Synthesis of Fused Imidazole-Containing Ring Systems *via* Dual Oxidative Amination of C(sp^3)-H bonds

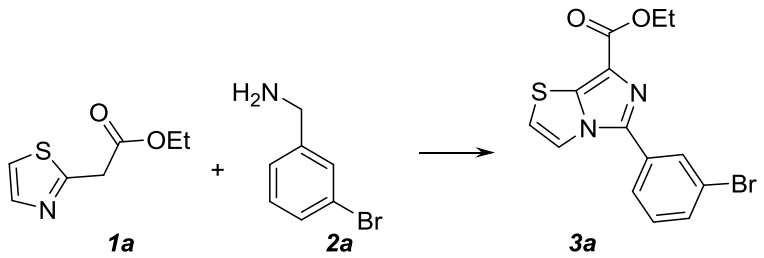
Georgette Castanedo,* Yanzhou Liu, James J. Crawford and Marie-Gabrielle Braun

Discovery Chemistry, Genentech, Inc., South San Francisco, CA 94080

SUPPORTING INFORMATION

Table of Contents

Reaction Optimization using ethyl 2-thiazol-2-ylacetate and 3-bromobenzylamine:



SI Table 1: Halogen Source Optimization

Entry	Iodine Source	Yield of compound *3a* (%)[a,b]	*% conversion of 1a*
1	Iodine	64	100
2	NIS	84	100
3	Bu_4NI	23	100
4	KI	25	100

[a] Yield of ***3a***, determined by LCMS using naphthalene as a quantitative internal standard.

[b] Correction factor of 1.05 applied to LCMS yields of ***3a*** after determining difference in ratios of

product to starting material by LCMS/NMR

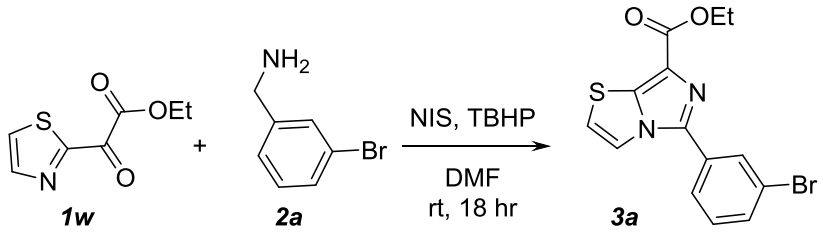
SI Table 2: Solvent Optimization

Entry	Solvent	Yield of compound *3a* (%)[a,b]	*% conversion of 1a*
1	DMA	85	100
2	DMF	87	100
3	DMSO	86	100
4	ACN	92	100

[a] Yield of ***3a***, determined by LCMS using naphthalene as a quantitative internal standard

[b] Correction factor of 1.05 applied to LCMS yields of ***3a*** after determining difference in ratios of product to starting material by LCMS/NMR

SI Table 3: β-Keto ester as substrate



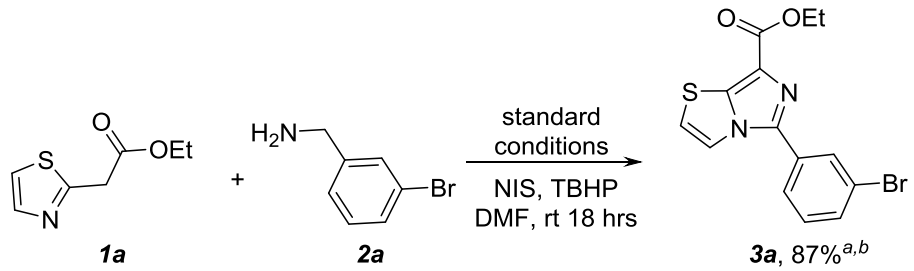
1w ***2a*** ***3a***

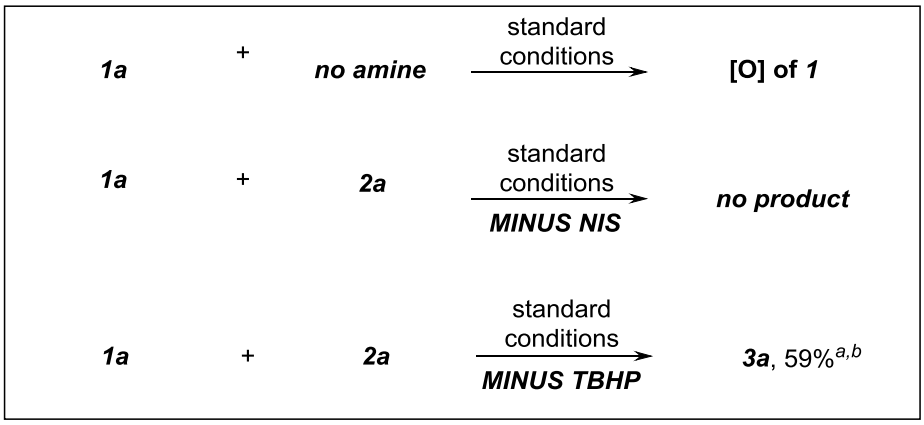
Entry	Substrate	Yield of compound *3a* (%)[a,b]	*% conversion of 1w*
1	***1w***	89	100

[a] Yield of ***3***, determined by LCMS using naphthalene as a quantitative internal standard

[b] Correction factor of 1.05 applied to LCMS yields of ***3a*** after determining difference in ratios of product to starting material by LCMS/NMR

SI Table 4: Control Experiments





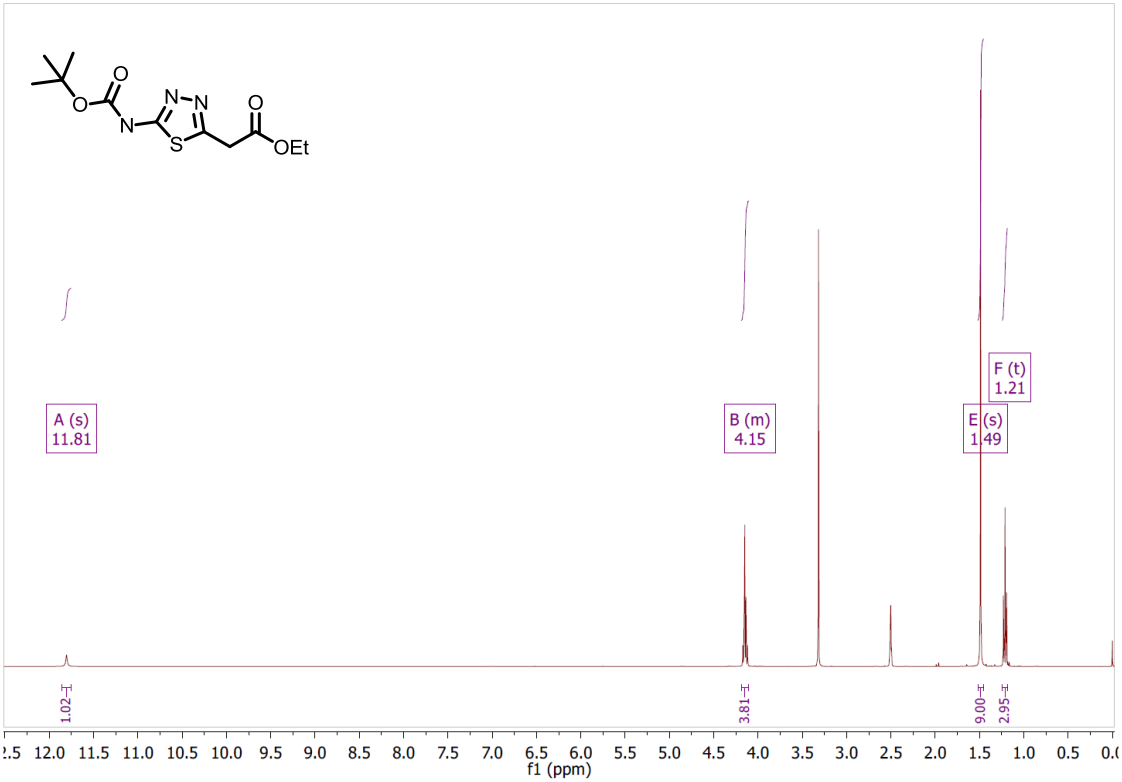
Entry	Reagent Missing	Yield of compound *3a* (%)[a,b]	*% conversion of 1*
1	No Amine	0	95[c]
2	No NIS	0	72
3	No TBHP	59	75

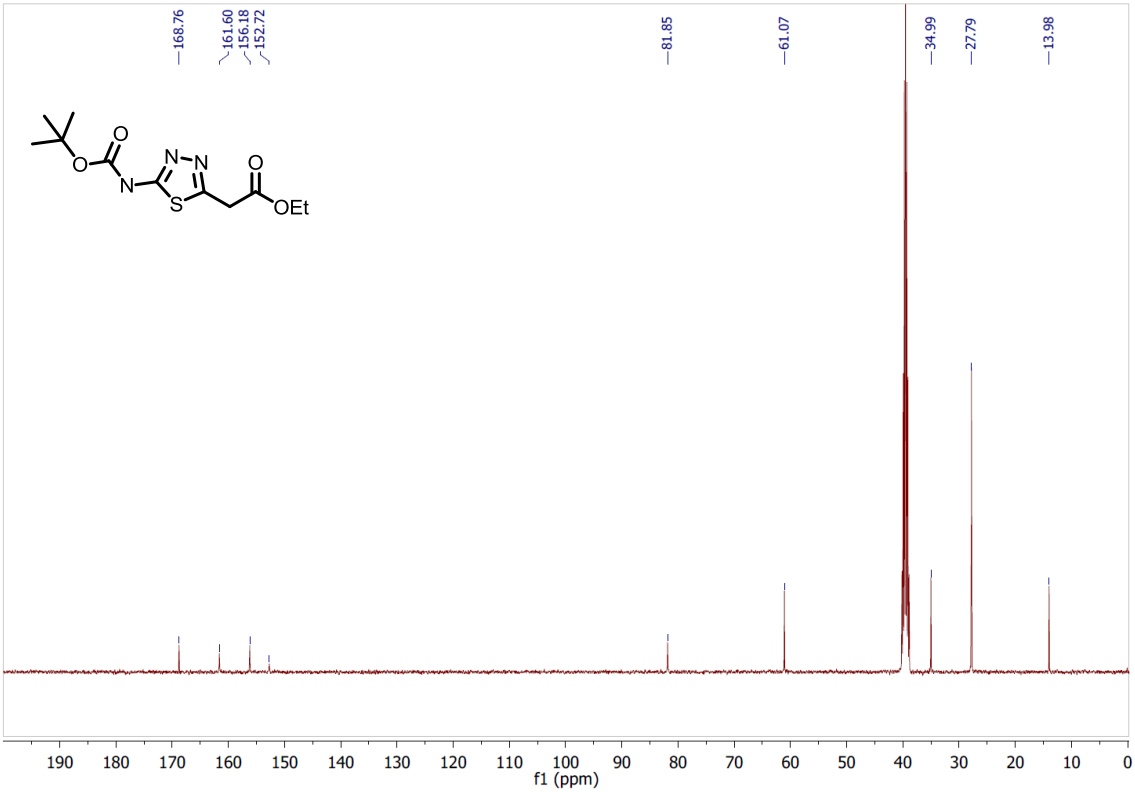
[a] Yield of ***3a***, determined by LCMS using naphthalene as a quantitative internal standard

[b] Correction factor of 1.05 applied to LCMS yields of ***3a*** after determining difference in ratios of product to starting material by LCMS/NMR

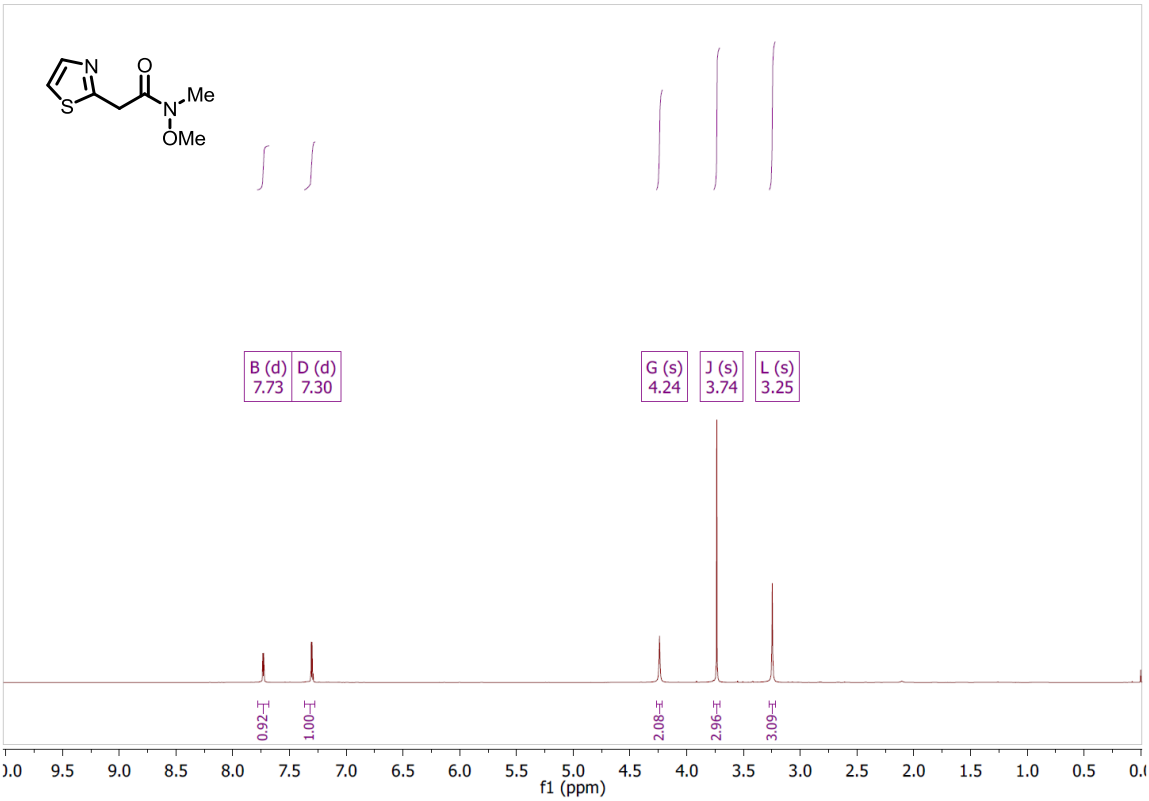
[c] Mass for oxidation of ***1a*** to ***1w*** was seen by mass spec which is consistent with observations from Mohan, D.; Rao, S.; Ravi, C.; and Adimurthy, S. *Org. Biomol. Chem*. **2015**, *13*, 5602.

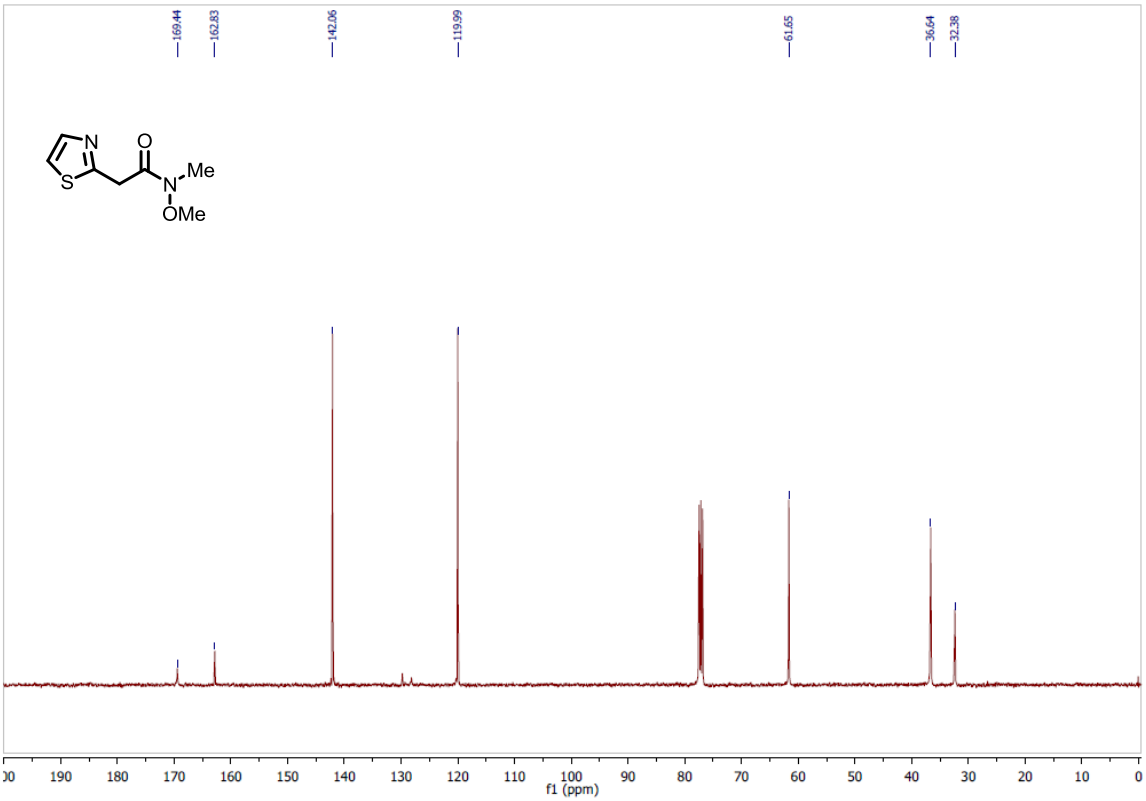
NMR Characterization Data
Starting Material *1e*



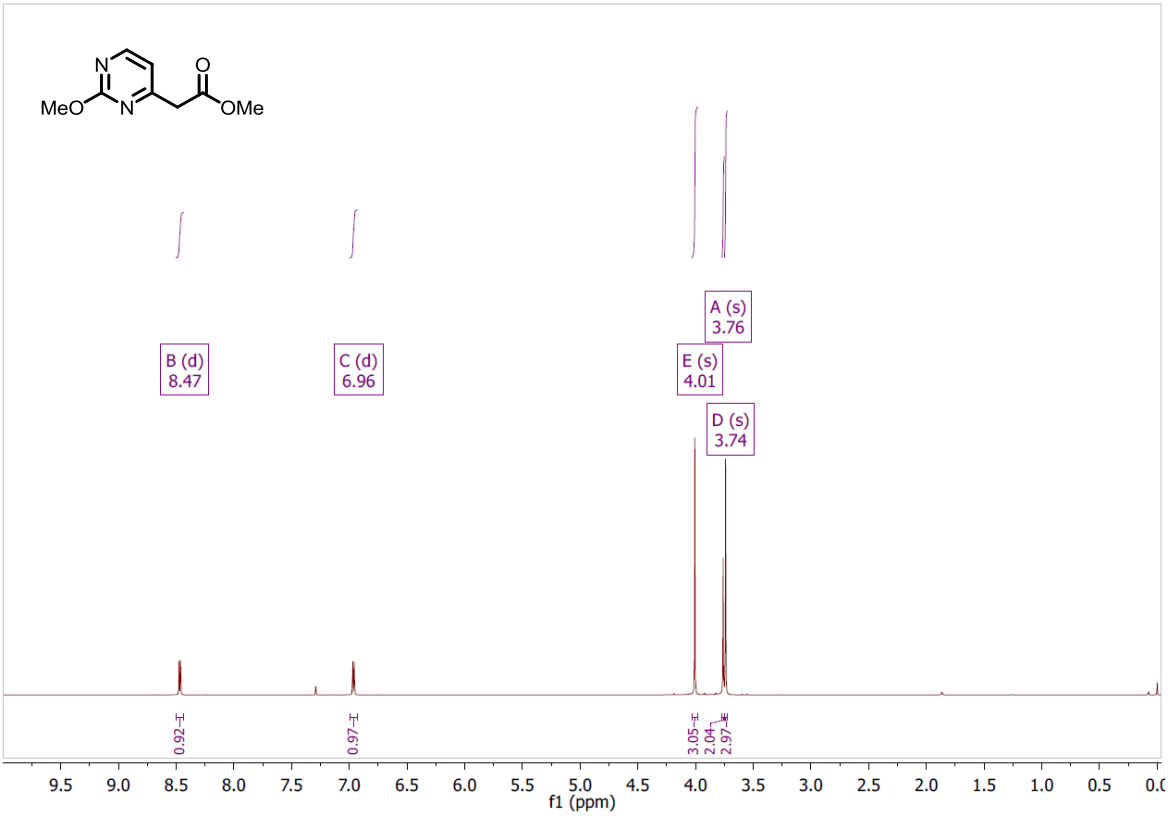


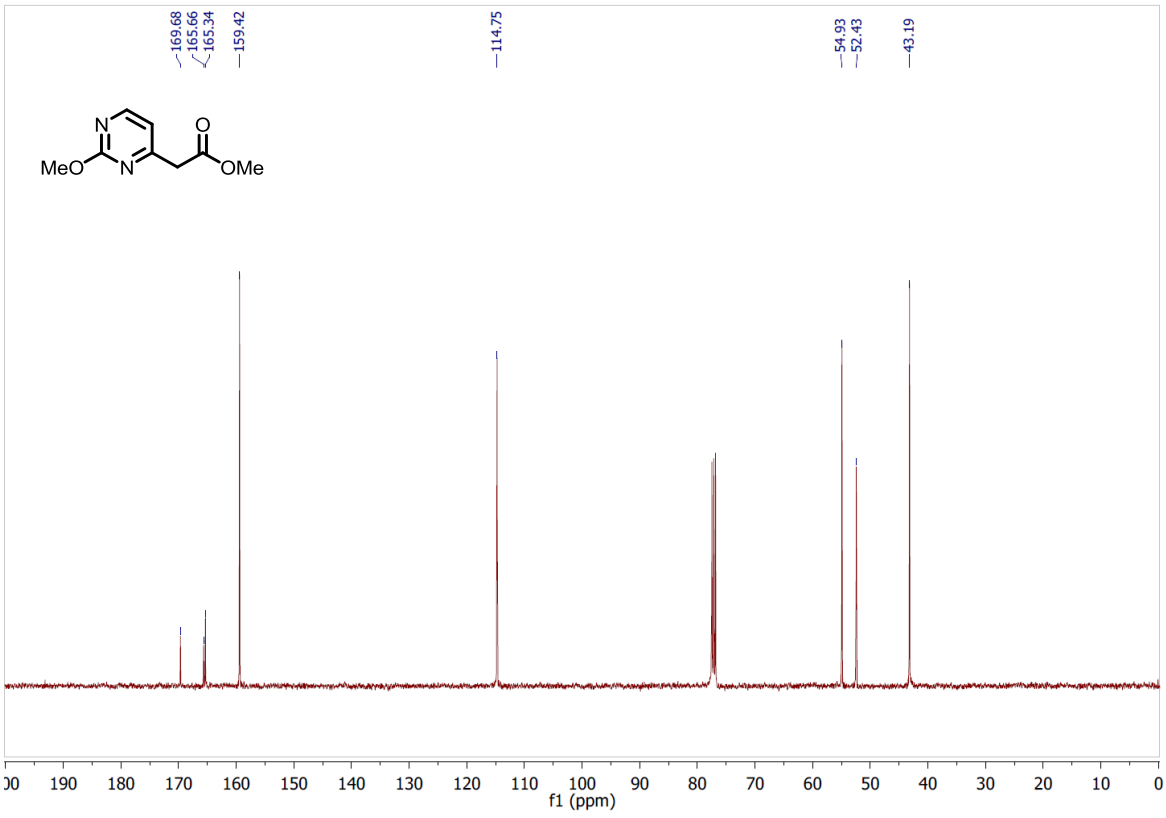
Starting Material *1h*



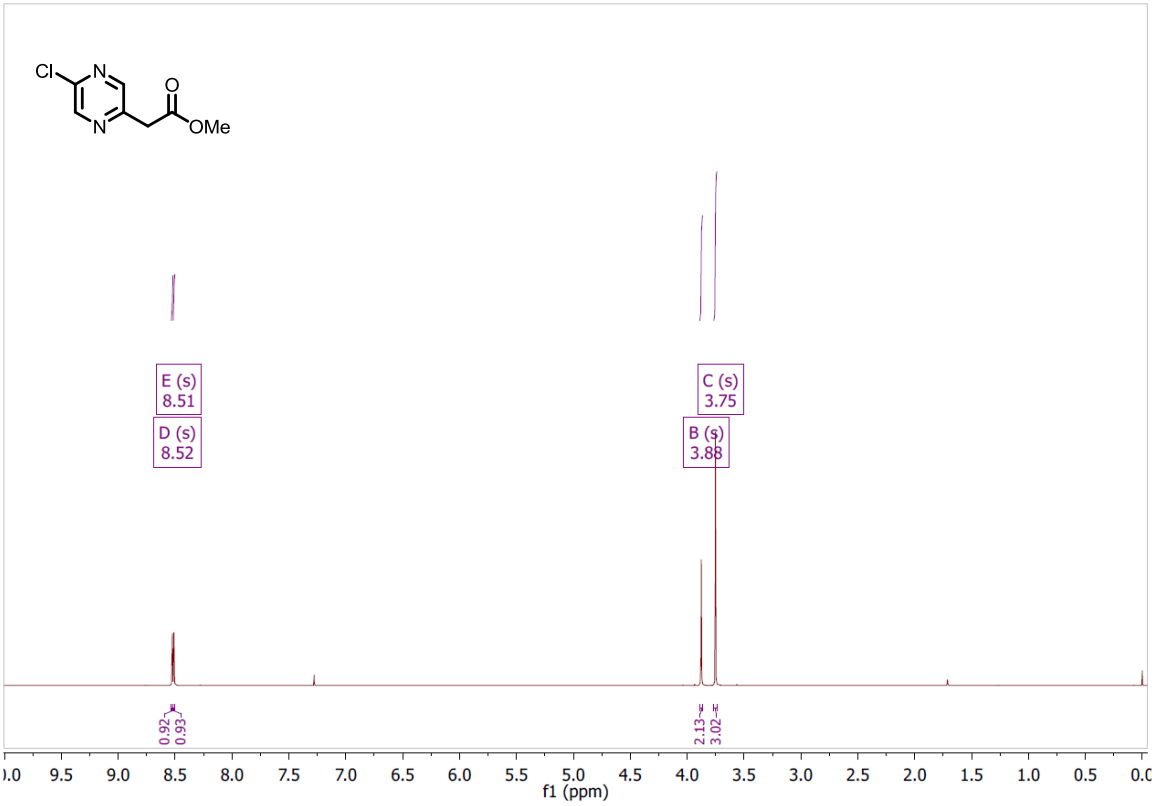


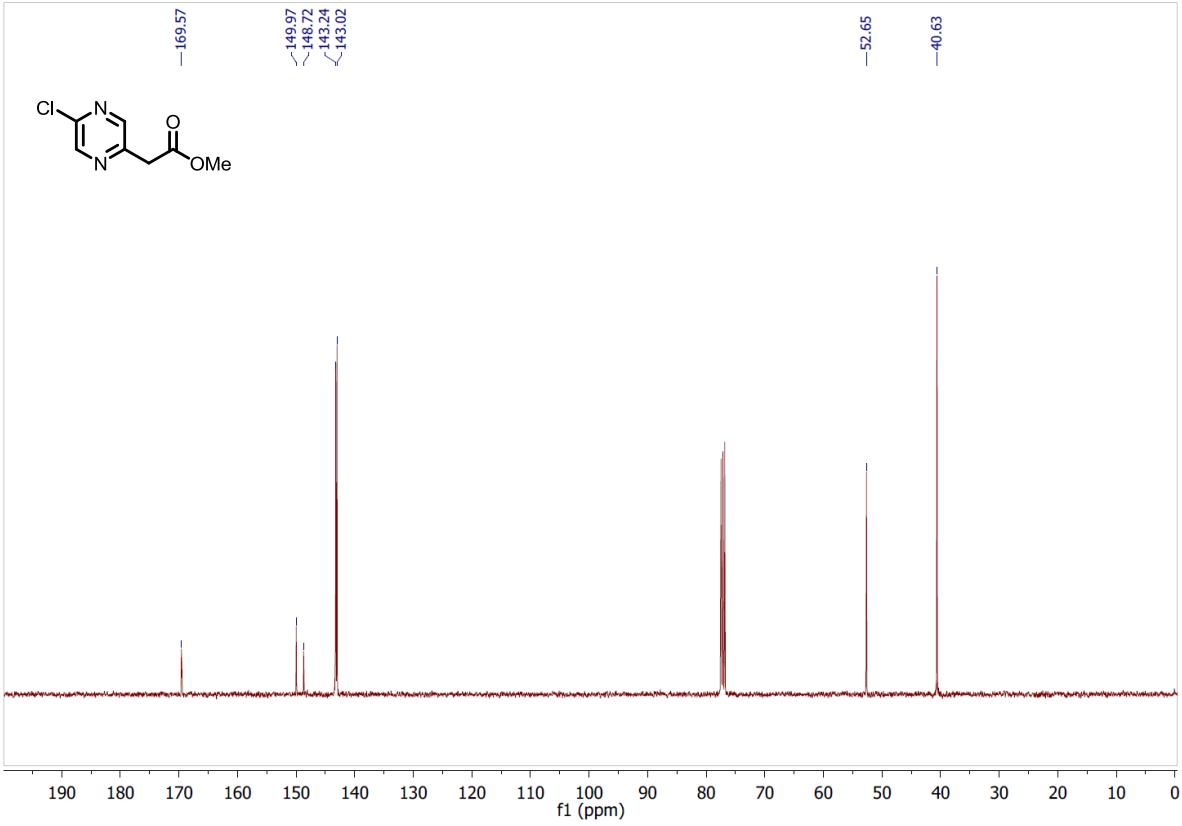
Starting Material *1p*



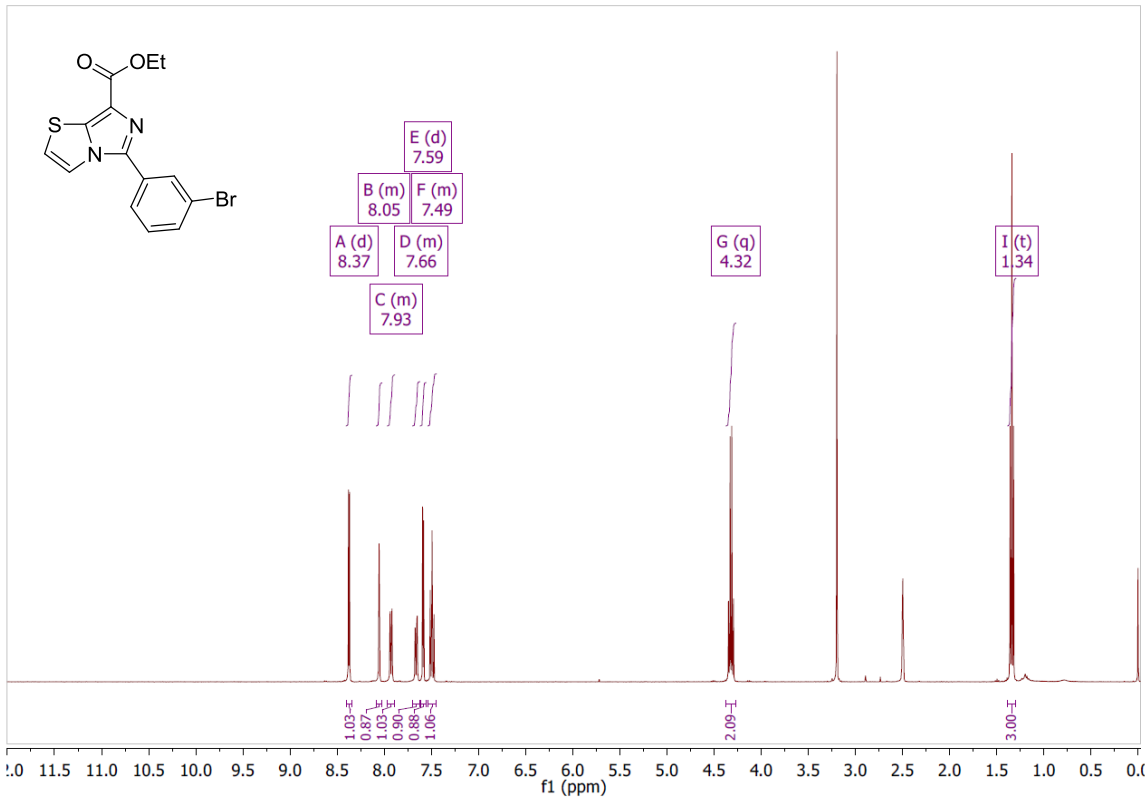


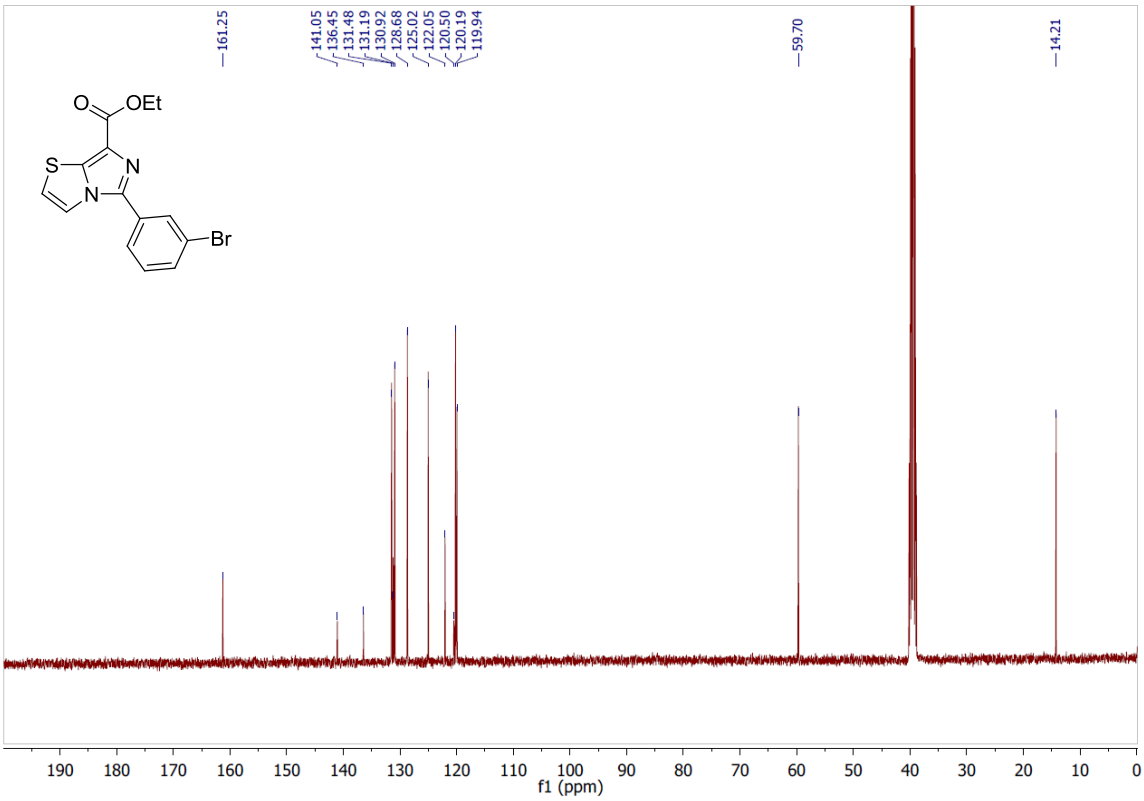
Starting Material *1q*



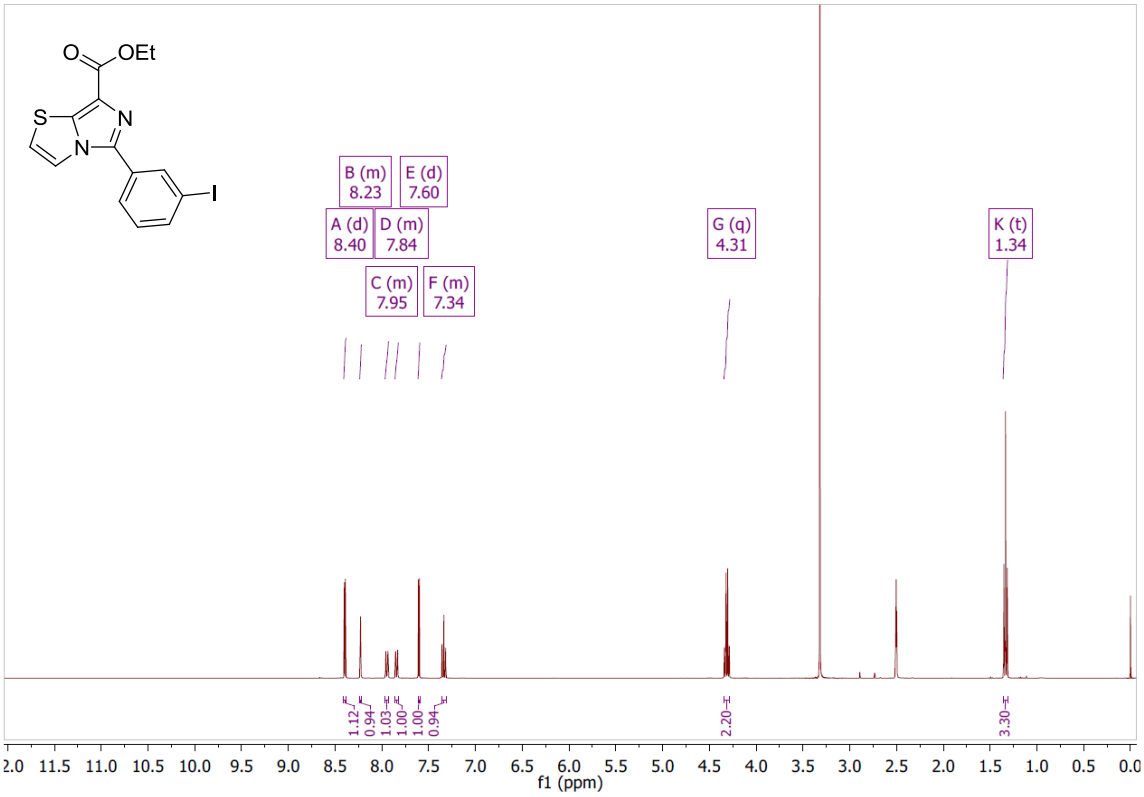


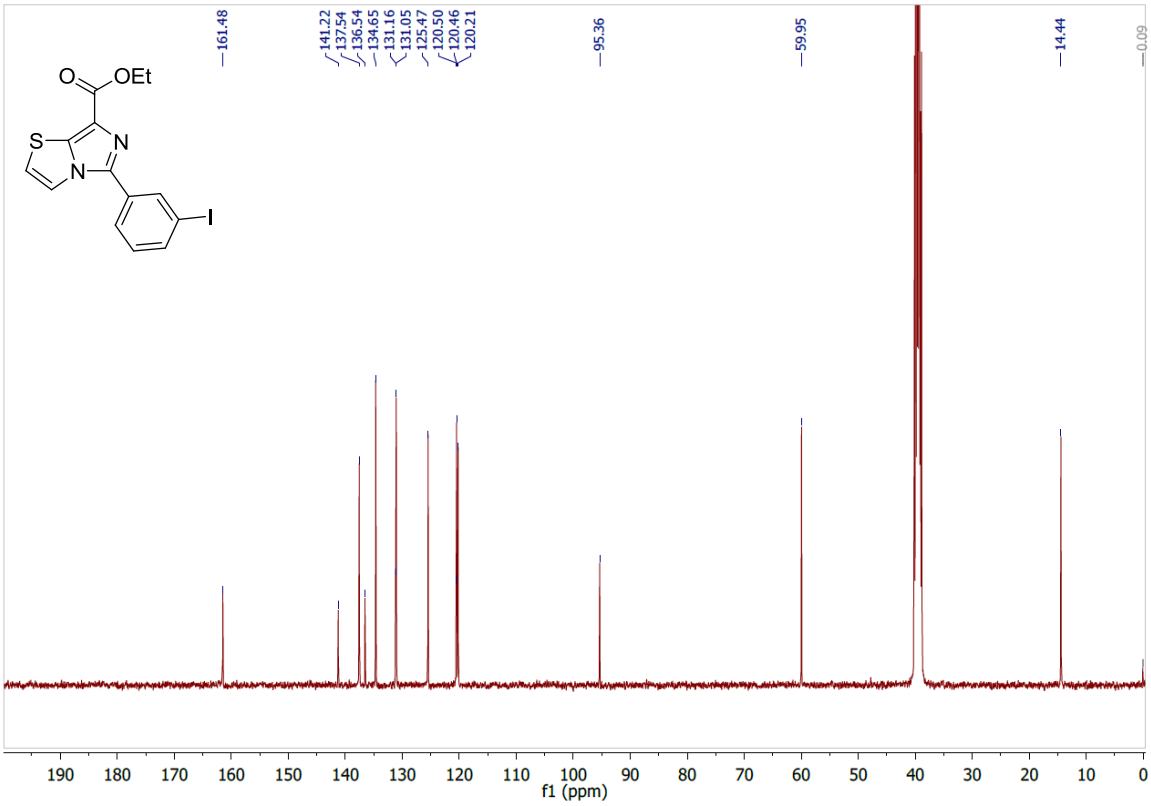
Compound *3a*


O
OEt
S
N
N
Br
E (d)
7.59
B (m)
8.05
F (m)
7.49
A (d)
8.37
D (m)
7.66
C (m)
7.93
G (q)
4.32
I (t)
1.34
1.03
0.87
1.03
0.90
0.88
1.06
2.09
3.00
f1 (ppm)

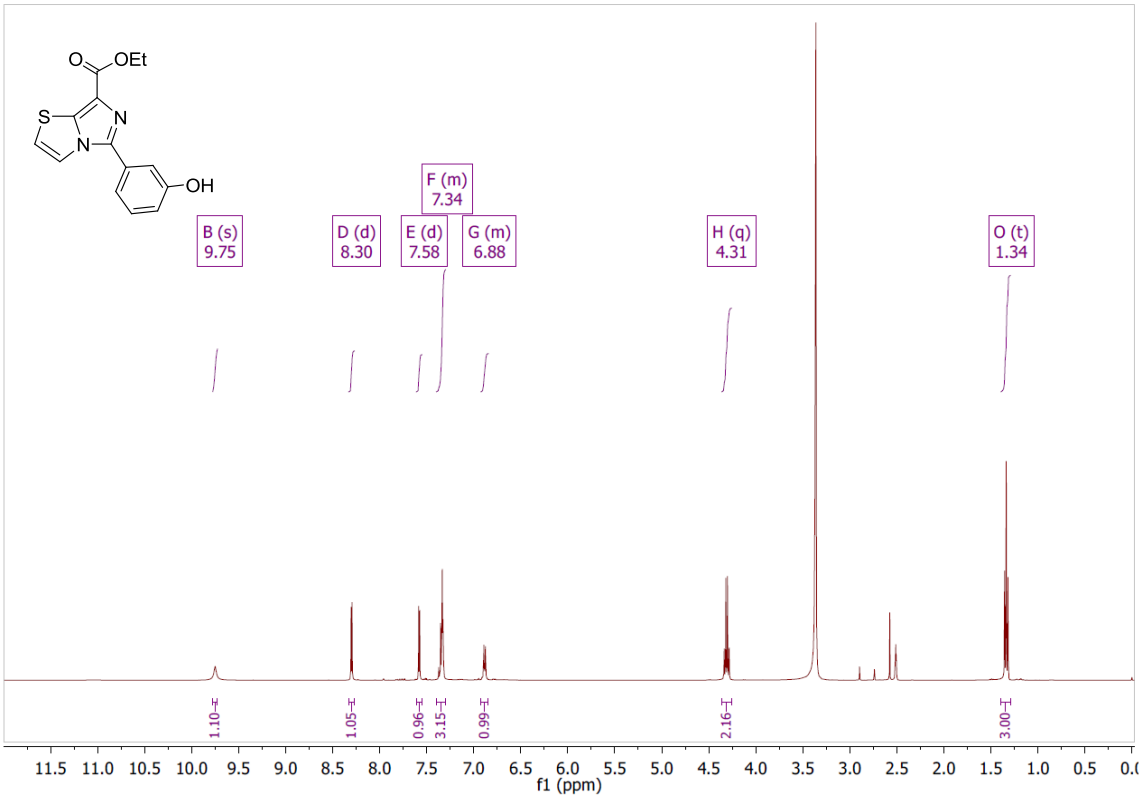

161.25
141.05
136.45
131.48
131.19
130.92
128.68
125.02
122.05
120.50
120.19
119.94
59.70
14.21
O
OEt
S
N
N
Br
f1 (ppm)

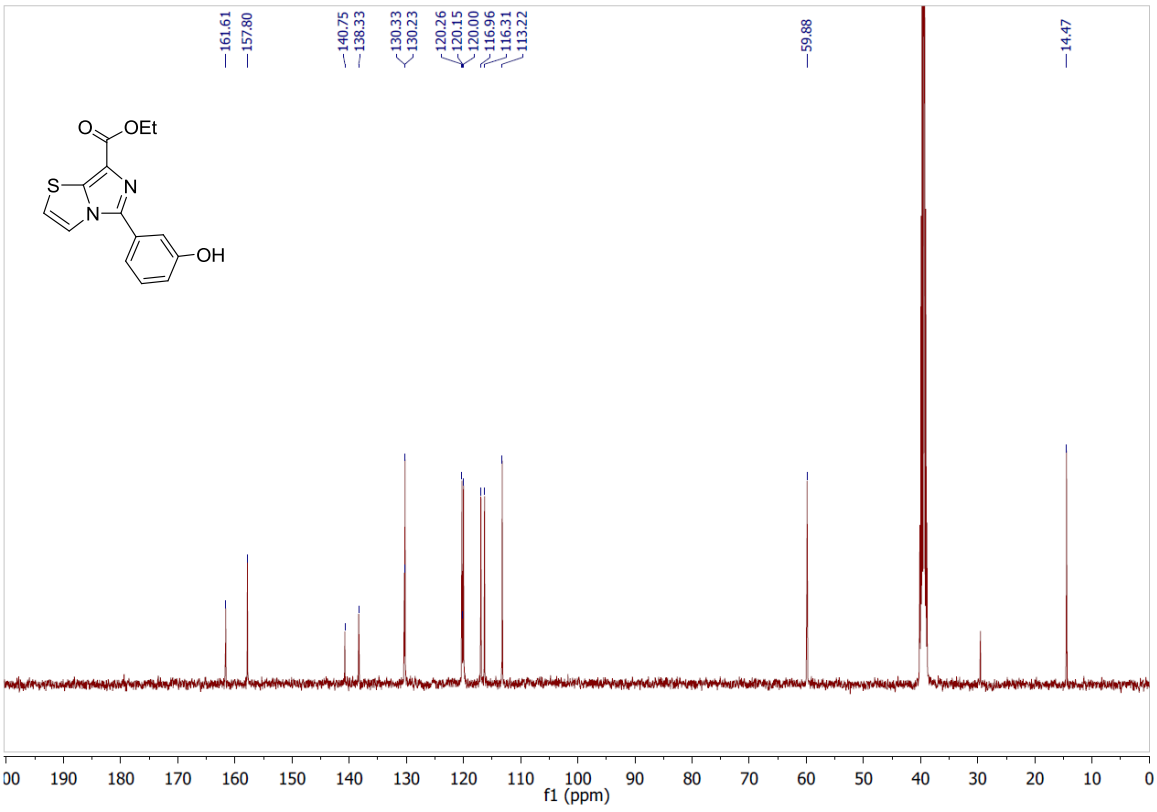
Compound *3b*


O
OEt
S
N
N
I
B (m) 8.23
E (d) 7.60
A (d) 8.40
D (m) 7.84
C (m) 7.95
F (m) 7.34
G (q) 4.31
K (t) 1.34
1.12
0.94
1.03
1.00
1.00
0.94
2.20
3.30
f1 (ppm)

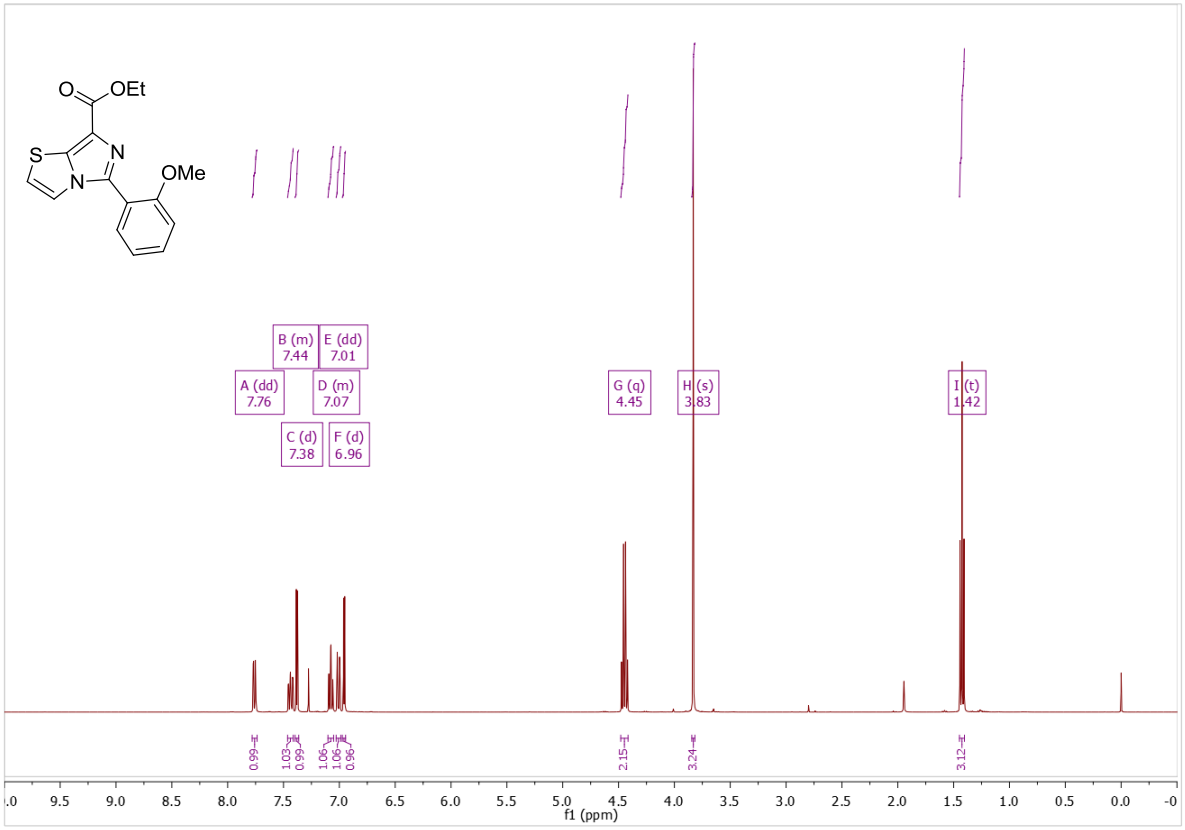

O
OEt
S
N
N
I
161.48
141.22
137.54
136.54
134.65
131.16
131.05
125.47
120.50
120.46
120.21
95.36
59.95
14.44
0.09
f1 (ppm)

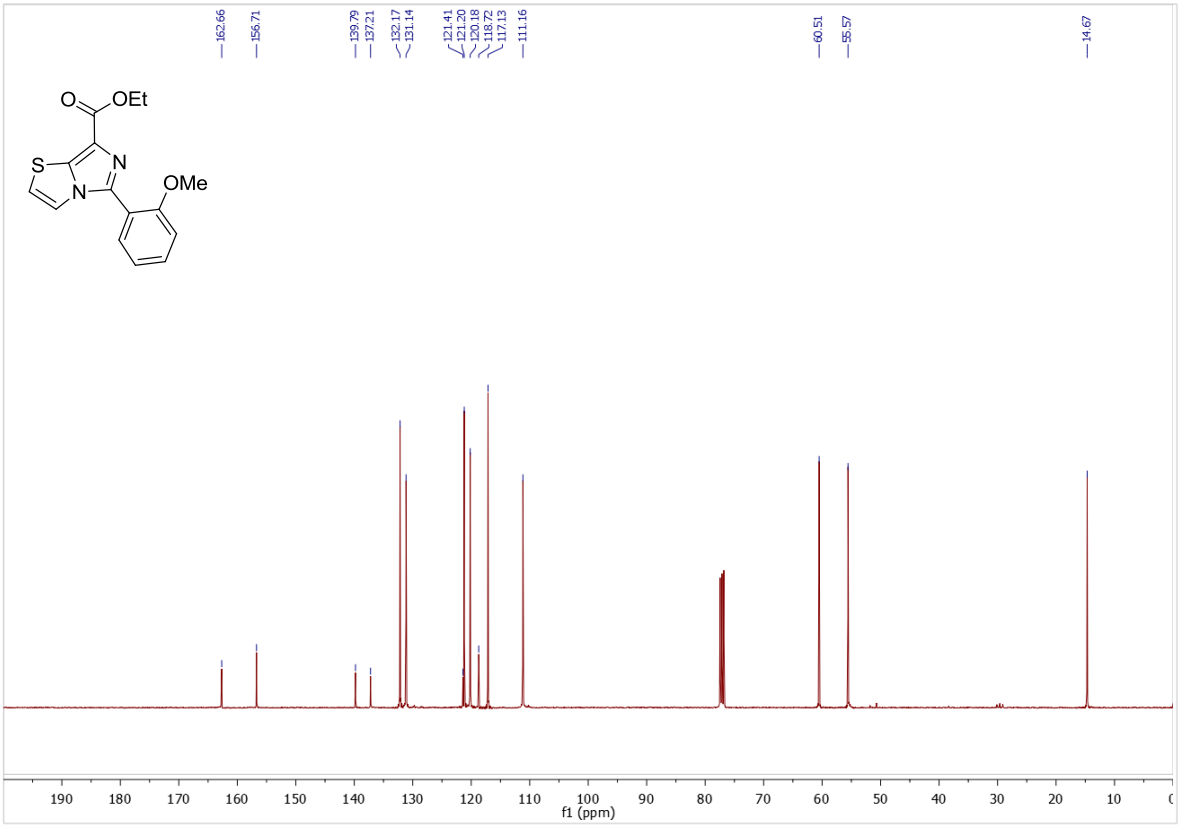
Compound *3c*


O
OEt
S
N
N
OH
B (s)
9.75
D (d)
8.30
F (m)
7.34
E (d)
7.58
G (m)
6.88
H (q)
4.31
O (t)
1.34
1.10
1.05
0.96
3.15
0.99
2.16
3.00
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
f1 (ppm)

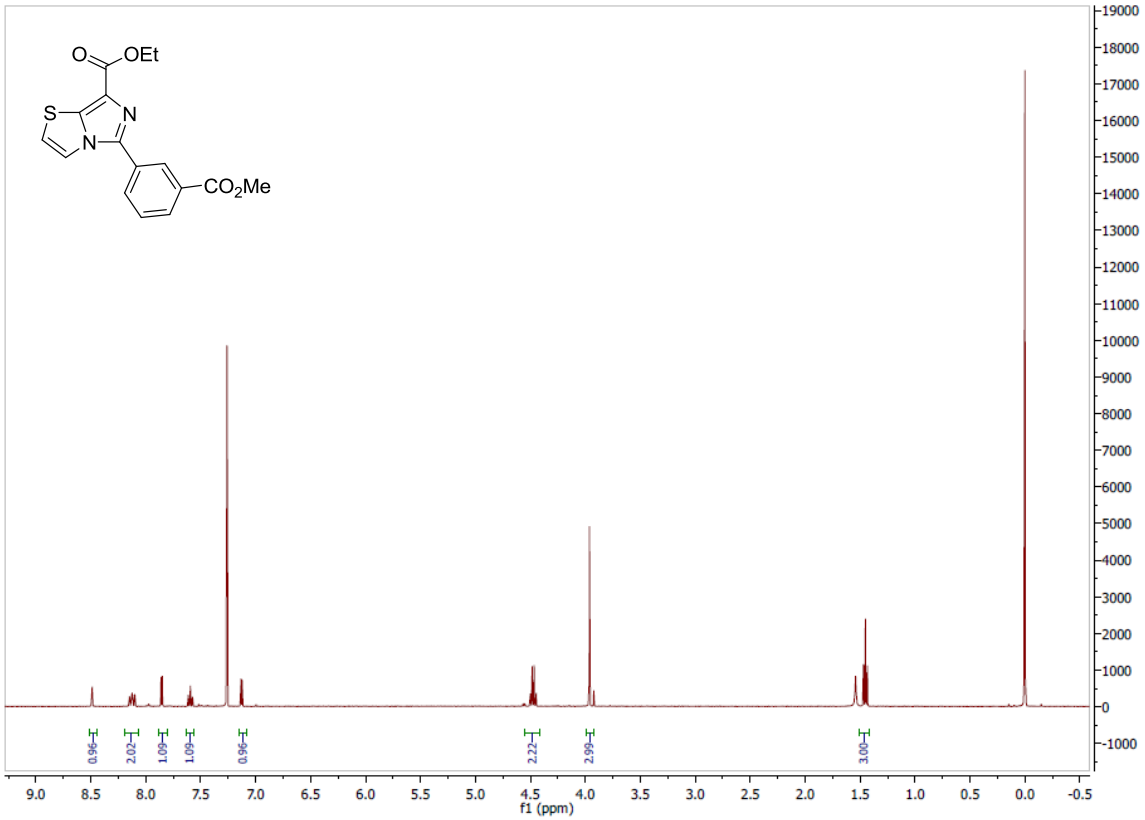

161.61
157.80
140.75
138.33
130.33
130.23
120.26
120.15
120.00
116.96
116.31
113.22
59.88
14.47
O
OEt
S
N
N
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

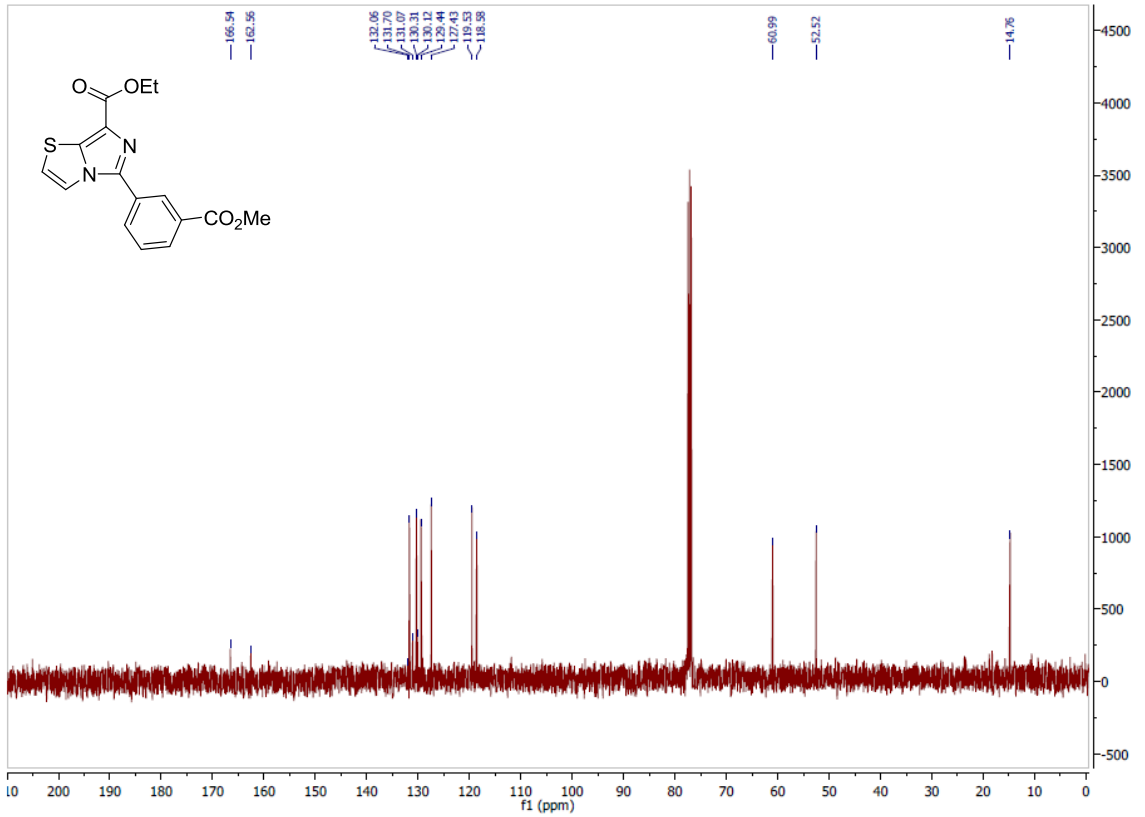
Compound *3d*


O
OEt
S
N
N
OMe
B (m) 7.44
E (dd) 7.01
A (dd) 7.76
D (m) 7.07
C (d) 7.38
F (d) 6.96
G (q) 4.45
H (s) 3.83
I (t) 1.42
0.99
1.03
0.99
1.06
1.06
0.96
2.15
3.24
3.12
f1 (ppm)

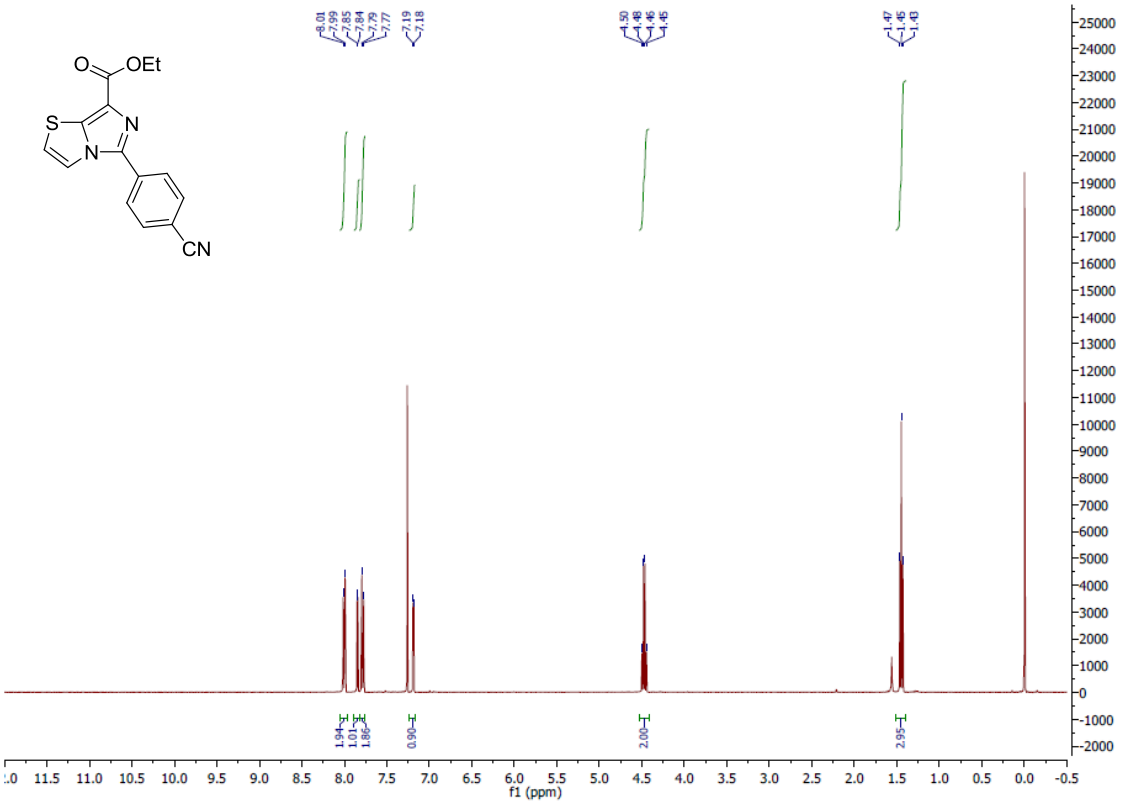

162.66
156.71
139.79
137.21
132.17
131.14
121.41
121.20
120.18
118.72
117.13
111.16
60.51
55.57
14.67
O
OEt
S
N
N
OMe
f1 (ppm)

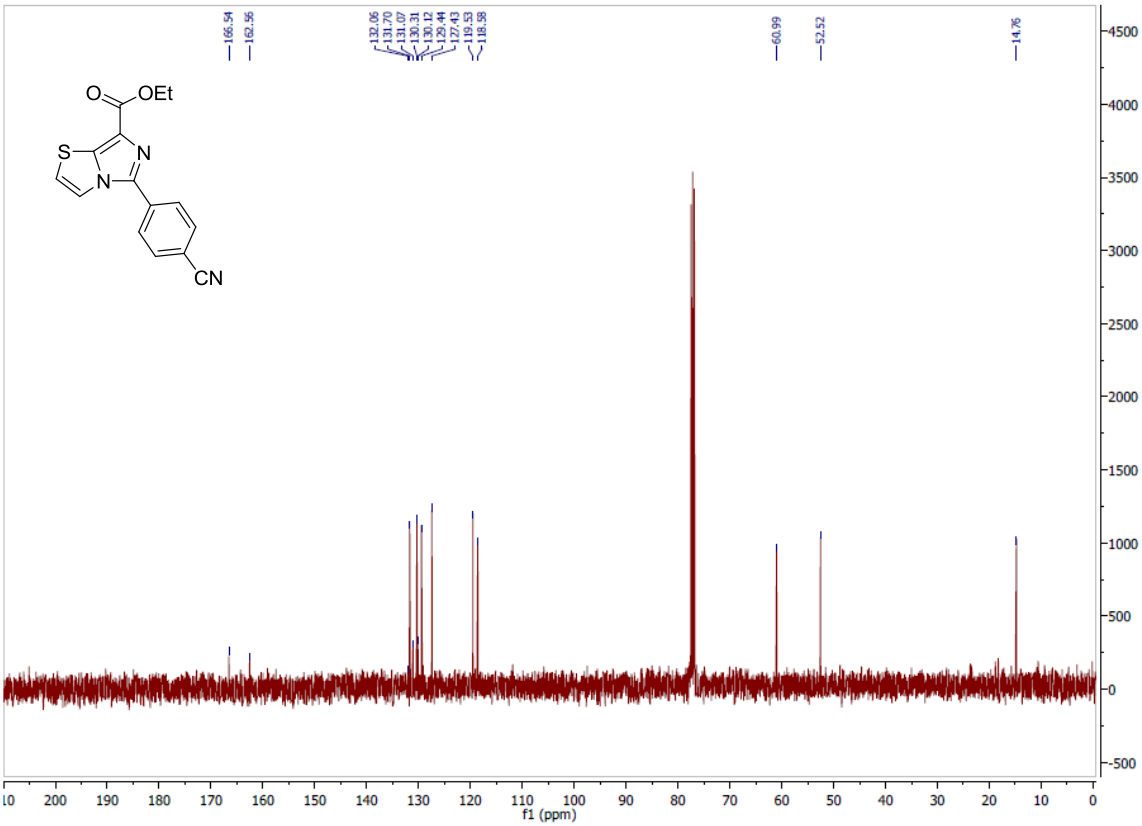
Compound *3e*


O
OEt
S
N
N
CO2Me
0.96
2.02
1.09
1.09
0.96
2.22
2.99
3.00
f1 (ppm)

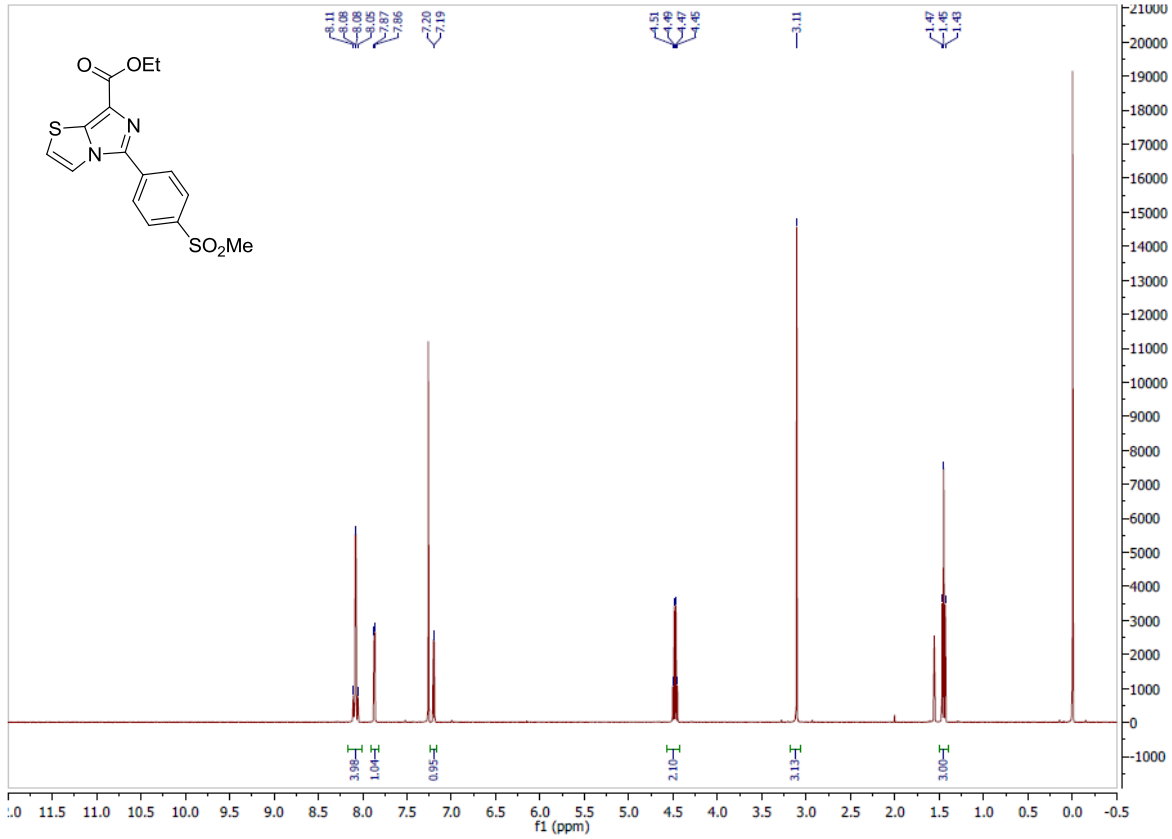

166.54
162.56
132.06
131.70
131.07
130.31
130.12
129.44
127.43
119.53
118.58
60.99
52.52
14.76
O
OEt
S
N
N
CO2Me
f1 (ppm)

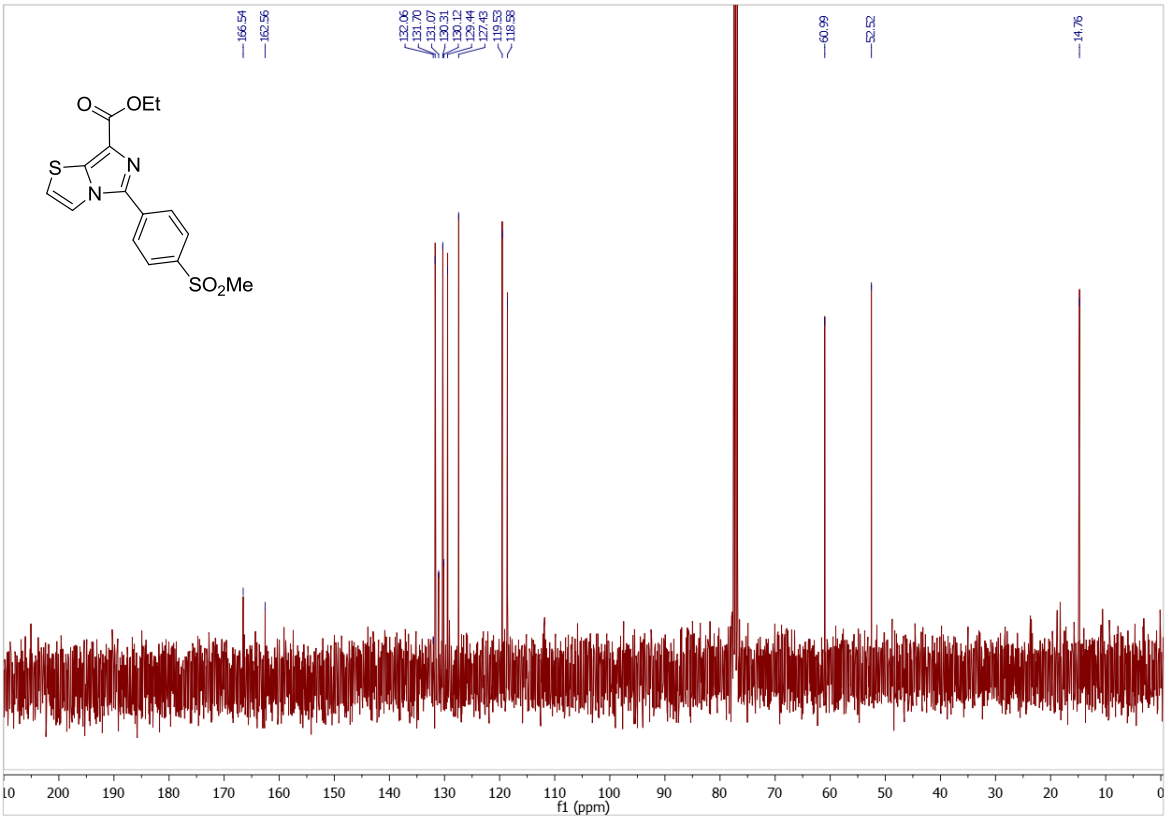
Compound *3f*


8.01
7.99
7.85
7.84
7.79
7.77
7.19
7.18
4.50
4.48
4.46
4.45
1.47
1.45
1.43
1.94
1.01
1.86
0.90
2.00
2.95
f1 (ppm)

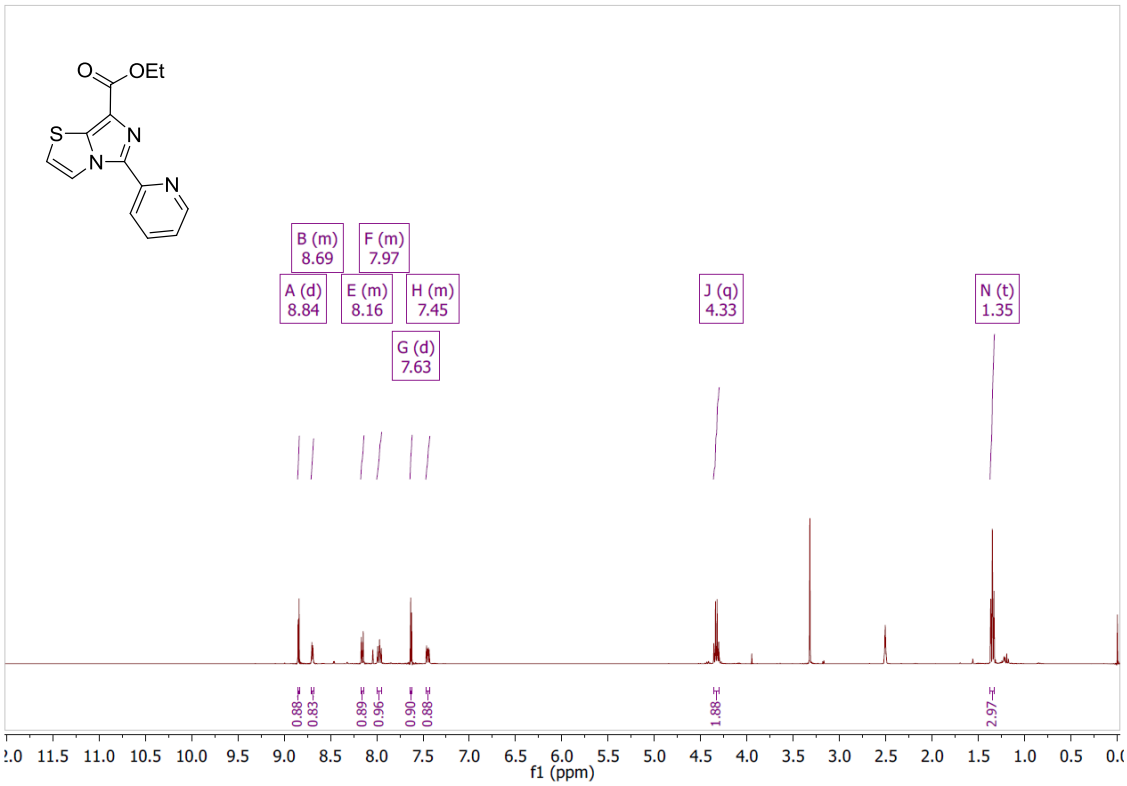

166.54
162.56
132.06
131.70
131.07
130.31
130.12
129.44
127.43
119.53
118.58
60.99
52.52
14.76
f1 (ppm)

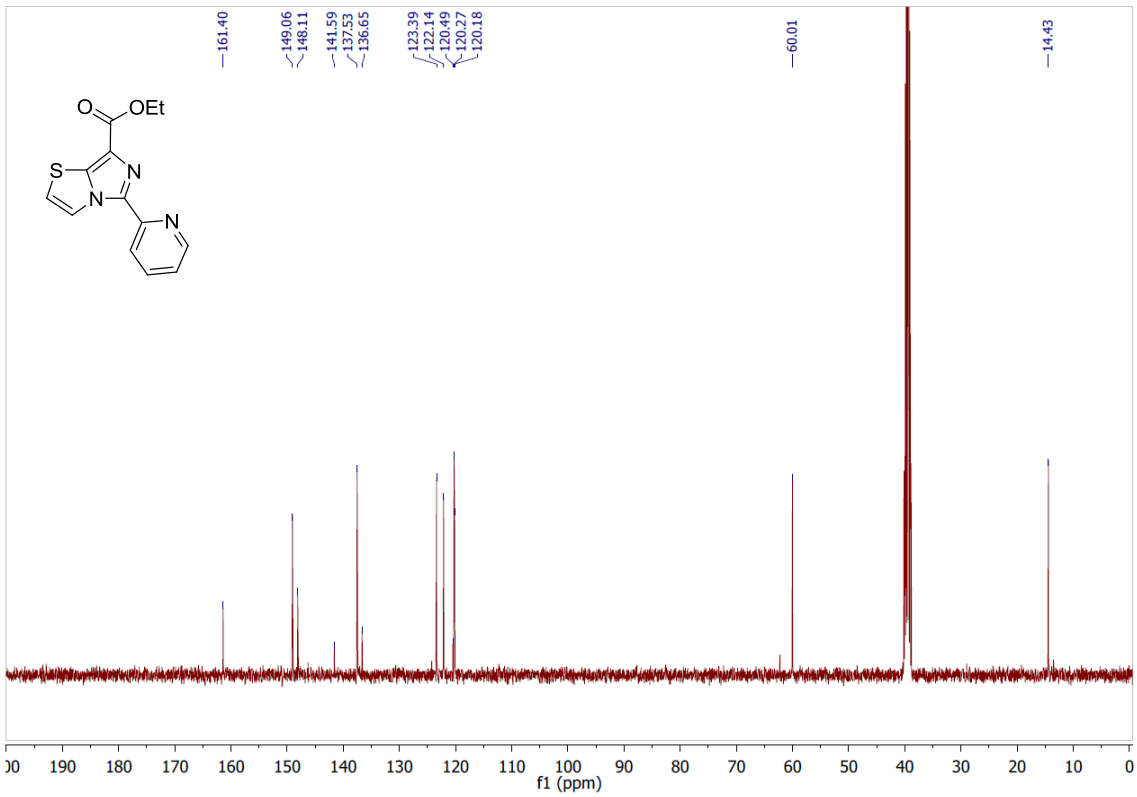
Compound *3g*


8.11
8.08
8.08
8.05
7.87
7.86
7.20
7.19
4.51
4.49
4.47
4.45
3.11
1.47
1.45
1.43
O
OEt
S
N
N
SO2Me
3.98
1.04
0.95
2.10
3.13
3.00
f1 (ppm)

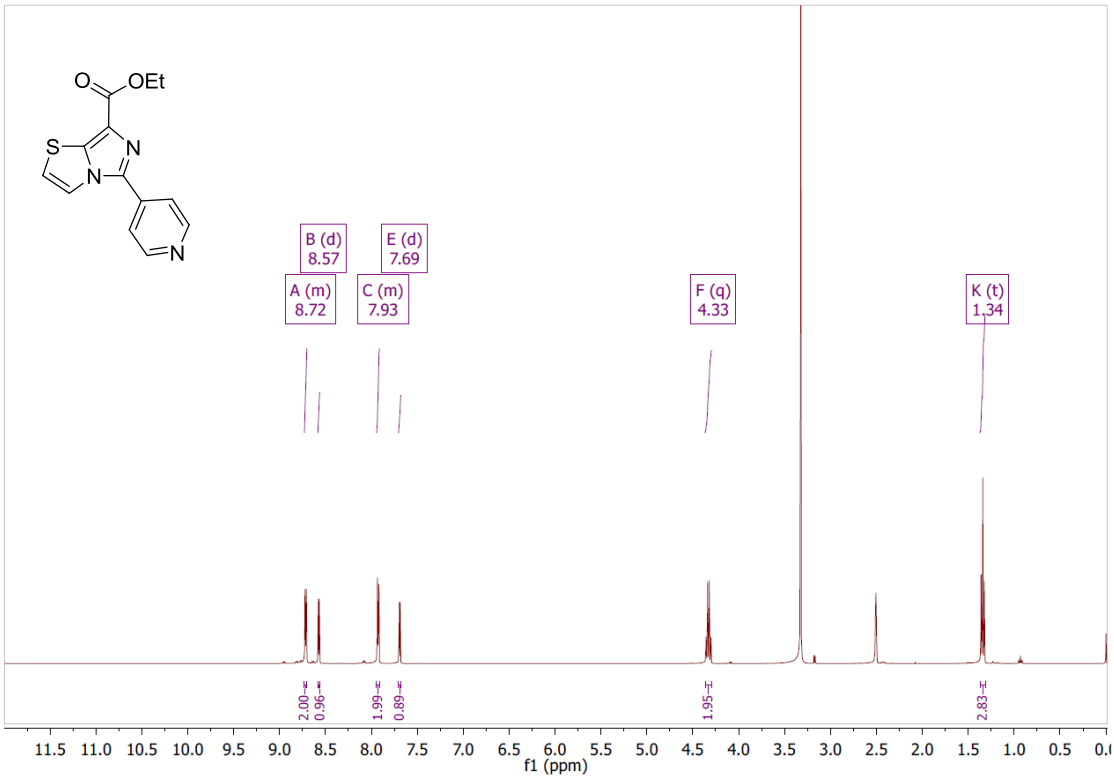

166.54
162.56
132.06
131.70
131.07
130.31
130.12
129.44
127.43
119.53
118.98
60.99
52.52
14.76
O
OEt
S
N
N
SO2Me
f1 (ppm)

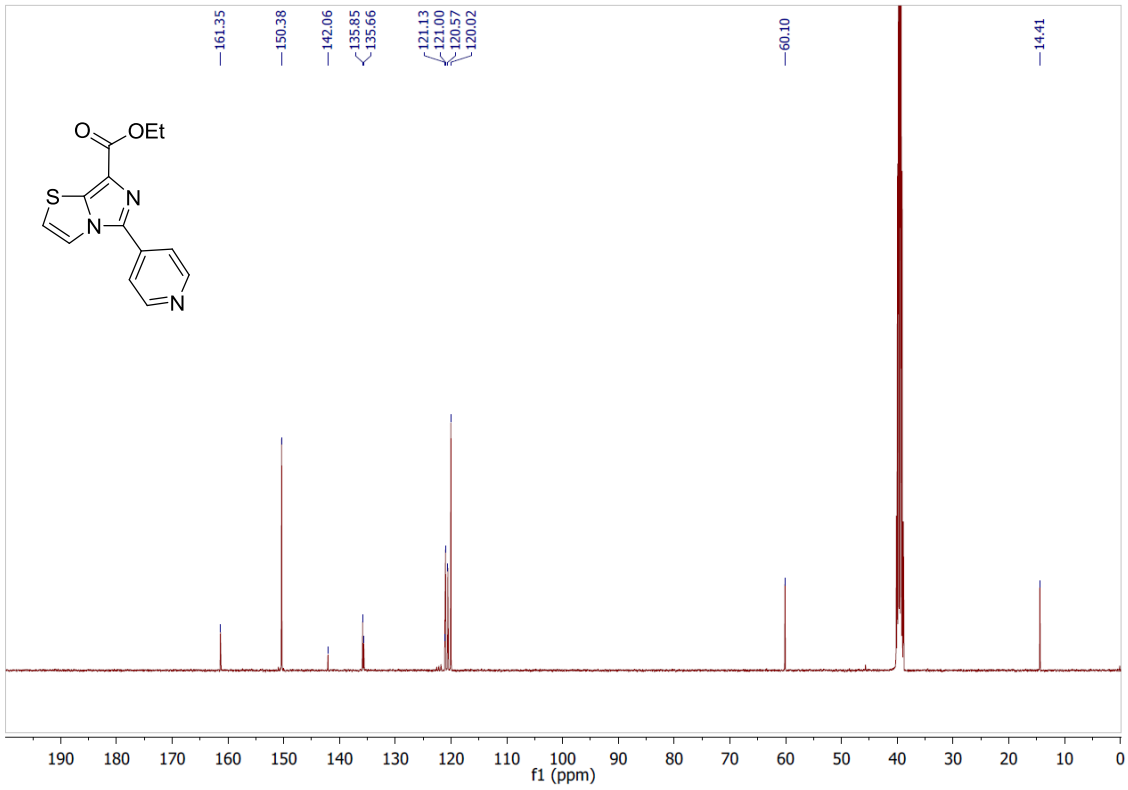
Compound *3h*


O
OEt
S
N
N
N
B (m)
8.69
F (m)
7.97
A (d)
8.84
E (m)
8.16
H (m)
7.45
G (d)
7.63
J (q)
4.33
N (t)
1.35
0.88
0.83
0.89
0.96
0.90
0.88
1.88
2.97
f1 (ppm)

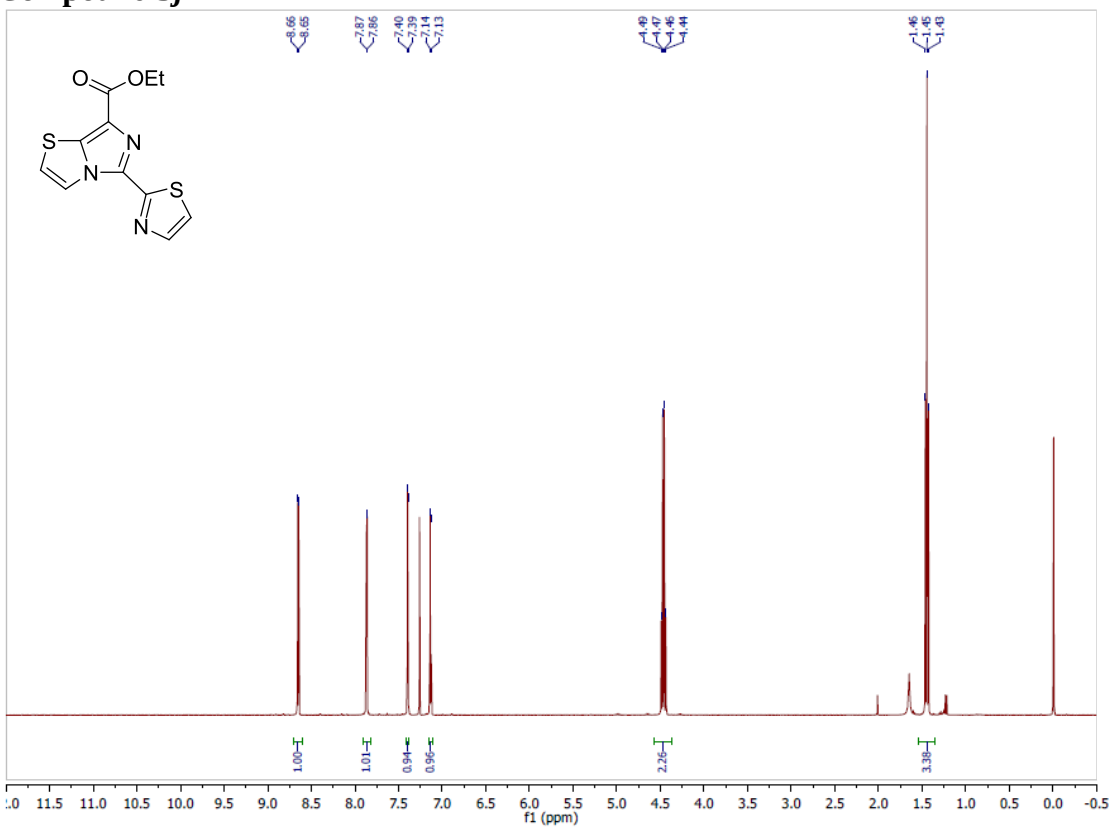

161.40
149.06
148.11
141.59
137.53
136.65
123.39
122.14
120.49
120.27
120.18
60.01
14.43
O
OEt
S
N
N
N
f1 (ppm)

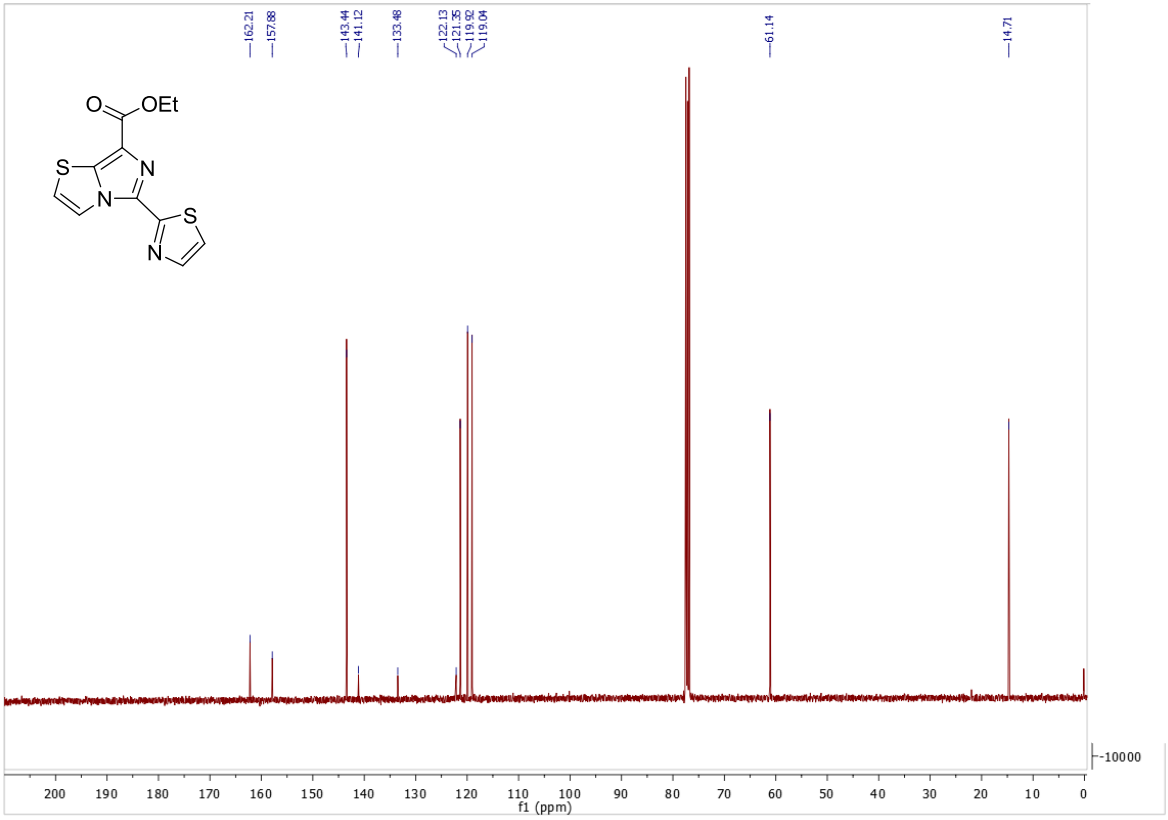
Compound *3i*


O
OEt
S
N
N
N
B (d)
8.57
E (d)
7.69
A (m)
8.72
C (m)
7.93
F (q)
4.33
K (t)
1.34
2.00
0.96
1.99
0.89
1.95
2.83
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
f1 (ppm)

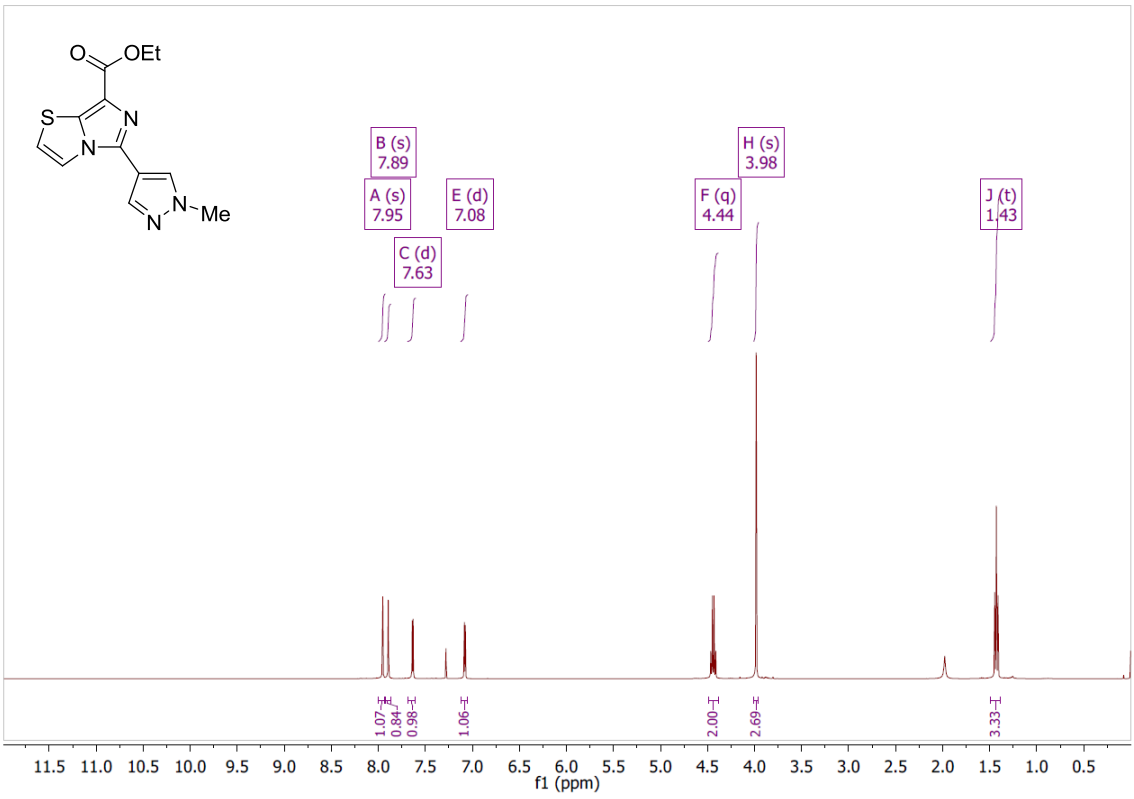

161.35
150.38
142.06
135.85
135.66
121.13
121.00
120.57
120.02
60.10
14.41
O
OEt
S
N
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

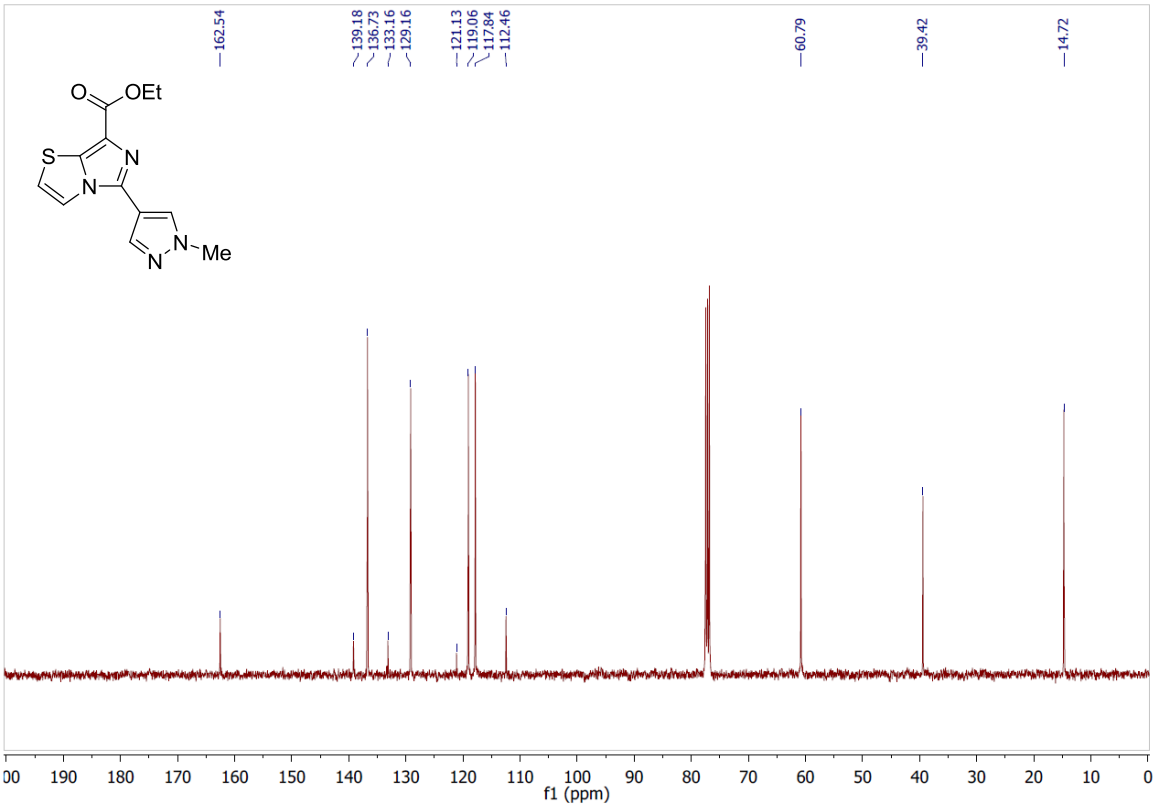
Compound *3j*


8.66
8.65
7.87
7.86
7.40
7.39
7.14
7.13
1.49
1.47
1.46
1.44
1.46
1.45
1.43
O
OEt
S
N
N
S
N
1.00
1.01
0.94
0.96
2.26
3.38
f1 (ppm)

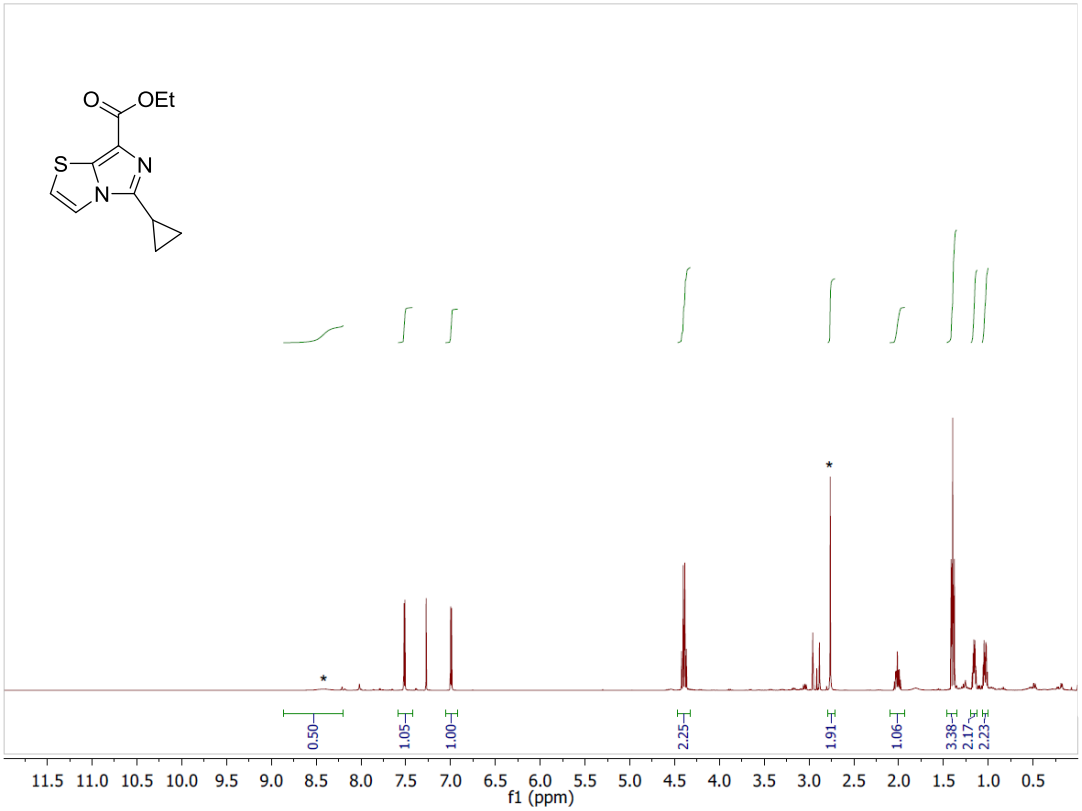

162.21
157.88
143.44
141.12
133.48
122.13
121.35
119.92
119.04
61.14
14.71
O
OEt
S
N
N
S
N
10000
f1 (ppm)

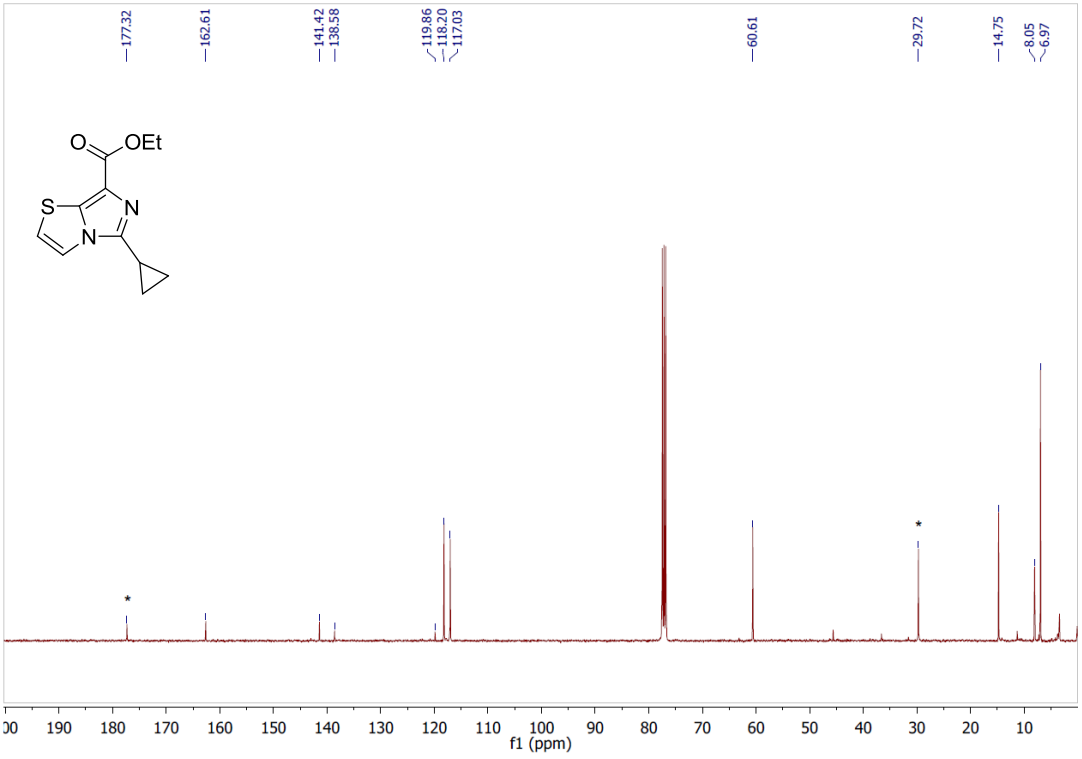
Compound *3k*


O
OEt
S
N
N
N
N
Me
B (s)
7.89
A (s)
7.95
C (d)
7.63
E (d)
7.08
H (s)
3.98
F (q)
4.44
J (t)
1.43
1.07
0.84
0.98
1.06
2.00
2.69
3.33
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
f1 (ppm)

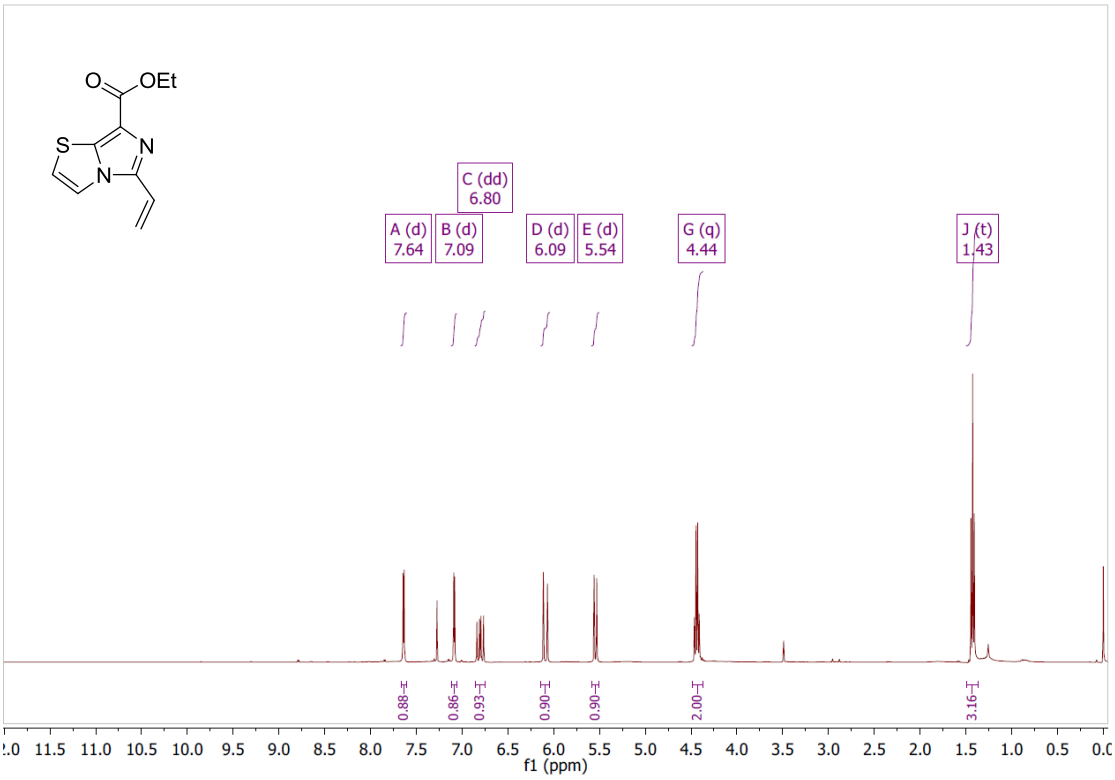

162.54
139.18
136.73
133.16
129.16
121.13
119.06
117.84
112.46
60.79
39.42
14.72
O
OEt
S
N
N
N
N
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

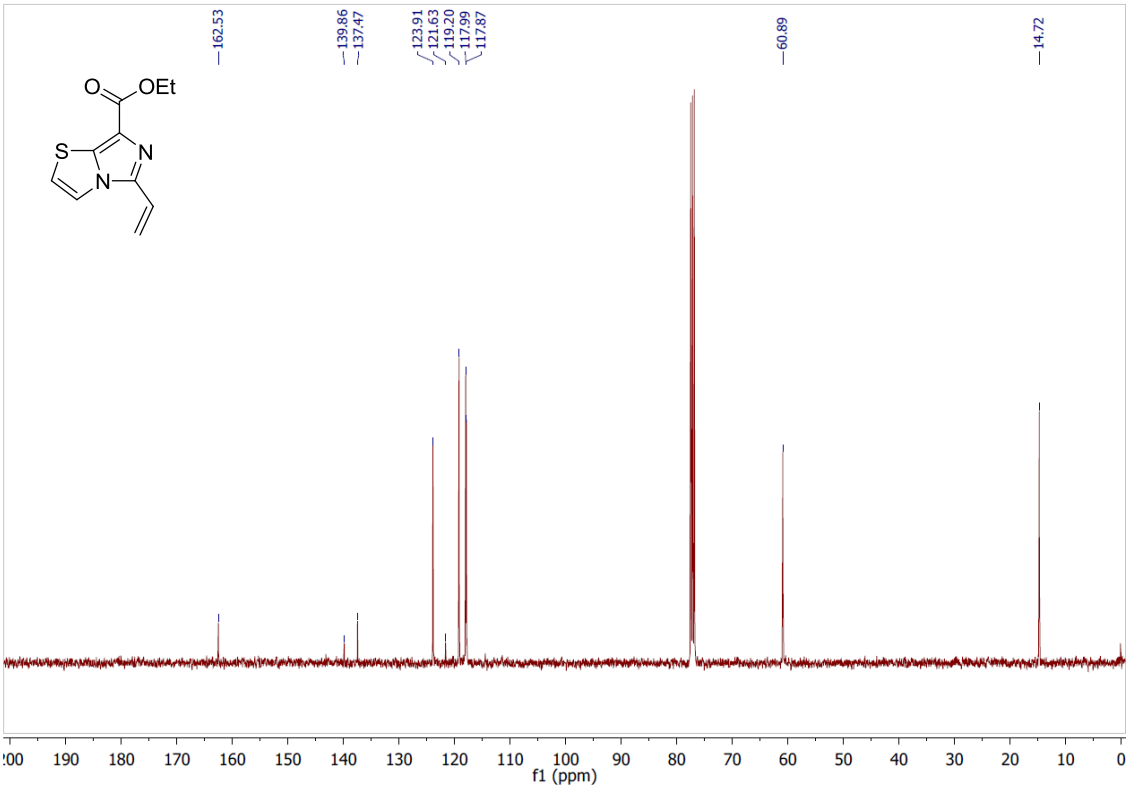
Compound *3l*


O
OEt
S
N
N
0.50
1.05
1.00
2.25
1.91
1.06
3.38
2.17
2.23
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
f1 (ppm)

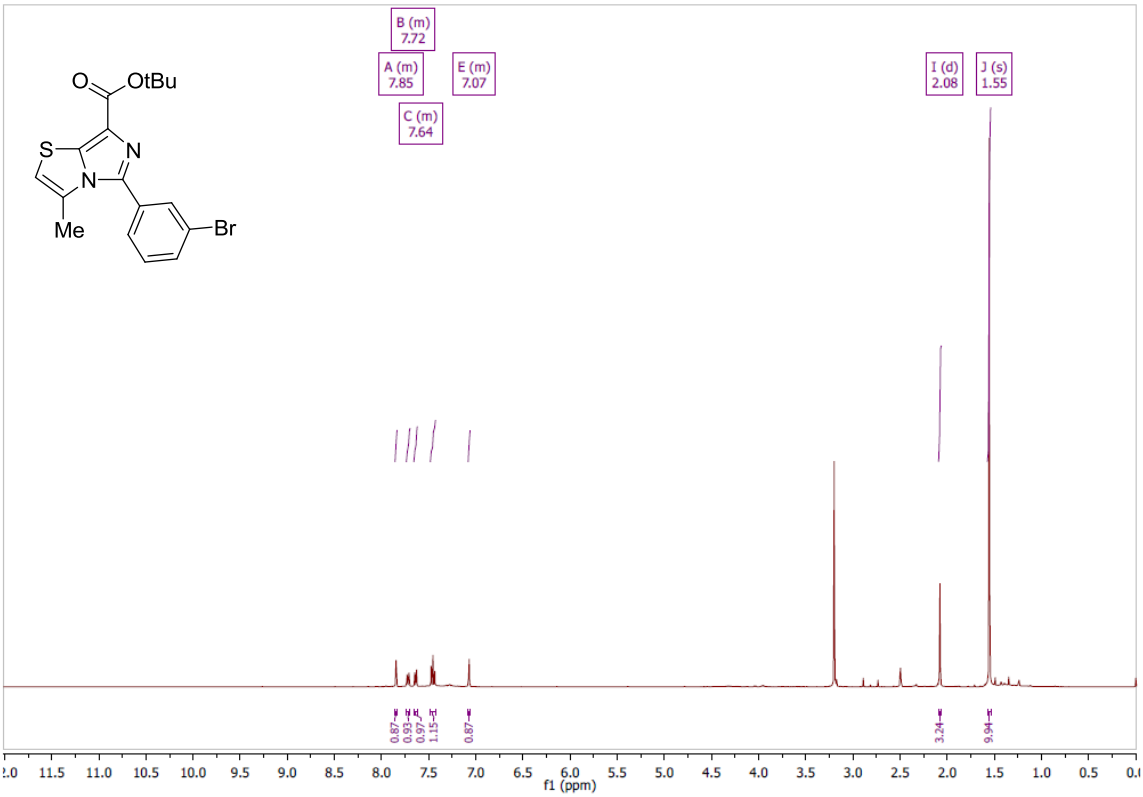

177.32
162.61
141.42
138.58
119.86
118.20
117.03
60.61
29.72
14.75
8.05
6.97
O
OEt
S
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

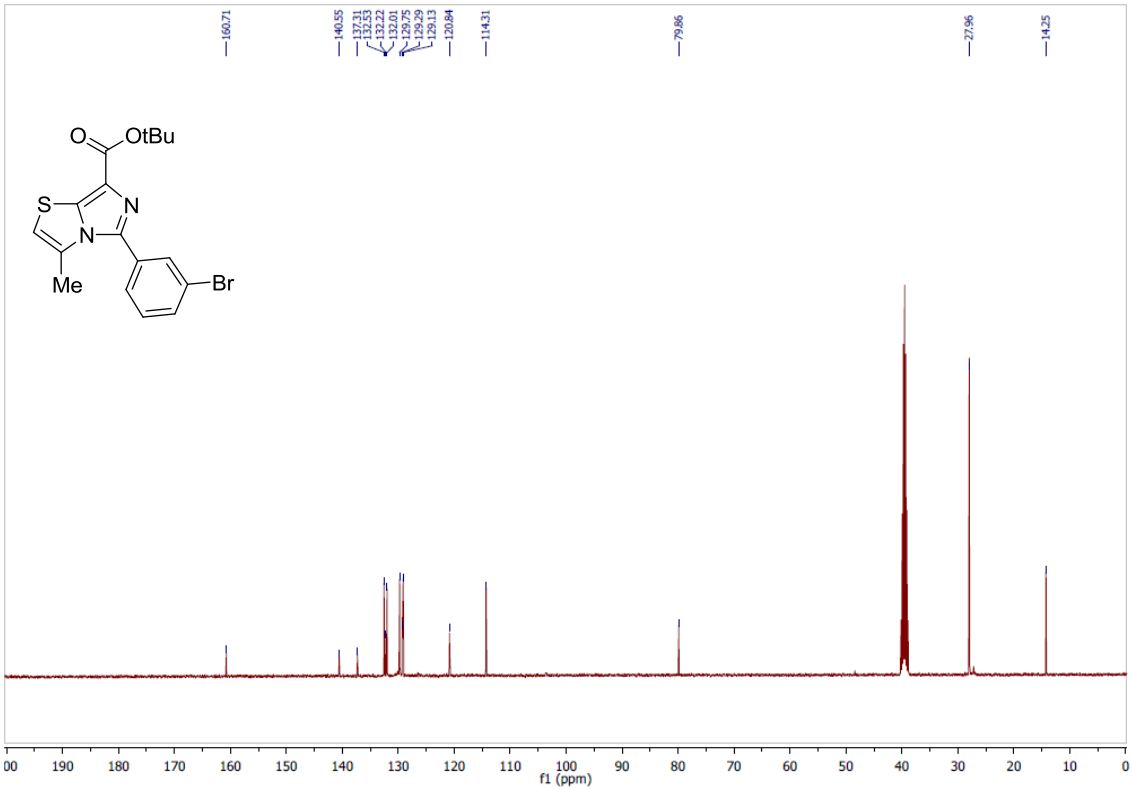
Compound *3m*


O
OEt
S
N
N
C (dd)
6.80
A (d)
7.64
B (d)
7.09
D (d)
6.09
E (d)
5.54
G (q)
4.44
J (t)
1.43
0.88
0.86
0.93
0.90
0.90
2.00
3.16
f1 (ppm)

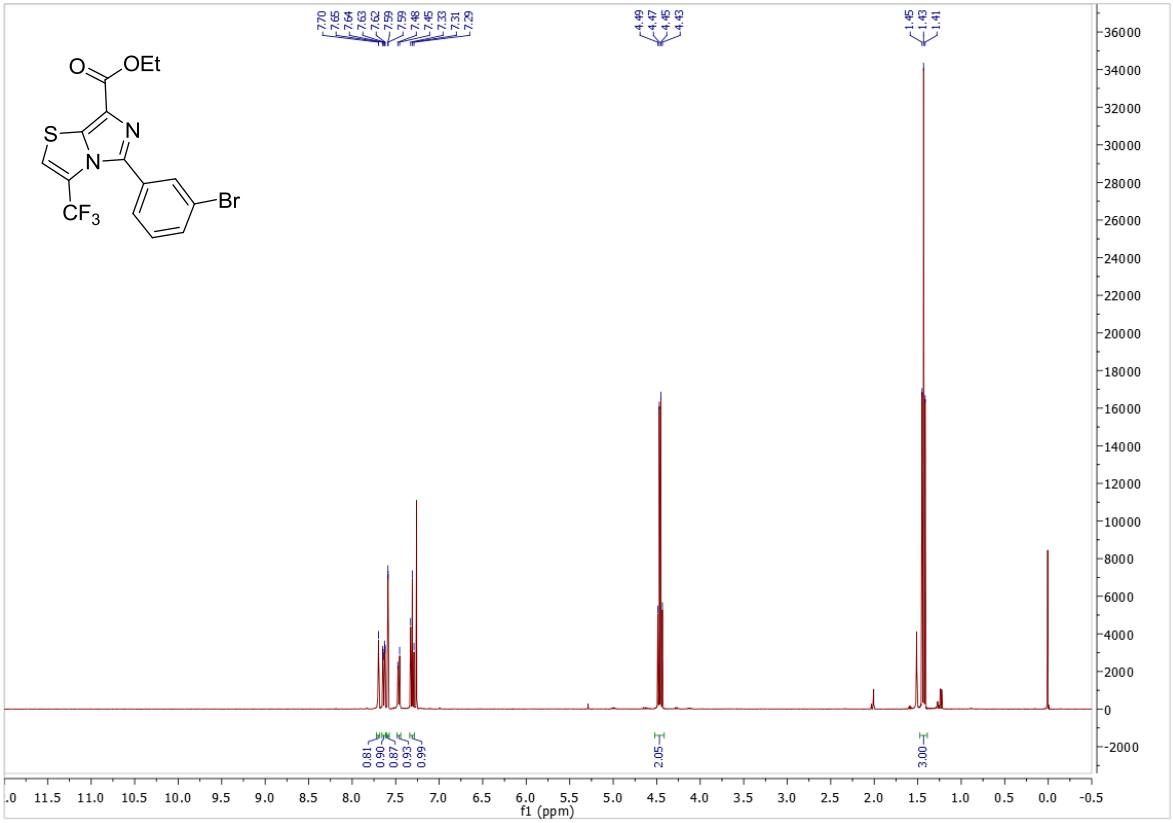

162.53
139.86
137.47
123.91
121.63
119.20
117.99
117.87
60.89
14.72
O
OEt
S
N
N
f1 (ppm)

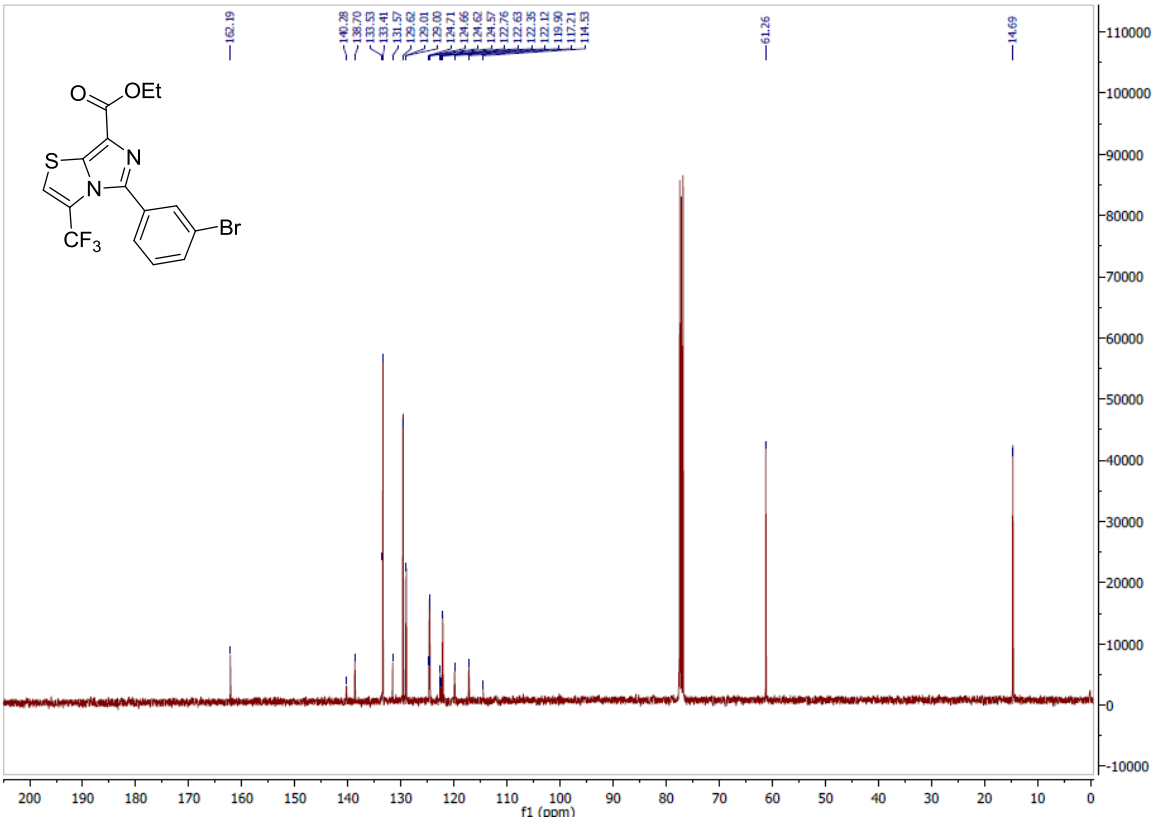
Compound *4b*


B (m)
7.72
A (m)
7.85
E (m)
7.07
C (m)
7.64
I (d)
2.08
J (s)
1.55
O
OtBu
S
N
N
Me
Br
f1 (ppm)

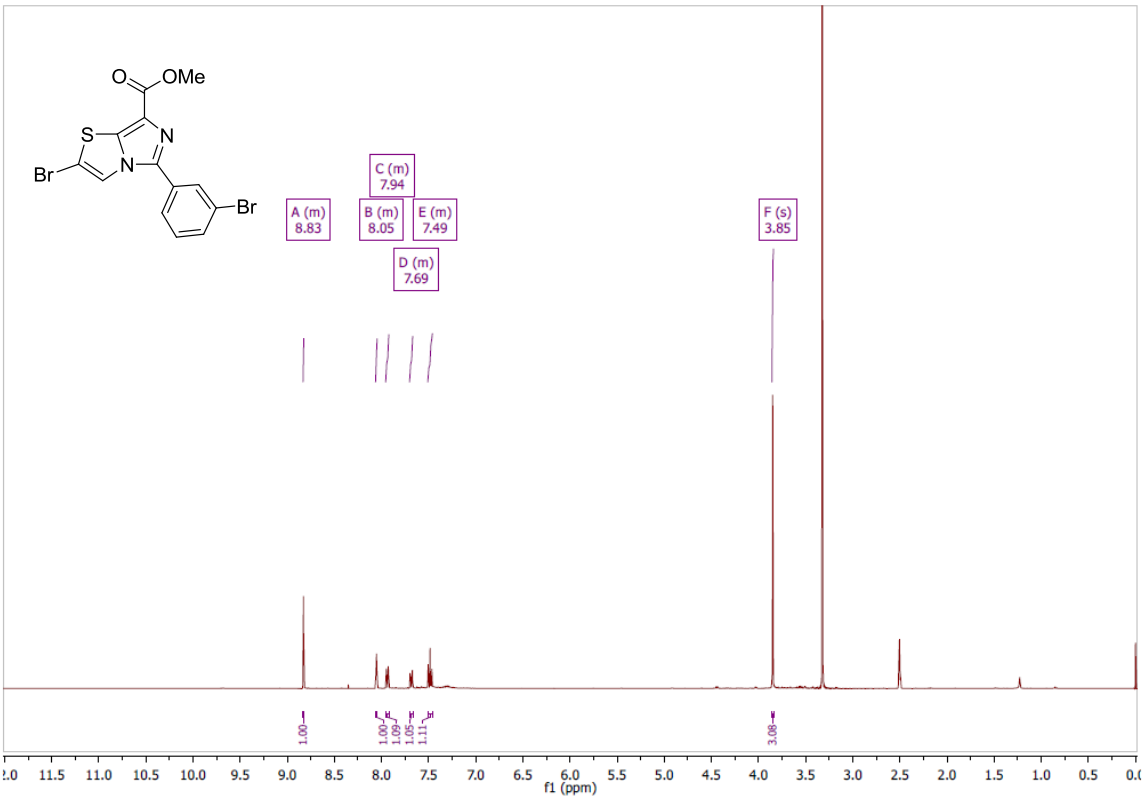

160.71
140.55
137.31
133.53
132.22
132.01
129.75
129.29
129.13
120.84
114.31
79.86
27.96
14.25
O
OtBu
S
N
N
Me
Br
f1 (ppm)

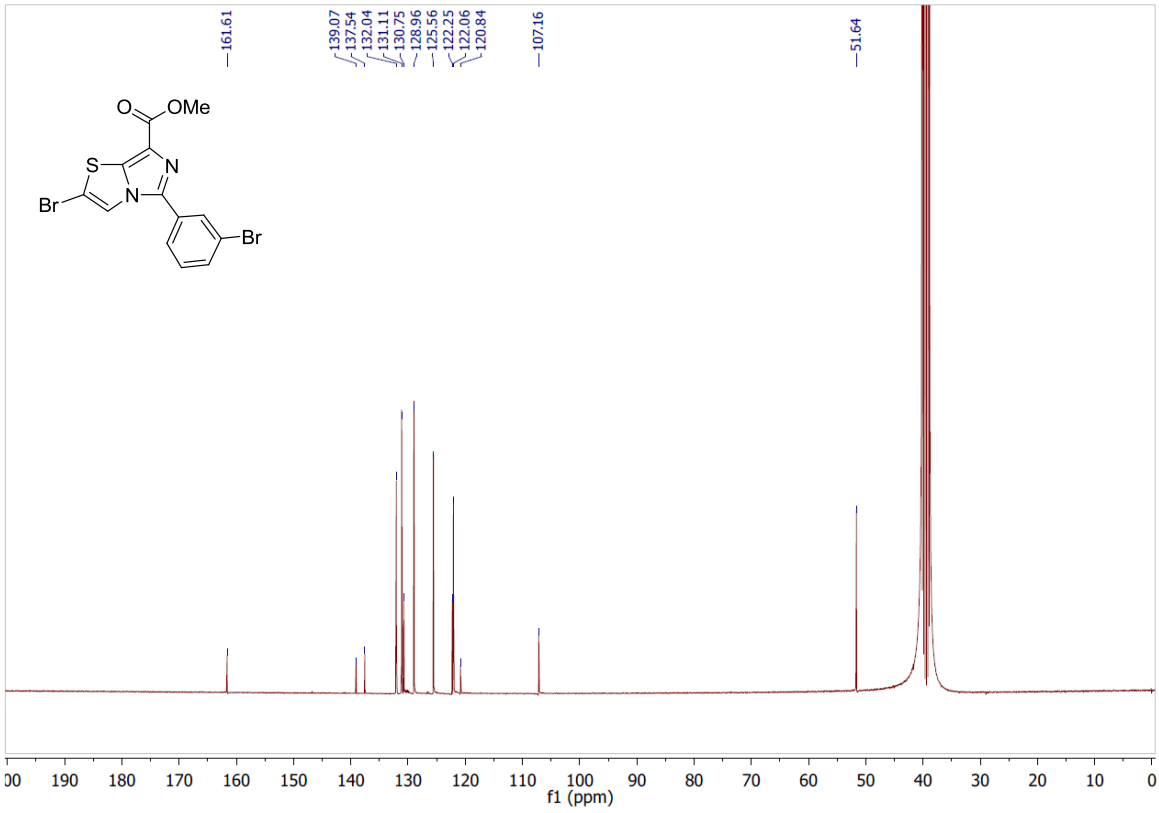
Compound *4c*


7.70
7.65
7.64
7.63
7.62
7.59
7.59
7.48
7.45
7.33
7.31
7.29
4.49
4.47
4.45
4.43
1.45
1.43
1.41
O
OEt
S
N
N
CF3
Br
0.81
0.90
0.87
0.93
0.99
2.05
3.00
f1 (ppm)

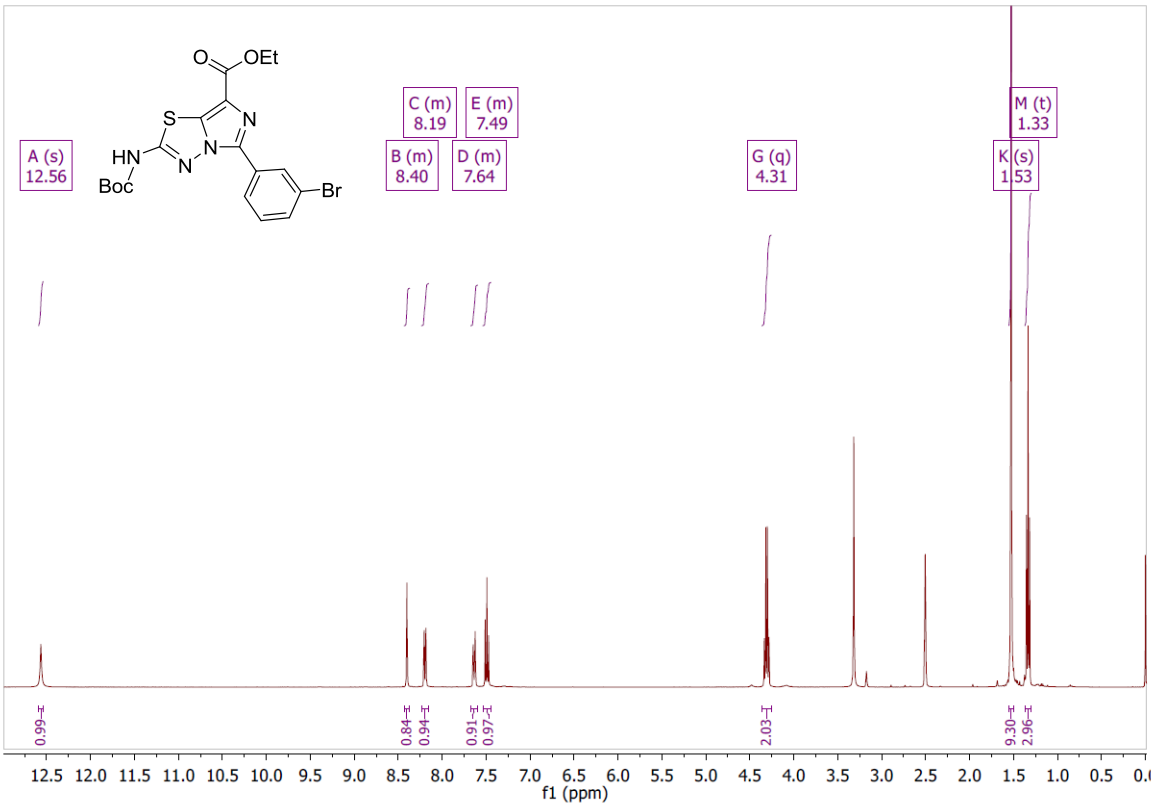

162.19
140.28
138.70
133.53
133.41
131.57
129.62
129.01
129.00
124.71
124.66
124.62
124.57
122.76
122.63
122.35
122.12
119.90
117.21
114.53
61.26
14.69
O
OEt
S
N
N
CF3
Br
f1 (ppm)

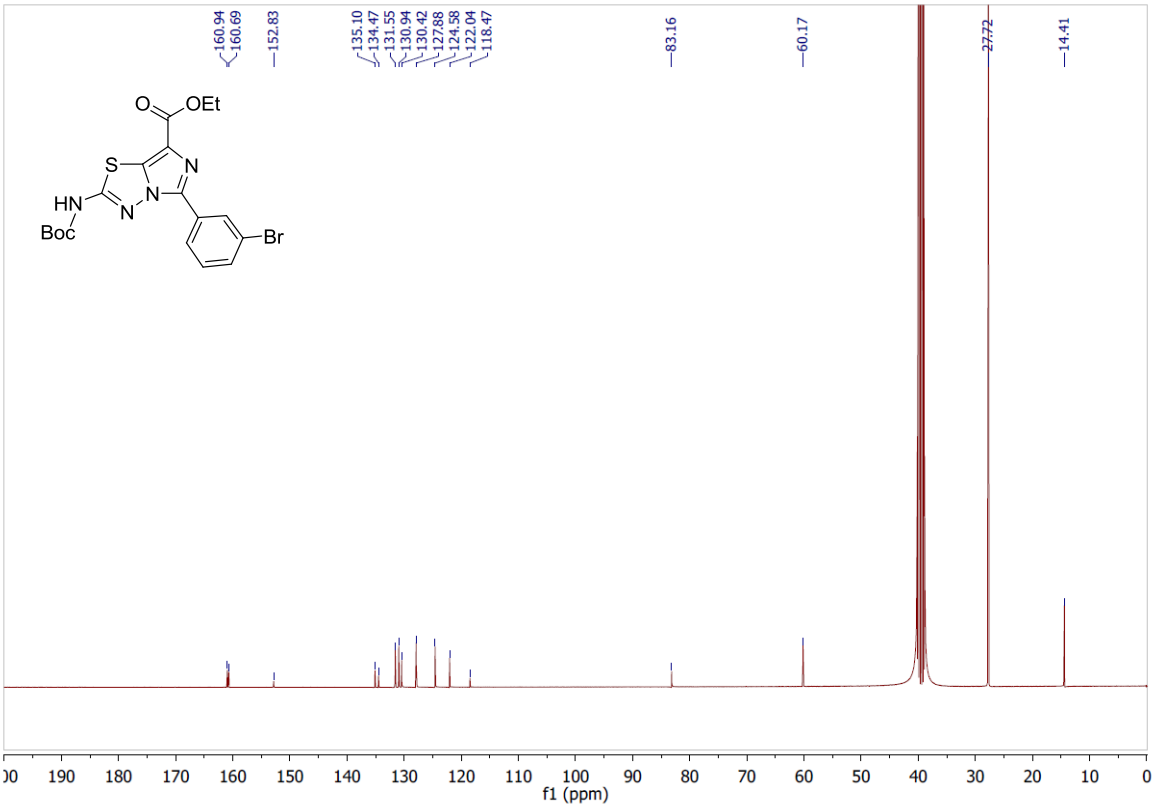
Compound *4d*


O
OMe
S
N
N
Br
Br
A (m)
8.83
B (m)
8.05
C (m)
7.94
D (m)
7.69
E (m)
7.49
F (s)
3.85
1.00
1.00
1.09
1.05
1.11
3.08
f1 (ppm)

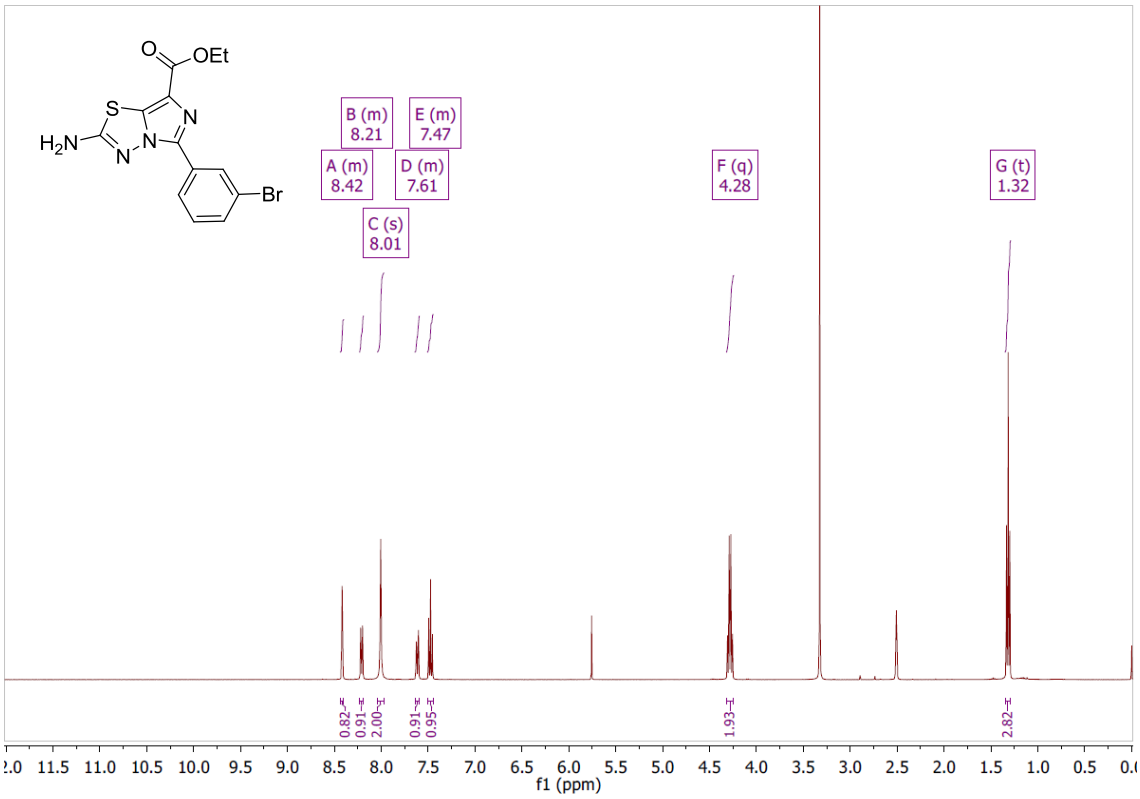

161.61
139.07
137.54
132.04
131.11
130.75
128.96
125.56
122.25
122.06
120.84
107.16
51.64
O
OMe
S
N
N
Br
Br
f1 (ppm)

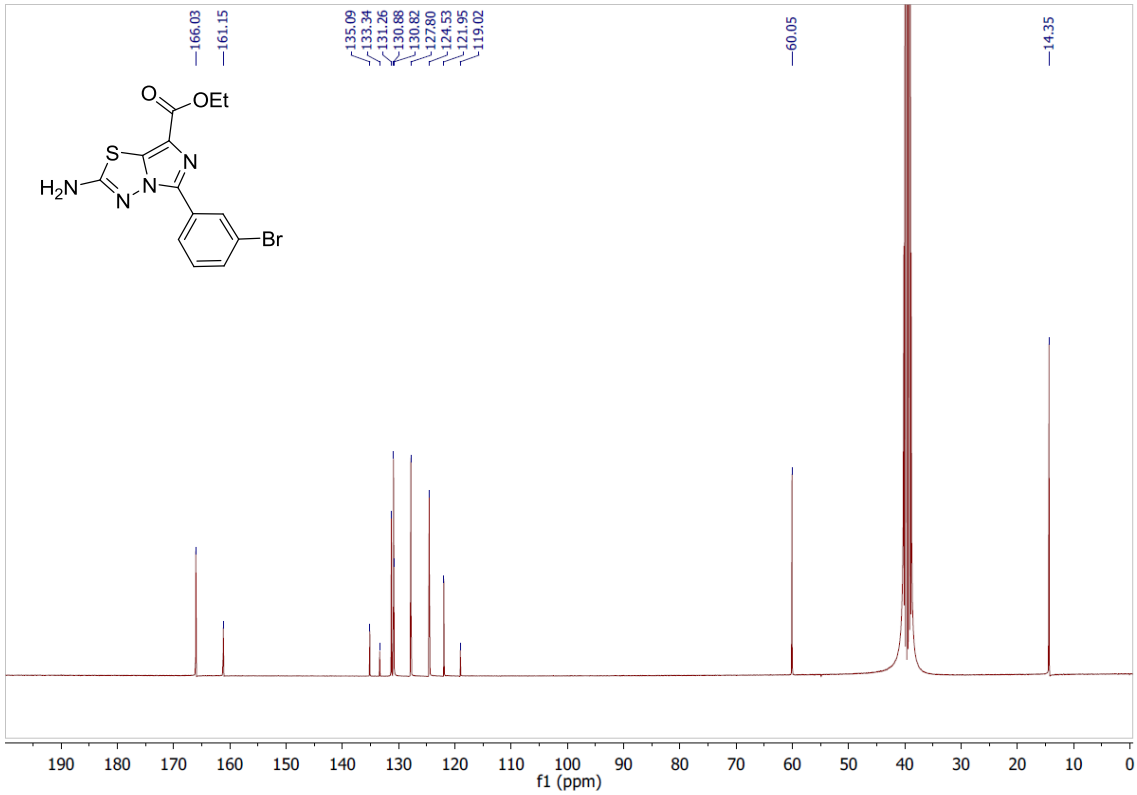
Compound *4e*


A (s)
12.56
B (m)
8.40
C (m)
8.19
D (m)
7.64
E (m)
7.49
G (q)
4.31
K (s)
1.53
M (t)
1.33
0.99
0.84
0.94
0.91
0.97
2.03
9.30
2.96
f1 (ppm)

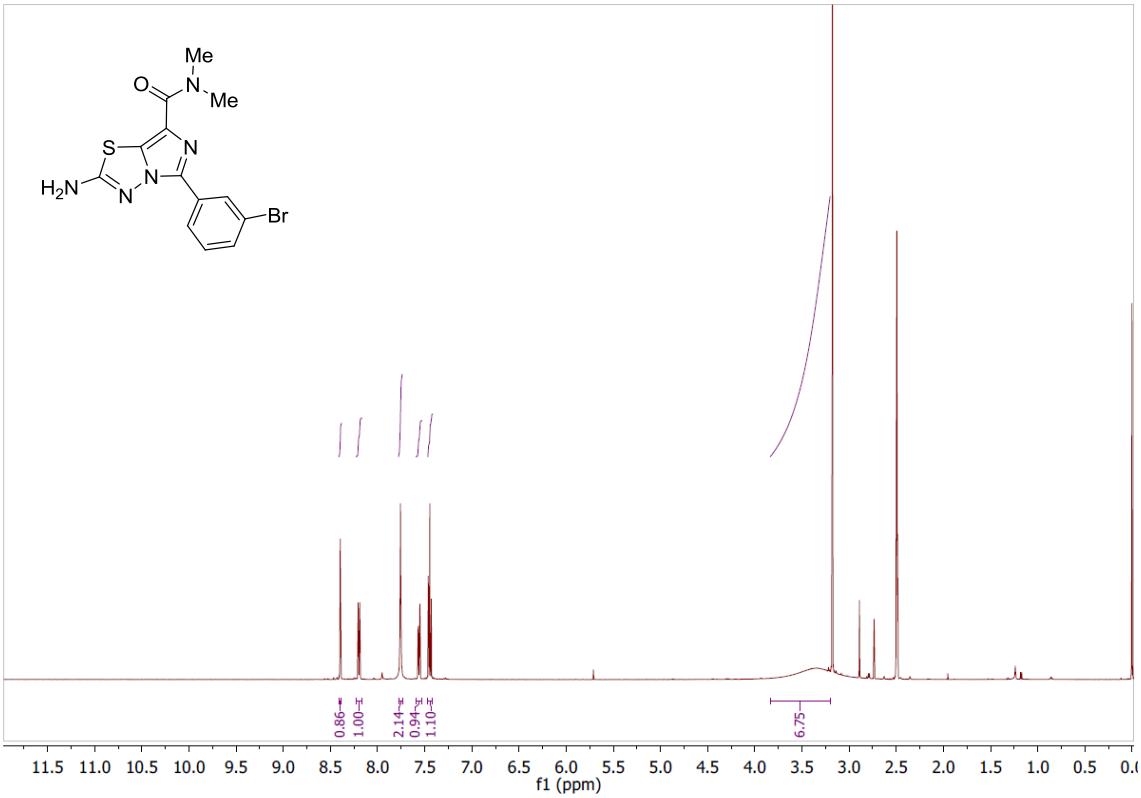

160.94
160.69
152.83
135.10
134.47
131.55
130.94
130.42
127.88
124.58
122.04
118.47
83.16
60.17
27.72
14.41
f1 (ppm)

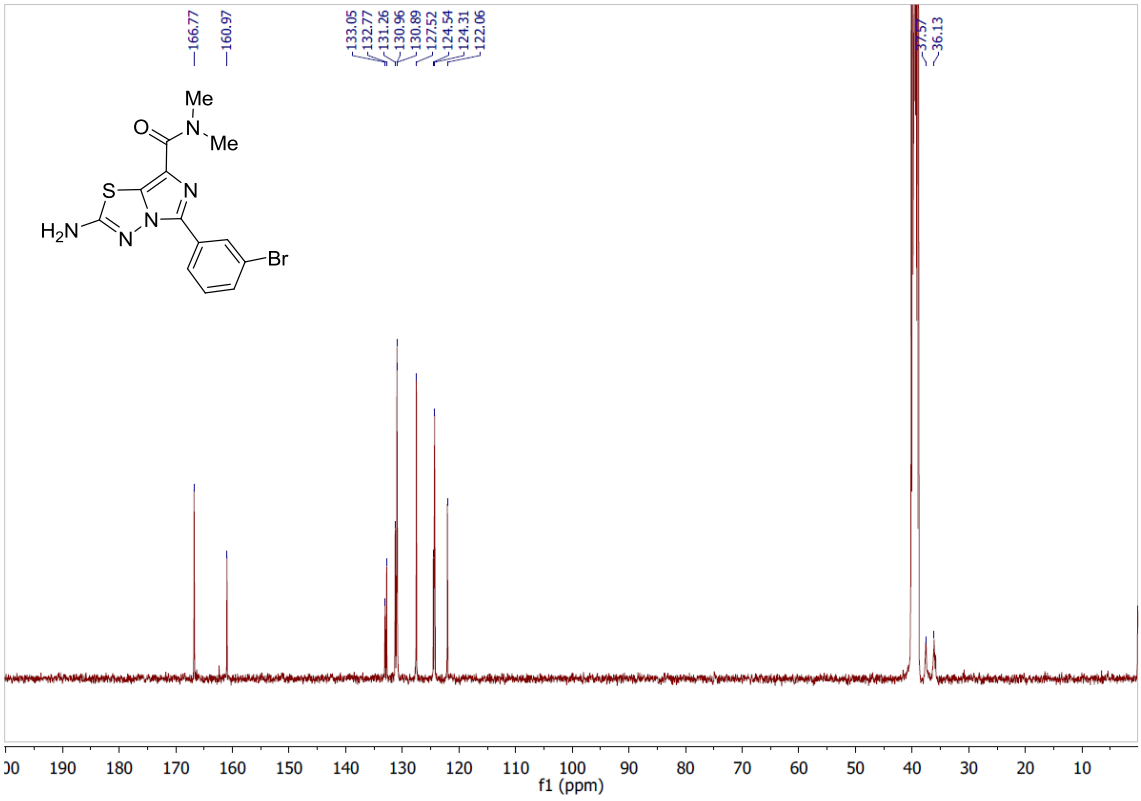
Compound *4f*


O
OEt
S
N
N
N
H2N
Br
B (m)
8.21
E (m)
7.47
A (m)
8.42
D (m)
7.61
C (s)
8.01
F (q)
4.28
G (t)
1.32
0.82
0.91
2.00
0.91
0.95
1.93
2.82
f1 (ppm)

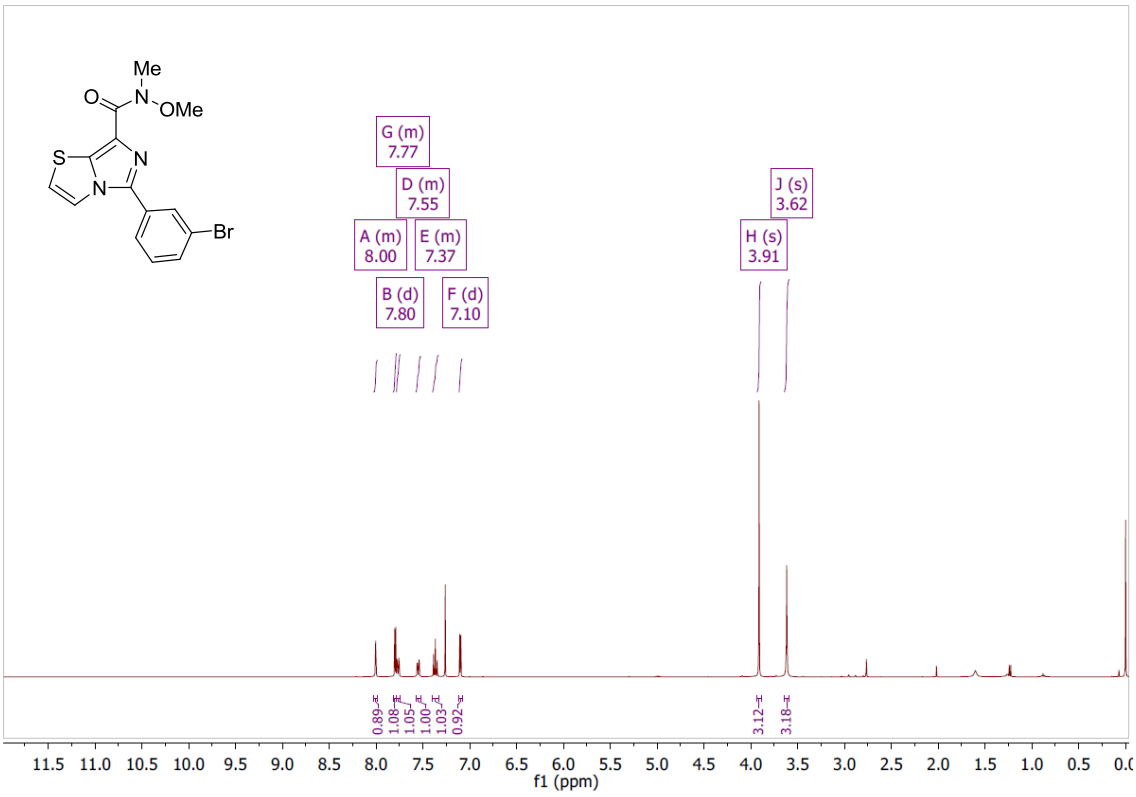

166.03
161.15
135.09
133.34
131.26
130.88
130.82
127.80
124.53
121.95
119.02
60.05
14.35
O
OEt
S
N
N
N
H2N
Br
f1 (ppm)

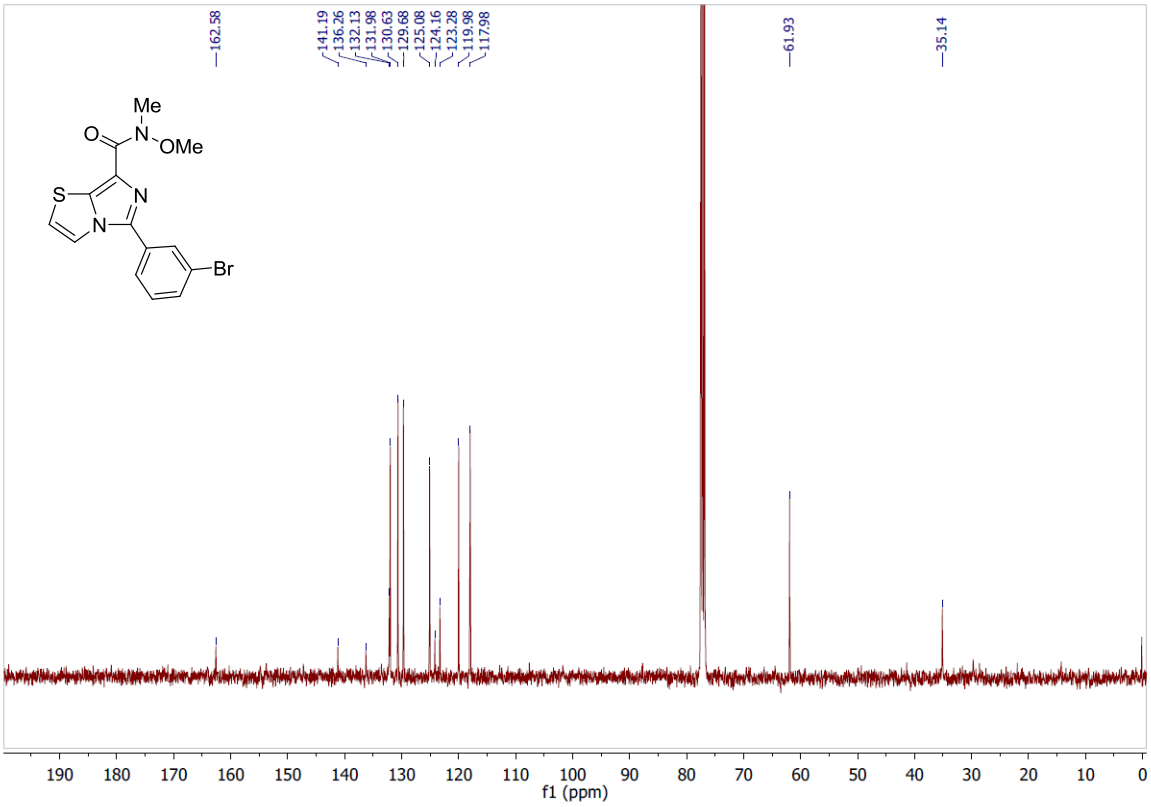
Compound *4g*


Me
O
N
Me
S
N
N
N
H2N
Br
0.86
1.00
2.14
0.94
1.10
6.75
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
f1 (ppm)

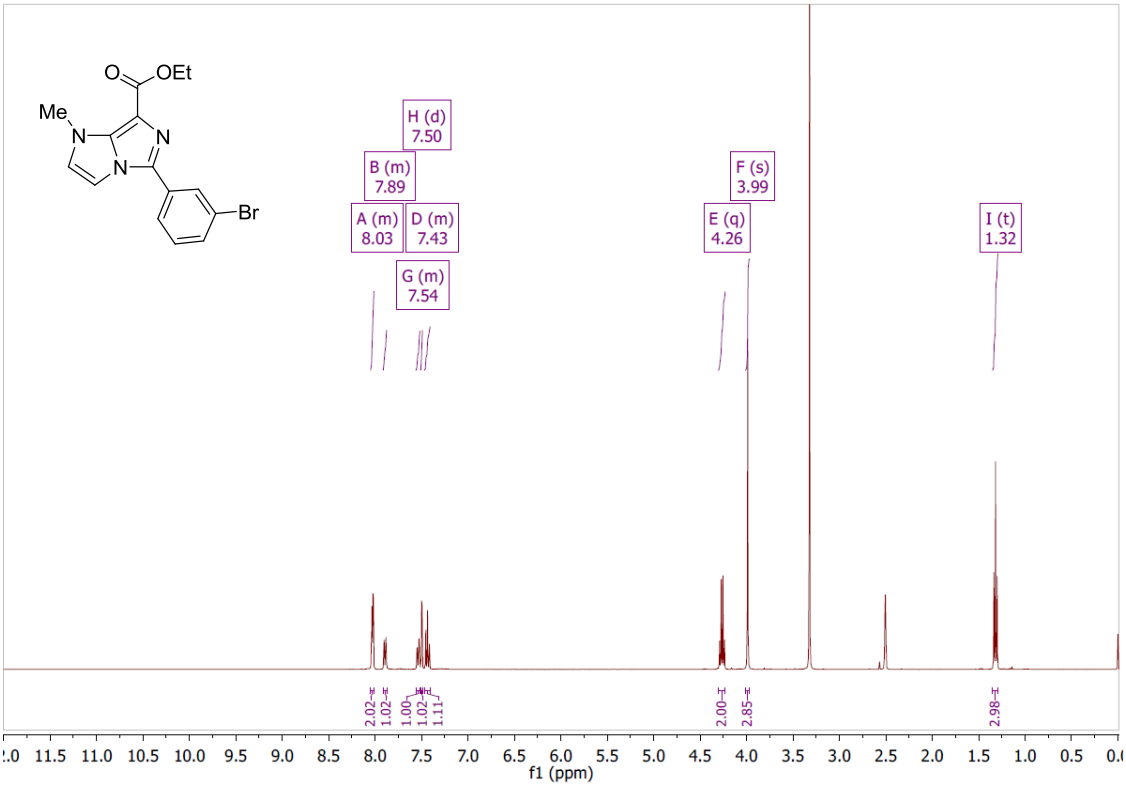

166.77
160.97
133.05
132.77
131.26
130.96
130.89
127.52
124.54
124.31
122.06
37.57
36.13
Me
O
N
Me
S
N
N
N
H2N
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

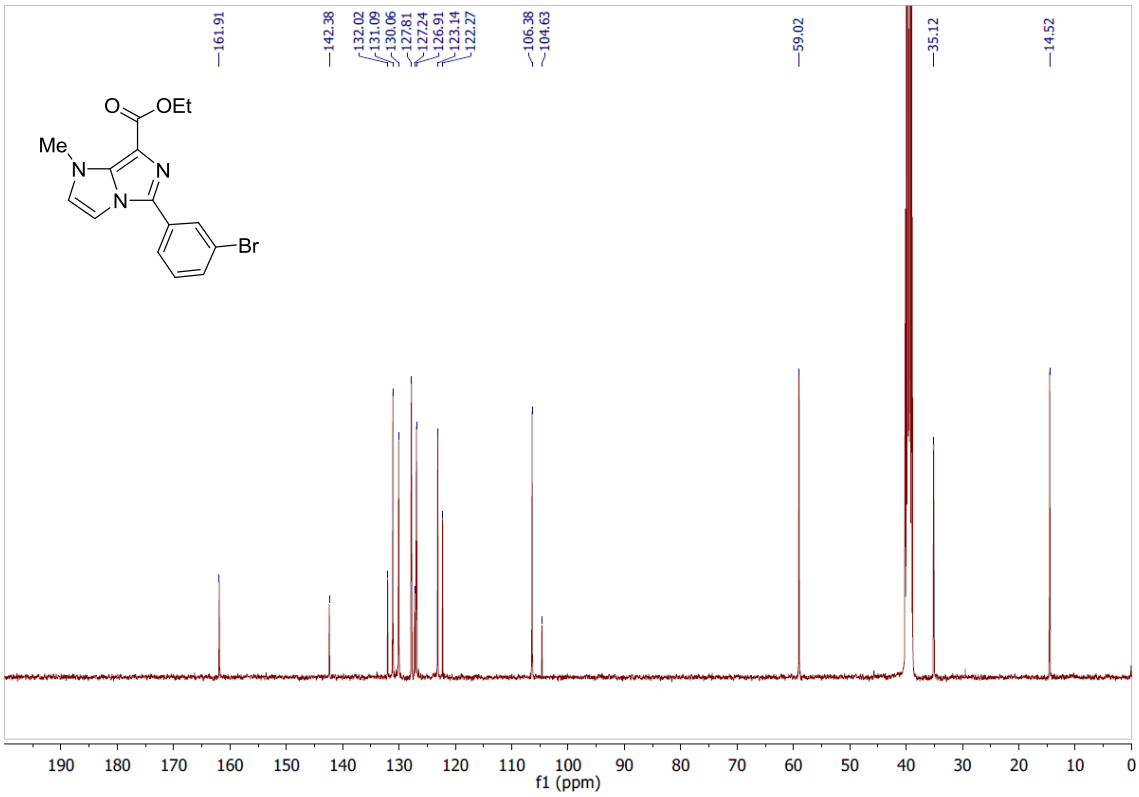
Compound *4h*


Me
O
N
OMe
S
N
N
Br
G (m)
7.77
D (m)
7.55
A (m)
8.00
E (m)
7.37
B (d)
7.80
F (d)
7.10
J (s)
3.62
H (s)
3.91
0.89
1.08
1.05
1.00
1.03
0.92
3.12
3.18
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)

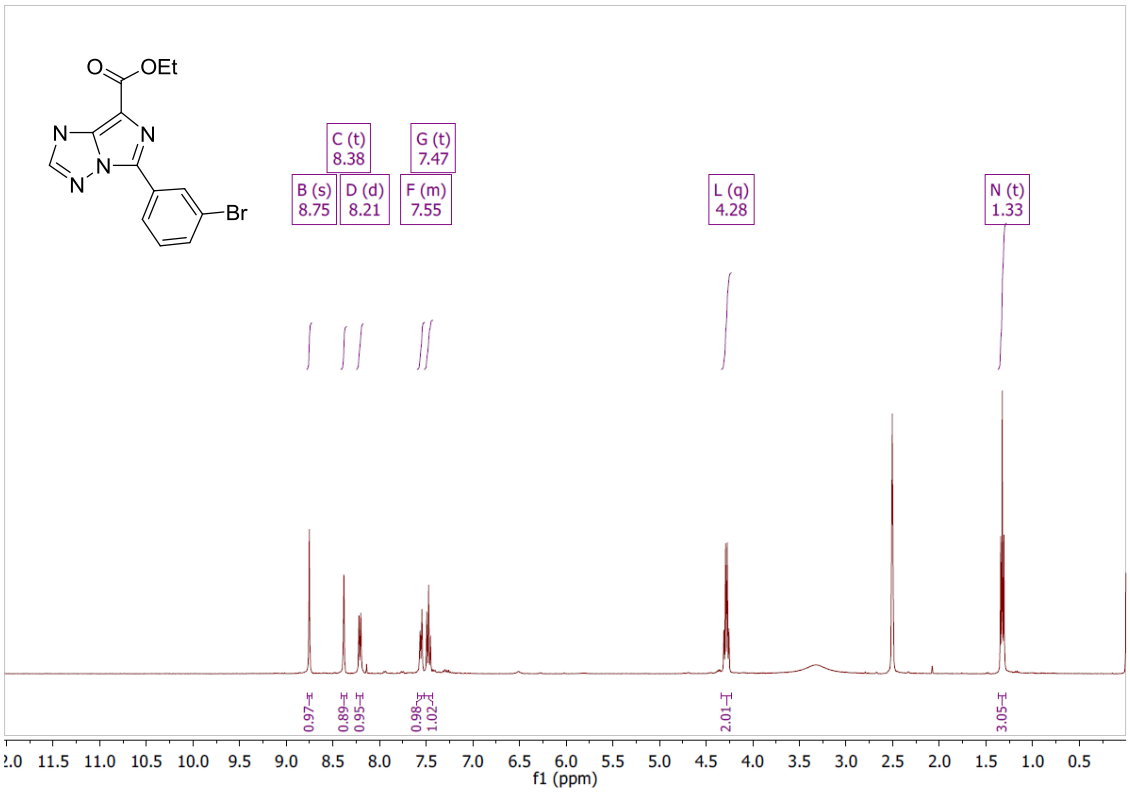

162.58
141.19
136.26
132.13
131.98
130.63
129.68
125.08
124.16
123.28
119.98
117.98
61.93
35.14
Me
O
N
OMe
S
N
N
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

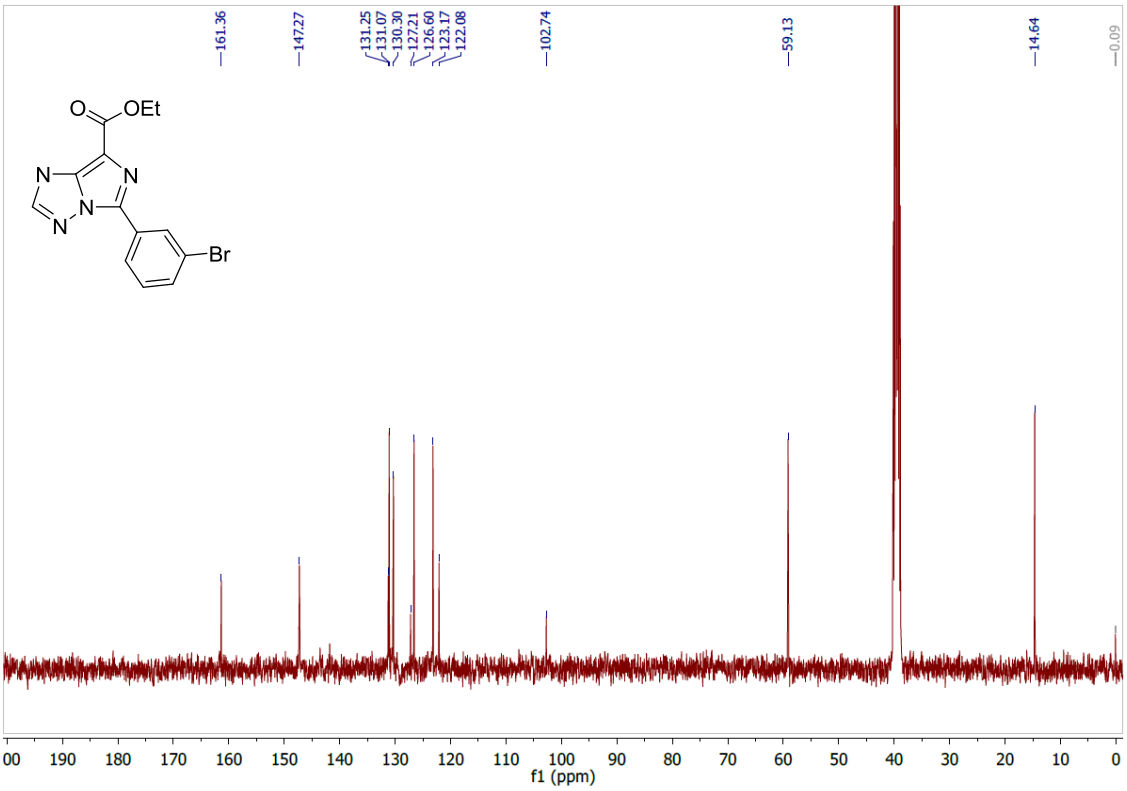
Compound *4i*


O
OEt
Me
N
N
N
Br
H (d)
7.50
B (m)
7.89
A (m)
8.03
D (m)
7.43
G (m)
7.54
F (s)
3.99
E (q)
4.26
I (t)
1.32
2.02
1.02
1.00
1.02
1.11
2.00
2.85
2.98
f1 (ppm)

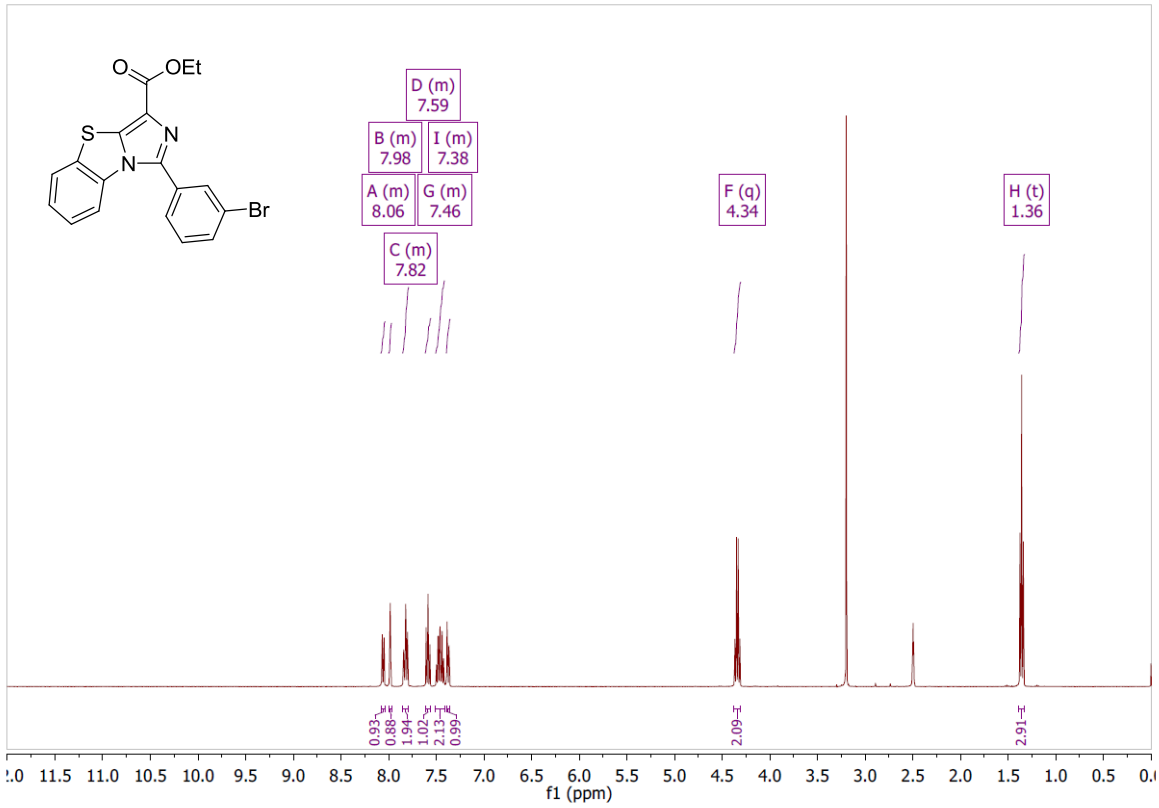

161.91
142.38
132.02
131.09
130.06
127.81
127.24
126.91
123.14
122.27
106.38
104.63
59.02
35.12
14.52
O
OEt
Me
N
N
N
Br
f1 (ppm)

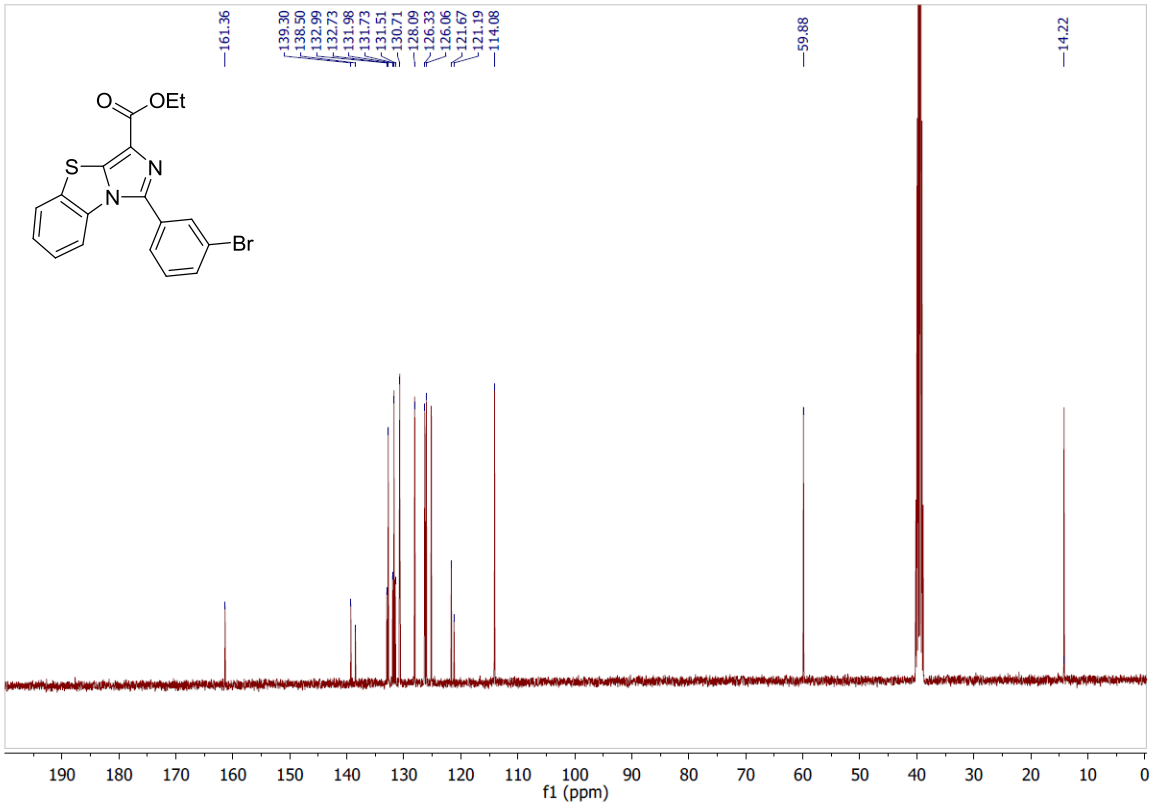
Compound *4j*


O
OEt
N
N
N
N
Br
C (t)
8.38
G (t)
7.47
B (s)
8.75
D (d)
8.21
F (m)
7.55
L (q)
4.28
N (t)
1.33
0.97
0.89
0.95
0.98
1.02
2.01
3.05
f1 (ppm)

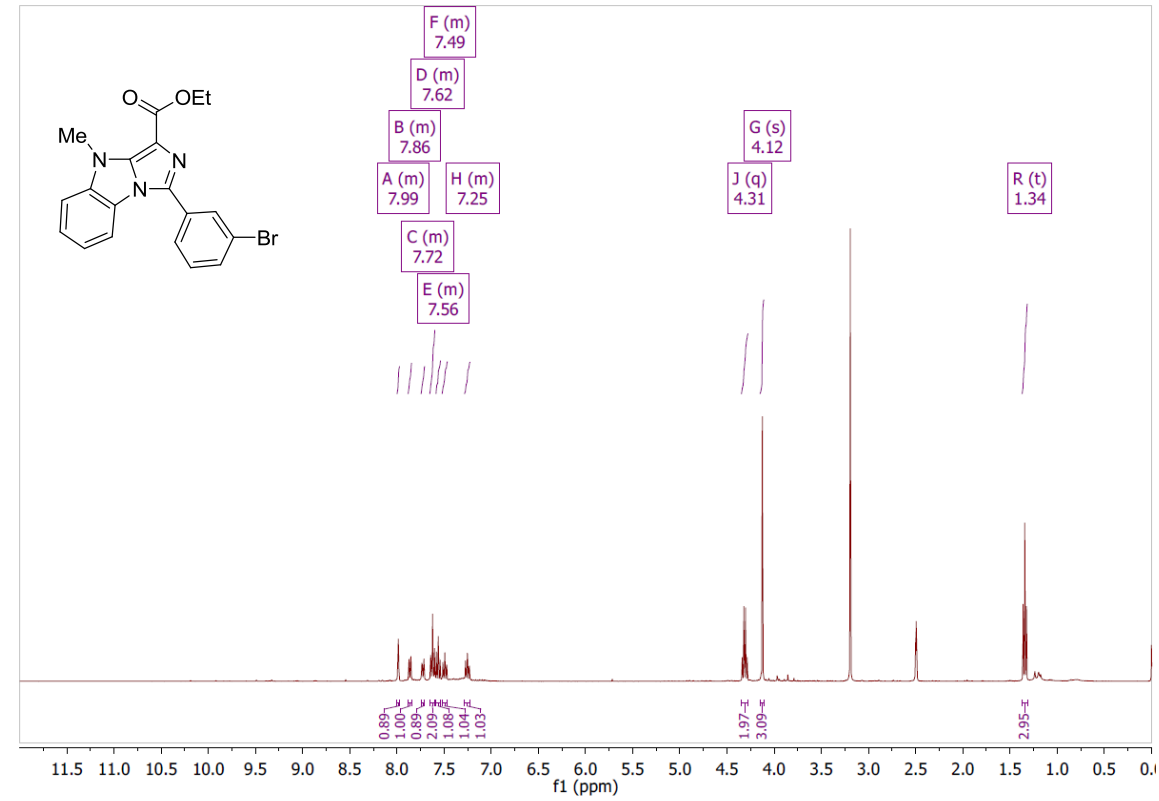

161.36
147.27
131.25
131.07
130.30
127.21
126.60
123.17
122.08
102.74
59.13
14.64
0.09
O
OEt
N
N
N
N
Br
f1 (ppm)

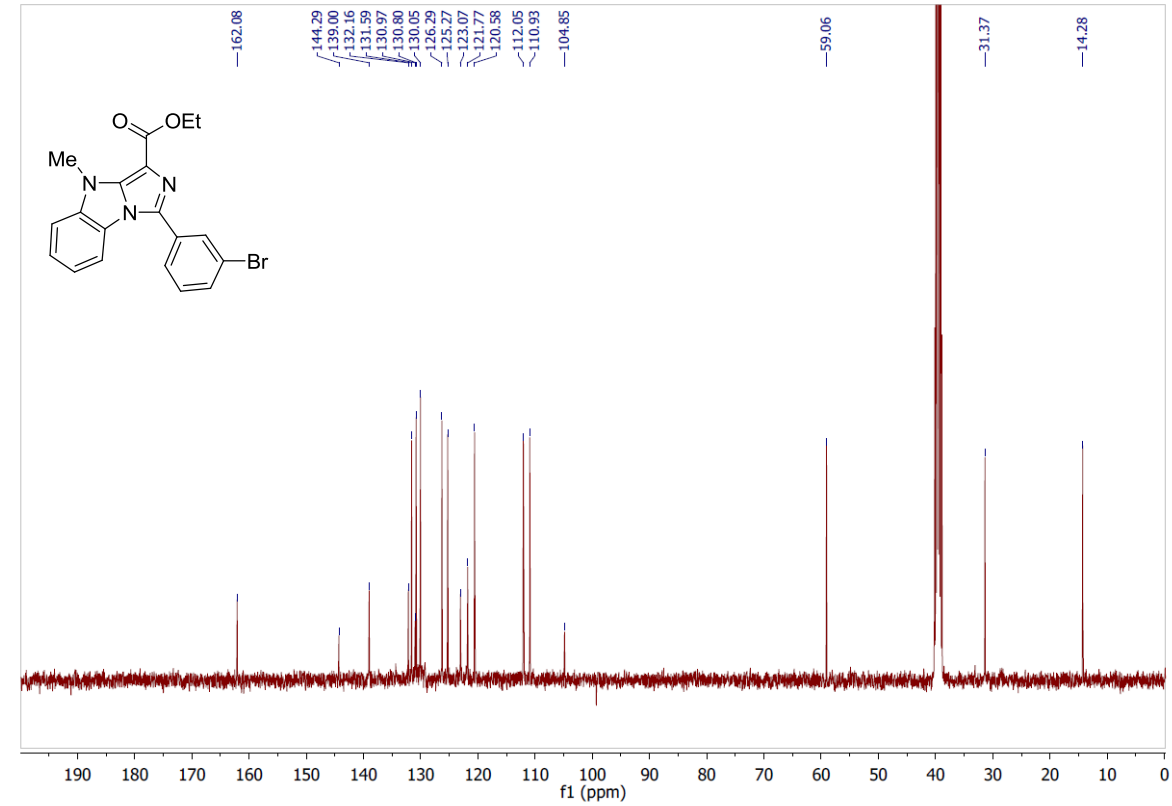
Compound *4k*


O
OEt
S
N
N
Br
D (m)
7.59
B (m)
7.98
I (m)
7.38
A (m)
8.06
G (m)
7.46
C (m)
7.82
F (q)
4.34
H (t)
1.36
0.93
0.88
1.94
1.02
2.13
0.99
2.09
2.91
f1 (ppm)

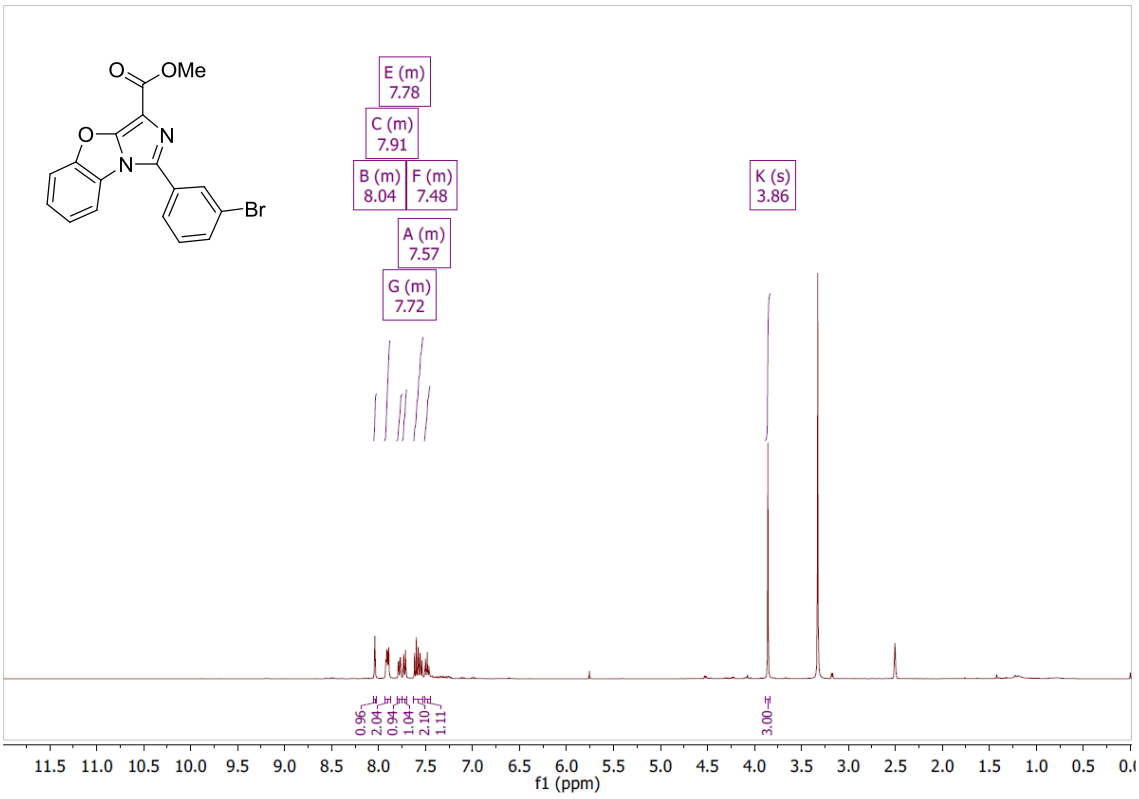

161.36
139.30
138.50
132.99
132.73
131.98
131.73
131.51
130.71
128.09
126.33
126.06
121.67
121.19
114.08
59.88
14.22
O
OEt
S
N
N
Br
f1 (ppm)

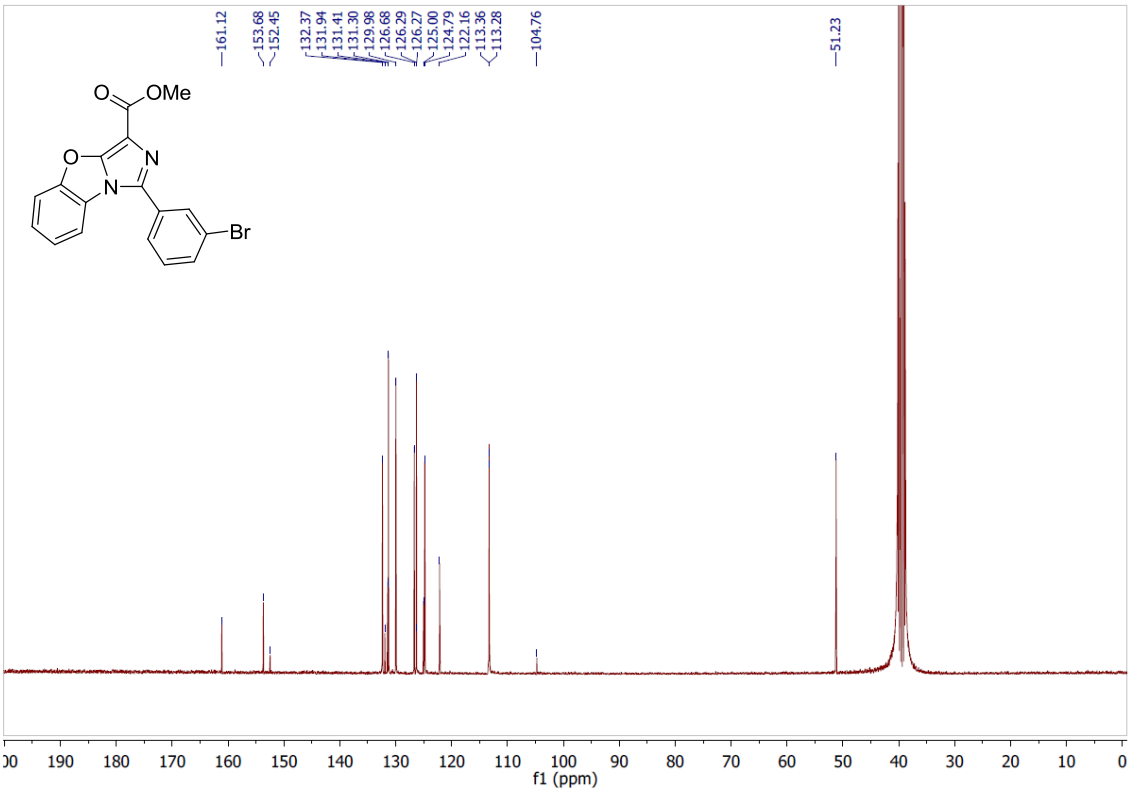
Compound *4l*


F (m)
7.49
D (m)
7.62
B (m)
7.86
A (m)
7.99
H (m)
7.25
C (m)
7.72
E (m)
7.56
G (s)
4.12
J (q)
4.31
R (t)
1.34
O
OEt
Me
N
N
N
Br
0.89
1.00
0.89
2.09
1.08
1.04
1.03
1.97
3.09
2.95
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
f1 (ppm)

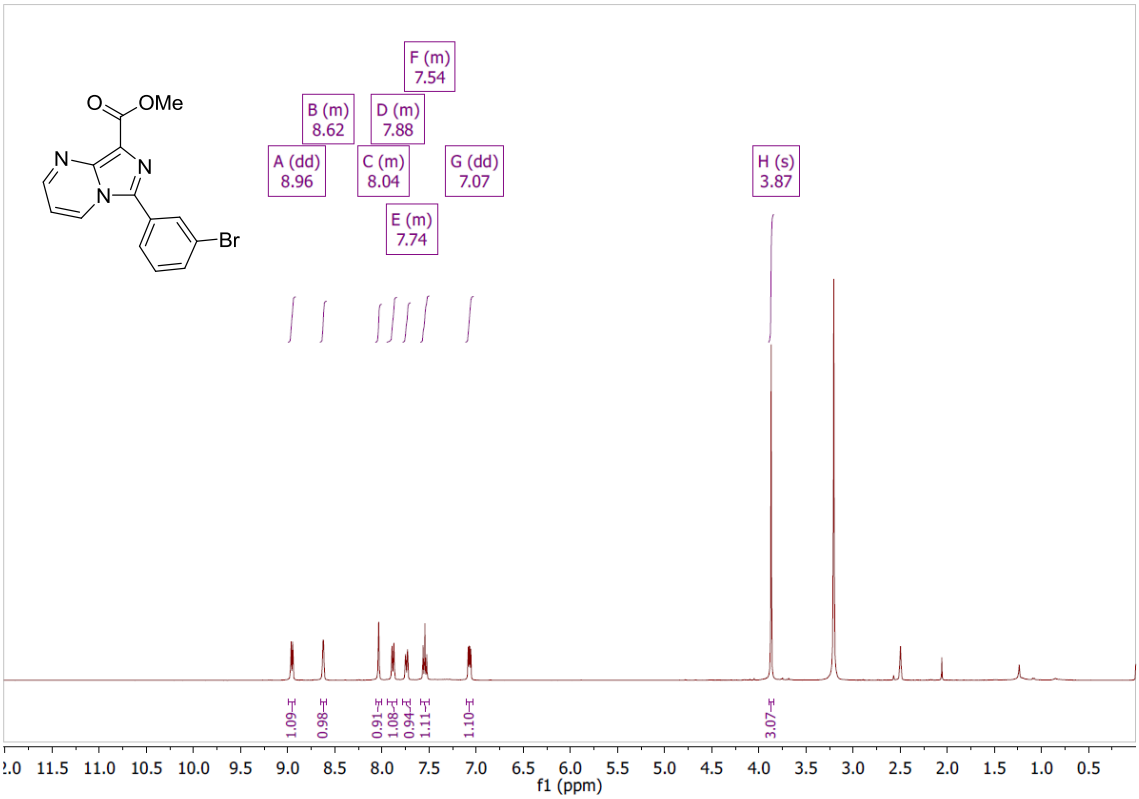

162.08
144.29
139.00
132.16
131.59
130.97
130.80
130.05
126.29
125.27
123.07
121.77
120.58
112.05
110.93
104.85
59.06
31.37
14.28
O
OEt
Me
N
N
N
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

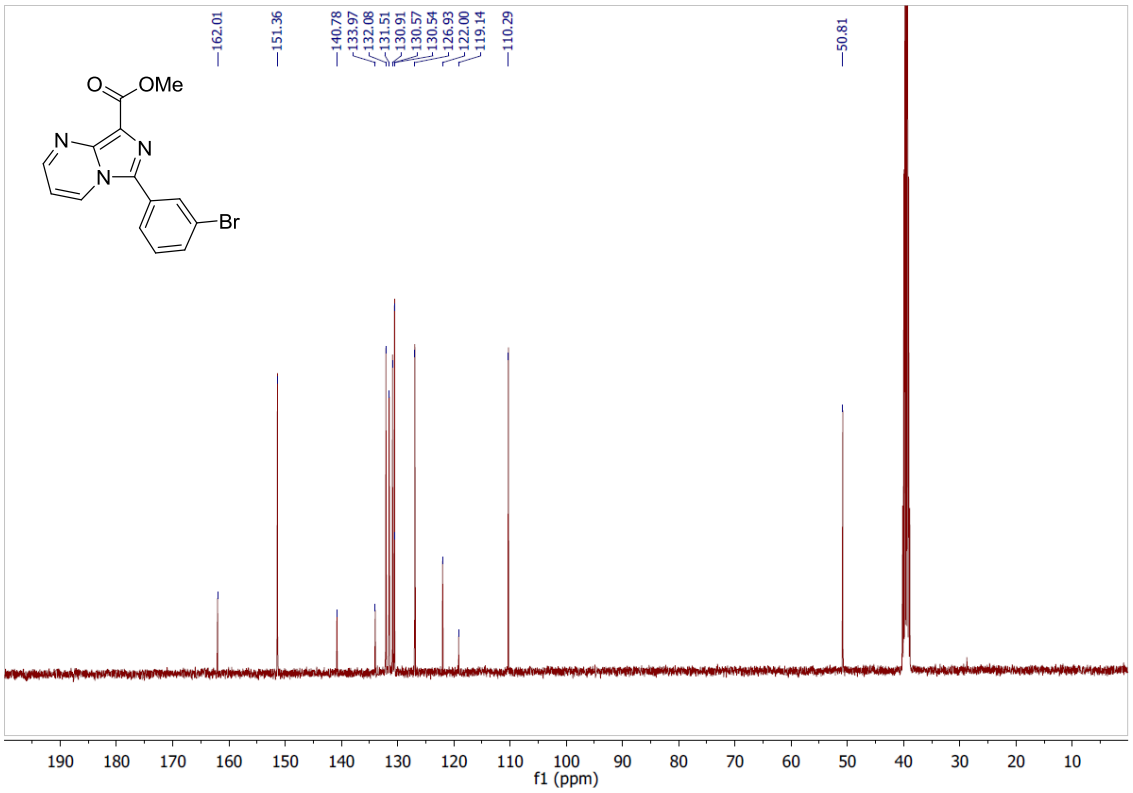
Compound *4m*


O
OMe
O
N
N
Br
E (m)
7.78
C (m)
7.91
B (m)
8.04
F (m)
7.48
A (m)
7.57
G (m)
7.72
K (s)
3.86
0.96
2.04
0.94
1.04
2.10
1.11
3.00
f1 (ppm)

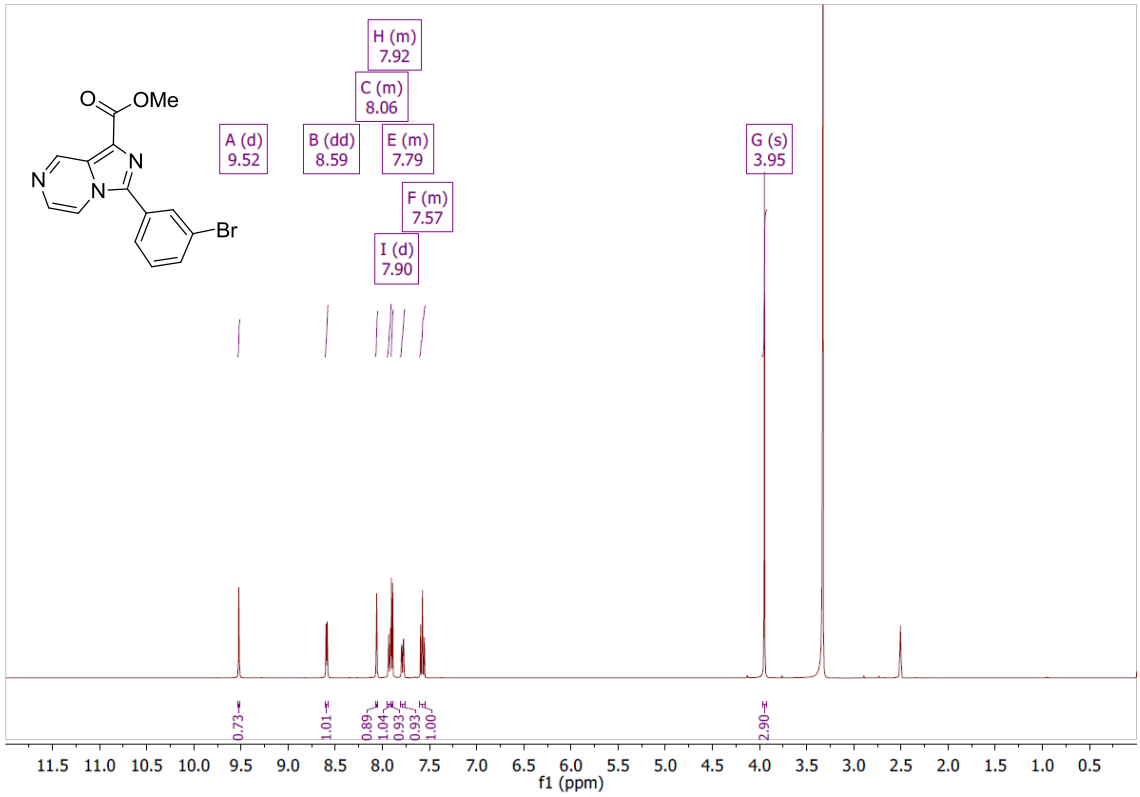

161.12
153.68
152.45
132.37
131.94
131.41
131.30
129.98
126.68
126.29
126.27
125.00
124.79
122.16
113.36
113.28
104.76
51.23
O
OMe
O
N
N
Br
f1 (ppm)

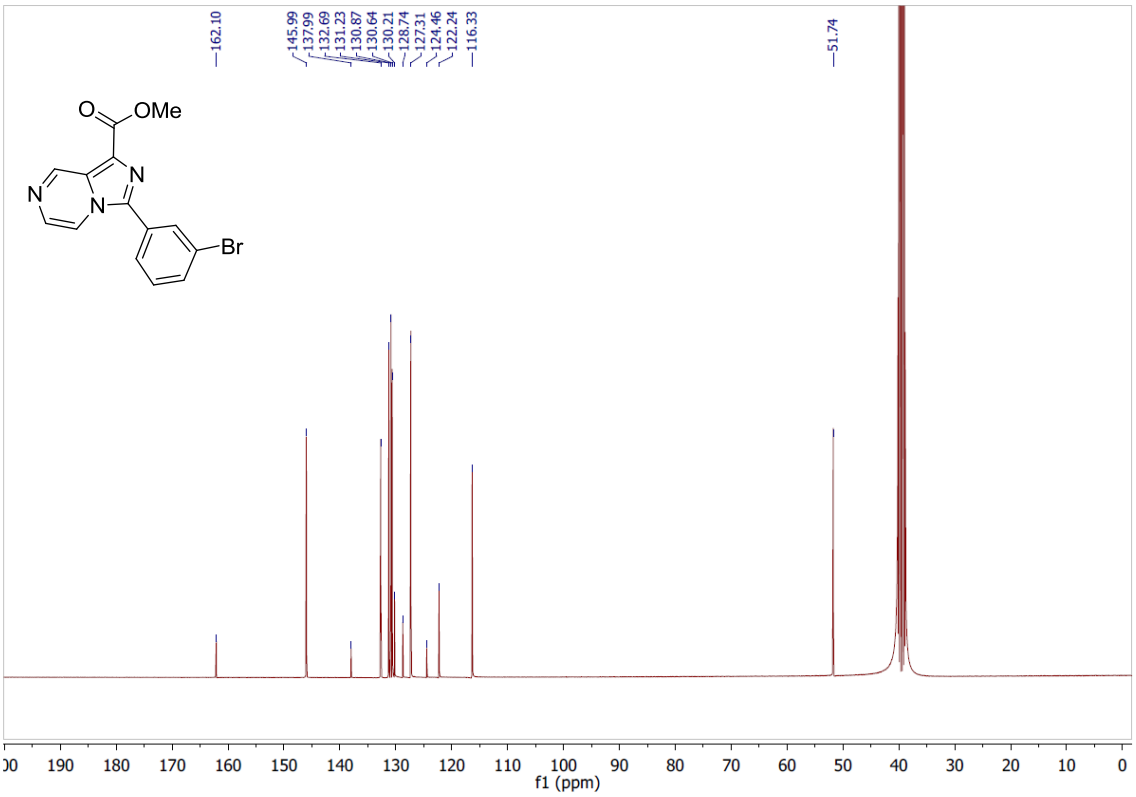
Compound *4n*


F (m)
7.54
B (m)
8.62
D (m)
7.88
A (dd)
8.96
C (m)
8.04
G (dd)
7.07
H (s)
3.87
E (m)
7.74
O
OMe
N
N
N
Br
1.09
0.98
0.91
1.08
0.94
1.11
1.10
3.07
f1 (ppm)

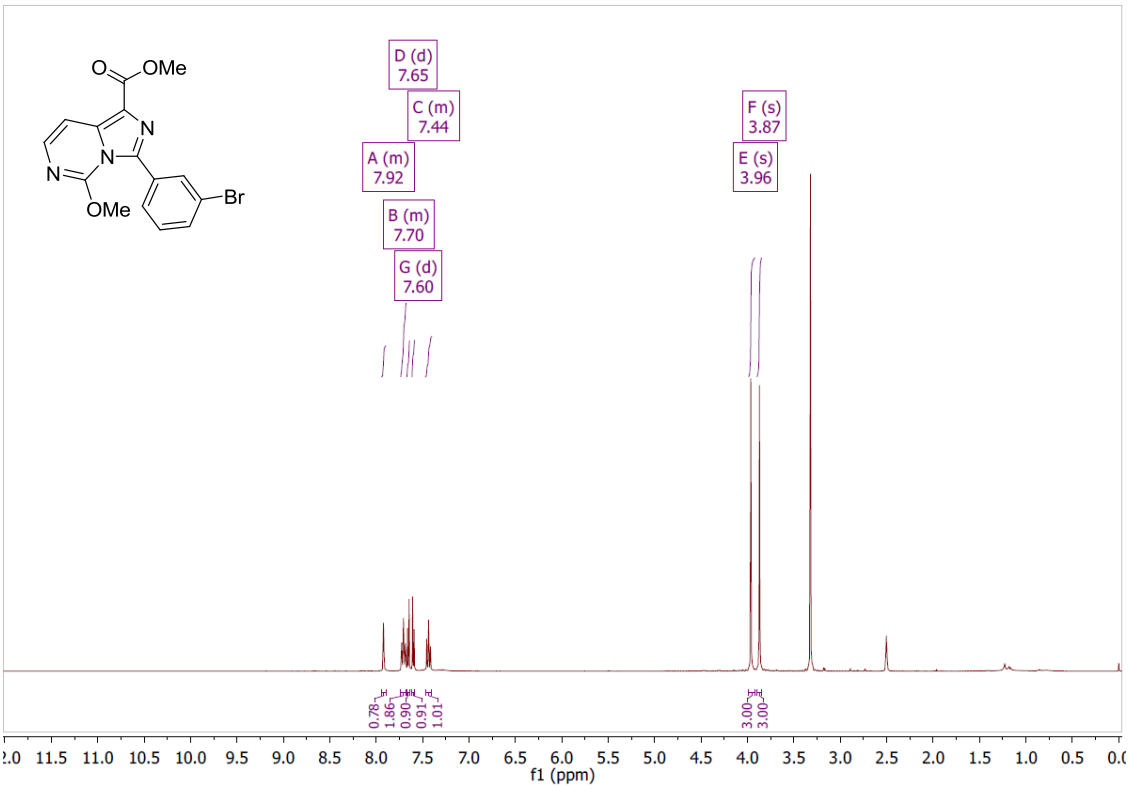

162.01
151.36
140.78
133.97
132.08
131.51
130.91
130.57
130.54
126.93
122.00
119.14
110.29
50.81
O
OMe
N
N
N
Br
f1 (ppm)

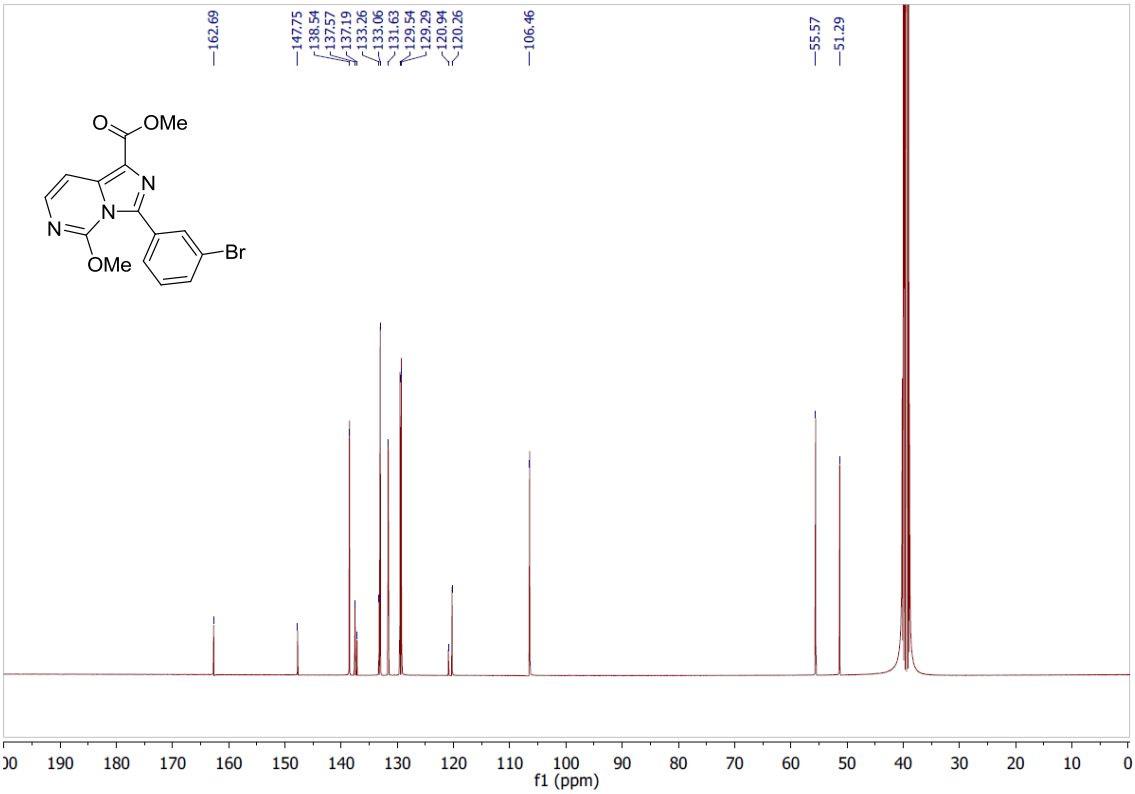
Compound *4o*


H (m)
7.92
C (m)
8.06
A (d)
9.52
B (dd)
8.59
E (m)
7.79
G (s)
3.95
F (m)
7.57
I (d)
7.90
O
OMe
N
N
N
Br
0.73
1.01
0.89
1.04
0.93
0.93
1.00
2.90
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
f1 (ppm)

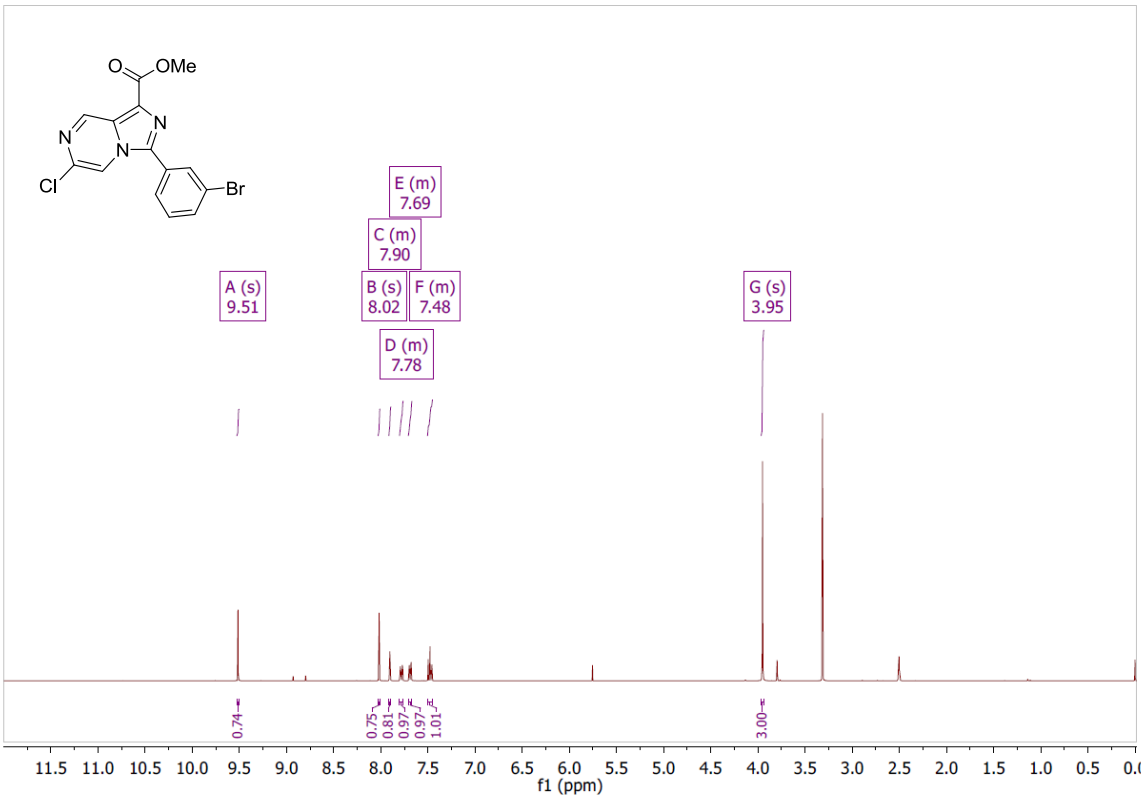

162.10
145.99
137.99
132.69
131.23
130.87
130.64
130.21
128.74
127.31
124.46
122.24
116.33
51.74
O
OMe
N
N
N
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

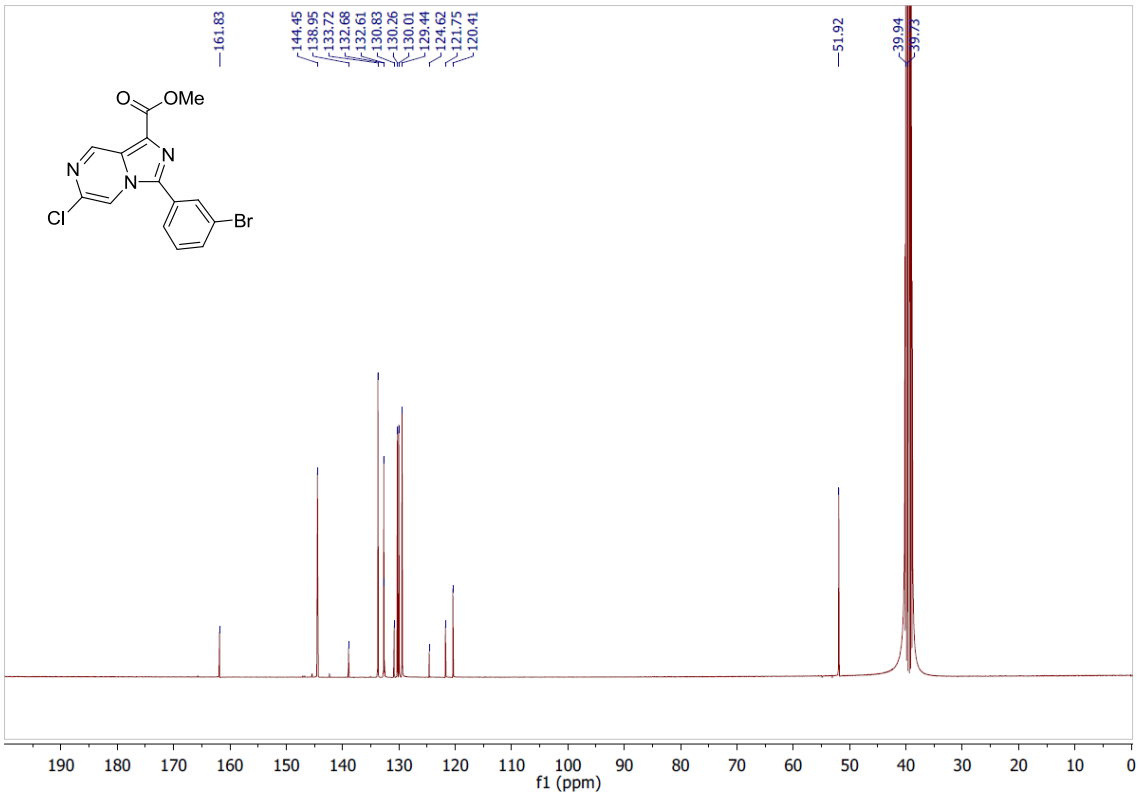
Compound *4p*


D (d)
7.65
C (m)
7.44
A (m)
7.92
B (m)
7.70
G (d)
7.60
F (s)
3.87
E (s)
3.96
0.78
1.86
0.90
0.91
1.01
3.00
3.00
f1 (ppm)

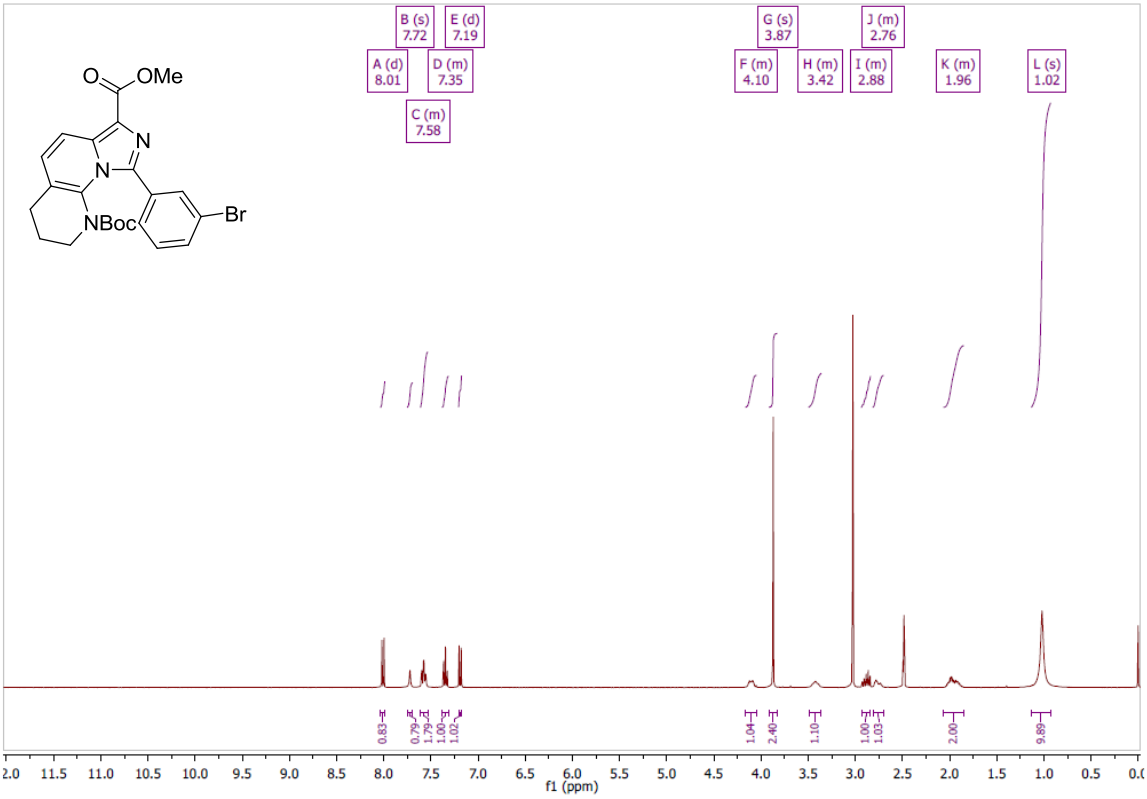

162.69
147.75
138.54
137.57
137.19
133.26
133.06
131.63
129.54
129.29
120.94
120.26
106.46
55.57
51.29
f1 (ppm)

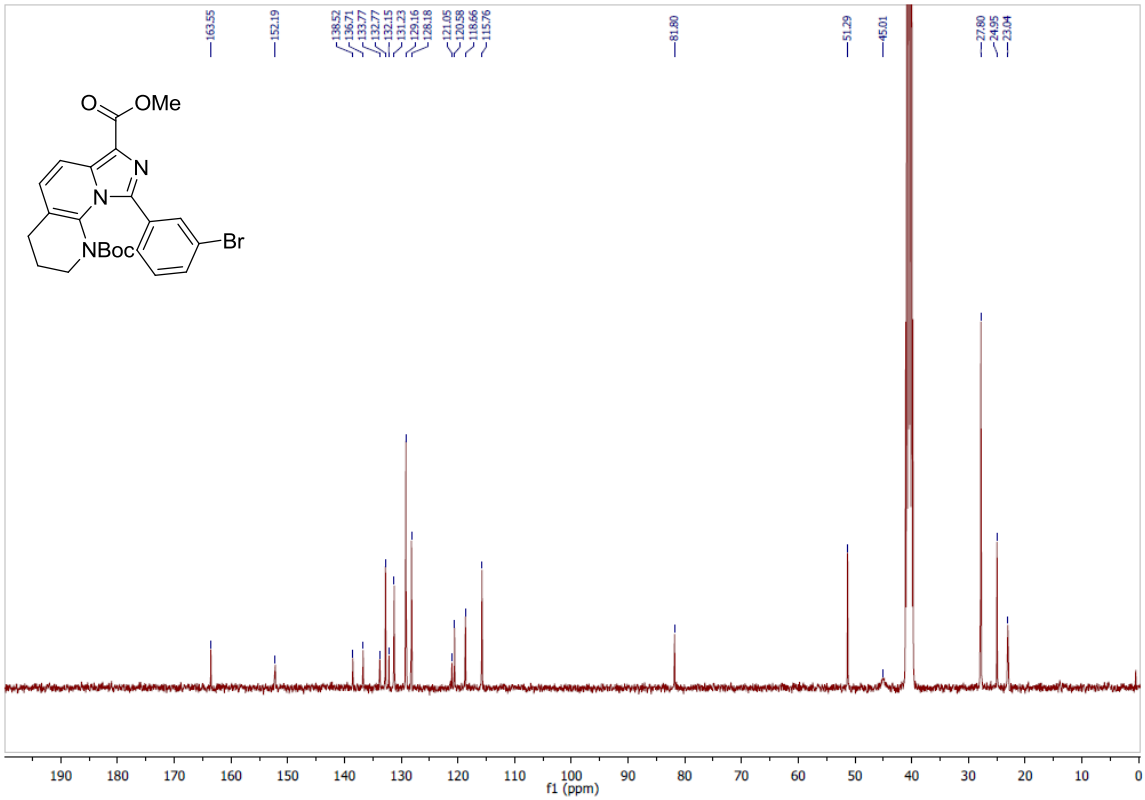
Compound *4q*


O
OMe
N
N
N
Cl
Br
A (s)
9.51
B (s)
8.02
C (m)
7.90
D (m)
7.78
E (m)
7.69
F (m)
7.48
G (s)
3.95
0.74
0.75
0.81
0.97
0.97
1.01
3.00
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
f1 (ppm)

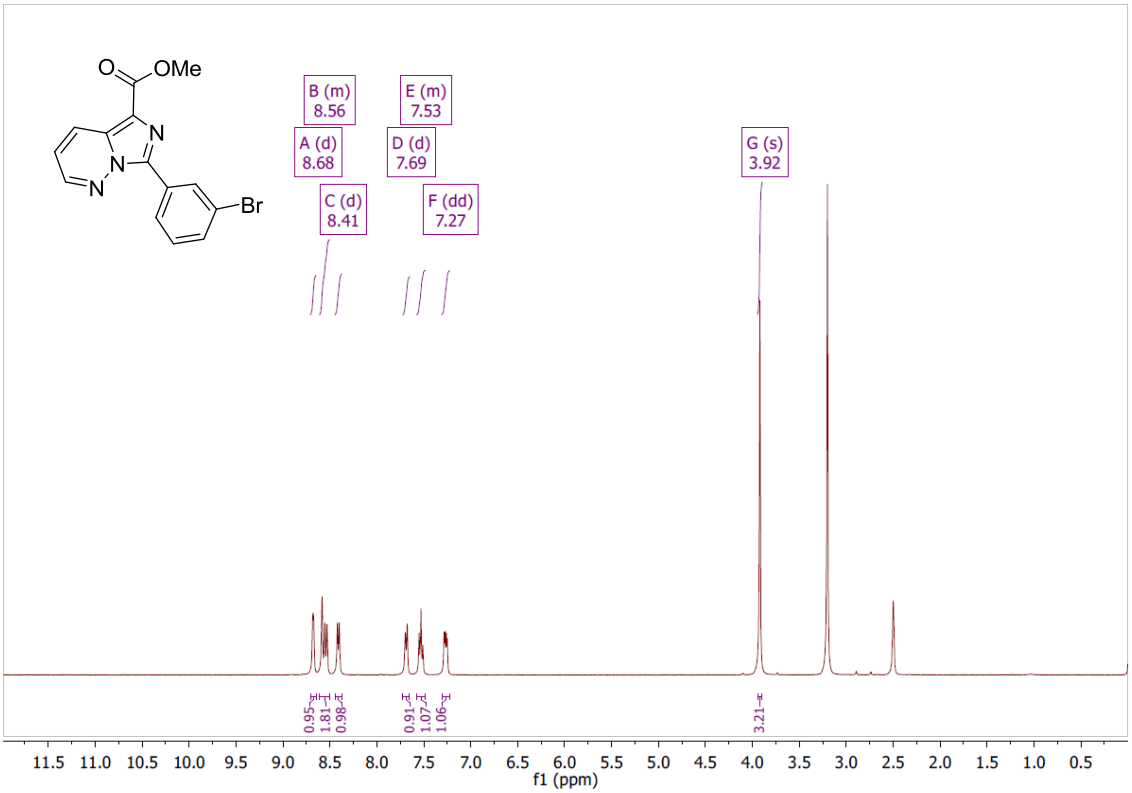

161.83
144.45
138.95
133.72
132.68
132.61
130.83
130.26
130.01
129.44
124.62
121.75
120.41
51.92
39.94
39.73
O
OMe
N
N
N
Cl
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

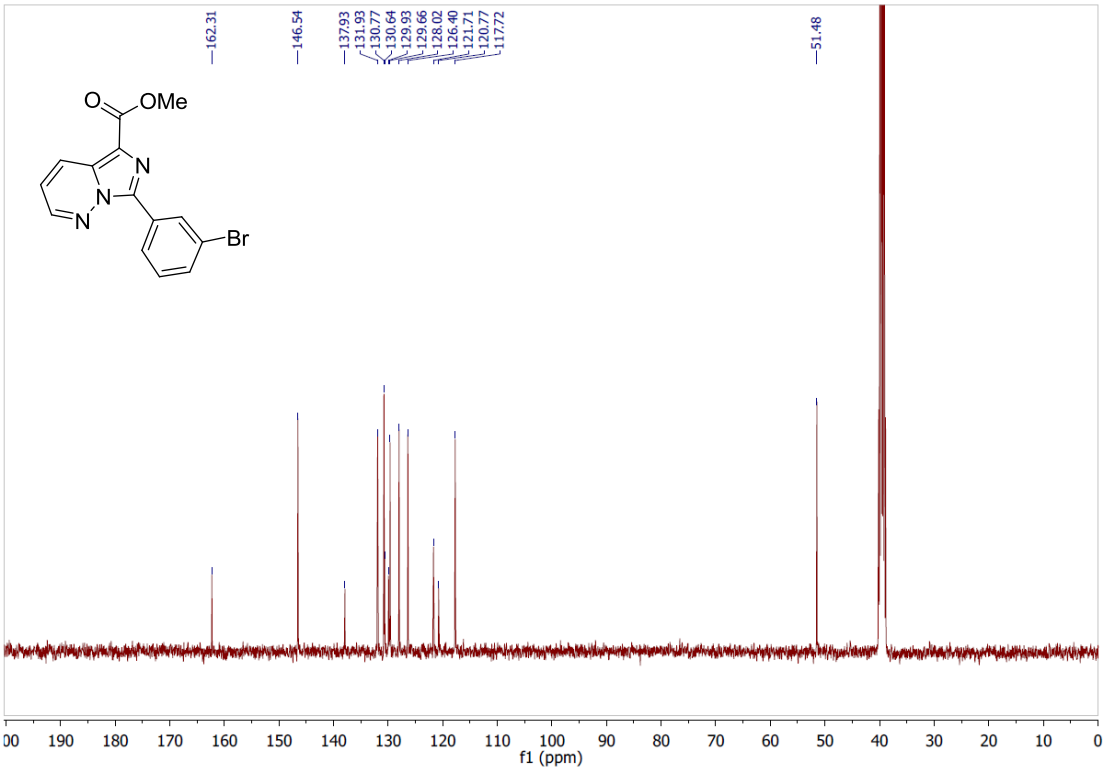
Compound *4r*


B (s) 7.72
E (d) 7.19
A (d) 8.01
D (m) 7.35
C (m) 7.58
G (s) 3.87
J (m) 2.76
F (m) 4.10
H (m) 3.42
I (m) 2.88
K (m) 1.96
L (s) 1.02
O
OMe
N
N
NBoc
Br
0.83
0.79
1.79
1.00
1.02
1.04
2.40
1.10
1.00
1.03
2.00
9.89
f1 (ppm)

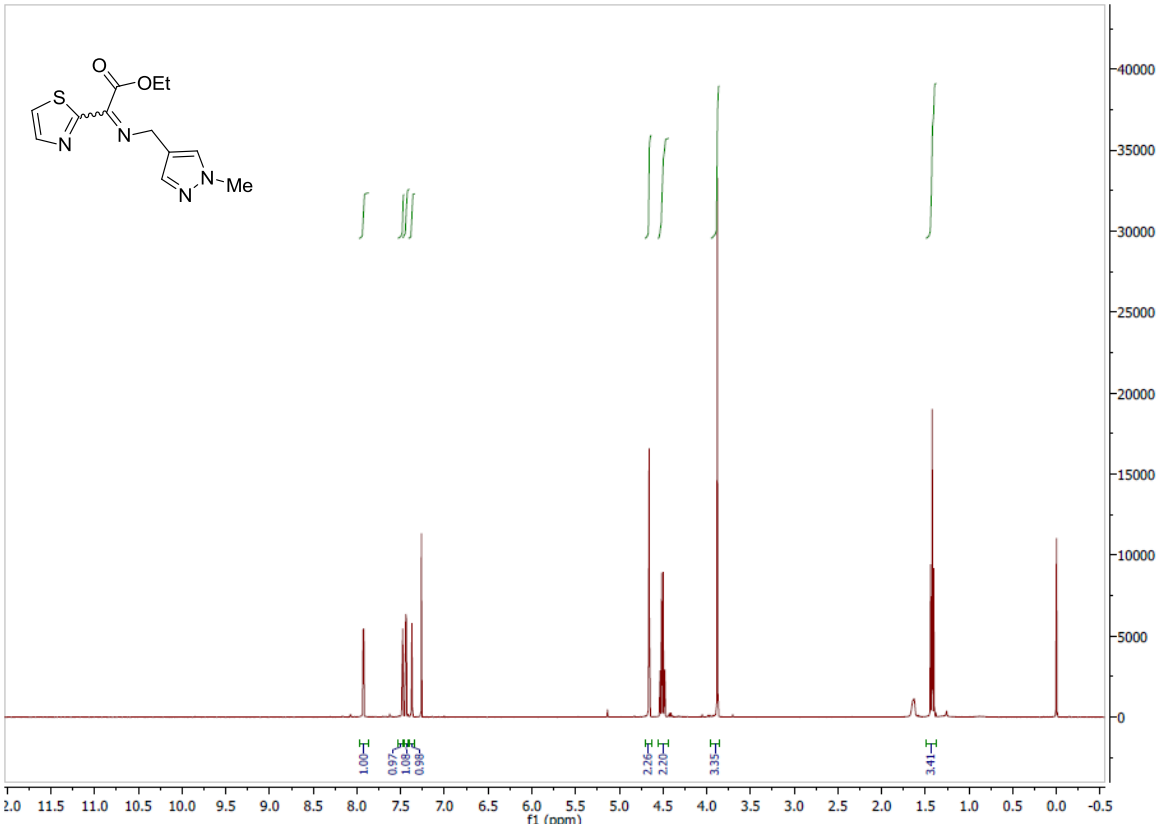

163.55
152.19
138.52
136.71
133.77
132.77
132.15
131.23
129.16
128.18
121.05
120.58
118.66
115.76
81.80
51.29
45.01
27.80
24.95
23.04
O
OMe
N
N
NBoc
Br
f1 (ppm)

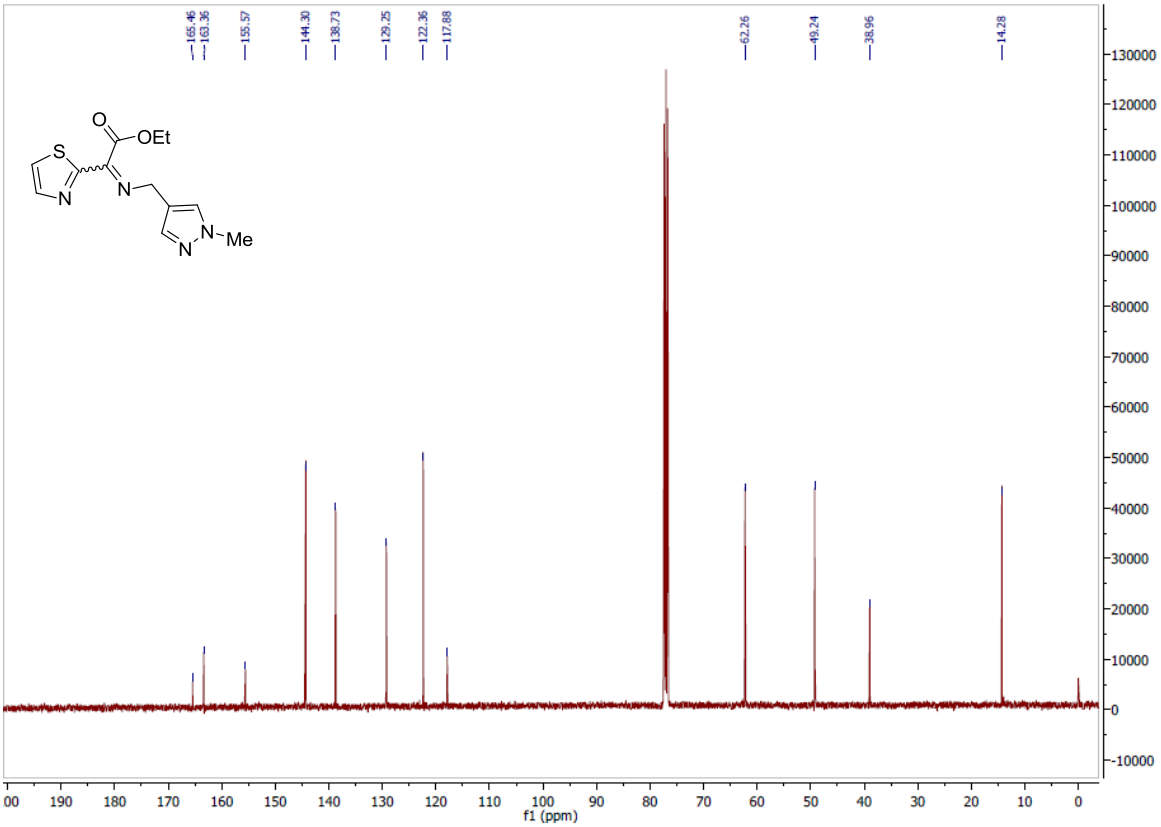
Compound *4t*


O
OMe
N
N
N
Br
B (m)
8.56
E (m)
7.53
A (d)
8.68
D (d)
7.69
C (d)
8.41
F (dd)
7.27
G (s)
3.92
0.95
1.81
0.98
0.91
1.07
1.06
3.21
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
f1 (ppm)

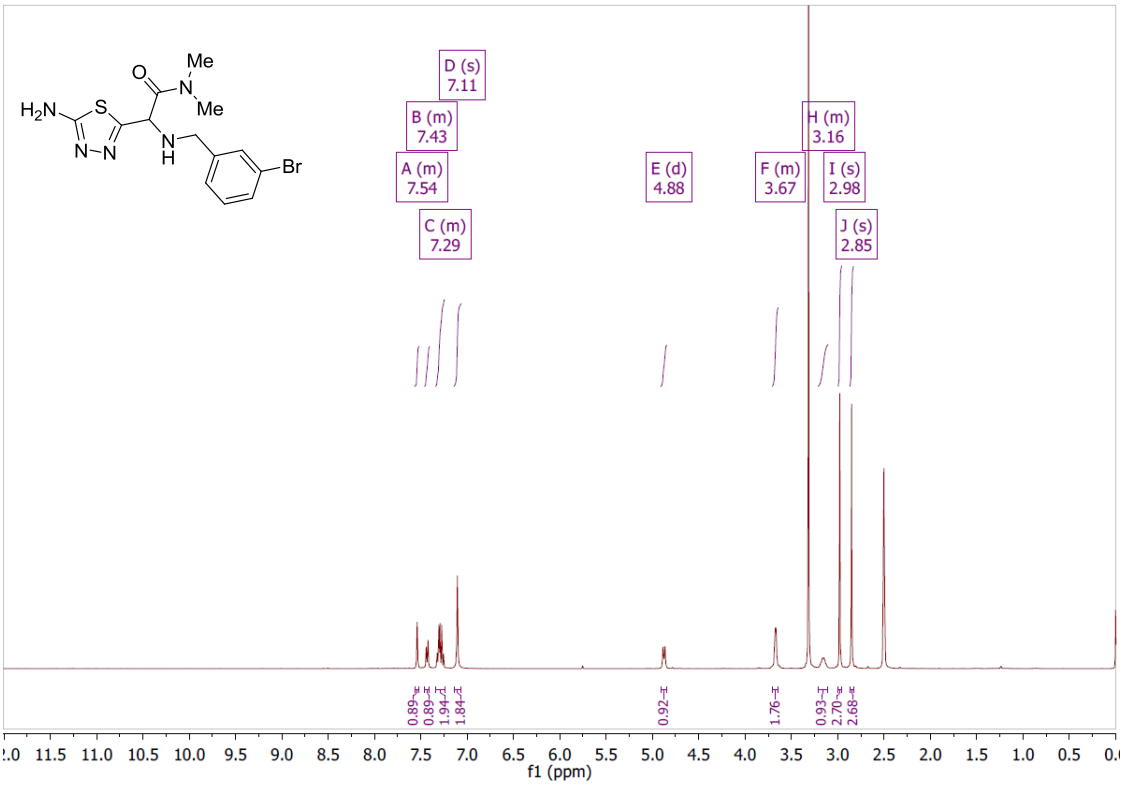

162.31
146.54
137.93
131.93
130.77
130.64
129.93
129.66
128.02
126.40
121.71
120.77
117.72
51.48
O
OMe
N
N
N
Br
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

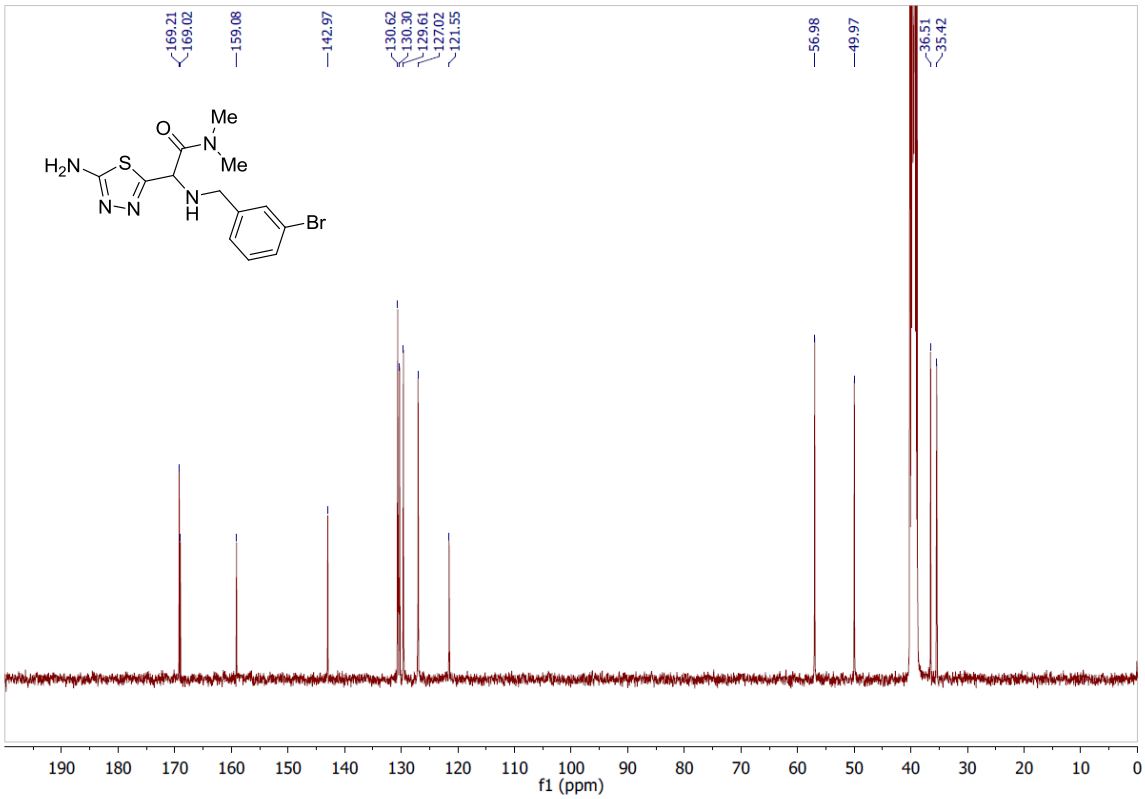
Compound *5*


O
OEt
S
N
N
N
N
Me
1.00
0.97
1.08
0.98
2.26
2.20
3.35
3.41
f1 (ppm)

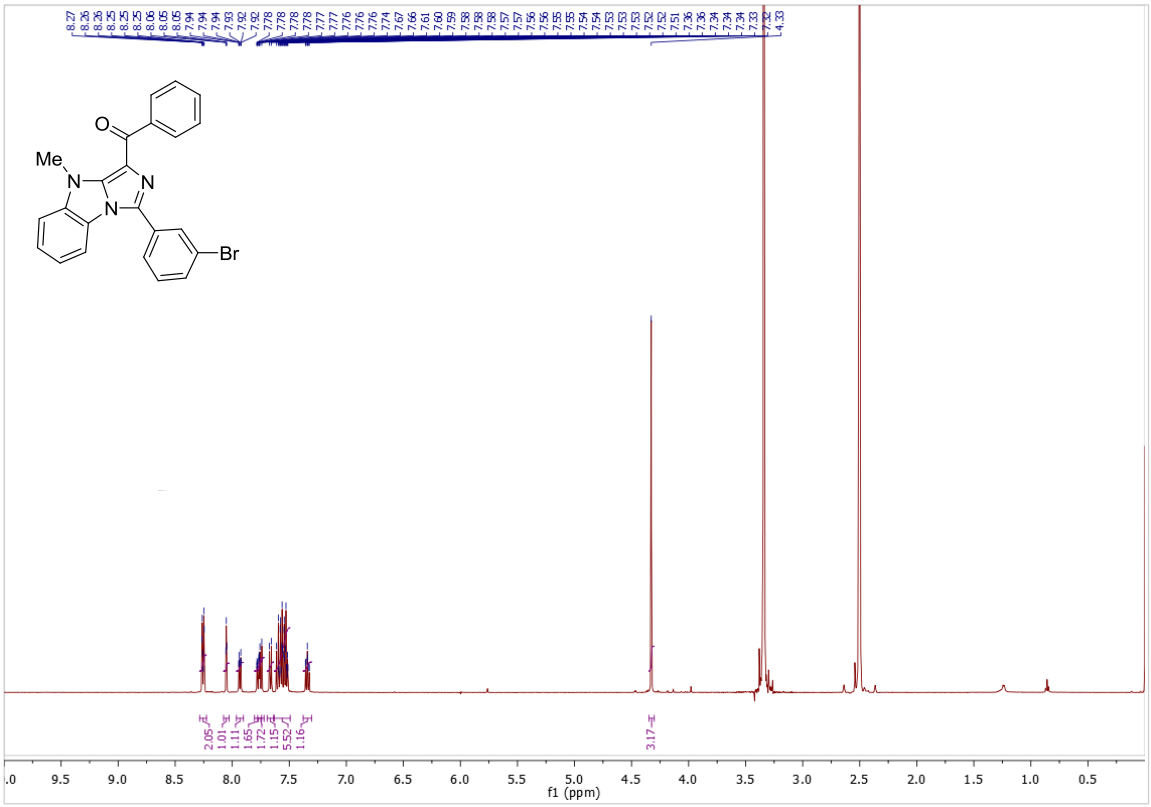

165.46
163.36
155.57
144.30
138.73
129.25
122.36
117.88
62.26
49.24
38.96
14.28
O
OEt
S
N
N
N
N
Me
f1 (ppm)

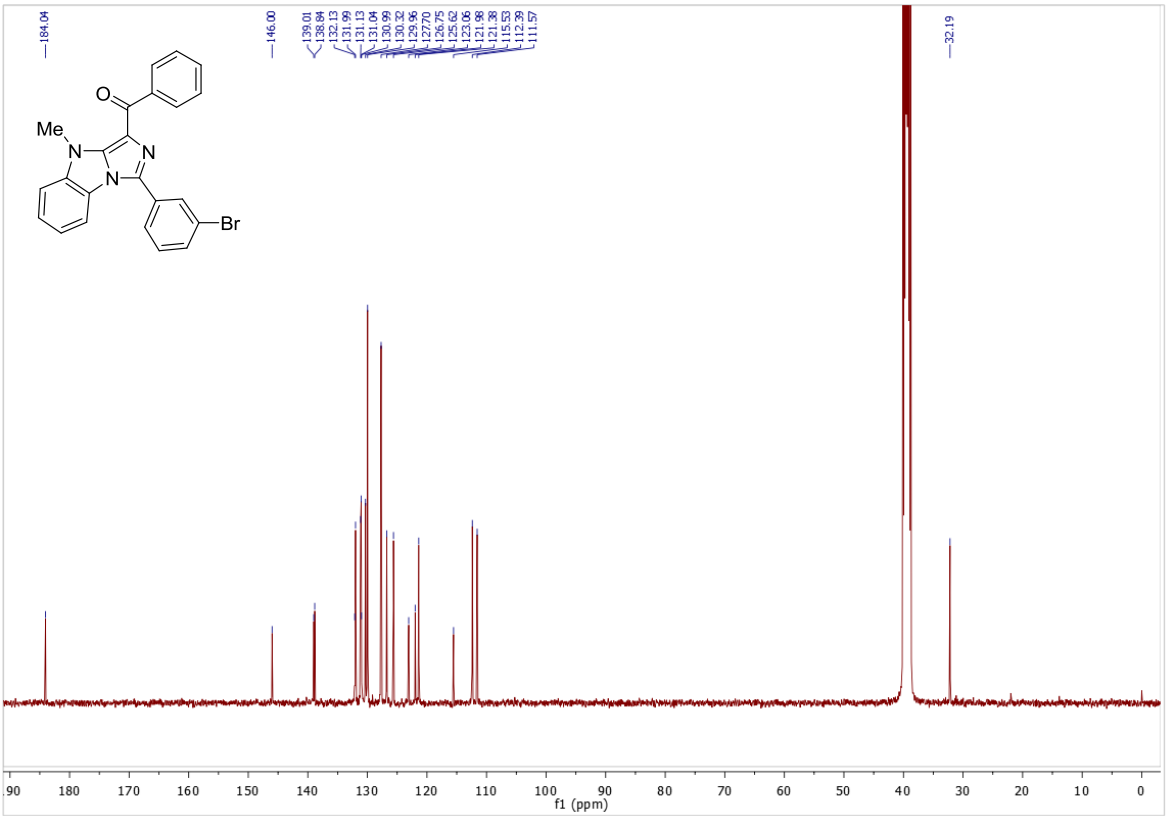
Compound *6*


D (s)
7.11
B (m)
7.43
A (m)
7.54
C (m)
7.29
E (d)
4.88
F (m)
3.67
H (m)
3.16
I (s)
2.98
J (s)
2.85
f1 (ppm)

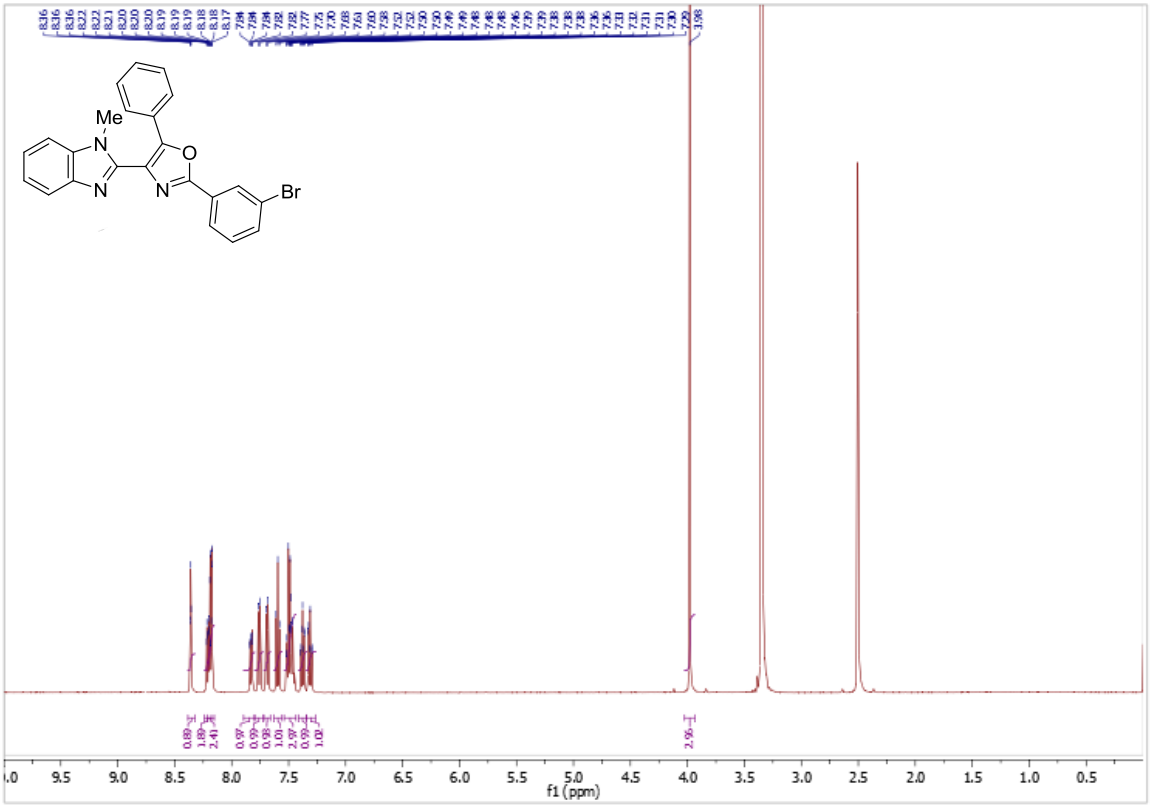

169.21
169.02
159.08
142.97
130.62
130.30
129.61
127.02
121.55
56.98
49.97
36.51
35.42
f1 (ppm)

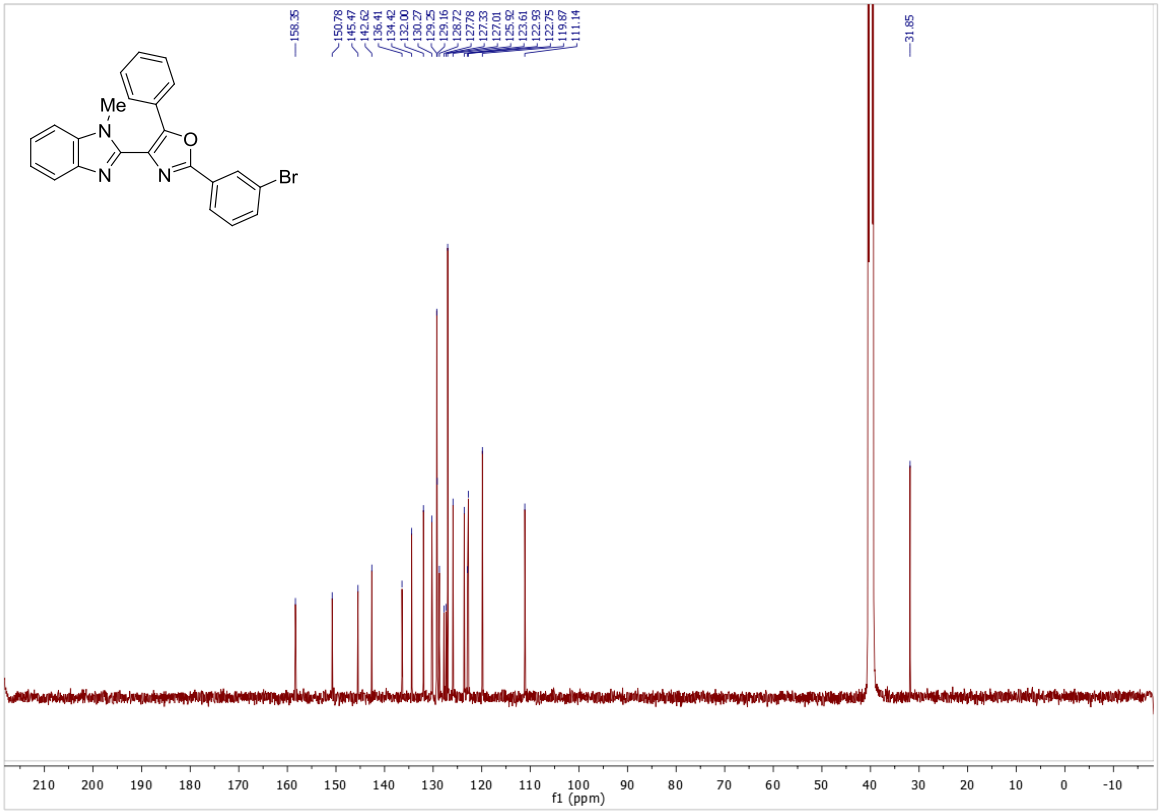
Compound *4u*


O
Me
N
N
N
Br
f1 (ppm)

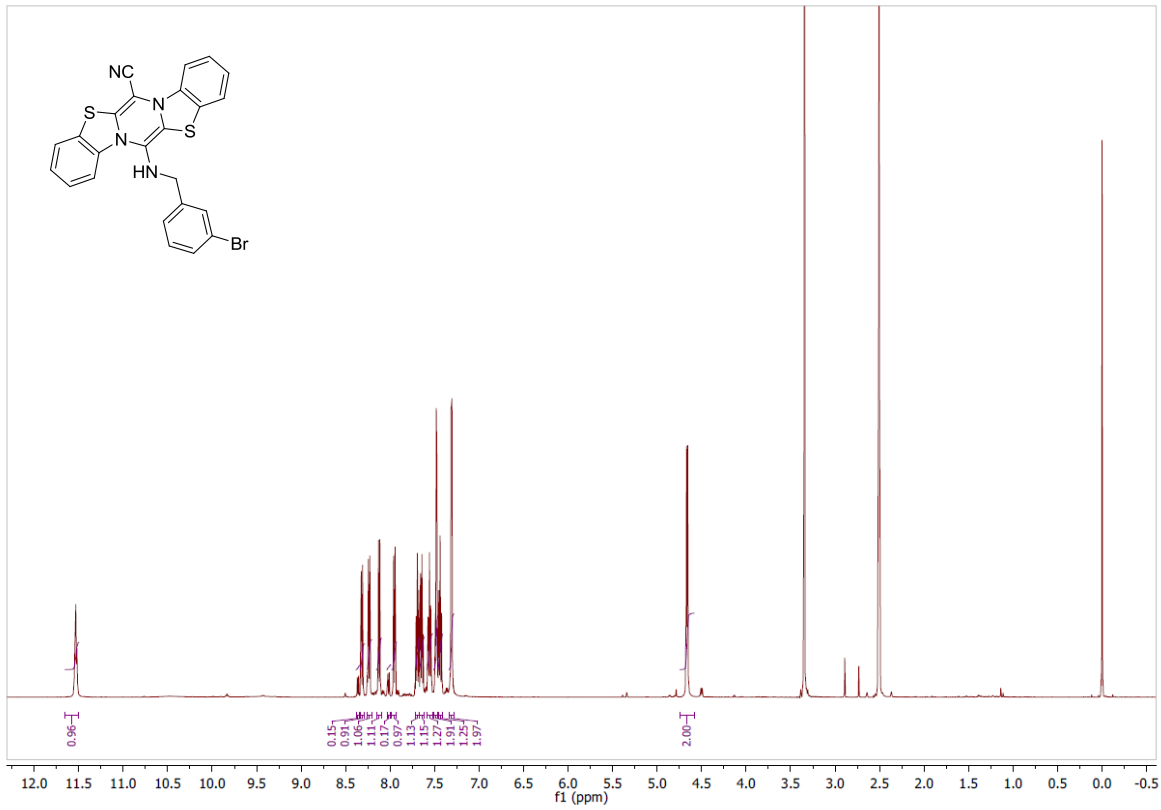

184.04
146.00
139.01
138.84
132.13
131.99
131.13
131.04
130.99
130.32
129.96
127.70
126.75
125.62
123.06
121.38
121.38
115.53
115.29
111.57
32.19
O
Me
N
N
N
Br
f1 (ppm)

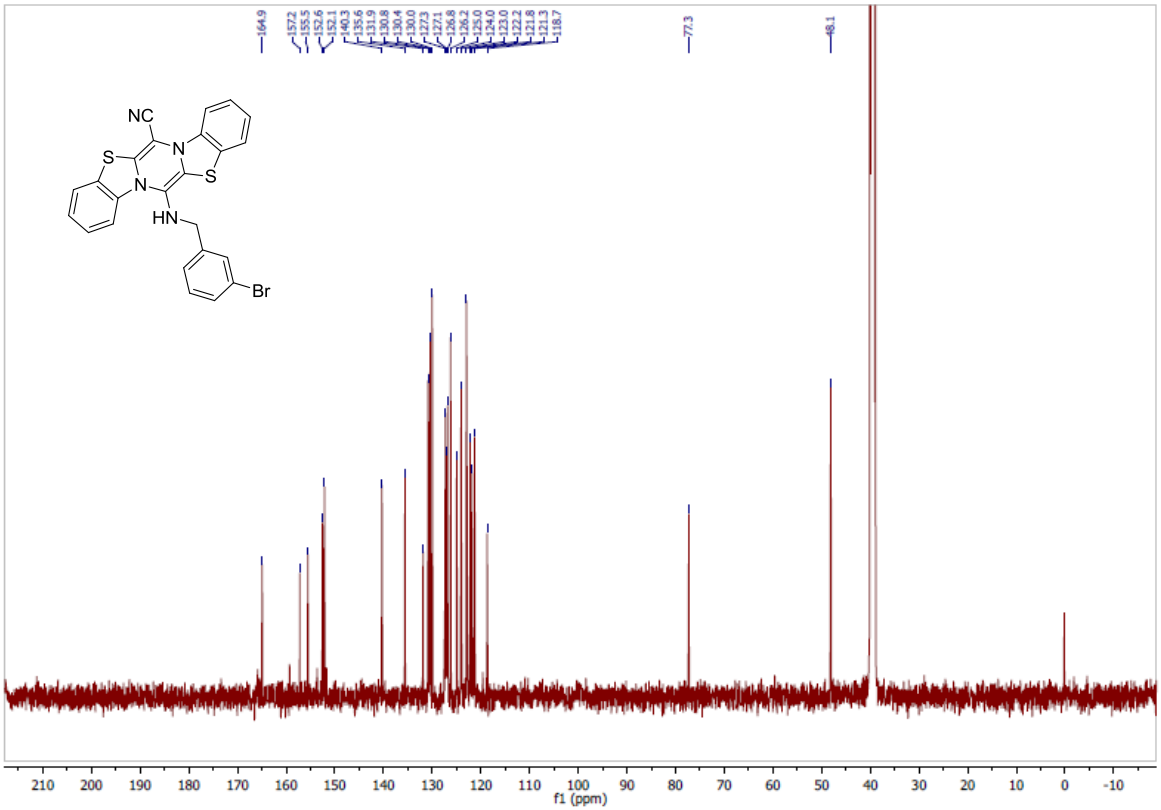
Compound *7*


Me
N
N
O
N
Br
f1 (ppm)


158.35
150.78
145.47
142.62
136.41
134.42
132.00
130.27
129.25
129.16
128.72
127.78
127.33
127.01
125.92
123.61
122.93
122.75
119.87
111.14
31.85
Me
N
N
O
N
Br
f1 (ppm)

Compound *8*


NC
S
N
N
S
HN
Br
0.96
0.15
0.91
1.06
1.11
0.17
0.97
1.13
1.15
1.27
1.91
1.25
1.97
2.00
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)


164.9
157.2
155.5
152.6
152.1
140.3
135.6
131.9
130.8
130.4
130.0
127.3
127.1
126.8
126.2
125.0
124.0
123.0
122.2
121.8
121.3
118.7
77.3
48.1
NC
S
N
N
S
HN
Br
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)