# Supporting Information

## *N*-[1,3-Dialkyl(aryl)-2-oxoimidazolidin-4-ylidene]-aryl(alkyl)sulphonamides as novel selective human cannabinoid type 2 receptor (hCB2R) ligands. Insights into the mechanism of receptor activation/deactivation.

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**Figure S1.** Competition radioligand binding assay of **10d** (A), **10e** (B), **10f** (C), **10g** (D), **10h** (E), **12a** (F), **12b** (G), **12e** (H) and **13** (I) at hCB2R, using [$^3$H]CP55 940. Data are reported as mean ± SE of three independent experiments conducted in duplicate.

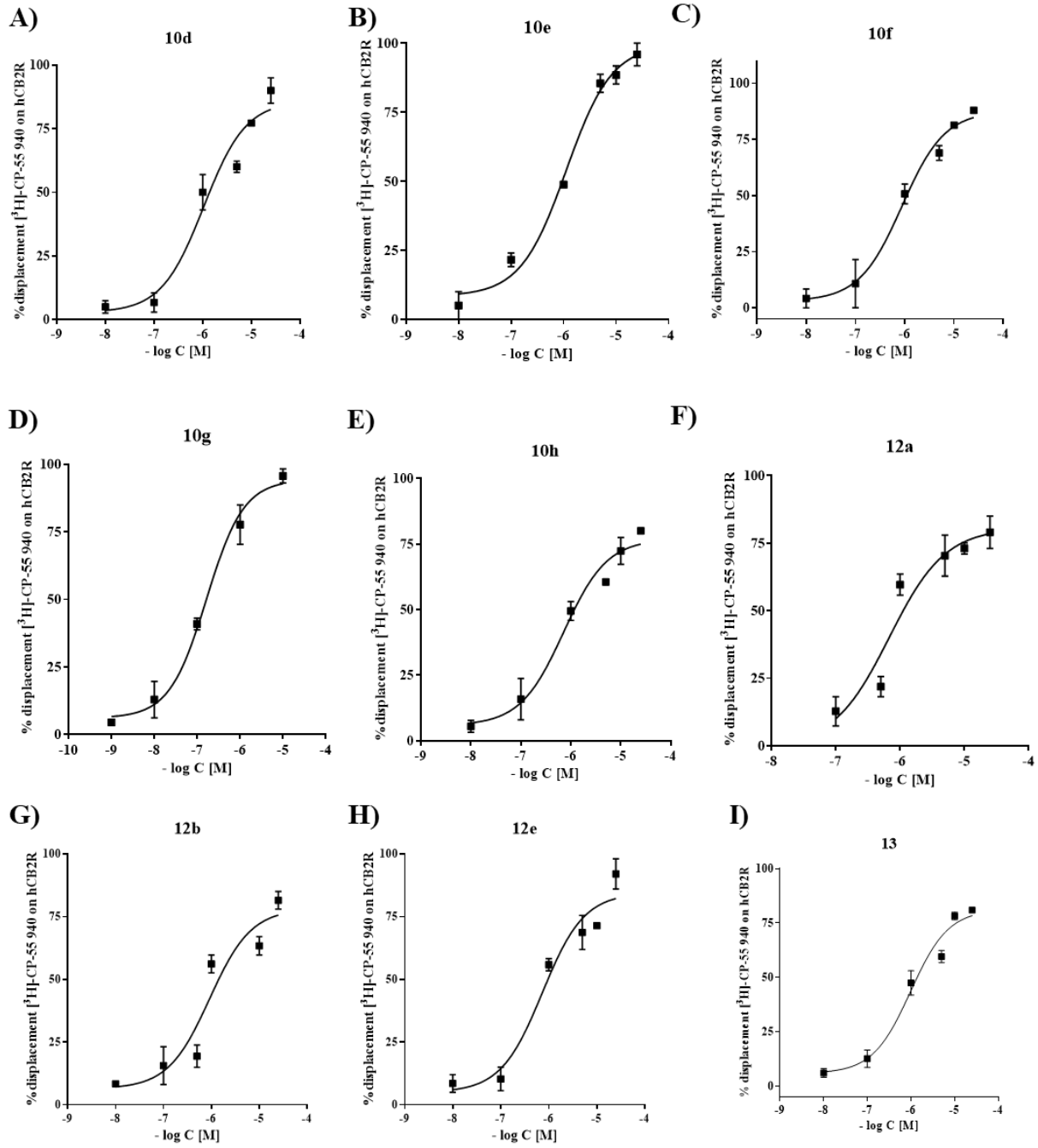


**Figure S2.** Chemical structure of compounds 47 (a), 49 (b), 51 (c) and 53 (d) from Mugnaini et al. [12].

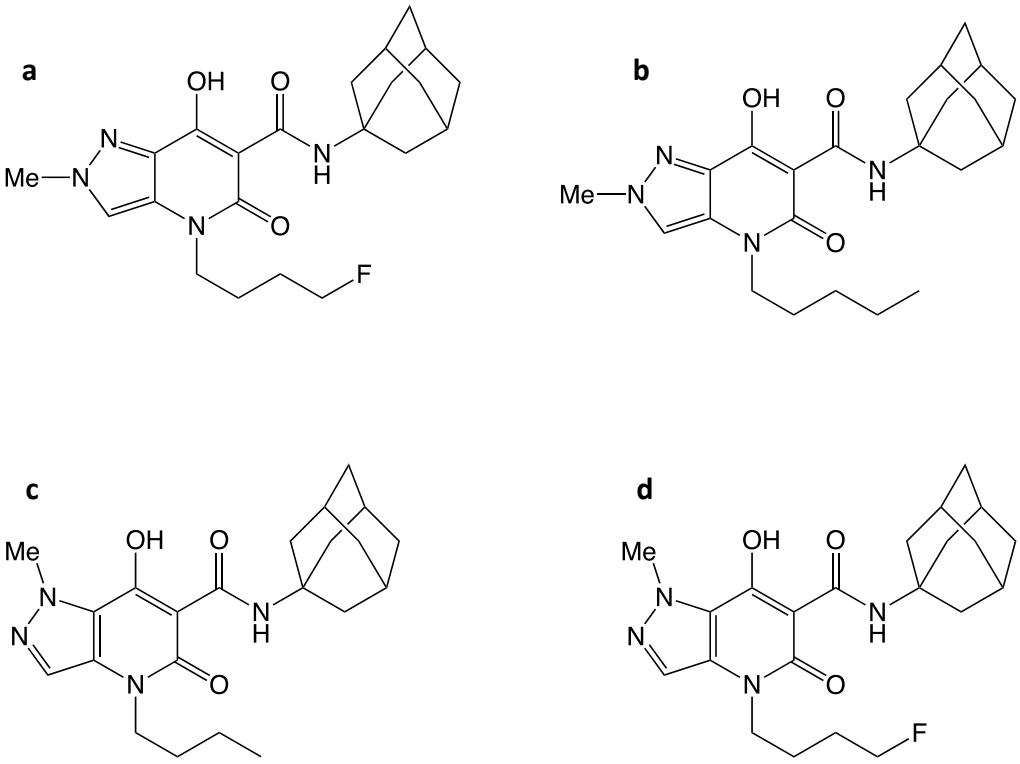


**Figure S3.** Docking poses of compound 49 (dark teal sticks, **a**) and compound 47 (grey sticks, **b**) in the antagonist conformation of hCB2R (PDB ID 5zty, light orange cartoon), and compound 51 (lilac sticks, **c**) and compound 53 (magenta sticks, **d**) in the agonist conformation of hCB2R (PDB ID 6kpc, light green cartoon). Compounds have been reported and described by Mugnaini et al. [12]. Residues lining the binding site are represented as capped sticks and labelled, helices are numbered as TM1-7.

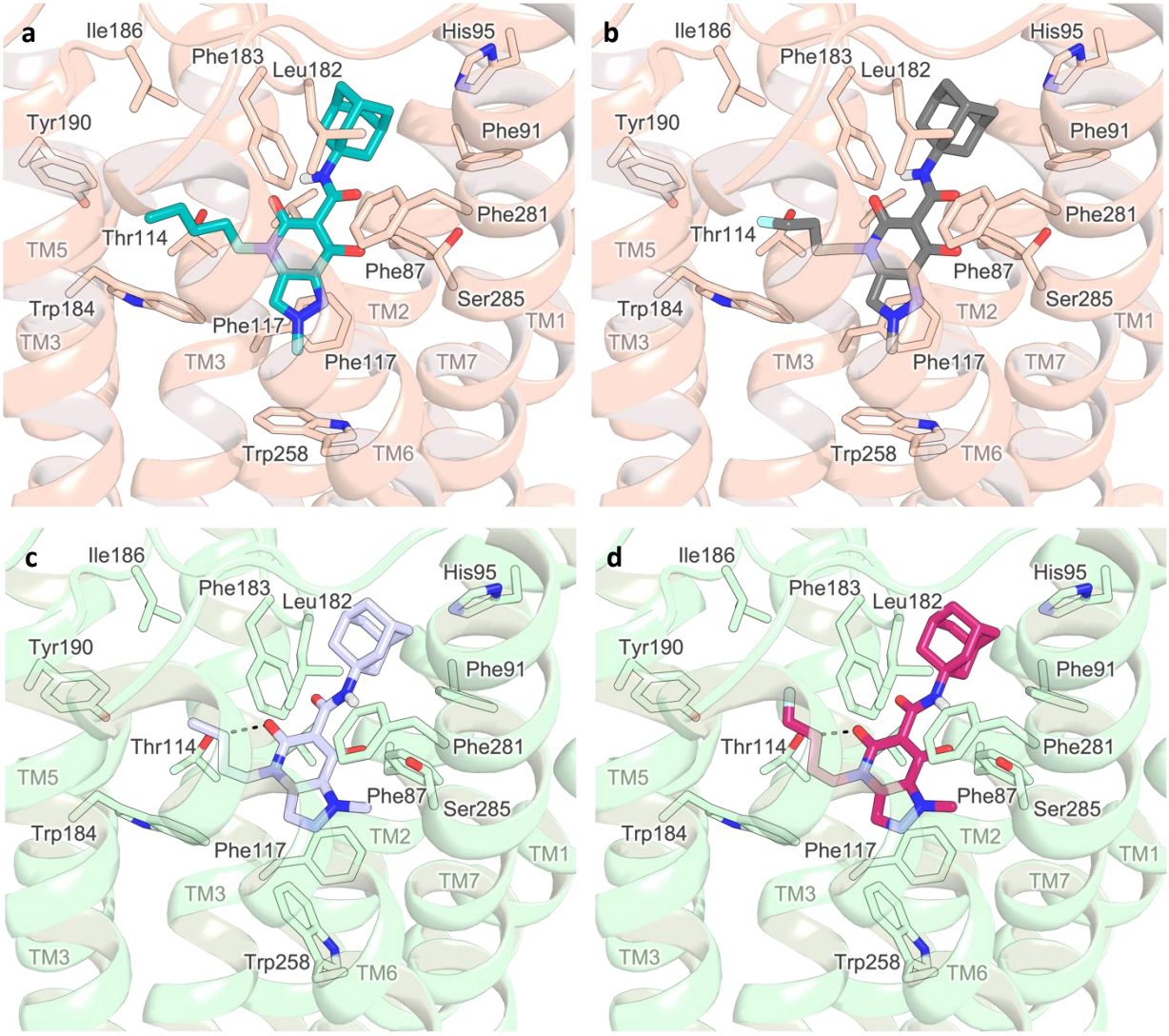


**Figure S4.** Docking poses of compounds **10e** (salmon pink, **a**) and **10g** (cyan, **b**) in the agonist conformation of hCB2R receptor (PDB ID: 6kpc, light green cartoon). Residues lining the binding site are represented as capped sticks and labelled, helices are numbered as TM1-7. Hydrogen bonds are represented as black dashed lines.

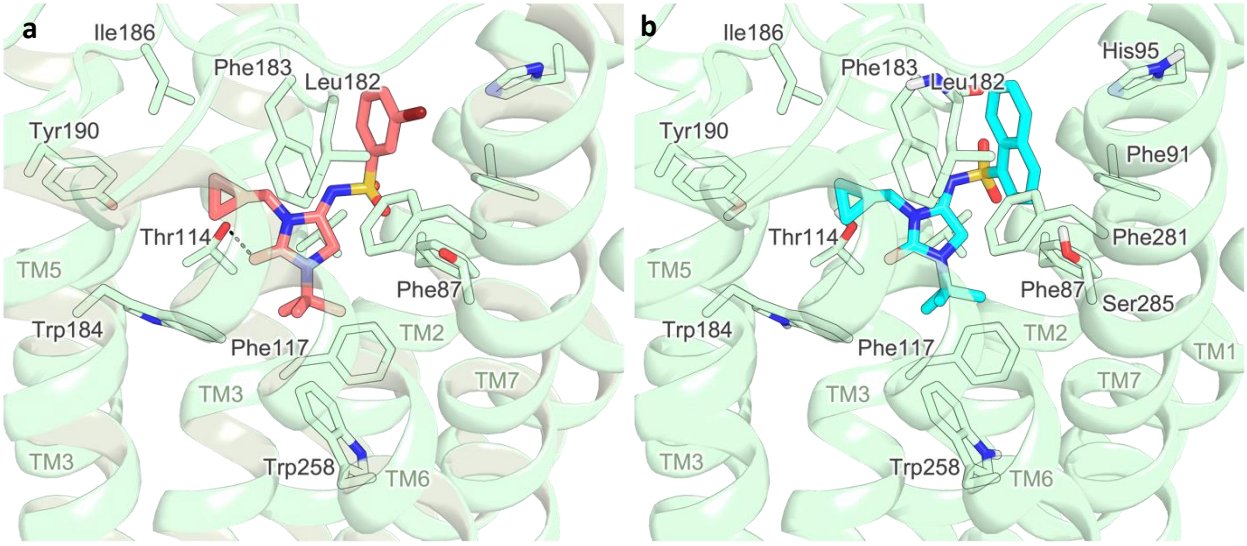


**Figure S5.** Docking poses of compound **12b** in the antagonist conformation of CB2R receptor (PDB ID 5zty). Residues lining the binding site are represented as capped sticks and labelled, transmembrane helices are numbered as TM1-7. Hydrogen bonds are represented as black dashed lines.

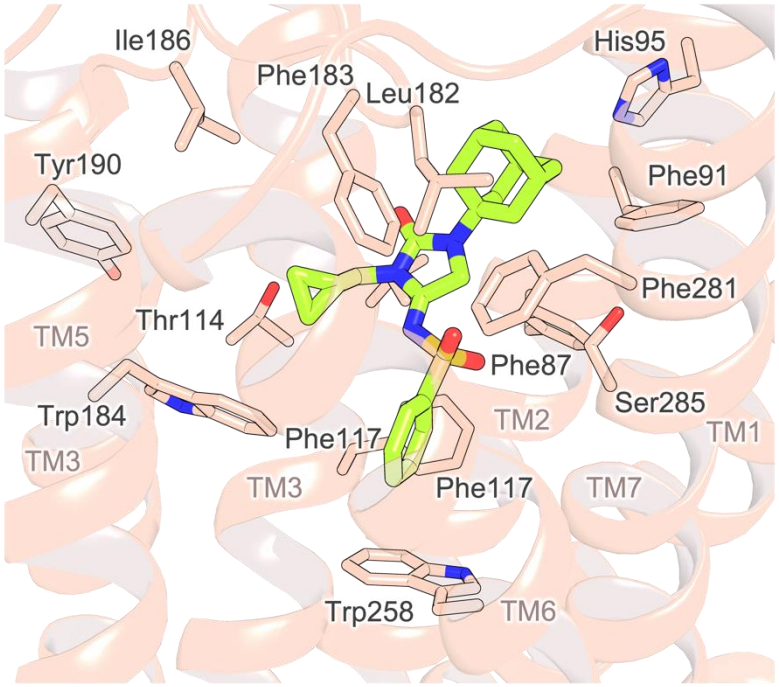
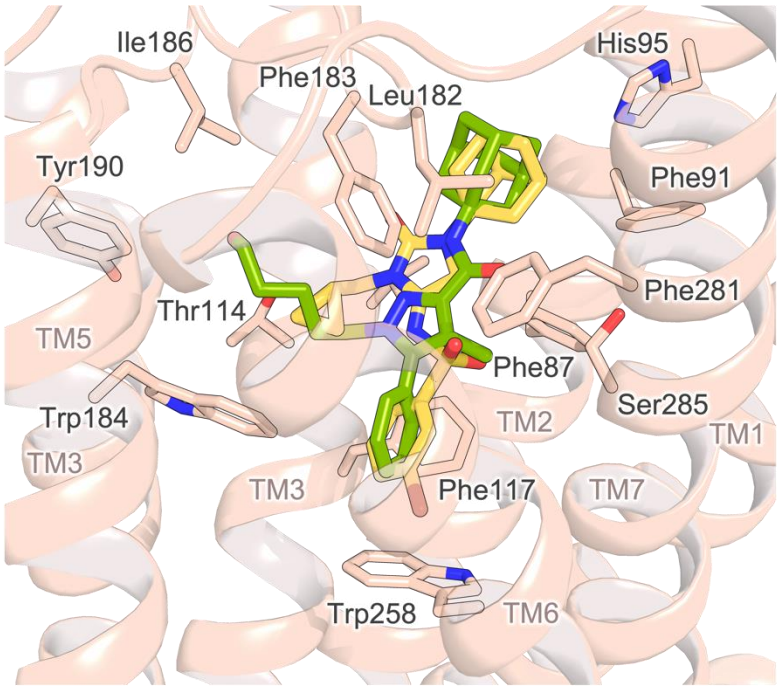
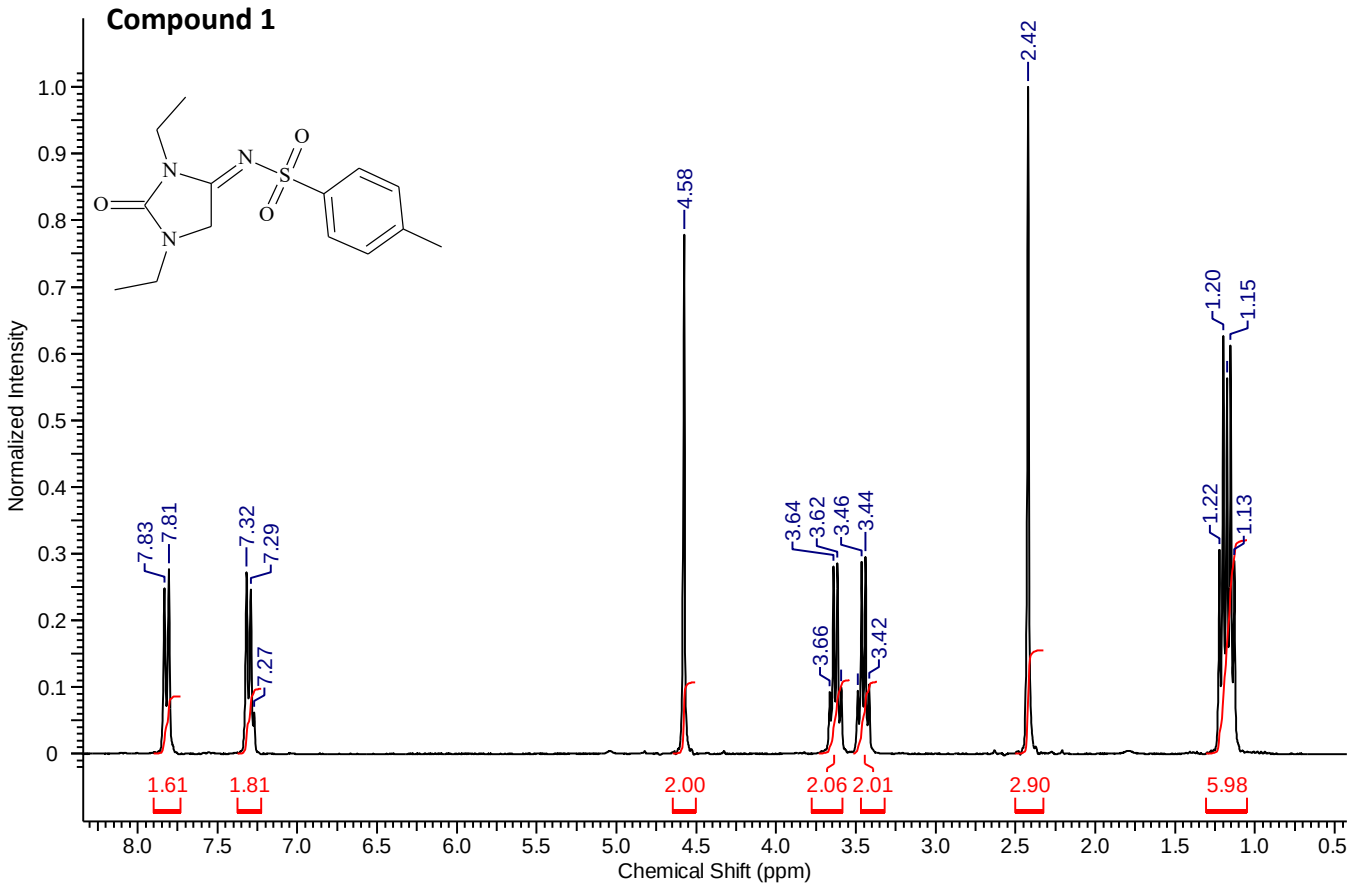


**Figure S6.** Alignment of **12e** docking pose (yellow) and antagonist AM10257 (green) in the antagonist-like state (PDB ID 5zty). Protein is coloured in light orange cartoon, residues lining the binding site are represented as capped sticks and labelled, helices are numbered as TM1-7.




Compound 1
Normalized Intensity
Chemical Shift (ppm)
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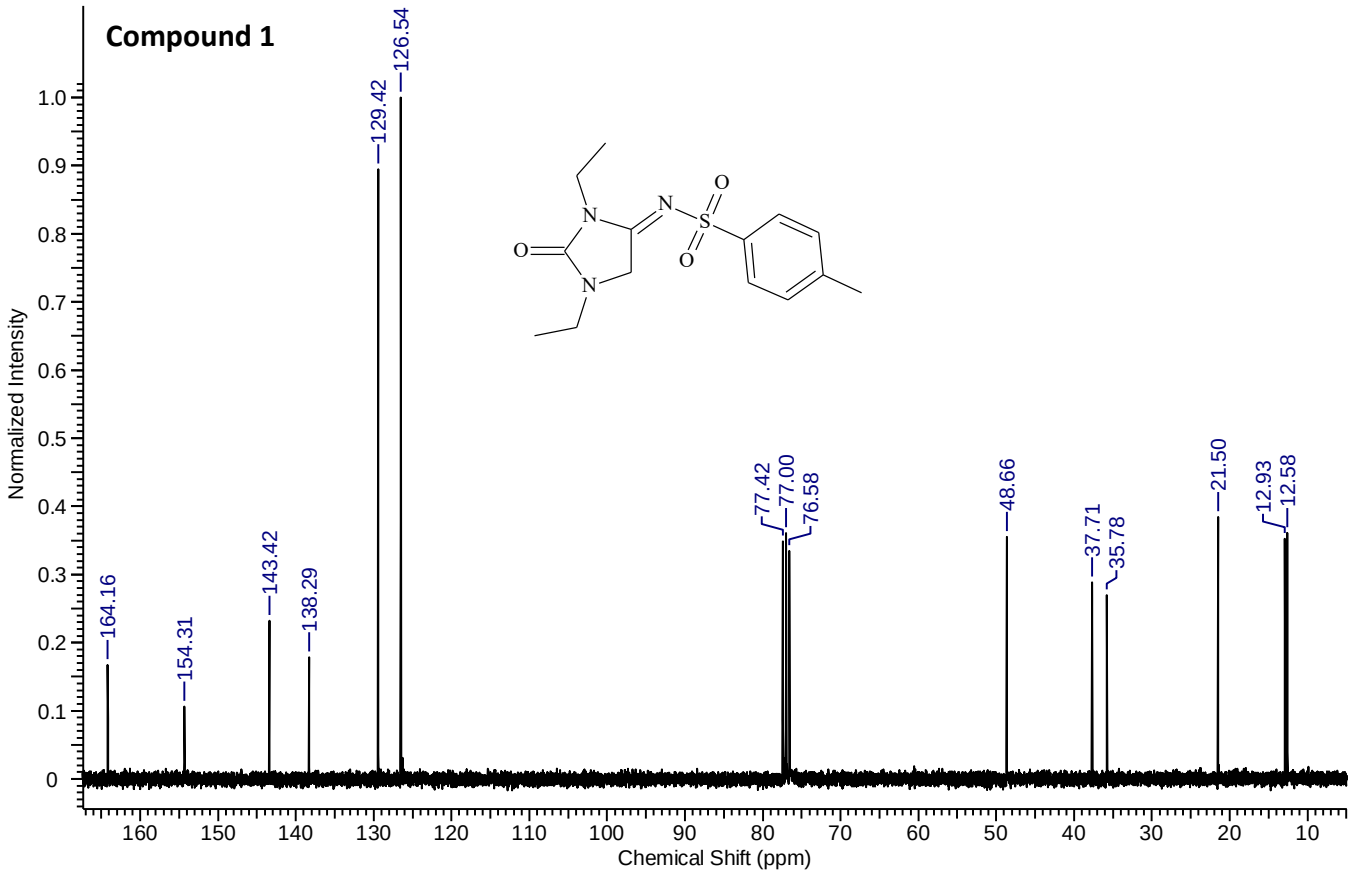
7.81
7.32
7.29
7.27
4.58
3.64
3.62
3.46
3.44
3.66
3.42
2.42
1.20
1.15
1.22
1.13
1.61
1.81
2.00
2.06
2.01
2.90
5.98


Compound 1
Normalized Intensity
Chemical Shift (ppm)
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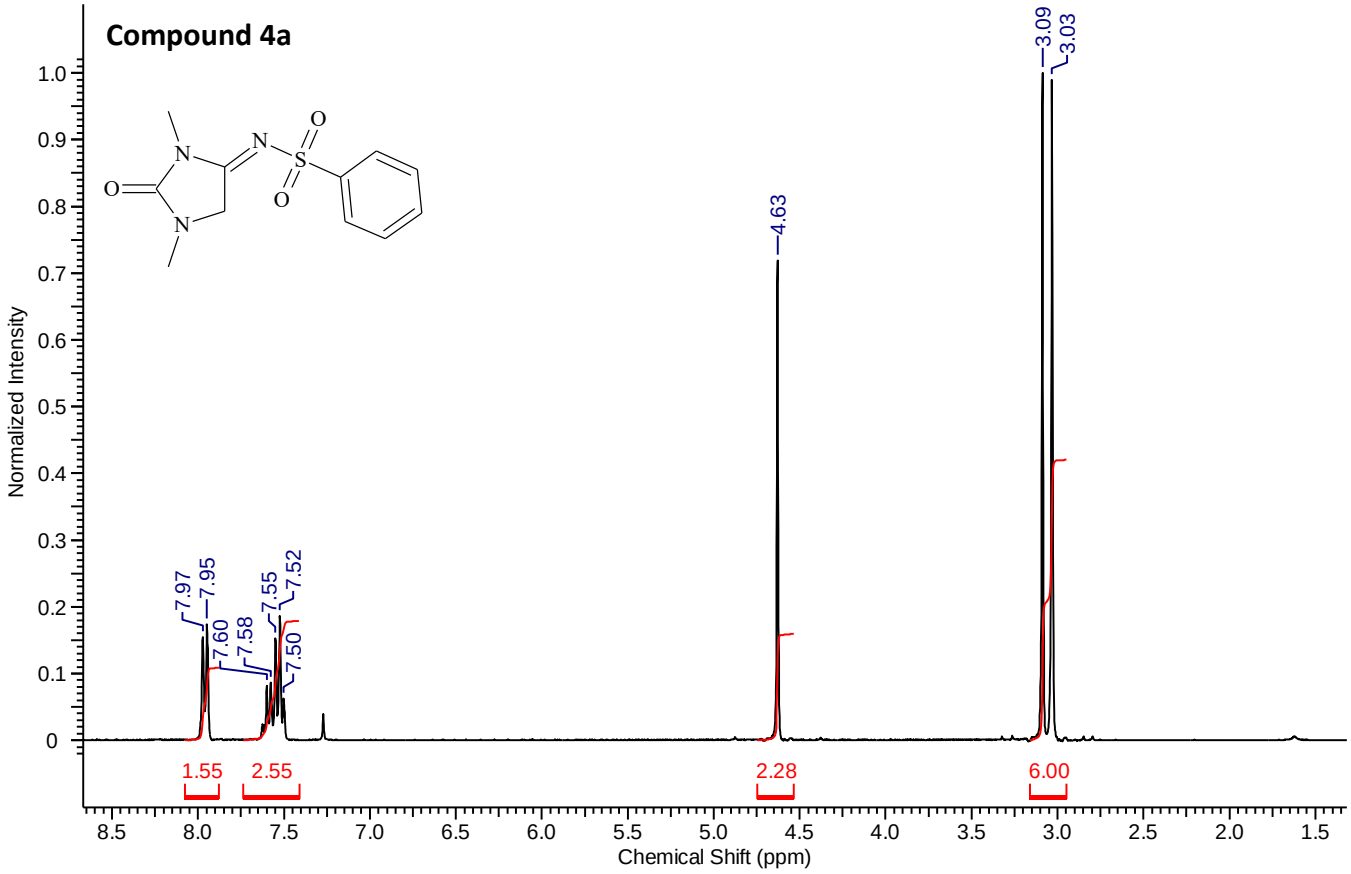
37.71
35.78
21.50
12.93
12.58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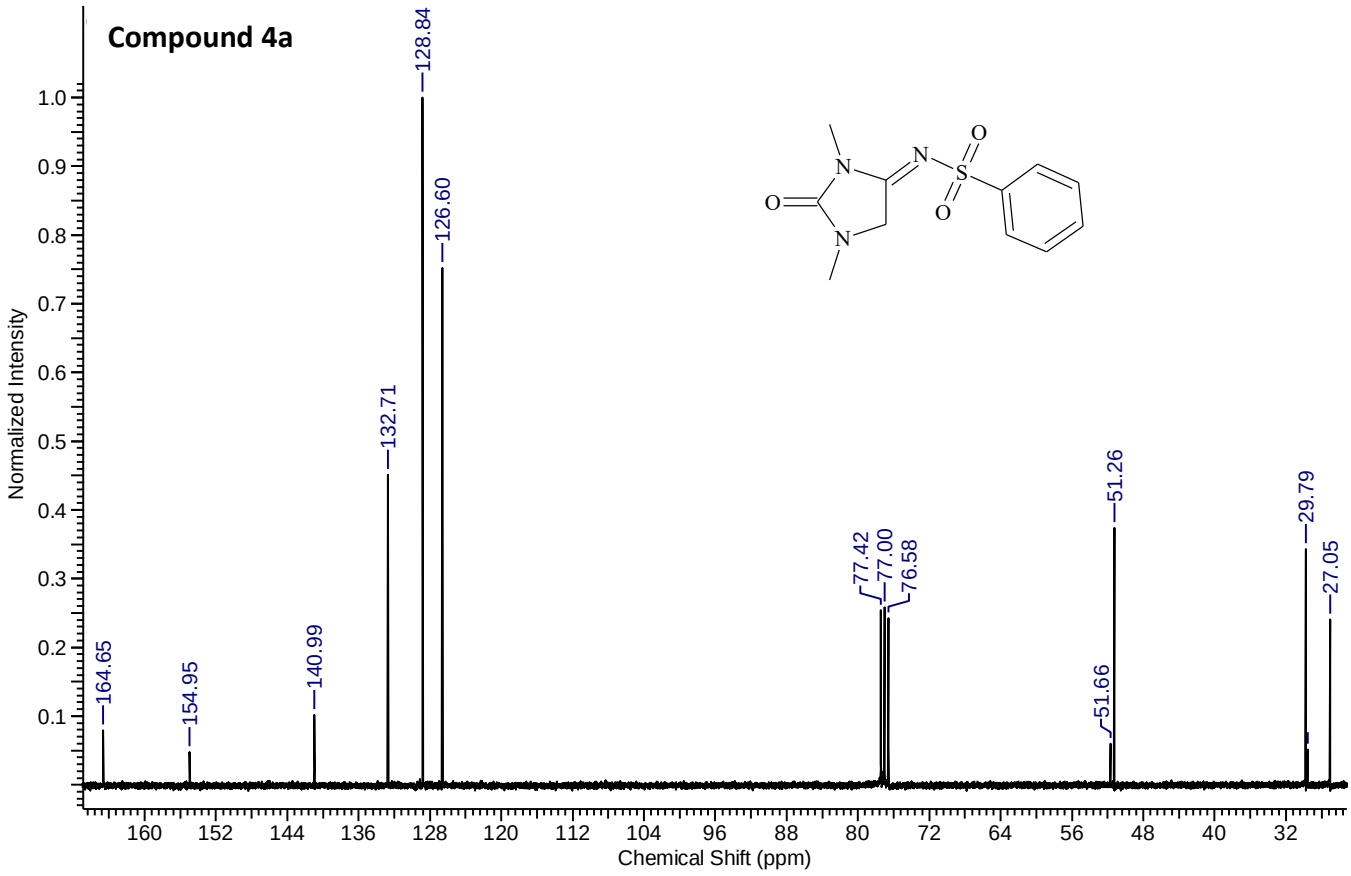
6.00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Normalized Intensity
Chemical Shift (ppm)
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76.58
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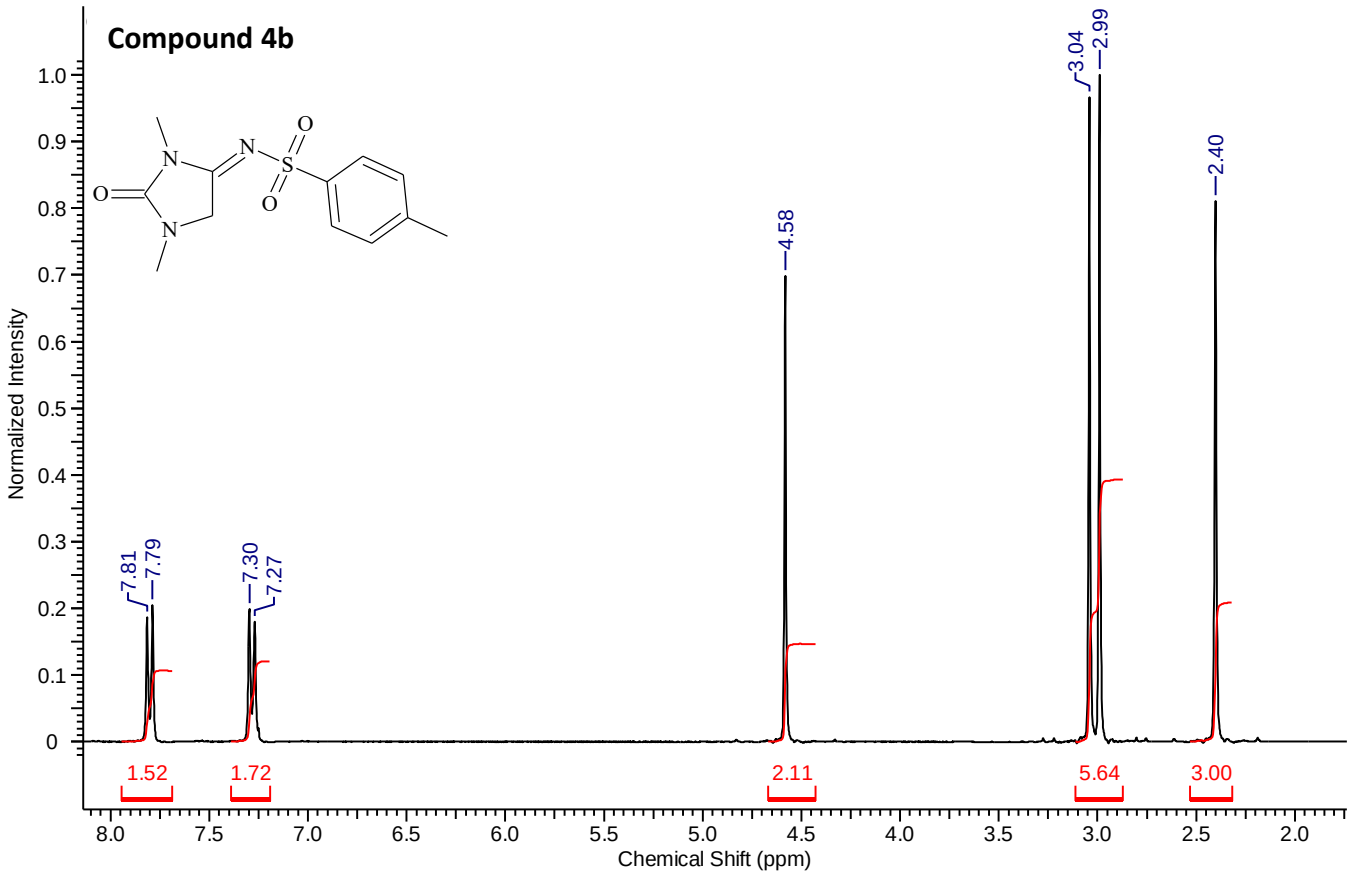
51.26
29.79
27.05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Normalized Intensity
Chemical Shift (ppm)
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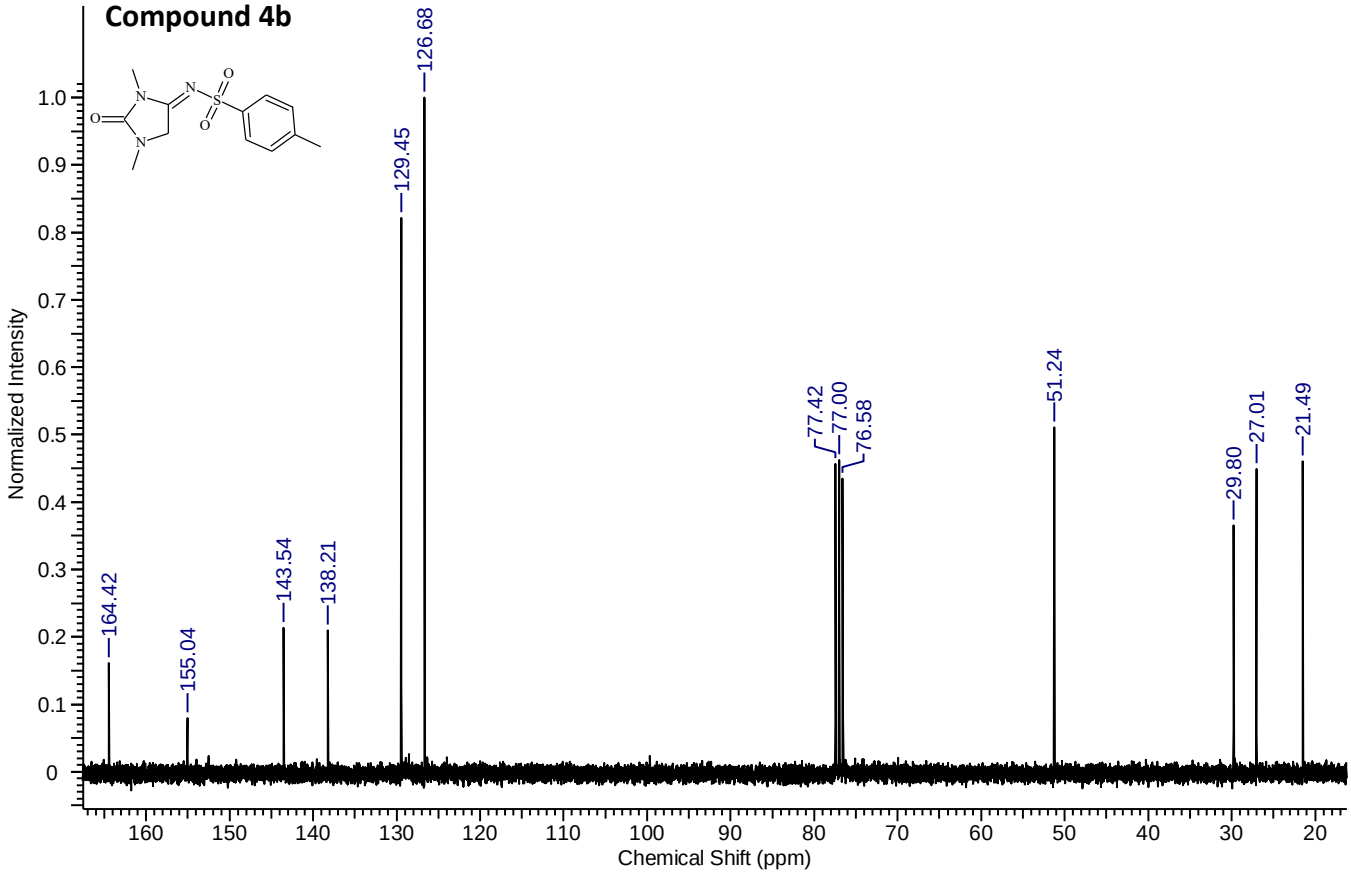
3.00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Normalized Intensity
Chemical Shift (ppm)
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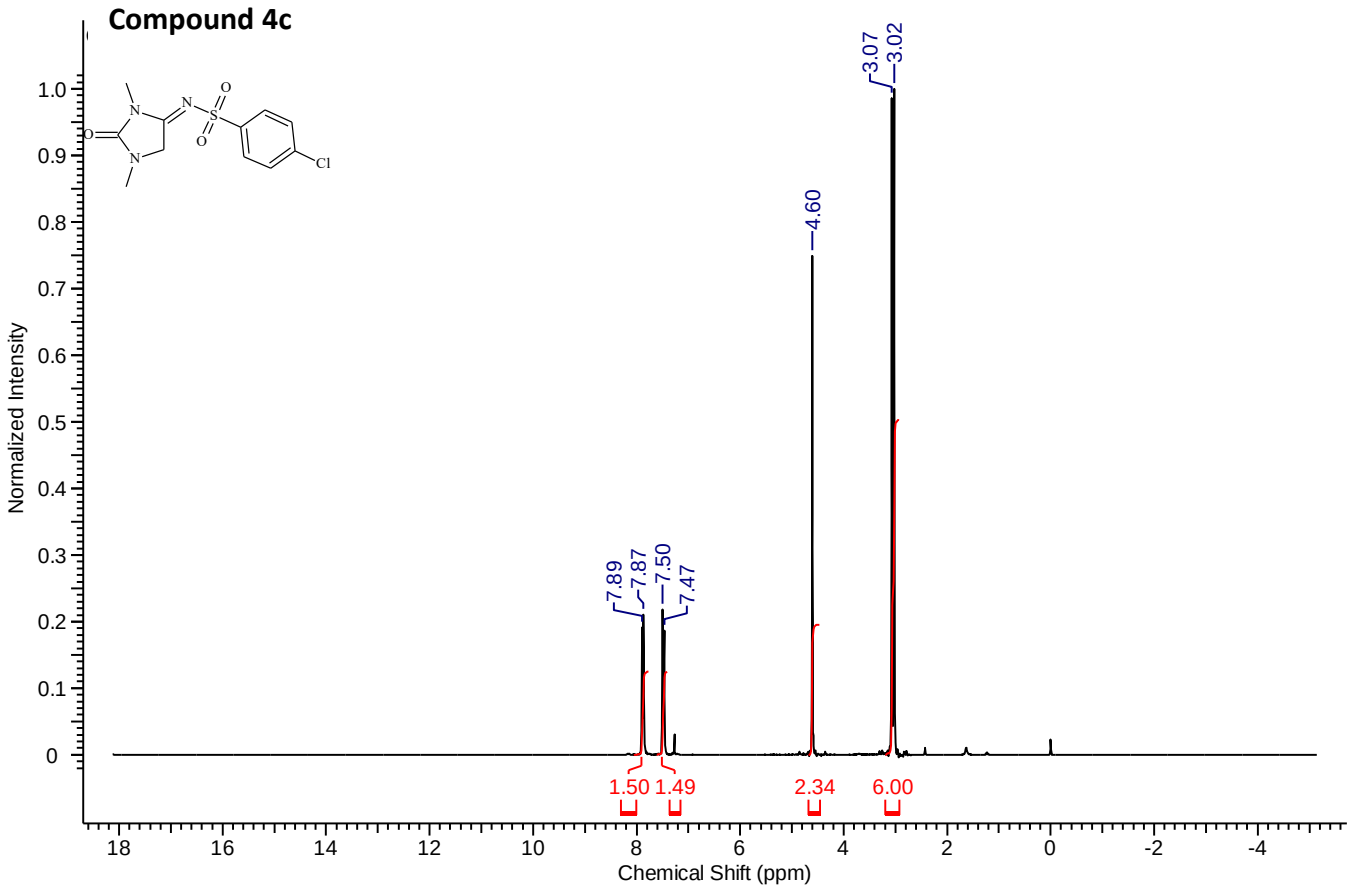
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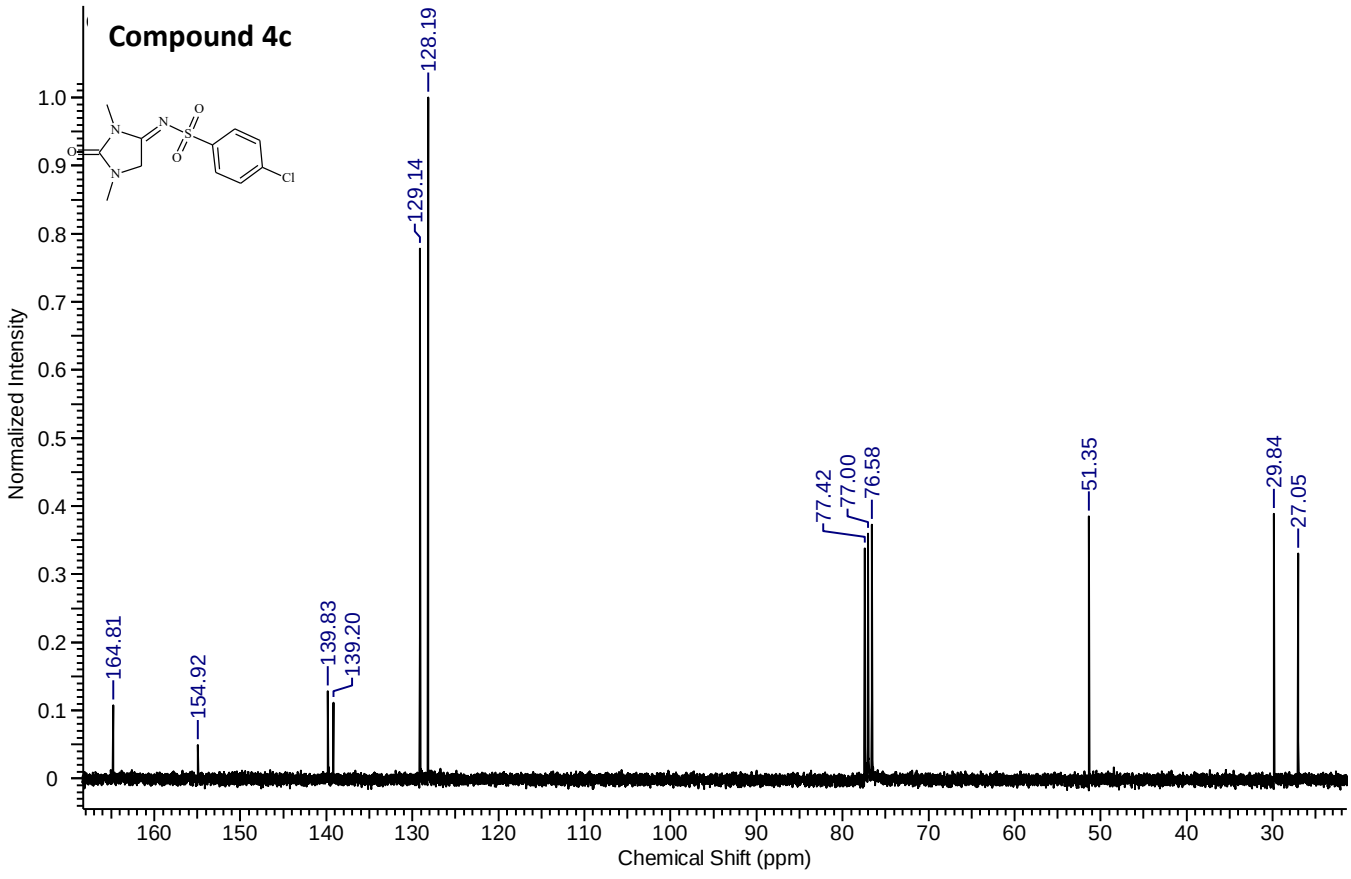
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Normalized Intensity
Chemical Shift (ppm)
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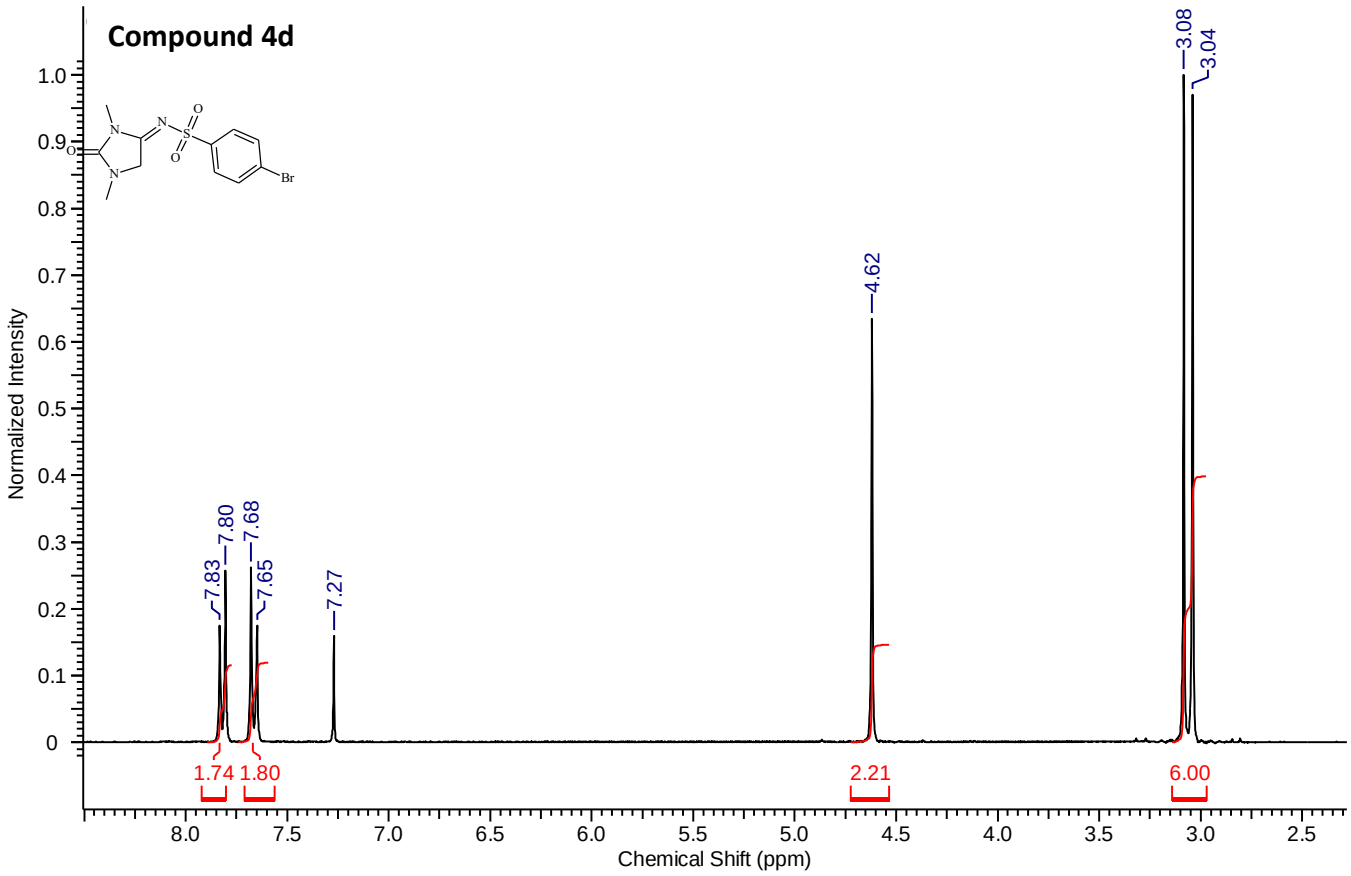
76.58
51.35
29.84
27.05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Chemical Shift (ppm)
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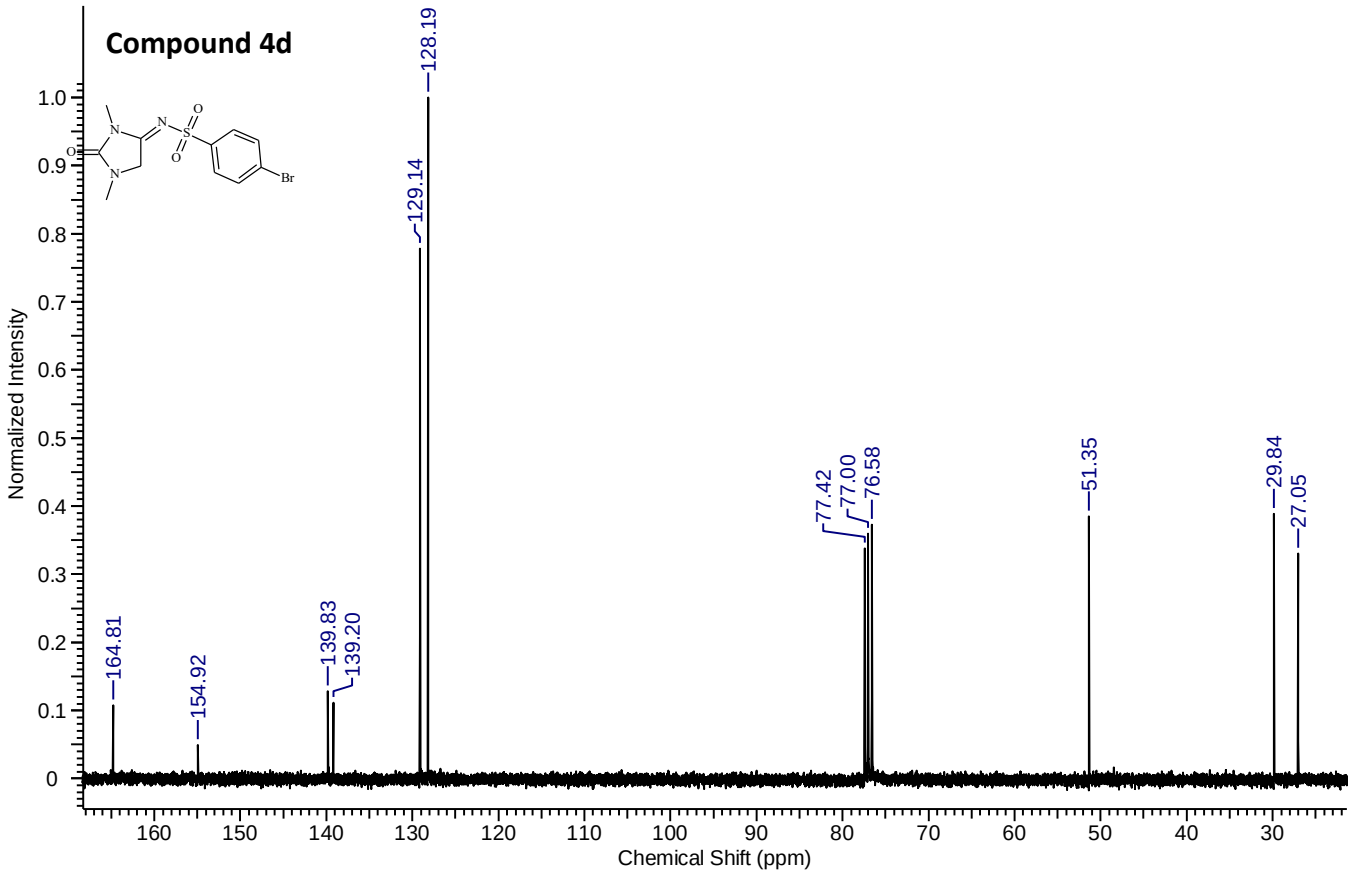
1.80
2.21
6.00


Compound 4d
Normalized Intensity
Chemical Shift (ppm)
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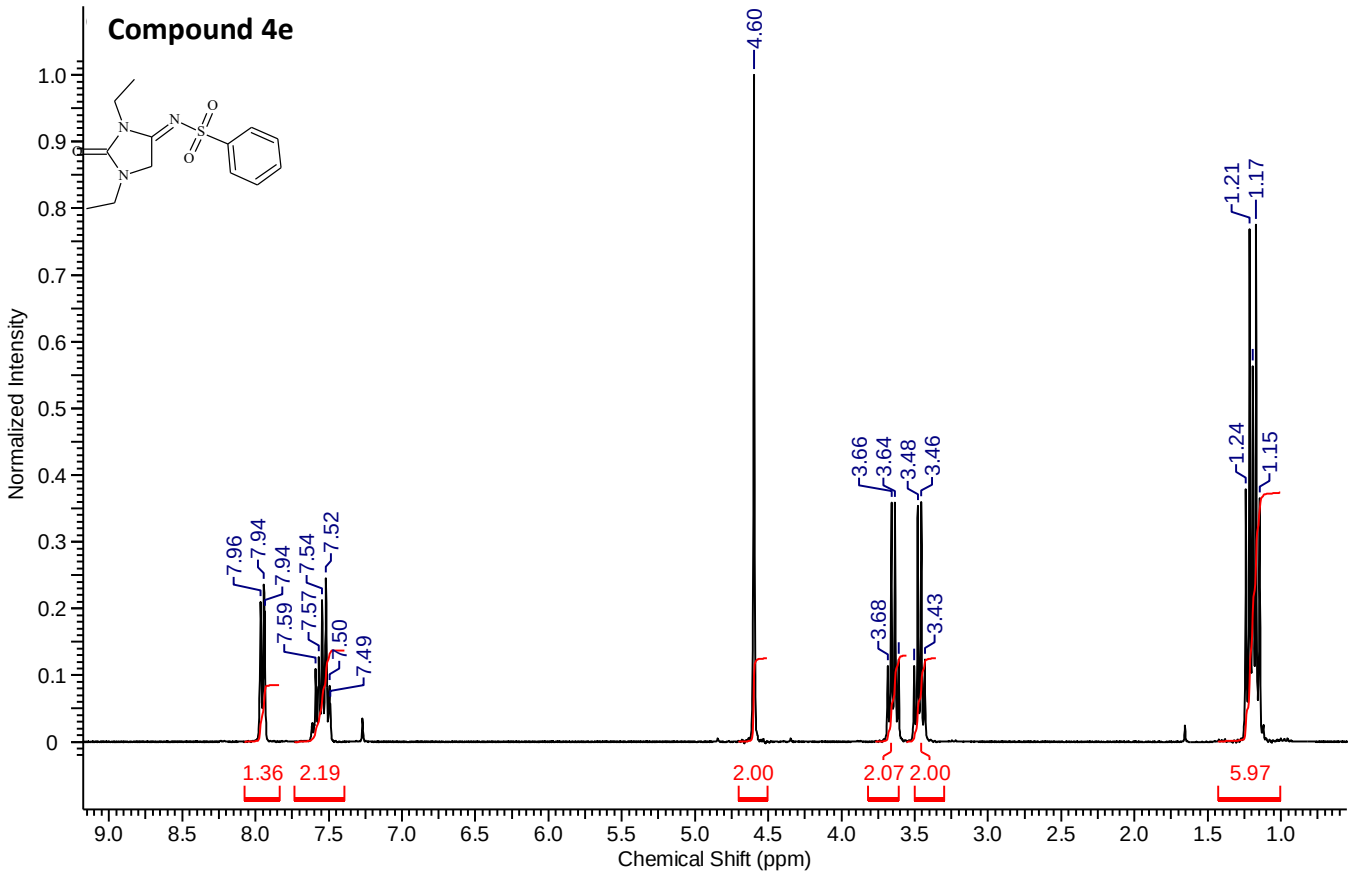
154.92
139.83
139.20
129.14
128.19
77.42
77.00
76.58
51.35
29.84
27.05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Normalized Intensity
Chemical Shift (ppm)
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1.36
2.19
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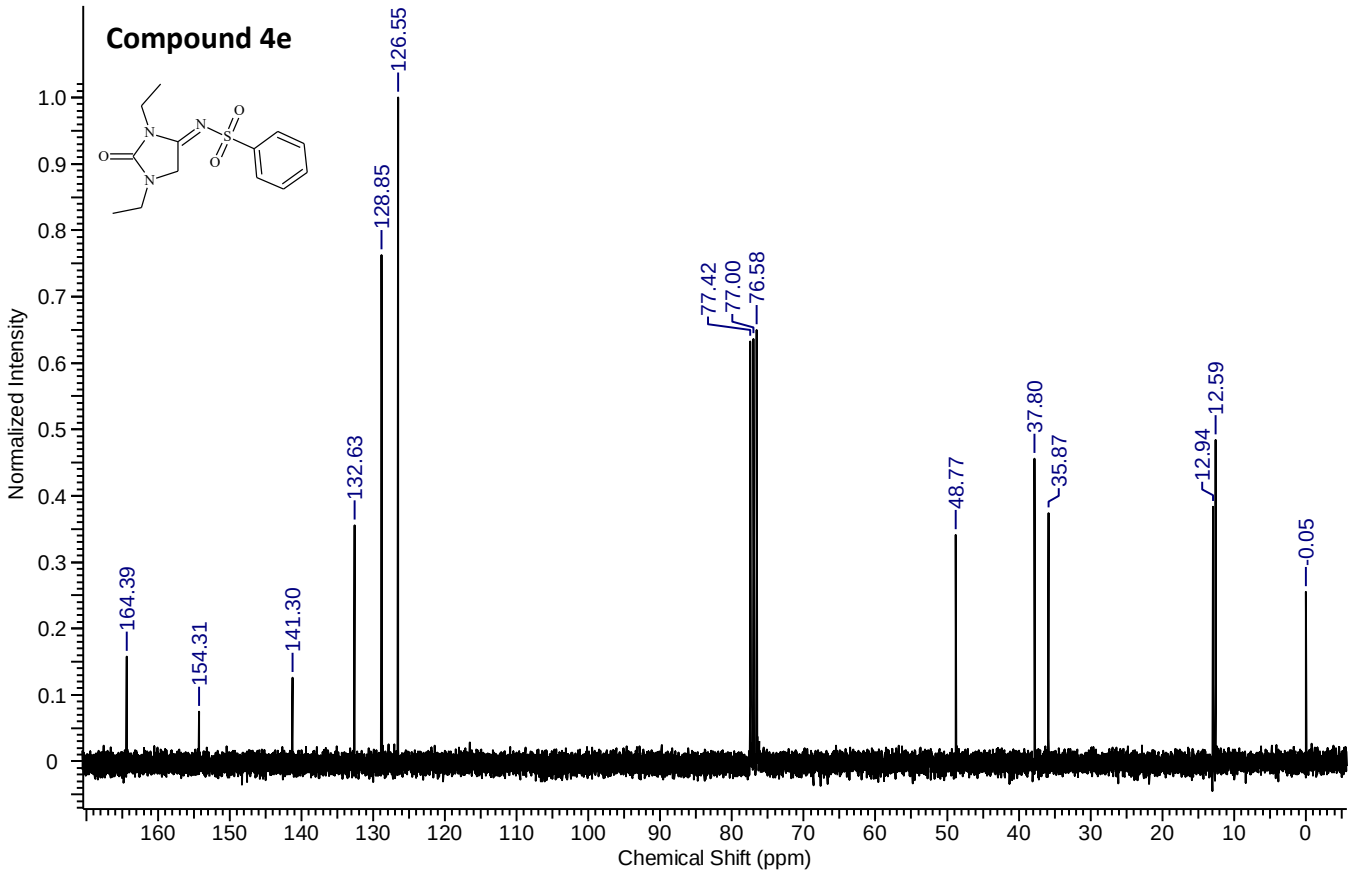
2.07
2.00
5.97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Chemical Shift (ppm)
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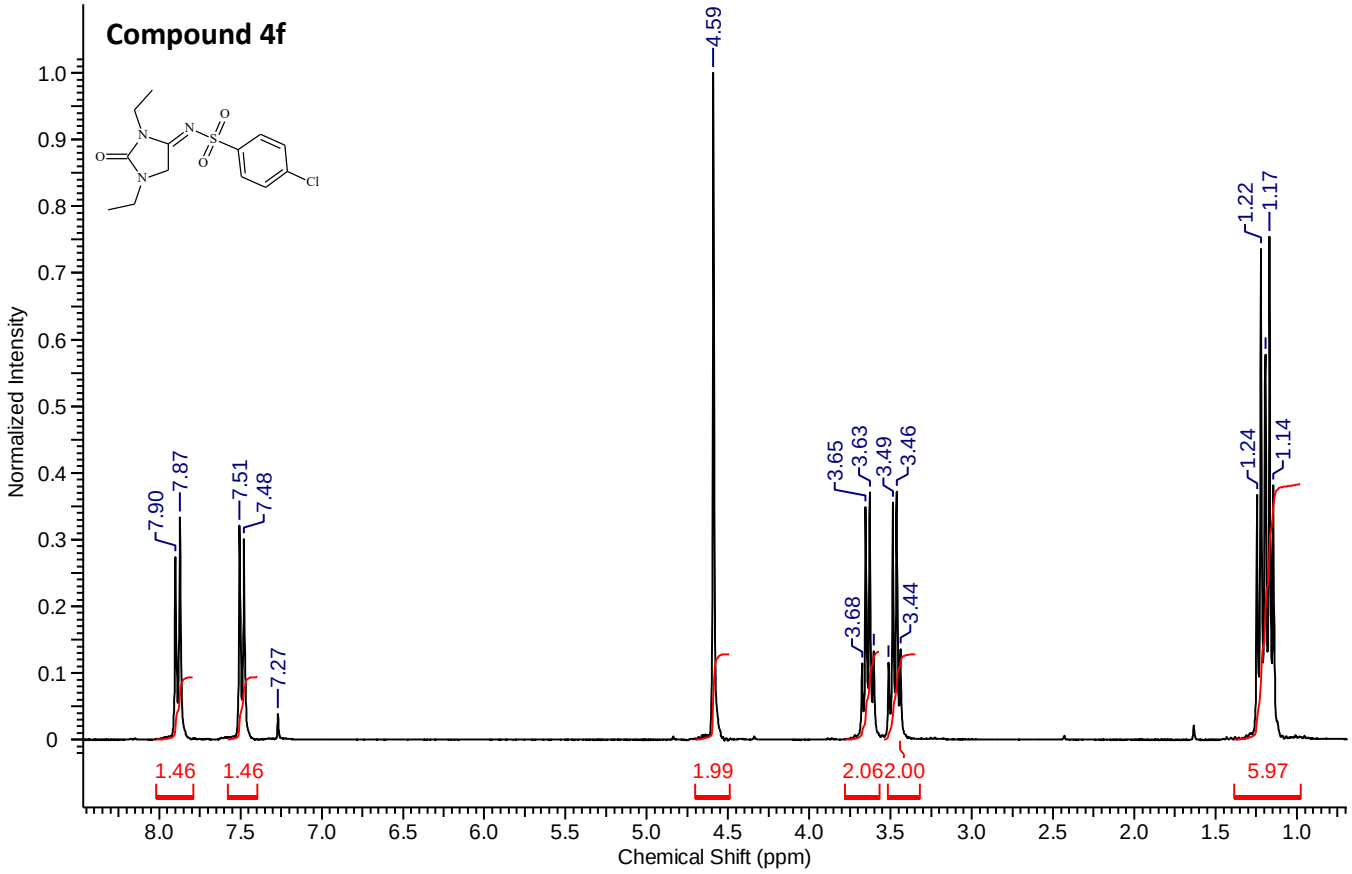
37.80
35.87
12.94
12.59
-0.05


Compound 4f
Normalized Intensity
Chemical Shift (ppm)
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7.27
4.59
3.65
3.63
3.49
3.46
3.68
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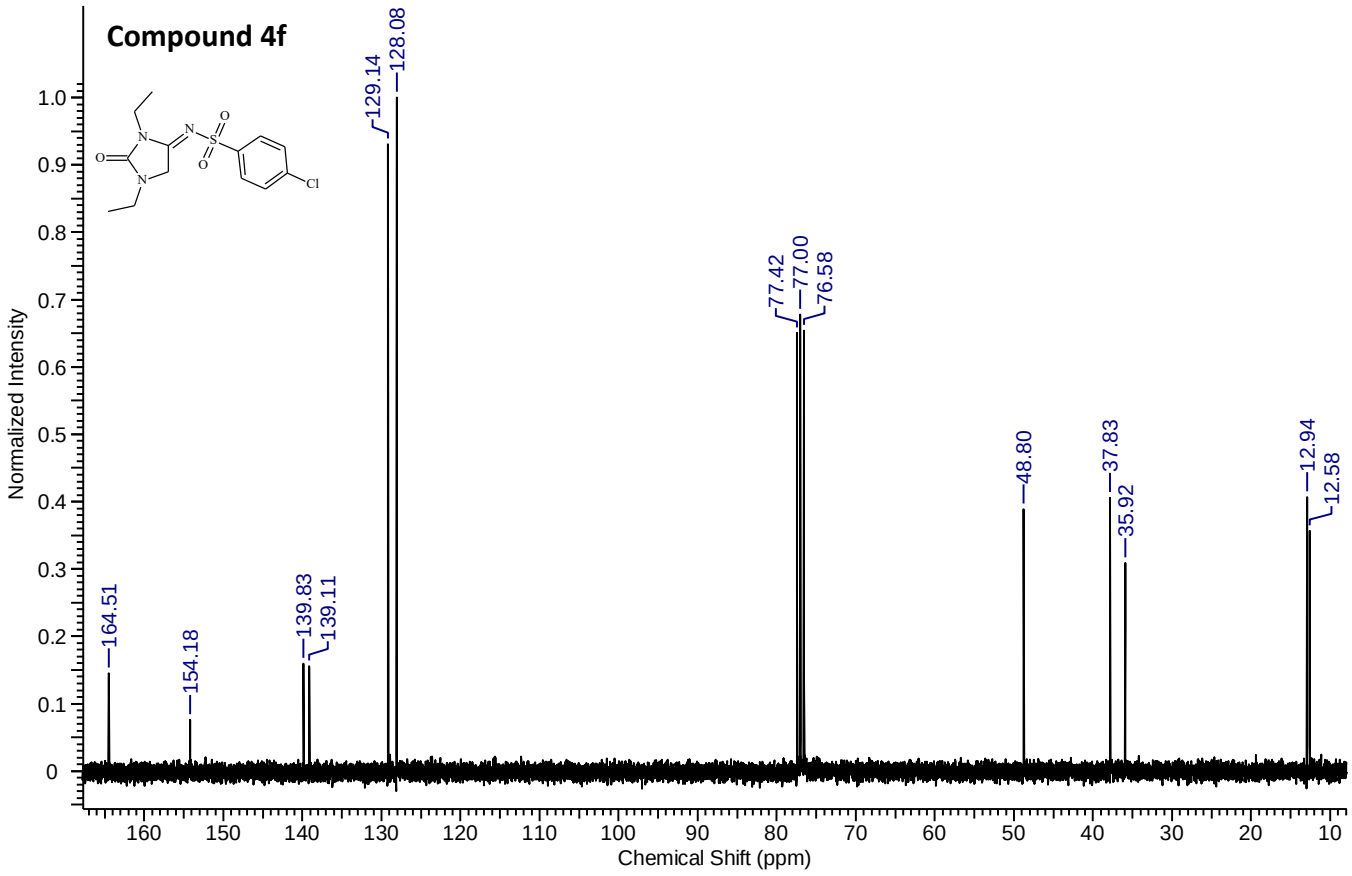
1.17
1.24
1.14
1.46
1.46
1.99
2.06
2.00
5.97


Compound 4f
Normalized Intensity
Chemical Shift (ppm)
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128.08
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76.58
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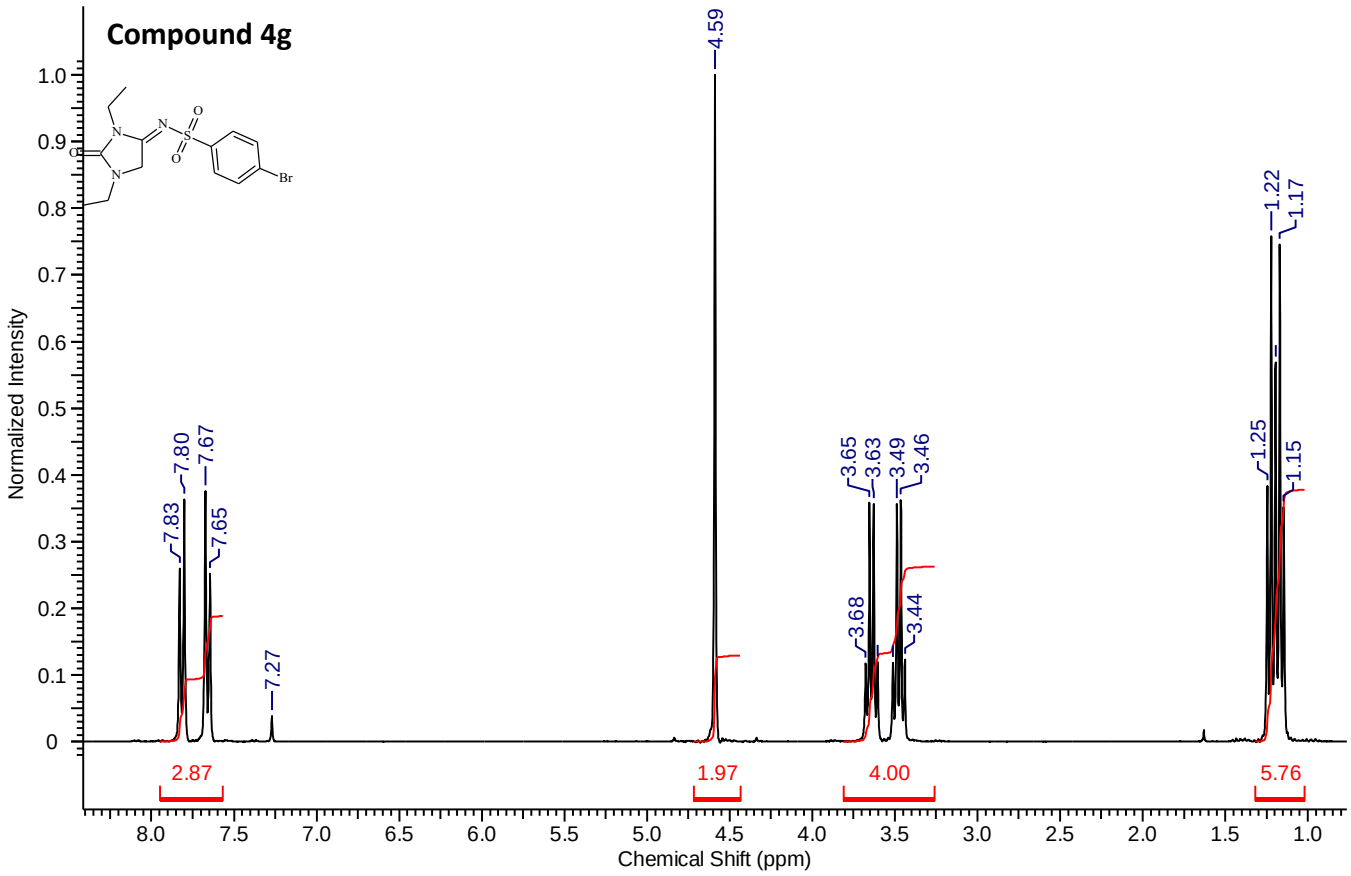
139.11
48.80
37.83
35.92
12.94
12.58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Normalized Intensity
Chemical Shift (ppm)
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7.80
7.67
7.65
7.27
3.68
3.65
3.63
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3.44
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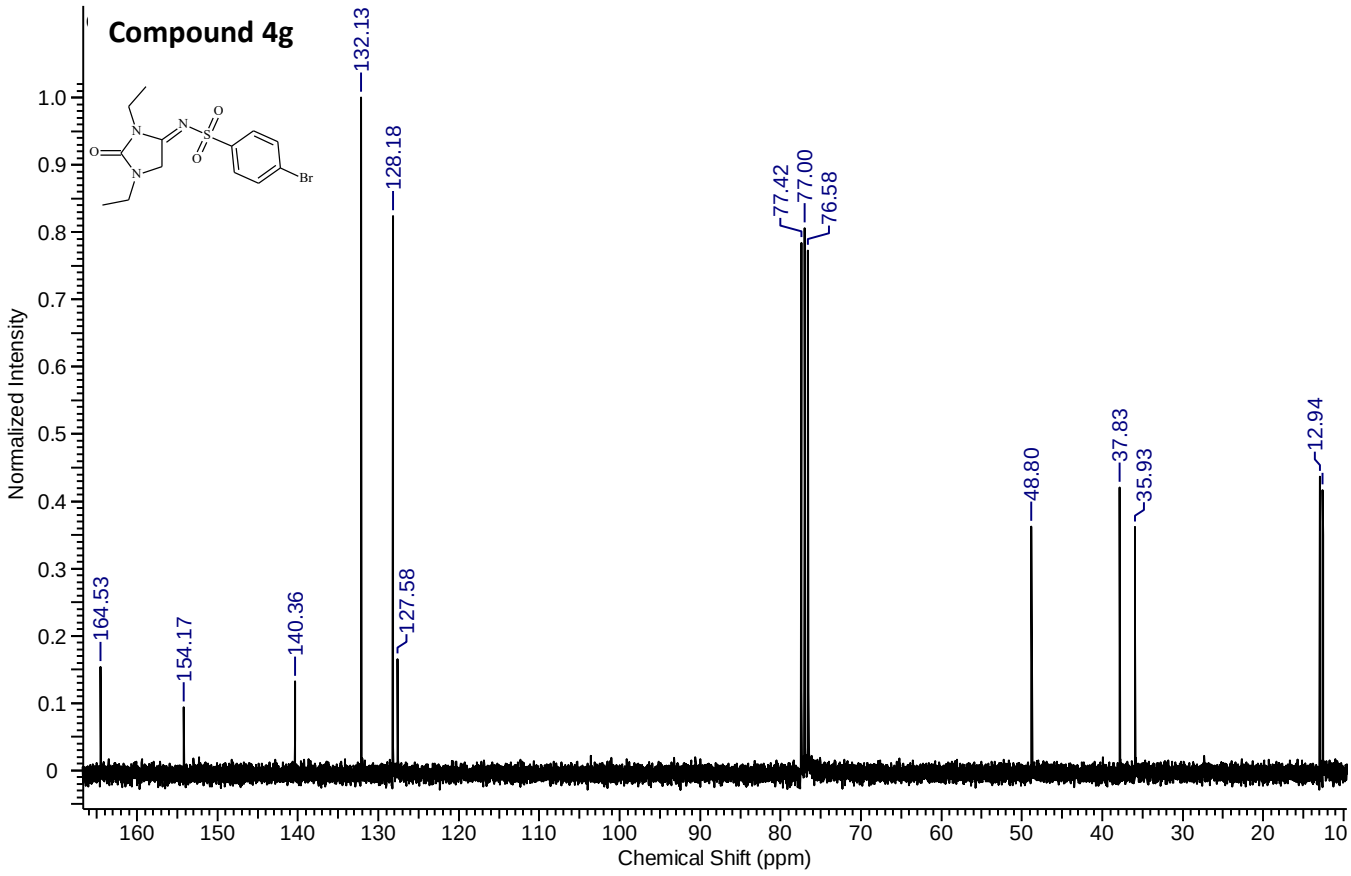
1.17
1.15
2.87
1.97
4.00
5.76


Compound 4g
Normalized Intensity
Chemical Shift (ppm)
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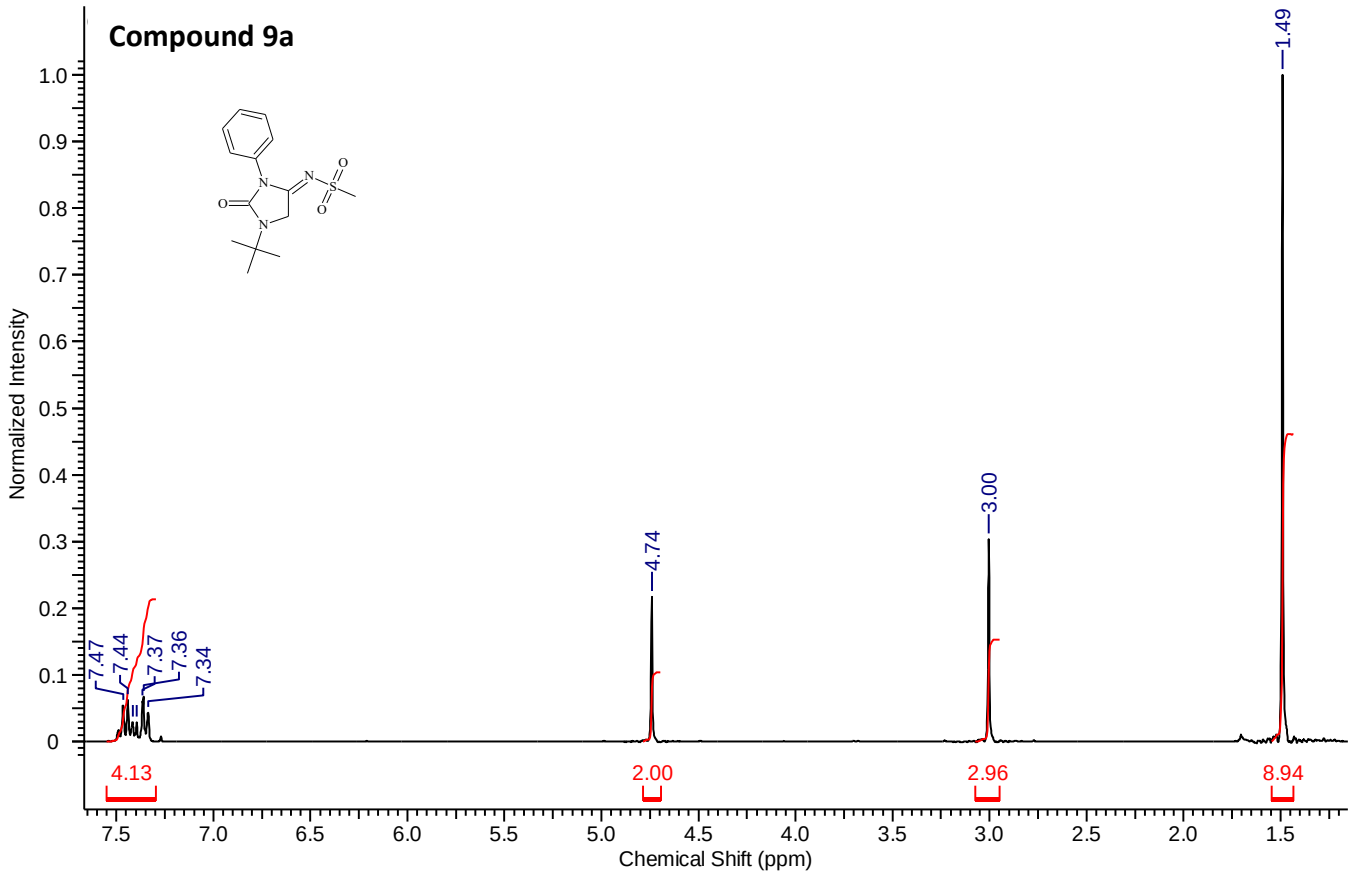
76.58
48.80
37.83
35.93
12.94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Normalized Intensity
Chemical Shift (ppm)
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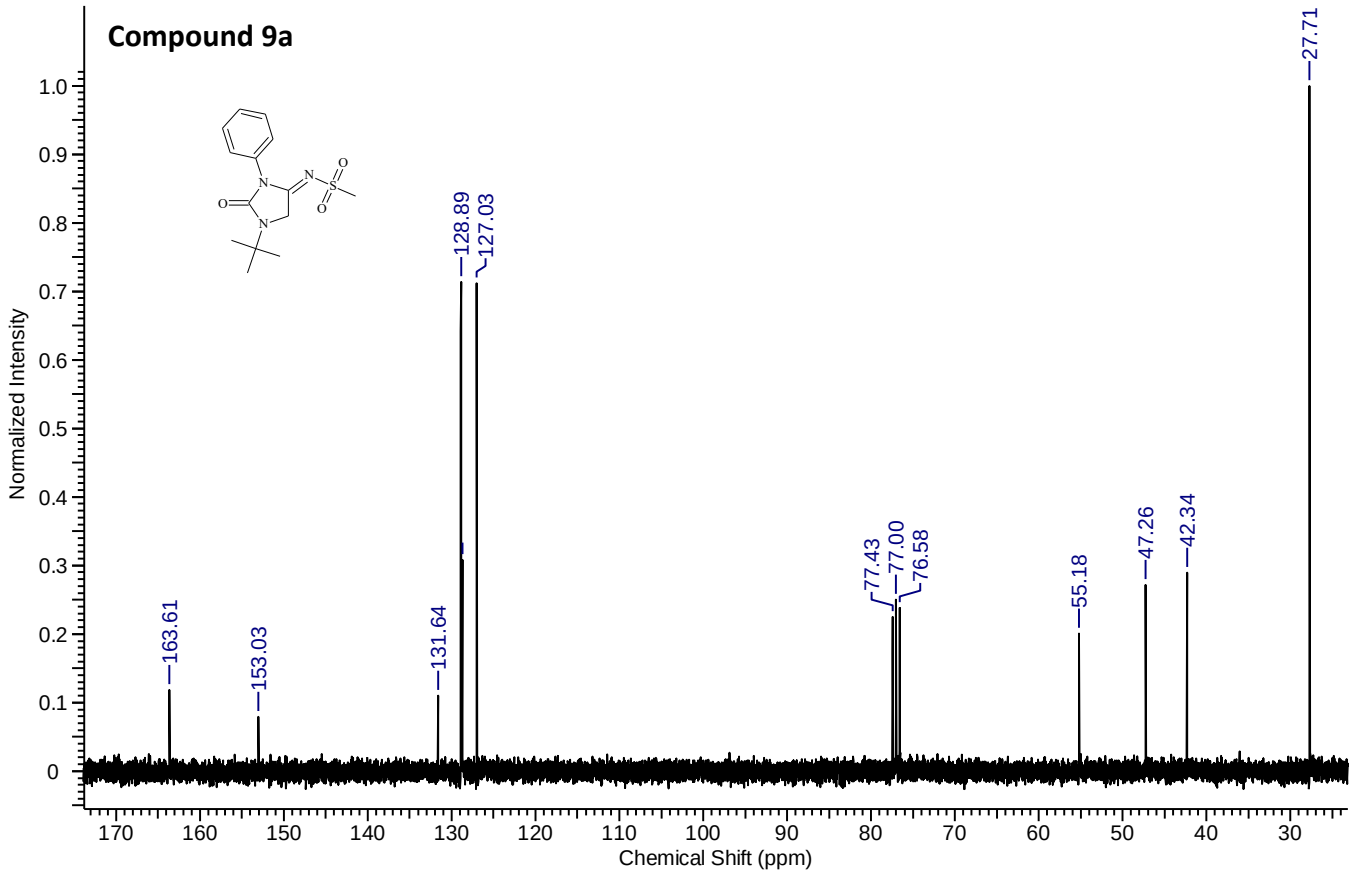
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Normalized Intensity
Chemical Shift (ppm)
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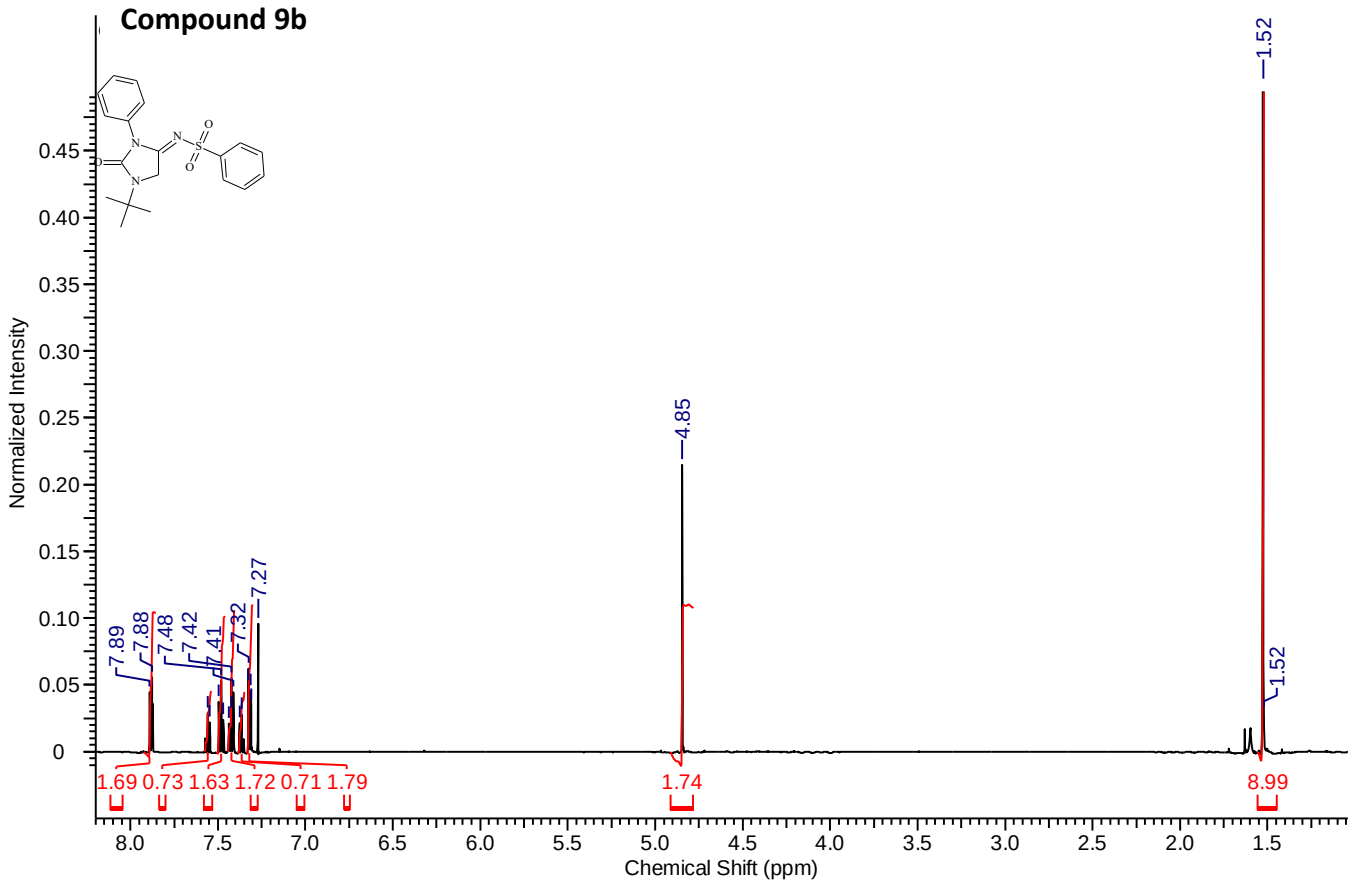
47.26
42.34


Compound 9b
Normalized Intensity
Chemical Shift (ppm)
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7.89
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7.32
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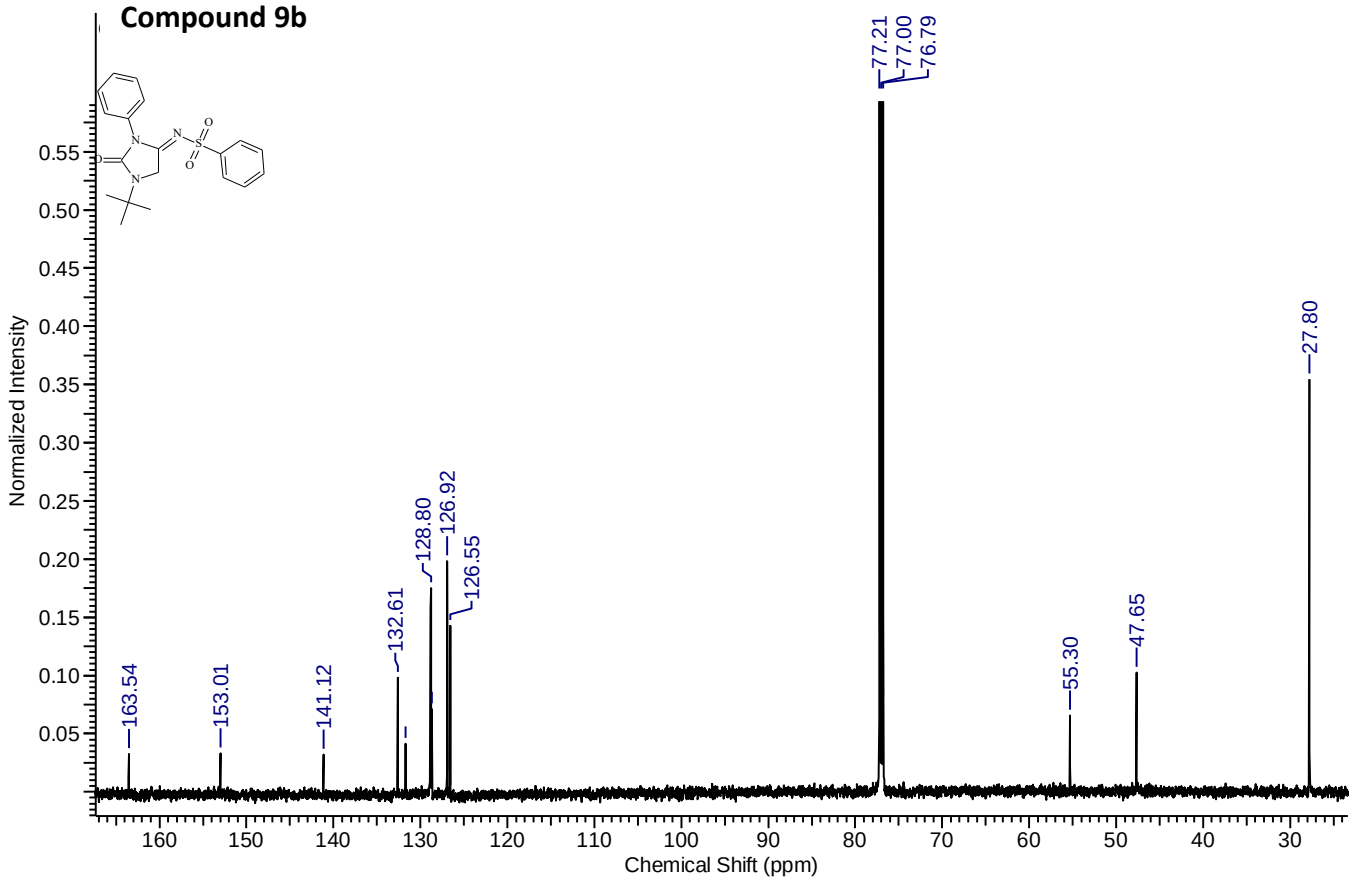
1.74
8.99


Compound 9b
Normalized Intensity
Chemical Shift (ppm)
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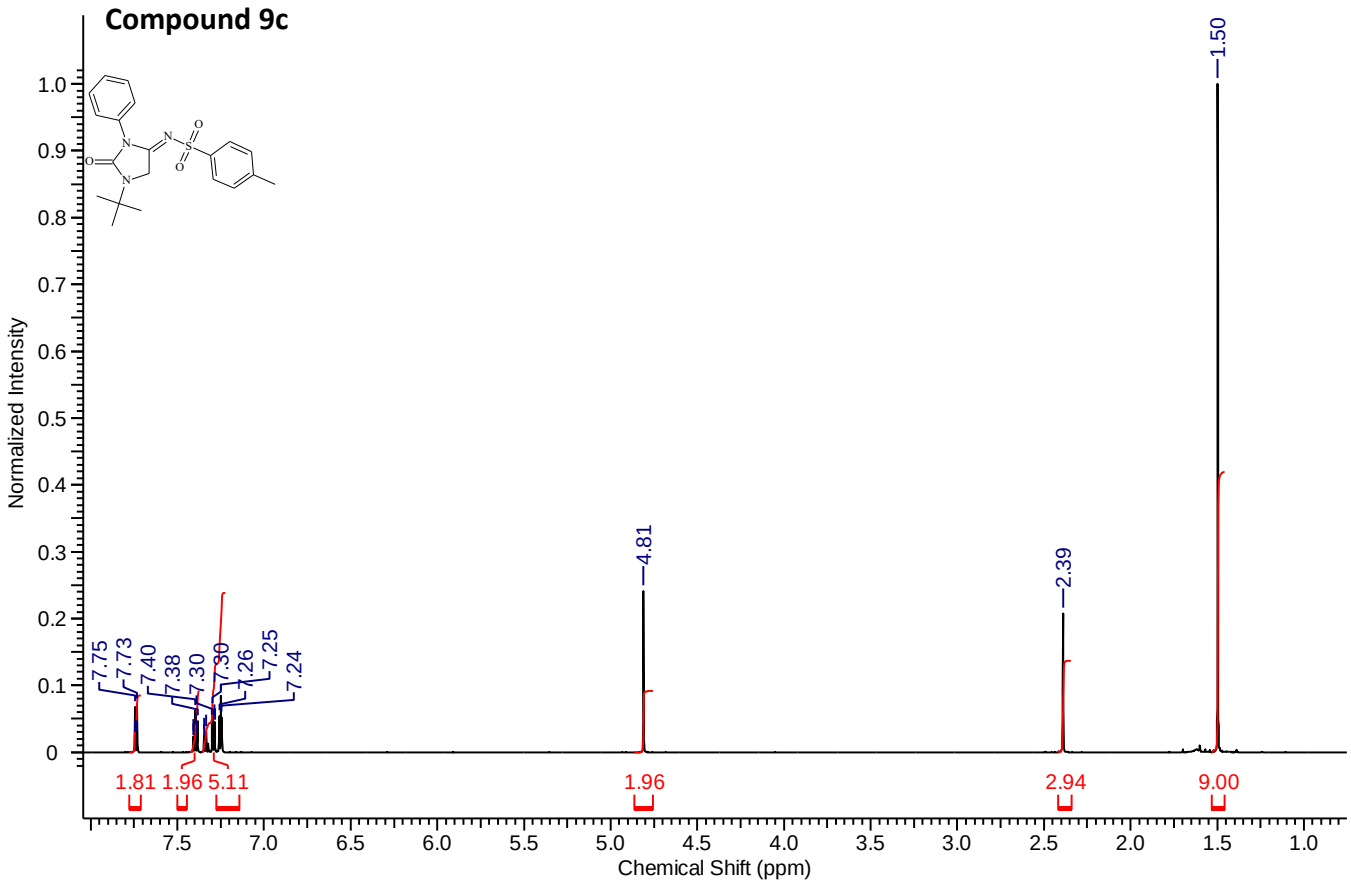
128.80
126.92
126.55
55.30
47.65
27.80


Compound 9c
Normalized Intensity
Chemical Shift (ppm)
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7.30
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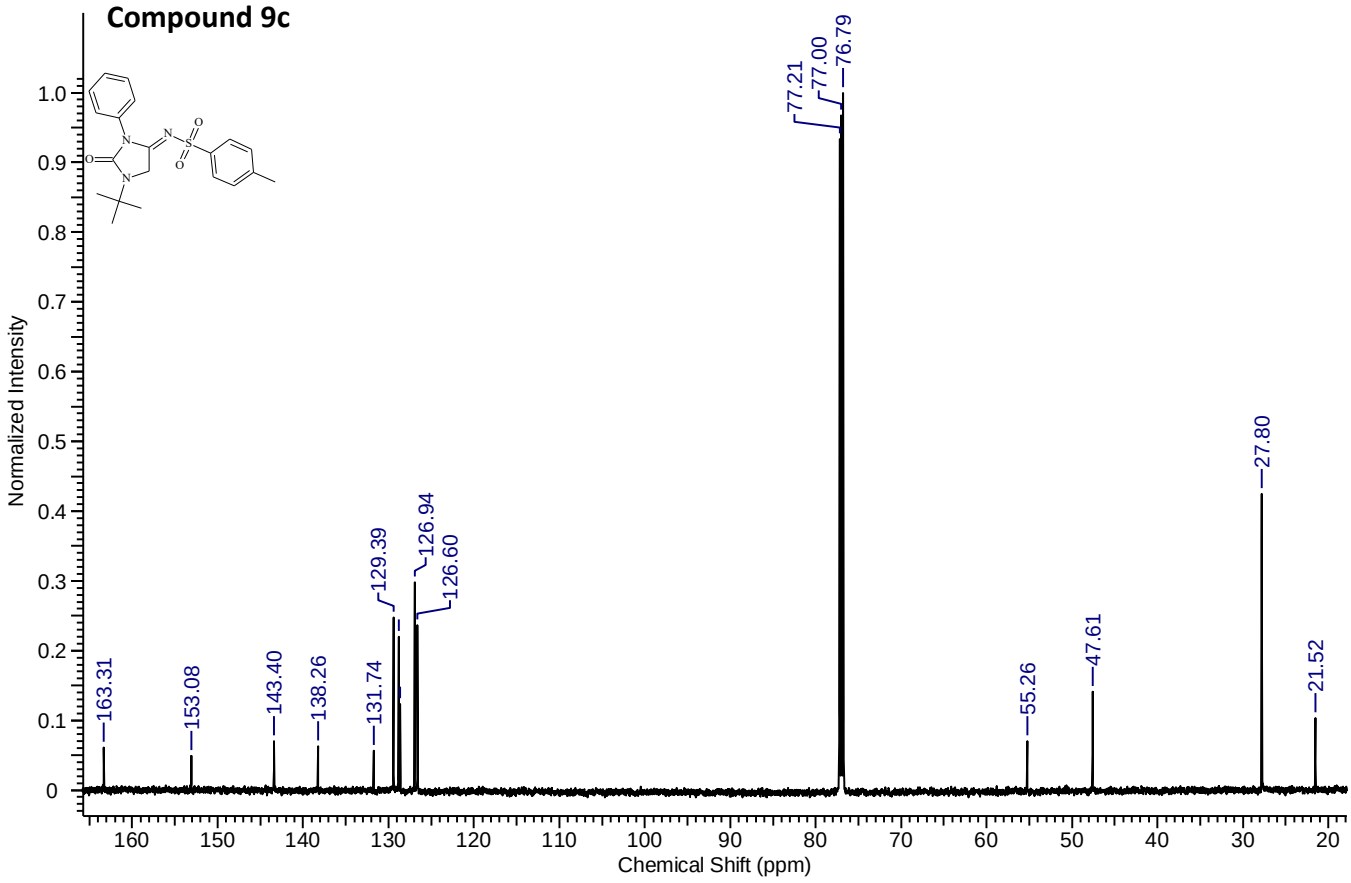
1.81
1.96
5.11
1.96
2.94
9.00


Compound 9c
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
163.31
153.08
143.40
138.26
131.74
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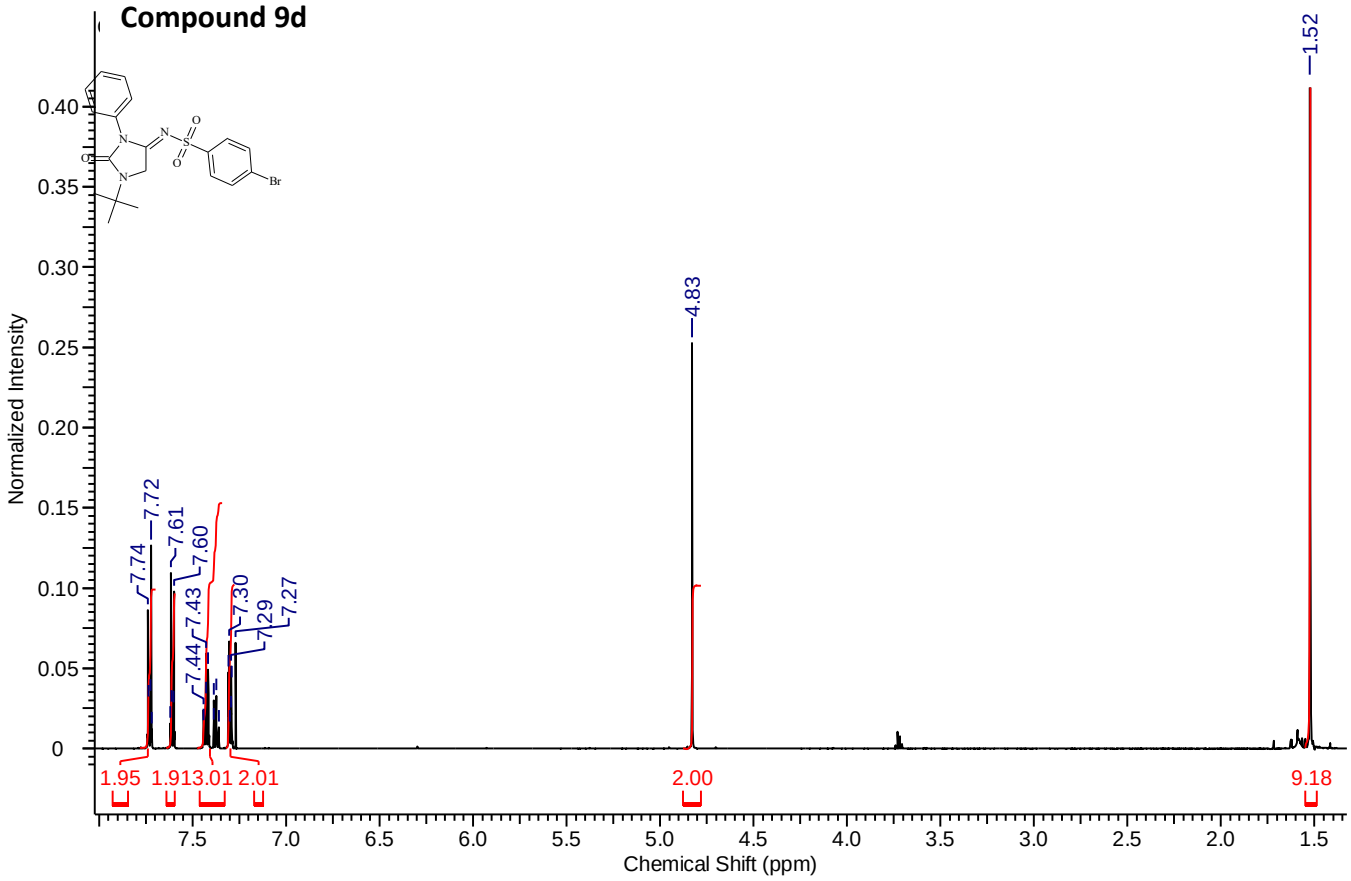
126.94
126.60
55.26
47.61
27.80
21.52


Compound 9d
Normalized Intensity
Chemical Shift (ppm)
7.74
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7.61
7.60
7.43
7.44
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7.29
7.27
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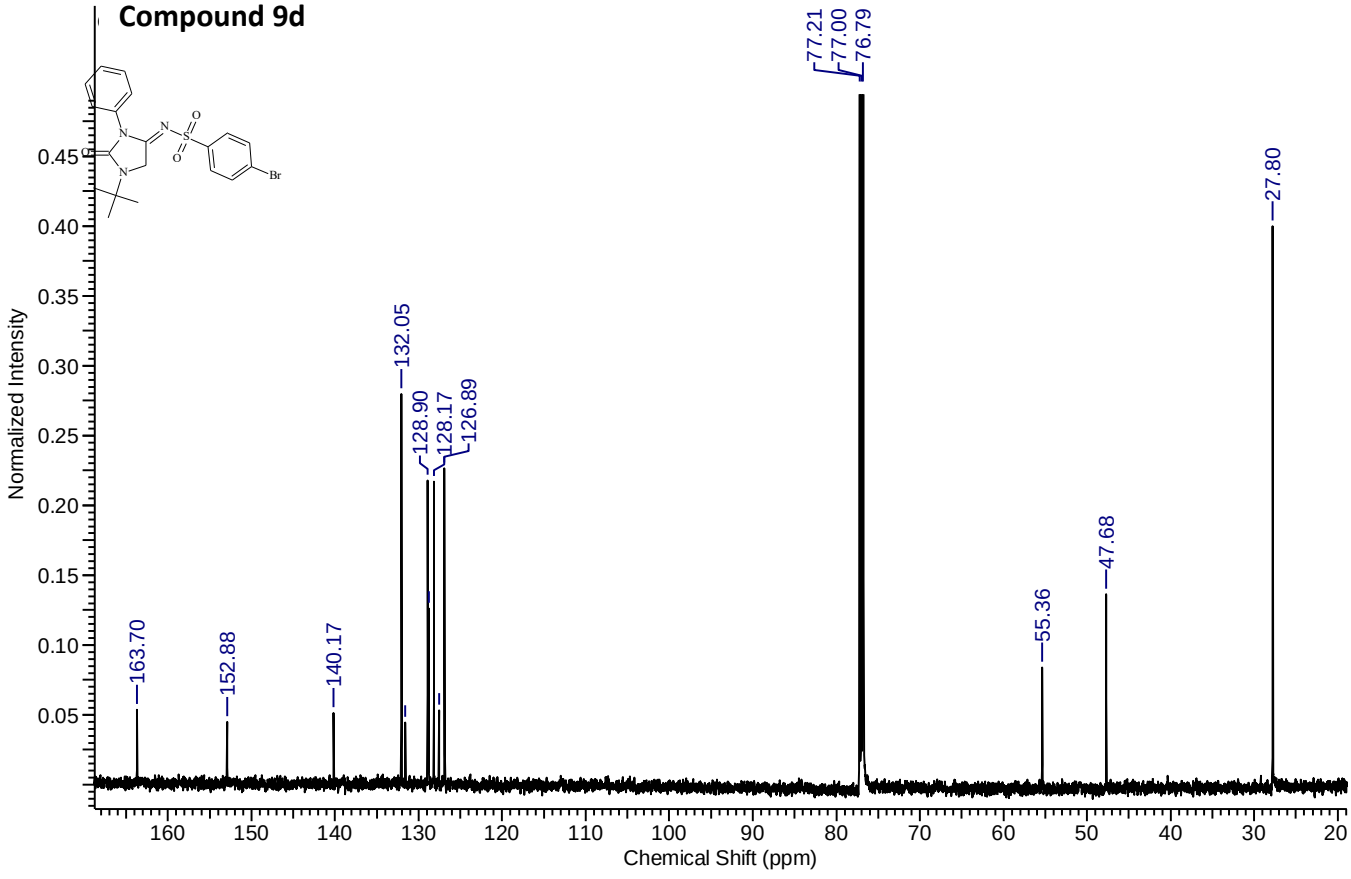
1.95
1.91
3.01
2.01
2.00
9.18


Compound 9d
Normalized Intensity
Chemical Shift (ppm)
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76.79
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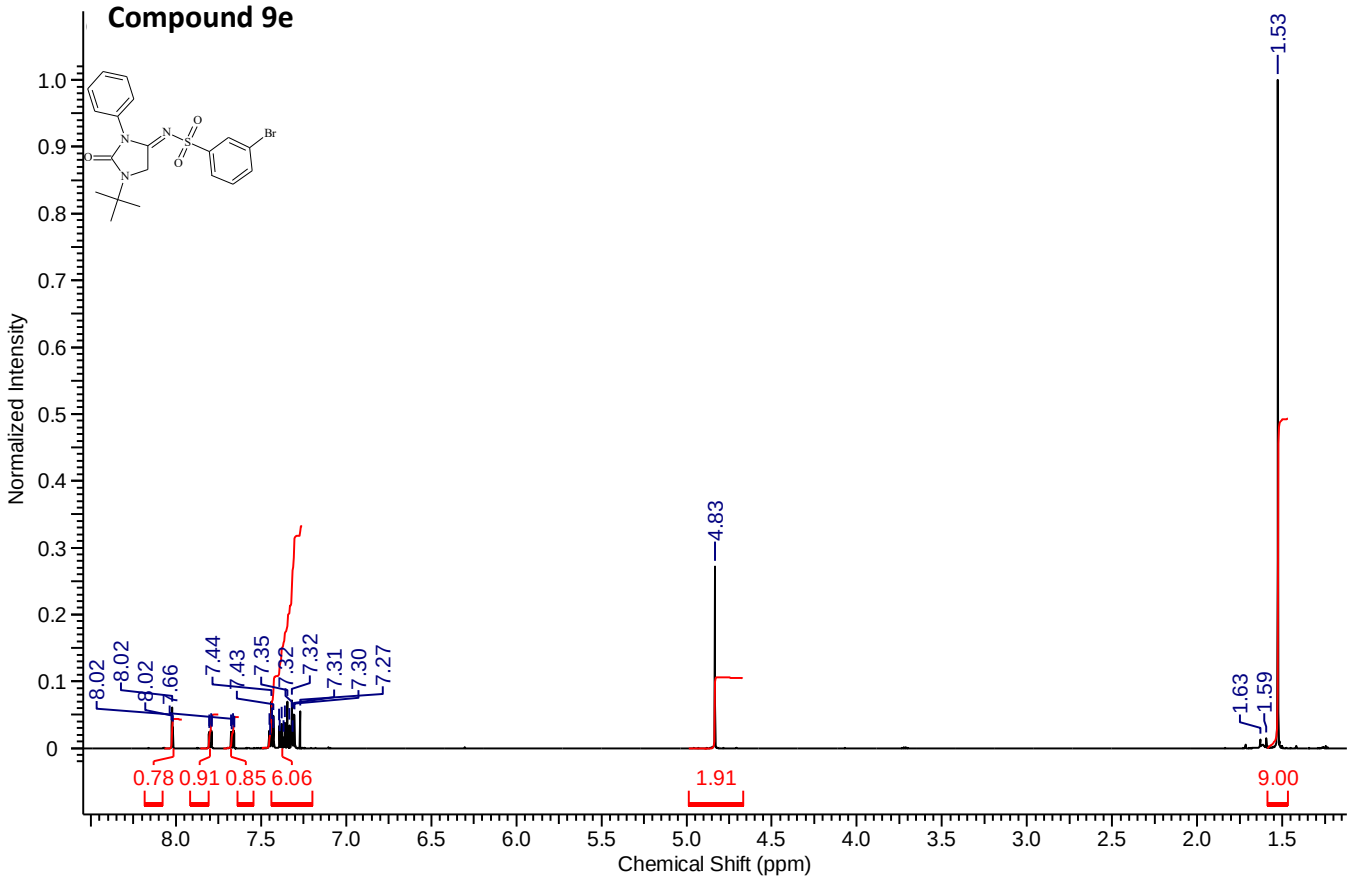
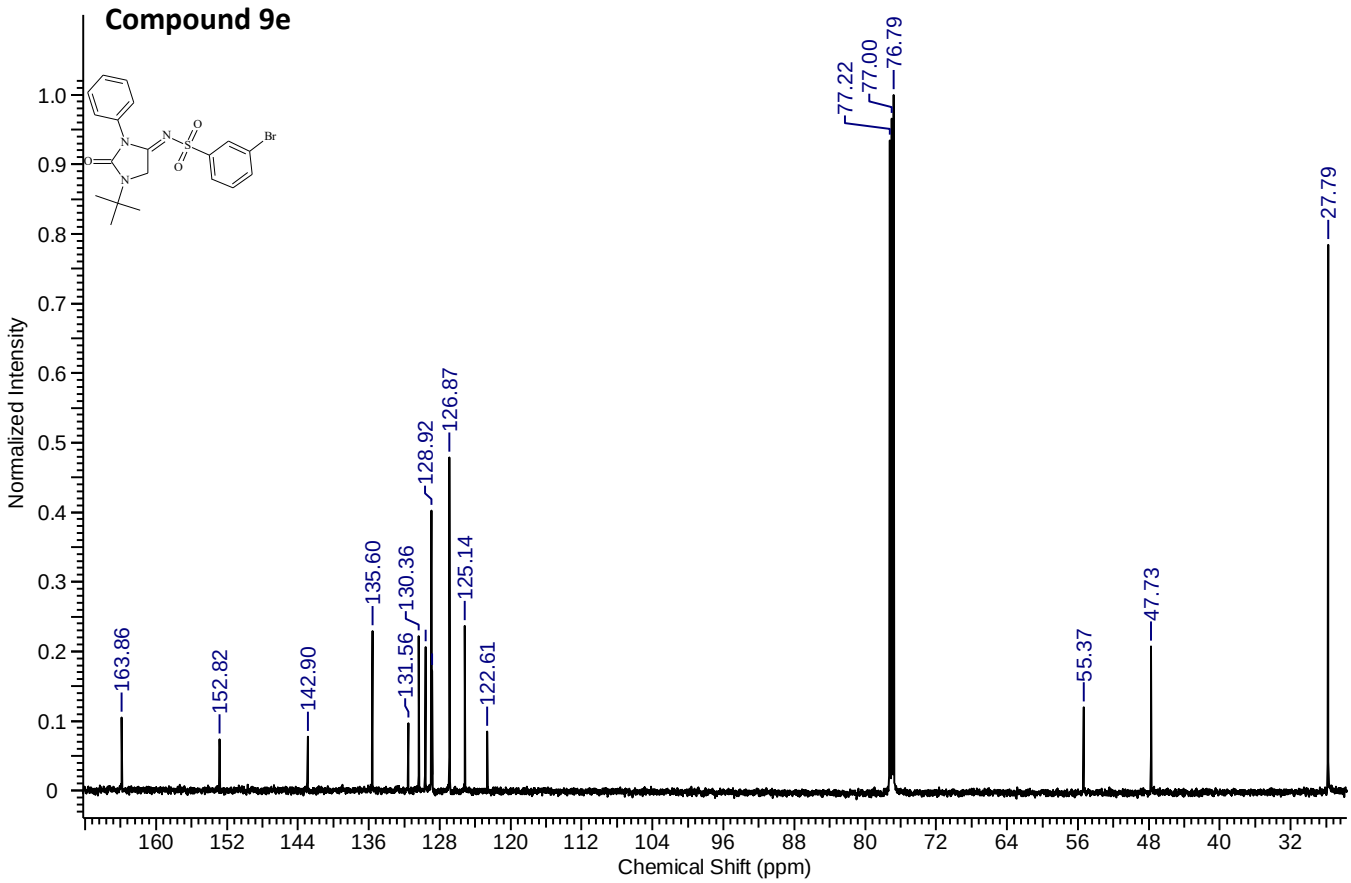
152.88
140.17
55.36
47.68
27.80


Compound 9e
Normalized Intensity
Chemical Shift (ppm)
8.02
8.02
8.02
7.66
7.44
7.43
7.35
7.32
7.32
7.31
7.30
7.27
4.83
1.63
1.59
1.53
0.78
0.91
0.85
6.06
1.91
9.00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Normalized Intensity
Chemical Shift (ppm)
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135.60
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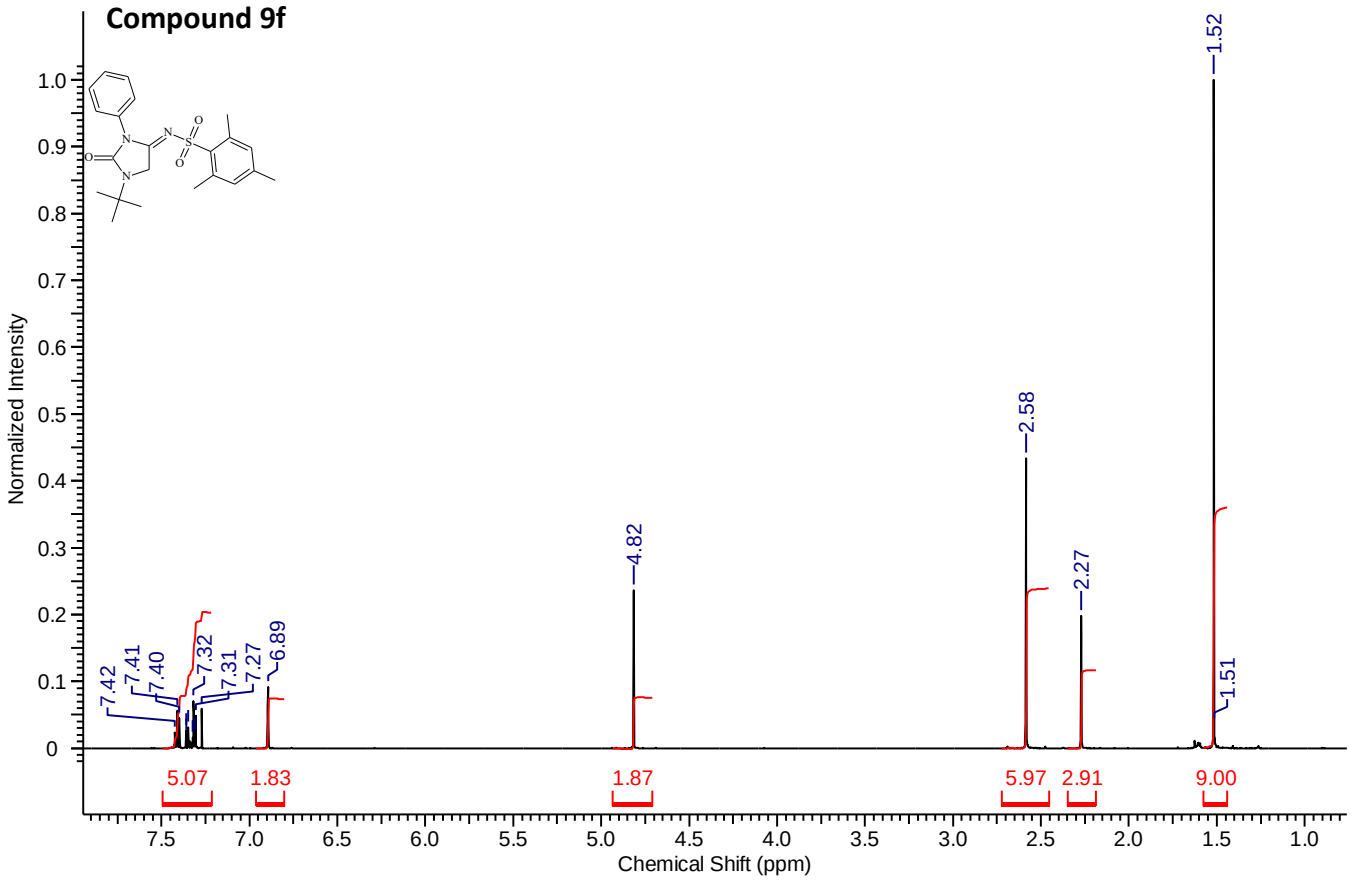
76.79
55.37
47.73
27.79


Compound 9f
Normalized Intensity
Chemical Shift (ppm)
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2.58
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7.42
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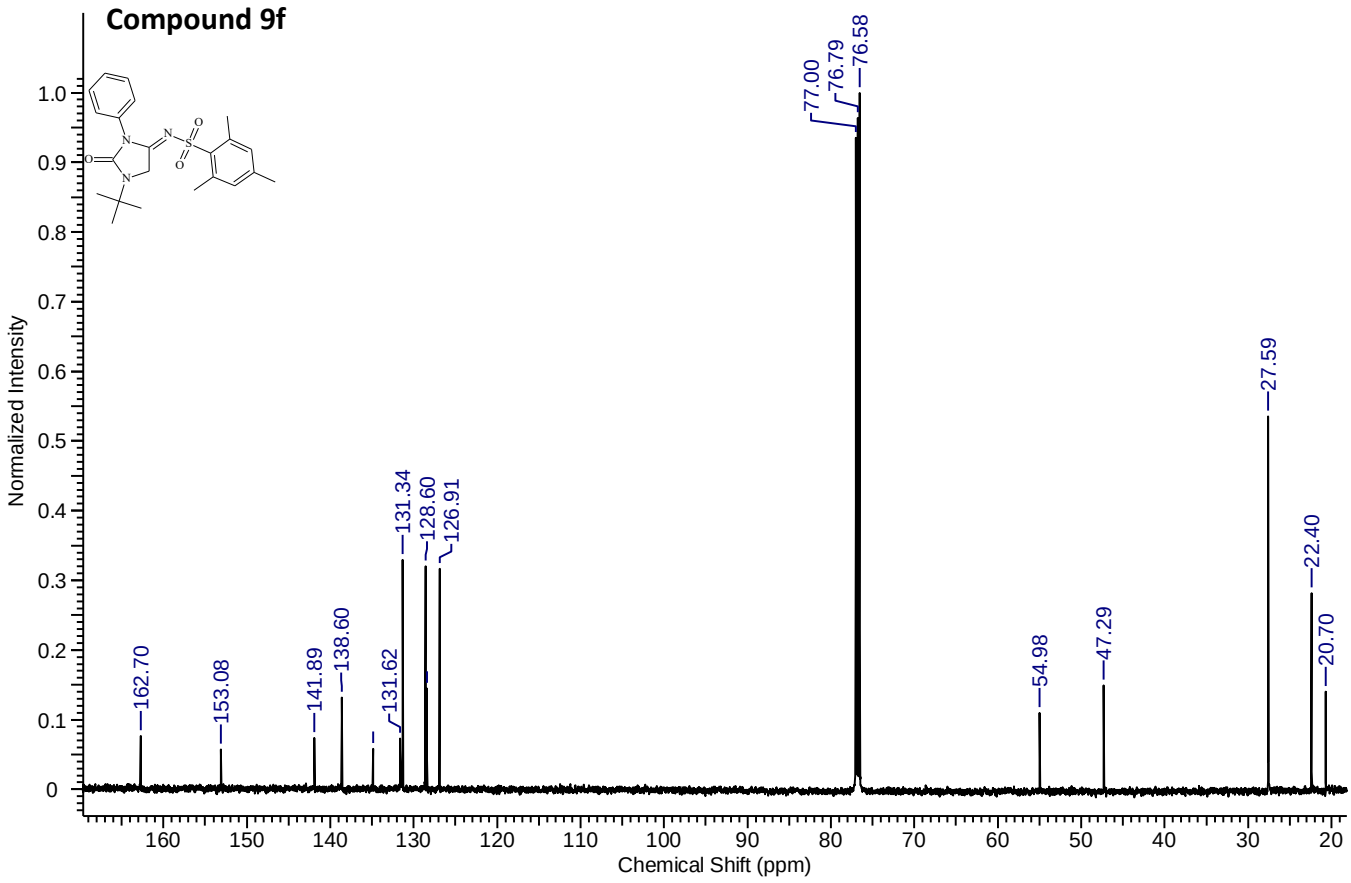
2.91
9.00


Compound 9f
Normalized Intensity
Chemical Shift (ppm)
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76.79
76.58
131.34
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131.62
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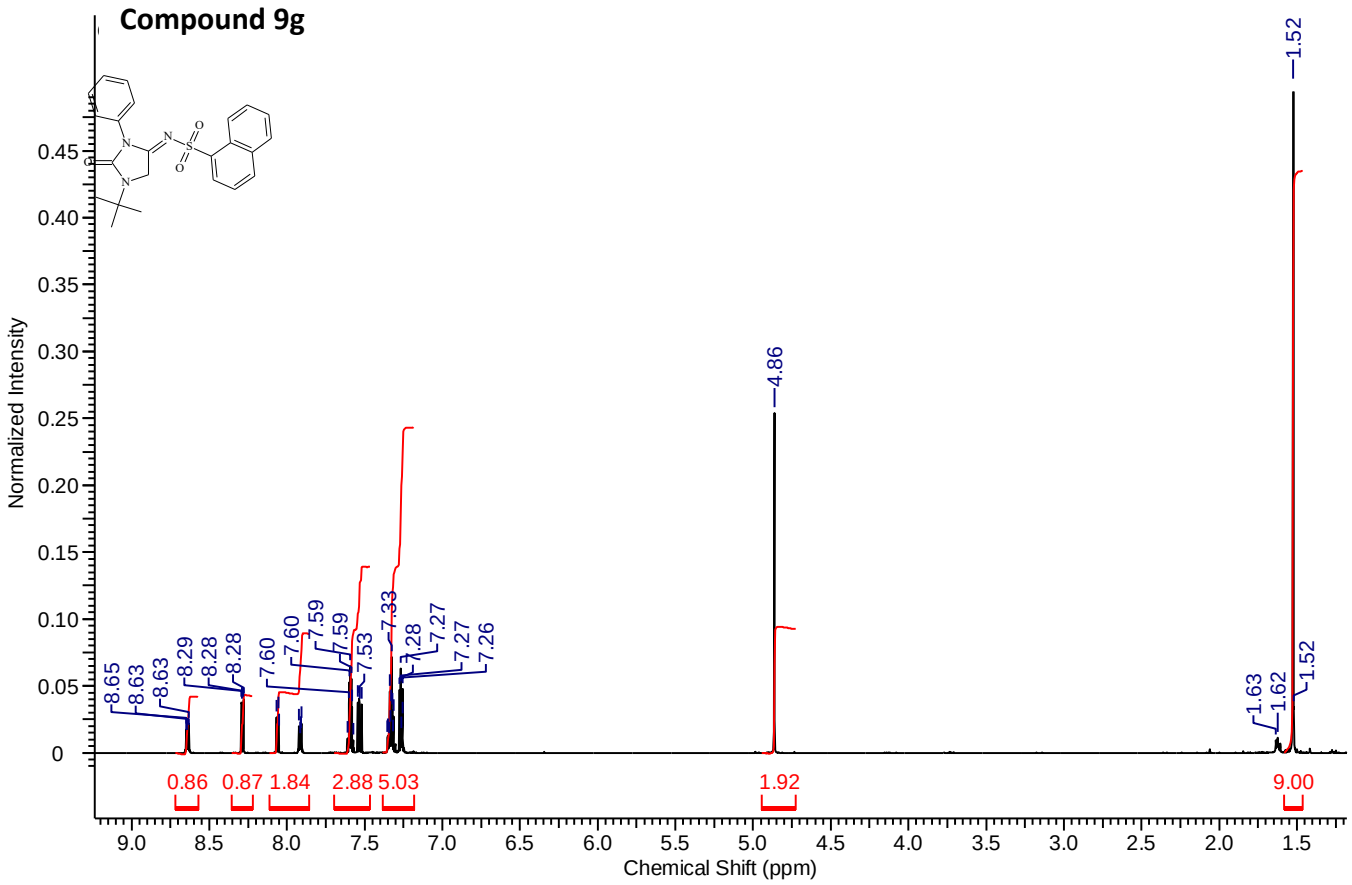
47.29
27.59
22.40
20.70


Compound 9g
Normalized Intensity
Chemical Shift (ppm)
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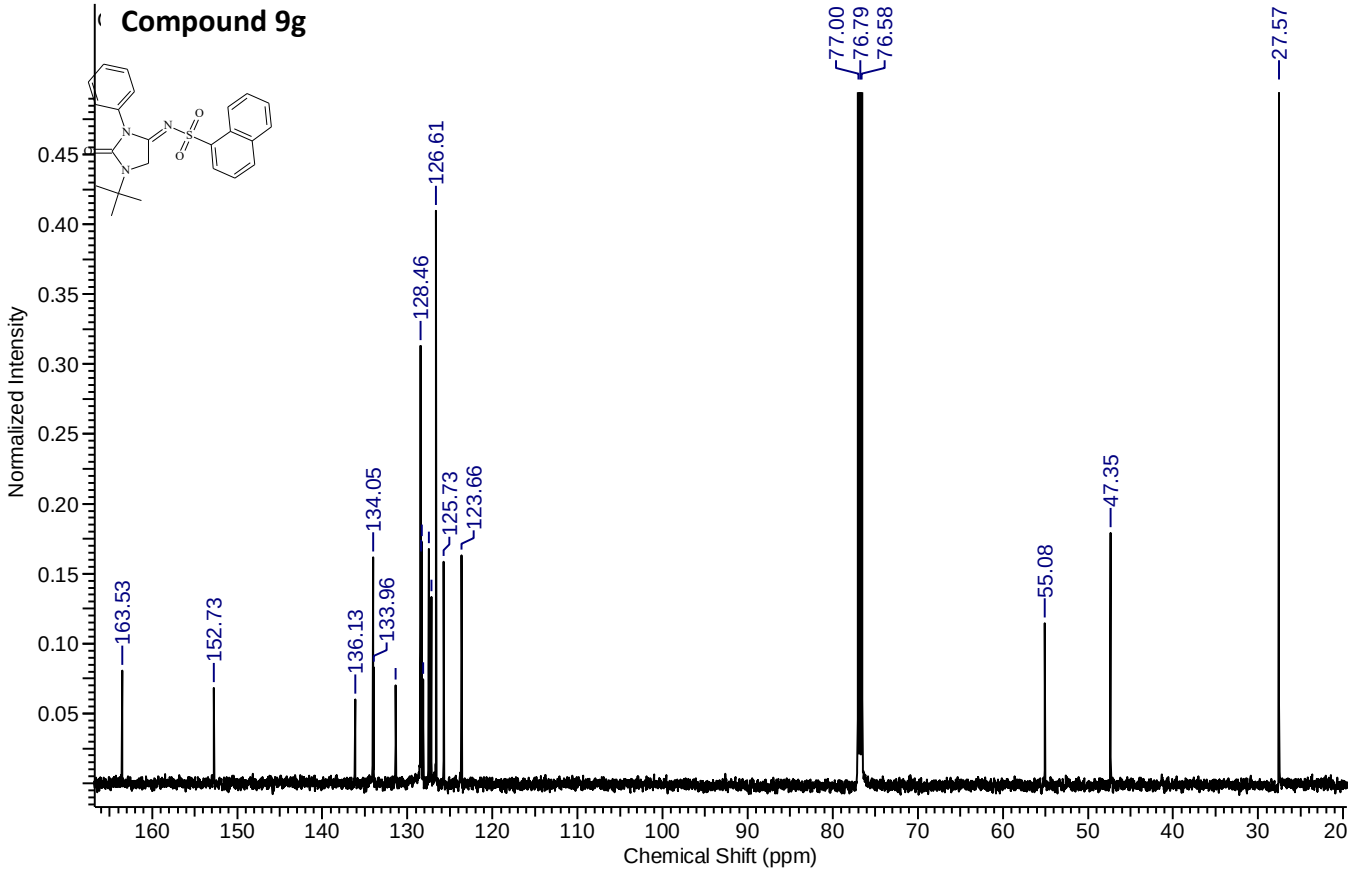
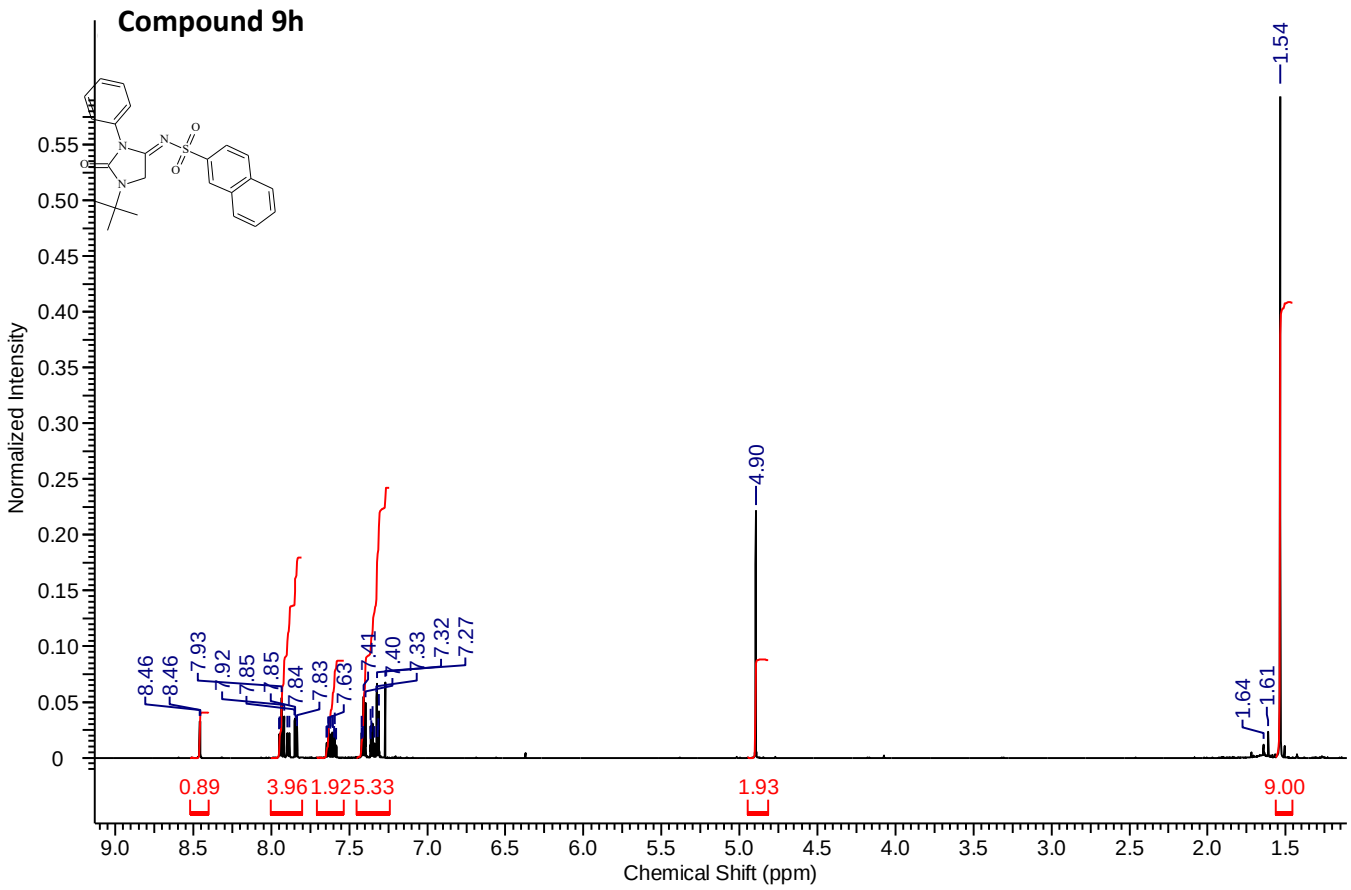
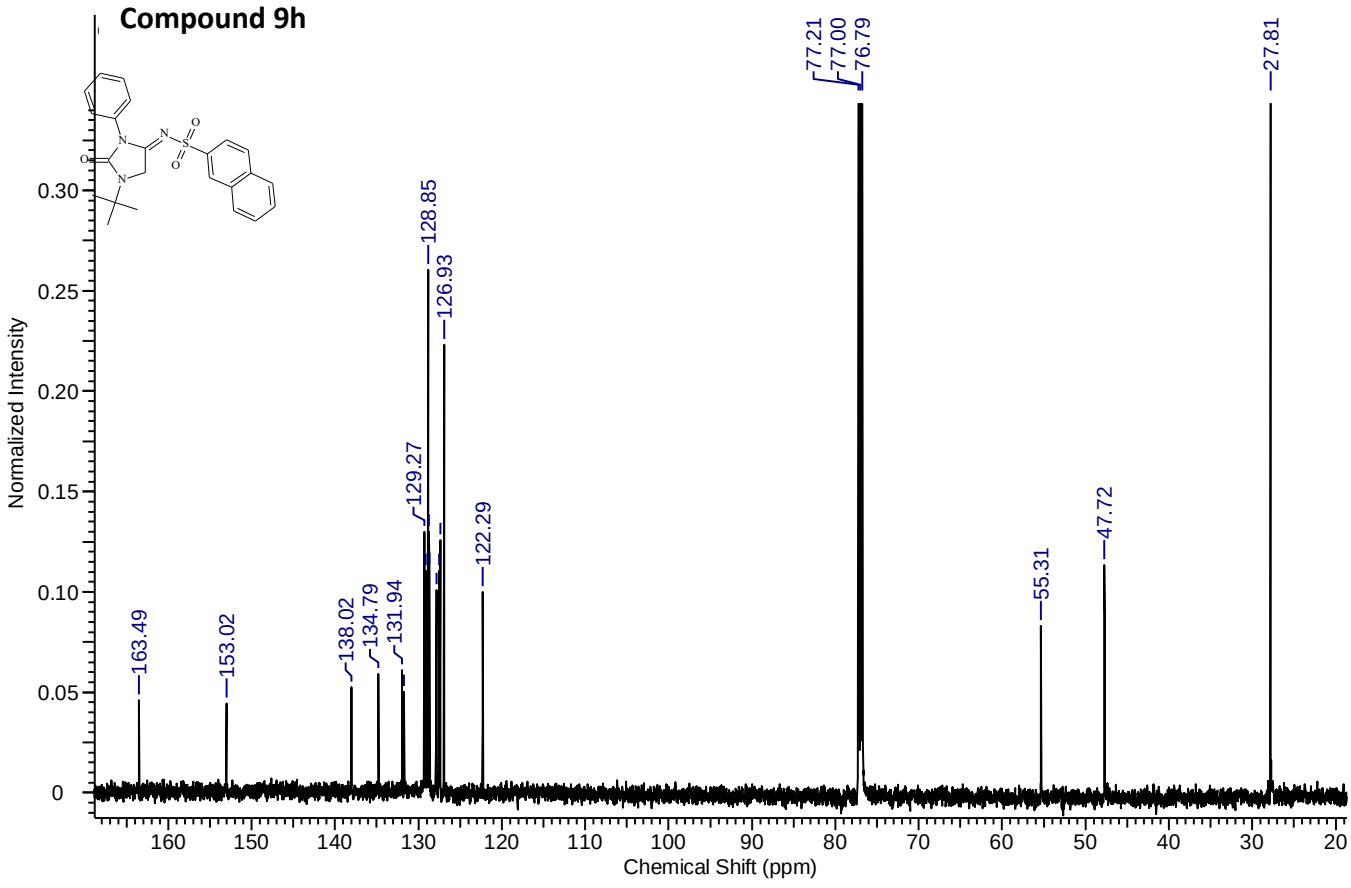
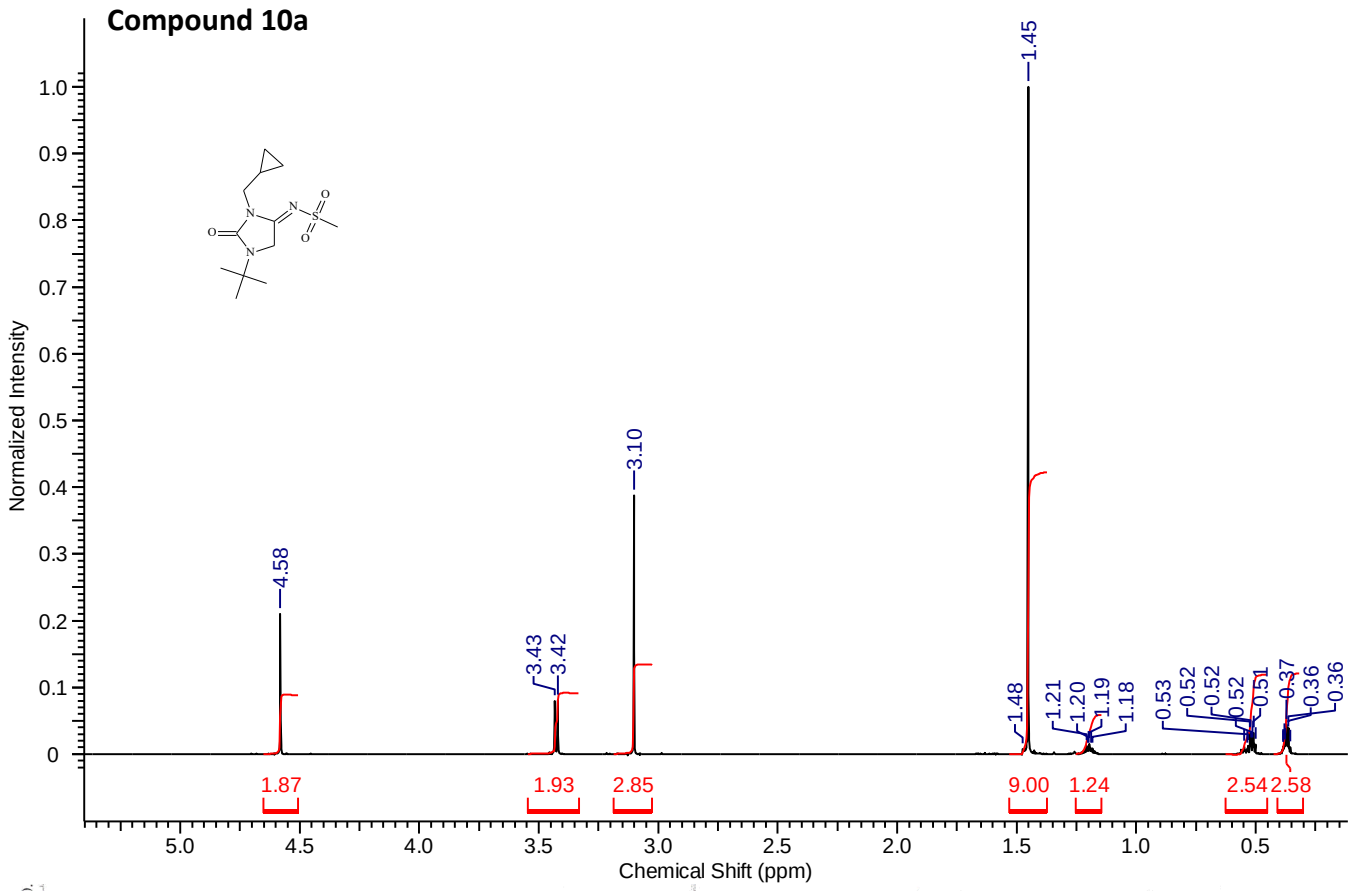
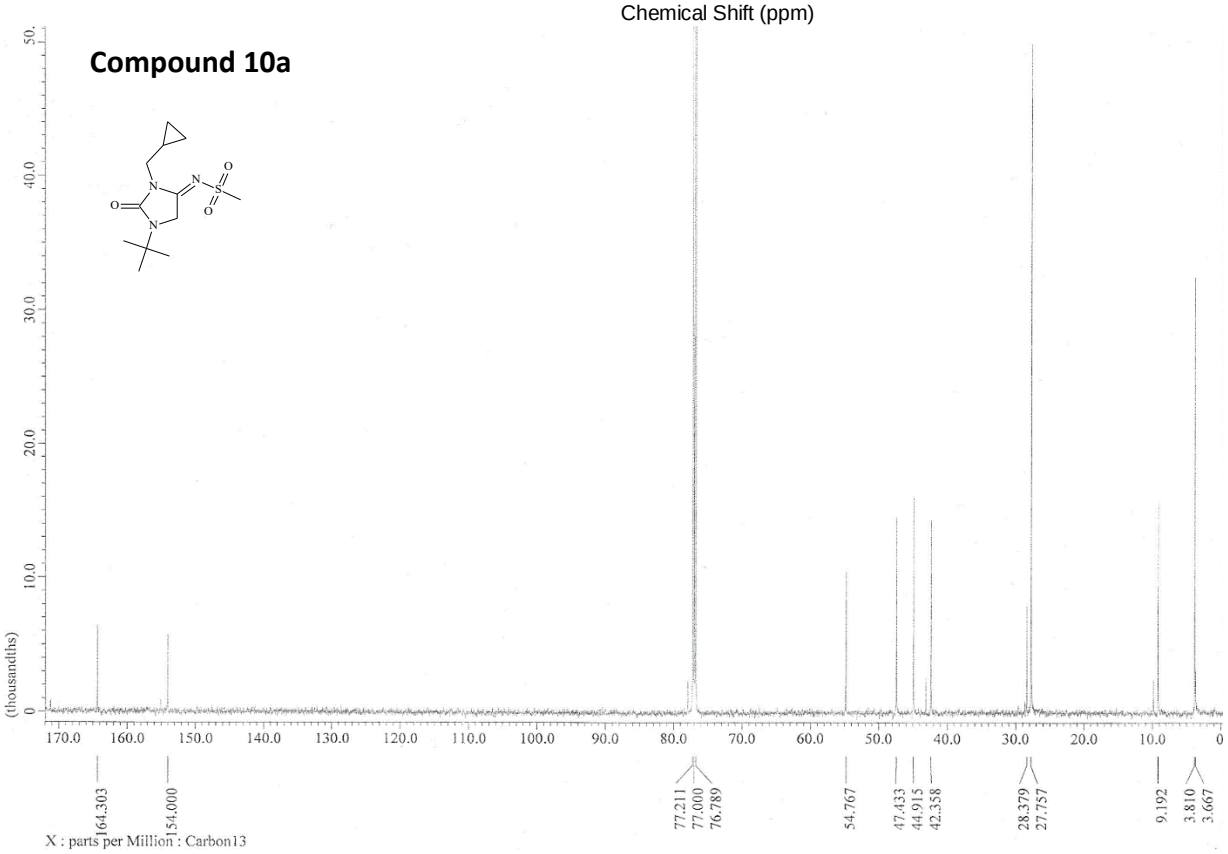
8.63
8.63
8.29
8.28
8.28
7.60
7.60
7.59
7.59
7.53
7.33
7.28
7.27
7.27
7.26
4.86
1.63
1.62
1.52
1.52
0.86
0.87
1.84
2.88
5.03
1.92
9.00

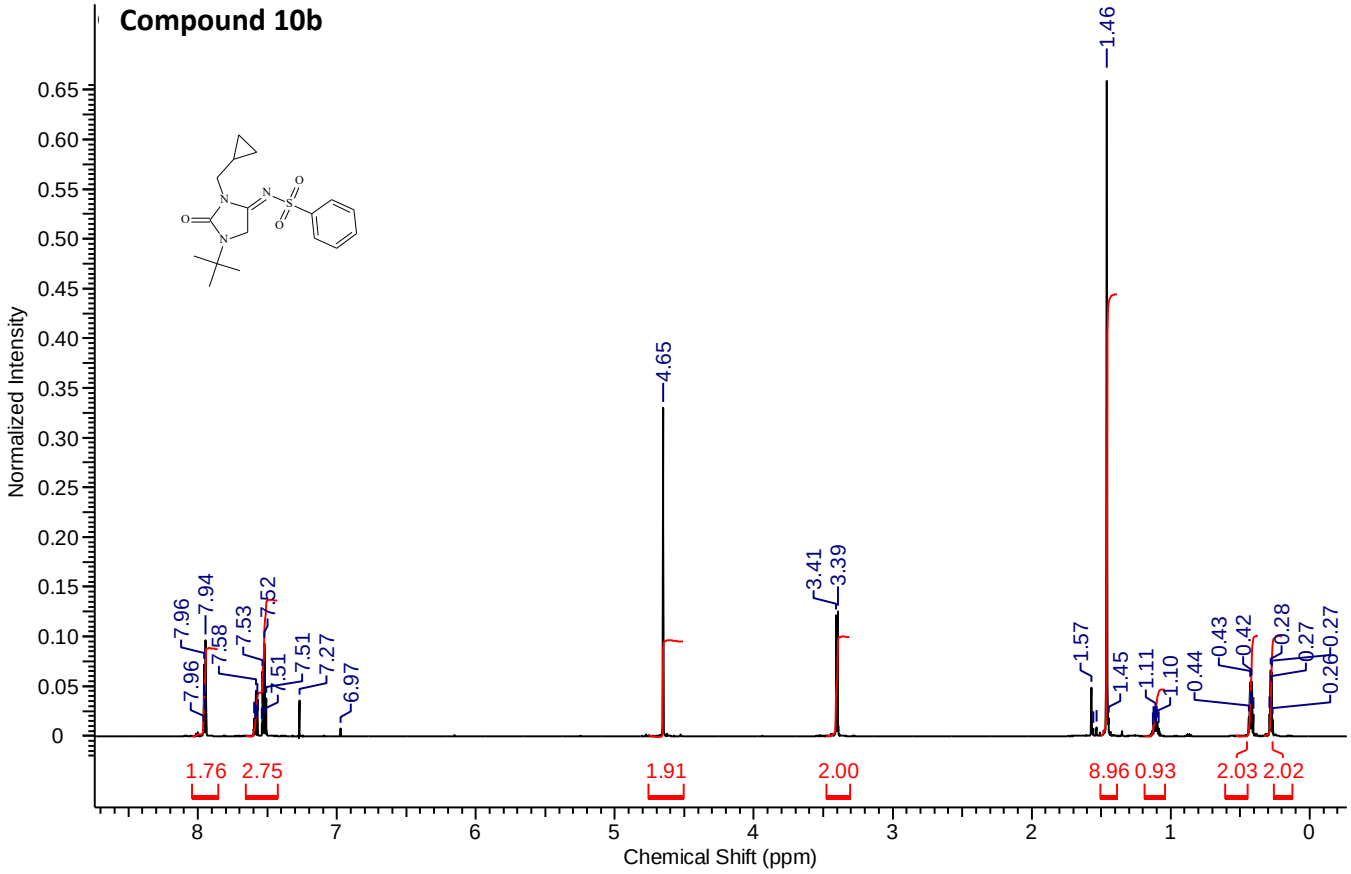

Compound 9g
Normalized Intensity
Chemical Shift (ppm)
163.53
152.73
136.13
134.05
133.96
128.46
126.61
125.73
123.66
77.00
76.79
76.58
55.08
47.35
27.57

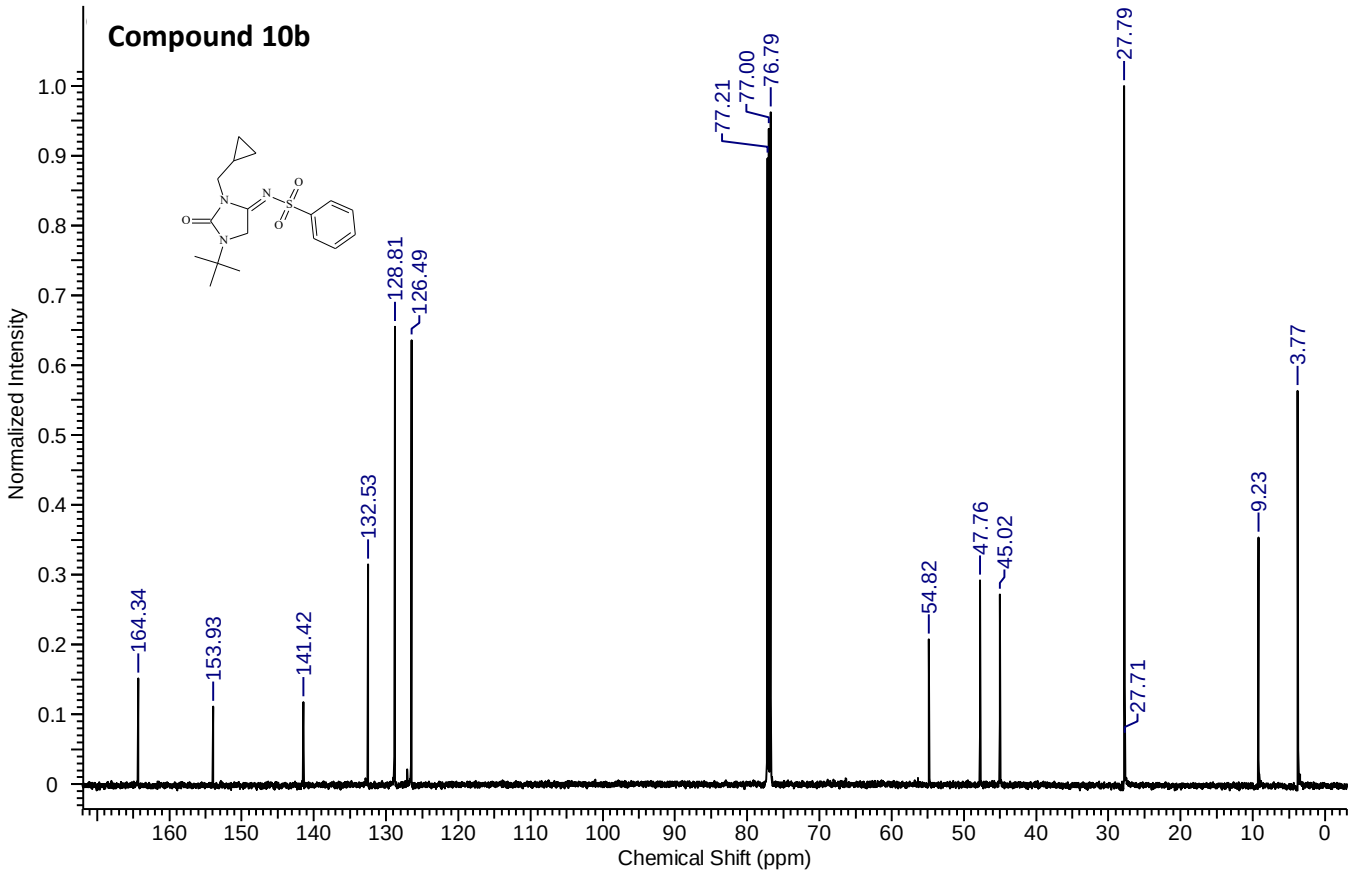

Compound 9h
Normalized Intensity
Chemical Shift (ppm)
8.46
8.46
7.93
7.92
7.85
7.85
7.84
7.83
7.63
7.41
7.40
7.33
7.32
7.27
4.90
1.64
1.61
1.54
0.89
3.96
1.92
5.33
1.93
9.00

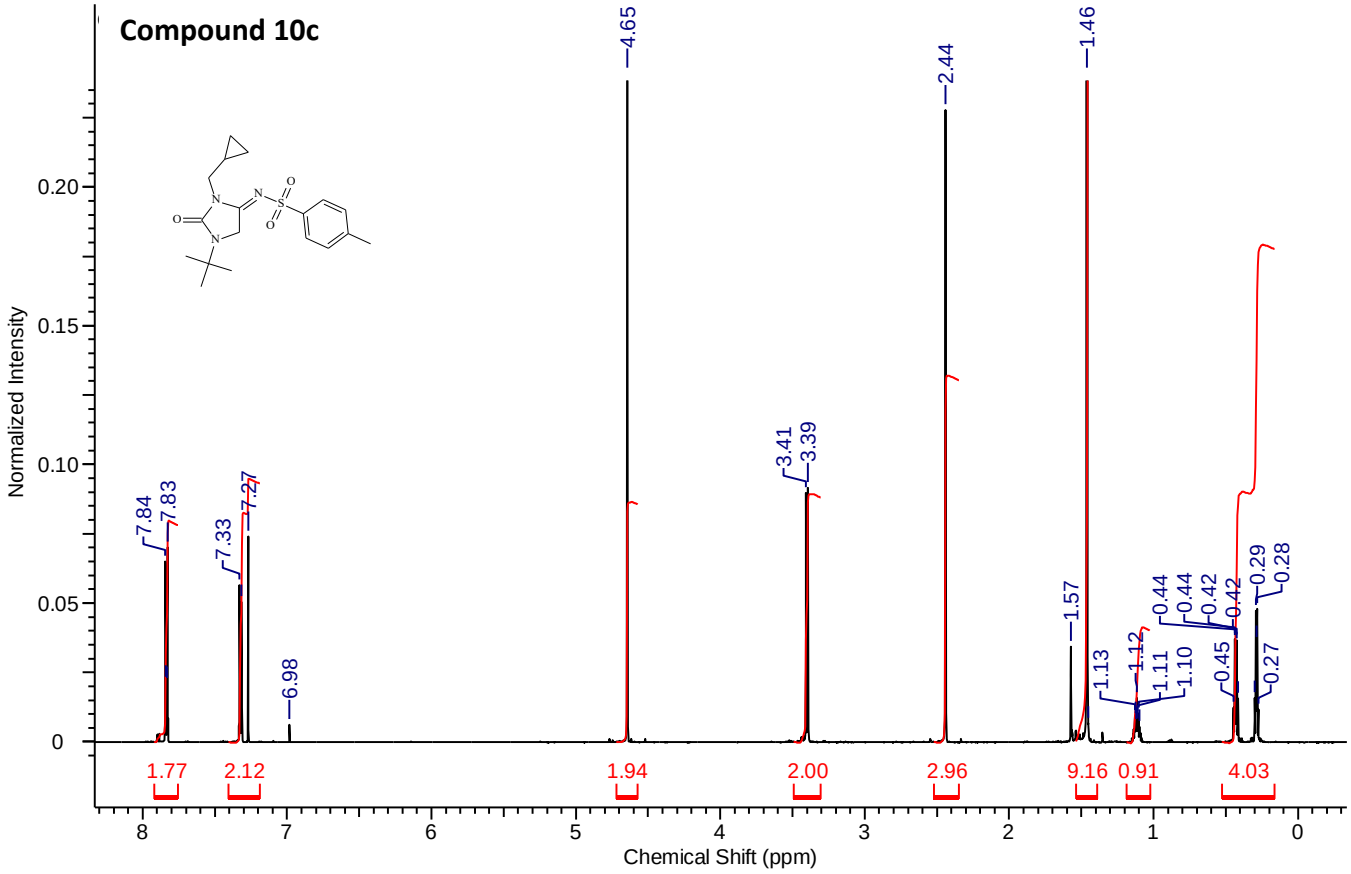

Compound 9h
Normalized Intensity
Chemical Shift (ppm)
163.49
153.02
138.02
134.79
131.94
129.27
128.85
126.93
122.29
77.21
77.00
76.79
55.31
47.72
27.81

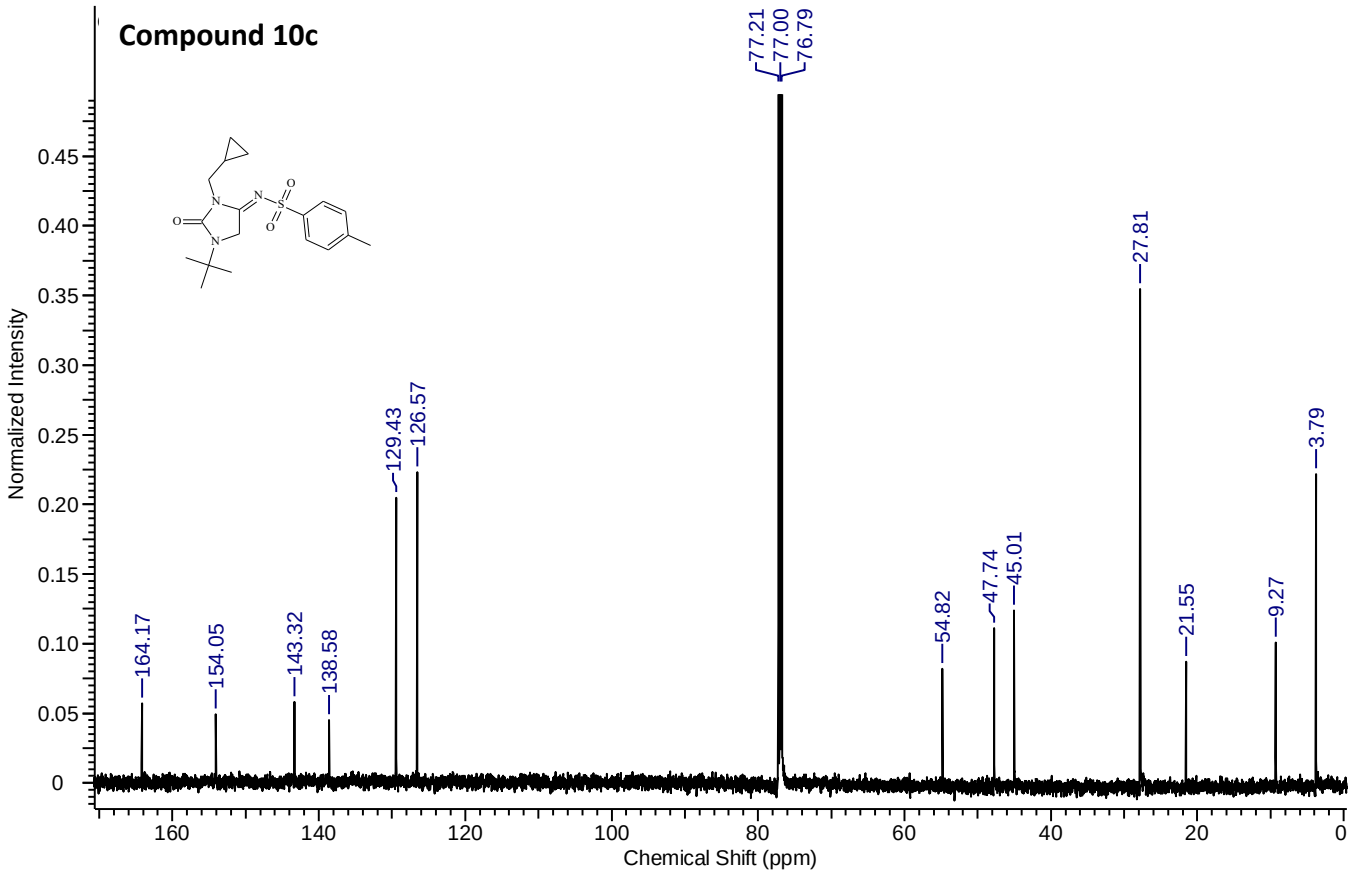

Compound 10a
Normalized Intensity
Chemical Shift (ppm)
4.58
3.43
3.42
3.10
1.48
1.45
1.21
1.20
1.19
1.18
0.53
0.52
0.52
0.52
0.51
0.37
0.36
0.36
1.87
1.93
2.85
9.00
1.24
2.54
2.58

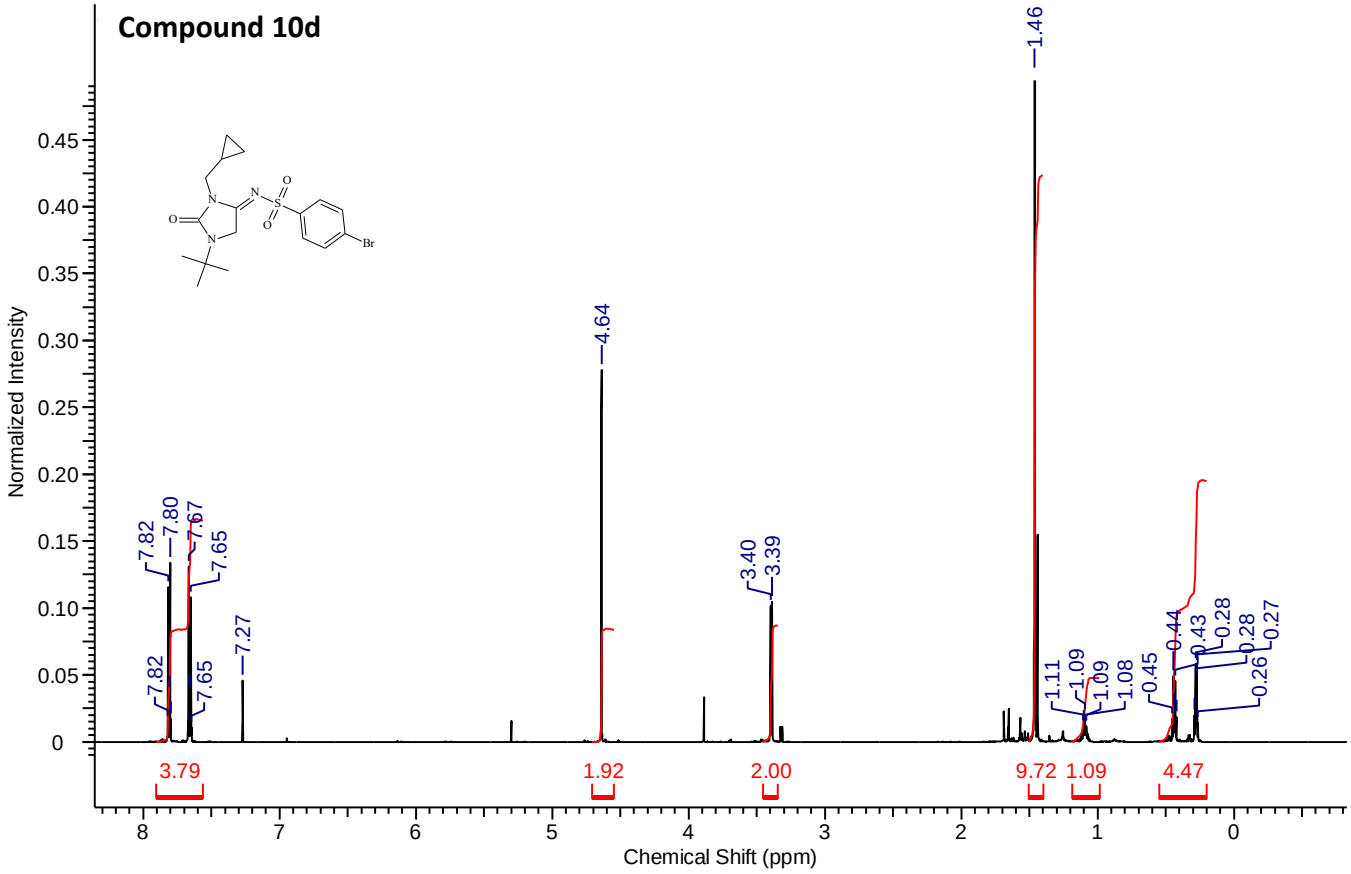

Compound 10a
(thousandths)
164.303
154.000
77.211
77.000
76.789
54.767
47.433
44.915
42.358
28.379
27.757
9.192
3.810
3.667
X : parts per Million : Carbon13

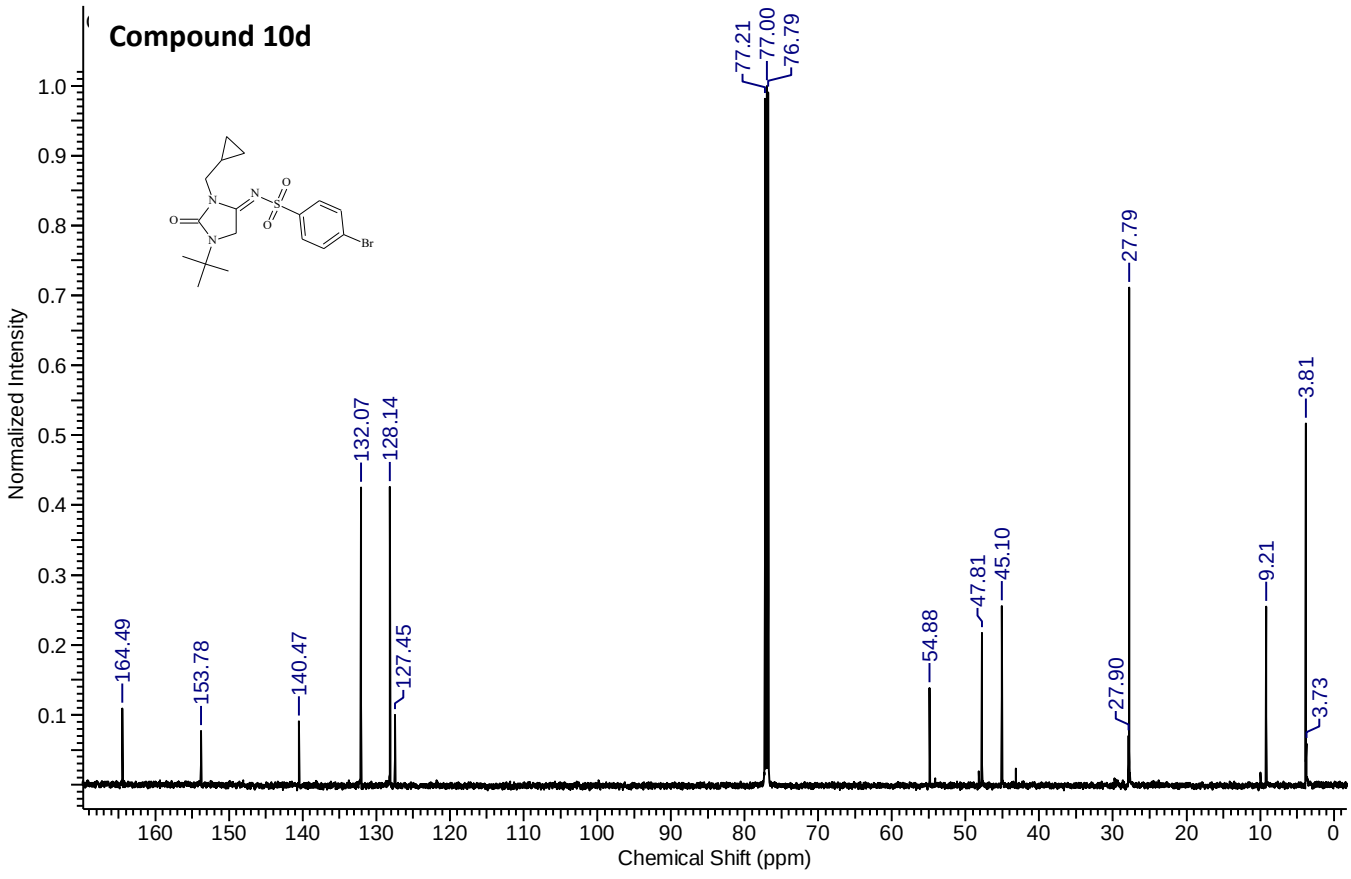

Compound 10b
Normalized Intensity
Chemical Shift (ppm)
1.46
4.65
3.41
3.39
7.96
7.94
7.58
7.53
7.52
7.51
7.27
6.97
1.57
1.45
1.11
1.10
0.44
0.43
0.42
0.28
0.27
0.26
0.27
1.76
2.75
1.91
2.00
8.96
0.93
2.03
2.02

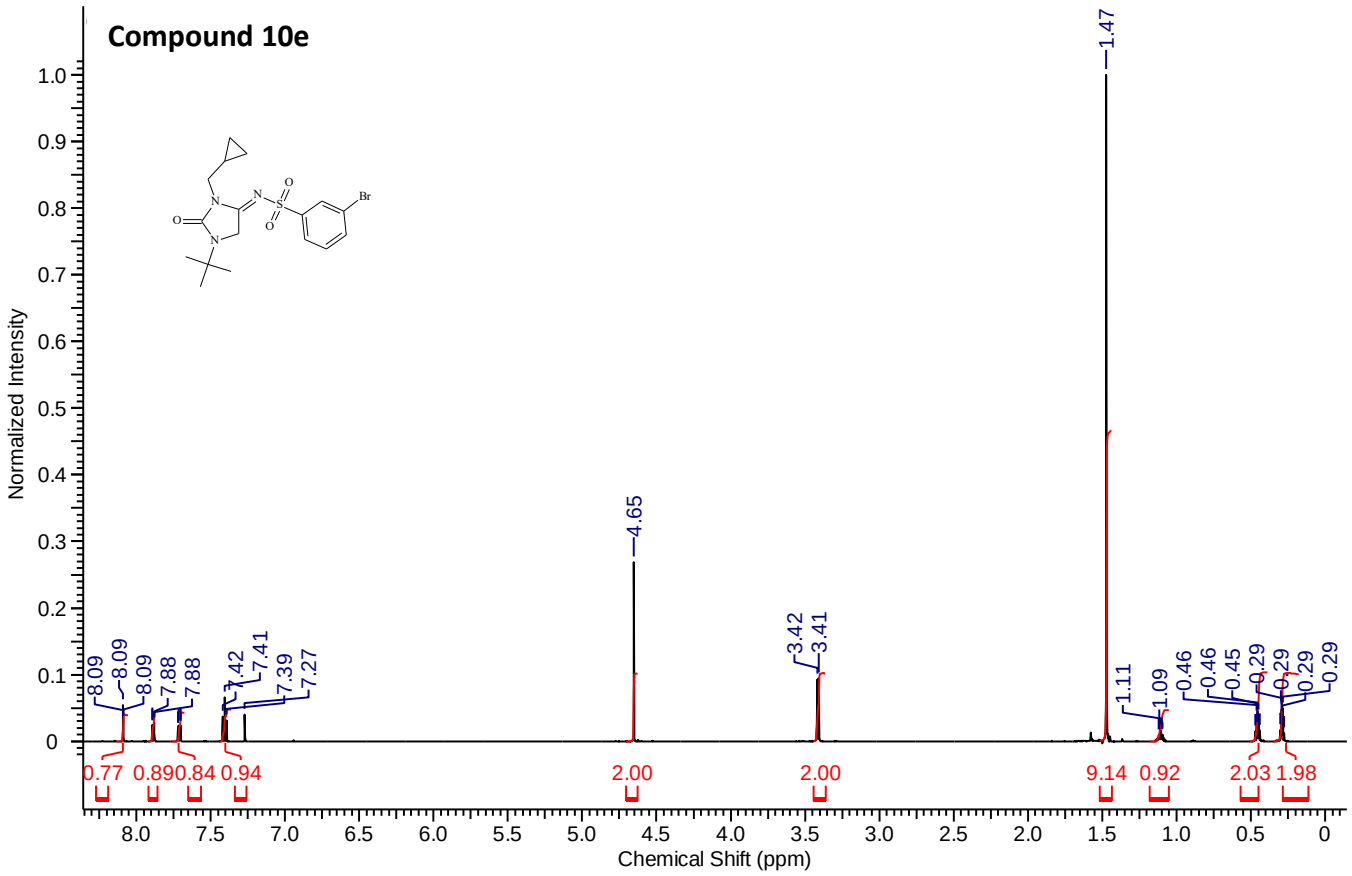

Compound 10b
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
27.79
128.81
126.49
164.34
153.93
141.42
132.53
54.82
47.76
45.02
27.71
9.23
3.77

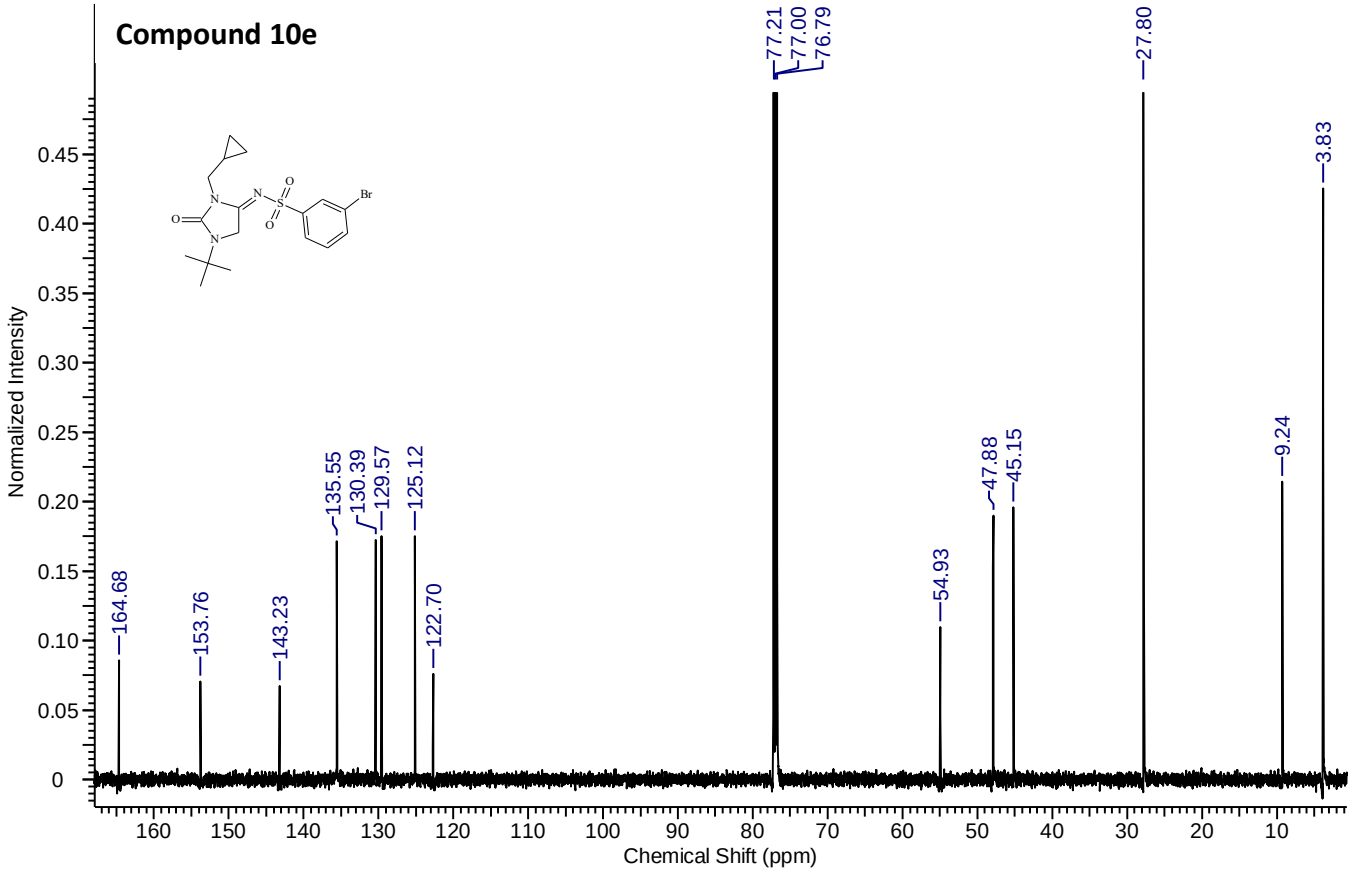

Compound 10c
Normalized Intensity
Chemical Shift (ppm)
4.65
2.44
1.46
3.41
3.39
7.84
7.83
7.33
7.27
6.98
1.57
1.13
1.12
1.11
1.10
0.44
0.44
0.42
0.42
0.45
0.29
0.28
0.27
1.77
2.12
1.94
2.00
2.96
9.16
0.91
4.03

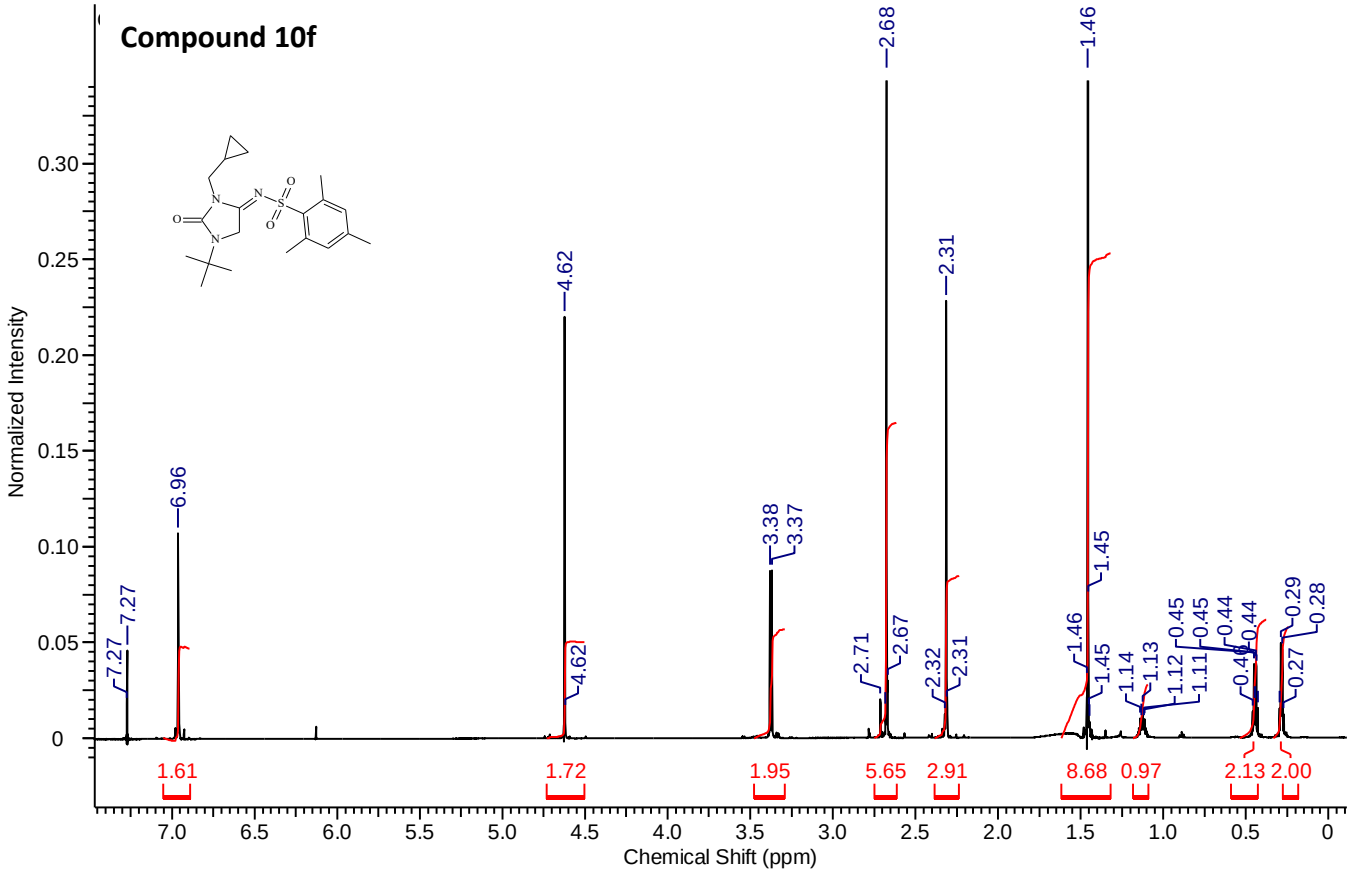

Compound 10c
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
27.81
3.79
129.43
126.57
164.17
154.05
143.32
138.58
54.82
47.74
45.01
21.55
9.27

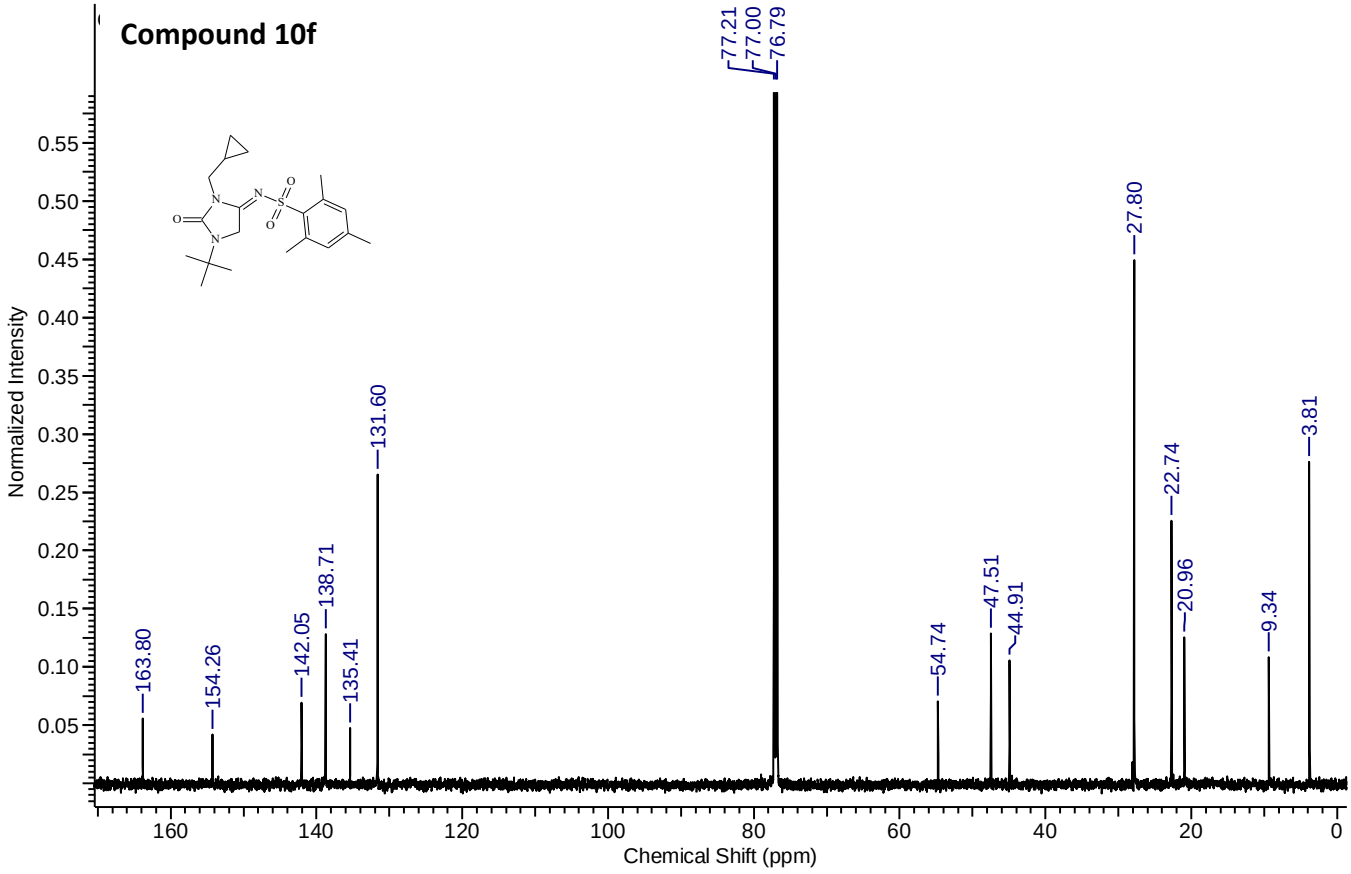

Compound 10d
Normalized Intensity
Chemical Shift (ppm)
1.46
4.64
3.40
3.39
7.82
7.80
7.67
7.65
7.27
1.11
1.09
1.09
1.08
0.45
0.44
0.43
0.28
0.28
0.26
0.27
3.79
1.92
2.00
9.72
1.09
4.47

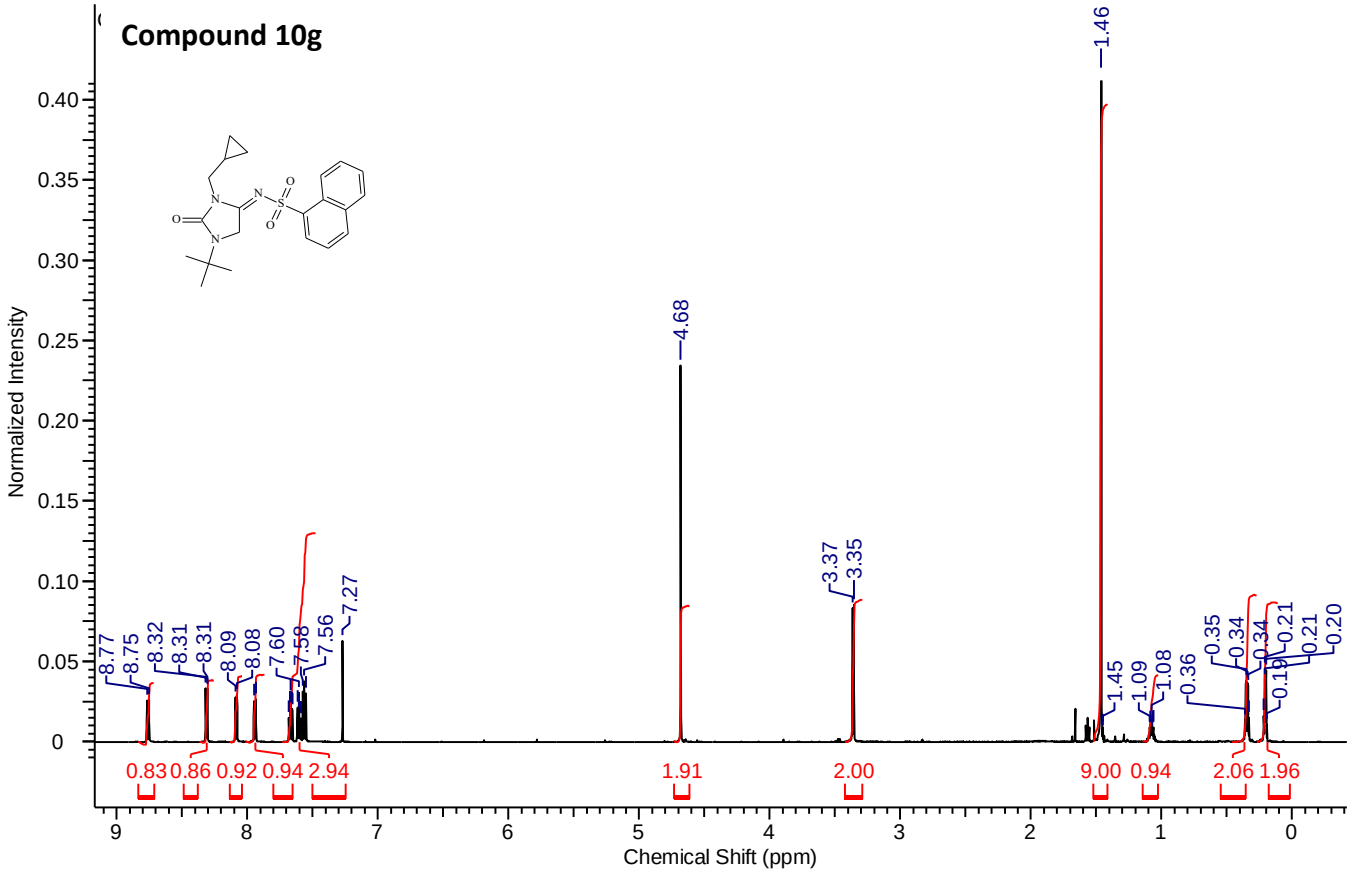

Compound 10d
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
132.07
128.14
164.49
153.78
140.47
127.45
54.88
47.81
45.10
27.79
27.90
9.21
3.81
3.73

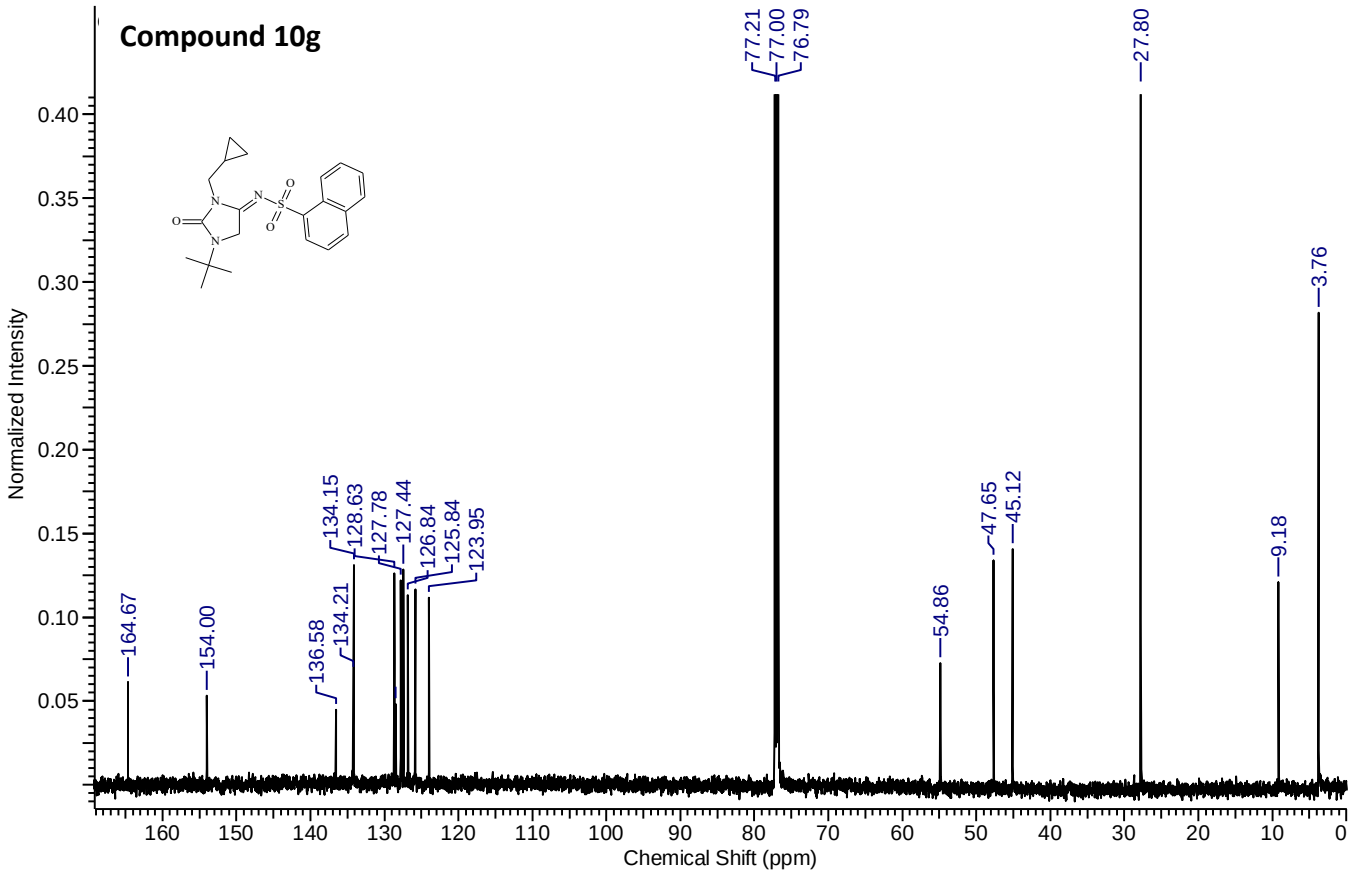

Compound 10e
Normalized Intensity
Chemical Shift (ppm)
8.09
8.09
8.09
7.88
7.88
7.42
7.41
7.39
7.27
4.65
3.42
3.41
1.47
1.11
1.09
0.46
0.46
0.45
0.29
0.29
0.29
0.29
0.77
0.89
0.84
0.94
2.00
2.00
9.14
0.92
2.03
1.98

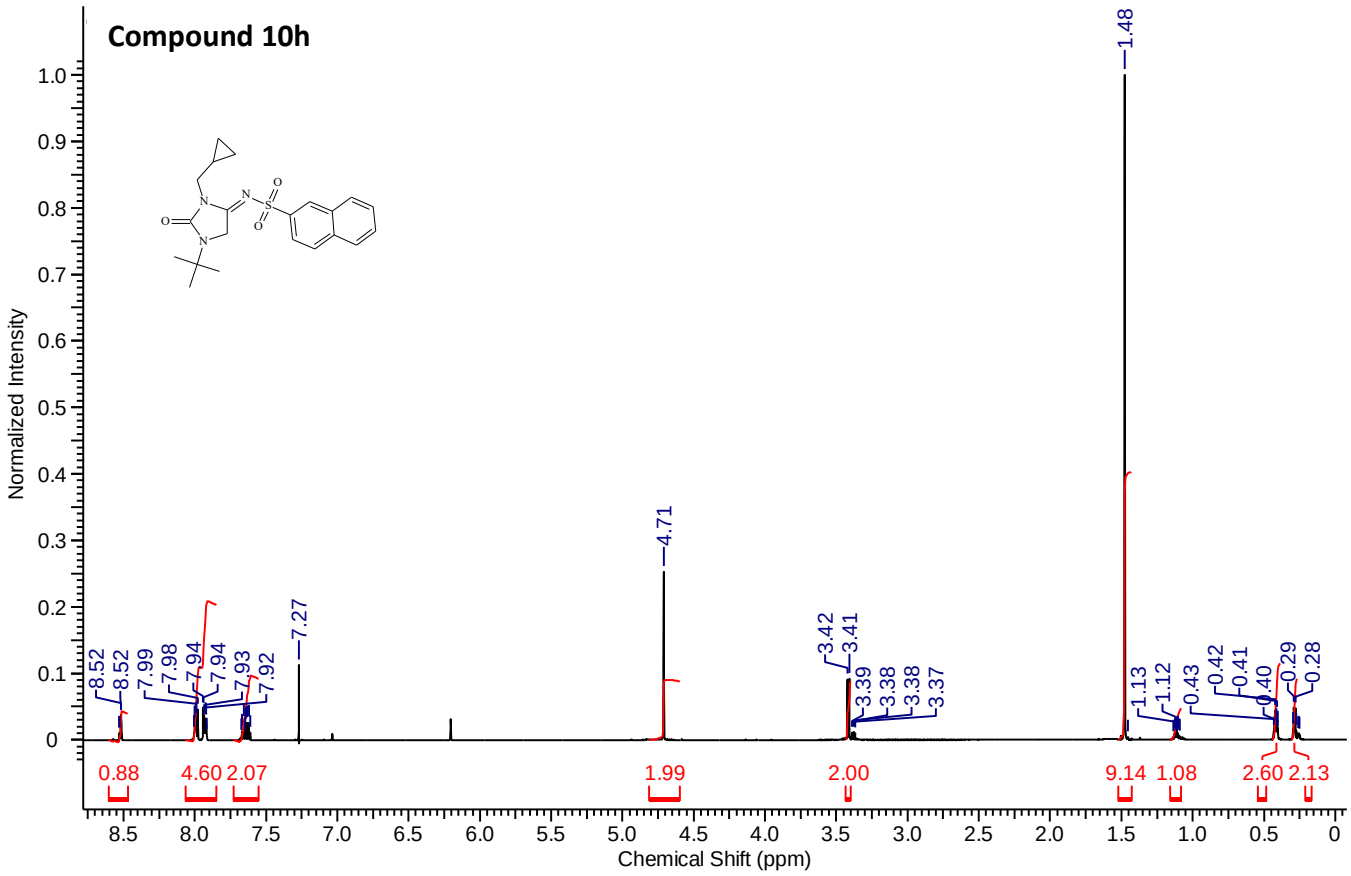

Compound 10e
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
27.80
3.83
164.68
153.76
143.23
135.55
130.39
129.57
125.12
122.70
54.93
47.88
45.15
9.24

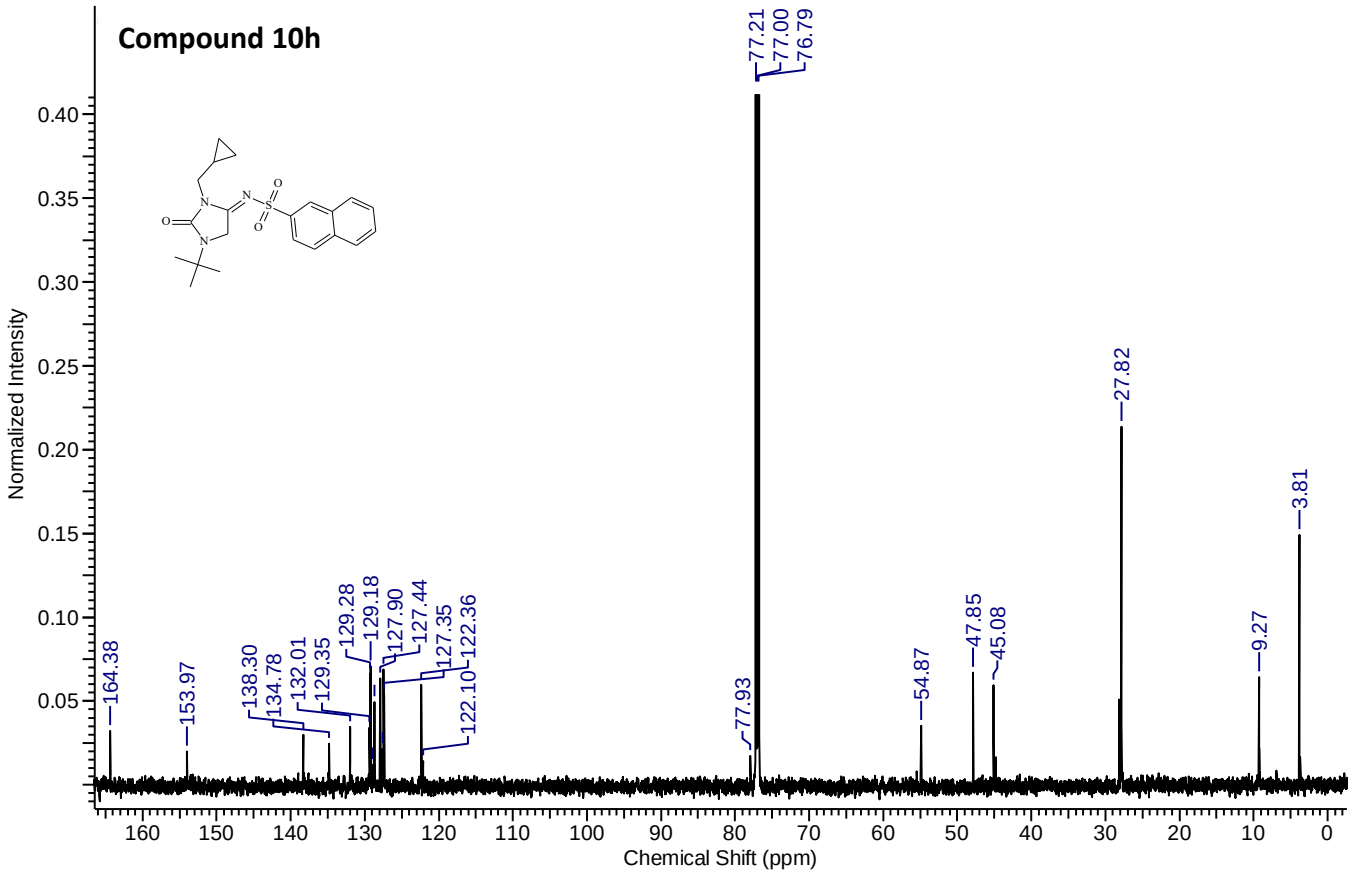

Compound 10f
Normalized Intensity
Chemical Shift (ppm)
7.27
6.96
4.62
3.38
3.37
2.71
2.68
2.67
2.32
2.31
1.46
1.45
1.14
1.13
1.12
1.11
0.45
0.45
0.44
0.44
0.46
0.29
0.28
0.27
1.61
1.72
1.95
5.65
2.91
8.68
0.97
2.13
2.00

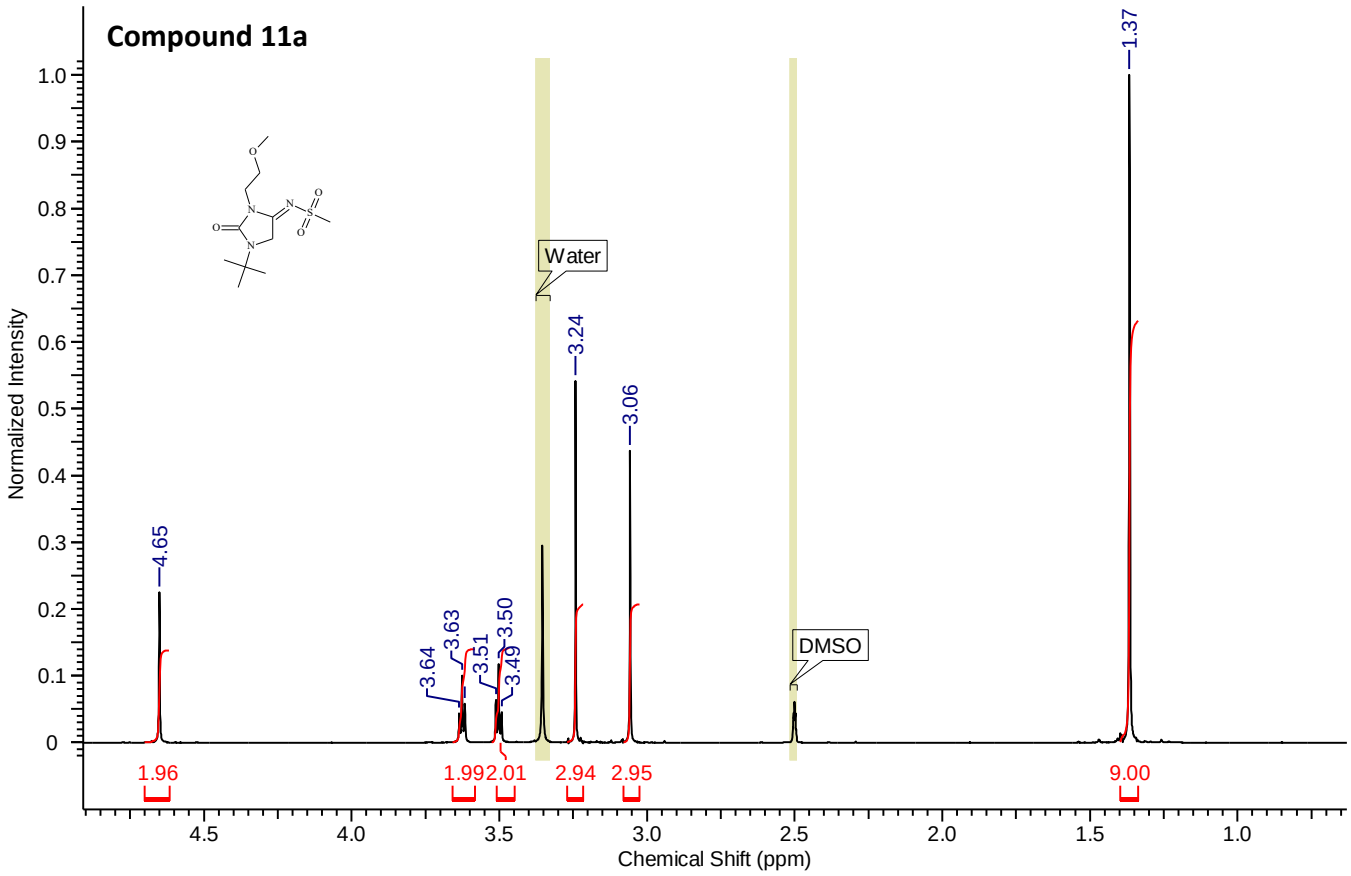

Compound 10f
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
163.80
154.26
142.05
138.71
135.41
131.60
54.74
47.51
44.91
27.80
22.74
20.96
9.34
3.81

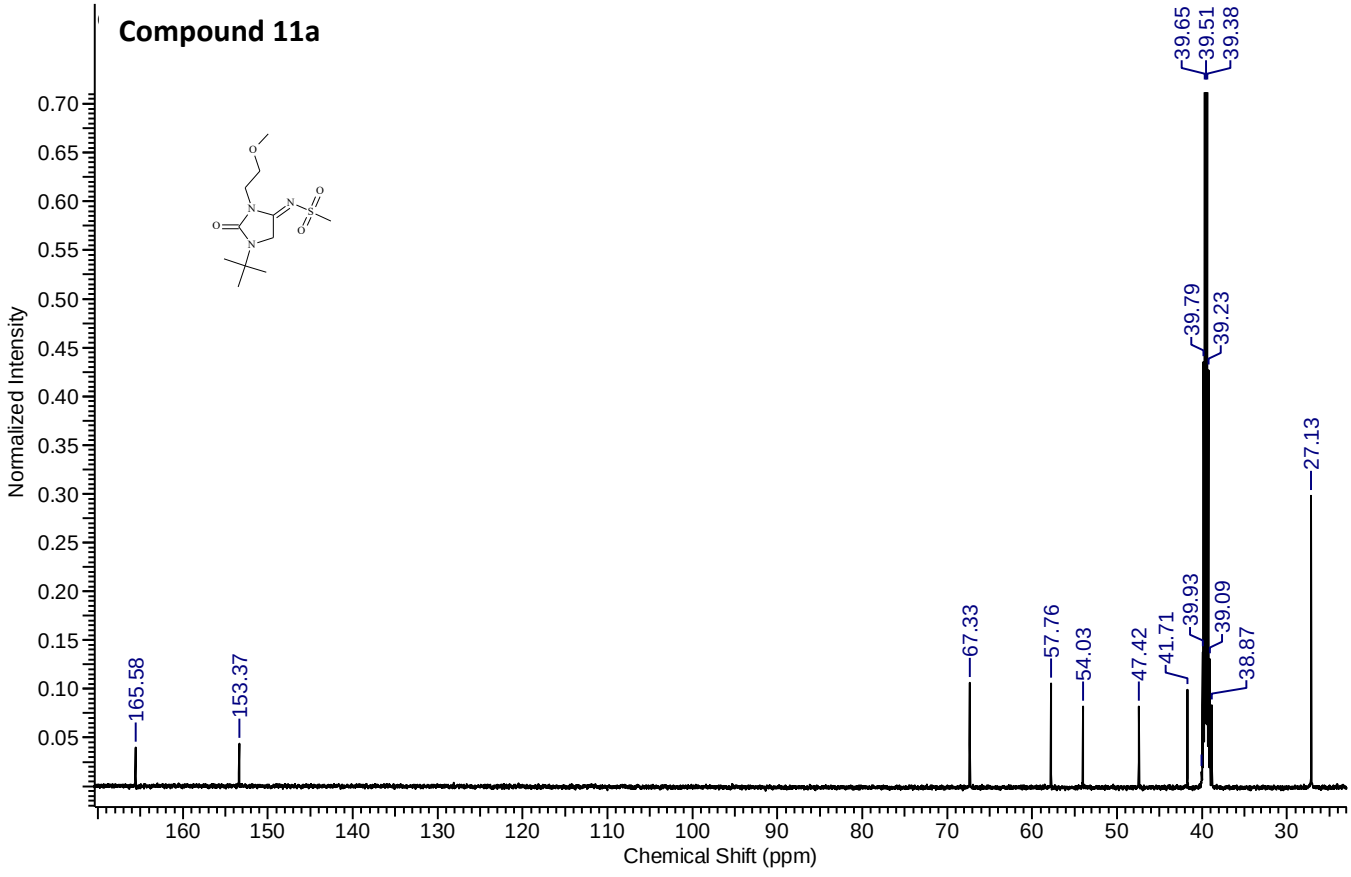

Compound 10g
Normalized Intensity
Chemical Shift (ppm)
8.77
8.75
8.32
8.31
8.31
8.09
8.08
7.60
7.58
7.56
7.27
4.68
3.37
3.35
1.46
1.45
1.09
1.08
0.36
0.35
0.34
0.34
0.19
0.21
0.21
0.20
0.83 0.86 0.92 0.94 2.94
1.91
2.00
9.00 0.94
2.06 1.96

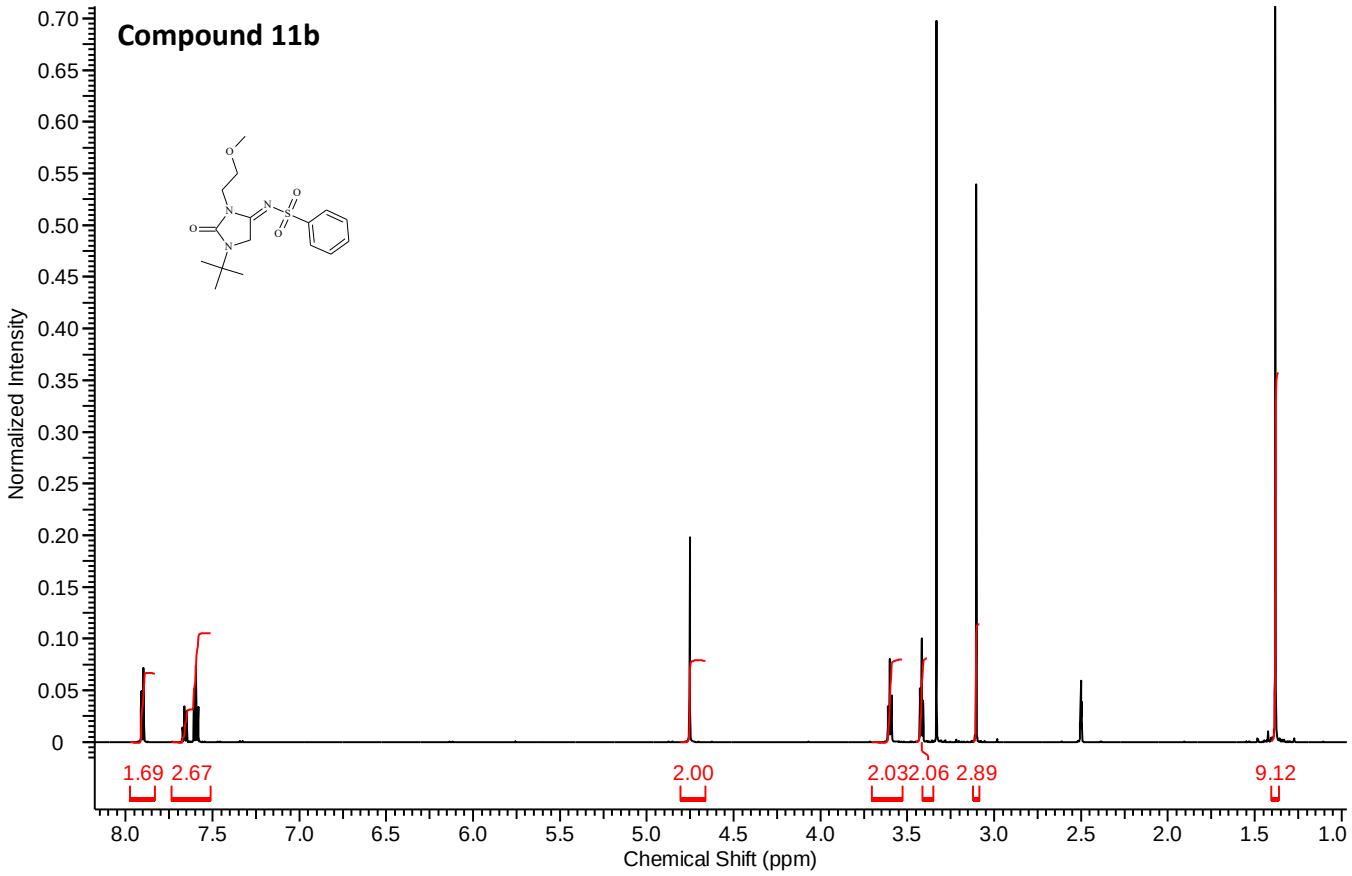

Compound 10g
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
27.80
3.76
164.67
154.00
136.58
134.21
134.15
128.63
127.78
127.44
126.84
125.84
123.95
54.86
47.65
45.12
9.18

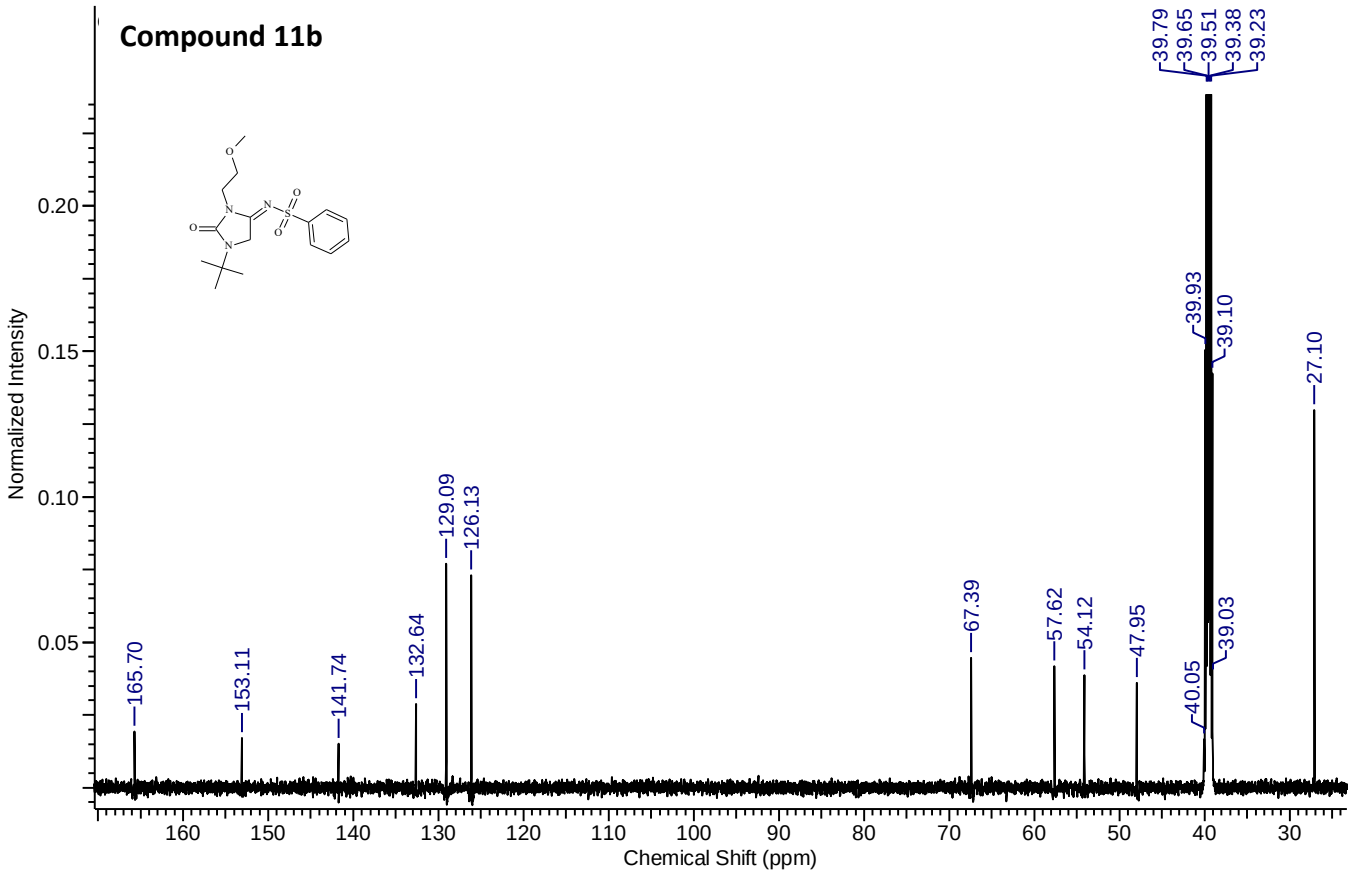

Compound 10h
Normalized Intensity
Chemical Shift (ppm)
1.48
4.71
7.27
8.52
8.52
7.99
7.98
7.94
7.94
7.93
7.92
3.42
3.41
3.39
3.38
3.38
3.37
1.13
1.12
0.43
0.42
0.41
0.40
0.29
0.28
0.88
4.60
2.07
1.99
2.00
9.14
1.08
2.60
2.13

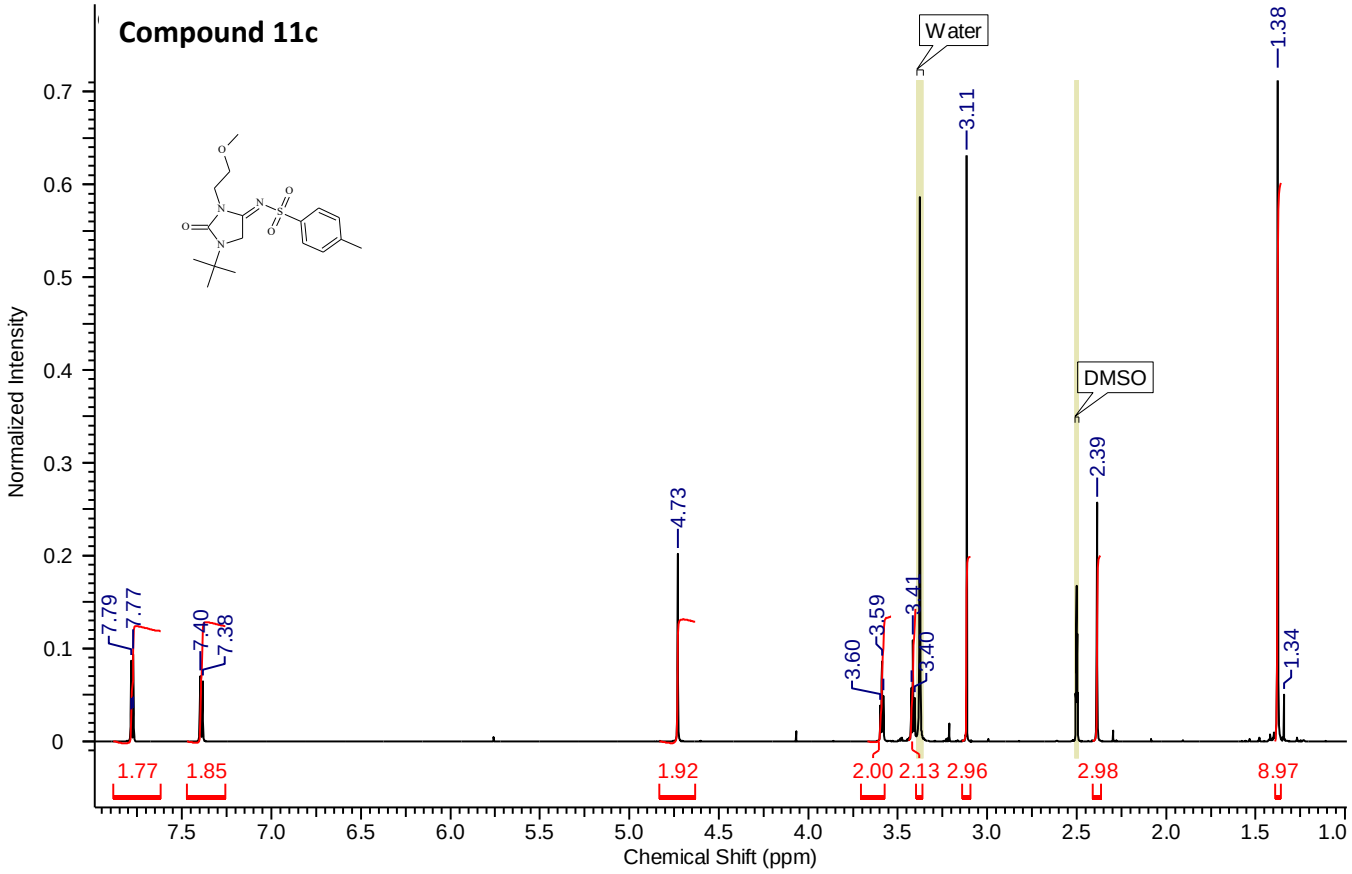

Compound 10h
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.79
27.82
3.81
164.38
153.97
138.30
134.78
132.01
129.35
129.28
129.18
127.90
127.44
127.35
122.36
122.10
77.93
54.87
47.85
45.08
9.27

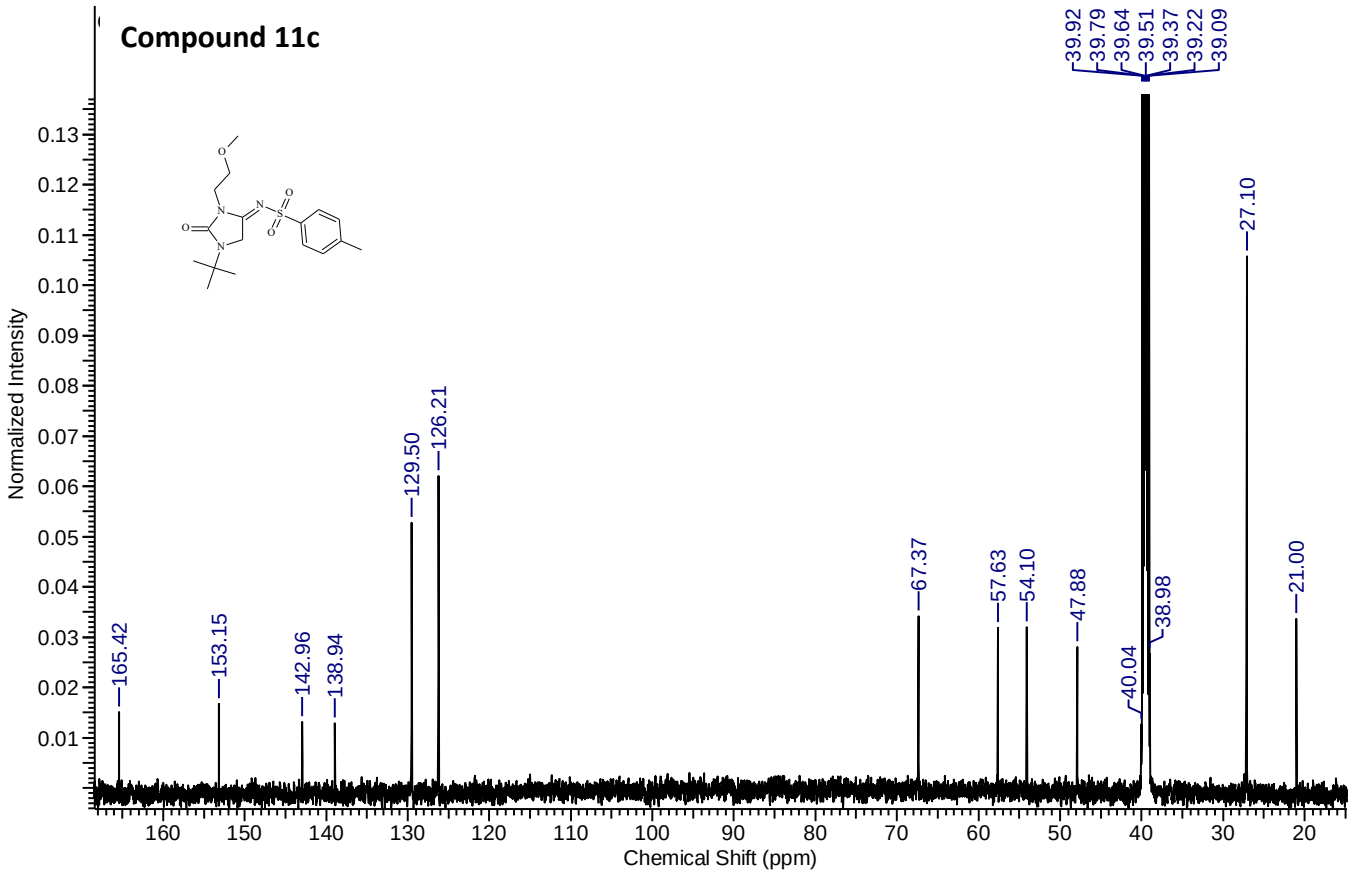

Compound 11a
Normalized Intensity
Chemical Shift (ppm)
Water
DMSO
4.65
3.64
3.63
3.51
3.50
3.49
3.24
3.06
1.37
1.96
1.99
2.01
2.94
2.95
9.00

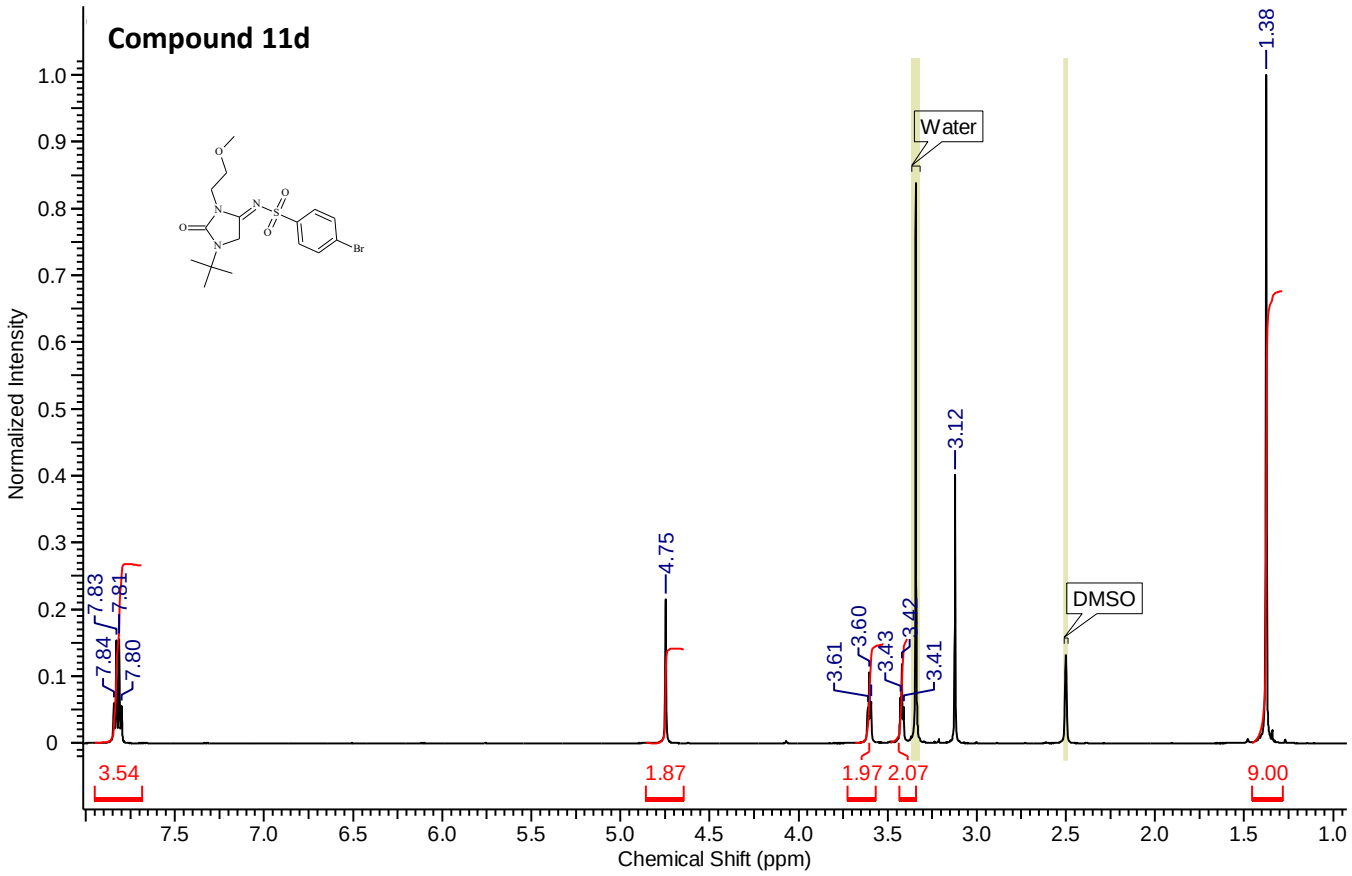

Compound 11a
Normalized Intensity
Chemical Shift (ppm)
165.58
153.37
67.33
57.76
54.03
47.42
41.71
39.93
39.79
39.65
39.51
39.38
39.23
39.09
38.87
27.13

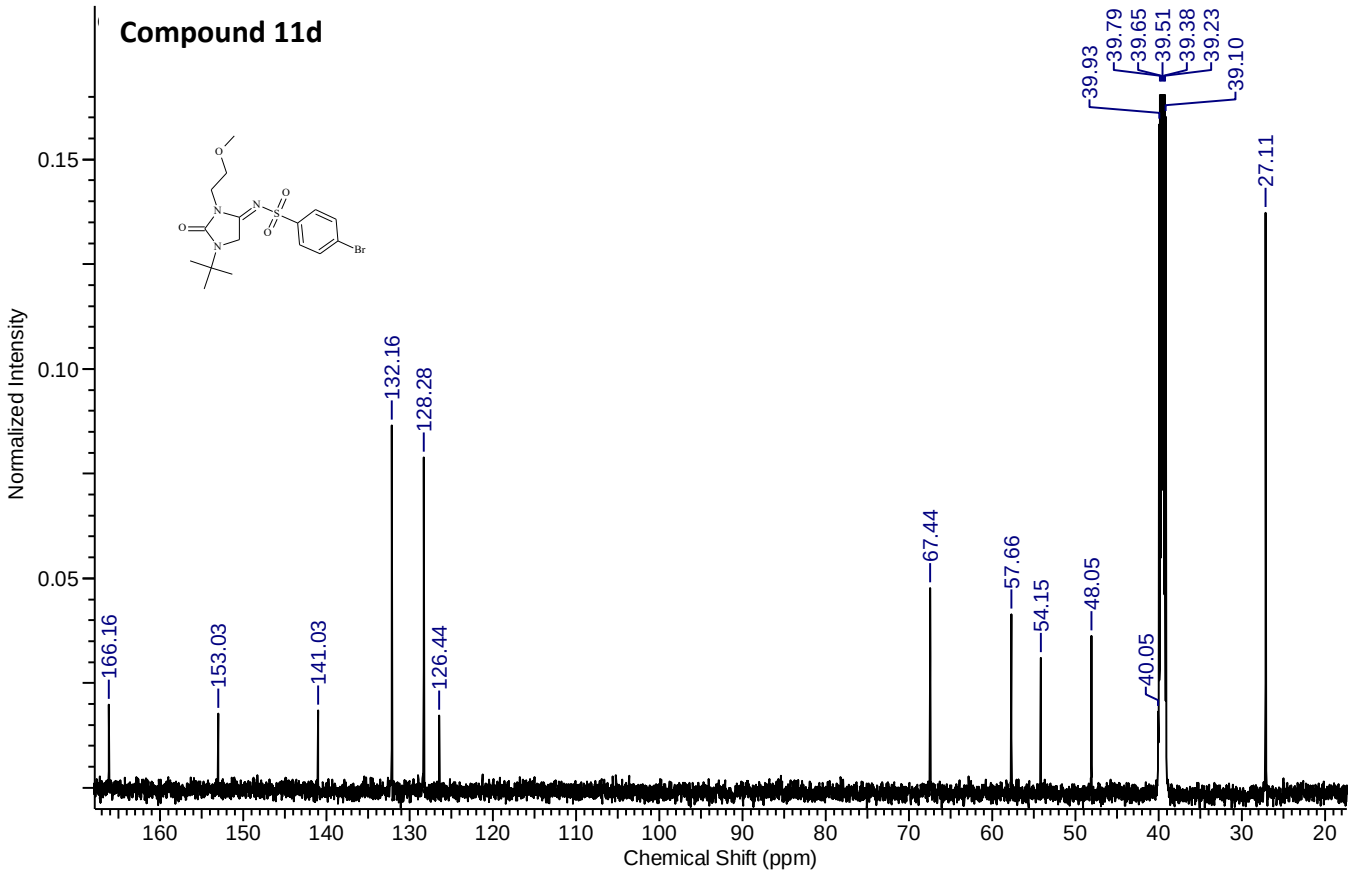

Compound 11b
Normalized Intensity
Chemical Shift (ppm)
1.69
2.67
2.00
2.03
2.06
2.89
9.12

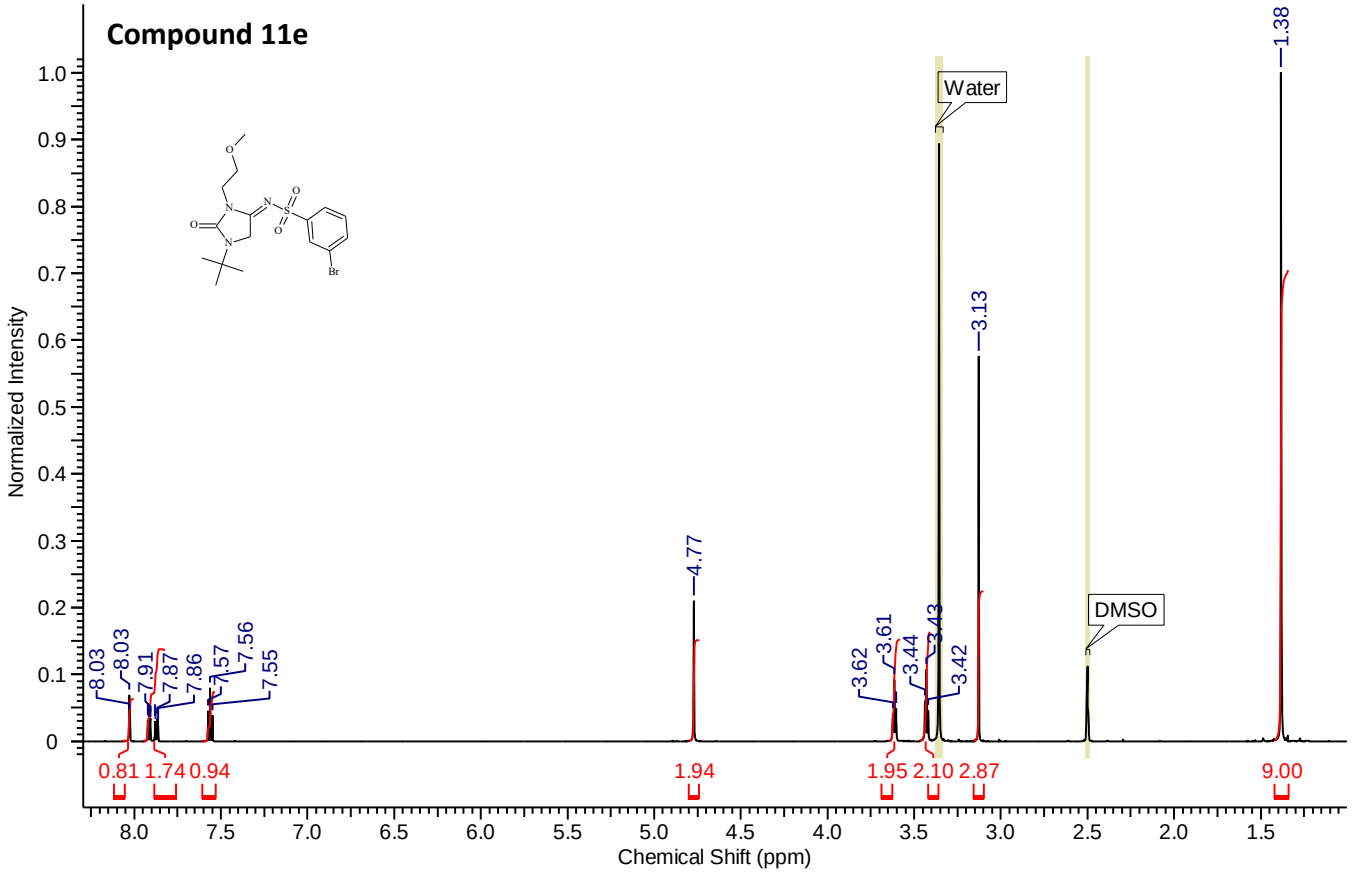

Compound 11b
Normalized Intensity
Chemical Shift (ppm)
165.70
153.11
141.74
132.64
129.09
126.13
67.39
57.62
54.12
47.95
40.05
39.93
39.79
39.65
39.51
39.38
39.23
39.10
39.03
27.10

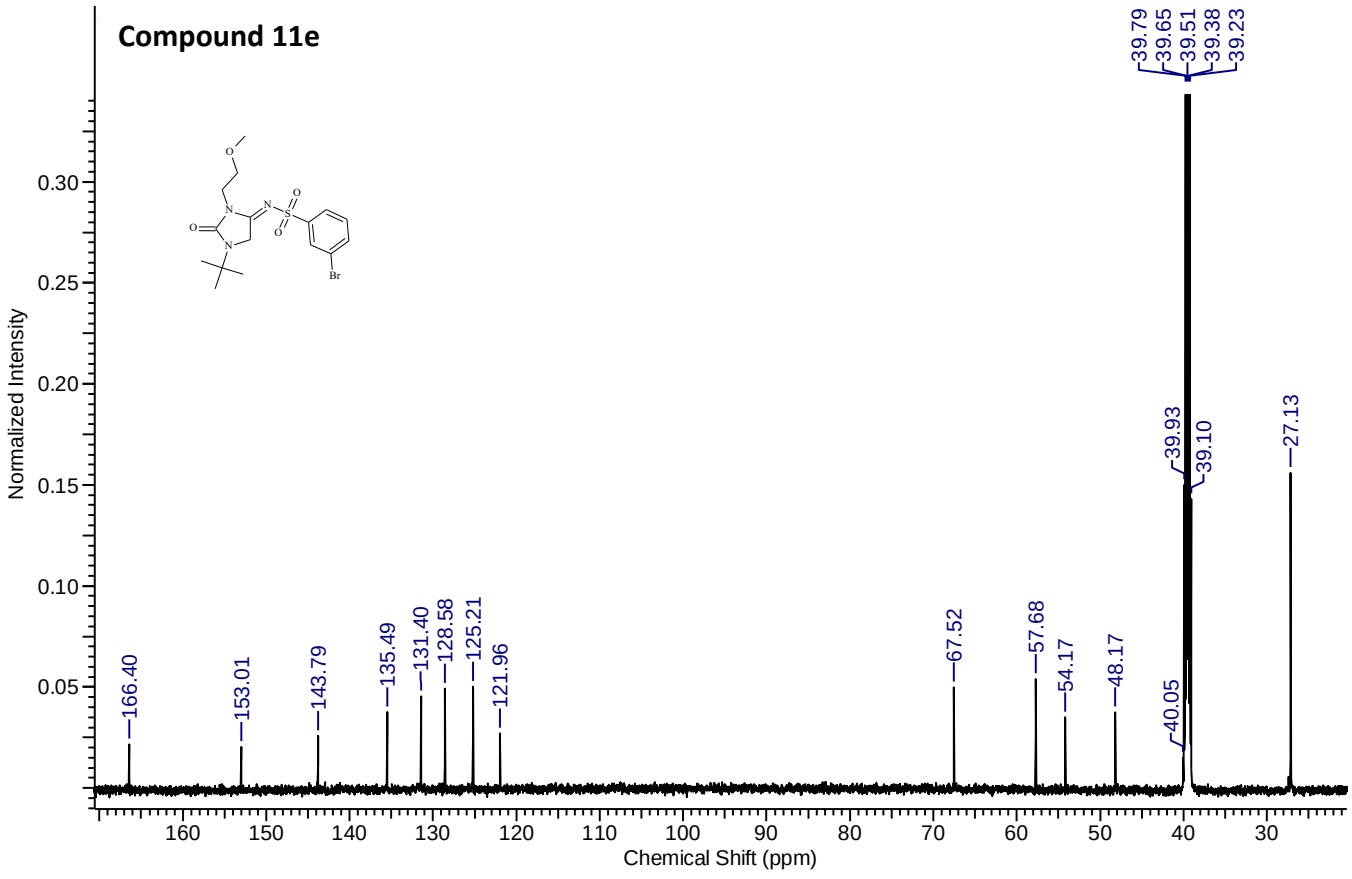

Compound 11c
Water
DMSO
7.79
7.77
7.40
7.38
4.73
3.60
3.59
3.41
3.40
3.11
2.39
1.38
1.34
1.77
1.85
1.92
2.00
2.13
2.96
2.98
8.97
Normalized Intensity
Chemical Shift (ppm)

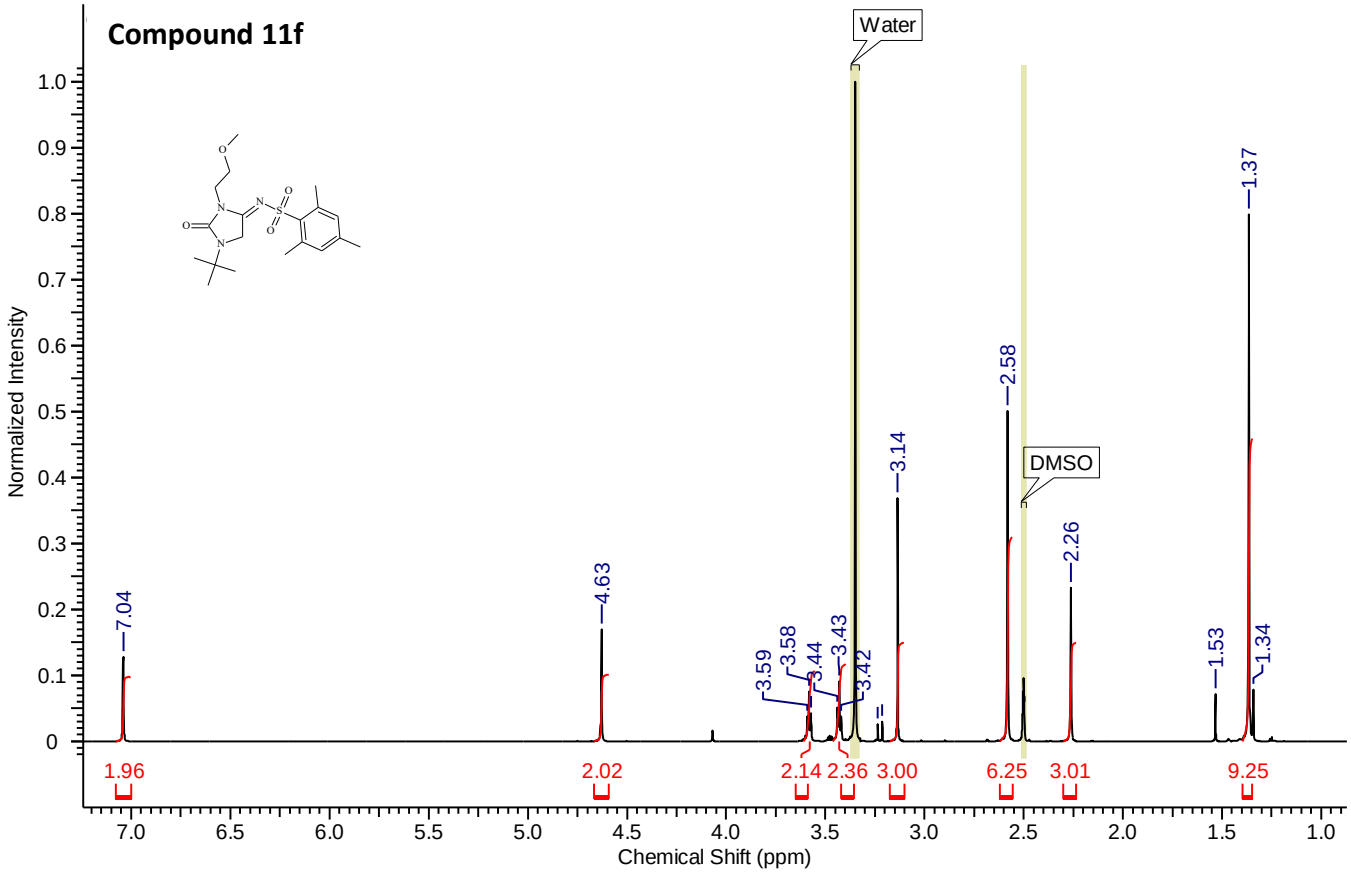

Compound 11c
39.92
39.79
39.64
39.51
39.37
39.22
39.09
165.42
153.15
142.96
138.94
129.50
126.21
67.37
57.63
54.10
47.88
40.04
38.98
27.10
21.00
Normalized Intensity
Chemical Shift (ppm)

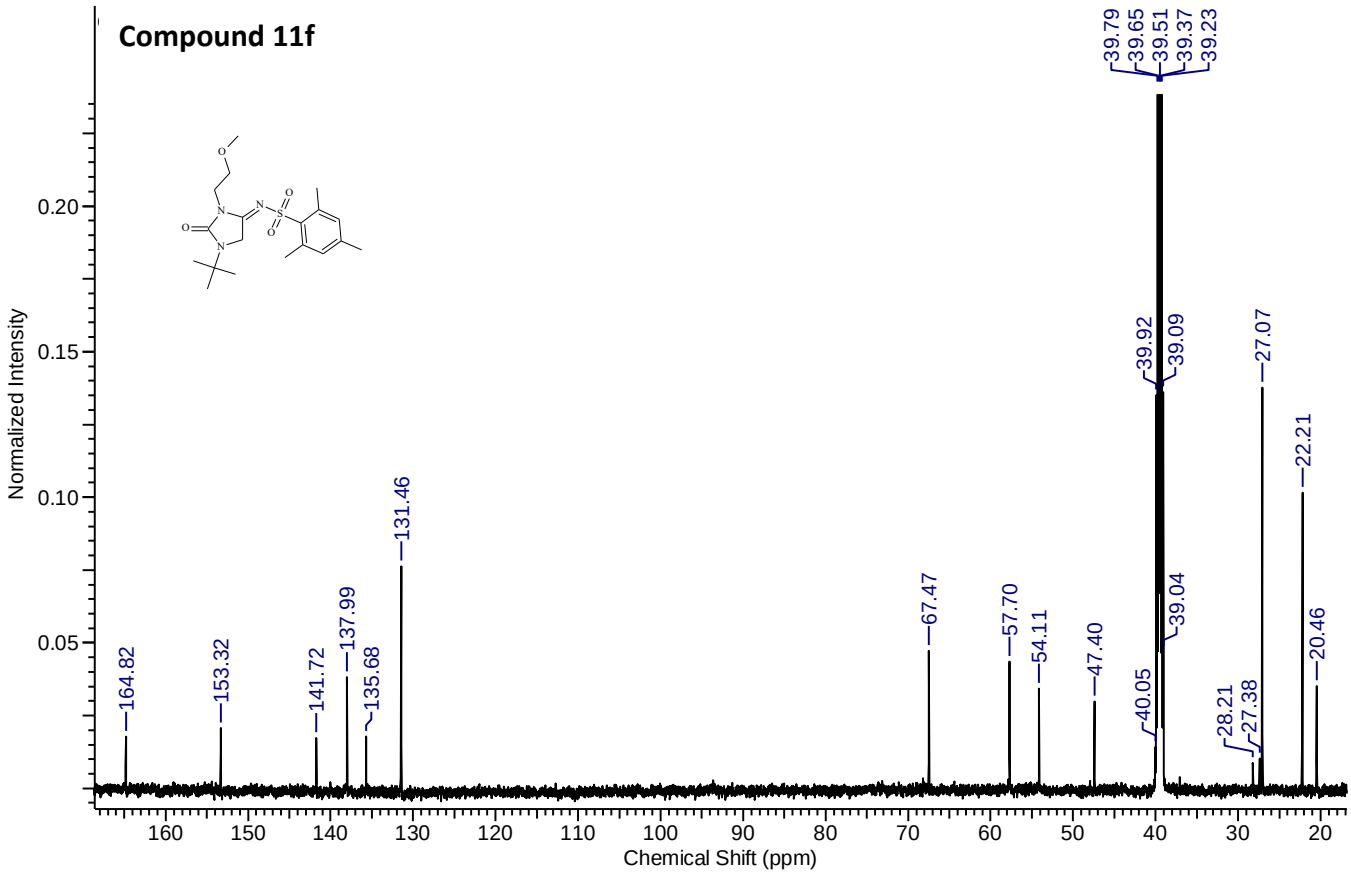

Compound 11d
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
7.83
7.81
7.84
7.80
4.75
3.61
3.60
3.43
3.42
3.41
3.12
1.38
3.54
1.87
1.97
2.07
9.00

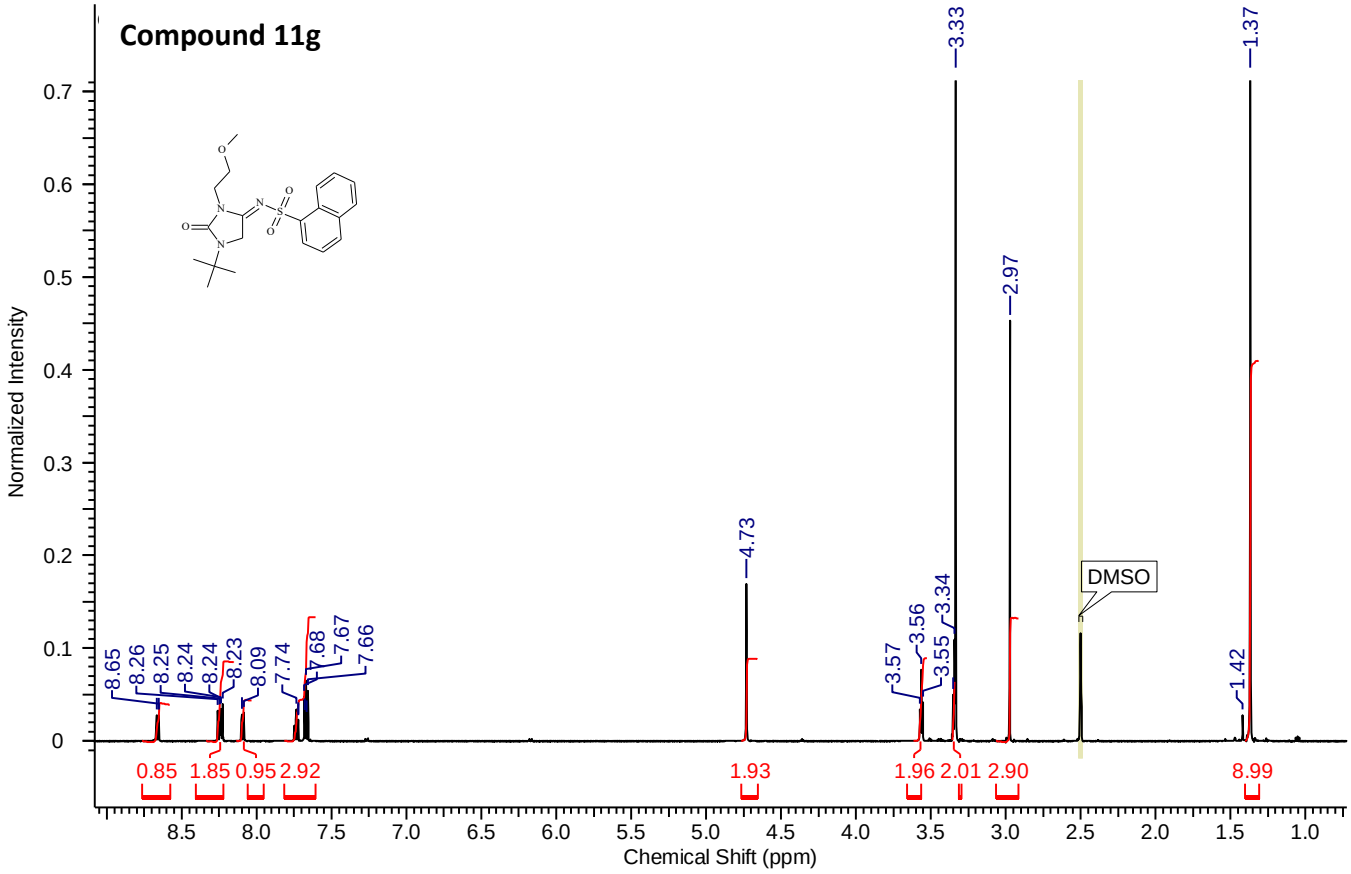

Compound 11d
Normalized Intensity
Chemical Shift (ppm)
166.16
153.03
141.03
132.16
128.28
126.44
67.44
57.66
54.15
48.05
40.05
39.93
39.79
39.65
39.51
39.38
39.23
39.10
27.11

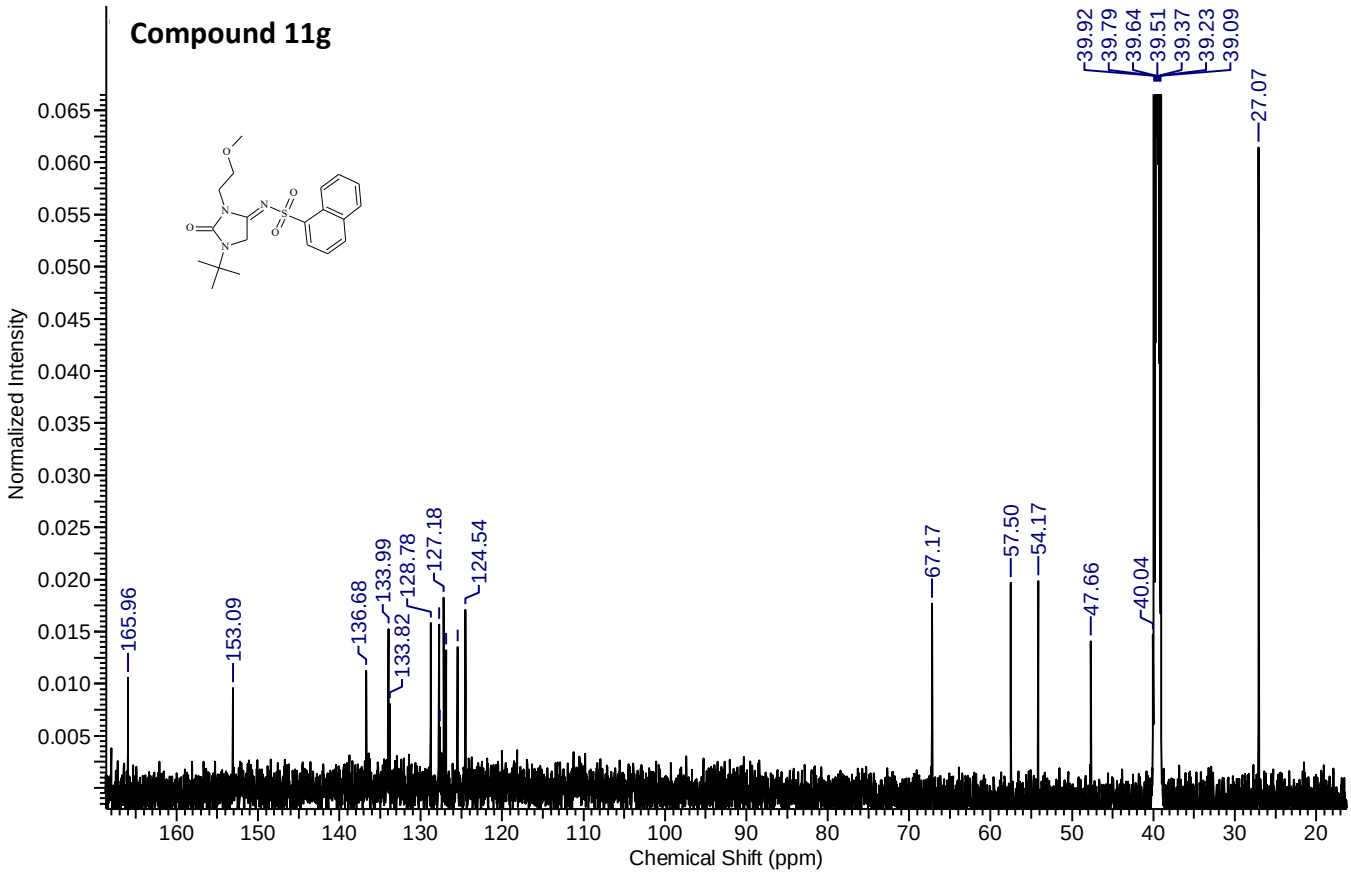

Compound 11e
Water
DMSO
1.38
3.13
4.77
8.03
8.03
7.91
7.87
7.86
7.57
7.56
7.55
3.62
3.61
3.44
3.43
3.42
0.81
1.74
0.94
1.94
1.95
2.10
2.87
9.00
Normalized Intensity
Chemical Shift (ppm)

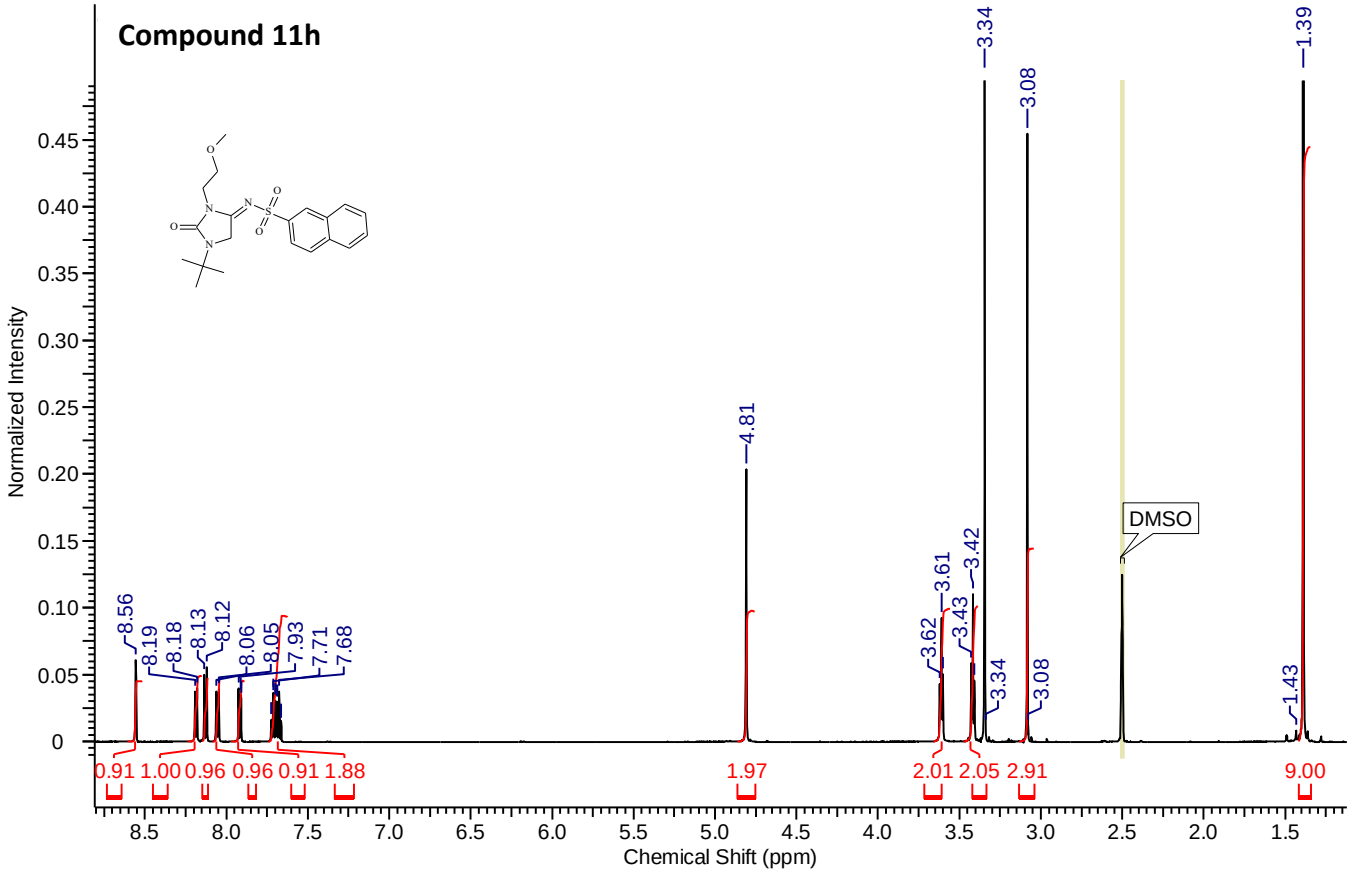

Compound 11e
39.79
39.65
39.51
39.38
39.23
39.93
39.10
27.13
166.40
153.01
143.79
135.49
131.40
128.58
125.21
121.96
67.52
57.68
54.17
48.17
40.05
Normalized Intensity
Chemical Shift (ppm)

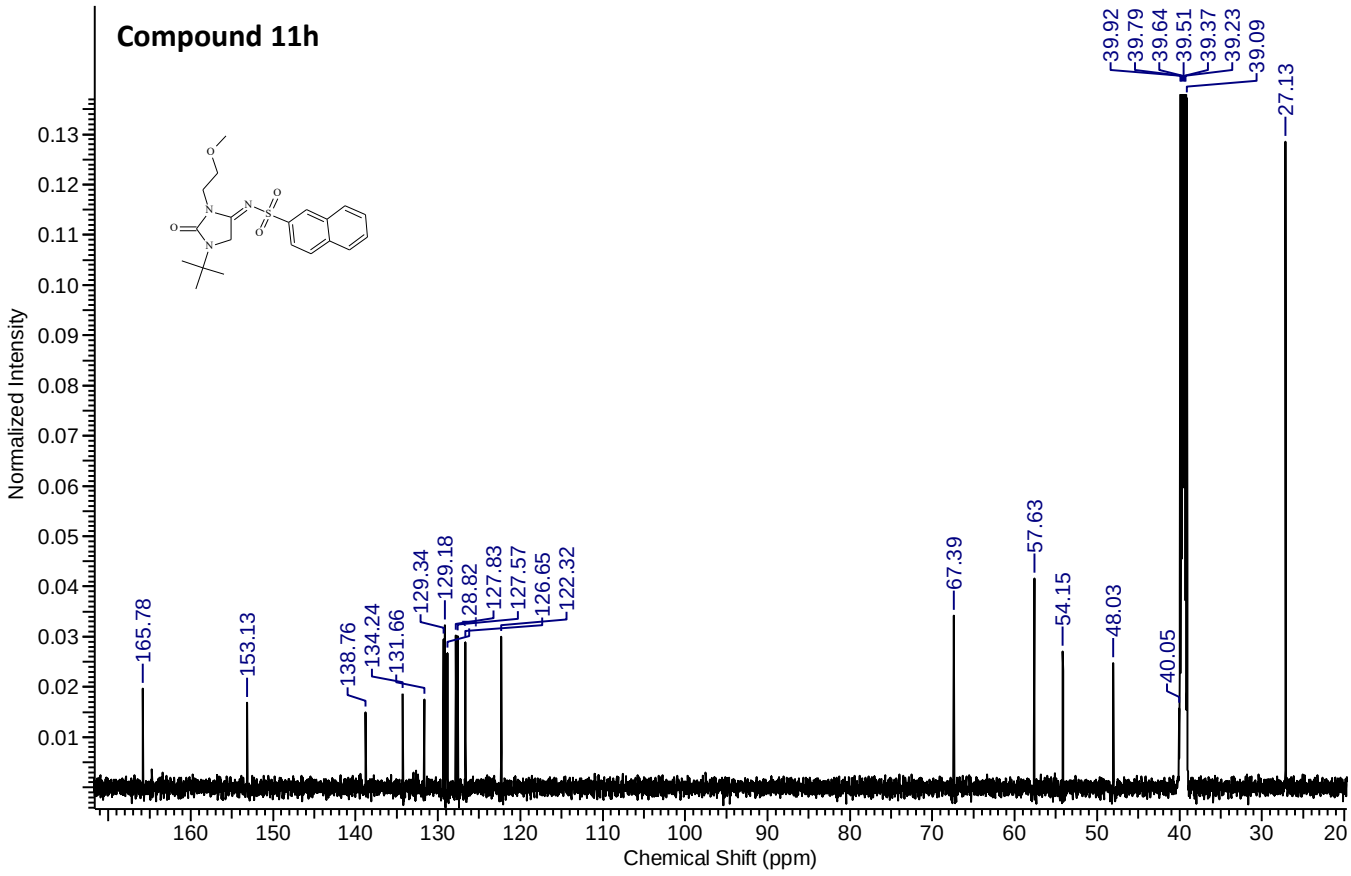

Compound 11f
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
7.04
4.63
3.59
3.58
3.44
3.43
3.42
3.14
2.58
2.26
1.53
1.37
1.34
1.96
2.02
2.14
2.36
3.00
6.25
3.01
9.25

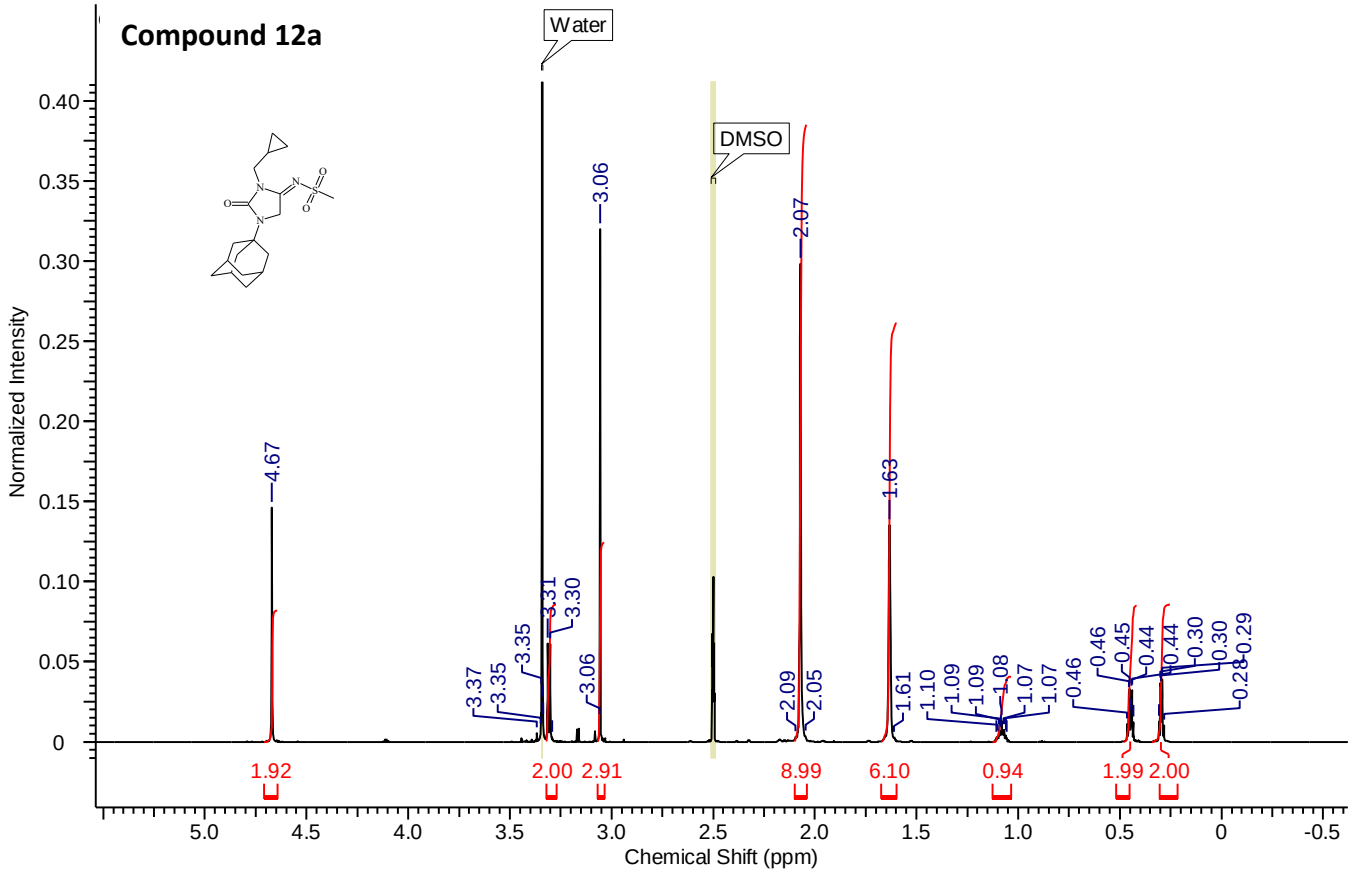

Compound 11f
Normalized Intensity
Chemical Shift (ppm)
164.82
153.32
141.72
137.99
135.68
131.46
67.47
57.70
54.11
47.40
40.05
39.92
39.79
39.65
39.51
39.37
39.23
39.09
39.04
28.21
27.38
27.07
22.21
20.46

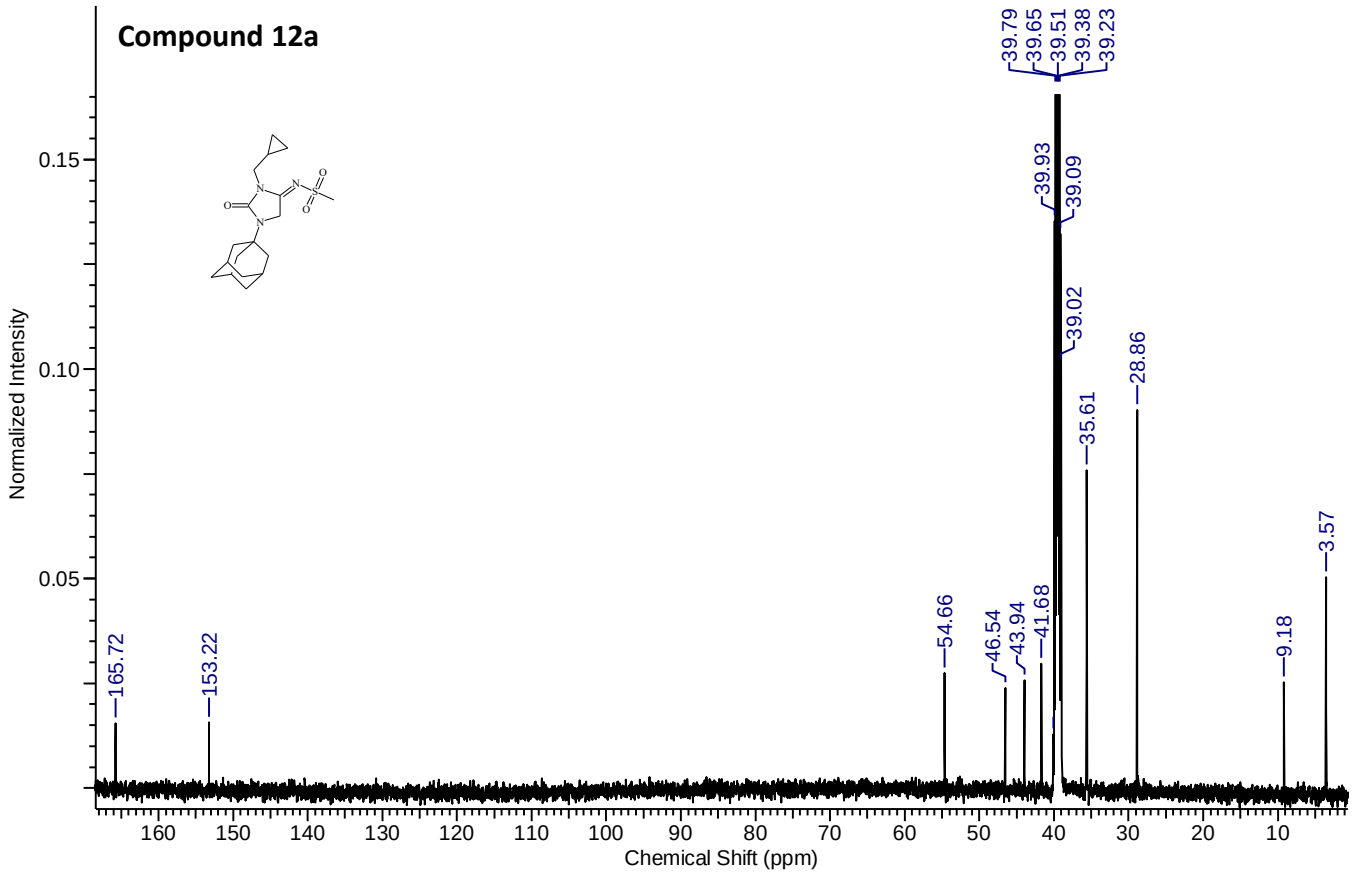

Compound 11g
Normalized Intensity
Chemical Shift (ppm)
8.65
8.26
8.25
8.24
8.24
8.23
8.09
7.74
7.68
7.67
7.66
4.73
3.57
3.56
3.55
3.34
3.33
2.97
DMSO
1.42
1.37
0.85
1.85
0.95
2.92
1.93
1.96
2.01
2.90
8.99

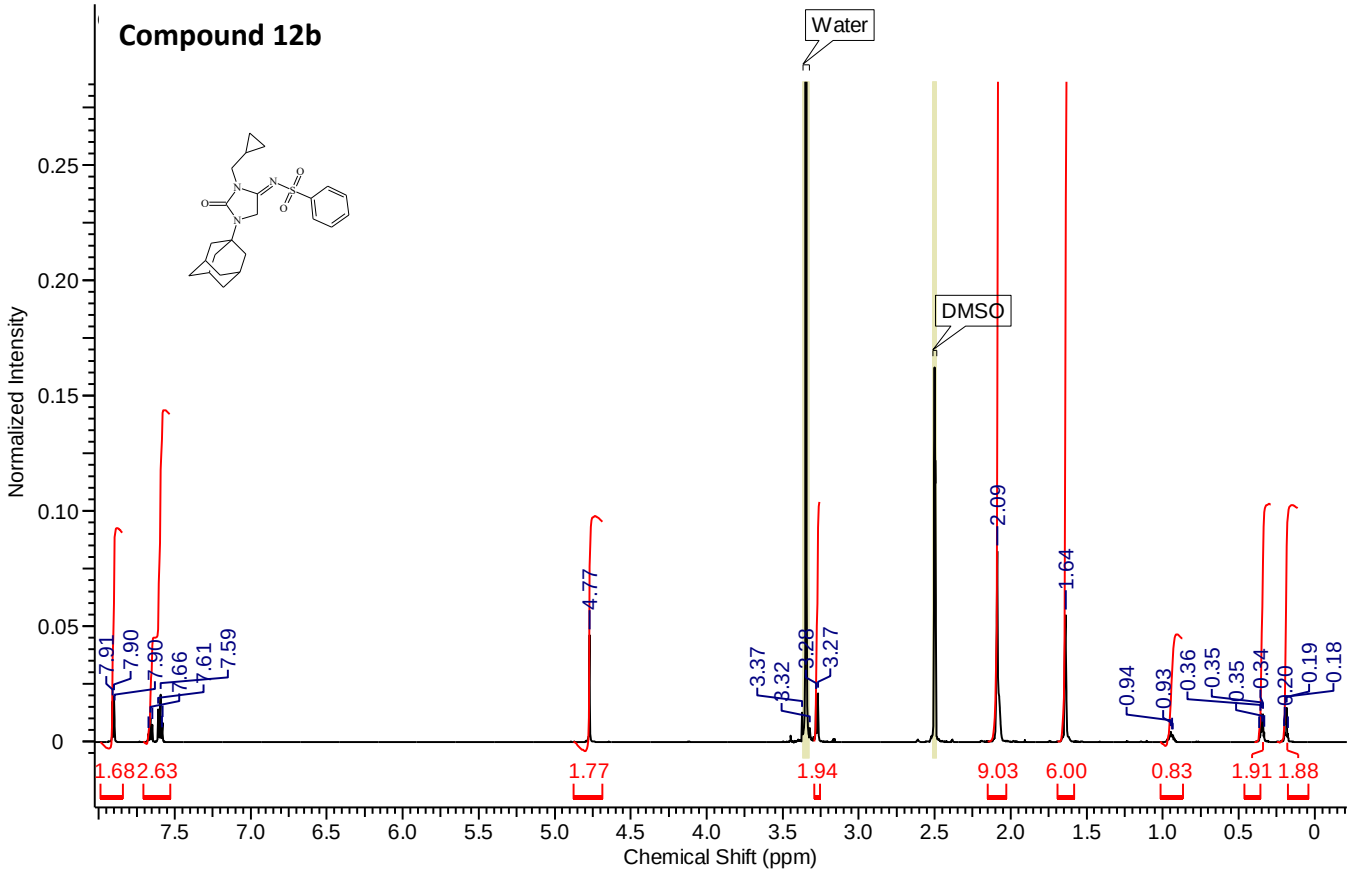

Compound 11g
Normalized Intensity
Chemical Shift (ppm)
165.96
153.09
136.68
133.99
133.82
128.78
127.18
124.54
67.17
57.50
54.17
47.66
40.04
39.92
39.79
39.64
39.51
39.37
39.23
39.09
27.07

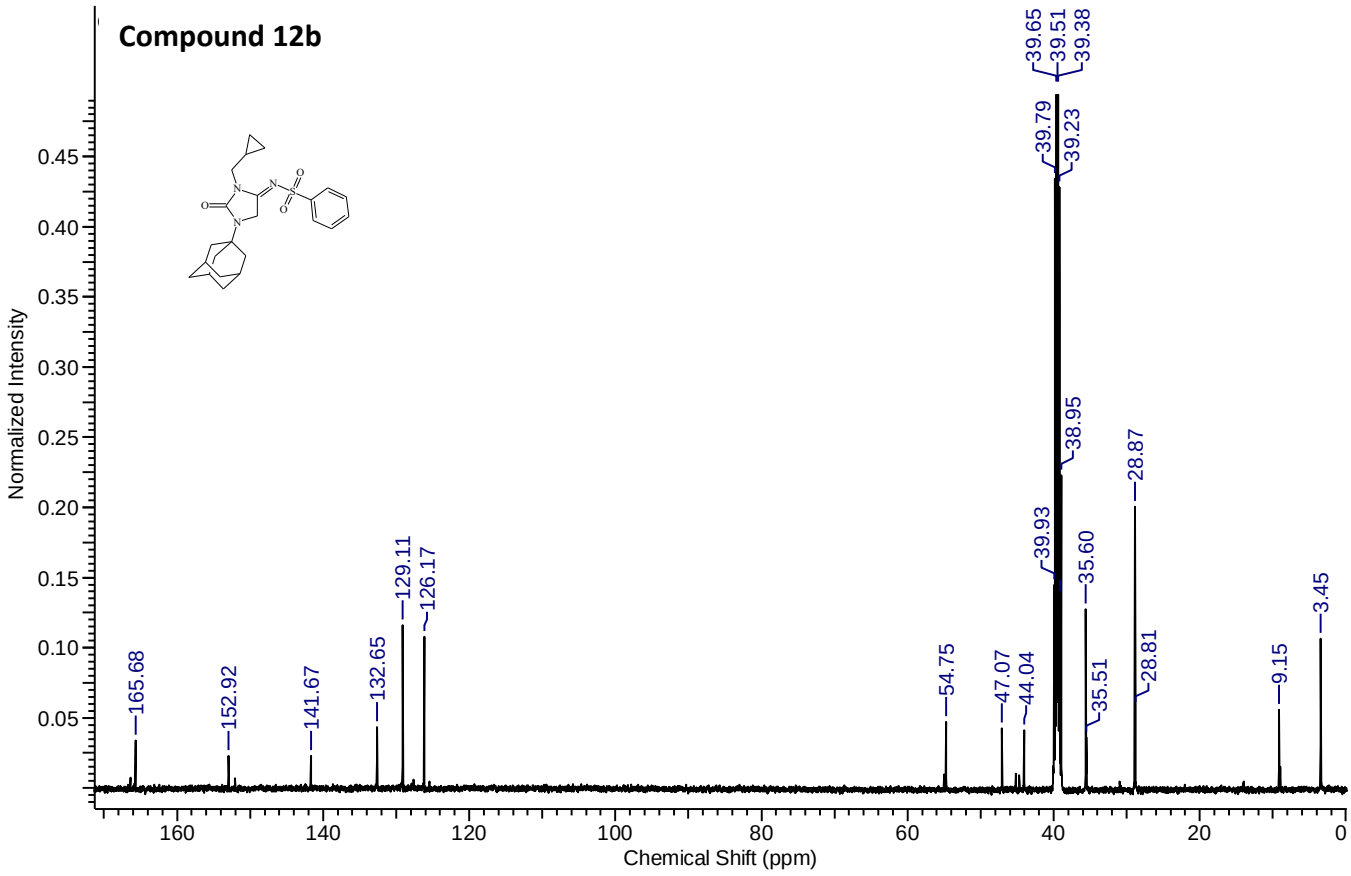

Compound 11h
Normalized Intensity
Chemical Shift (ppm)
8.56
8.19
8.18
8.13
8.12
8.06
8.05
7.93
7.71
7.68
4.81
3.62
3.61
3.43
3.42
3.34
3.08
DMSO
1.43
1.39
0.91 1.00 0.96 0.96 0.91 1.88
1.97
2.01 2.05 2.91
9.00

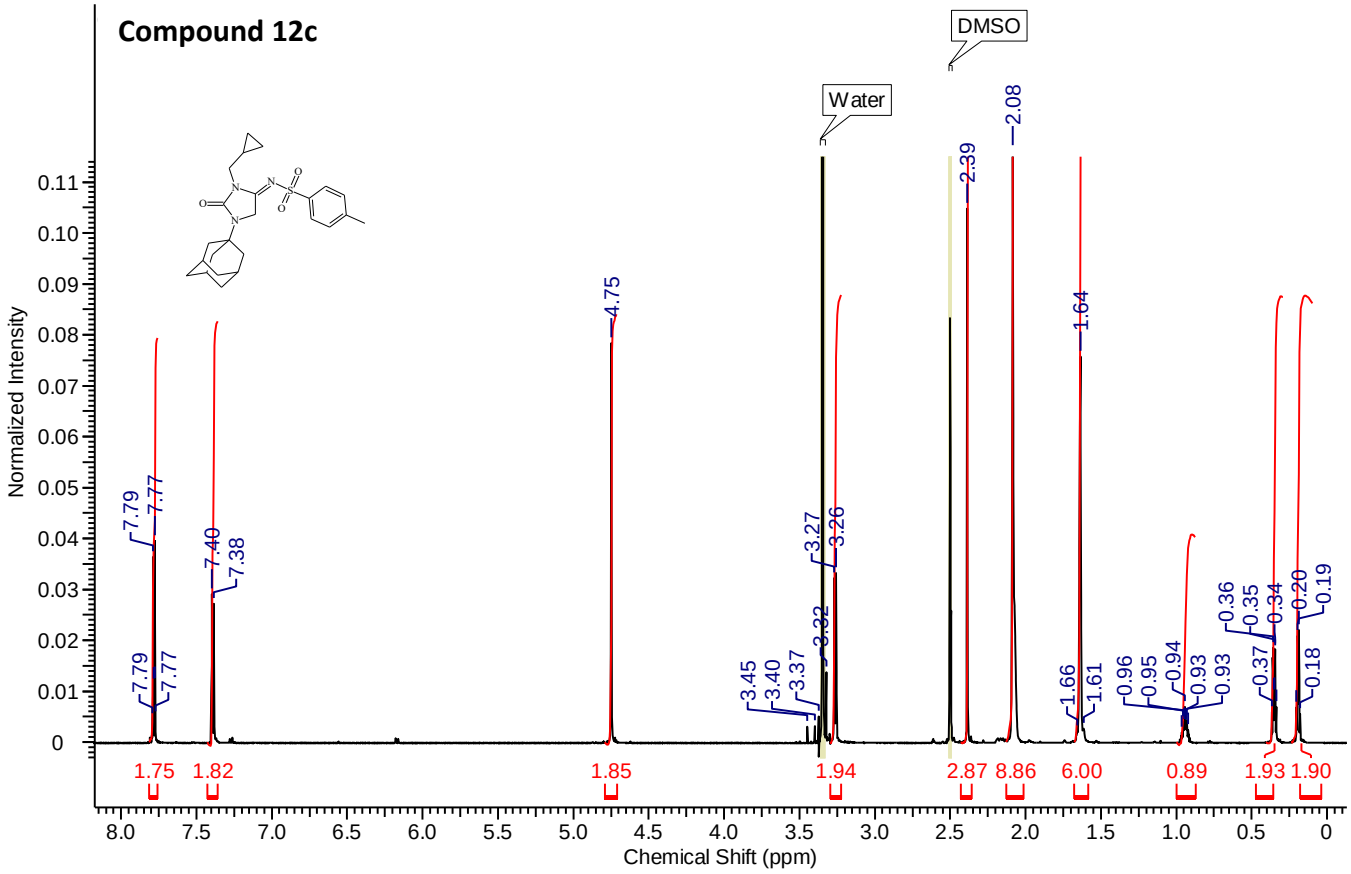

Compound 11h
Normalized Intensity
Chemical Shift (ppm)
165.78
153.13
138.76
134.24
131.66
129.34
129.18
128.82
127.83
127.57
126.65
122.32
67.39
57.63
54.15
48.03
40.05
39.92
39.79
39.64
39.51
39.37
39.23
39.09
27.13

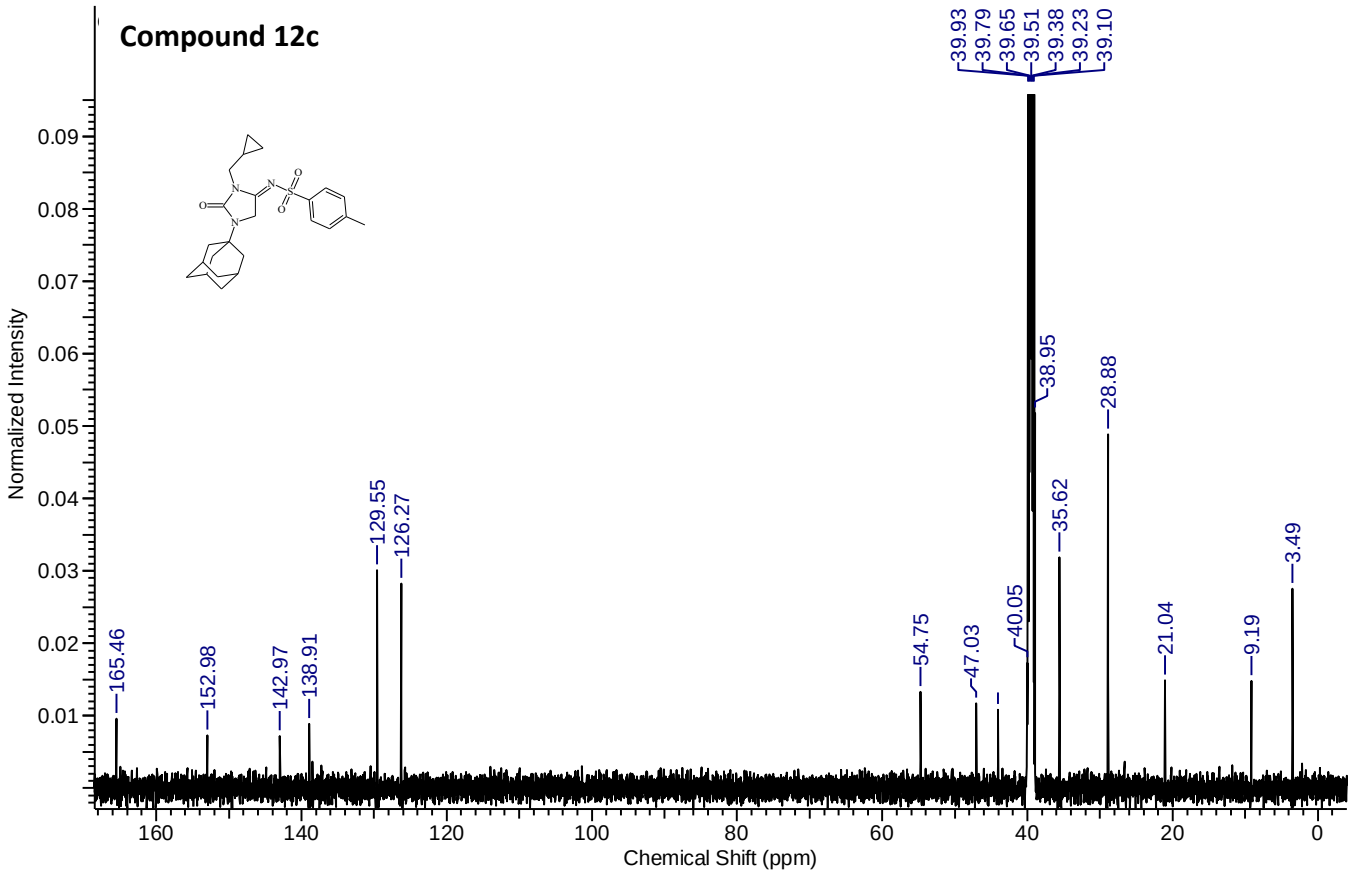

Compound 12a
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
4.67
3.37
3.35
3.35
3.31
3.30
3.06
3.06
2.09
2.07
2.05
1.63
1.61
1.10
1.09
1.09
1.08
1.07
1.07
0.46
0.46
0.45
0.44
0.44
0.30
0.30
0.29
0.28
1.92
2.00
2.91
8.99
6.10
0.94
1.99
2.00

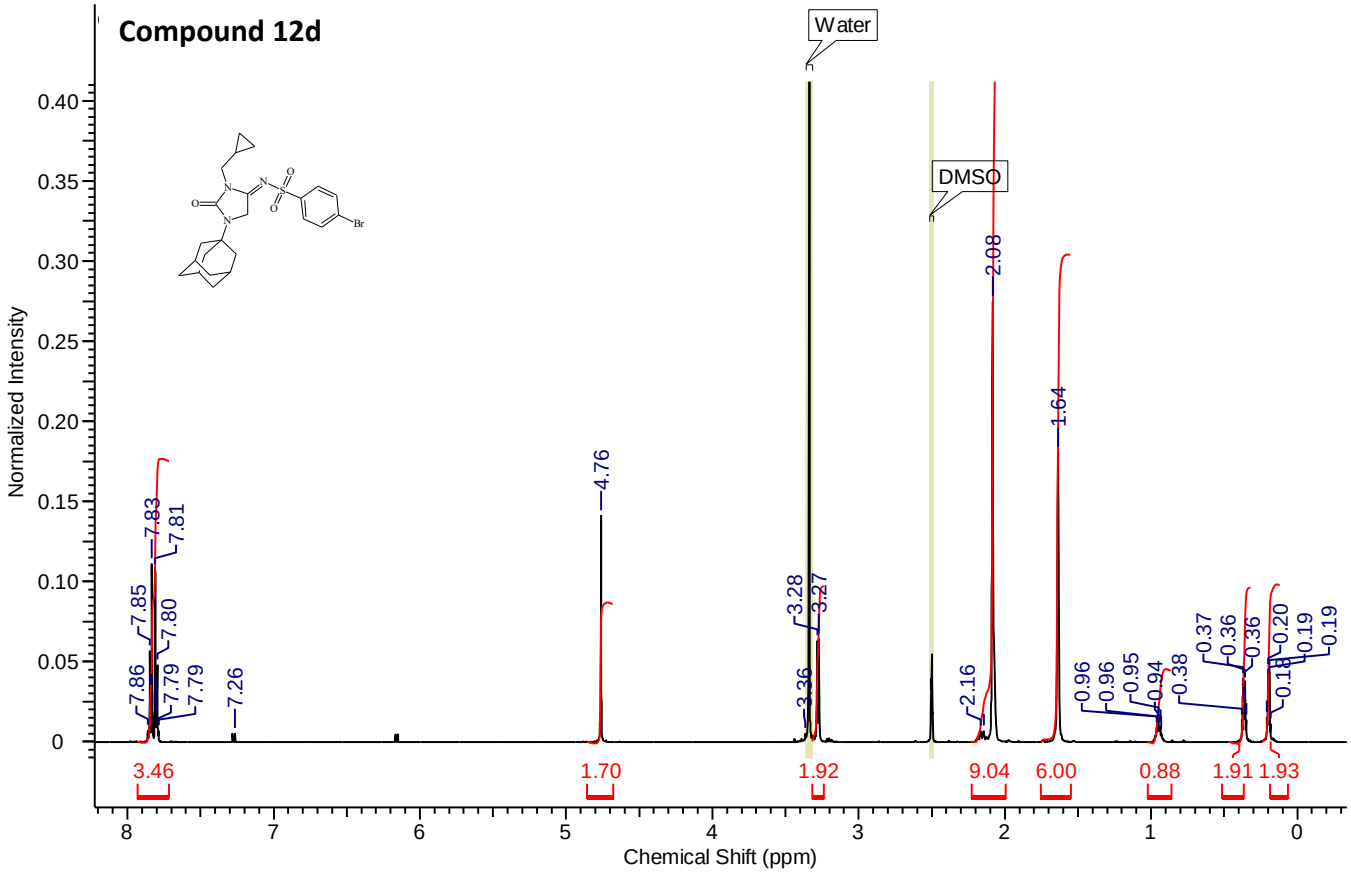

Compound 12a
Normalized Intensity
Chemical Shift (ppm)
39.79
39.65
39.51
39.38
39.23
39.93
39.09
39.02
28.86
35.61
3.57
54.66
46.54
43.94
41.68
9.18
165.72
153.22

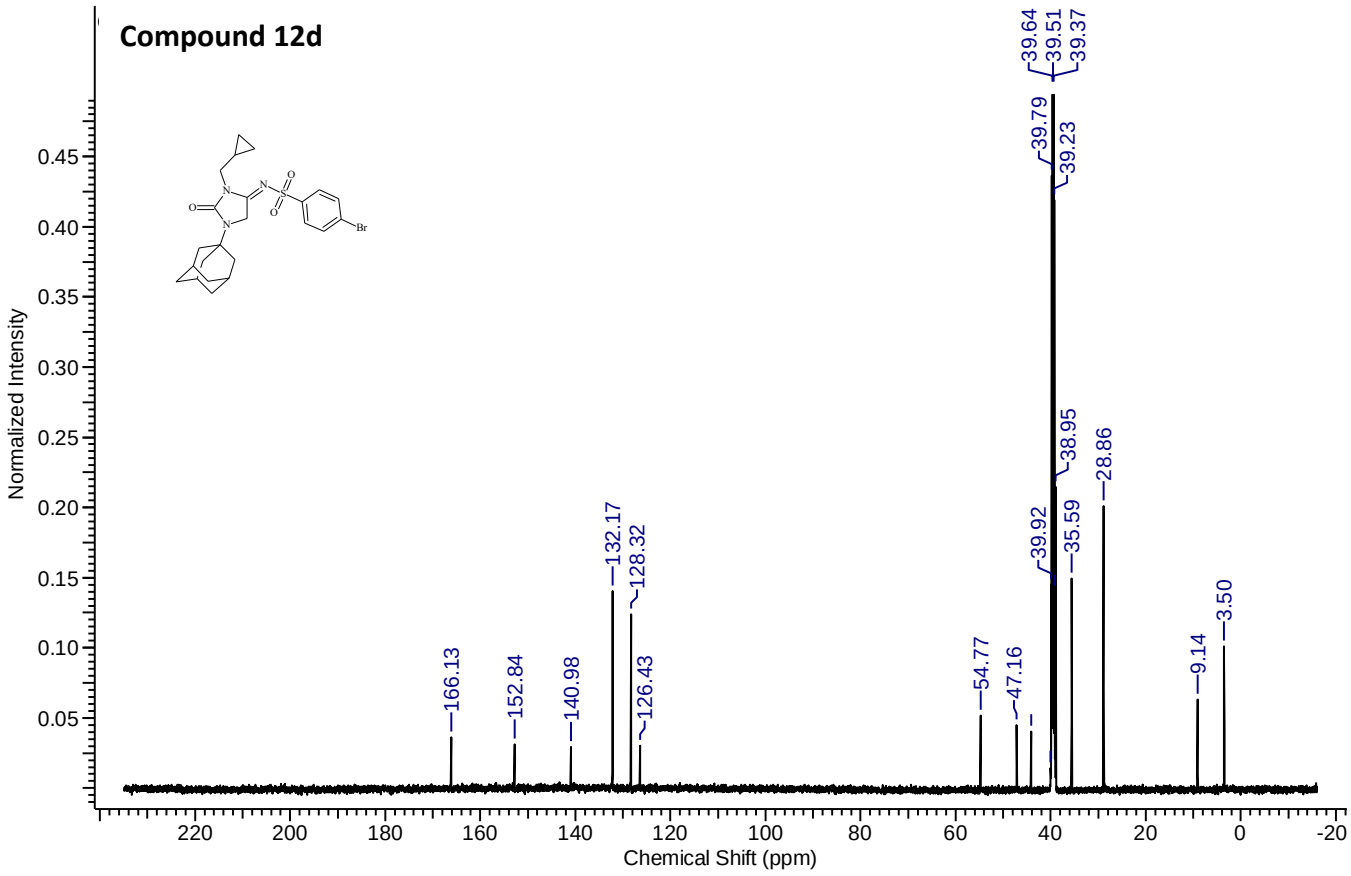

Compound 12b
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
7.91
7.90
7.90
7.66
7.61
7.59
4.77
3.37
3.32
3.28
3.27
2.09
1.64
0.94
0.93
0.36
0.35
0.35
0.34
0.20
0.19
0.18
1.68
2.63
1.77
1.94
9.03
6.00
0.83
1.91
1.88

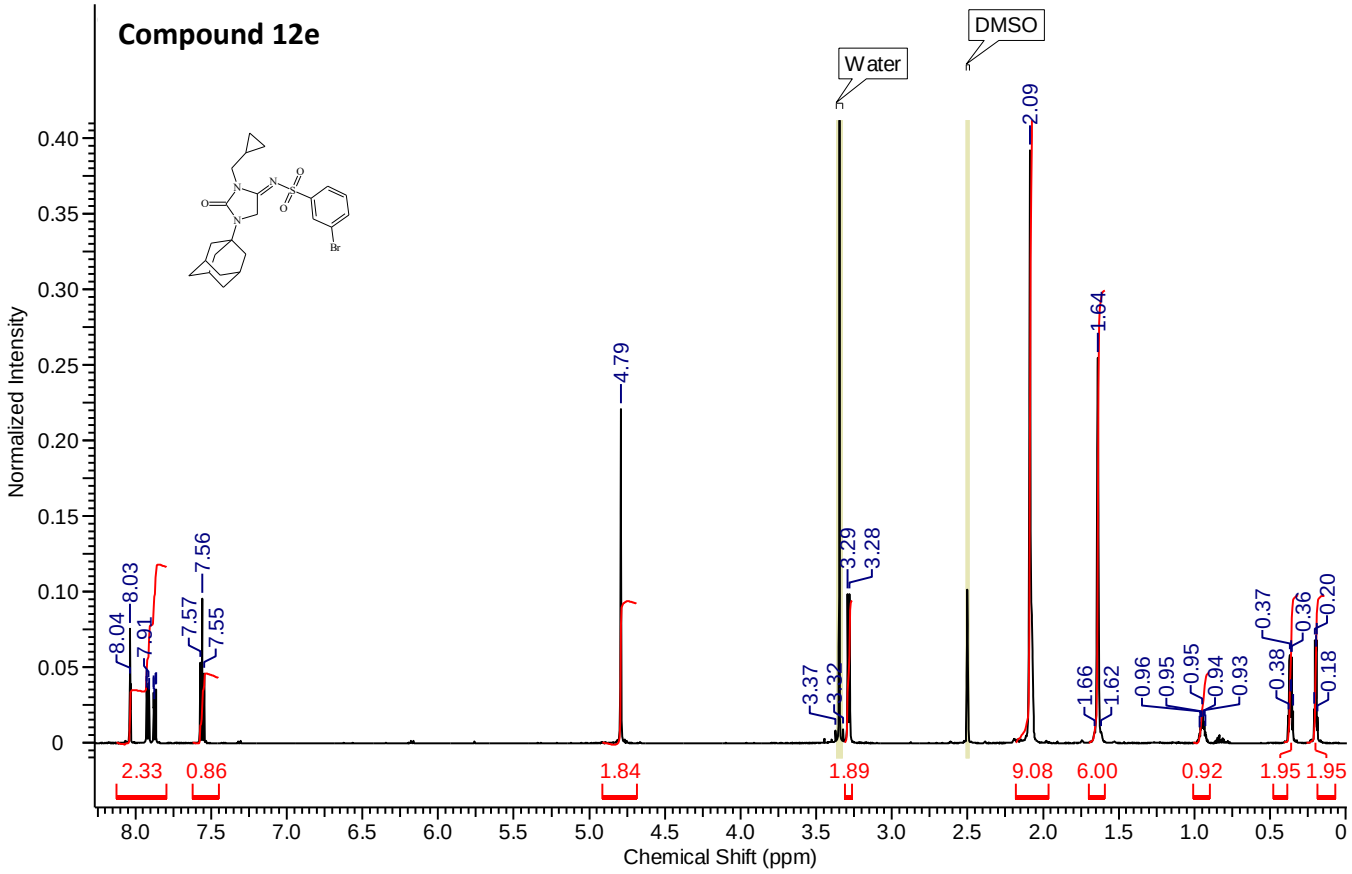

Compound 12b
Normalized Intensity
Chemical Shift (ppm)
165.68
152.92
141.67
132.65
129.11
126.17
54.75
47.07
44.04
39.93
39.79
39.65
39.51
39.38
39.23
38.95
35.60
35.51
28.87
28.81
9.15
3.45

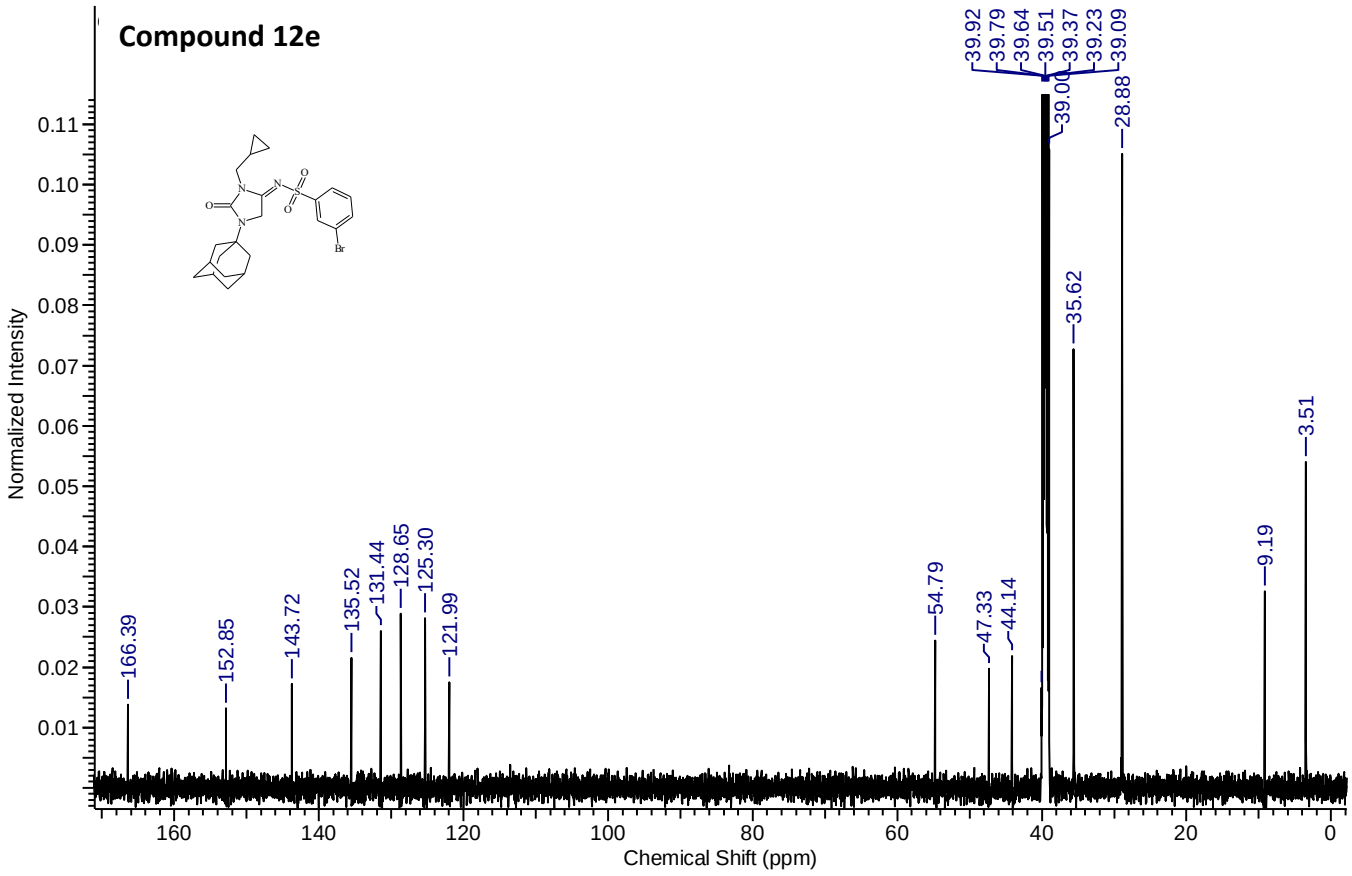

Compound 12c
DMSO
Water
Normalized Intensity
Chemical Shift (ppm)
7.79
7.77
7.40
7.38
4.75
3.45
3.40
3.37
3.32
3.27
3.26
2.39
2.08
1.66
1.64
1.61
0.96
0.95
0.94
0.93
0.93
0.37
0.36
0.35
0.34
0.20
0.19
0.18
1.75
1.82
1.85
1.94
2.87
8.86
6.00
0.89
1.93
1.90

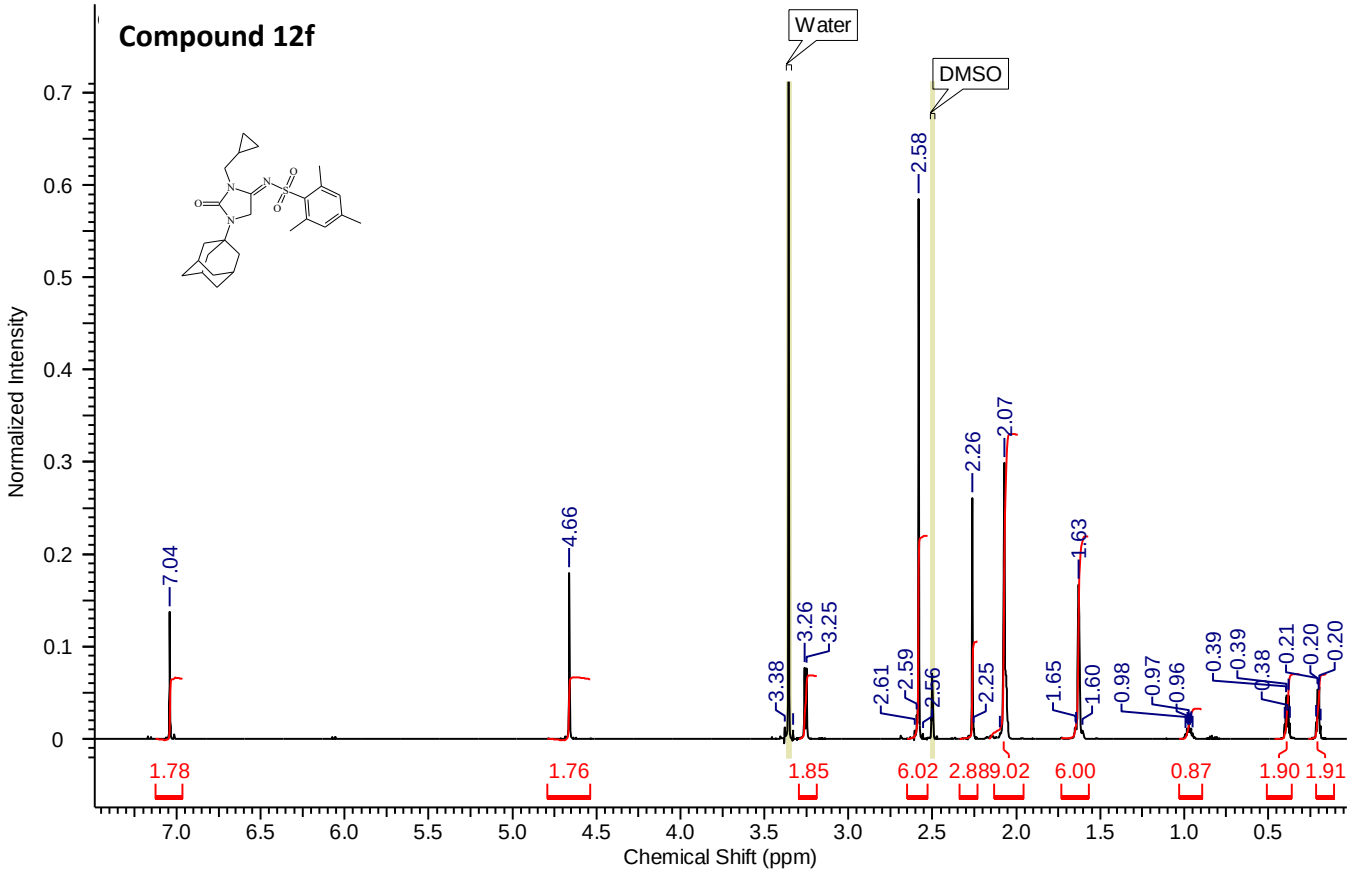

Compound 12c
Normalized Intensity
Chemical Shift (ppm)
165.46
152.98
142.97
138.91
129.55
126.27
54.75
47.03
40.05
39.93
39.79
39.65
39.51
39.38
39.23
39.10
38.95
35.62
28.88
21.04
9.19
3.49

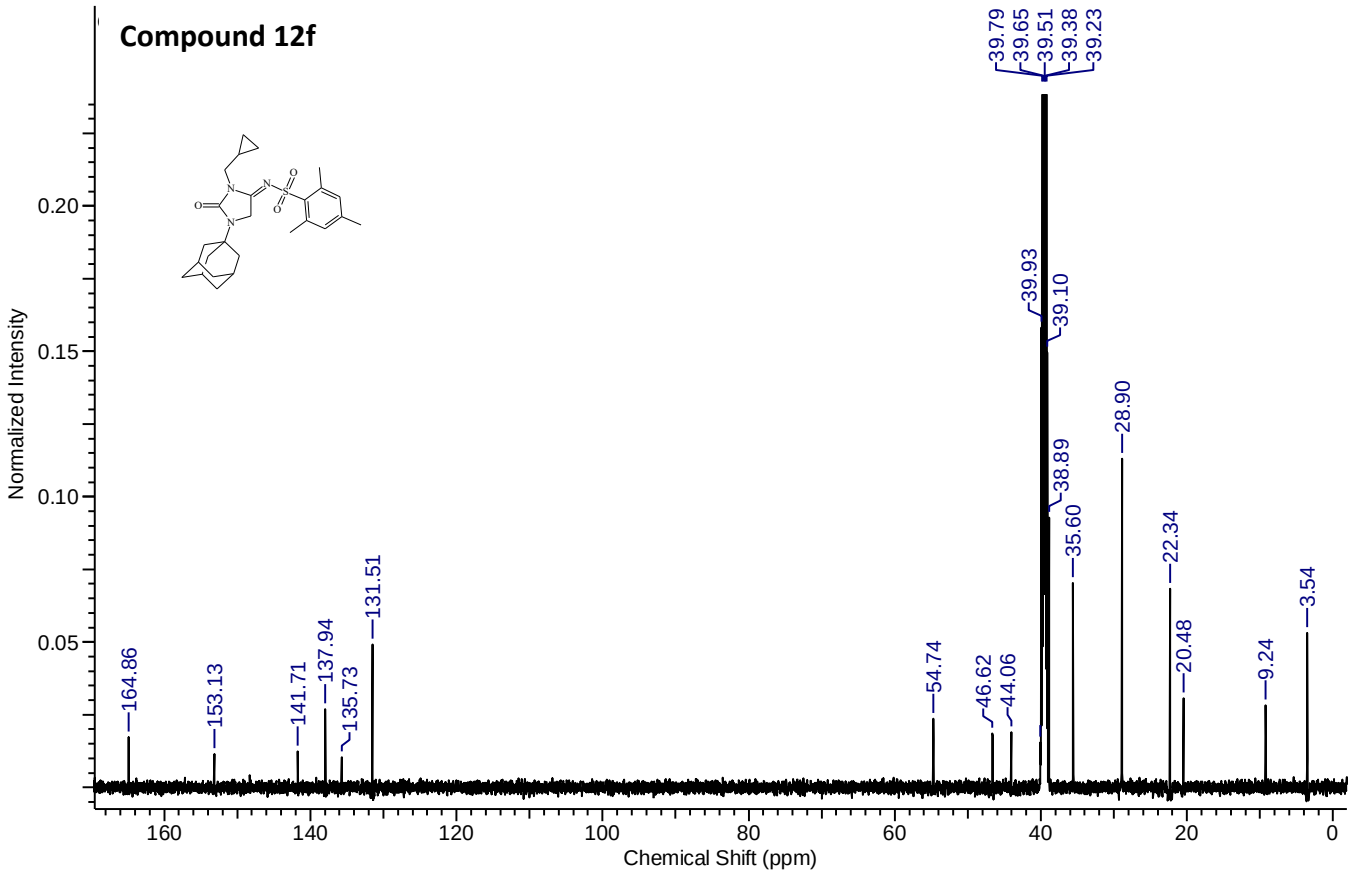

Compound 12d
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
7.86
7.85
7.83
7.81
7.80
7.79
7.79
7.26
4.76
3.36
3.28
3.27
2.16
2.08
1.64
0.96
0.96
0.95
0.94
0.38
0.37
0.36
0.36
0.20
0.19
0.19
0.18
3.46
1.70
1.92
9.04
6.00
0.88
1.91
1.93

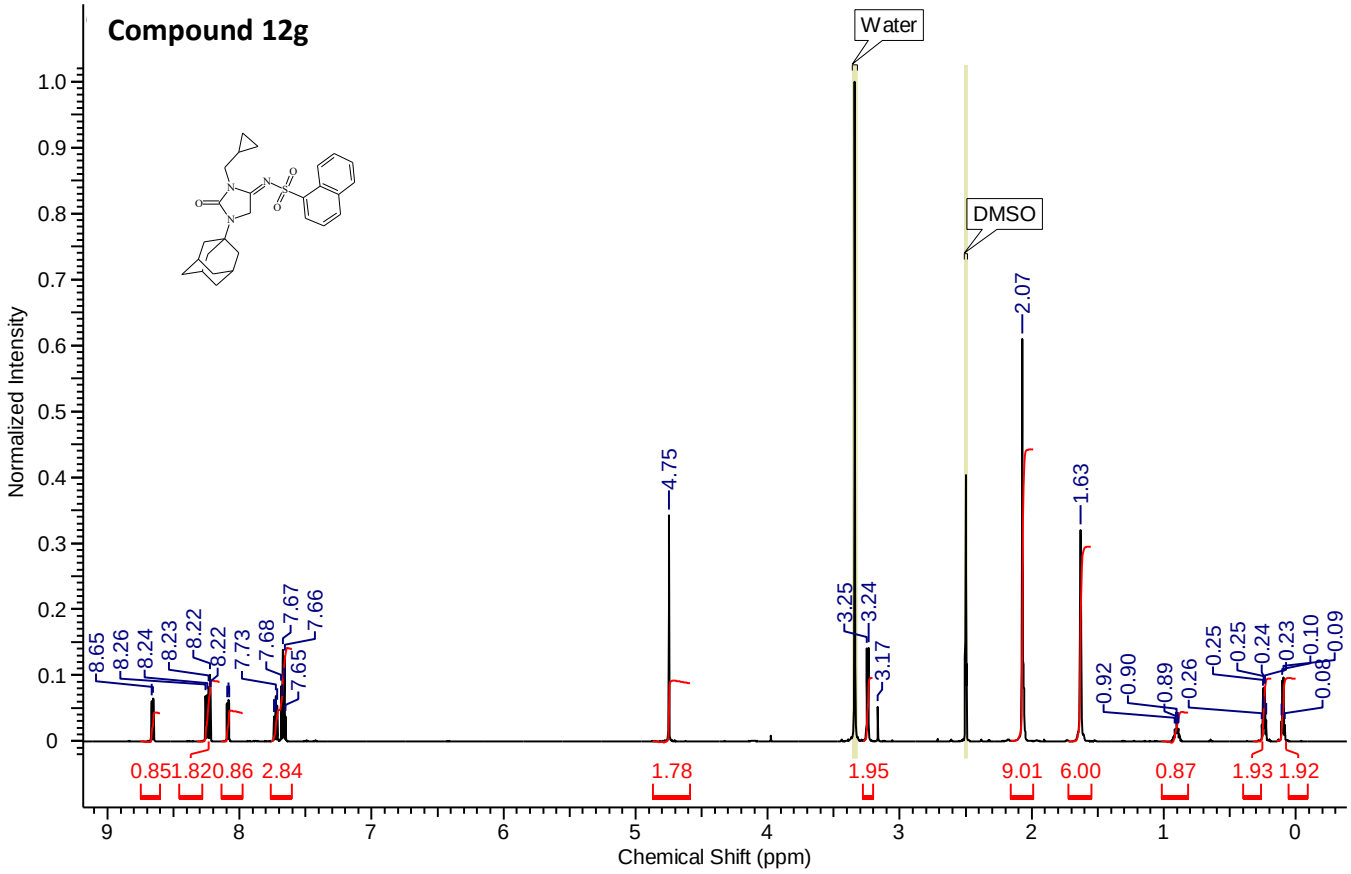

Compound 12d
Normalized Intensity
Chemical Shift (ppm)
166.13
152.84
140.98
132.17
128.32
126.43
54.77
47.16
39.92
39.79
39.64
39.51
39.37
39.23
38.95
35.59
28.86
9.14
3.50

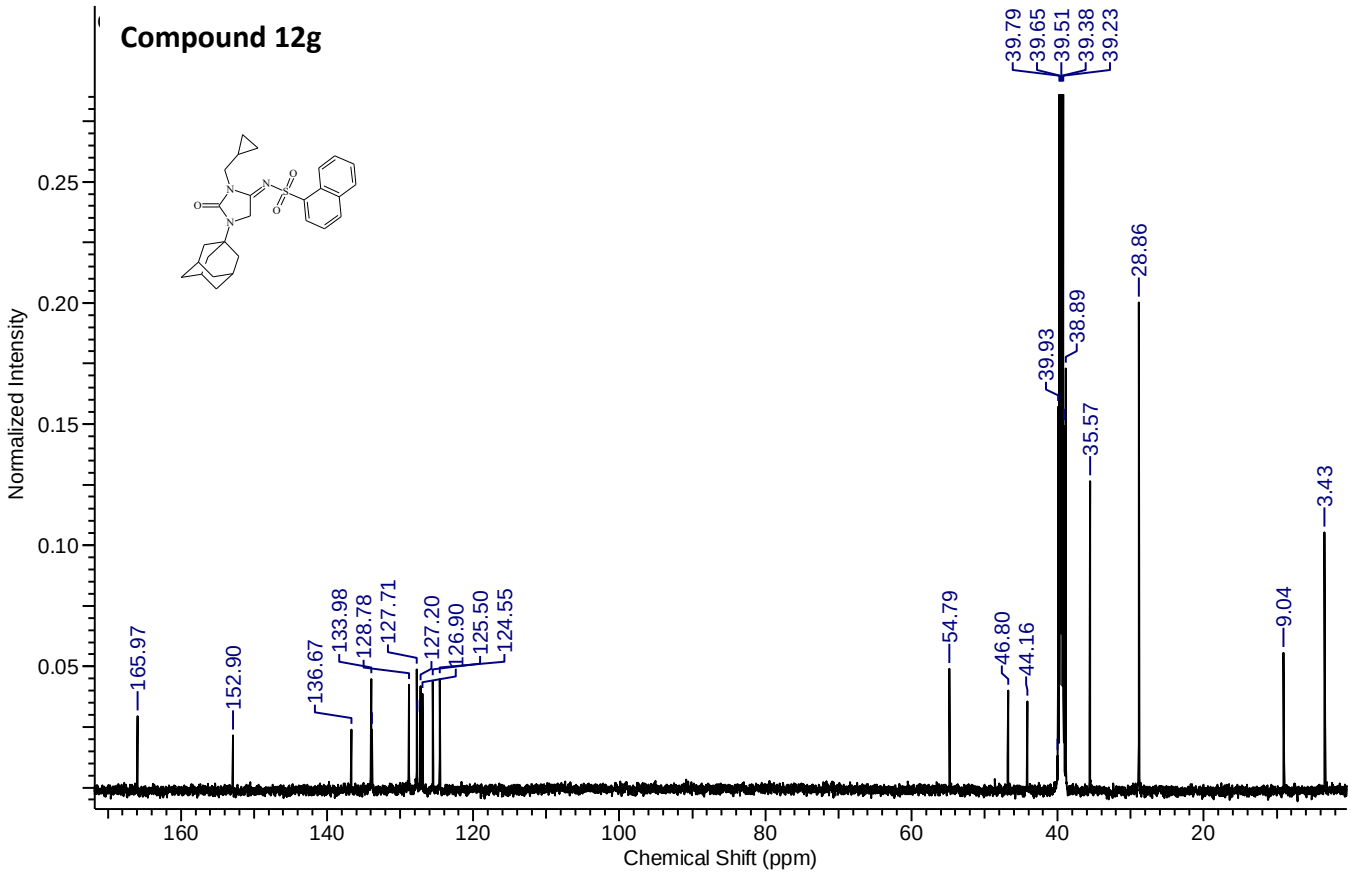

Compound 12e
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
8.04
8.03
7.91
7.57
7.56
7.55
4.79
3.37
3.32
3.29
3.28
2.09
1.66
1.64
1.62
0.96
0.95
0.95
0.94
0.93
0.38
0.37
0.36
0.20
0.18
2.33
0.86
1.84
1.89
9.08
6.00
0.92
1.95
1.95

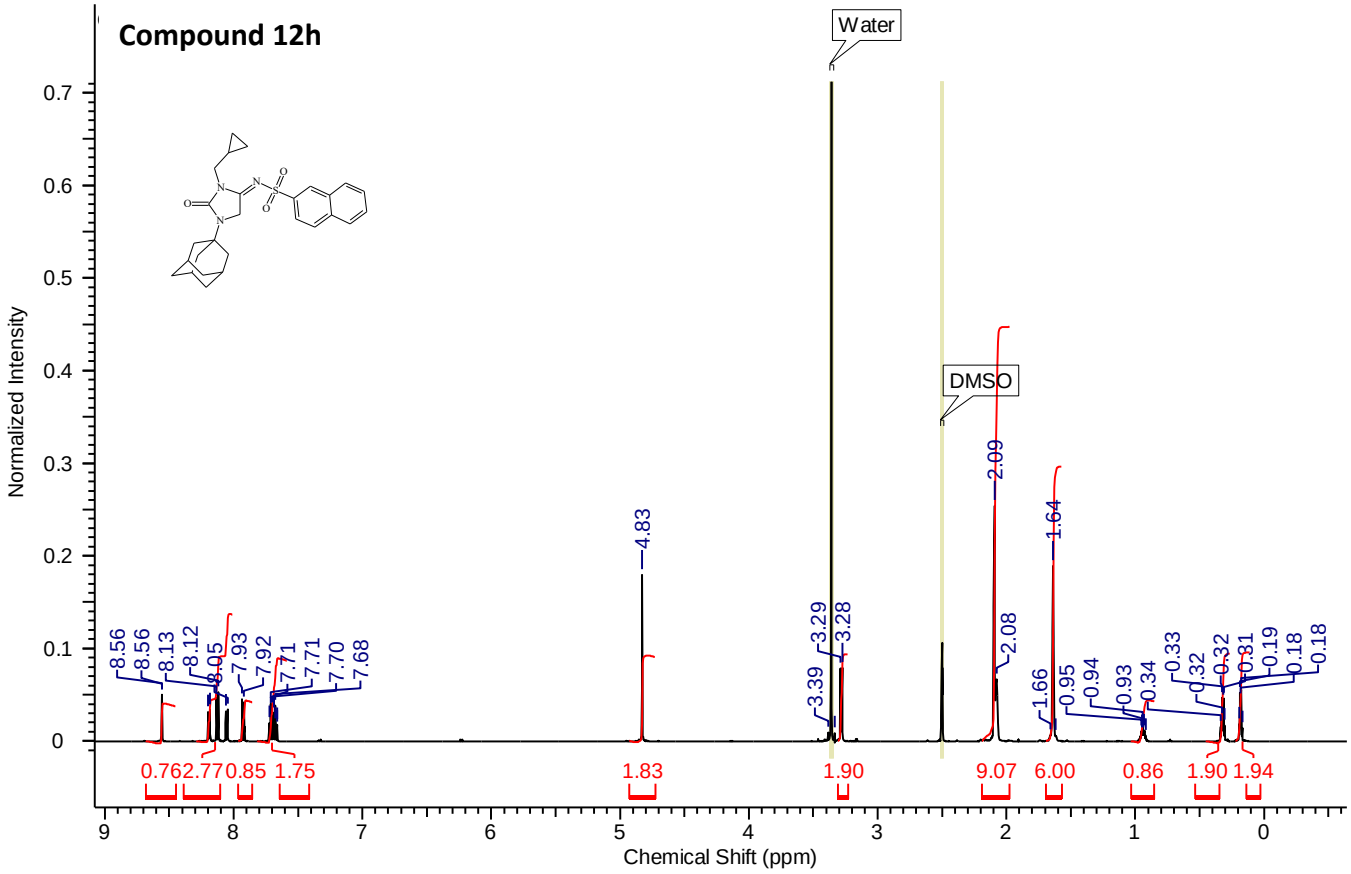

Compound 12e
Normalized Intensity
Chemical Shift (ppm)
166.39
152.85
143.72
135.52
131.44
128.65
125.30
121.99
54.79
47.33
44.14
39.92
39.79
39.64
39.51
39.37
39.23
39.09
39.00
35.62
28.88
9.19
3.51

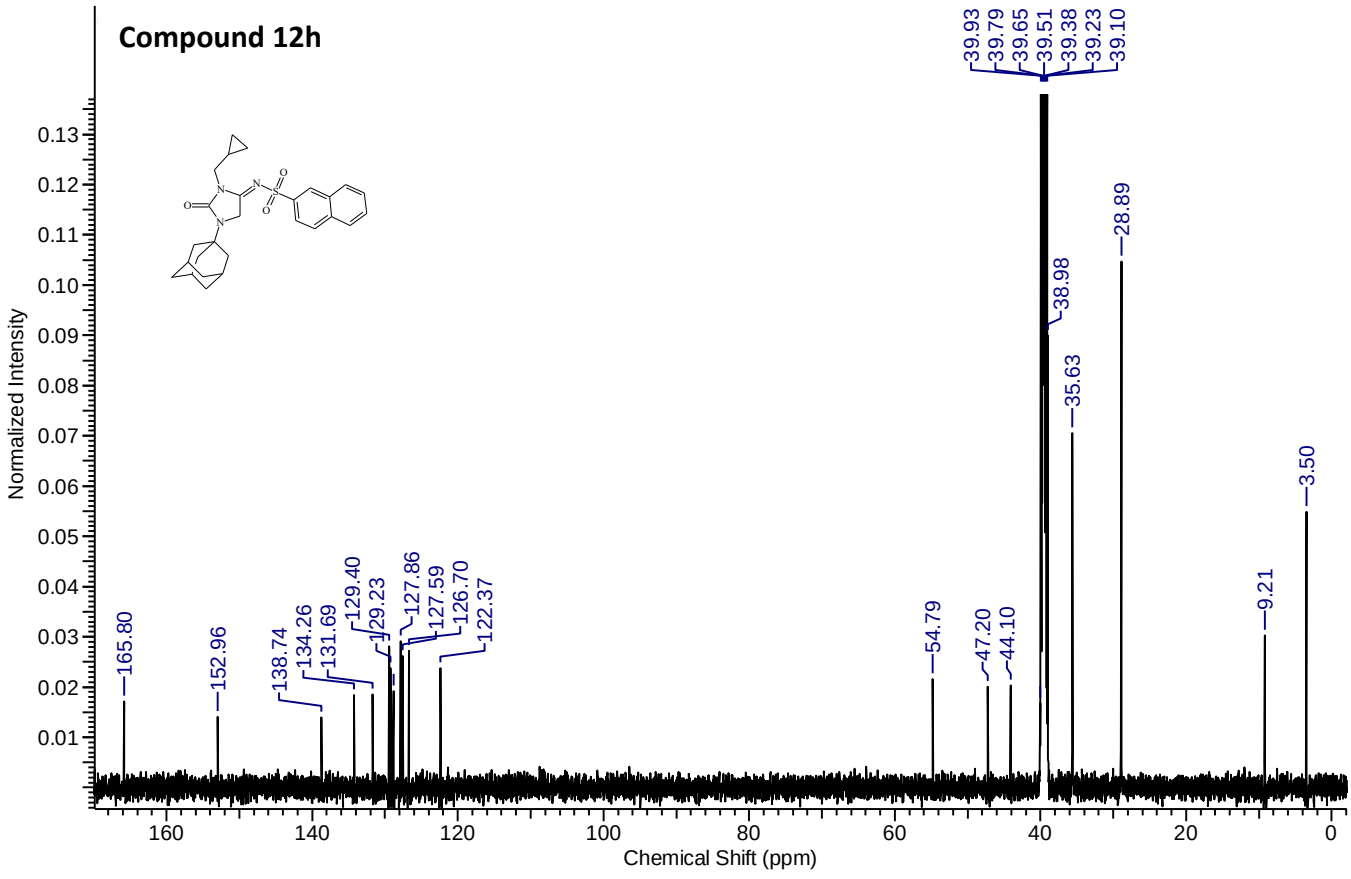

Compound 12f
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
7.04
4.66
3.38
3.26
3.25
2.61
2.59
2.56
2.58
2.25
2.26
2.07
1.65
1.63
1.60
0.98
0.97
0.96
0.39
0.39
0.38
0.21
0.20
0.20
1.78
1.76
1.85
6.02
2.88
9.02
6.00
0.87
1.90
1.91

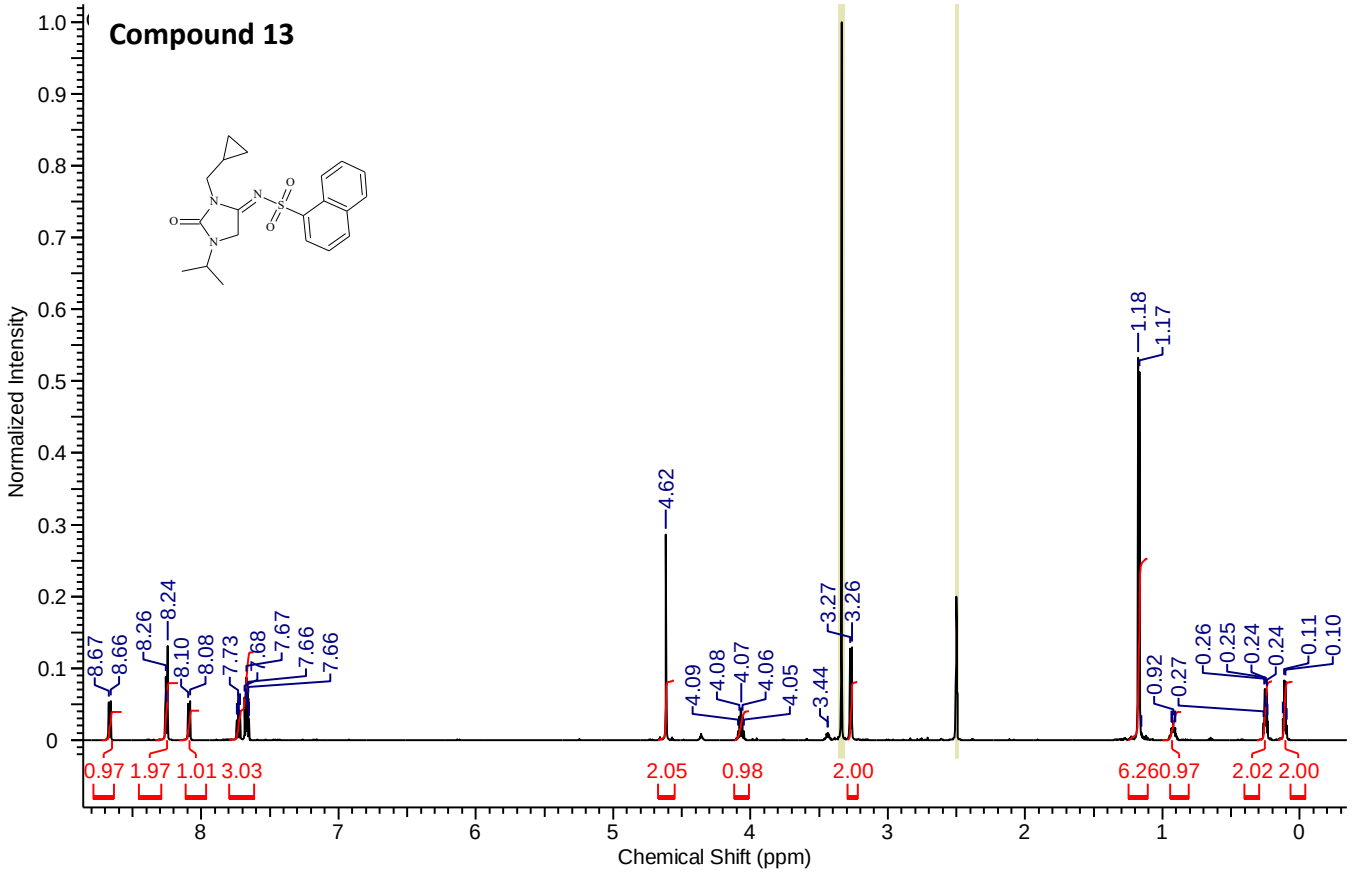

Compound 12f
Normalized Intensity
Chemical Shift (ppm)
164.86
153.13
141.71
137.94
135.73
131.51
54.74
46.62
44.06
39.79
39.65
39.51
39.38
39.23
39.93
39.10
38.89
35.60
28.90
22.34
20.48
9.24
3.54

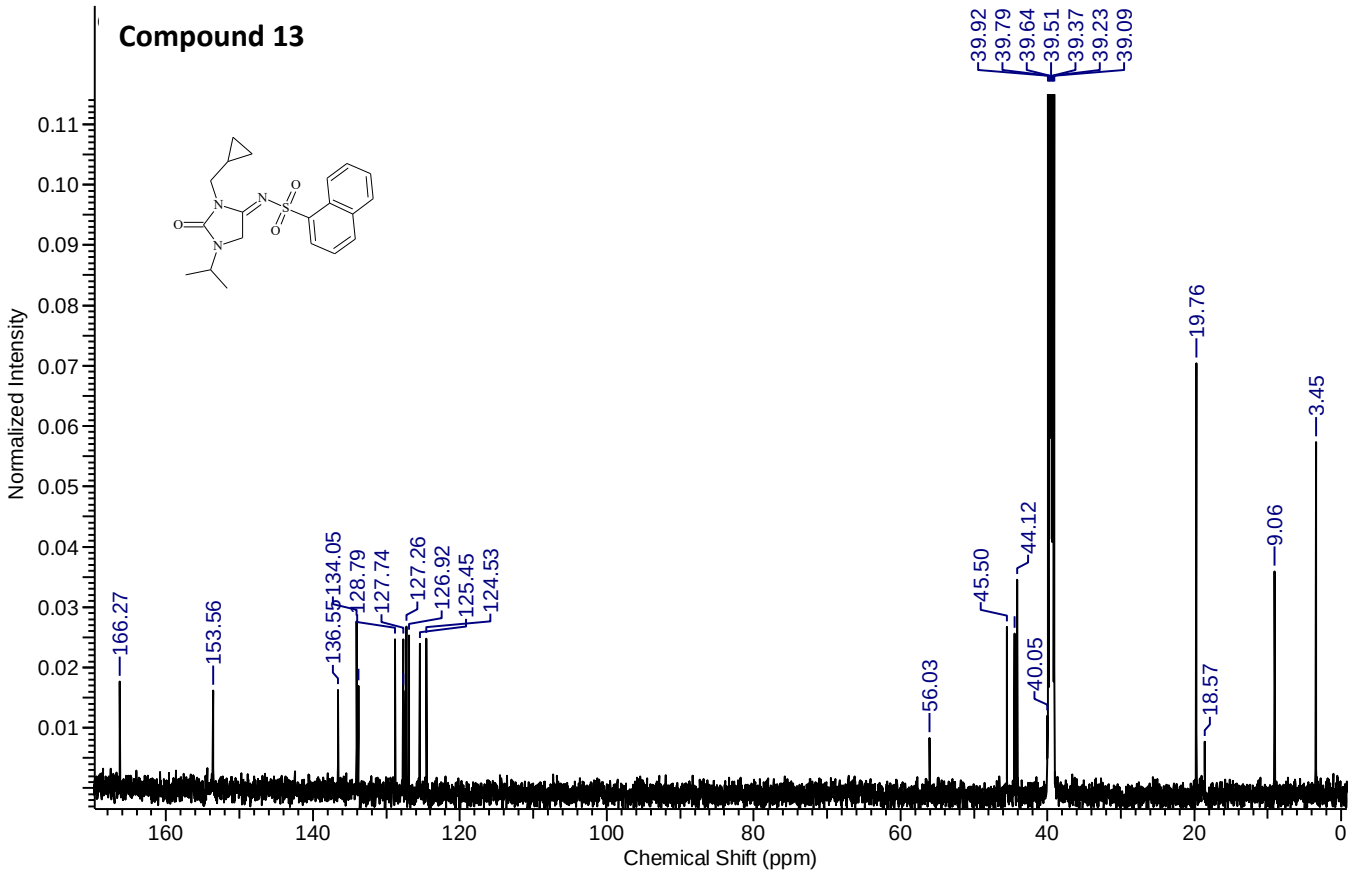

Compound 12g
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
8.65
8.26
8.24
8.23
8.22
8.22
7.73
7.68
7.67
7.66
7.65
4.75
3.25
3.24
3.17
2.07
1.63
0.92
0.90
0.89
0.26
0.25
0.25
0.24
0.23
0.10
0.09
0.08
0.85
1.82
0.86
2.84
1.78
1.95
9.01
6.00
0.87
1.93
1.92

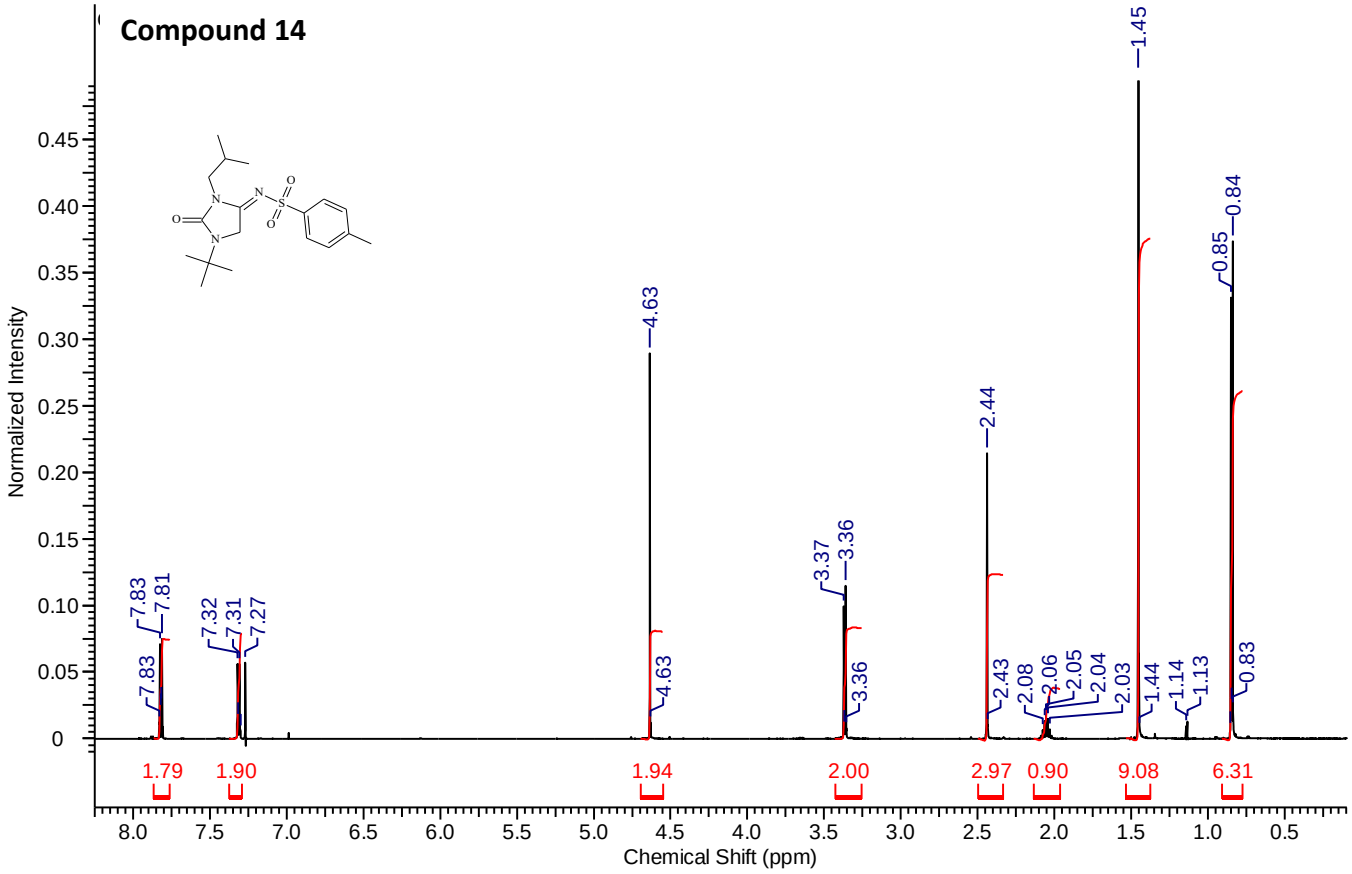

Compound 12g
Normalized Intensity
Chemical Shift (ppm)
39.79
39.65
39.51
39.38
39.23
28.86
39.93
38.89
35.57
3.43
9.04
54.79
46.80
44.16
165.97
152.90
136.67
133.98
128.78
127.71
127.20
126.90
125.50
124.55

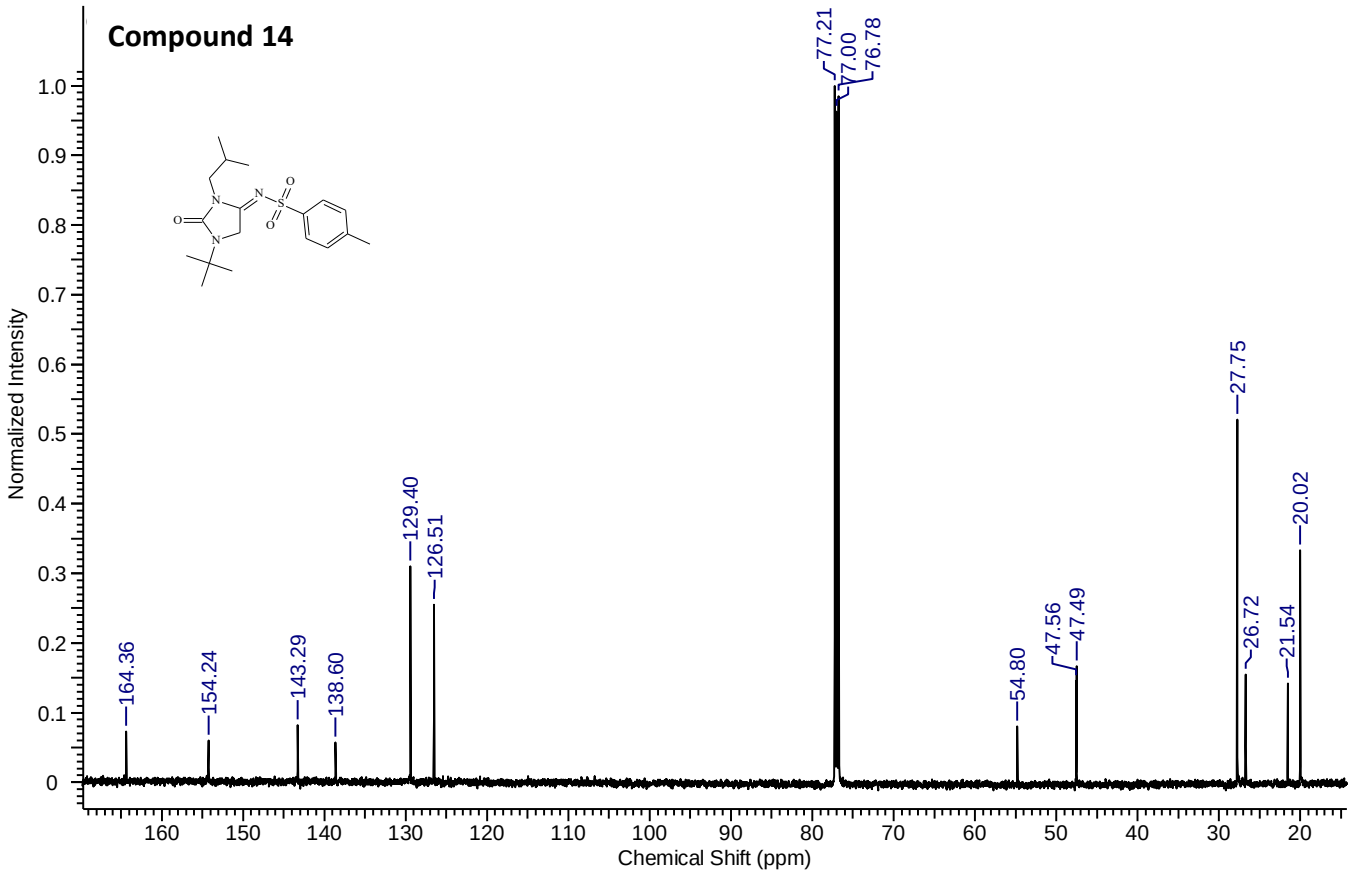

Compound 12h
Water
DMSO
Normalized Intensity
Chemical Shift (ppm)
8.56
8.56
8.13
8.12
8.05
7.93
7.92
7.71
7.71
7.70
7.68
4.83
3.29
3.28
3.39
2.09
2.08
1.64
1.66
0.95
0.94
0.93
0.34
0.33
0.32
0.81
0.19
0.18
0.18
0.76
2.77
0.85
1.75
1.83
1.90
9.07
6.00
0.86
1.90
1.94

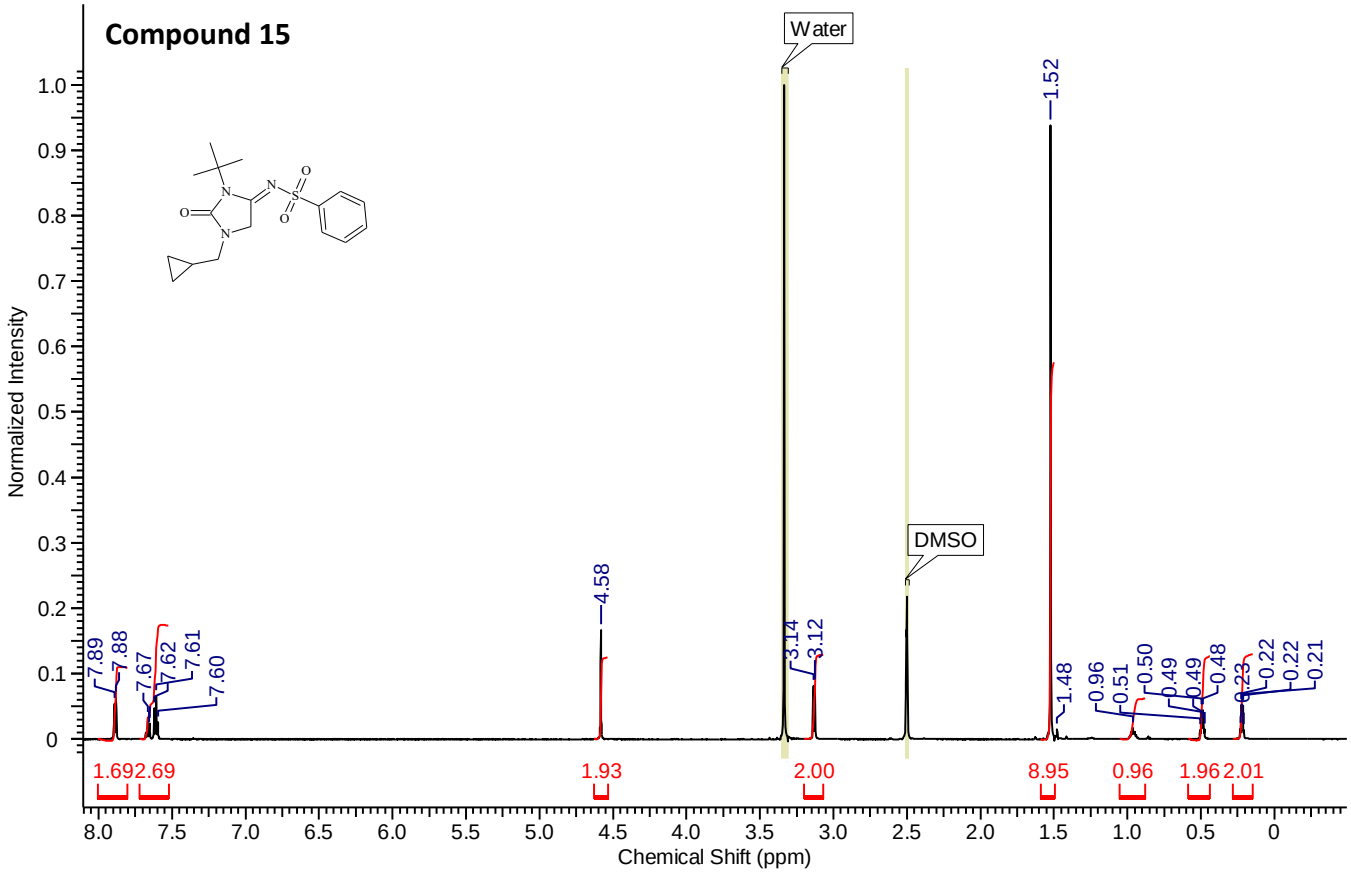

Compound 12h
Normalized Intensity
Chemical Shift (ppm)
39.93
39.79
39.65
39.51
39.38
39.23
39.10
38.98
28.89
35.63
3.50
9.21
165.80
152.96
138.74
134.26
131.69
129.40
129.23
127.86
127.59
126.70
122.37
54.79
47.20
44.10

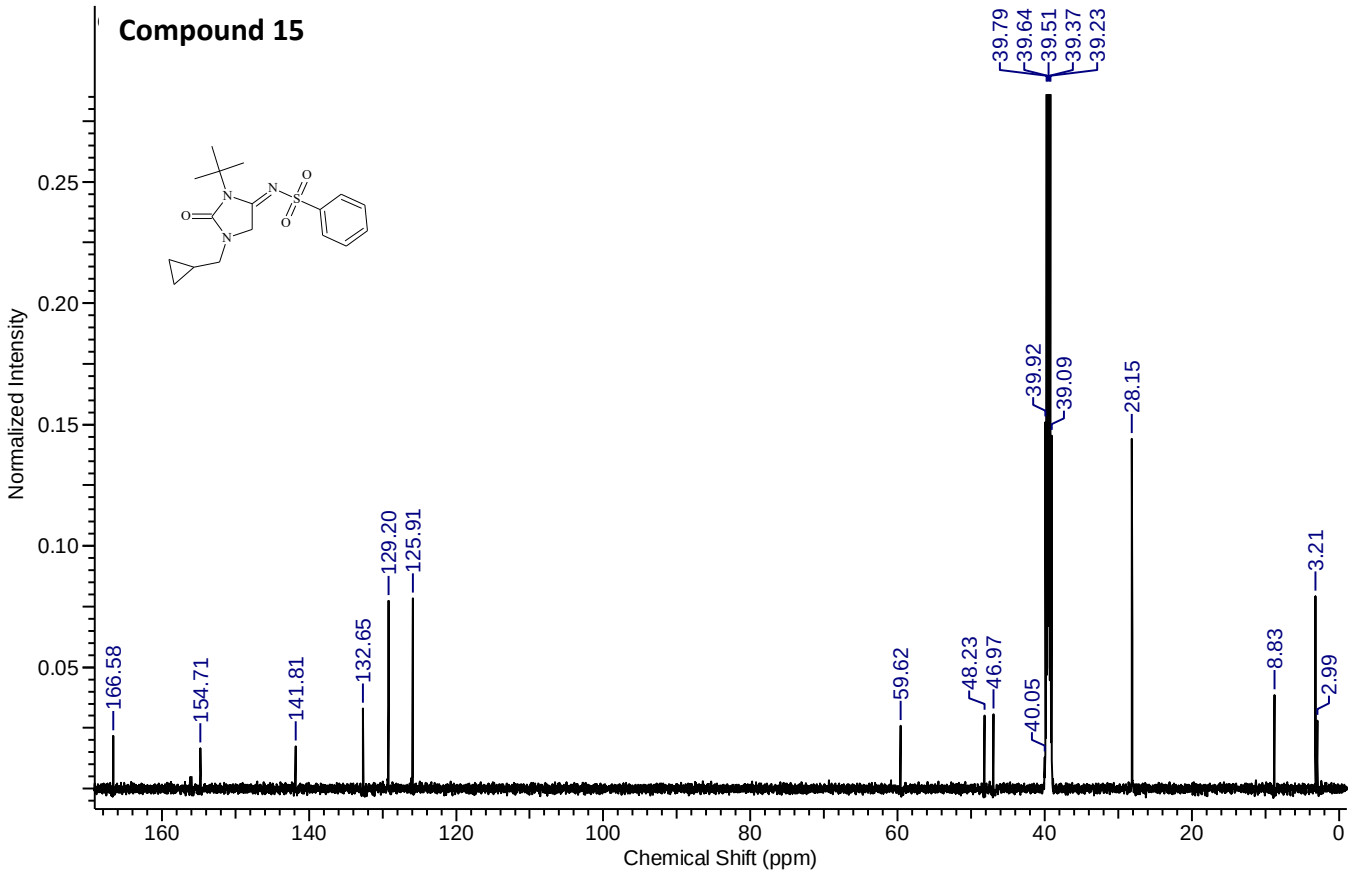

Compound 13
Normalized Intensity
Chemical Shift (ppm)
8.67
8.66
8.26
8.24
8.10
8.08
7.73
7.68
7.67
7.66
7.66
4.62
4.09
4.08
4.07
4.06
4.05
3.44
3.27
3.26
1.18
1.17
0.92
0.27
0.26
0.25
0.24
0.24
0.11
0.10
0.97
1.97
1.01
3.03
2.05
0.98
2.00
6.26
0.97
2.02
2.00


Compound 13
Normalized Intensity
Chemical Shift (ppm)
39.92
39.79
39.64
39.51
39.37
39.23
39.09
166.27
153.56
136.55
134.05
128.79
127.74
127.26
126.92
125.45
124.53
56.03
45.50
44.12
40.05
19.76
18.57
9.06
3.45


Compound 14
Normalized Intensity
Chemical Shift (ppm)
7.83
7.81
7.32
7.31
7.27
4.63
3.37
3.36
2.44
2.43
2.08
2.06
2.05
2.04
2.03
1.45
1.44
1.14
1.13
0.85
0.84
0.83
1.79
1.90
1.94
2.00
2.97
0.90
9.08
6.31


Compound 14
Normalized Intensity
Chemical Shift (ppm)
77.21
77.00
76.78
164.36
154.24
143.29
138.60
129.40
126.51
54.80
47.56
47.49
27.75
26.72
21.54
20.02


Compound 15
Water
DMSO
1.52
4.58
3.14
3.12
7.89
7.88
7.67
7.62
7.61
7.60
1.48
0.96
0.51
0.50
0.49
0.49
0.48
0.23
0.22
0.22
0.21
1.69
2.69
1.93
2.00
8.95
0.96
1.96
2.01
Normalized Intensity
Chemical Shift (ppm)


Compound 15
39.79
39.64
39.51
39.37
39.23
39.92
39.09
28.15
3.21
166.58
154.71
141.81
132.65
129.20
125.91
59.62
48.23
46.97
40.05
8.83
2.99
Normalized Intensity
Chemical Shift (ppm)