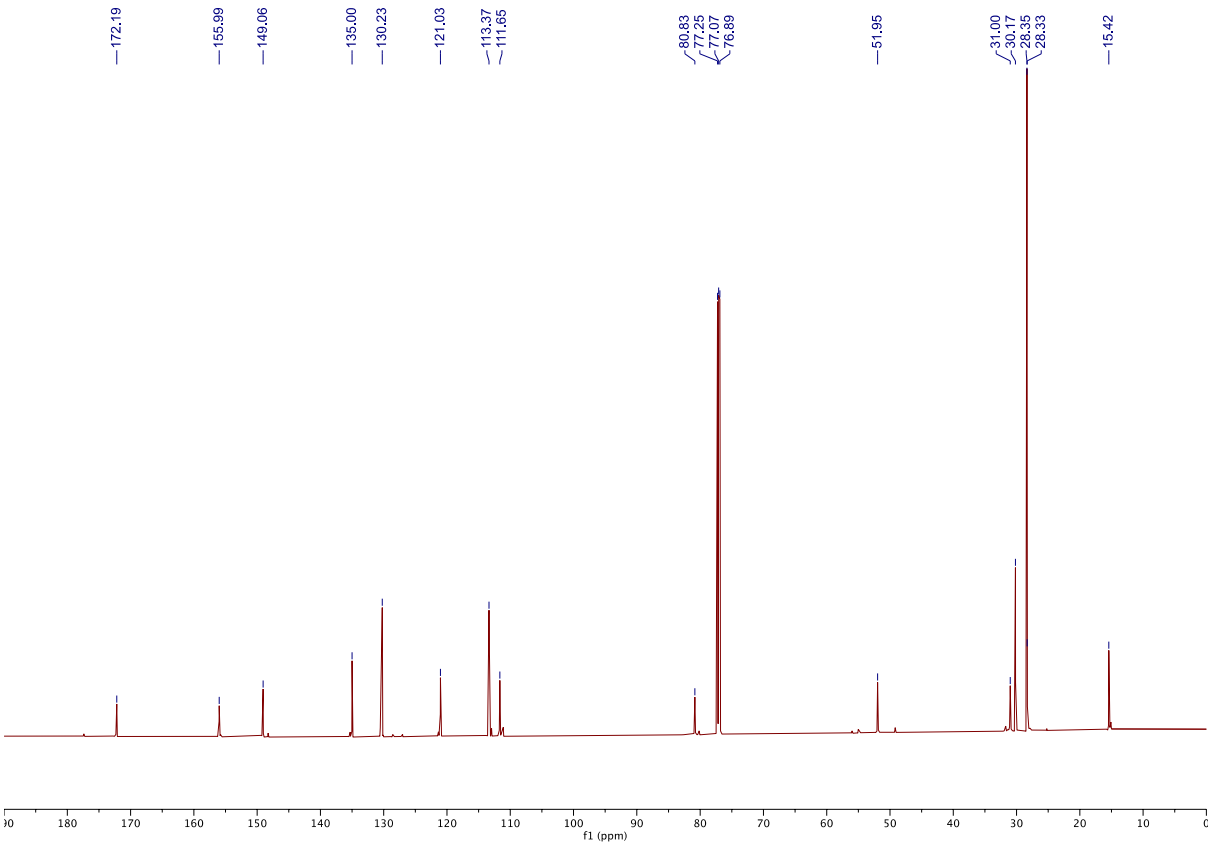
Compound 8


8.52
7.28 CDCl3
7.13
7.12
7.11
6.86
6.85
6.80
6.70
6.69
5.15
4.30
1.48
1.41
1.40
O
H
N
N
H
Cl
NH
O
O
0.84
1.06
1.24
1.06
1.13
0.88
1.02
9.09
3.00
f1 (ppm)

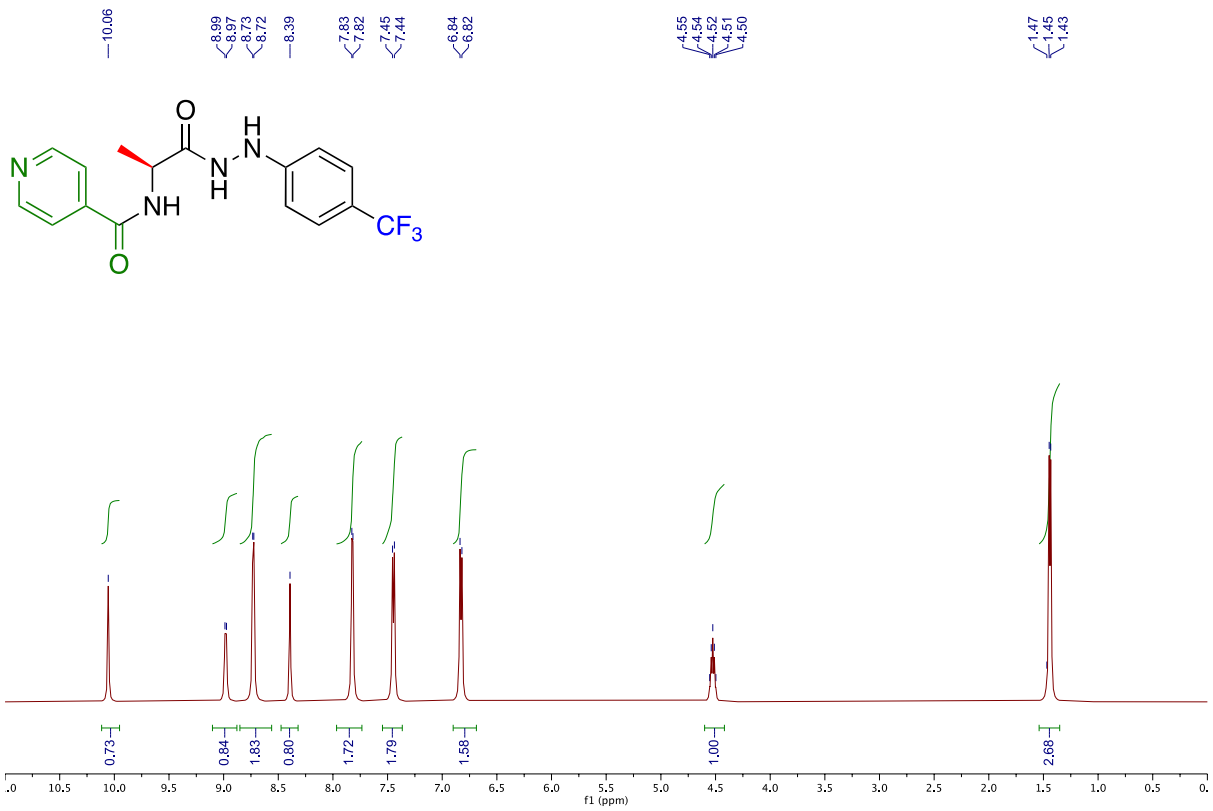

172.96
155.90
149.10
135.00
130.18
121.05
113.36
111.70
80.80
48.61
28.34
17.48
f1 (ppm)

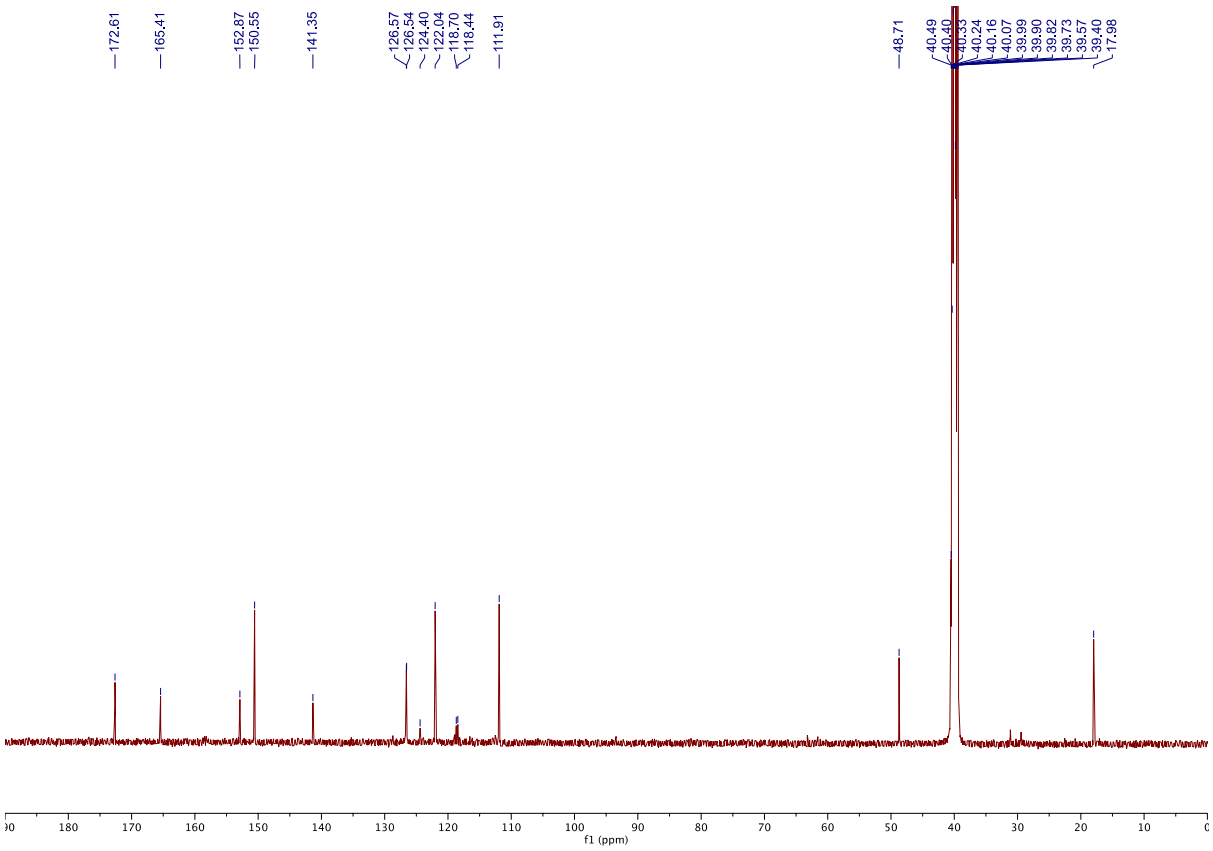
Compound 9


8.44
7.26 CDCl3
7.14
7.11
7.08
6.91
6.87
6.86
6.86
6.86
6.84
6.84
6.83
6.81
6.80
6.79
6.76
6.70
6.70
6.69
6.69
6.67
6.67
6.67
6.66
6.19
5.26
5.23
4.41
4.39
4.36
4.34
2.62
2.59
2.59
2.57
2.57
2.55
2.17
2.14
2.12
2.11
2.10
2.08
2.04
2.02
2.00
1.97
1.95
1.92
1.90
1.73 H2O
1.73 H2O
1.47
S
O
H
N
N
Cl
O
NH
O
0.73
1.23
1.27
1.11
1.12
0.80
0.80
1.00
2.04
5.91
9.30
f1 (ppm)

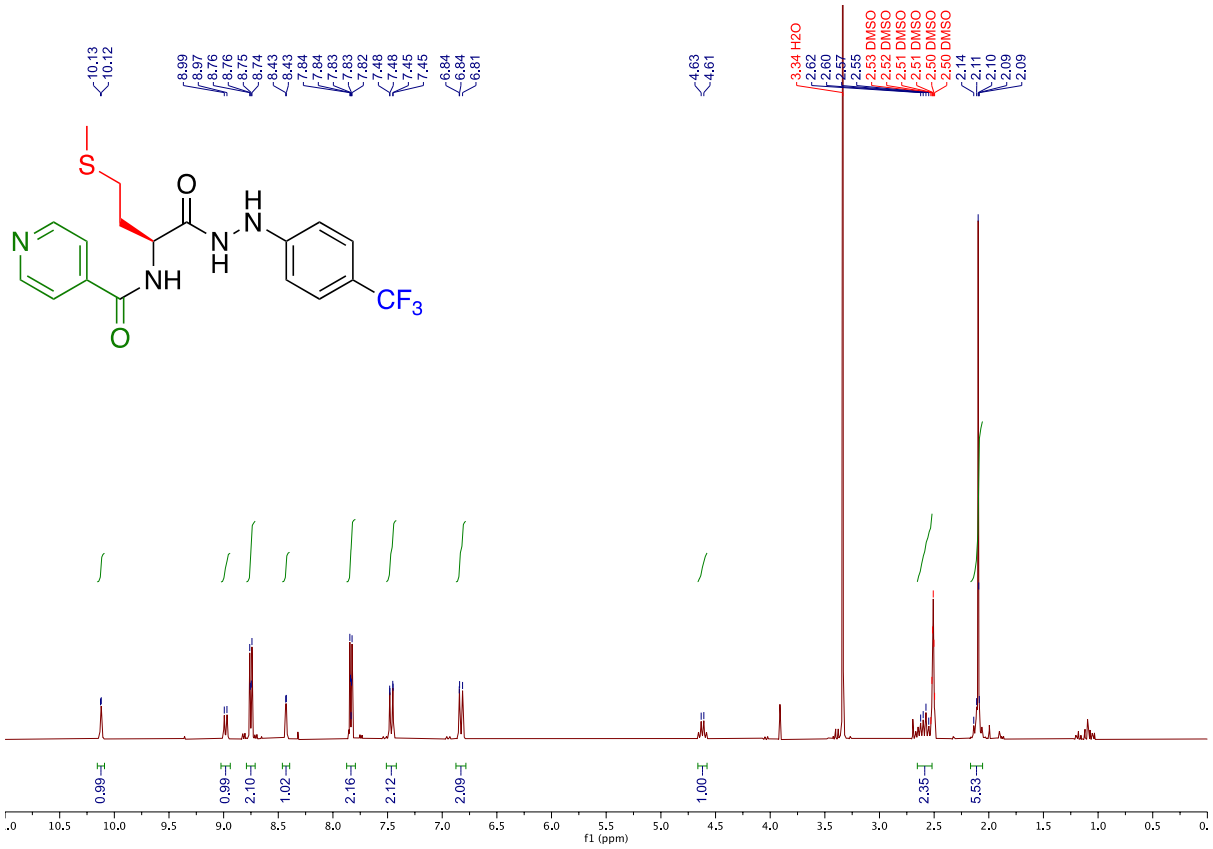

172.19
155.99
149.06
135.00
130.23
121.03
113.37
111.65
80.83
77.25
77.07
76.89
51.95
31.00
30.17
28.35
28.33
15.42
f1 (ppm)

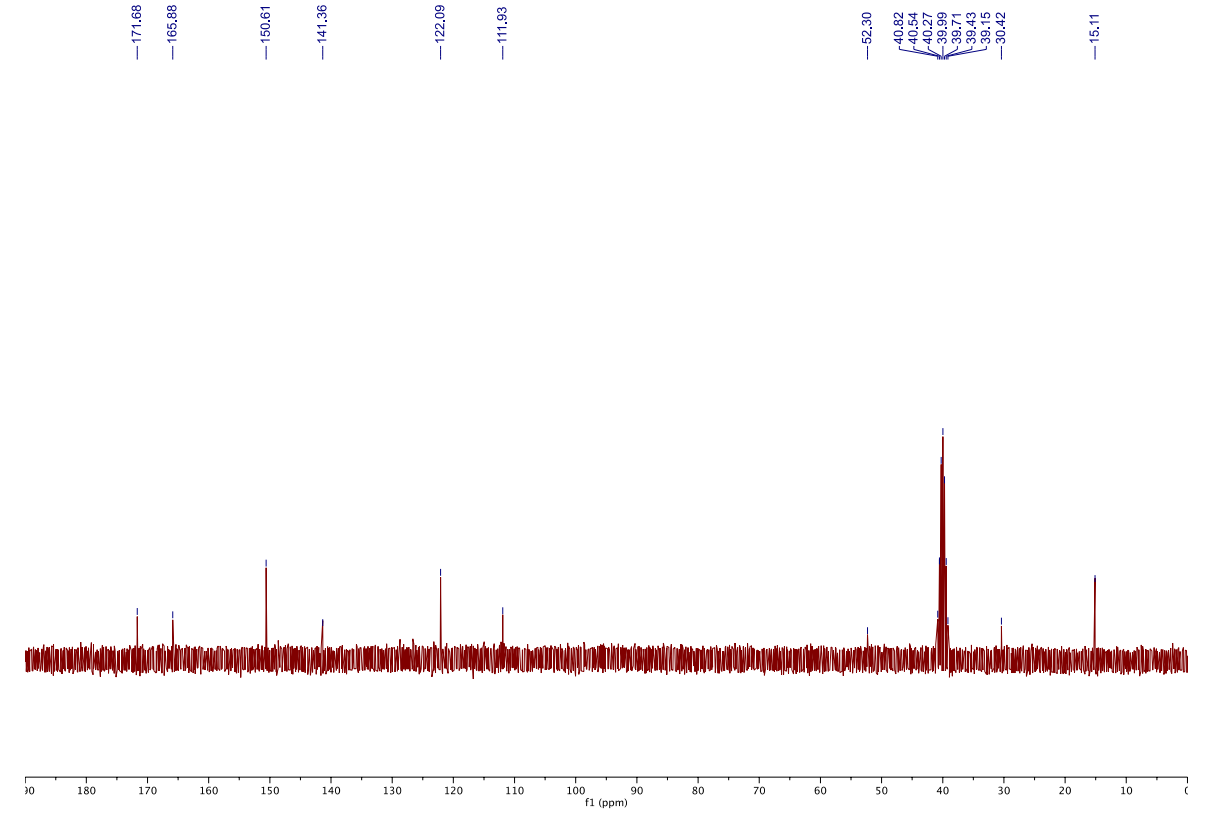
Compound 10


10.06
8.99
8.97
8.73
8.72
8.39
7.83
7.82
7.45
7.44
6.84
6.82
4.55
4.54
4.52
4.51
4.50
1.47
1.45
1.43
O
H
N
N
N
H
NH
O
CF3
0.73
0.84
1.83
0.80
1.72
1.79
1.58
1.00
2.68
f1 (ppm)

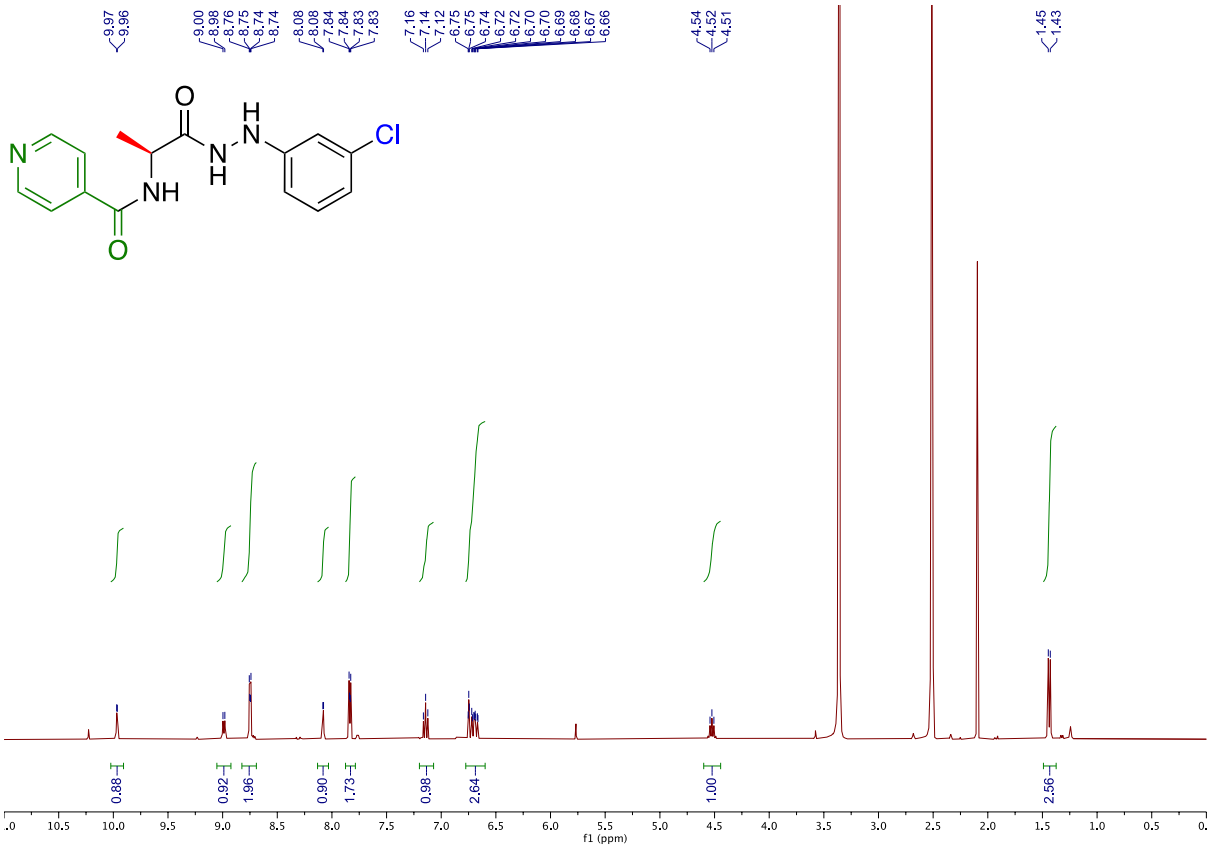

172.61
165.41
152.87
150.55
141.35
126.57
126.54
124.40
122.04
118.70
118.44
111.91
48.71
40.49
40.40
40.33
40.24
40.16
40.07
39.99
39.90
39.82
39.73
39.57
39.40
17.98
f1 (ppm)

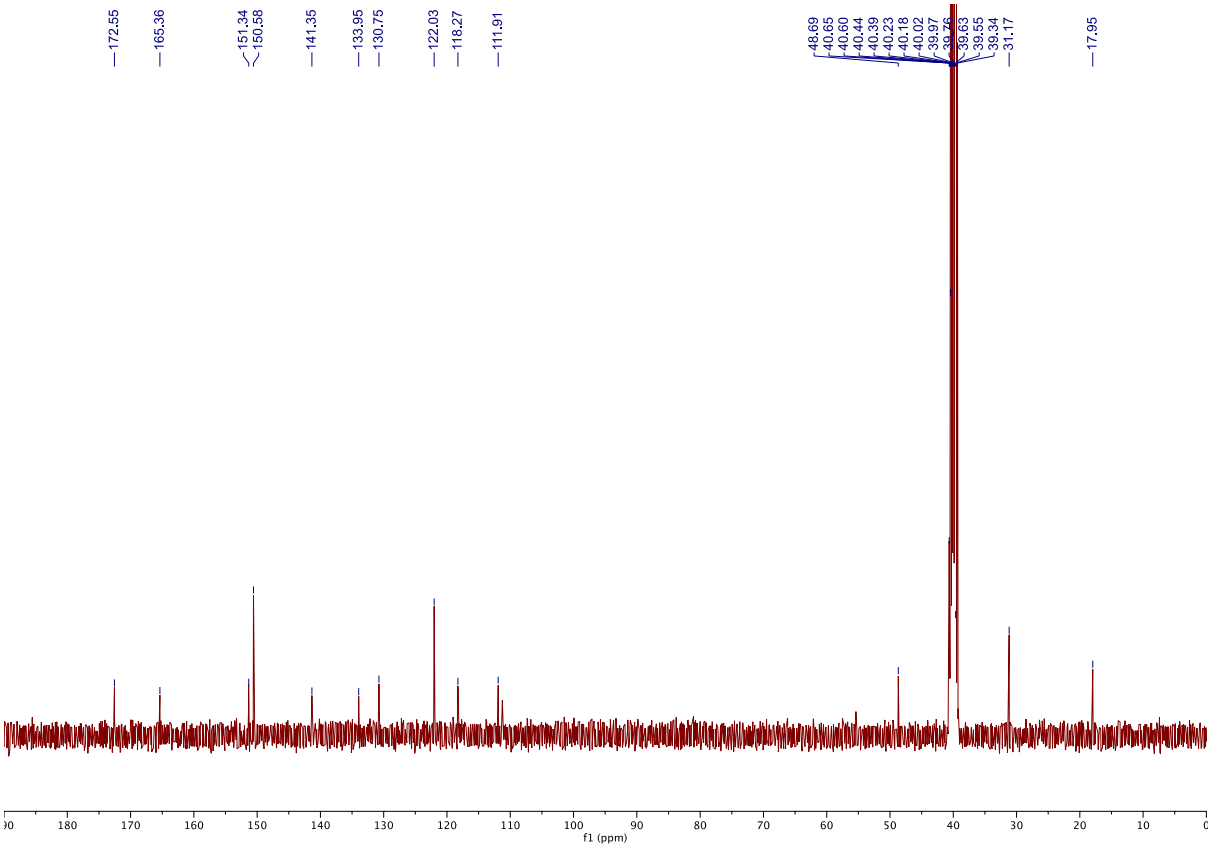
Compound 11


10.13
10.12
8.99
8.97
8.76
8.76
8.75
8.74
8.43
8.43
7.84
7.84
7.83
7.83
7.82
7.48
7.48
7.45
7.45
6.84
6.84
6.81
4.63
4.61
3.34 H2O
2.62
2.60
2.57
2.55
2.53 DMSO
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.14
2.11
2.10
2.09
2.09
S
O
H
N
N
N
NH
O
CF3
0.99
0.99
2.10
1.02
2.16
2.12
2.09
1.00
2.35
5.53
f1 (ppm)

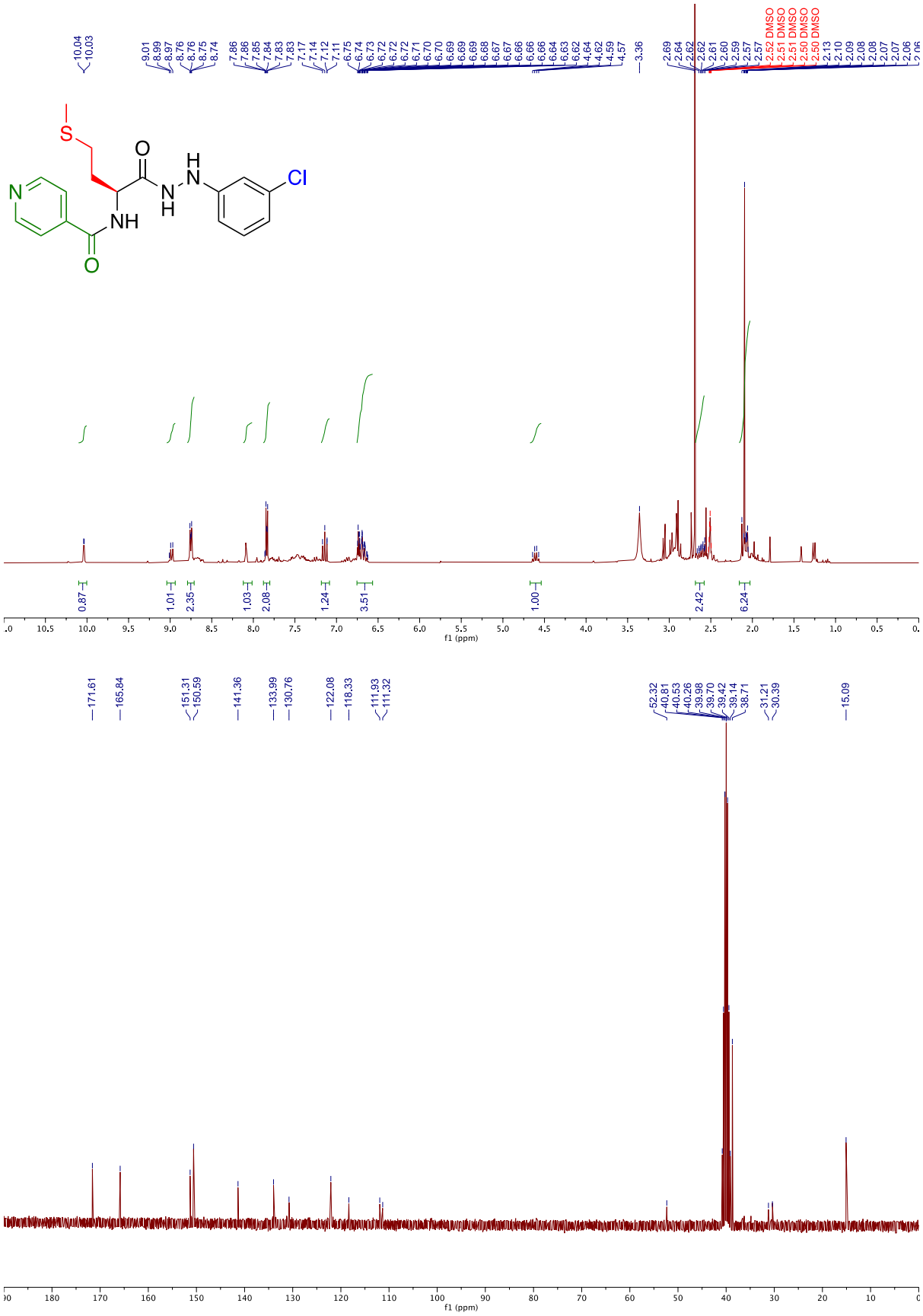

171.68
165.88
150.61
141.36
122.09
111.93
52.30
40.82
40.54
40.27
39.99
39.71
39.43
39.15
30.42
15.11
f1 (ppm)

Compound 12

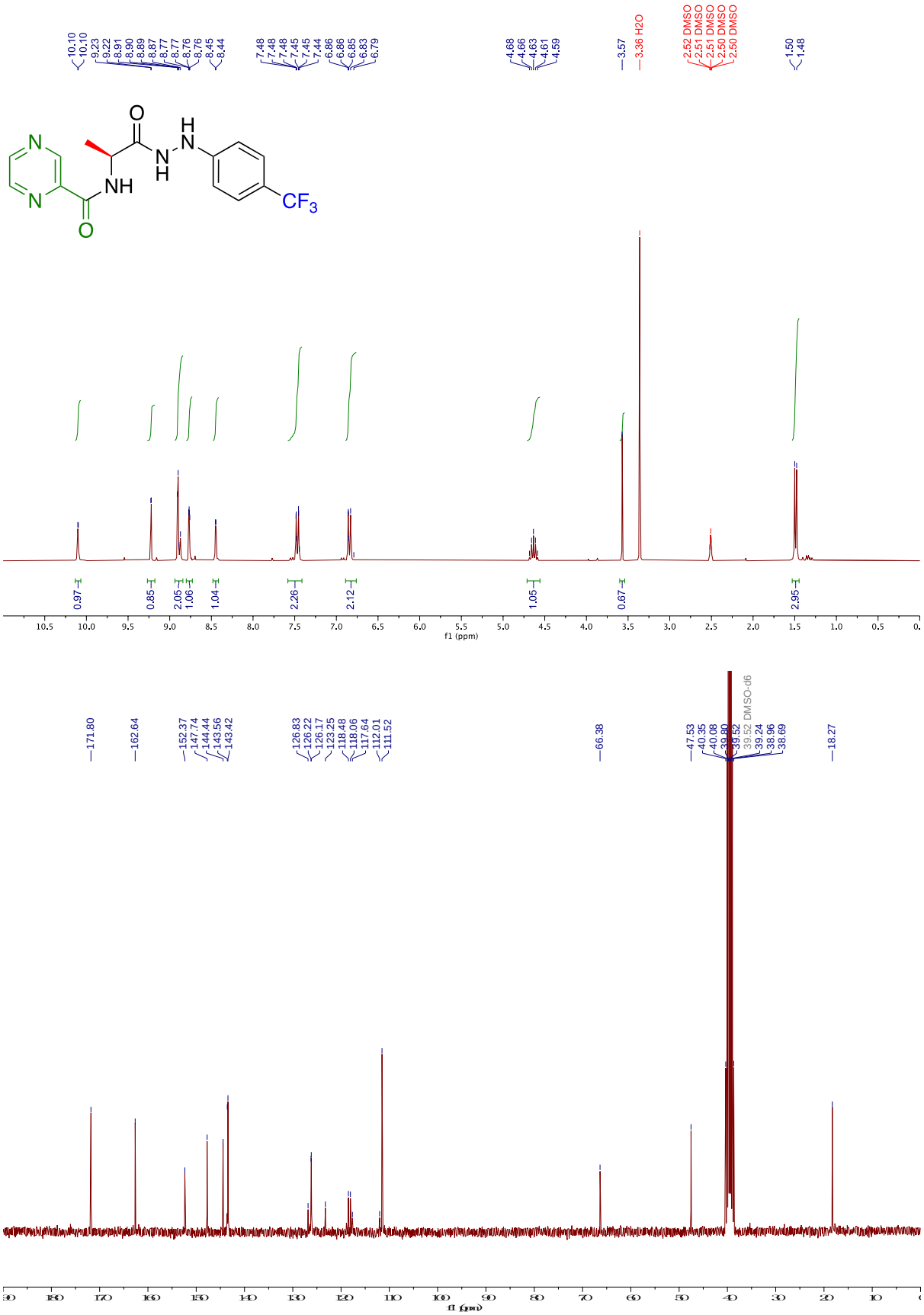

9.97
9.96
9.00
8.98
8.76
8.75
8.74
8.74
8.08
8.08
7.84
7.84
7.83
7.83
7.16
7.14
7.12
6.75
6.75
6.74
6.72
6.72
6.70
6.70
6.69
6.68
6.67
6.66
4.54
4.52
4.51
1.45
1.43
O
H
N
N
Cl
N
NH
O
0.88
0.92
1.96
0.90
1.73
0.98
2.64
1.00
2.56
f1 (ppm)


172.55
165.36
151.34
150.58
141.35
133.95
130.75
122.03
118.27
111.91
48.69
40.65
40.60
40.44
40.39
40.23
40.18
40.02
39.97
39.63
39.55
39.34
31.17
17.95
f1 (ppm)

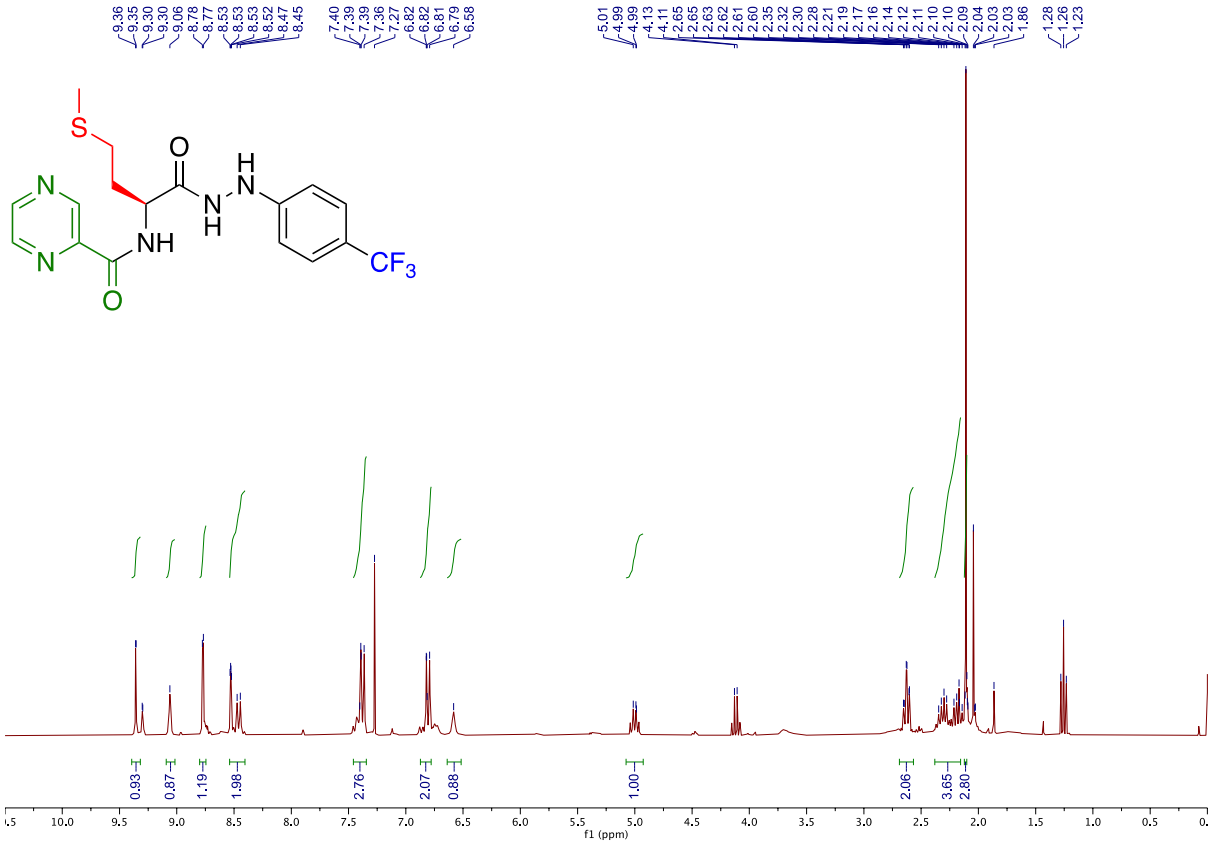
Compound 13

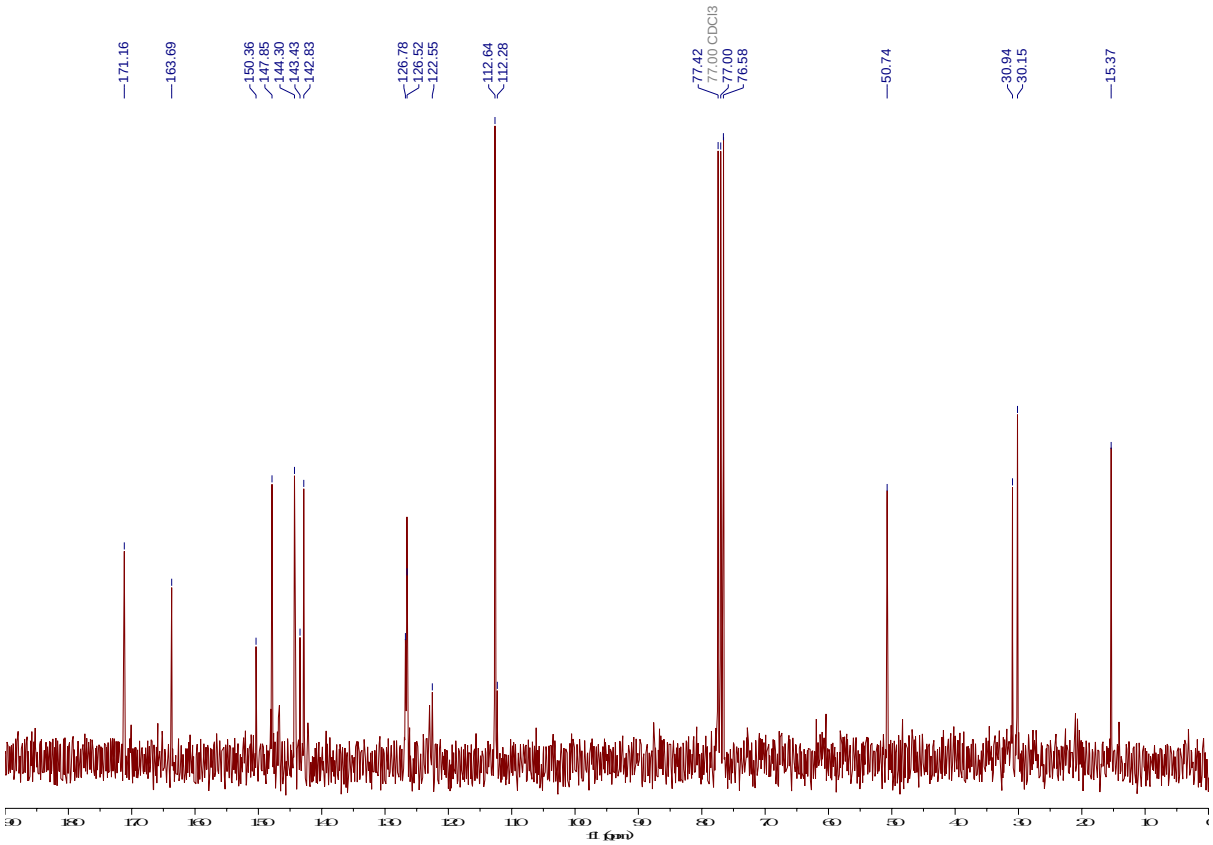

S
O
H
N
N
Cl
N
NH
O
10.04
10.03
9.01
8.99
8.97
8.76
8.76
8.75
8.74
7.86
7.86
7.85
7.84
7.83
7.83
7.17
7.14
7.12
7.11
6.75
6.74
6.73
6.72
6.72
6.72
6.71
6.70
6.70
6.69
6.69
6.69
6.68
6.67
6.67
6.66
6.66
6.66
6.64
6.63
6.62
4.64
4.62
4.59
4.57
3.36
2.69
2.64
2.62
2.62
2.61
2.60
2.59
2.57
2.57
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.13
2.10
2.09
2.08
2.08
2.07
2.07
2.06
0.87
1.01
2.35
1.03
2.08
1.24
3.51
1.00
2.42
6.24
f1 (ppm)
171.61
165.84
151.31
150.59
141.36
133.99
130.76
122.08
118.33
111.93
111.32
52.32
40.81
40.53
40.26
39.98
39.70
39.42
39.14
38.71
31.21
30.39
15.09
f1 (ppm)

Compound 14


10.10
10.10
9.23
9.22
8.91
8.90
8.89
8.87
8.77
8.77
8.76
8.76
8.45
8.44
7.48
7.48
7.48
7.45
7.45
7.44
6.86
6.86
6.85
6.83
6.79
4.68
4.66
4.63
4.61
4.59
3.57
3.36 H2O
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
1.50
1.48
O
H
N
N
N
NH
O
CF3
0.97
0.85
2.05
1.06
1.04
2.26
2.12
1.05
0.67
2.95
f1 (ppm)
171.80
162.64
152.37
147.74
144.44
143.56
143.42
126.83
126.22
126.17
123.25
118.48
118.06
117.64
112.01
111.52
66.38
47.53
40.35
40.08
39.80
39.52
39.52 DMSO-d6
39.24
38.96
38.69
18.27

Compound 15


9.36
9.35
9.30
9.30
9.06
8.78
8.77
8.53
8.53
8.52
8.47
8.45
7.40
7.39
7.39
7.36
7.27
6.82
6.82
6.81
6.79
6.58
5.01
4.99
4.99
4.13
4.11
2.65
2.65
2.63
2.62
2.61
2.60
2.35
2.32
2.30
2.28
2.21
2.19
2.17
2.16
2.14
2.12
2.11
2.10
2.10
2.09
2.04
2.03
2.03
1.86
1.28
1.26
1.23
S
O
N
H
N
N
N
H
NH
O
CF3
0.93
0.87
1.19
1.98
2.76
2.07
0.88
1.00
2.06
3.65
2.80
f1 (ppm)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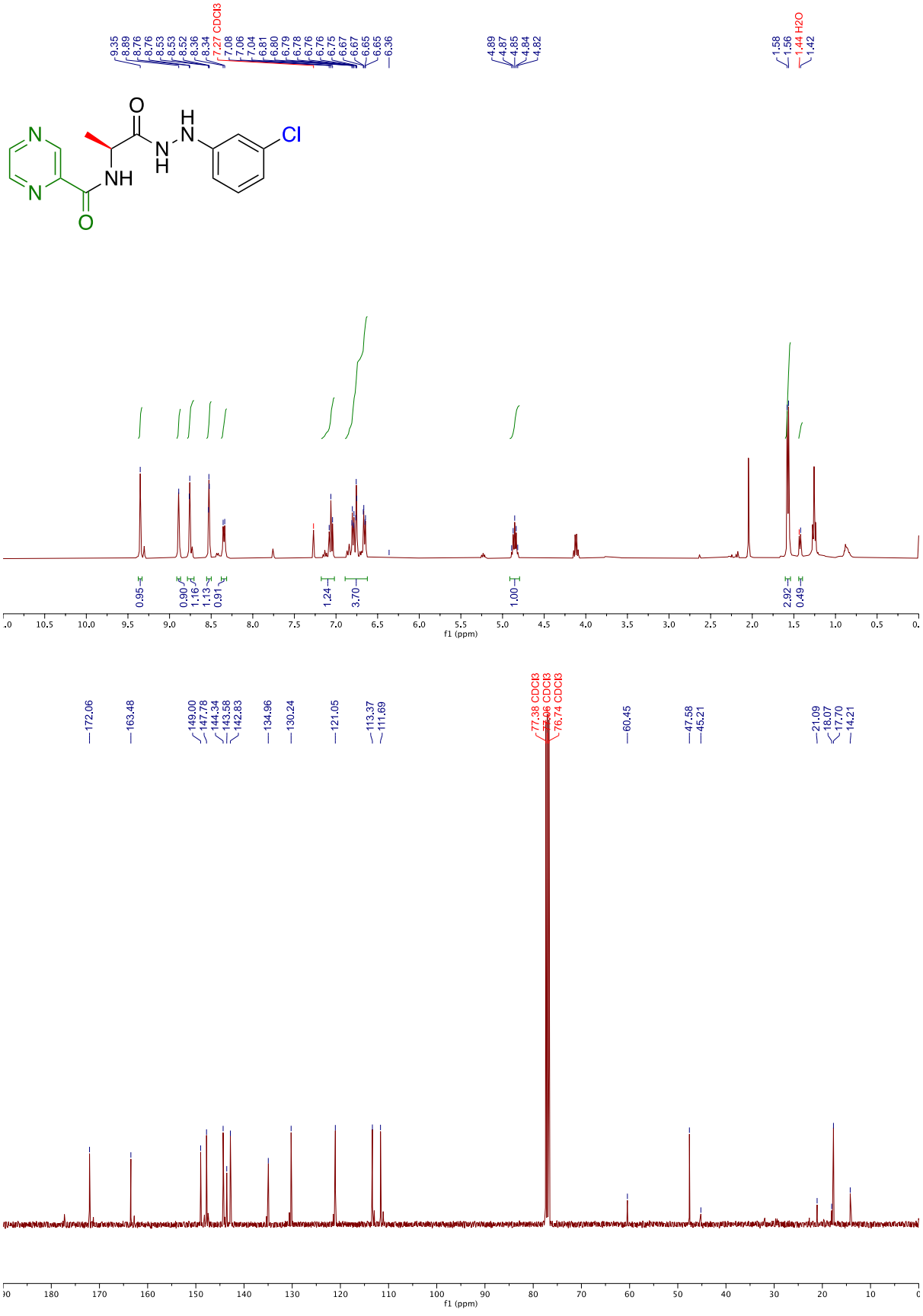
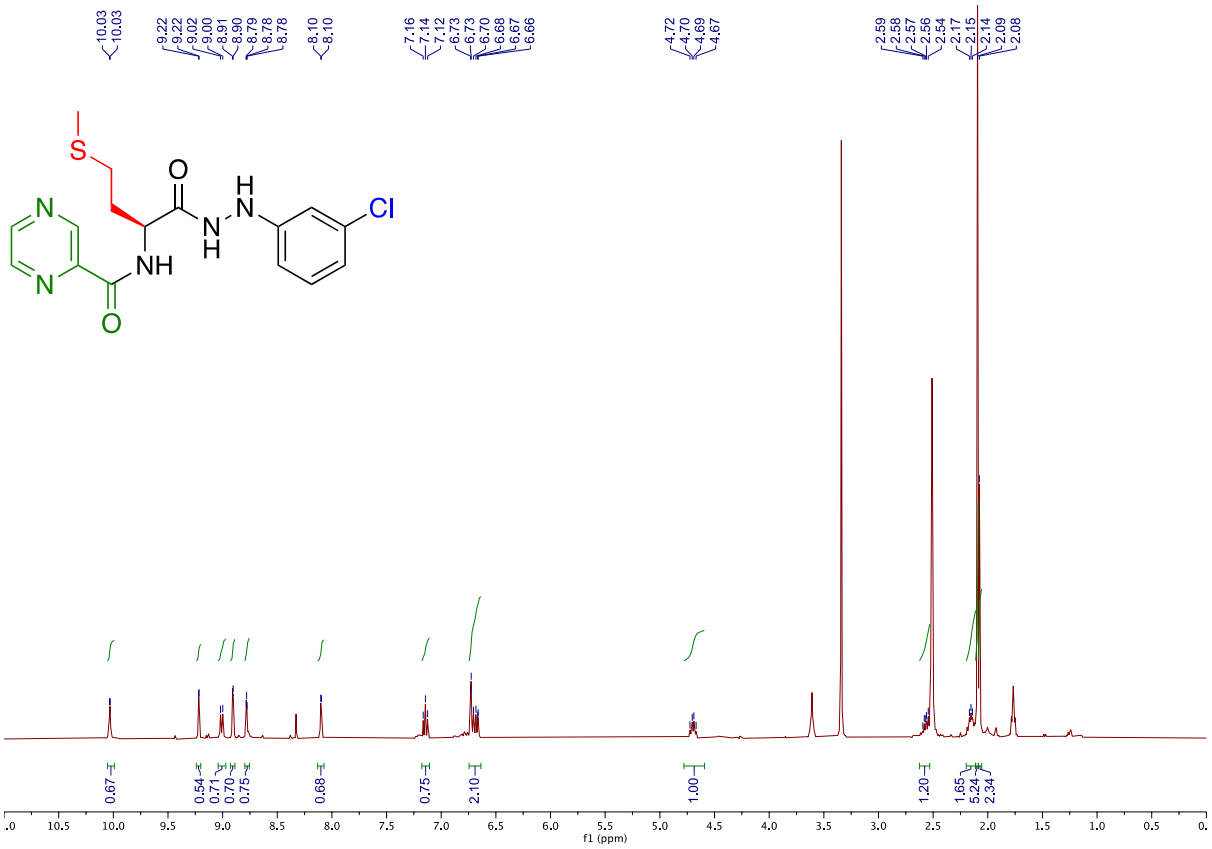
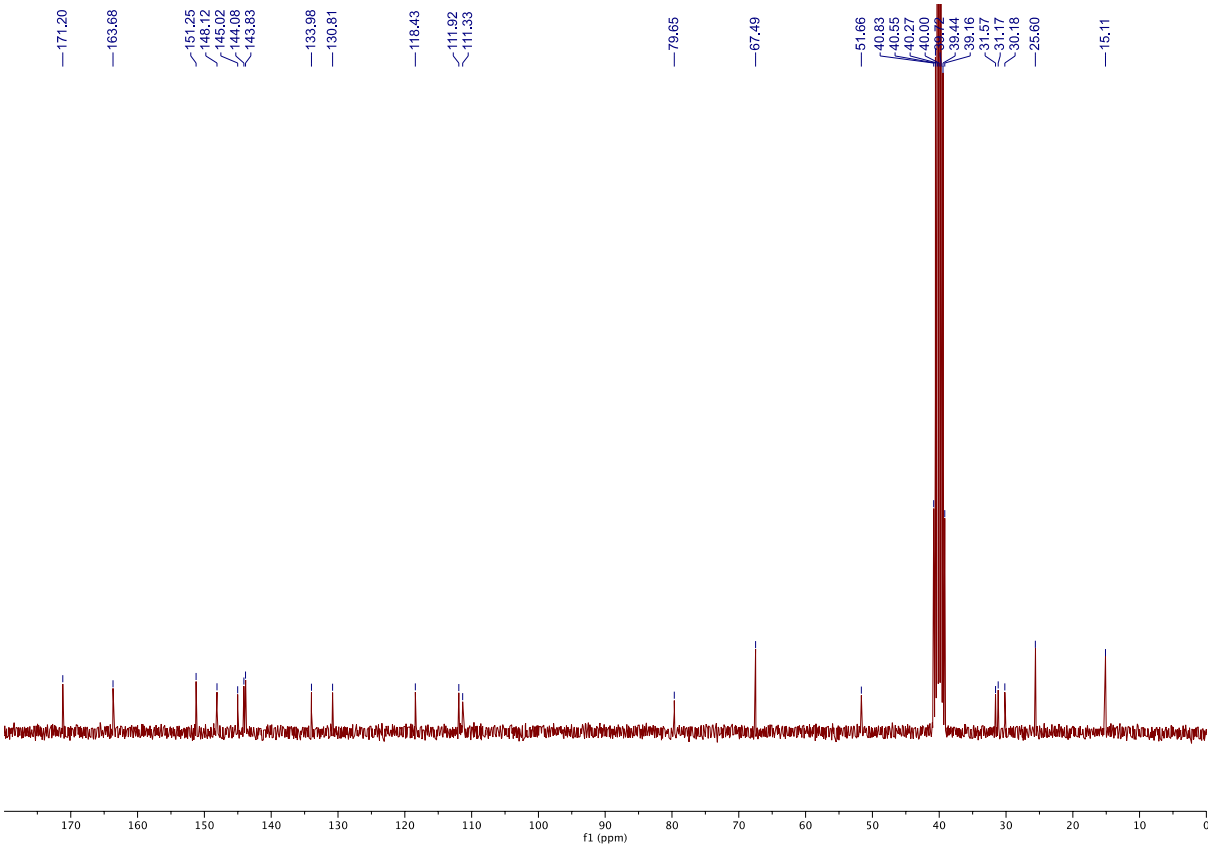
163.69
150.36
147.85
144.30
143.43
142.83
126.78
126.52
122.55
112.64
112.28
77.42
77.00 CDCl3
77.00
76.58
50.74
30.94
30.15
15.37
f1 (ppm)

Compound 16

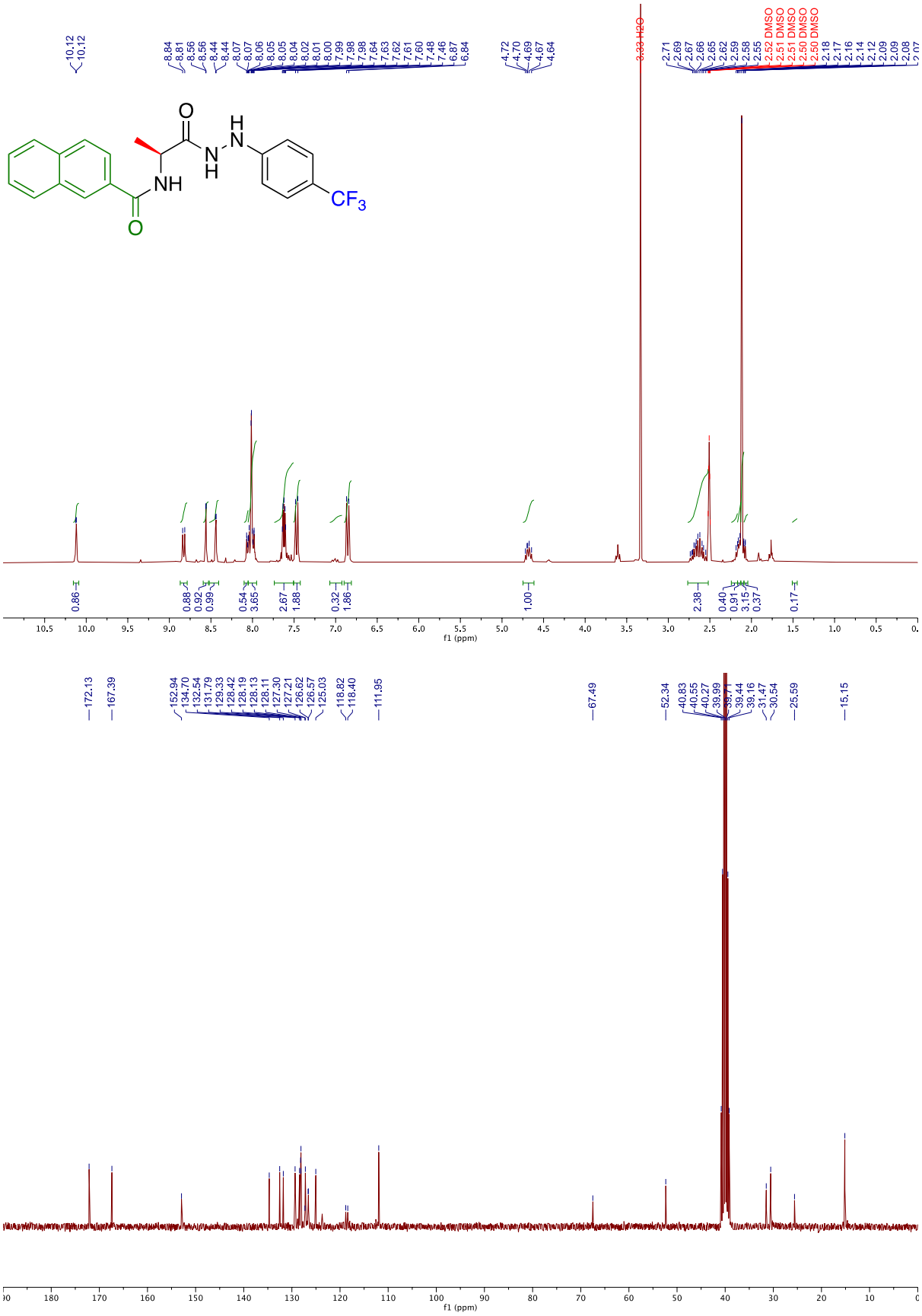

9.35
8.89
8.76
8.76
8.53
8.53
8.52
8.36
8.34
7.27 CDCl3
7.08
7.06
7.04
6.81
6.80
6.79
6.78
6.76
6.76
6.75
6.67
6.67
6.65
6.65
6.36
4.89
4.87
4.85
4.84
4.82
1.58
1.56
1.44 H2O
1.42
O
H
N
N
Cl
N
NH
N
O
0.95
0.90
1.16
1.13
0.91
1.24
3.70
1.00
2.92
0.49
f1 (ppm)
172.06
163.48
149.00
147.78
144.34
143.58
142.83
134.96
130.24
121.05
113.37
111.69
77.38 CDCl3
77.06 CDCl3
76.74 CDCl3
60.45
47.58
45.21
21.09
18.07
17.70
14.21
f1 (ppm)

Compound 17

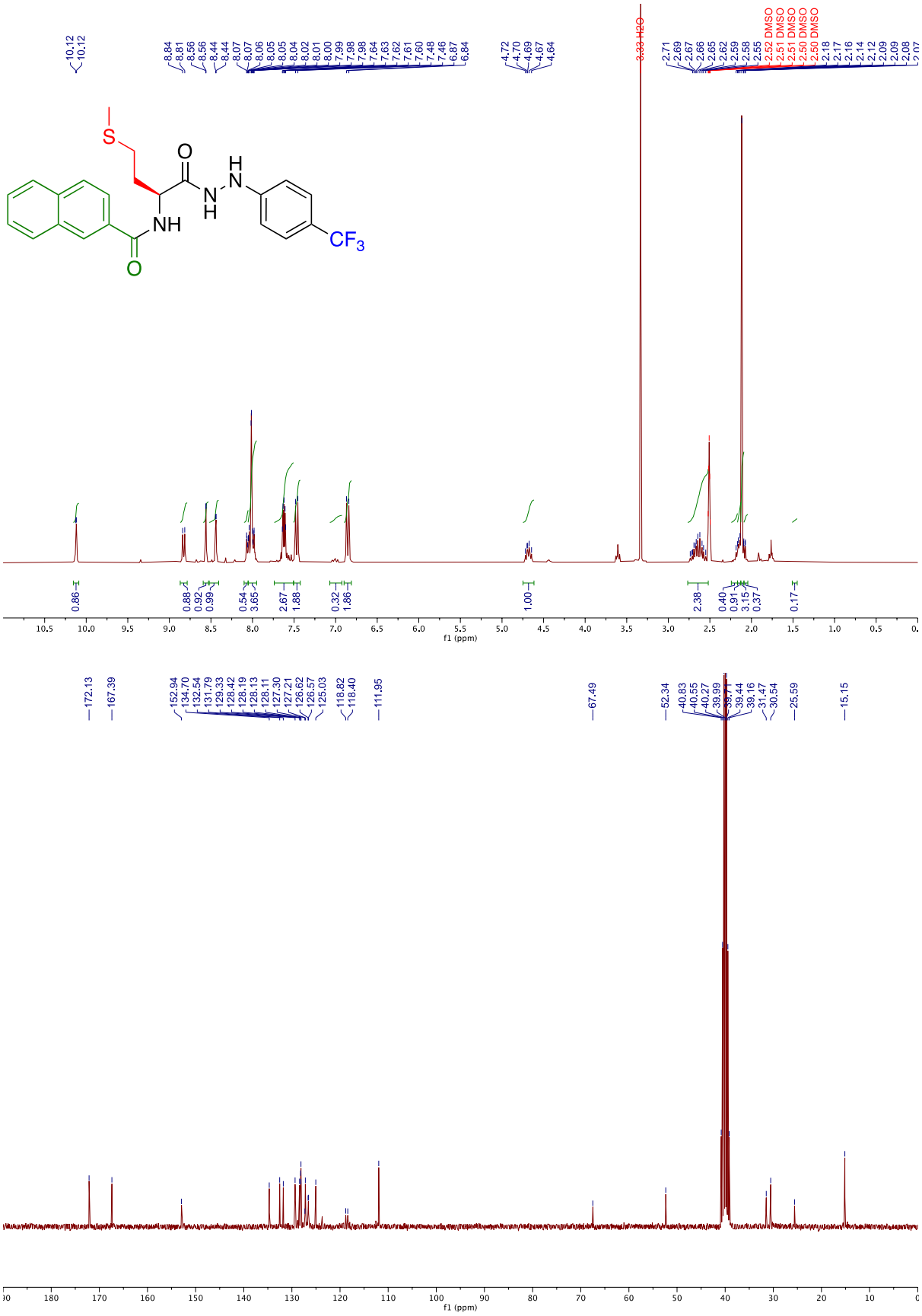

10.03
10.03
9.22
9.22
9.02
9.00
8.91
8.90
8.79
8.78
8.78
8.10
8.10
7.16
7.14
7.12
6.73
6.70
6.68
6.67
6.66
4.72
4.70
4.69
4.67
2.59
2.58
2.57
2.56
2.54
2.17
2.15
2.14
2.09
2.08
S
O
N
H
N
Cl
N
NH
N
O
0.67
0.54
0.71
0.70
0.75
0.68
0.75
2.10
1.00
1.20
1.65
5.24
2.34
f1 (ppm)


171.20
163.68
151.25
148.12
145.02
144.08
143.83
133.98
130.81
118.43
111.92
111.33
79.65
67.49
51.66
40.83
40.55
40.27
40.00
39.72
39.44
39.16
31.57
31.17
30.18
25.60
15.11
f1 (ppm)

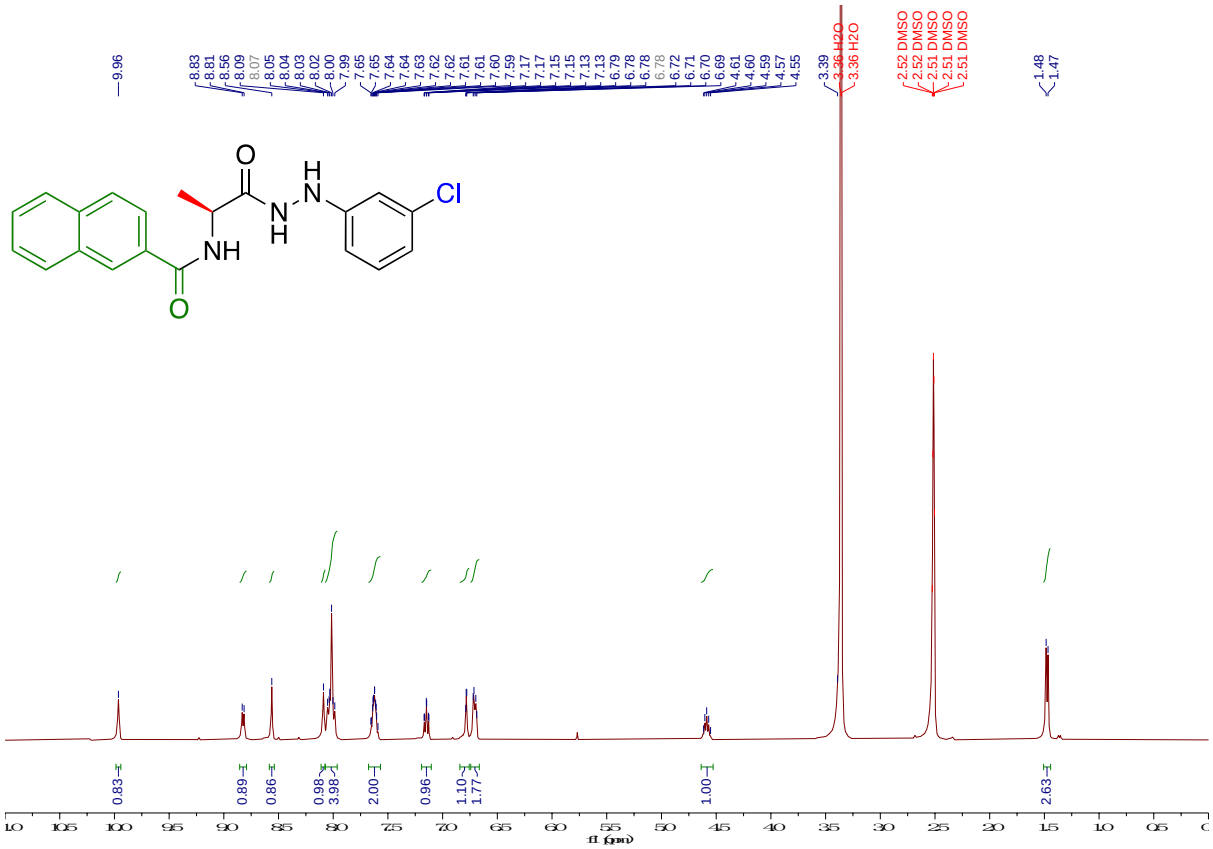
Compound 18

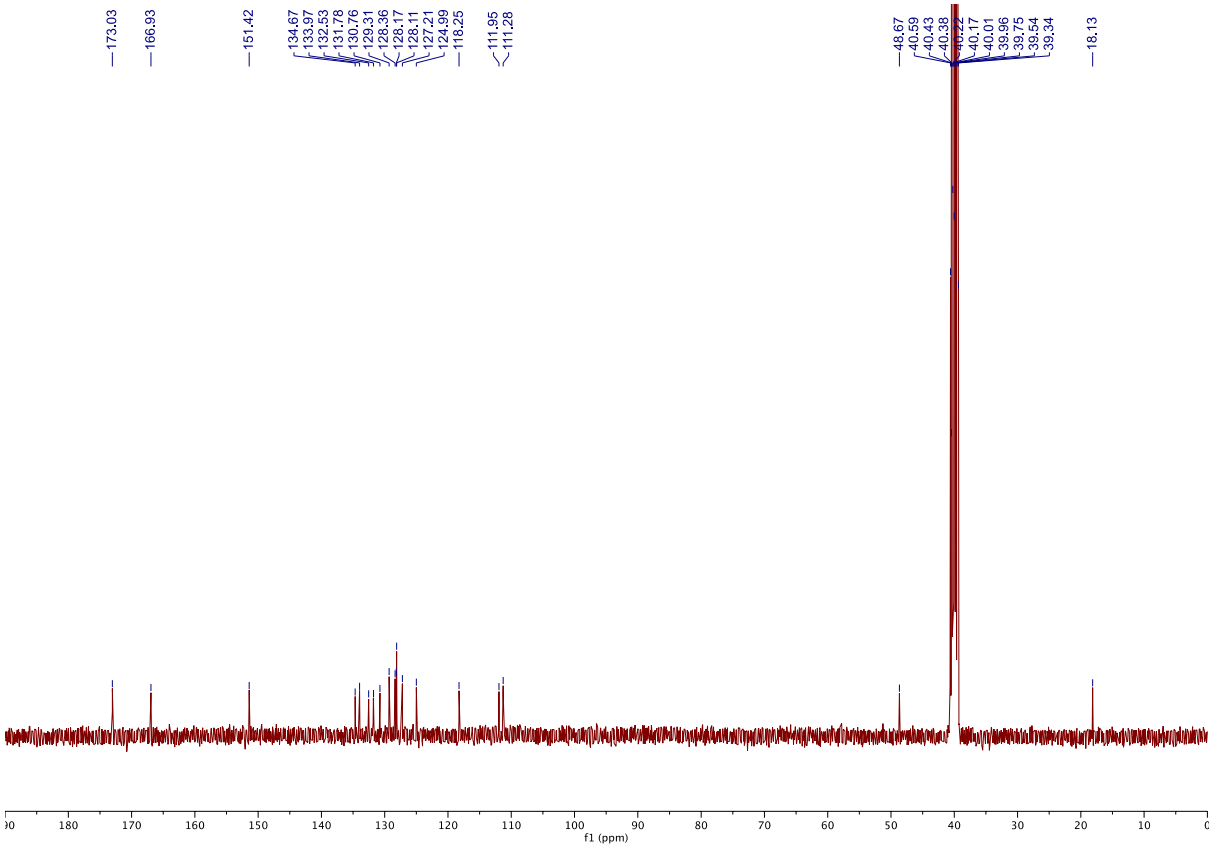

10.12
10.12
8.84
8.81
8.56
8.56
8.44
8.44
8.07
8.07
8.06
8.05
8.05
8.04
8.02
8.01
8.00
7.99
7.98
7.98
7.64
7.63
7.62
7.61
7.60
7.48
7.46
6.87
6.84
4.72
4.70
4.69
4.67
4.64
3.33 H2O
2.71
2.69
2.67
2.66
2.65
2.62
2.59
2.58
2.55
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.18
2.17
2.16
2.14
2.12
2.09
2.09
2.08
O
H
N
N
H
NH
O
CF3
0.86
0.88
0.92
0.99
0.54
3.65
2.67
1.88
0.32
1.86
1.00
2.38
0.40
0.91
3.15
0.37
0.17
f1 (ppm)
172.13
167.39
152.94
134.70
132.54
131.79
129.33
128.42
128.19
128.13
128.11
127.30
127.21
126.62
126.57
125.03
118.82
118.40
111.95
67.49
52.34
40.83
40.55
40.27
39.99
39.71
39.44
39.16
31.47
30.54
25.59
15.15
f1 (ppm)

Compound 19

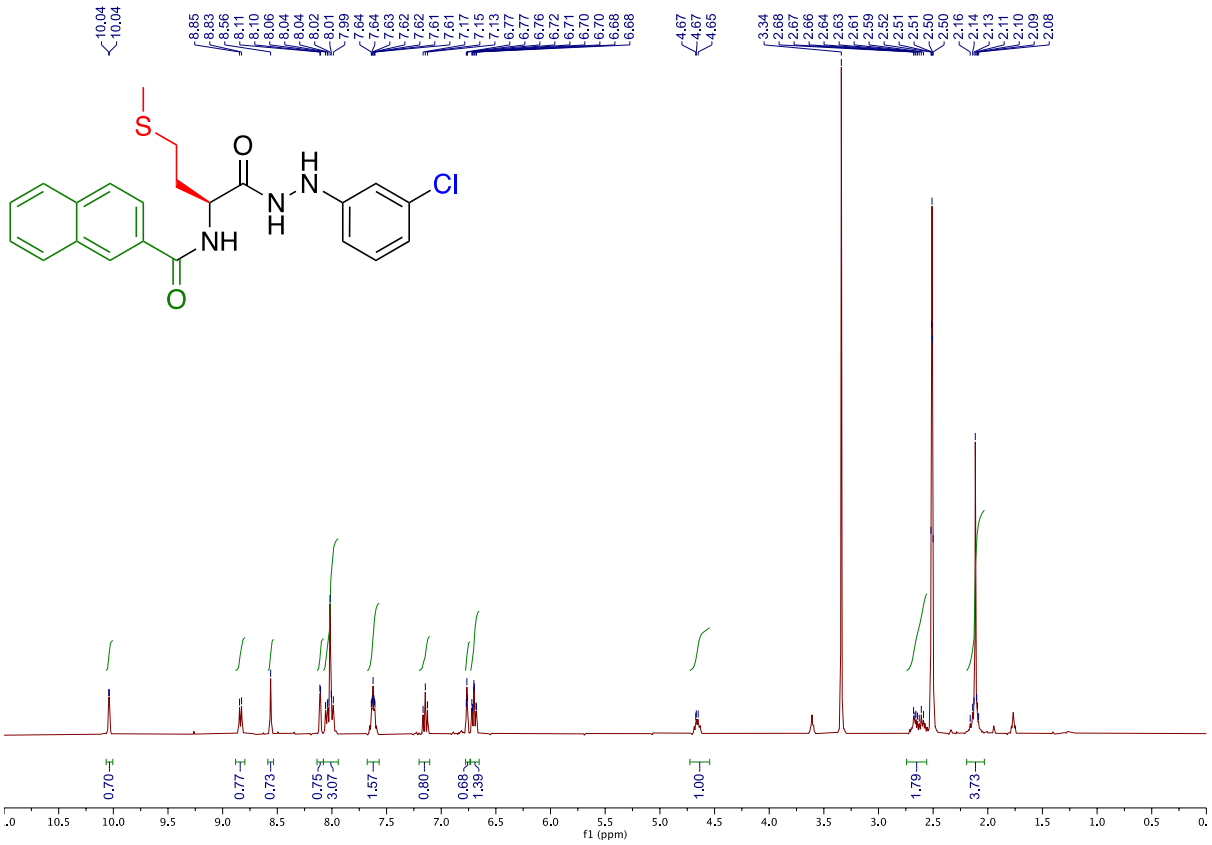

10.12
10.12
8.84
8.81
8.56
8.56
8.44
8.44
8.07
8.07
8.06
8.05
8.05
8.04
8.02
8.01
8.00
7.99
7.98
7.98
7.64
7.63
7.62
7.61
7.60
7.48
7.46
6.87
6.84
4.72
4.70
4.69
4.67
4.64
3.33 H2O
2.71
2.69
2.67
2.66
2.65
2.62
2.59
2.58
2.55
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.18
2.17
2.16
2.14
2.12
2.09
2.09
2.08
S
O
H
N
N
NH
O
CF3
0.86
0.88
0.92
0.99
0.54
3.65
2.67
1.88
0.32
1.86
1.00
2.38
0.40
0.91
3.15
0.37
0.17
f1 (ppm)
172.13
167.39
152.94
134.70
132.54
131.79
129.33
128.42
128.19
128.13
128.11
127.30
127.21
126.62
126.57
125.03
118.82
118.40
111.95
67.49
52.34
40.83
40.55
40.27
39.99
39.71
39.44
39.16
31.47
30.54
25.59
15.15
f1 (ppm)

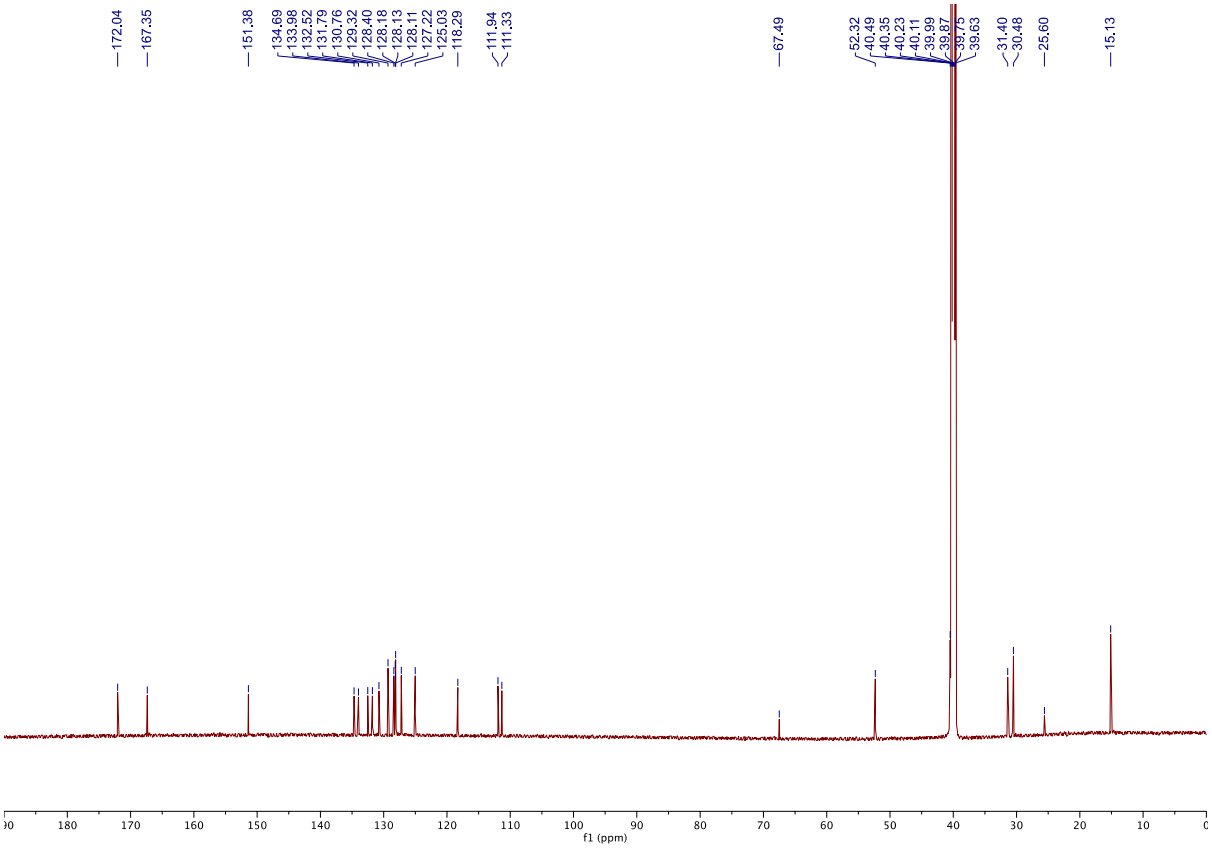
Compound 20


9.96
8.83
8.81
8.56
8.09
8.07
8.05
8.04
8.03
8.02
8.00
7.99
7.65
7.64
7.64
7.63
7.62
7.62
7.61
7.61
7.60
7.59
7.17
7.17
7.15
7.13
7.13
6.79
6.78
6.78
6.78
6.72
6.71
6.70
6.69
4.61
4.60
4.59
4.57
4.55
3.39
3.36 H2O
3.36 H2O
2.52 DMSO
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.51 DMSO
1.48
1.47
O
H
N
N
Cl
NH
O
0.83
0.89
0.86
0.98
3.98
2.00
0.96
1.10
1.77
1.00
2.63
f1 (ppm)

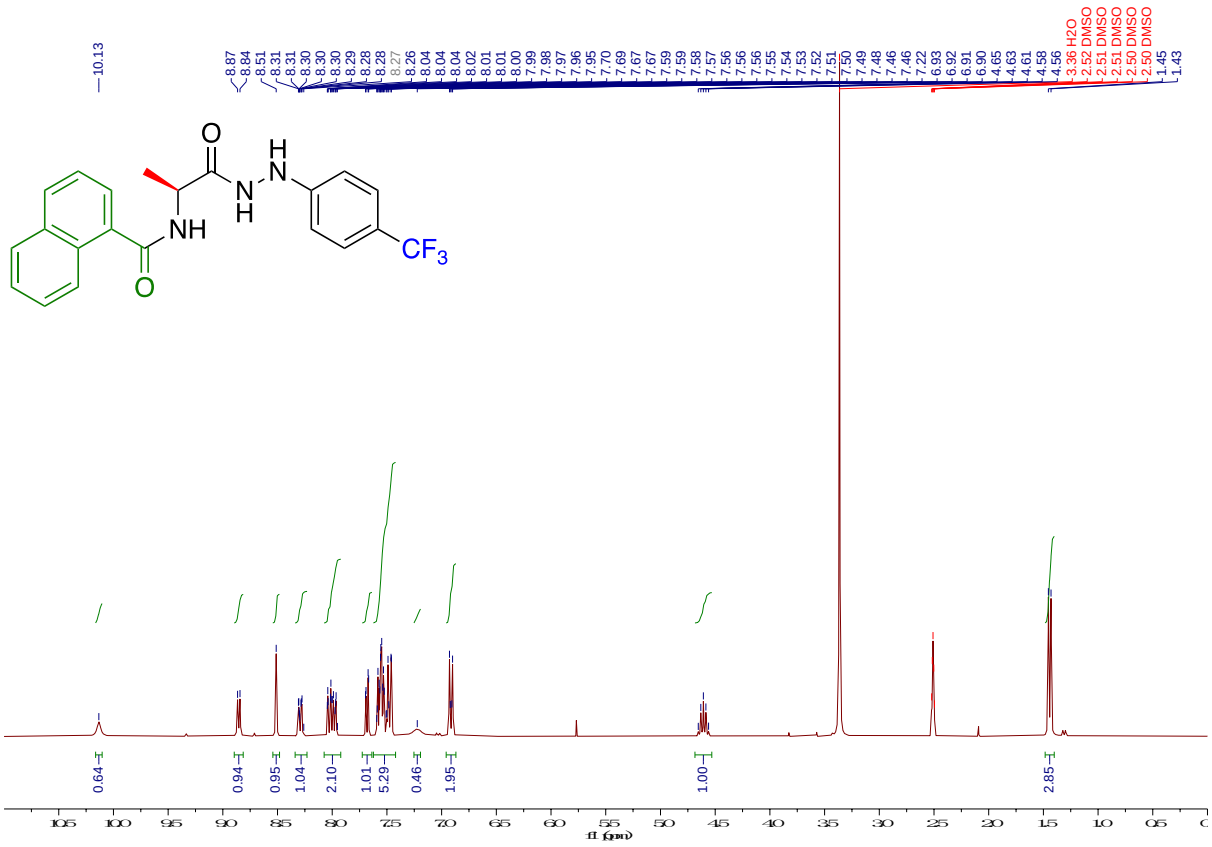

173.03
166.93
151.42
134.67
133.97
132.53
131.78
130.76
129.31
128.36
128.17
128.11
127.21
124.99
118.25
111.95
111.28
48.67
40.59
40.43
40.38
40.22
40.17
40.01
39.96
39.75
39.54
39.34
18.13
f1 (ppm)

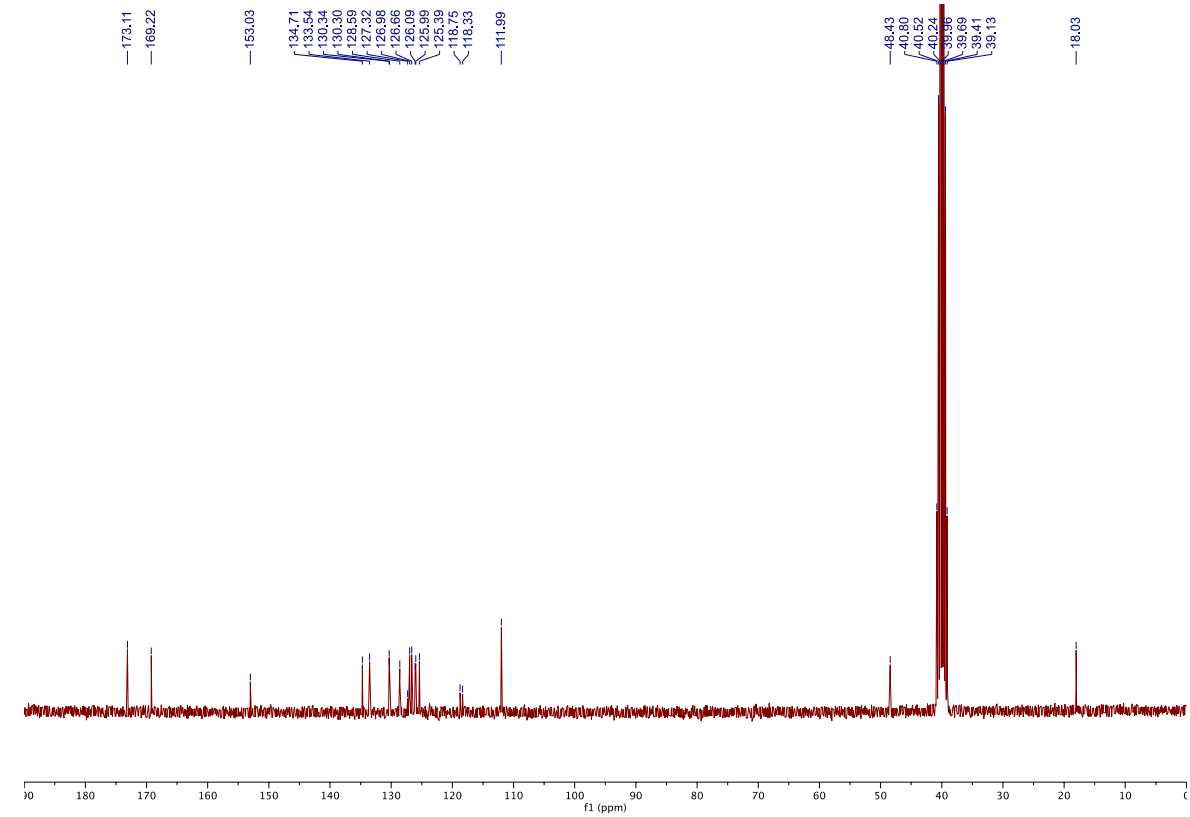
Compound 21


10.04
10.04
8.85
8.83
8.56
8.11
8.10
8.06
8.04
8.04
8.02
8.01
7.99
7.64
7.64
7.63
7.62
7.62
7.61
7.61
7.17
7.15
7.13
6.77
6.77
6.76
6.72
6.71
6.70
6.70
6.68
6.68
4.67
4.67
4.65
3.34
2.68
2.67
2.66
2.64
2.63
2.61
2.59
2.52
2.51
2.51
2.50
2.50
2.16
2.14
2.13
2.11
2.10
2.09
2.08
S
O
H
N
N
Cl
NH
O
0.70
0.77
0.73
0.75
3.07
1.57
0.80
0.68
1.39
1.00
1.79
3.73
f1 (ppm)

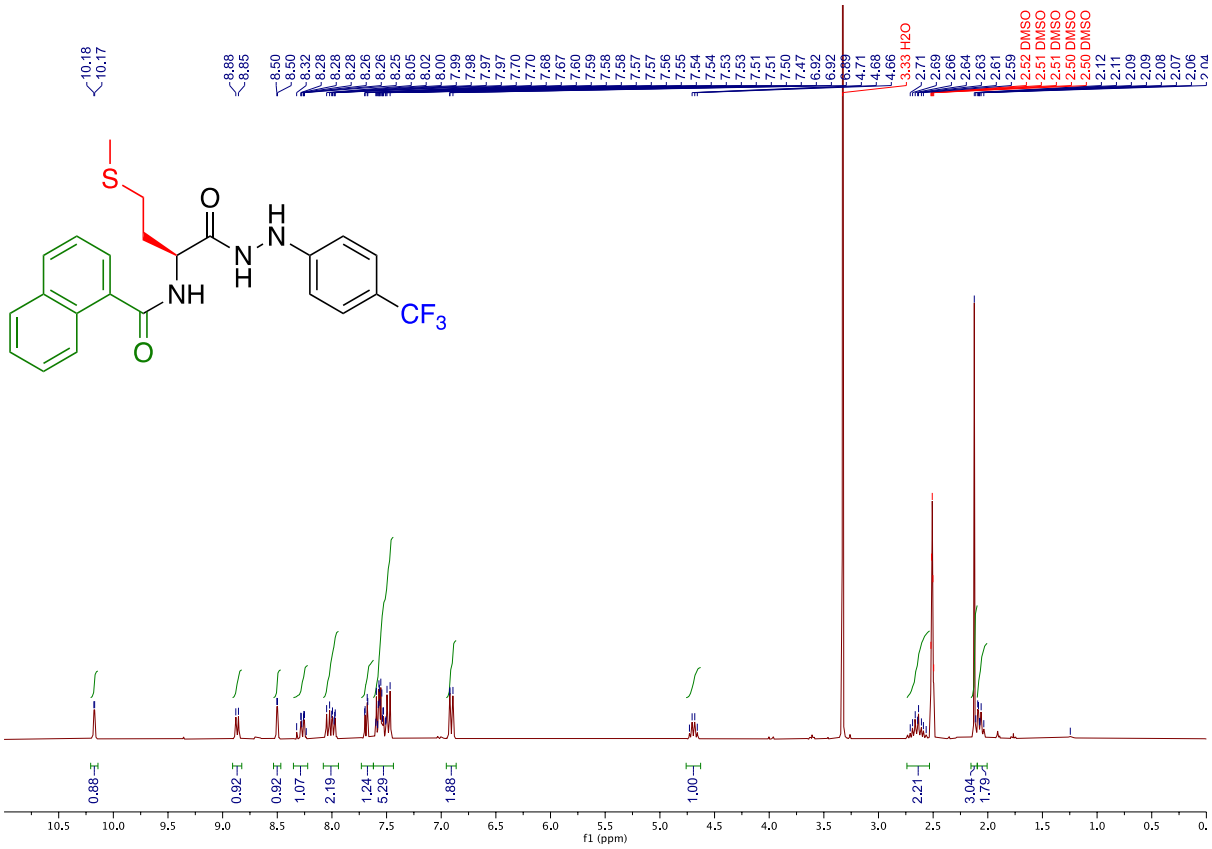

172.04
167.35
151.38
134.69
133.98
132.52
131.79
130.76
129.32
128.40
128.18
128.13
128.11
127.22
125.03
118.29
111.94
111.33
67.49
52.32
40.49
40.35
40.23
40.11
39.99
39.87
39.75
39.63
31.40
30.48
25.60
15.13
f1 (ppm)

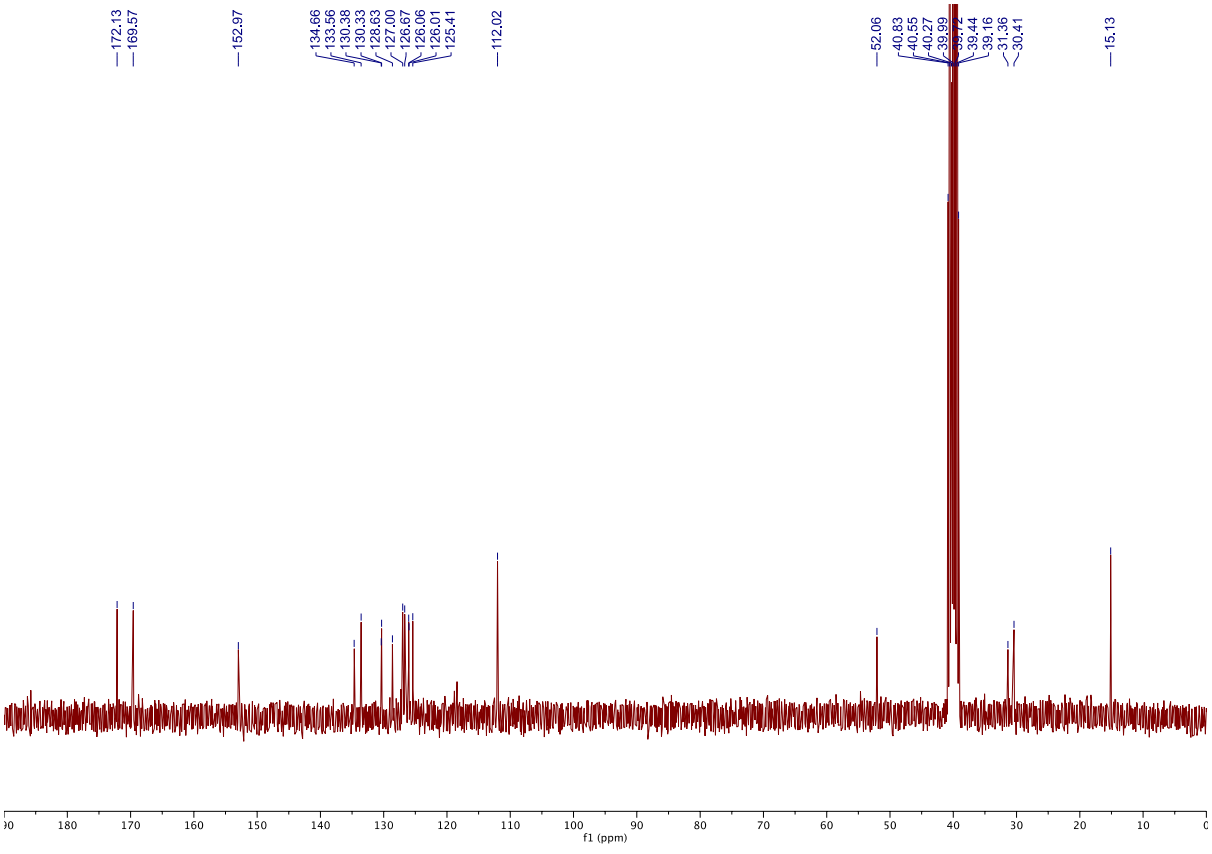
Compound 22


10.13
8.87
8.84
8.51
8.31
8.30
8.30
8.29
8.28
8.28
8.27
8.26
8.04
8.04
8.04
8.02
8.01
8.01
8.00
7.99
7.98
7.97
7.96
7.95
7.70
7.69
7.67
7.67
7.59
7.59
7.58
7.57
7.56
7.56
7.56
7.55
7.54
7.53
7.52
7.51
7.50
7.49
7.48
7.46
7.46
7.22
6.93
6.92
6.91
6.90
4.65
4.63
4.61
4.58
4.56
3.36 H2O
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
1.45
1.43
O
H
N
N
H
NH
O
CF3
0.64
0.94
0.95
1.04
2.10
1.01
5.29
0.46
1.95
1.00
2.85
f1 (ppm)

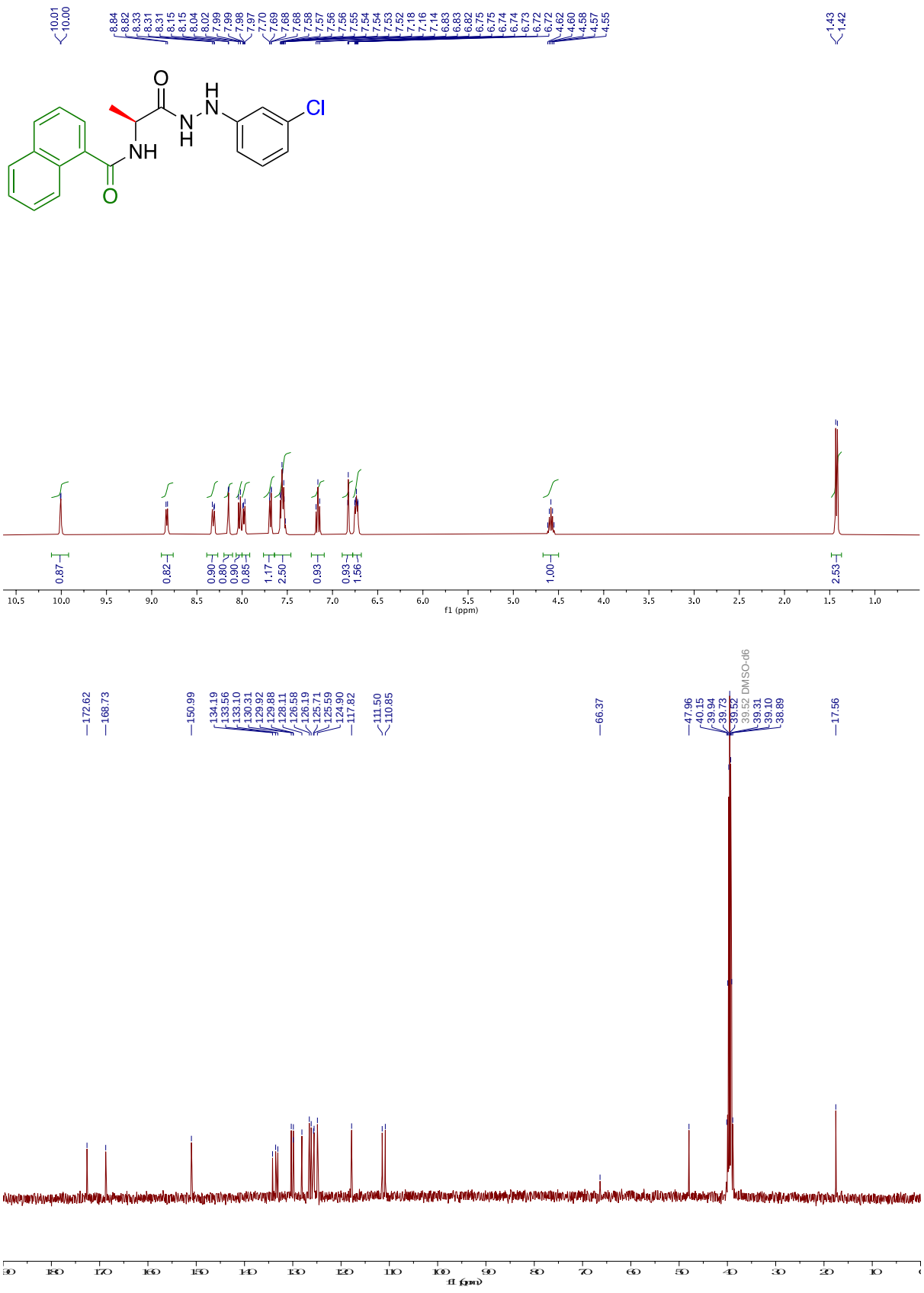

173.11
169.22
153.03
134.71
133.54
130.34
130.30
128.59
127.32
126.98
126.66
126.09
125.99
125.39
118.75
118.33
111.99
48.43
40.80
40.52
40.24
39.96
39.69
39.41
39.13
18.03
f1 (ppm)

Compound 23

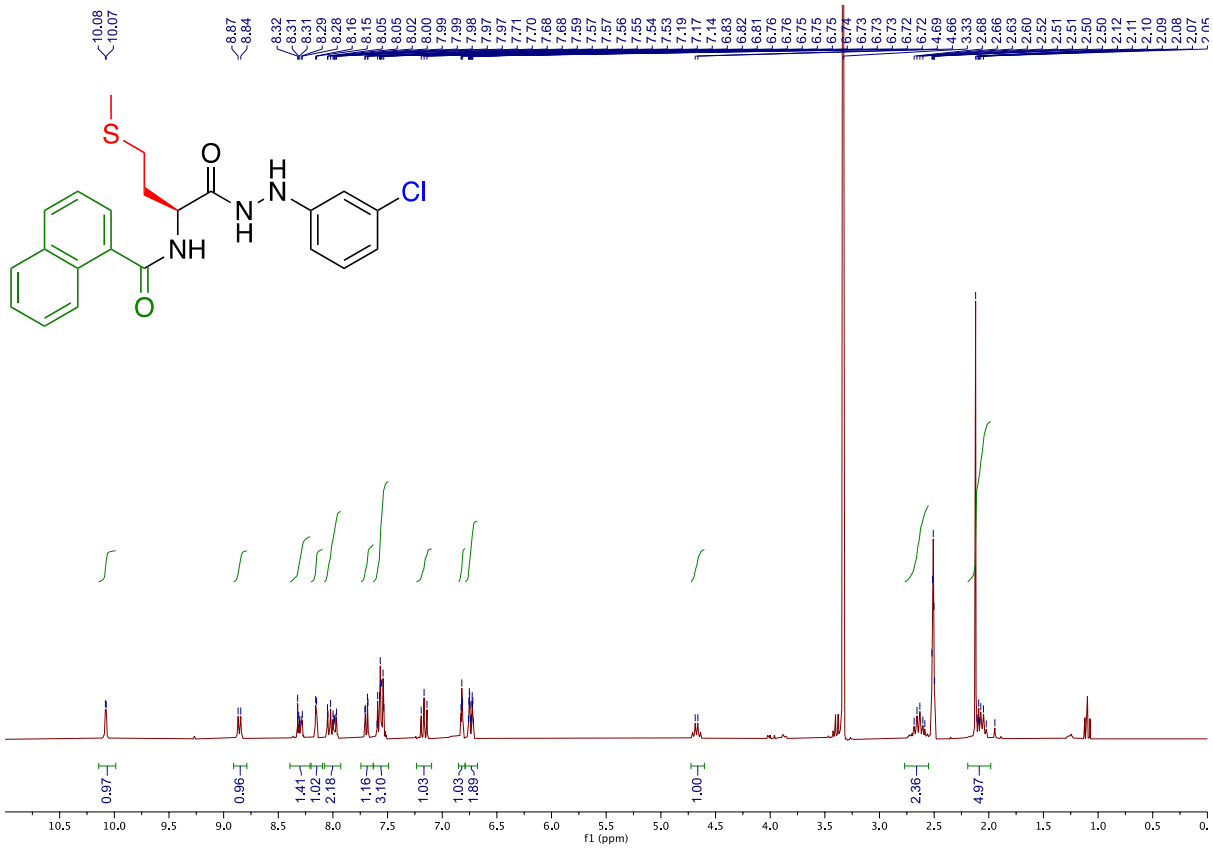

10.18
10.17
8.88
8.85
8.50
8.50
8.32
8.28
8.28
8.28
8.26
8.26
8.25
8.05
8.02
8.00
7.99
7.98
7.97
7.97
7.70
7.70
7.68
7.67
7.60
7.59
7.58
7.58
7.57
7.57
7.56
7.55
7.54
7.54
7.53
7.51
7.51
7.50
7.47
6.92
6.92
6.88
4.71
4.68
4.66
3.33 H2O
2.71
2.69
2.66
2.64
2.63
2.61
2.59
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.12
2.11
2.09
2.09
2.08
2.07
2.06
S
O
H
N
N
H
NH
O
CF3
0.88
0.92
0.92
1.07
2.19
1.24
5.29
1.88
1.00
2.21
3.04
1.79
f1 (ppm)

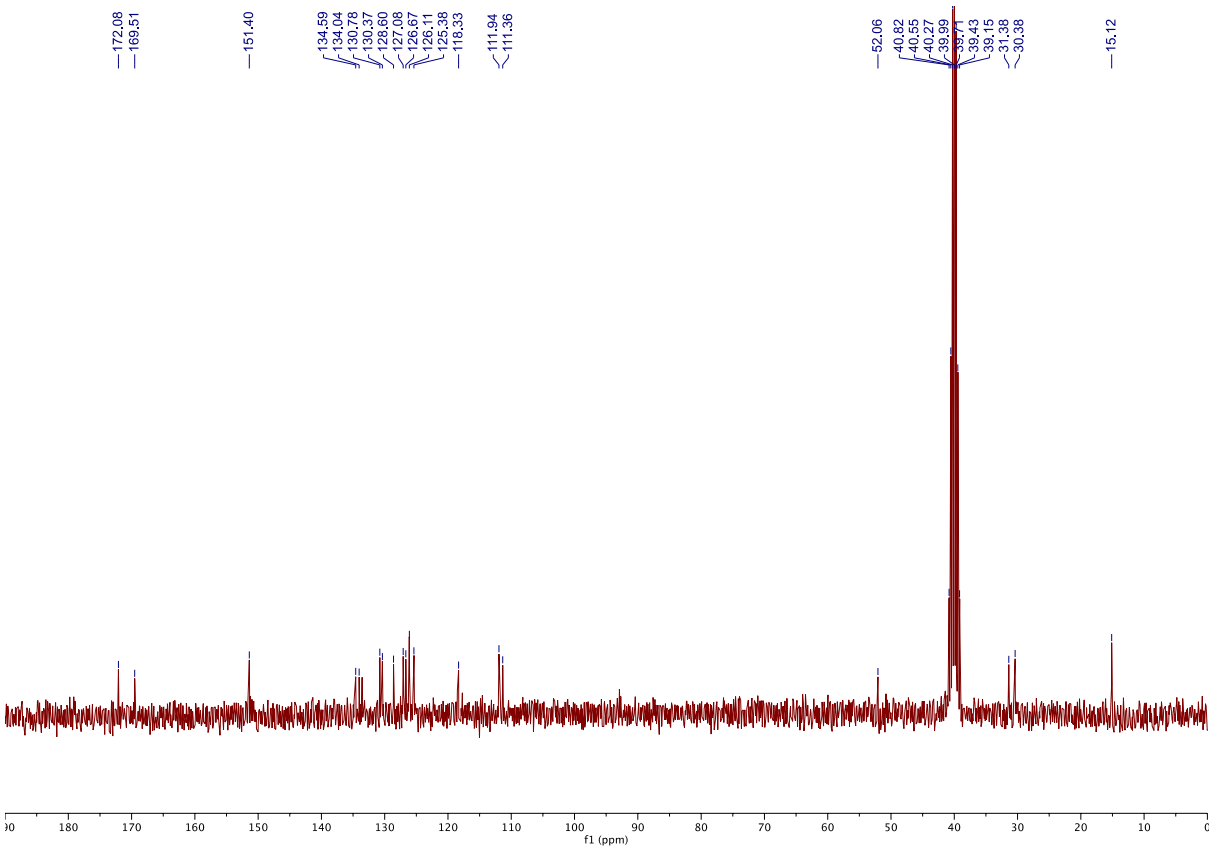

172.13
169.57
152.97
134.66
133.56
130.38
130.33
128.63
127.00
126.67
126.06
126.01
125.41
112.02
52.06
40.83
40.55
40.27
39.99
39.72
39.44
39.16
31.36
30.41
15.13
f1 (ppm)

Compound 24

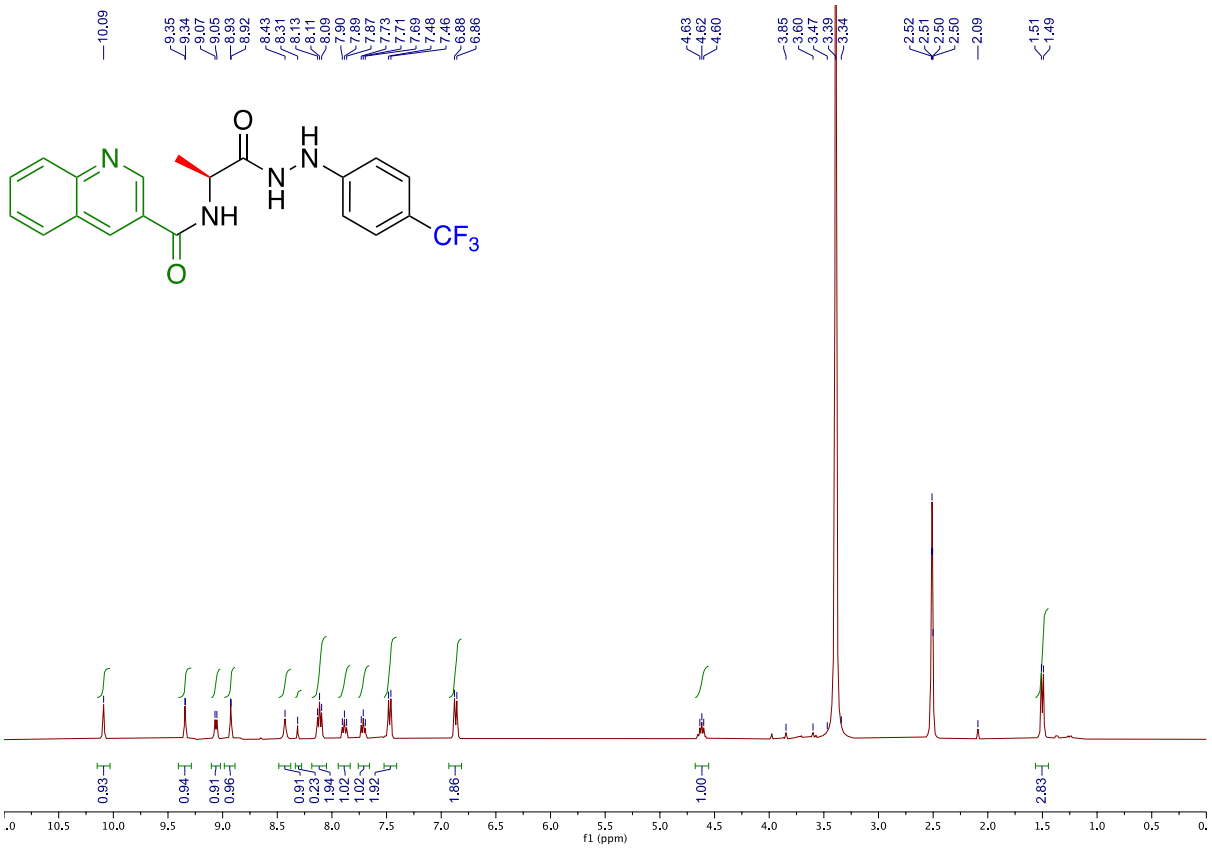

10.01
10.00
8.84
8.82
8.33
8.31
8.31
8.15
8.15
8.04
8.02
7.99
7.99
7.98
7.97
7.70
7.69
7.68
7.68
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.53
7.52
7.18
7.16
7.14
6.83
6.83
6.82
6.75
6.75
6.74
6.74
6.73
6.72
6.72
4.62
4.60
4.58
4.57
4.55
1.43
1.42
O
H
N
N
H
Cl
NH
O
0.87
0.82
0.90
0.80
0.90
0.85
1.17
2.50
0.93
0.93
1.56
1.00
2.53
f1 (ppm)
172.62
168.73
150.99
134.19
133.56
133.10
130.31
129.92
129.88
128.11
126.58
126.19
125.71
125.59
124.90
117.82
111.50
110.85
66.37
47.96
40.15
39.94
39.73
39.52
39.52 DMSO-d6
39.31
39.10
38.89
17.56

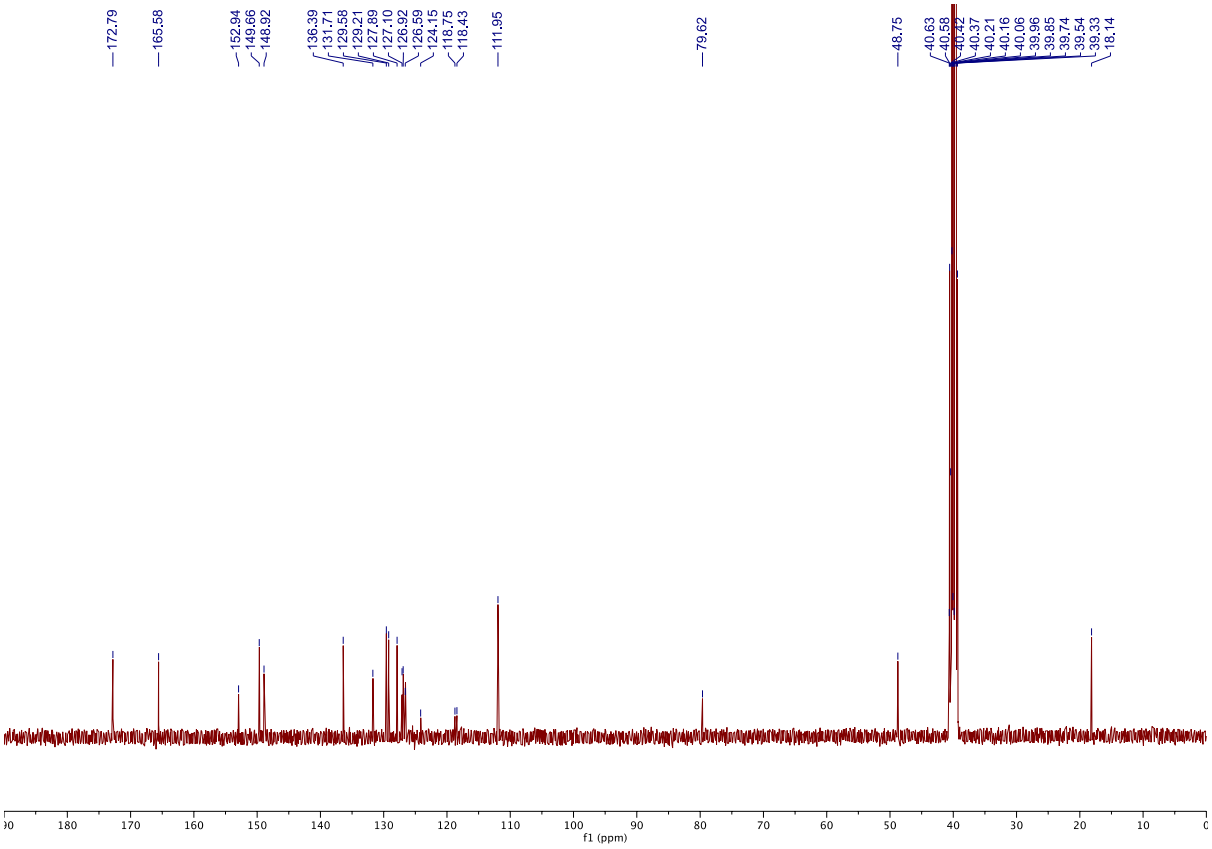
Compound 25



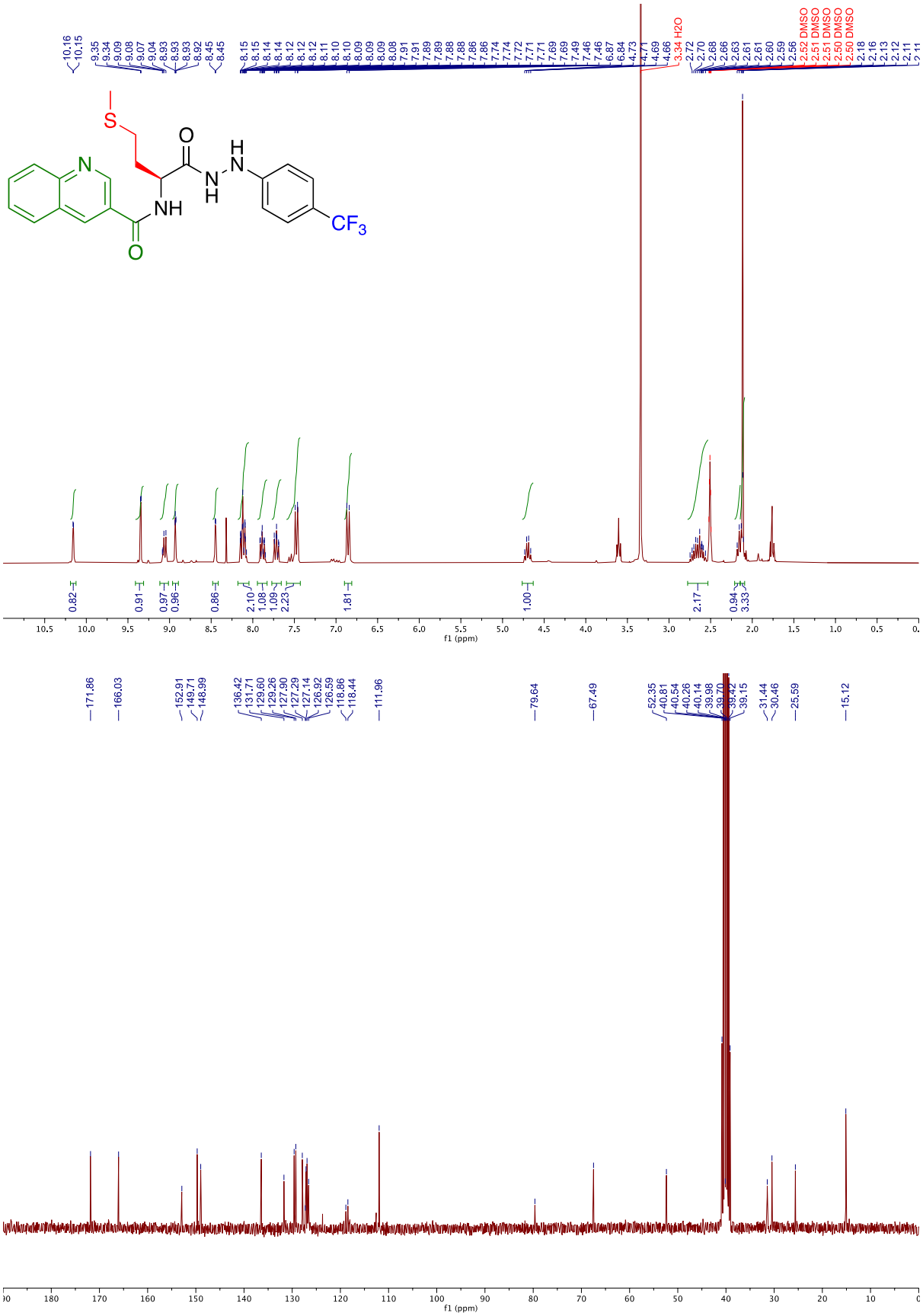


Compound 26

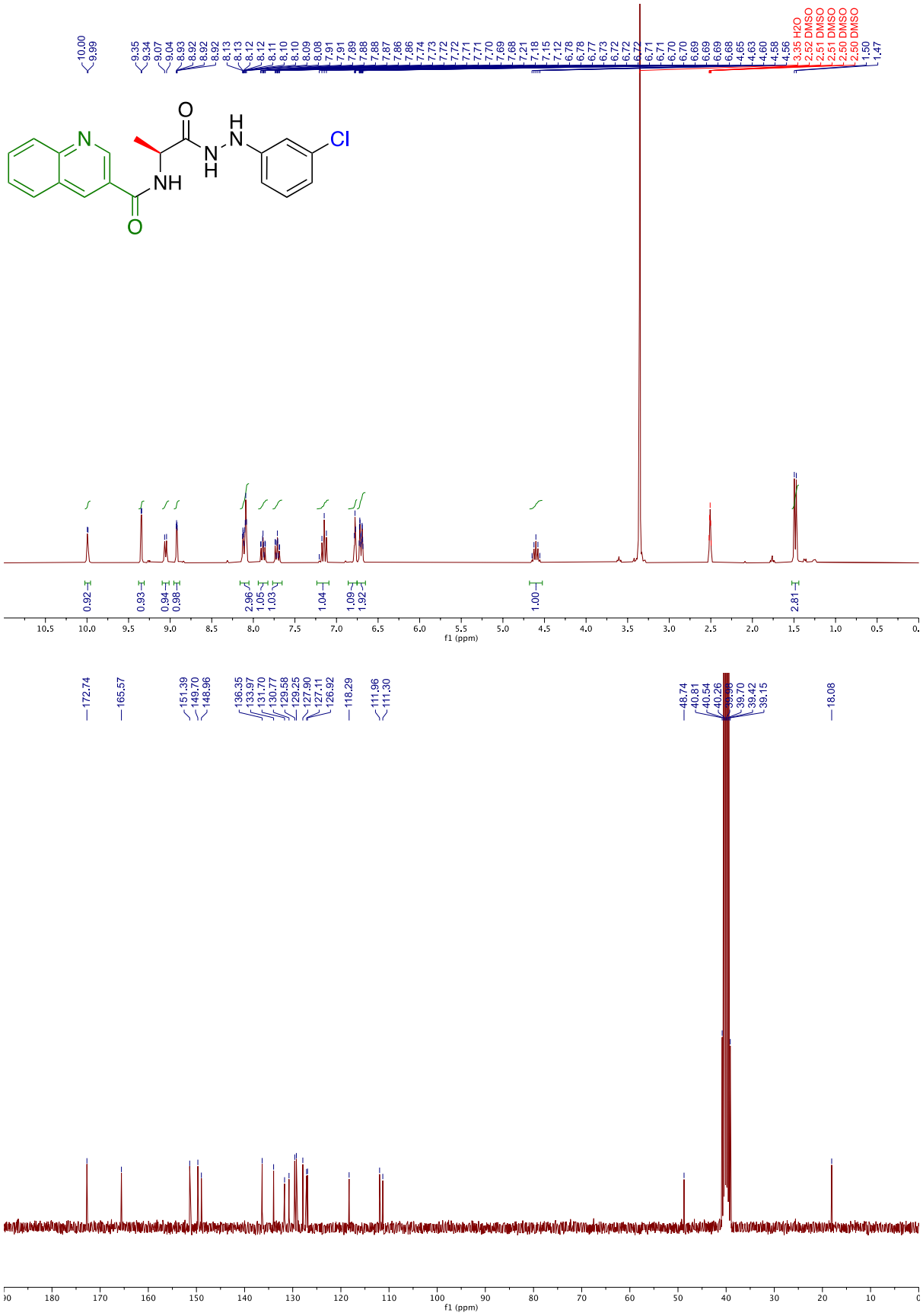

10.09
9.35
9.34
9.07
9.05
8.93
8.92
8.43
8.31
8.13
8.11
8.09
7.90
7.89
7.87
7.73
7.71
7.69
7.48
7.46
6.88
6.86
4.63
4.62
4.60
3.85
3.60
3.47
3.39
3.34
2.52
2.51
2.50
2.50
2.09
1.51
1.49
0.93
0.94
0.91
0.96
0.91
0.23
1.94
1.02
1.92
1.86
1.00
2.83
f1 (ppm)


172.79
165.58
152.94
149.66
148.92
136.39
131.71
129.58
129.21
127.89
127.10
126.92
126.59
124.15
118.75
118.43
111.95
79.62
48.75
40.63
40.58
40.42
40.37
40.21
40.16
40.06
39.96
39.85
39.74
39.54
39.33
18.14
f1 (ppm)

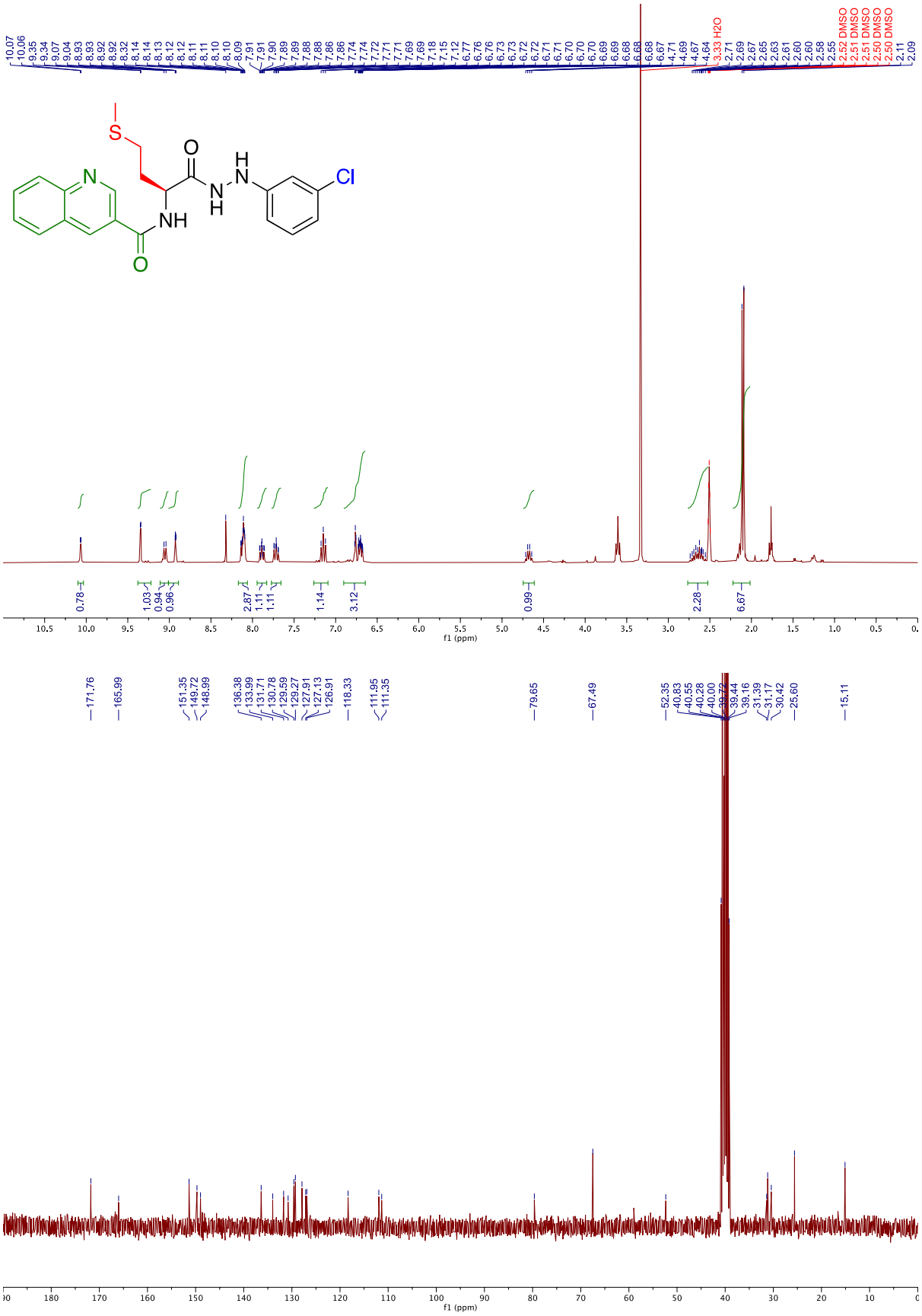
Compound 27


10.16
10.15
9.35
9.34
9.09
9.08
9.07
9.04
8.93
8.93
8.93
8.92
8.45
8.45
8.15
8.15
8.14
8.14
8.12
8.12
8.12
8.11
8.10
8.10
8.09
8.09
8.09
8.08
7.91
7.91
7.89
7.89
7.88
7.88
7.86
7.86
7.74
7.74
7.72
7.71
7.71
7.69
7.69
7.49
7.46
7.46
6.87
6.84
4.73
4.71
4.69
4.66
3.34 H2O
2.72
2.70
2.68
2.66
2.63
2.61
2.61
2.60
2.59
2.56
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.18
2.16
2.13
2.12
2.11
S
O
N
H
N
N
H
NH
O
CF3
0.82
0.91
0.97
0.96
0.86
2.10
1.08
1.09
2.23
1.81
1.00
2.17
0.94
3.33
f1 (ppm)
171.86
166.03
152.91
149.71
148.99
136.42
131.71
129.60
129.26
127.90
127.29
127.14
126.92
126.59
118.86
118.44
111.96
79.64
67.49
52.35
40.81
40.54
40.26
40.14
39.98
39.70
39.42
39.15
31.44
30.46
25.59
15.12
f1 (ppm)

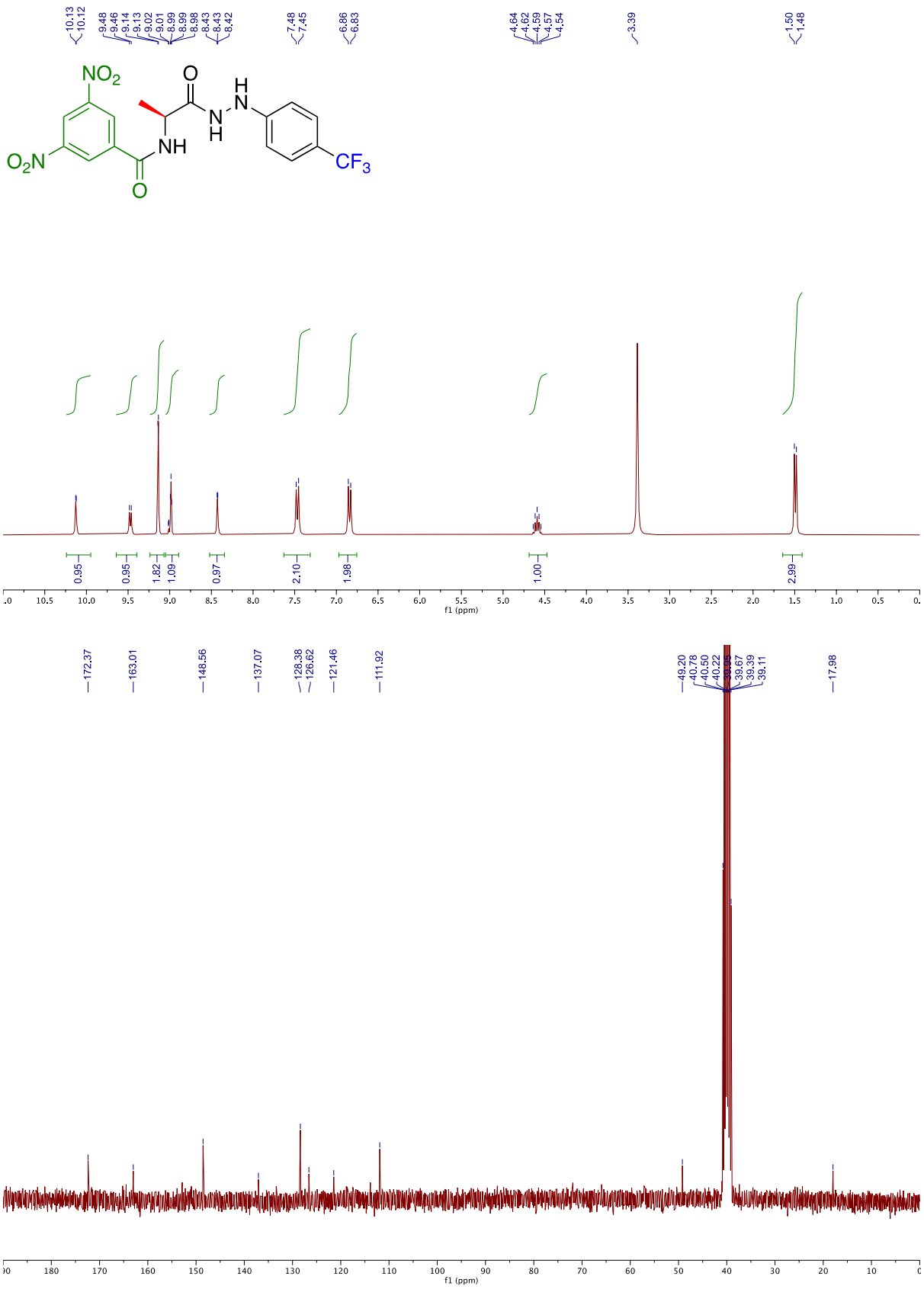
Compound 28


10.00
9.99
9.35
9.34
9.07
9.04
8.93
8.92
8.92
8.92
8.13
8.13
8.12
8.12
8.11
8.10
8.10
8.09
8.08
7.91
7.91
7.89
7.88
7.88
7.87
7.86
7.86
7.74
7.73
7.72
7.72
7.71
7.71
7.70
7.69
7.68
7.21
7.18
7.15
7.12
6.78
6.78
6.77
6.73
6.72
6.72
6.72
6.71
6.71
6.70
6.70
6.69
6.69
6.69
6.68
4.65
4.63
4.60
4.58
4.56
3.35 H2O
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
1.50
1.47
O
H
N
N
N
Cl
NH
O
0.92
0.93
0.94
0.98
2.96
1.05
1.03
1.04
1.09
1.92
1.00
2.81
f1 (ppm)
172.74
165.57
151.39
149.70
148.96
136.35
133.97
131.70
130.77
129.58
129.25
127.90
127.11
126.92
118.29
111.96
111.30
48.74
40.81
40.54
40.26
39.98
39.70
39.42
39.15
18.08
f1 (ppm)

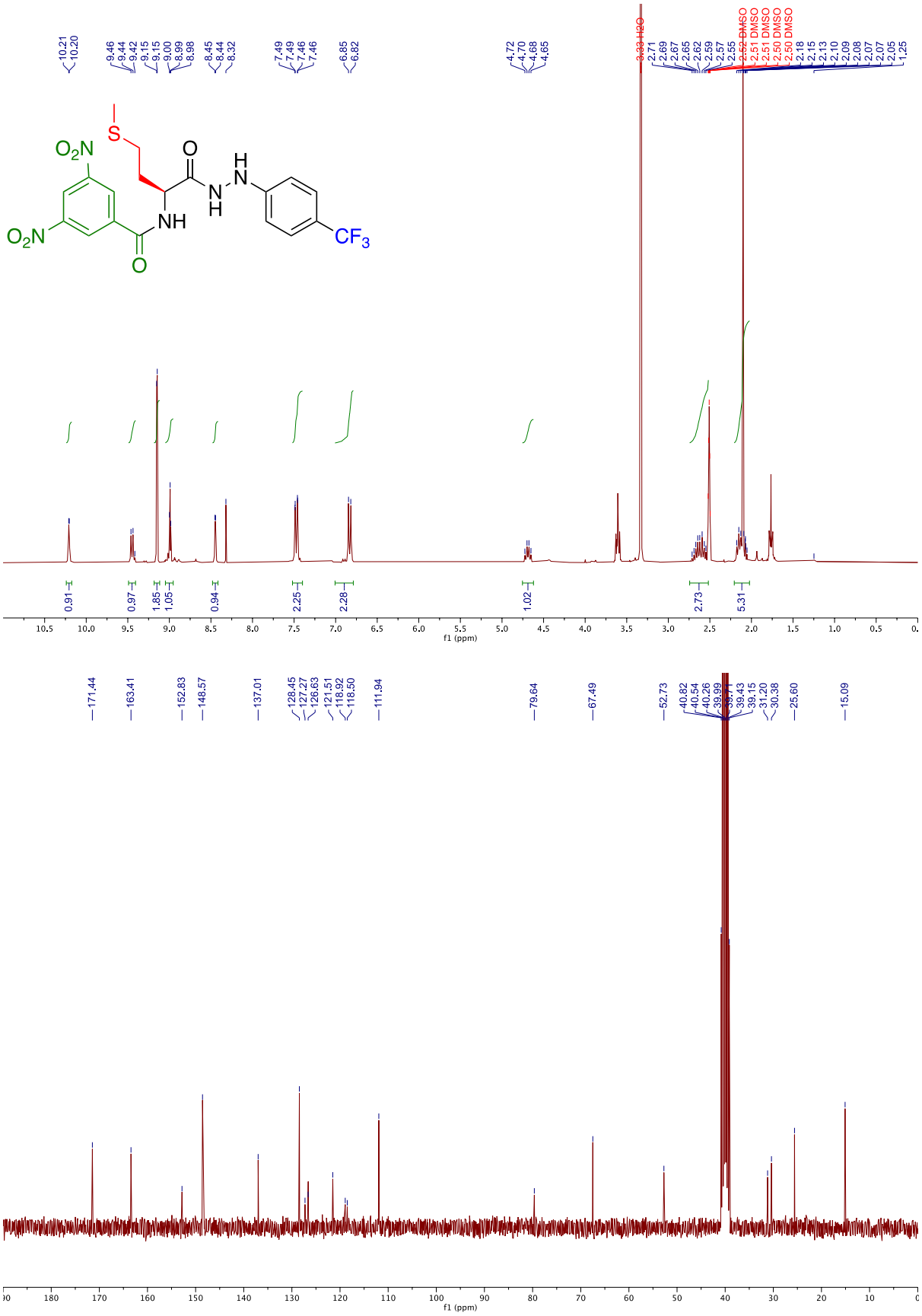
Compound 29


10.07 10.06 9.35 9.34 9.07 9.04 8.93 8.93 8.92 8.92 8.32 8.14 8.14 8.13 8.12 8.12 8.11 8.11 8.10 8.10 8.09 7.91 7.91 7.90 7.89 7.89 7.88 7.88 7.86 7.86 7.74 7.74 7.72 7.71 7.71 7.69 7.69 7.18 7.15 7.12 6.77 6.76 6.76 6.73 6.73 6.72 6.72 6.71 6.71 6.70 6.70 6.69 6.69 6.68 6.68 6.68 6.67 4.71 4.69 4.67 4.64 3.33 H2O 2.71 2.69 2.67 2.65 2.63 2.61 2.60 2.60 2.58 2.55 2.52 DMSO 2.51 DMSO 2.51 DMSO 2.50 DMSO 2.50 DMSO 2.11 2.09
S
O
H
N
N
N
H
Cl
NH
O
0.78 1.03 0.94 0.96 2.87 1.11 1.11 1.14 3.12 0.99 2.28 6.67
f1 (ppm)
171.76 165.99 151.35 149.72 148.99 136.38 133.99 131.71 130.78 129.59 129.27 127.91 127.13 126.91 118.33 111.95 111.35 79.65 67.49 52.35 40.83 40.55 40.28 40.00 39.72 39.44 39.16 31.39 31.17 30.42 25.60 15.11
f1 (ppm)

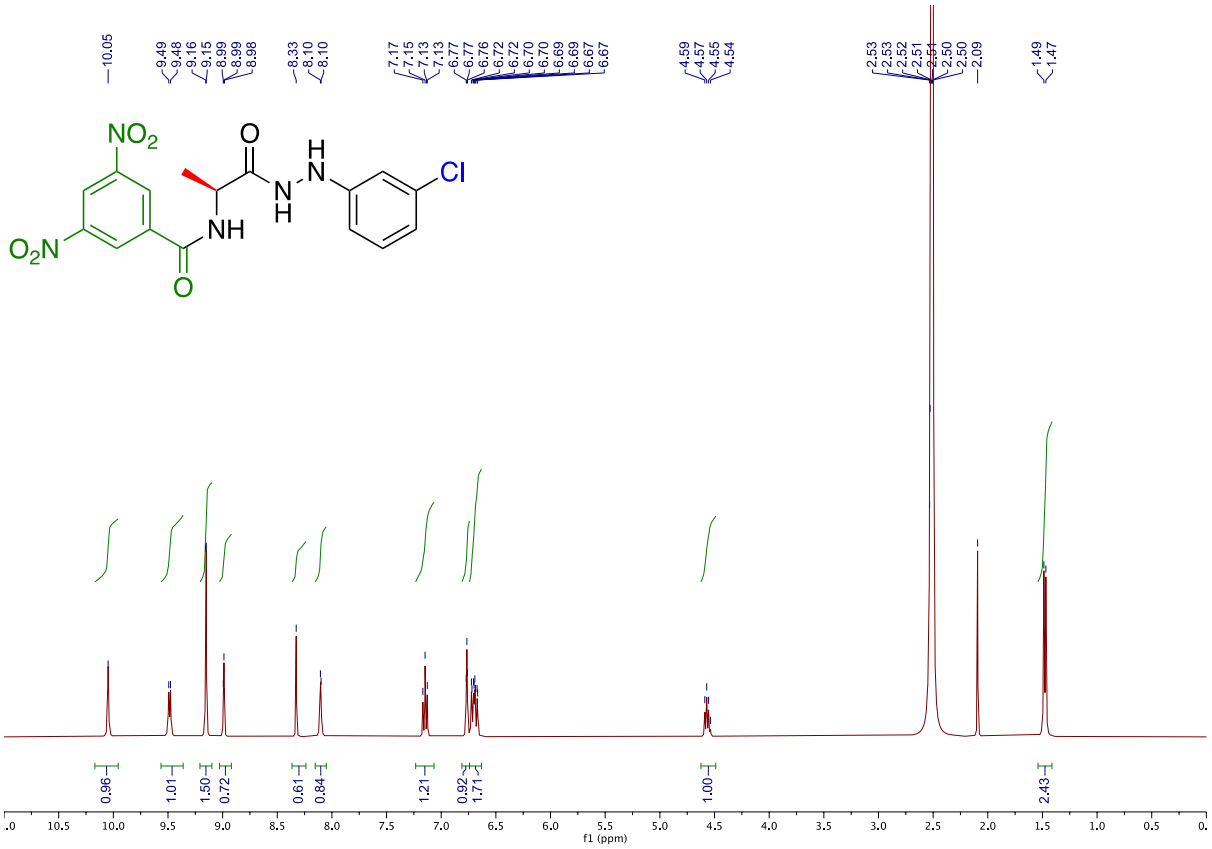
Compound 30

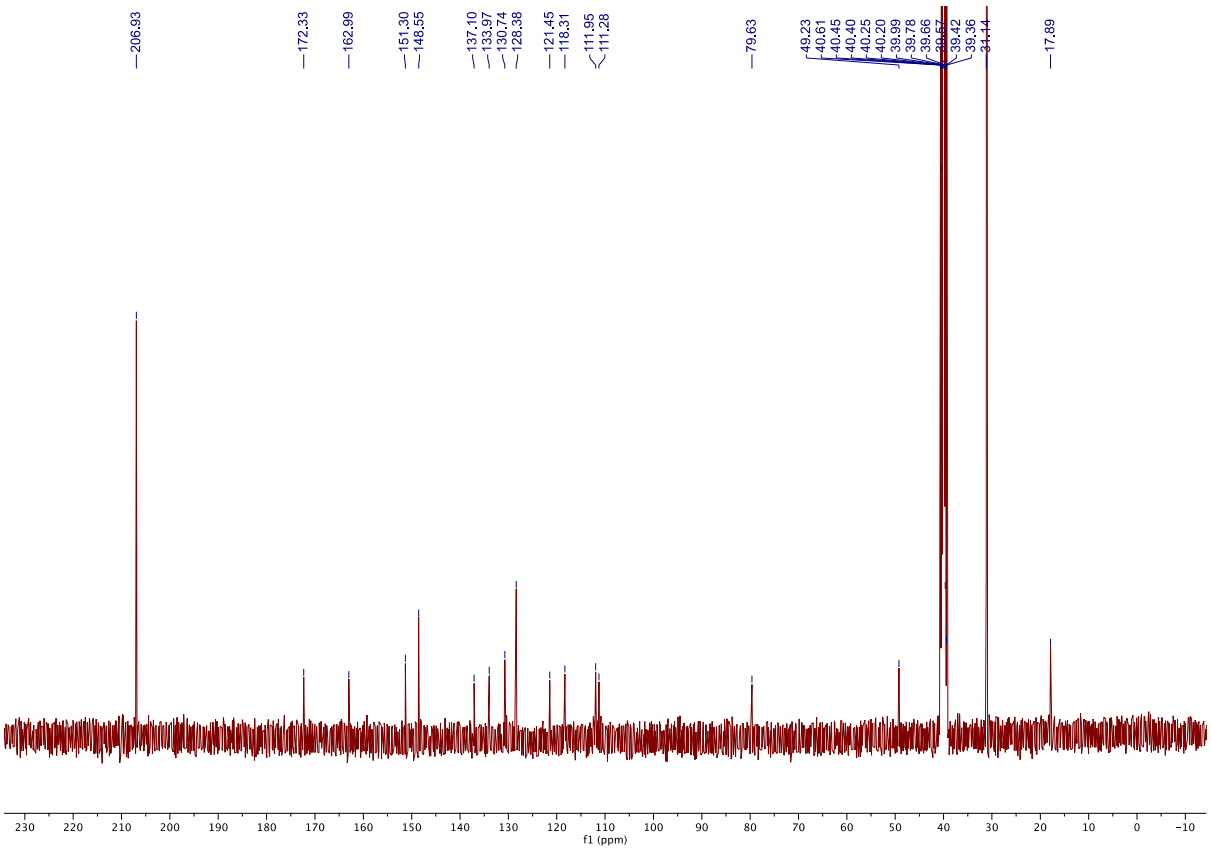

10.13
10.12
9.48
9.46
9.14
9.13
9.02
9.01
8.99
8.99
8.98
8.43
8.43
8.42
7.48
7.45
6.86
6.83
4.64
4.62
4.59
4.57
4.54
3.39
1.50
1.48
NO2
O2N
O
NH
O
N
H
N
H
CF3
0.95
0.95
1.82
1.09
0.97
2.10
1.98
1.00
2.99
f1 (ppm)
172.37
163.01
148.56
137.07
128.38
126.62
121.46
111.92
49.20
40.78
40.50
40.22
39.67
39.39
39.11
17.98
f1 (ppm)

Compound 31

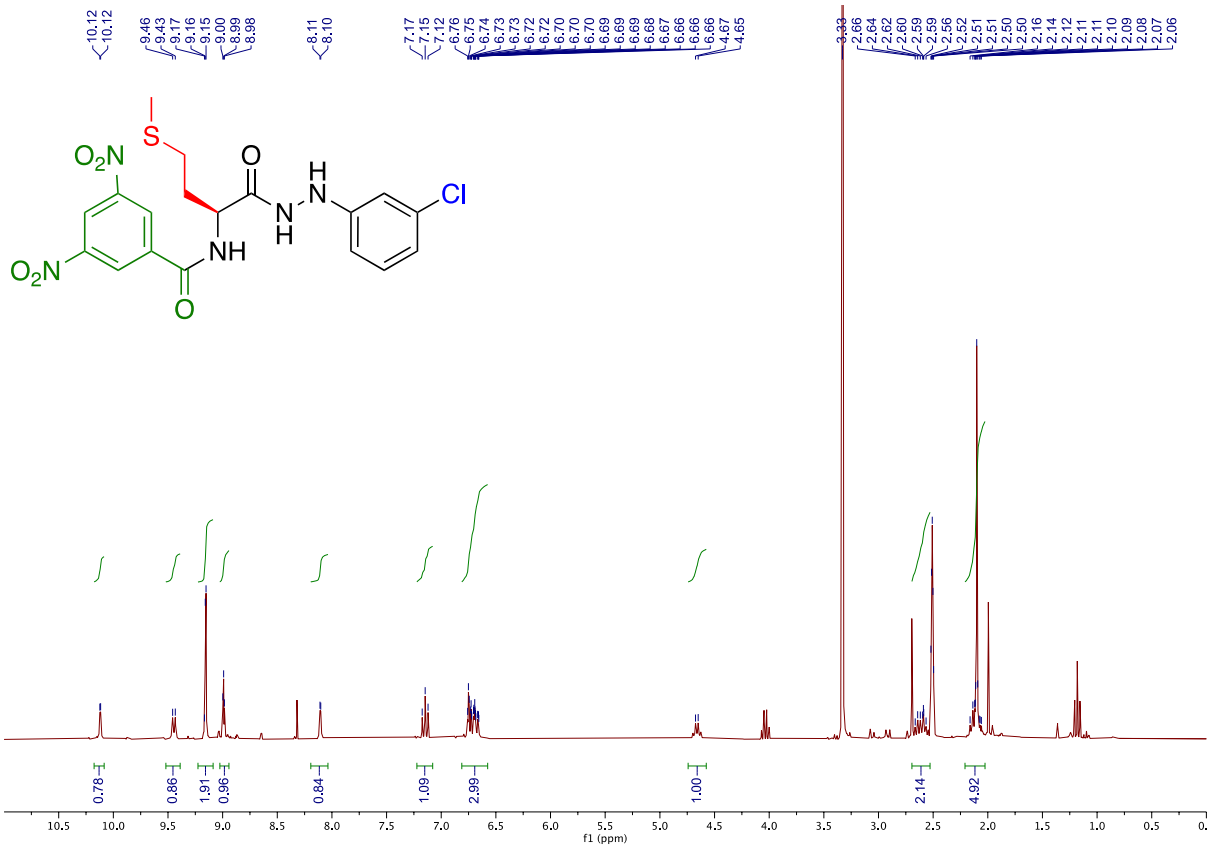

10.21
10.20
9.46
9.44
9.42
9.15
9.00
8.99
8.98
8.45
8.44
8.32
7.49
7.49
7.46
7.46
6.85
6.82
4.72
4.70
4.68
4.65
3.33 H2O
2.71
2.69
2.67
2.65
2.62
2.59
2.57
2.55
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.18
2.15
2.13
2.10
2.09
2.08
2.07
2.07
2.05
1.25
O2N
S
O
H
N
N
NH
O2N
O
CF3
0.91
0.97
1.85
1.05
0.94
2.25
2.28
1.02
2.73
5.31
f1 (ppm)
171.44
163.41
152.83
148.57
137.01
128.45
127.27
126.63
121.51
118.92
118.50
111.94
79.64
67.49
52.73
40.82
40.54
40.26
39.99
39.71
39.43
39.15
31.20
30.38
25.60
15.09
f1 (ppm)

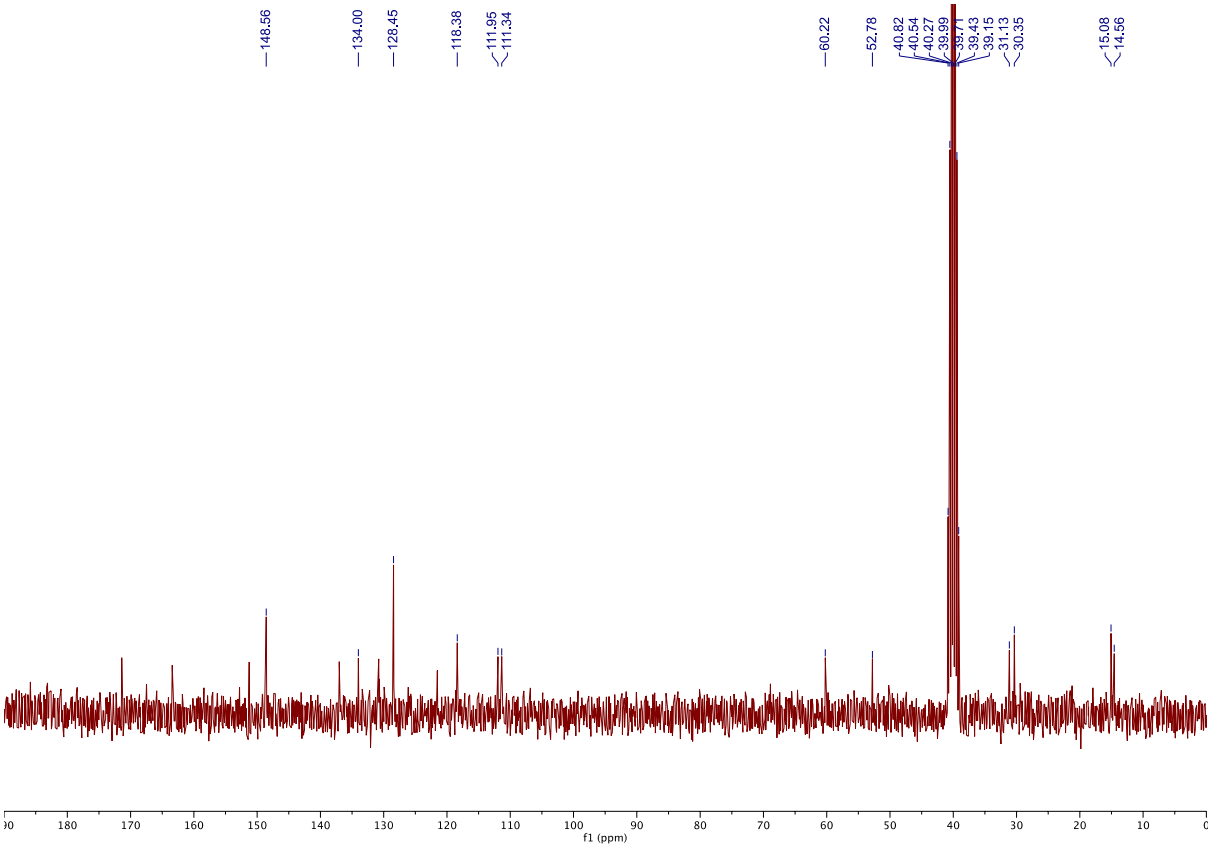
Compound 32


10.05
9.49
9.48
9.16
9.15
8.99
8.99
8.98
8.33
8.10
8.10
7.17
7.15
7.13
7.13
6.77
6.77
6.76
6.72
6.72
6.70
6.70
6.69
6.69
6.67
6.67
4.59
4.57
4.55
4.54
2.53
2.53
2.52
2.51
2.50
2.50
2.09
1.49
1.47
NO2
O2N
O
NH
N
H
H
N
Cl
O
0.96
1.01
1.50
0.72
0.61
0.84
1.21
0.92
1.71
1.00
2.43
f1 (ppm)

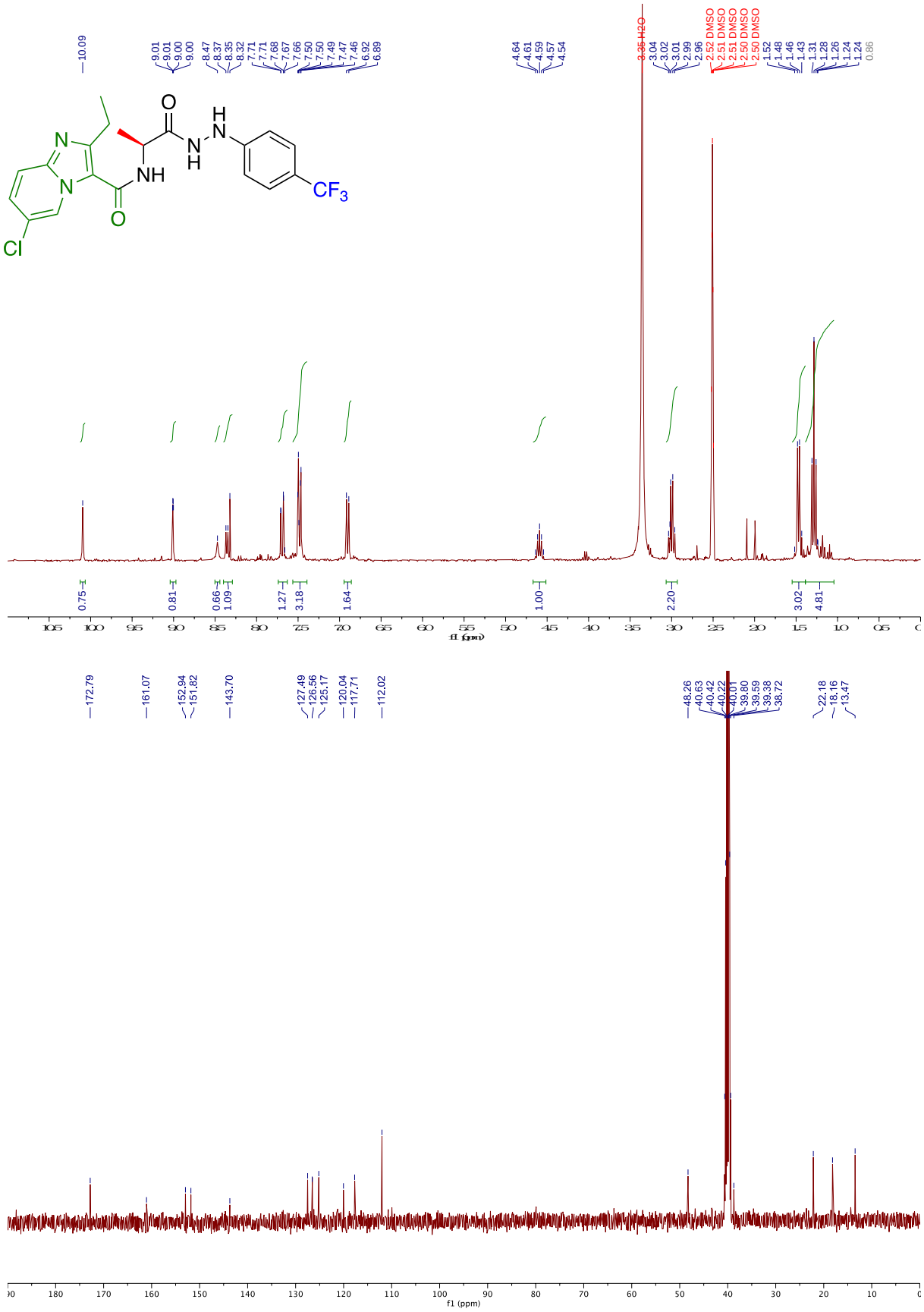

206.93
172.33
162.99
151.30
148.55
137.10
133.97
130.74
128.38
121.45
118.31
111.95
111.28
79.63
49.23
40.61
40.45
40.40
40.25
40.20
39.99
39.78
39.66
39.57
39.42
39.36
31.44
17.89
f1 (ppm)

Compound 33

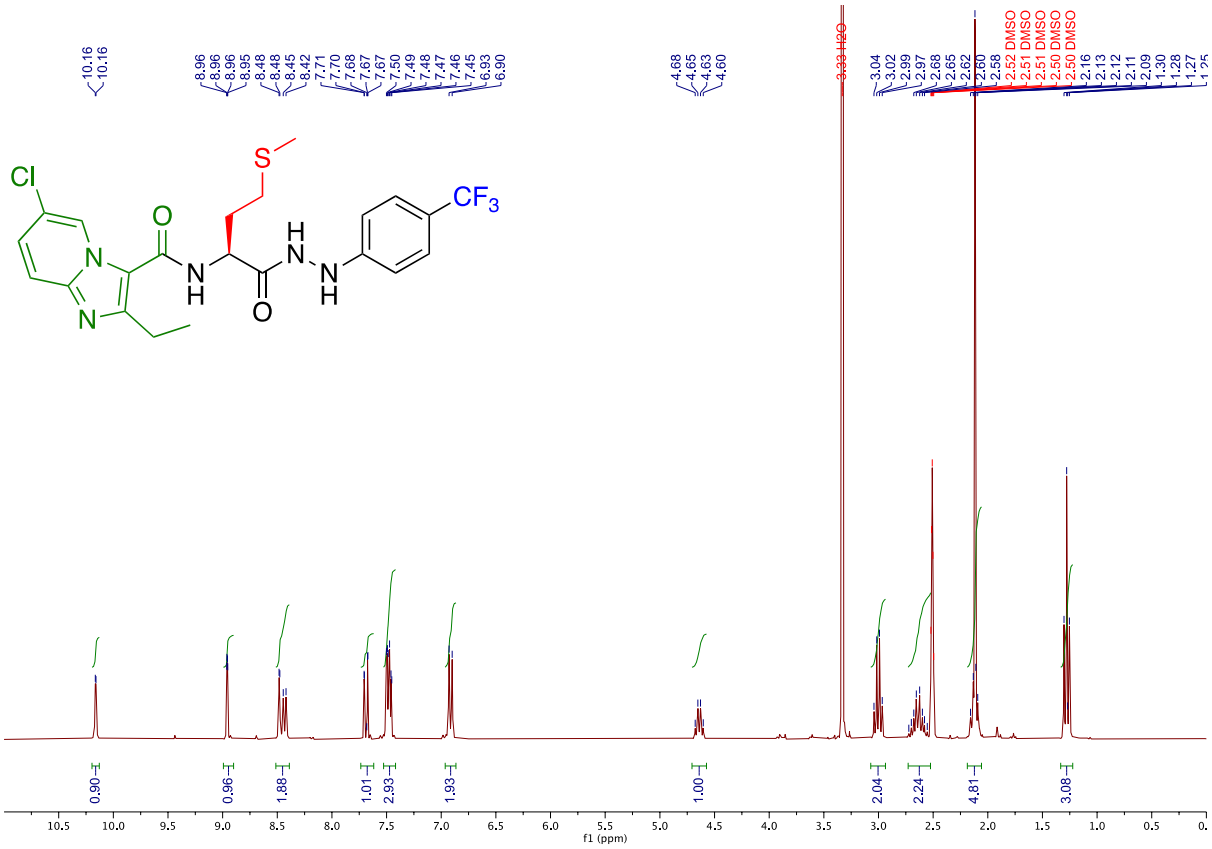

10.12
10.12
9.46
9.43
9.17
9.16
9.15
9.00
8.99
8.98
8.11
8.10
7.17
7.15
7.12
6.76
6.75
6.74
6.73
6.73
6.72
6.72
6.70
6.70
6.70
6.69
6.69
6.69
6.68
6.67
6.66
6.66
6.66
4.67
4.65
3.33
2.66
2.64
2.62
2.60
2.59
2.59
2.56
2.52
2.51
2.51
2.50
2.50
2.16
2.14
2.12
2.11
2.11
2.10
2.09
2.08
2.07
2.06
O2N
S
O
H
N
Cl
N
H
O2N
NH
O
0.78
0.86
1.91
0.96
0.84
1.09
2.99
1.00
2.14
4.92
f1 (ppm)

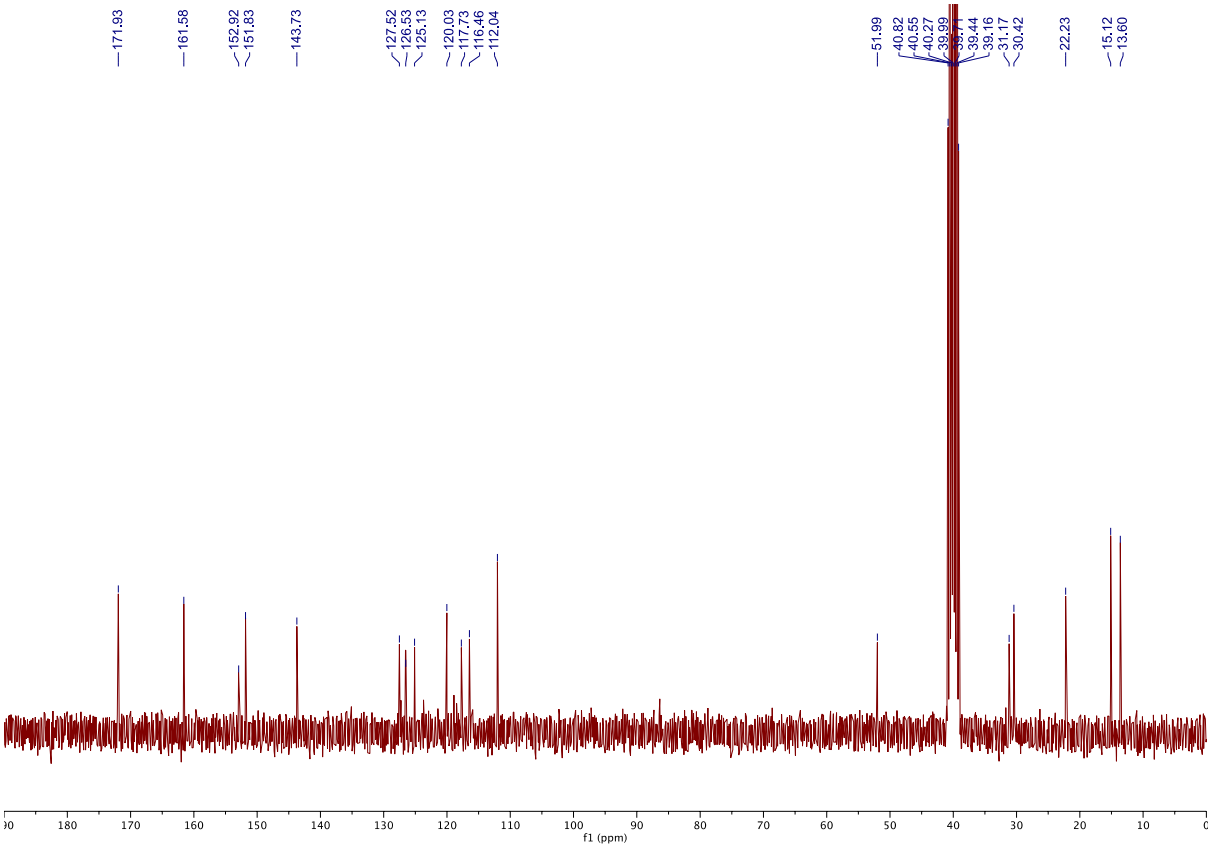

148.56
134.00
128.45
118.38
111.95
111.34
60.22
52.78
40.82
40.54
40.27
39.99
39.71
39.43
39.15
31.13
30.35
15.08
14.56
f1 (ppm)

Compound 34

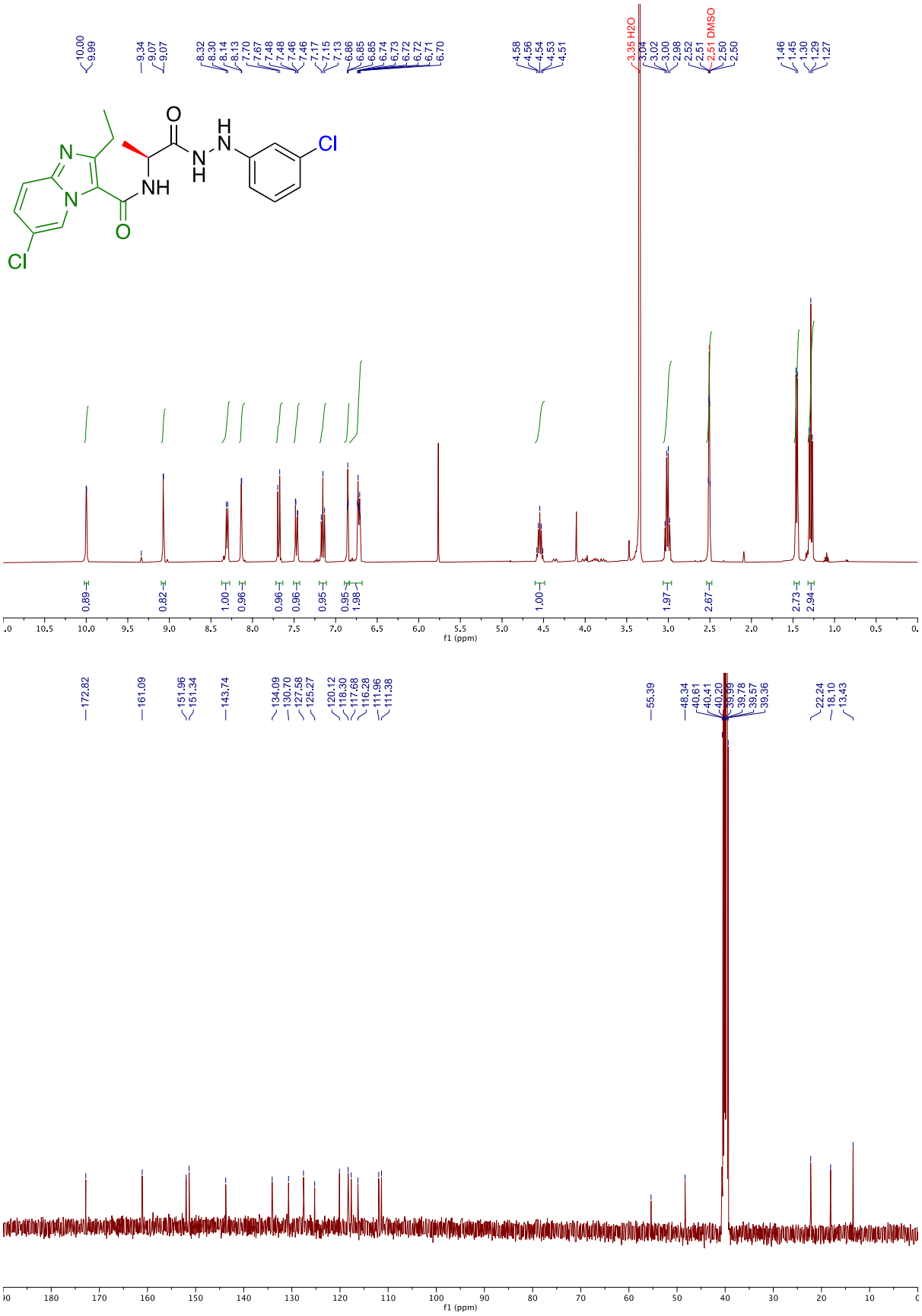

10.09
9.01
9.01
9.00
9.00
8.47
8.37
8.35
8.32
7.71
7.71
7.68
7.67
7.66
7.50
7.50
7.49
7.47
7.46
6.92
6.89
4.64
4.61
4.59
4.57
4.54
3.38 H2O
3.04
3.02
3.01
2.99
2.96
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
1.52
1.48
1.46
1.43
1.31
1.28
1.26
1.24
1.24
0.86
0.75
0.81
0.66
1.09
1.27
3.18
1.64
1.00
2.20
3.02
4.81
f1 (ppm)
172.79
161.07
152.94
151.82
143.70
127.49
126.56
125.17
120.04
117.71
112.02
48.26
40.63
40.42
40.22
40.01
39.80
39.59
39.38
38.72
22.18
18.16
13.47
f1 (ppm)

Compound 35

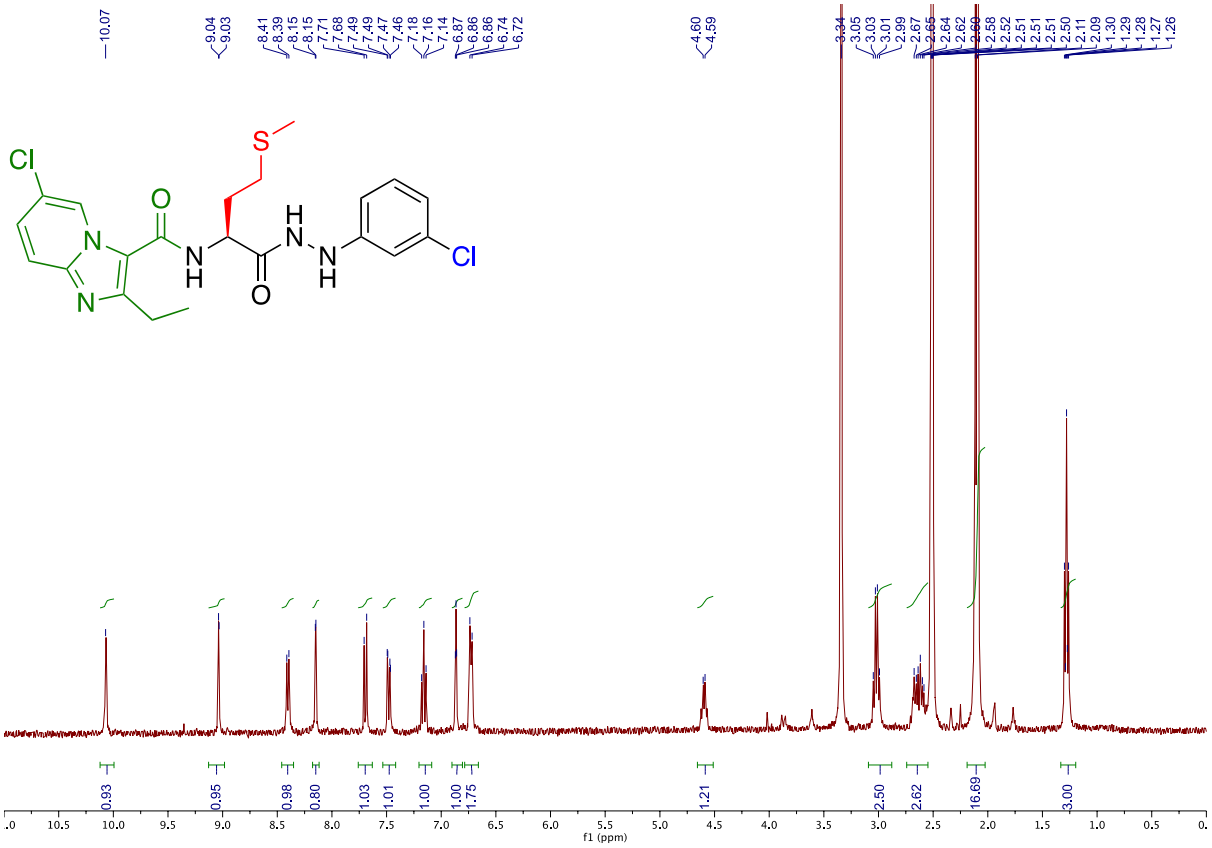

10.16
10.16
8.96
8.96
8.96
8.95
8.48
8.48
8.45
8.42
7.71
7.70
7.68
7.67
7.67
7.50
7.49
7.48
7.47
7.46
7.45
6.93
6.90
4.68
4.65
4.63
4.60
3.33 H2O
3.04
3.02
2.99
2.97
2.68
2.65
2.62
2.60
2.58
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.16
2.13
2.12
2.11
2.09
1.30
1.28
1.27
Cl
O
N
N
S
N
H
O
N
H
CF3
0.90
0.96
1.88
1.01
2.93
1.93
1.00
2.04
2.24
4.81
3.08
f1 (ppm)

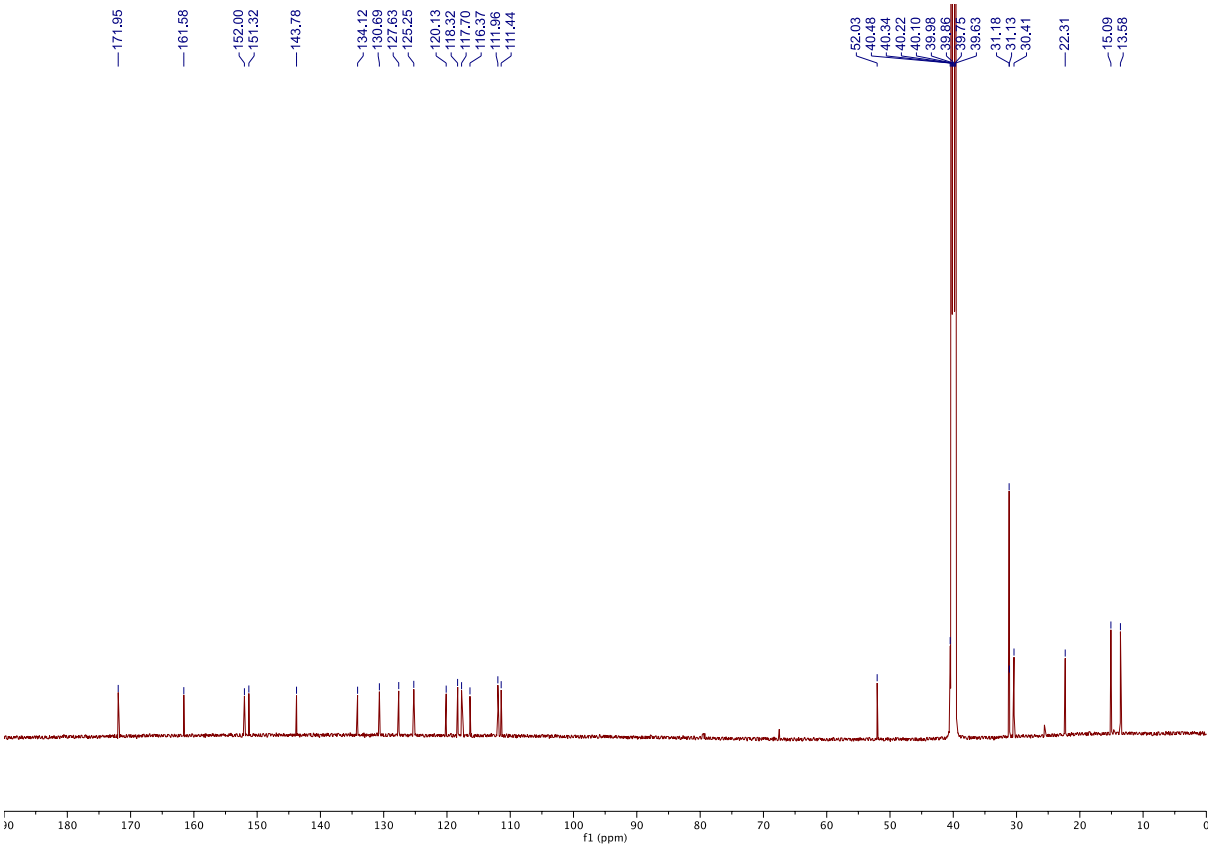

171.93
161.58
152.92
151.83
143.73
127.52
126.53
125.13
120.03
117.73
116.46
112.04
51.99
40.82
40.55
40.27
39.99
39.71
39.44
39.16
31.17
30.42
22.23
15.12
13.60
f1 (ppm)

Compound 36


10.00
9.99
9.34
9.07
9.07
8.32
8.30
8.14
8.13
7.70
7.67
7.48
7.48
7.46
7.46
7.17
7.15
7.13
6.86
6.85
6.74
6.73
6.72
6.72
6.71
6.70
4.58
4.56
4.54
4.53
4.51
3.35 H2O
3.04
3.02
3.00
2.98
2.52
2.51
2.51 DMSO
2.50
2.50
1.46
1.45
1.30
1.29
1.27
0.89
0.82
1.00
0.96
0.96
0.96
0.95
0.95
1.98
1.00
1.97
2.67
2.73
2.94
f1 (ppm)
172.82
161.09
151.96
151.34
143.74
134.09
130.70
127.58
125.27
120.12
118.30
117.68
116.28
111.96
111.38
55.39
48.34
40.61
40.41
40.20
39.99
39.78
39.57
39.36
22.24
18.10
13.43
f1 (ppm)

Compound 37


10.07
9.04
9.03
8.41
8.39
8.15
8.15
7.71
7.68
7.49
7.49
7.47
7.46
7.18
7.16
7.14
6.87
6.86
6.86
6.74
6.72
4.60
4.59
3.34
3.05
3.03
3.01
2.99
2.67
2.65
2.64
2.62
2.60
2.58
2.52
2.51
2.51
2.51
2.50
2.11
2.09
1.30
1.29
1.28
1.27
1.26
Cl
S
O
N
H
N
N
H
O
N
Cl
0.93
0.95
0.98
0.80
1.03
1.01
1.00
1.00
1.75
1.21
2.50
2.62
16.69
3.00
f1 (ppm)


171.95
161.58
152.00
151.32
143.78
134.12
130.69
127.63
125.25
120.13
118.32
117.70
116.37
111.96
111.44
52.03
40.48
40.34
40.22
40.10
39.98
39.86
39.75
39.63
31.18
31.13
30.41
22.31
15.09
13.58
f1 (ppm)