Supporting information

Chemoselective cyclization of N-sulfonyl ketimines with ethenesulfonyl fluorides: access to trans-cyclopropanes and fused-dihydropyrroles

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Crystallographic data: Single crystal X-ray structural of compound **3ea** was collected at 150(2) K using graphite monochromated Mo Kα radiation (λα = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structure was solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on *F2*. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2*Ueq* of their parent atoms. The crystal data are summarized in Table S1. The **CCDC** number of compound **3ea** (1881253**)** can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre,12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

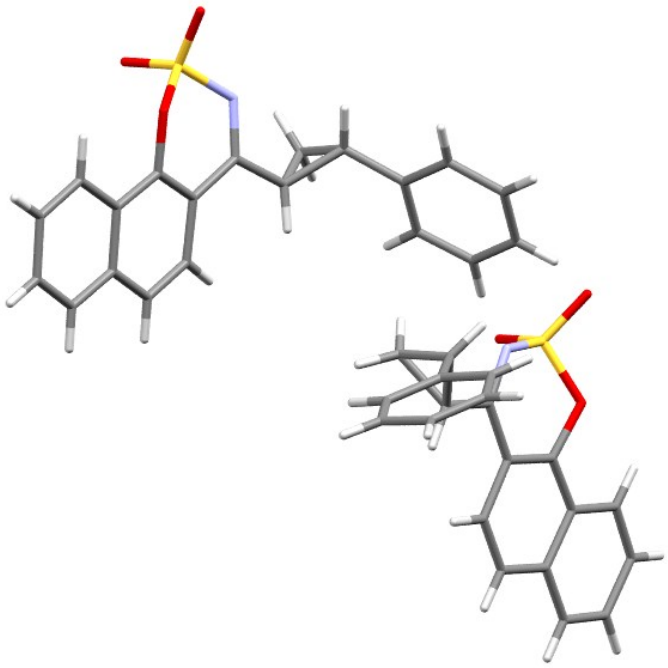


Figure S1. ORTEP diagram of compound **3ea (CCDC 1881253),** thermal ellipsoids drawn at the 50% probability level.

Table S1. Crystal data for compound 3ea.

Compound	**3ea**
Empirical formula	C40 H30 N2 O6 S2
Formula weight	698.78
Temperatute	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Triclinic, P -1
a (Å) *b* (Å)	a = 8.4665(8) A b = 9.9099(8) A

c (Å) *α* (°) *β* (°) *γ* (°)	c = 20.0858(16) A alpha = 94.466(7) deg. beta = 93.734(7) deg. gamma = 95.165(7) deg.
Volume (Å^3)	1668.9(2) A^3
Z, Calculated density (mg/m^3)	2, 1.391 Mg/m^3
Absorption coefficient (mm^{-1})	0.213 mm^-1
F(000)	728
Crystal size (mm)	0.320 x 0.260 x 0.210 mm
Θ range (deg)	3.027 to 28.833 deg.
Limiting indices	-11<=h<=11, -13<=k<=12, -26<=l<=27
Reflections collected / unique	15475 / 7546 [R(int) = 0.0545]
Completeness to Θ = 25.242	99.9 %
Max. and min. transmission	1.00000 and 0.64701
Absorption correction	Semi-empirical from equivalents
Data / restrains / parameters	7546 / 0 / 451
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0664, wR2 = 0.1426
R indices (all data)	R1 = 0.1371, wR2 = 0.1849
Extinction coefficient	n/a
Largest diff. peak and hole (e.A^{-3})	0.231 and -0.361 e.A^-3
CCDC	**1881253**

Crystallographic data: The crystal data are summarized in Table S2. The **CCDC** number of compound **3aj** (**1881255)** can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

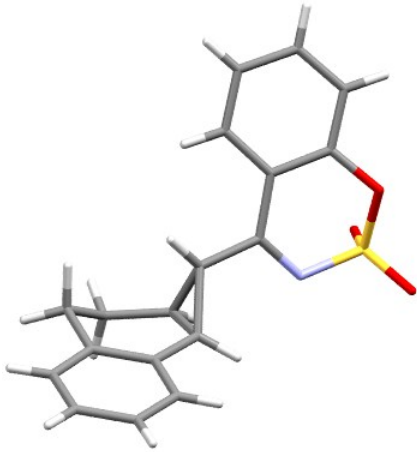


Figure S2. ORTEP diagram of 3aj, thermal ellipsoids drawn at the 50% probability level.

Table S2. Crystal data for compound 3aj.

Compound	**3aj**
Empirical formula	C18 H15 N O3 S
Formula weight	325.37
Temperatute	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
a (Å) *b* (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	a = 13.1858(4) A b = 8.0088(2) A c = 15.5088(4) A alpha = 90 deg. beta = 107.498(3) deg. gamma = 90 deg.
Volume ($Å^3$)	1561.98(8) A^3
Z, Calculated density (mg/m^3)	4, 1.384 Mg/m^3
Absorption coefficient (mm^{-1})	0.222 mm^-1
F(000)	680
Crystal size (mm)	0.230 x 0.180 x 0.130 m
Θ range (deg)	2.892 to 28.935 deg.
Limiting indices	-16<=h<=17, -9<=k<=10, -20<=l<=20
Reflections collected / unique	14747 / 3730 [R(int) = 0.0557]
Completeness to Θ = 25.242	99.9%
Max. and min. transmission	Semi-empirical from equivalents
Absorption correction	1.00000 and 0.89606
Data / restrains / parameters	3730 / 0 / 208
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0576, wR2 = 0.1391
R indices (all data)	R1 = 0.0955, wR2 = 0.1623
Extinction coefficient	n/a
Largest diff. peak and hole ($e.A^{-3}$)	0.203 and -0.413 e.A^-3
CCDC	**1881255**

Crystallographic data: The crystal data are summarized in Table S3. The **CCDC** number of compound **4aa** (**1881254)** can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

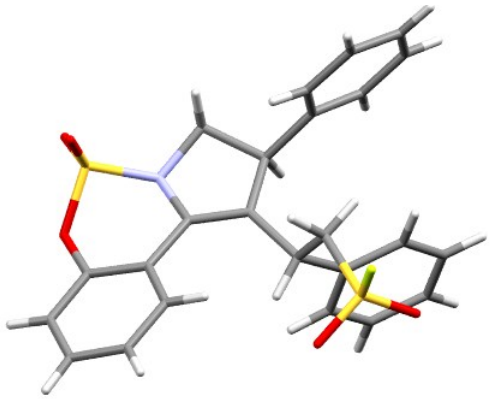
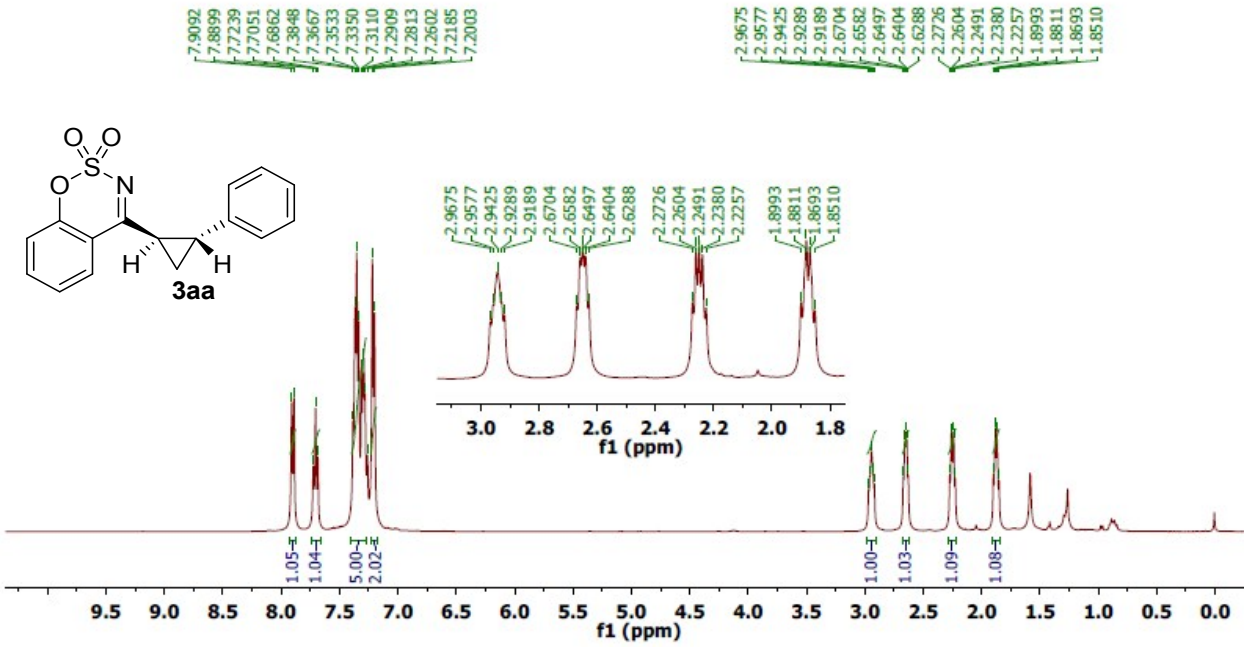


Figure **S3**. ORTEP diagram of **4aa**, thermal ellipsoids drawn at the 50% probability level.

Table **S3.** Crystal data of **4aa.**

Compound	**4aa**
Empirical formula	C24 H20 F N O5 S2
Formula weight	485.53
Temperatute	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
a (Å) *b* (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	a = 13.2102(5) A b = 11.1069(3) A c = 15.6812(6) A alpha = 90 deg. beta = 106.801(4) deg. gamma = 90 deg.
Volume ($Å^3$)	2202.60(14) A^3
Z, Calculated density (mg/m^3)	4, 1.464 Mg/m^3
Absorption coefficient (mm^{-1})	0.288 mm^-1
F(000)	1008

Crystal size (mm)	0.330 x 0.260 x 0.180 mm
Θ range (deg)	3.276 to 29.142 deg.
Limiting indices	-16<=h<=14, -14<=k<=14, -20<=l<=20
Reflections collected / unique	17722 / 5225 [R(int) = 0.0512]
Completeness to Θ = 25.242	99.7
Max. and min. transmission	1.00000 and 0.85714
Absorption correction	Semi-empirical from equivalents
Data / restrains / parameters	5225 / 0 / 298
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1392
R indices (all data)	R1 = 0.0758, wR2 = 0.1625
Extinction coefficient	n/a
Largest diff. peak and hole ($e.A^{-3}$)	0.335 and -0.542 e.A^-3
CCDC	1881254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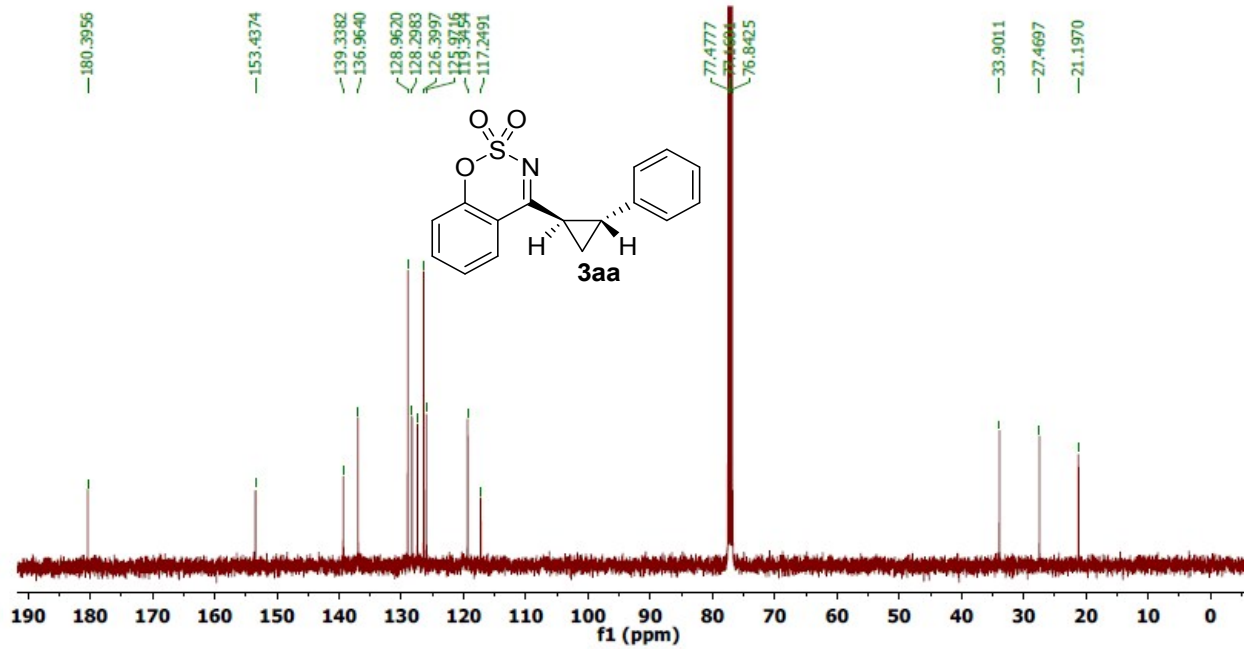
f1 (ppm)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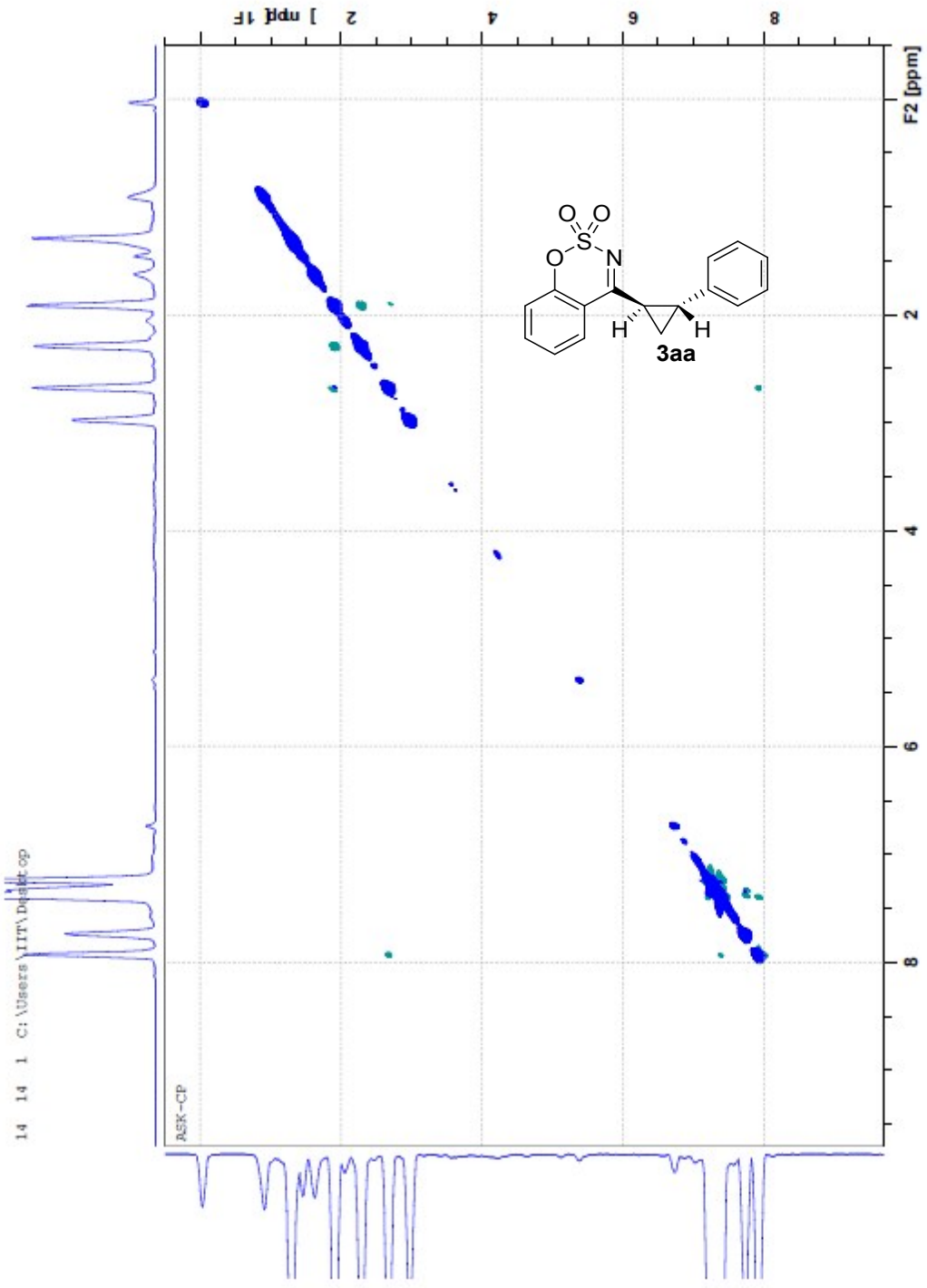
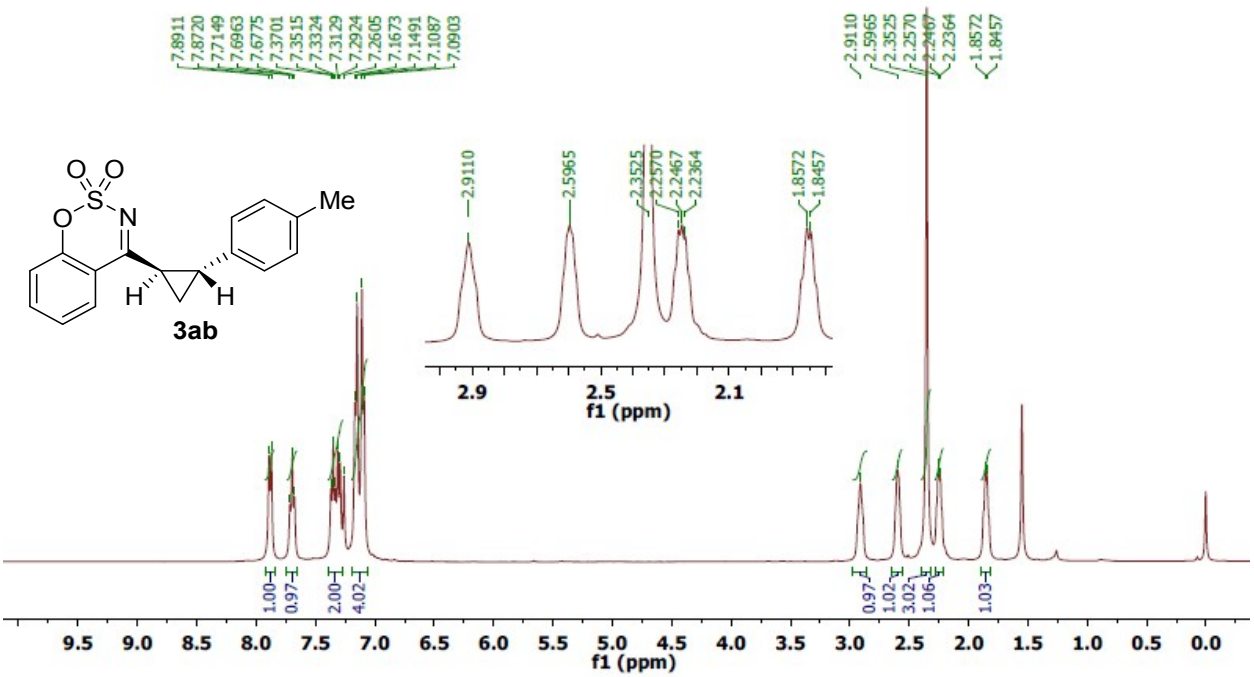
f1 (ppm)

NOESY Experiment

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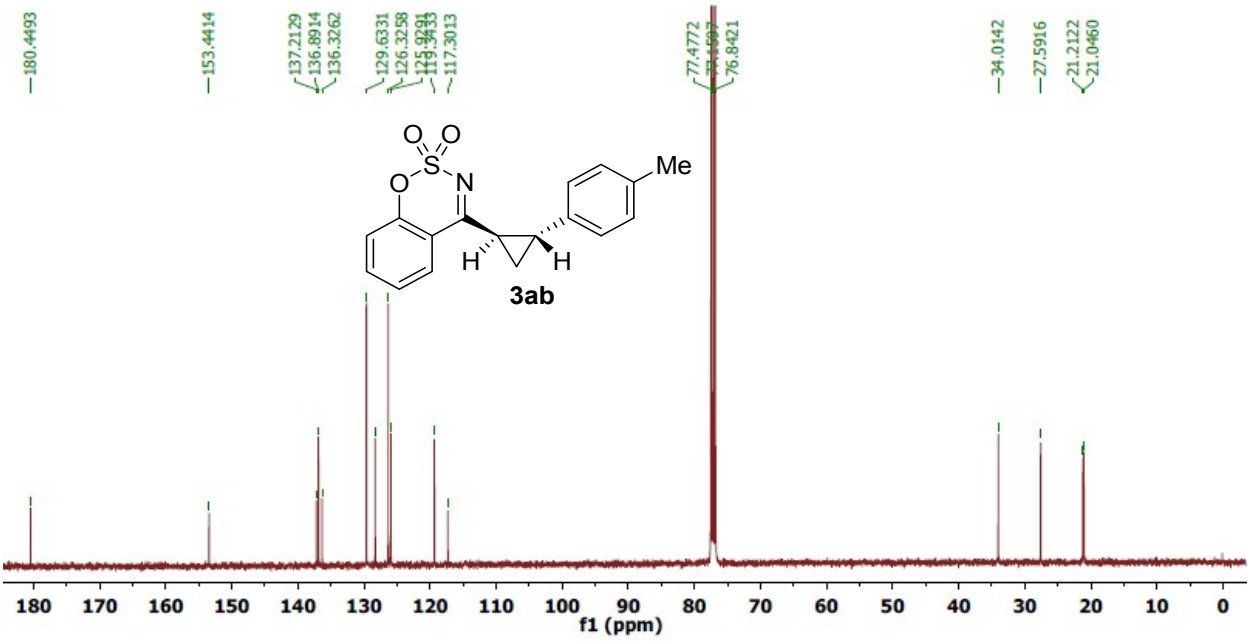
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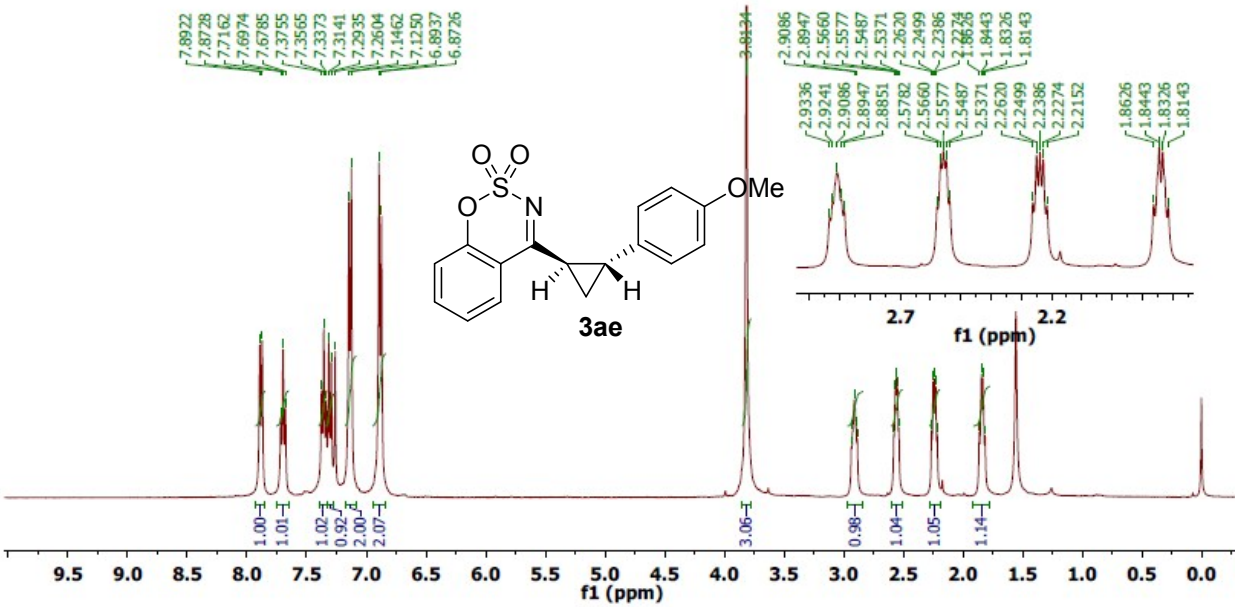
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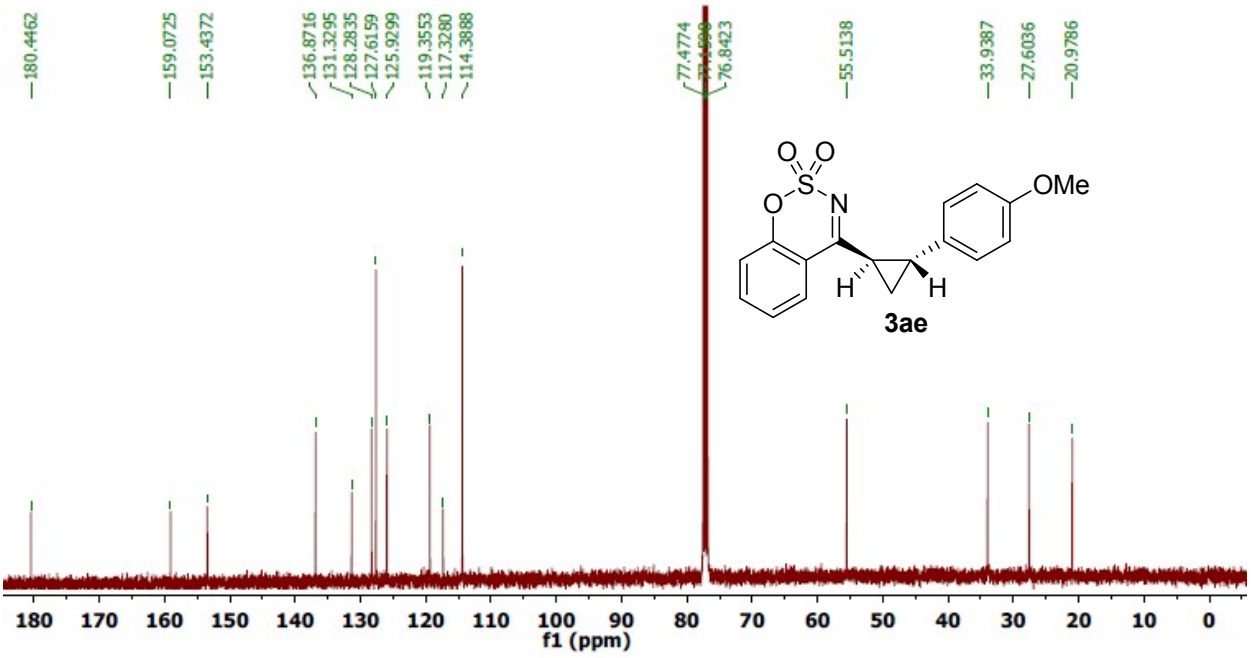
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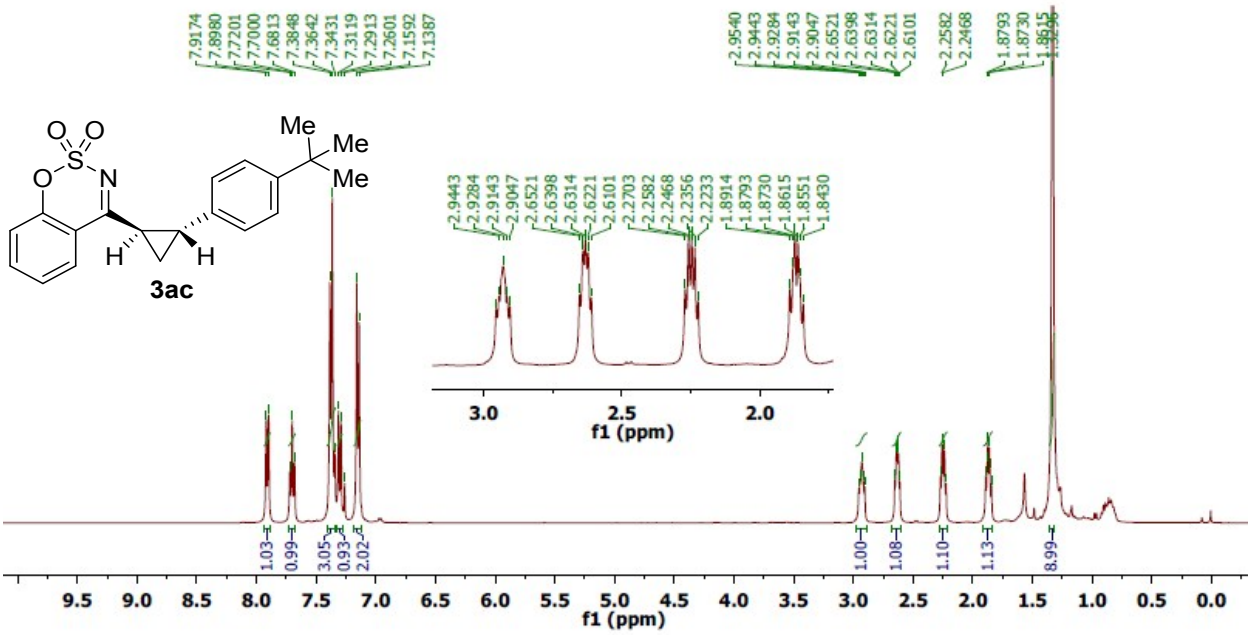
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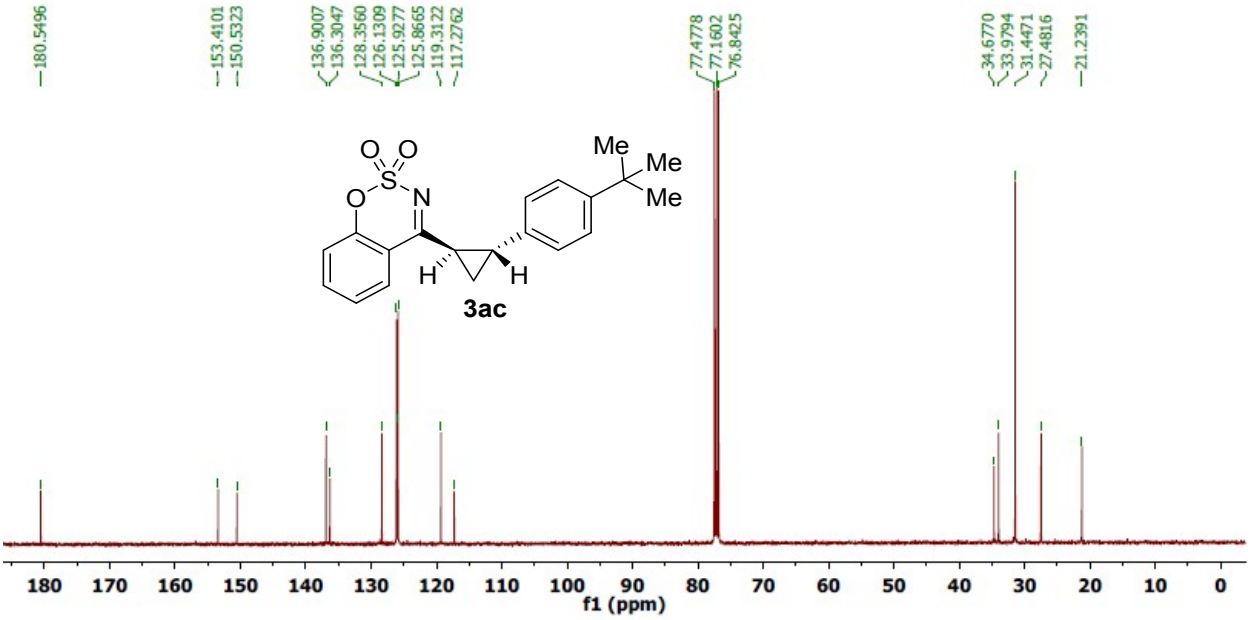
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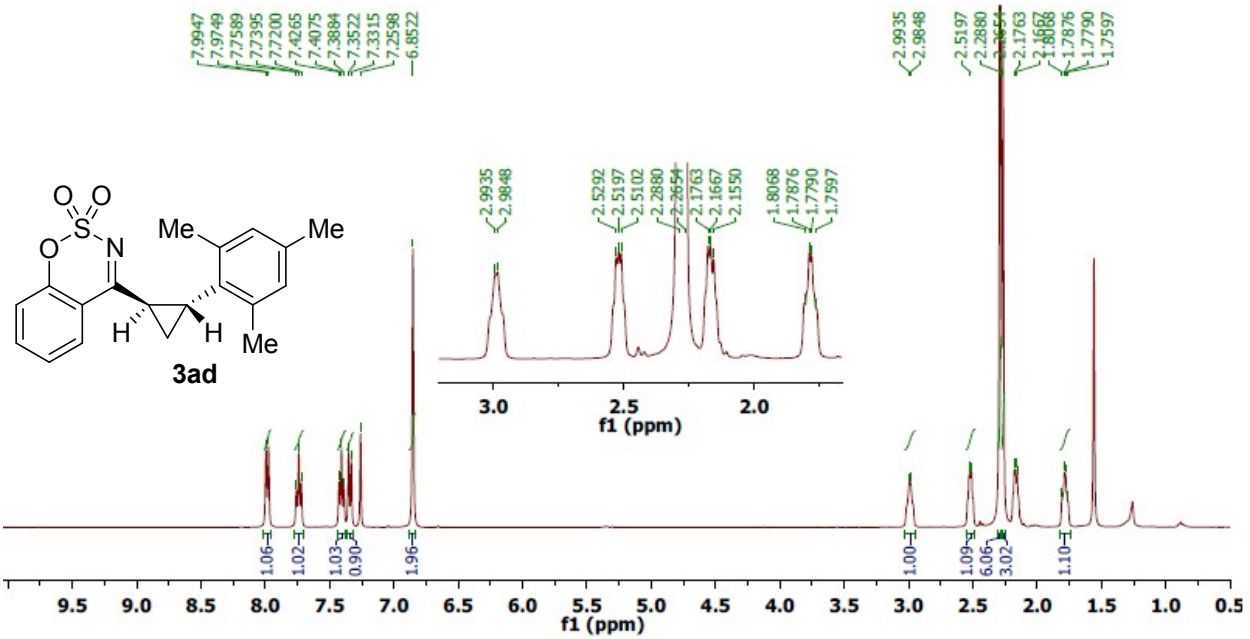
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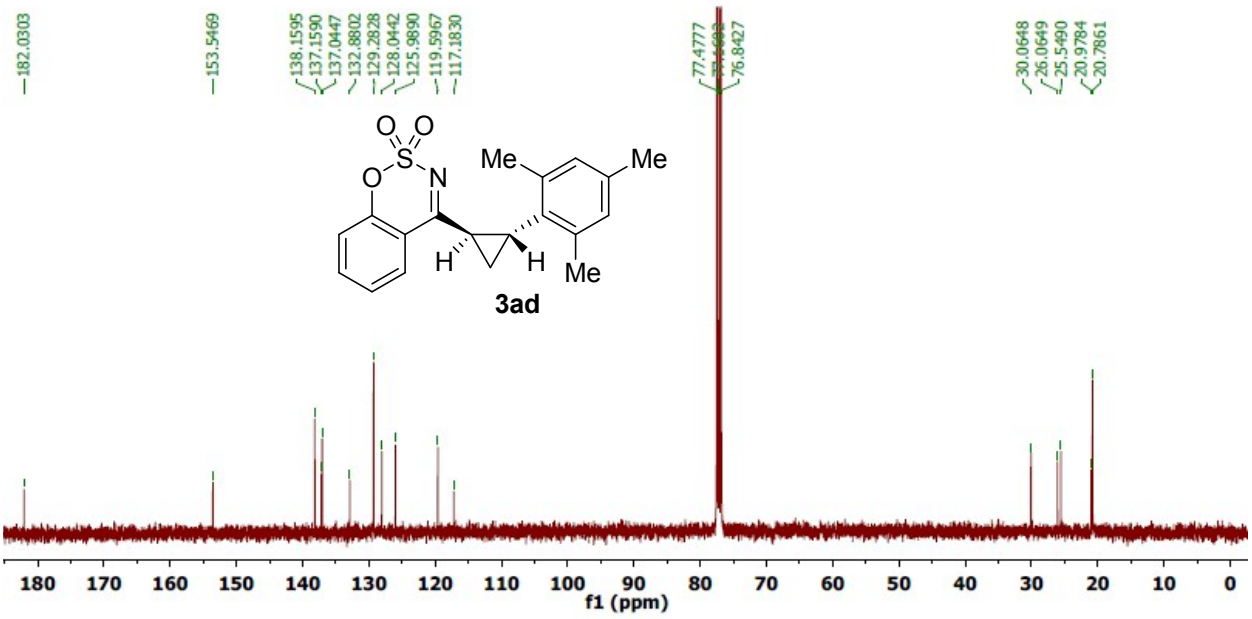
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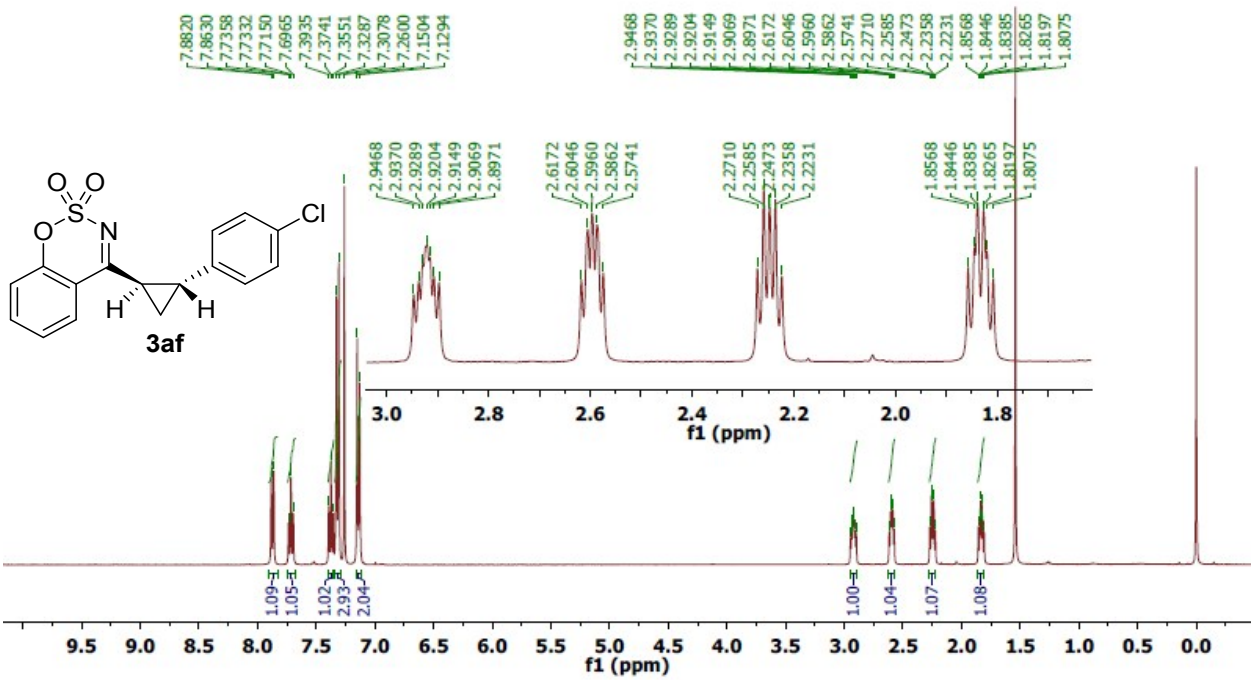
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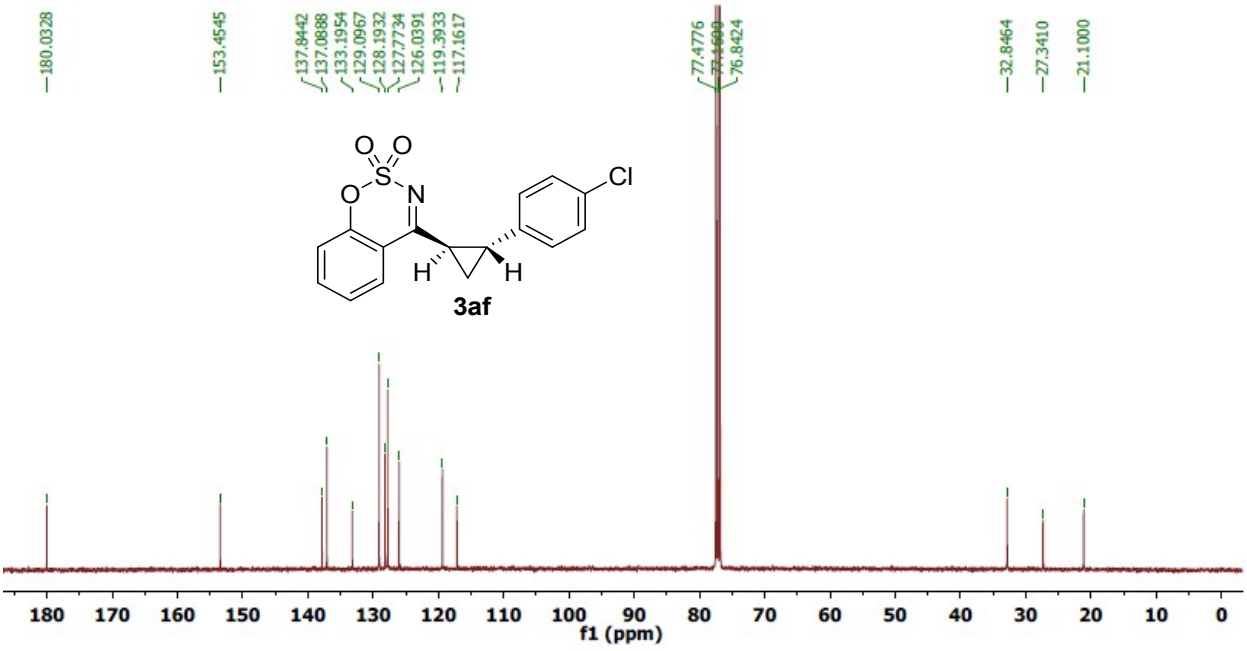
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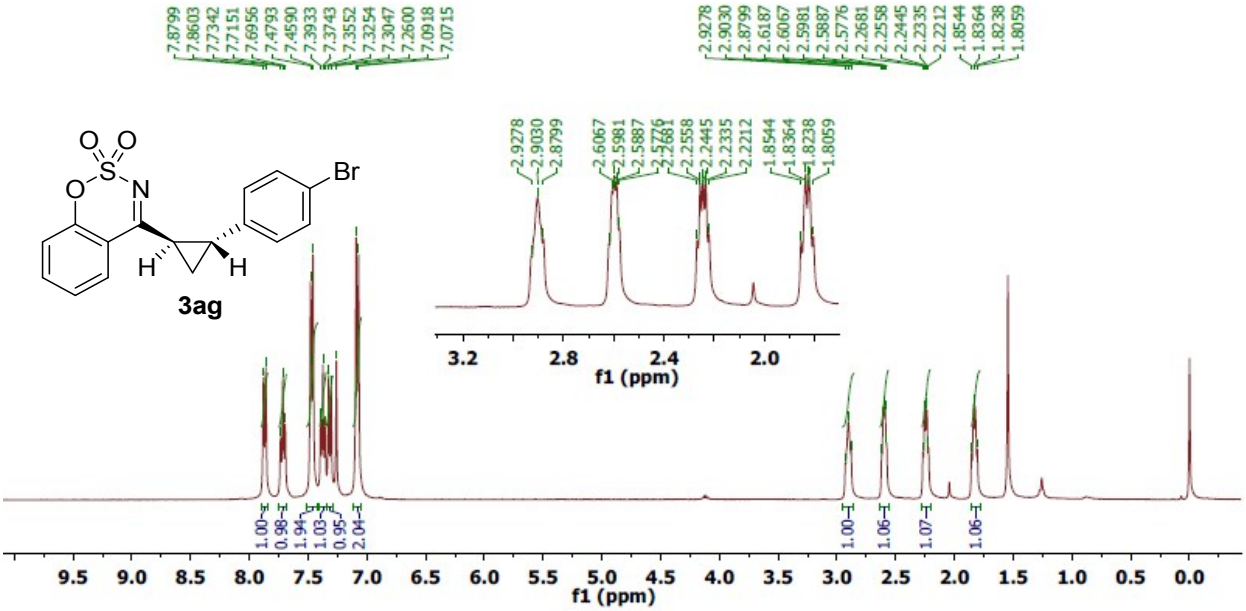
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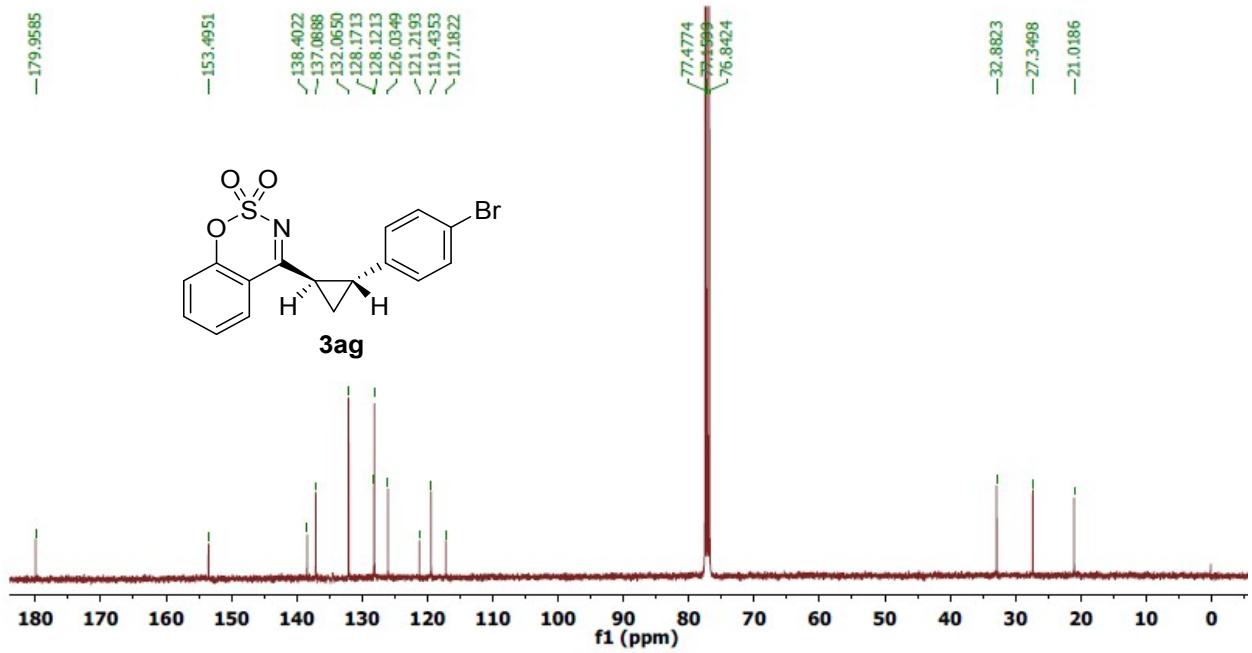
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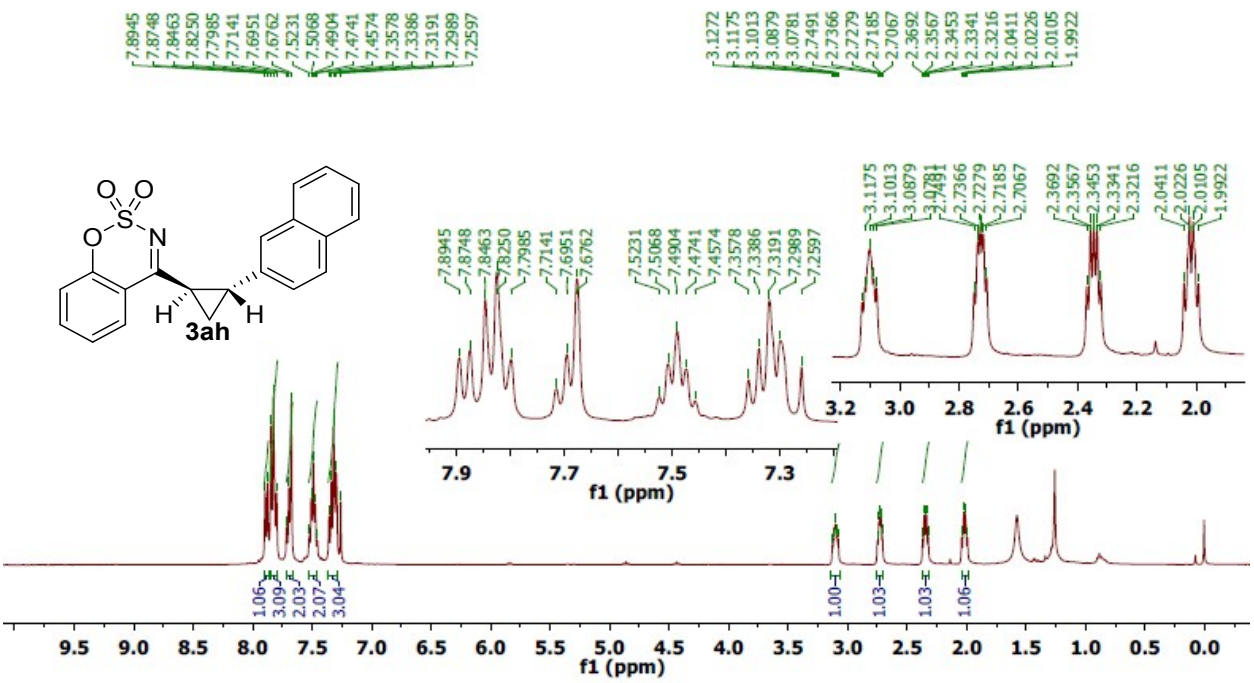
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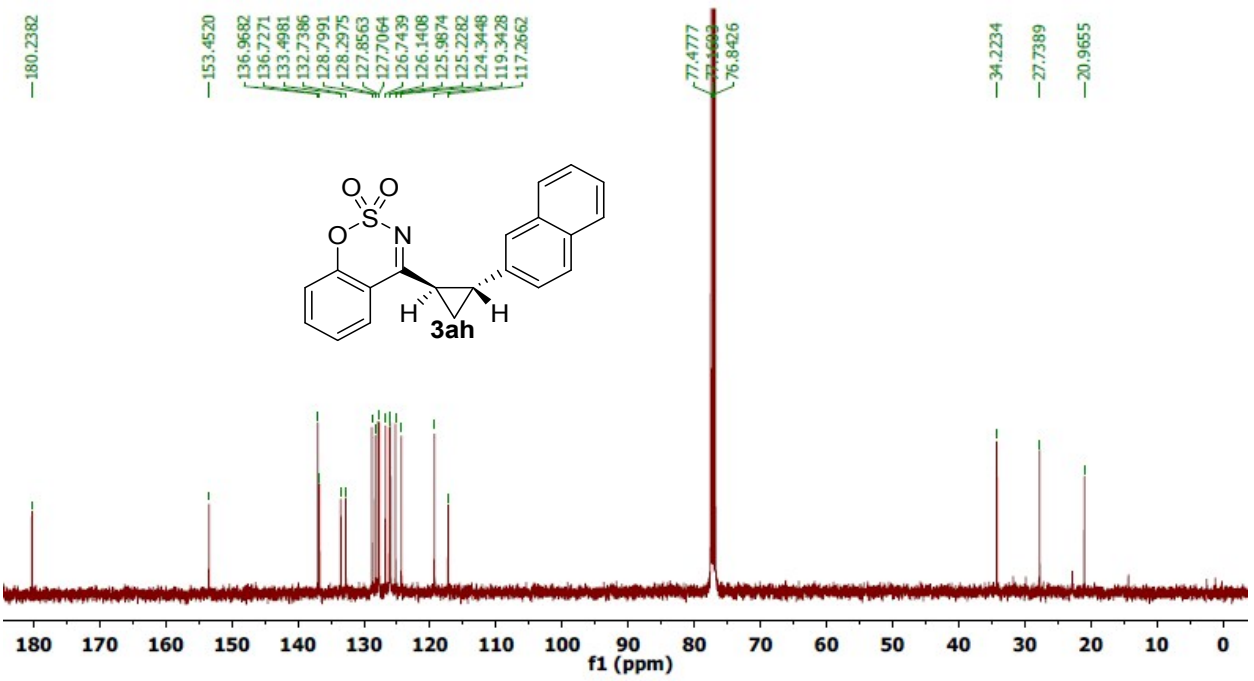
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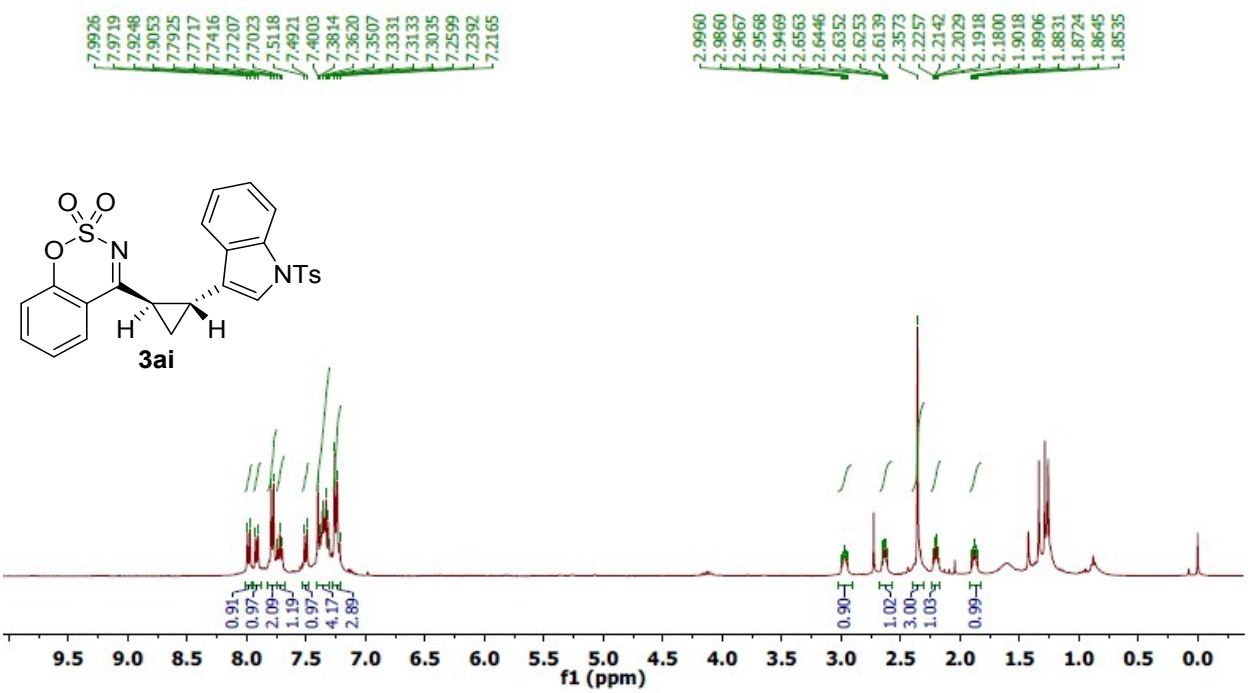
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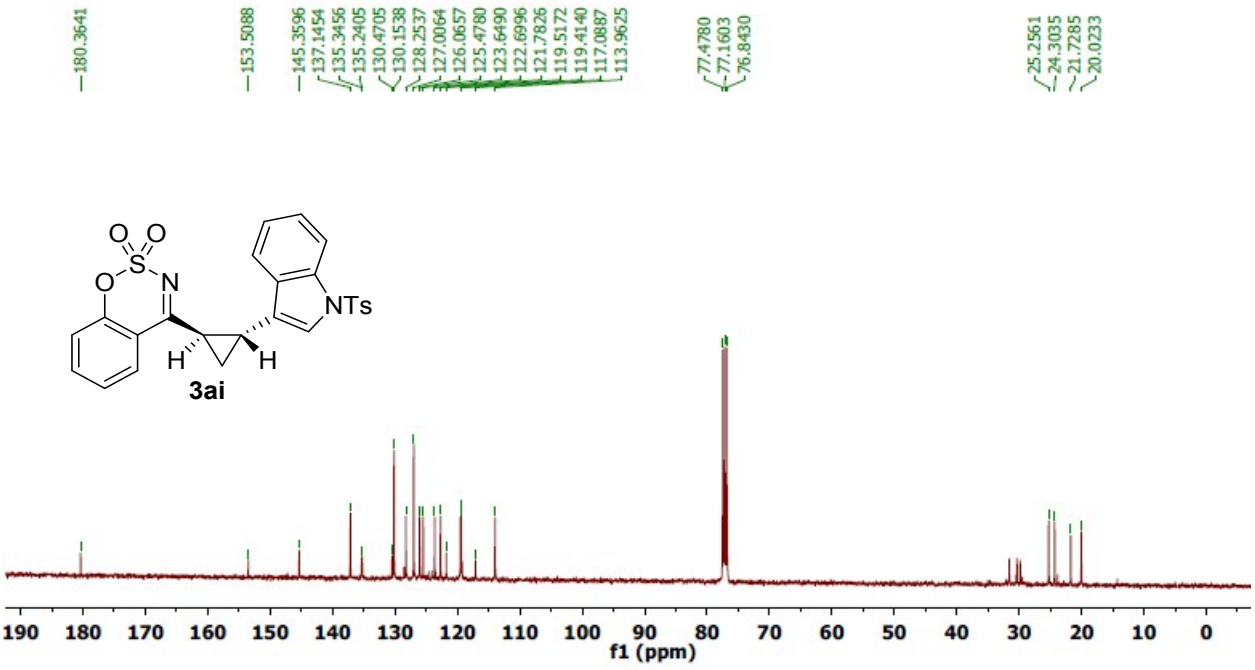
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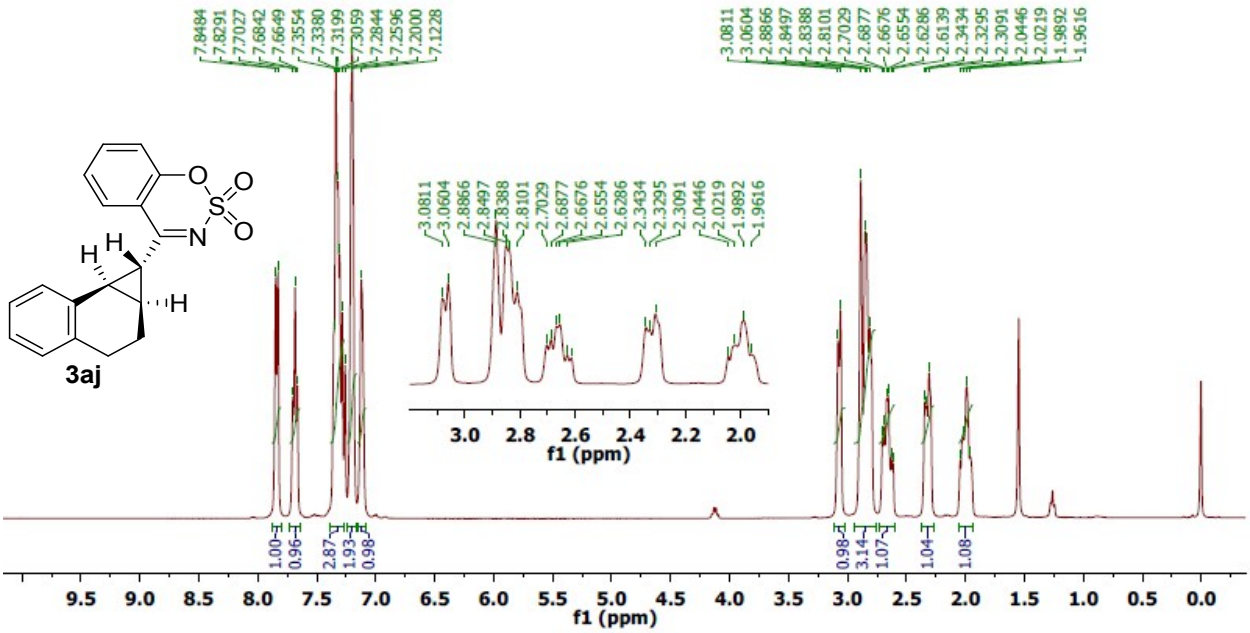
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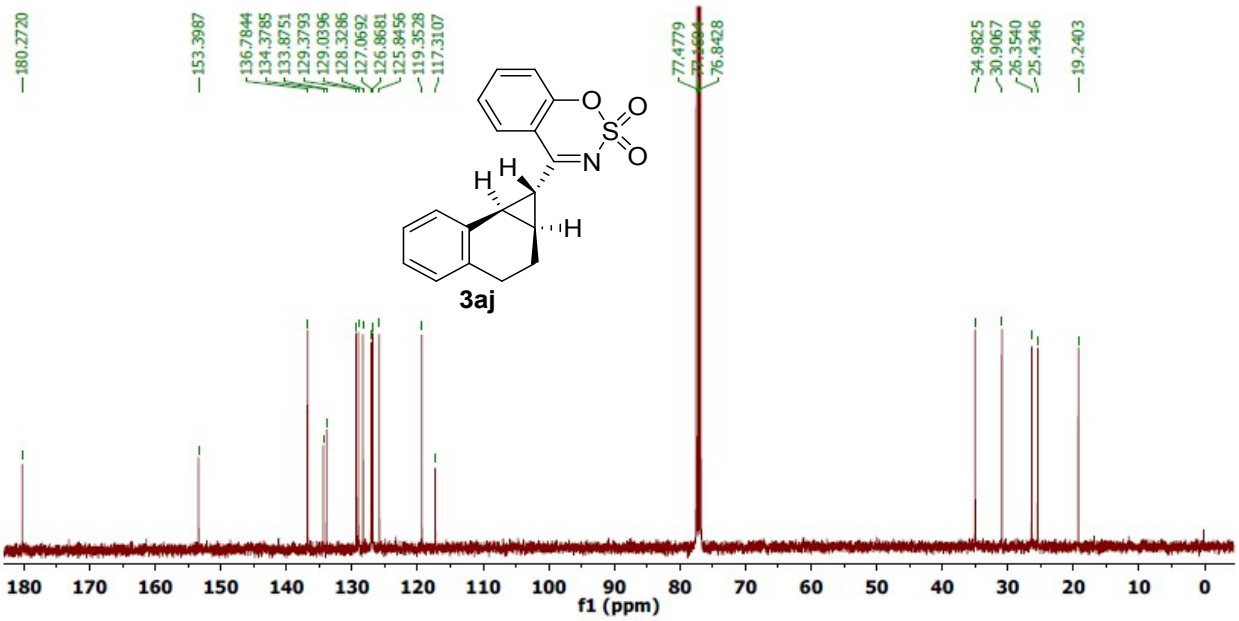
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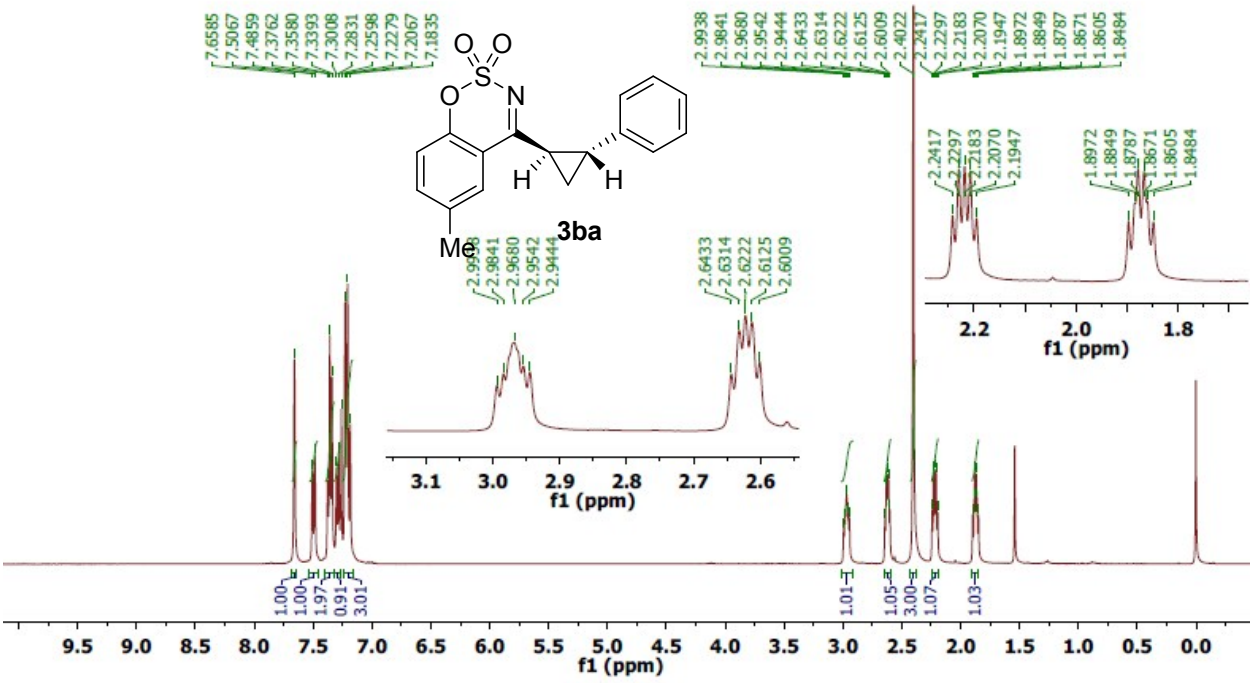
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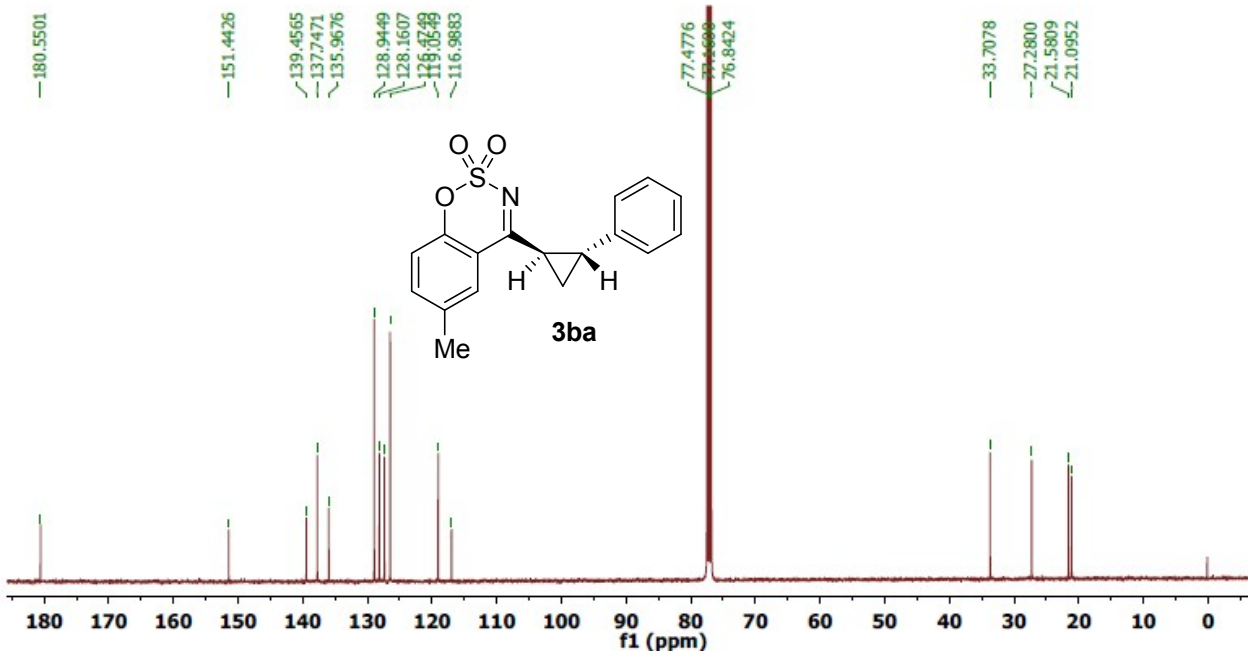
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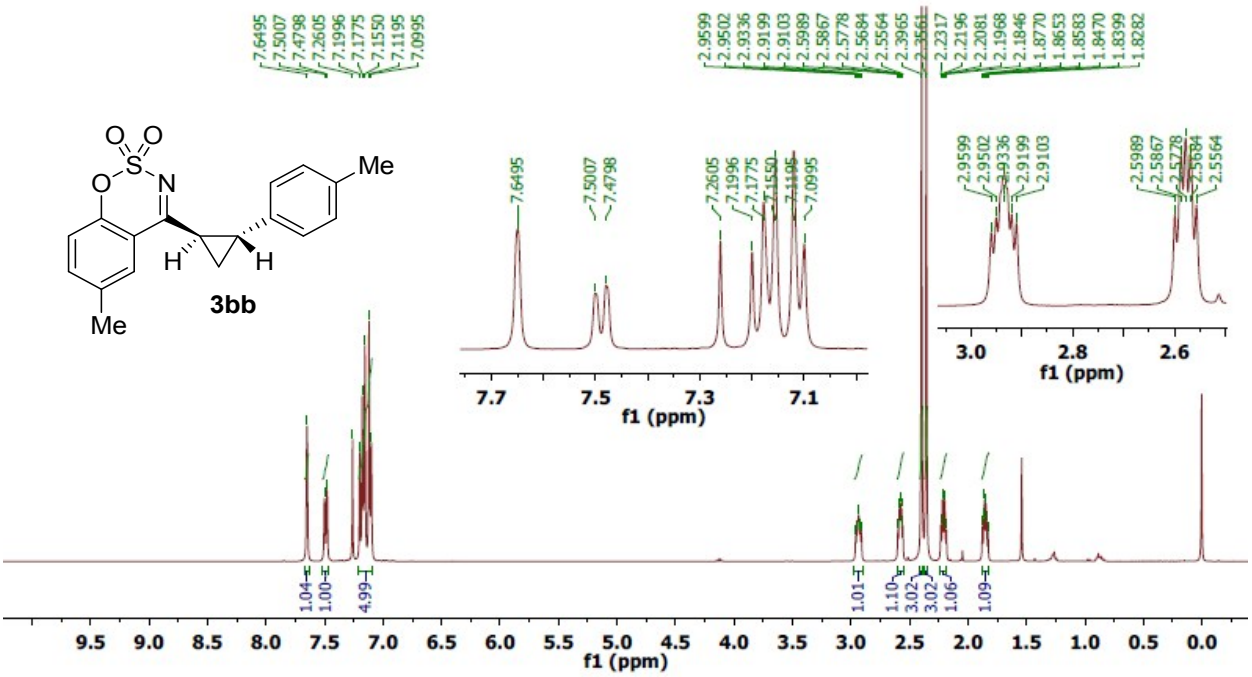
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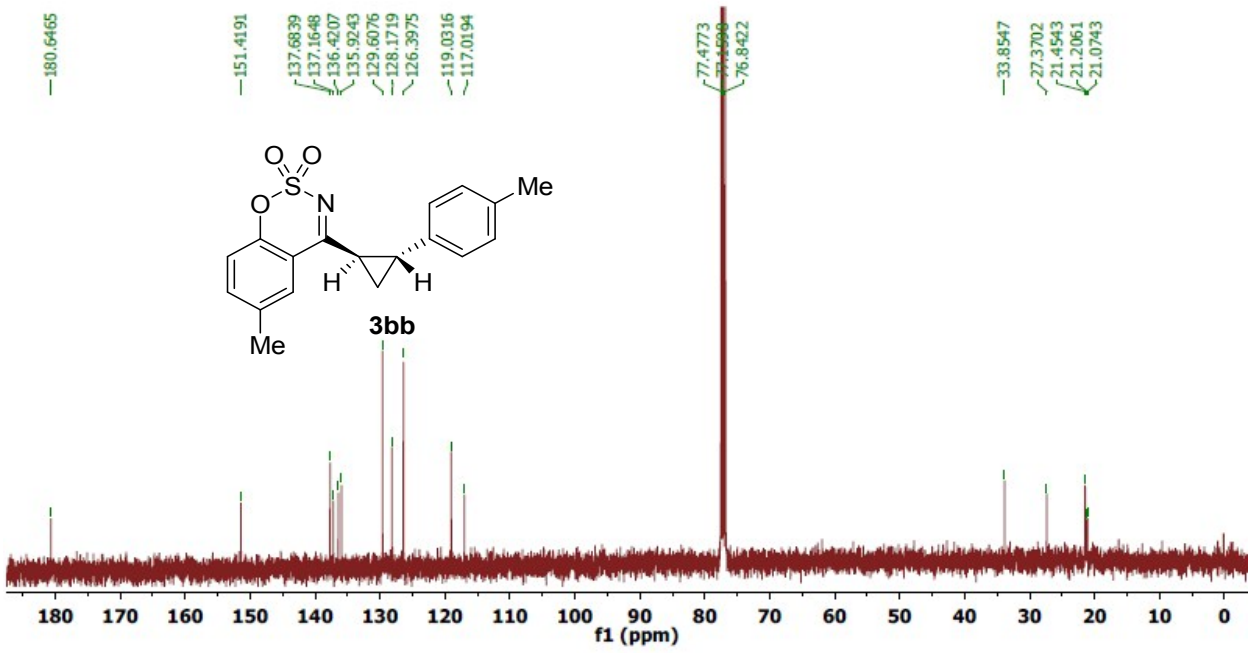
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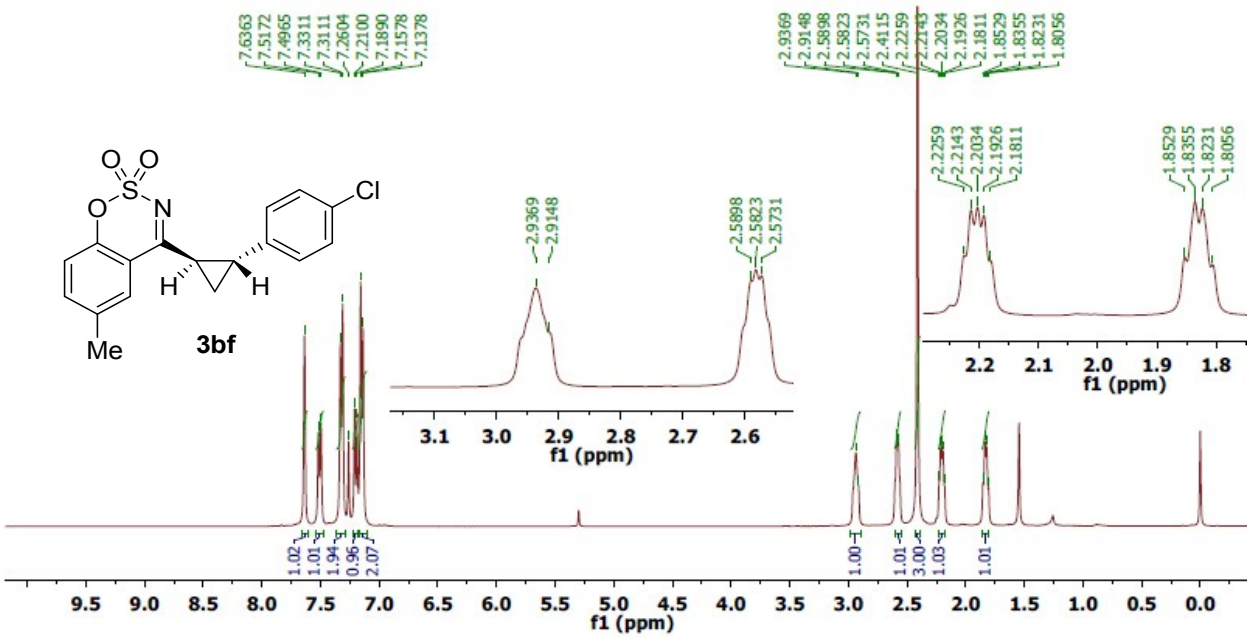
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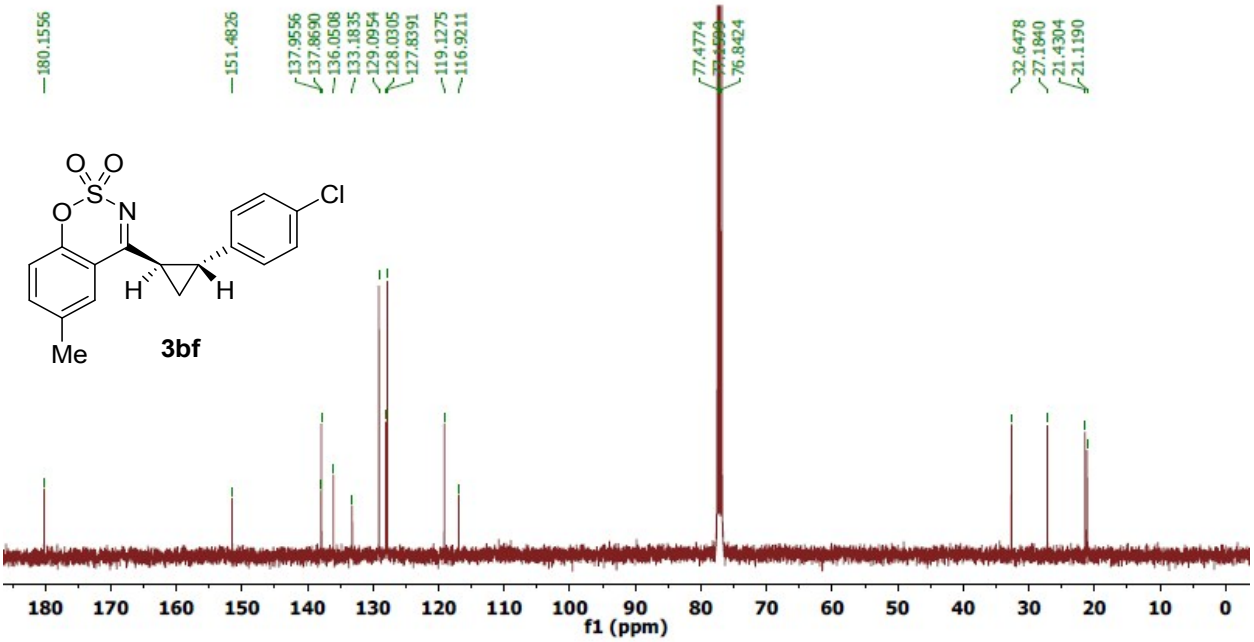
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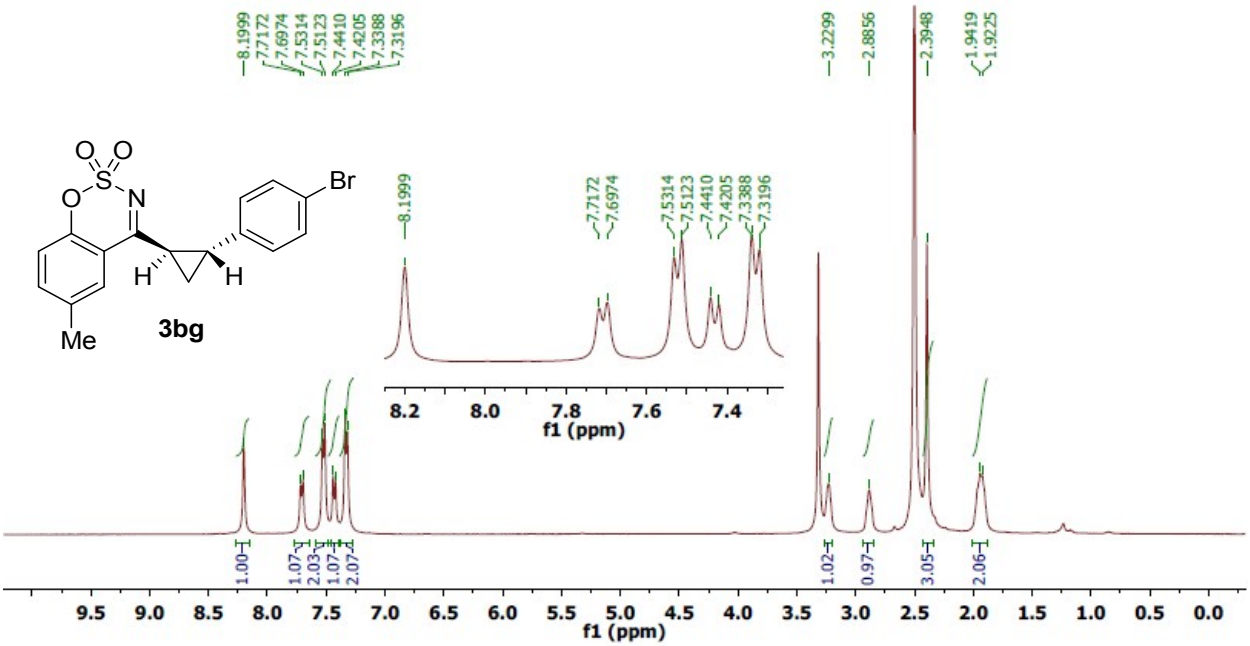
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7.6974
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7.5123
7.4410
7.4205
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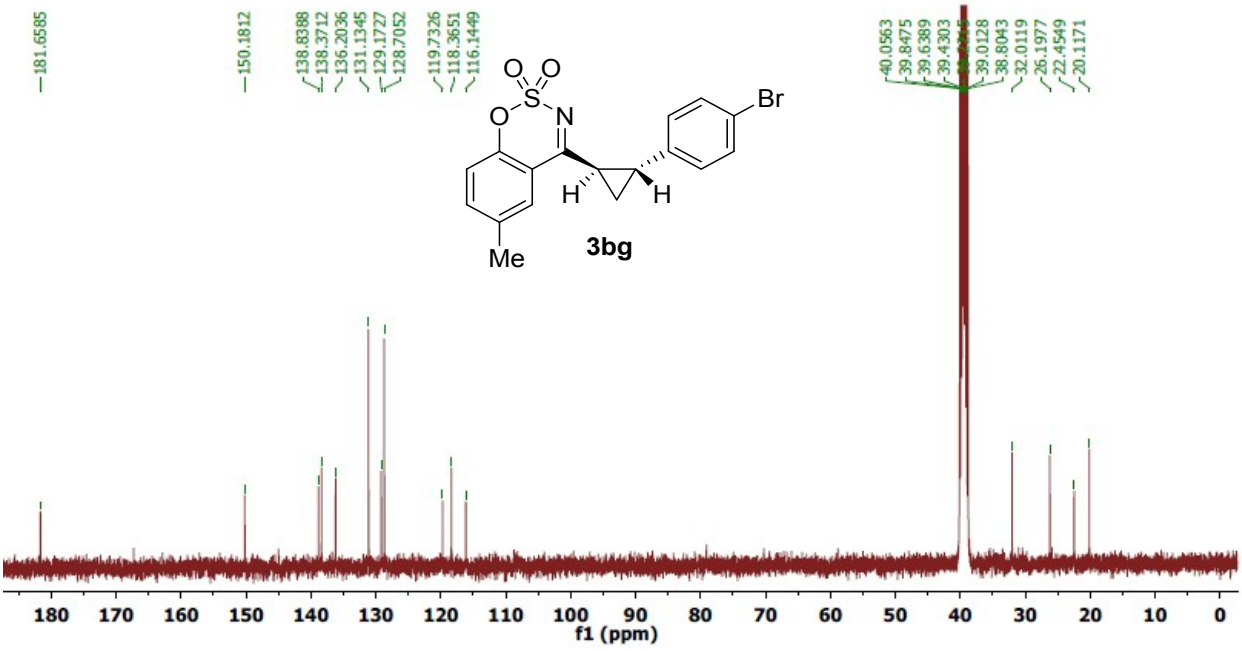
1.9225
Br
Me
3bg
f1 (ppm)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39.8475
39.6389
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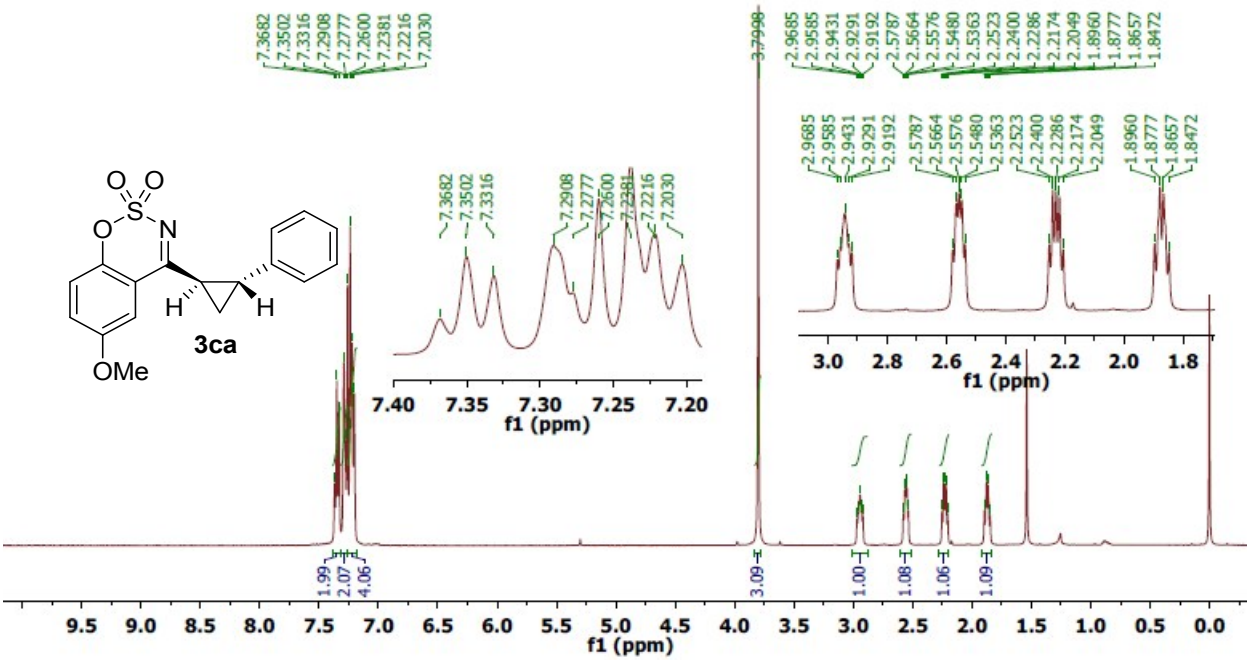
20.1171
Br
Me
3bg
f1 (ppm)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OMe
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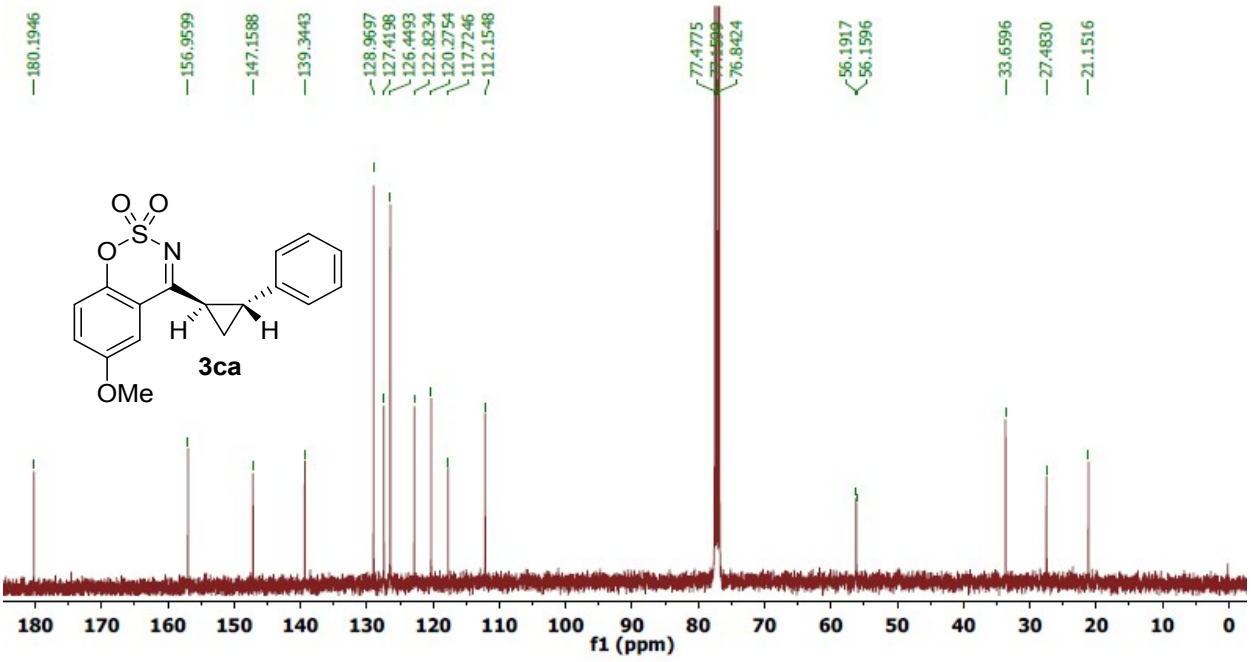
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OMe
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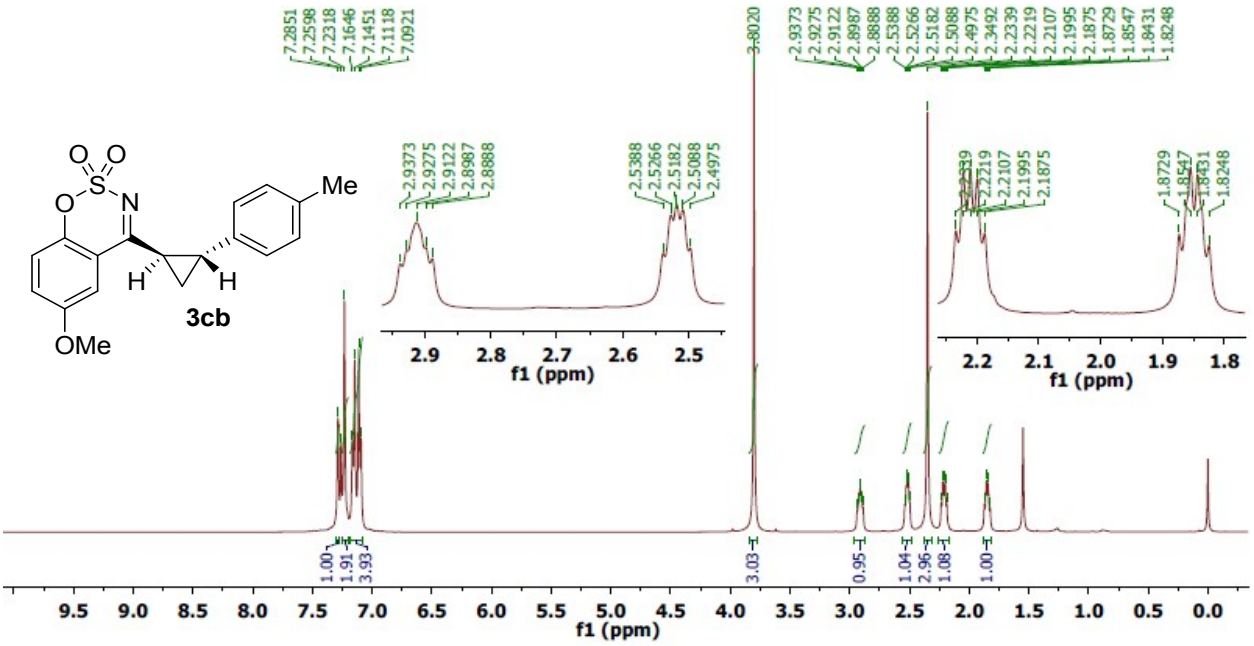
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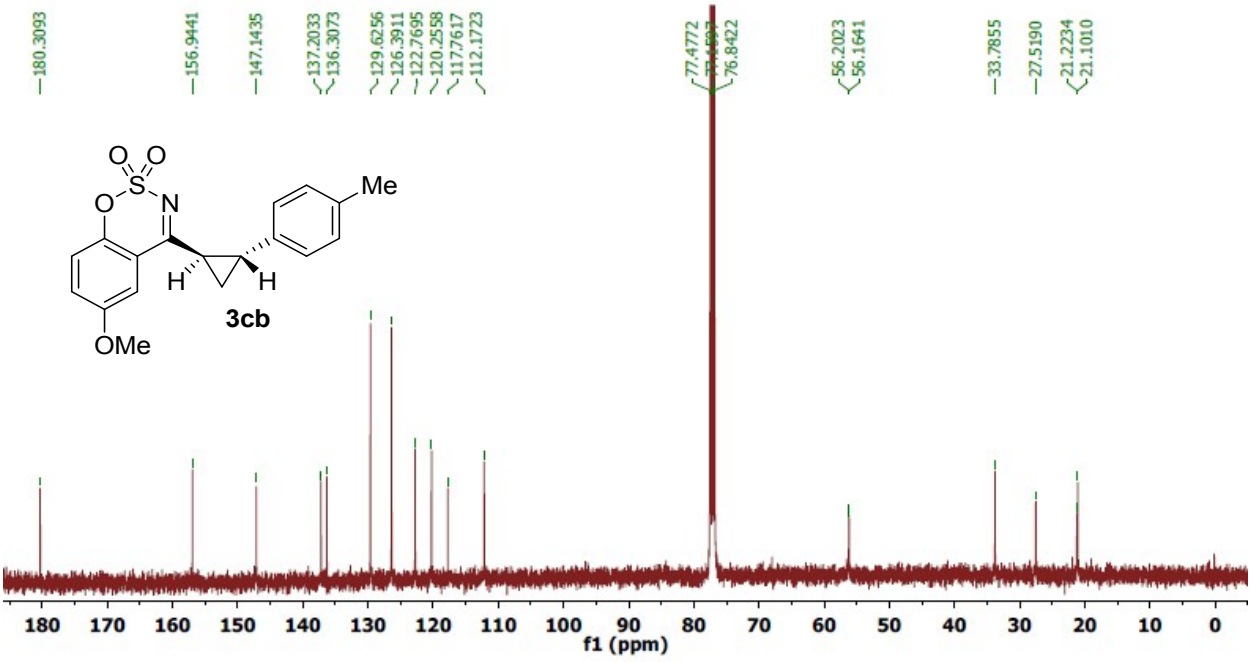
Me
OMe
f1 (ppm)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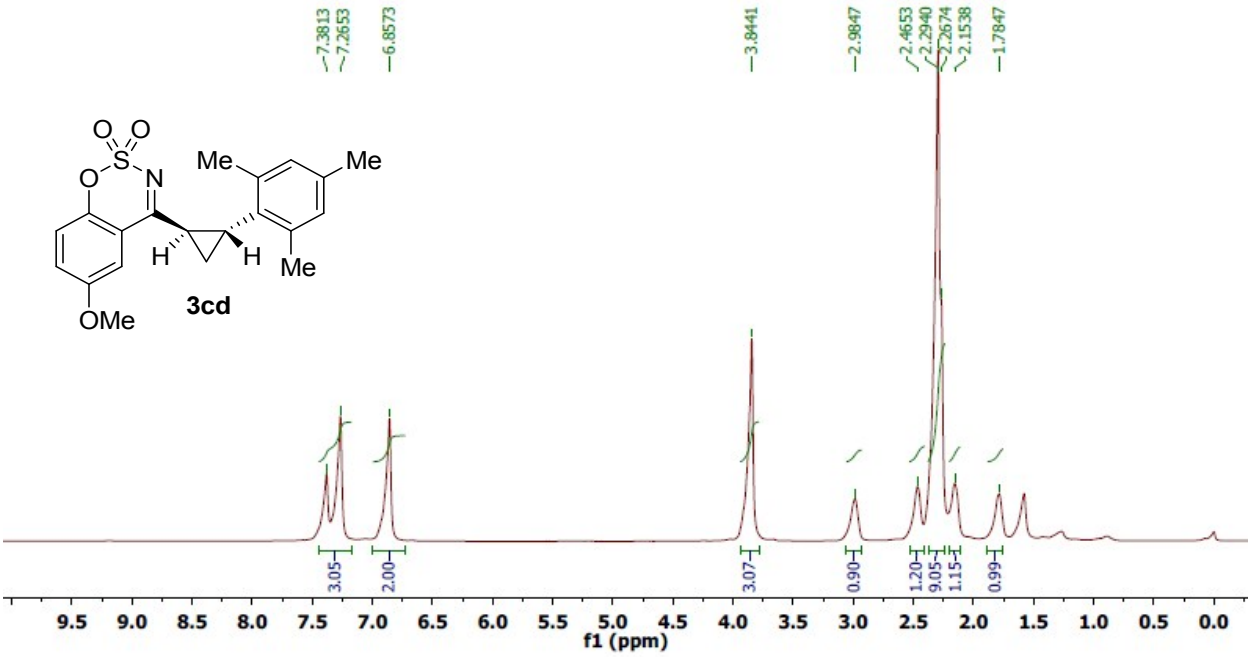
OMe
f1 (ppm)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2.2940
2.2674
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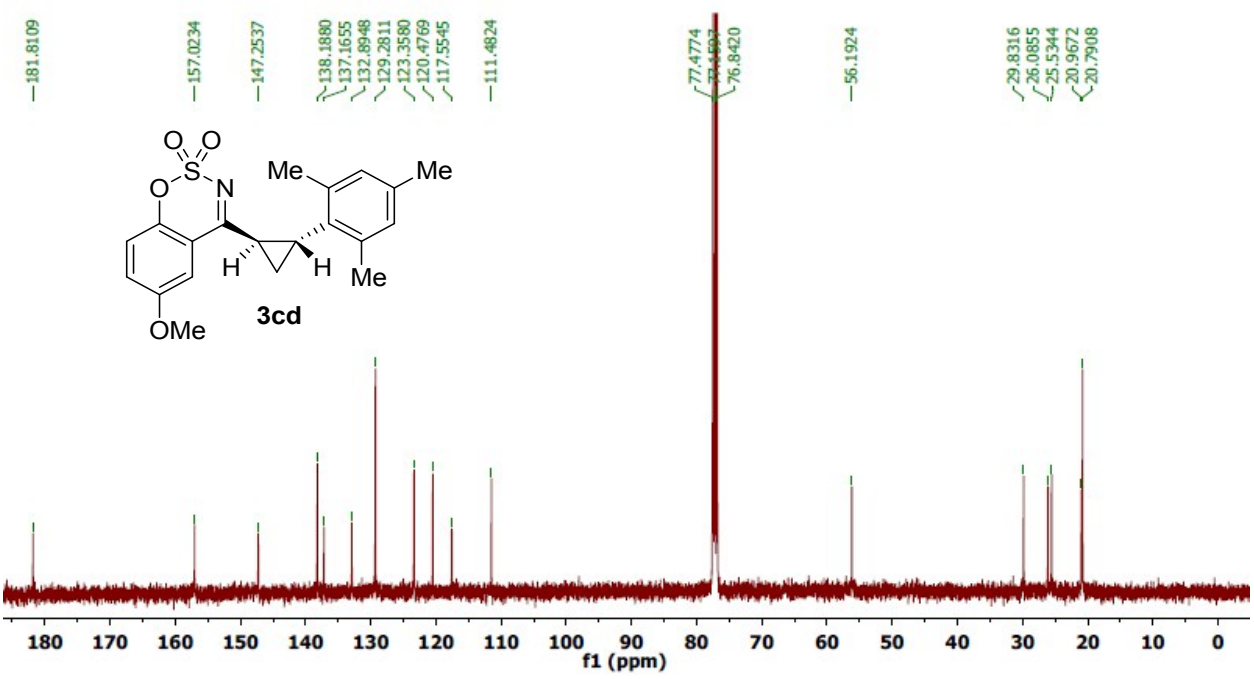
2.00
3.07
0.90
1.20
9.05
1.15
0.99
f1 (ppm)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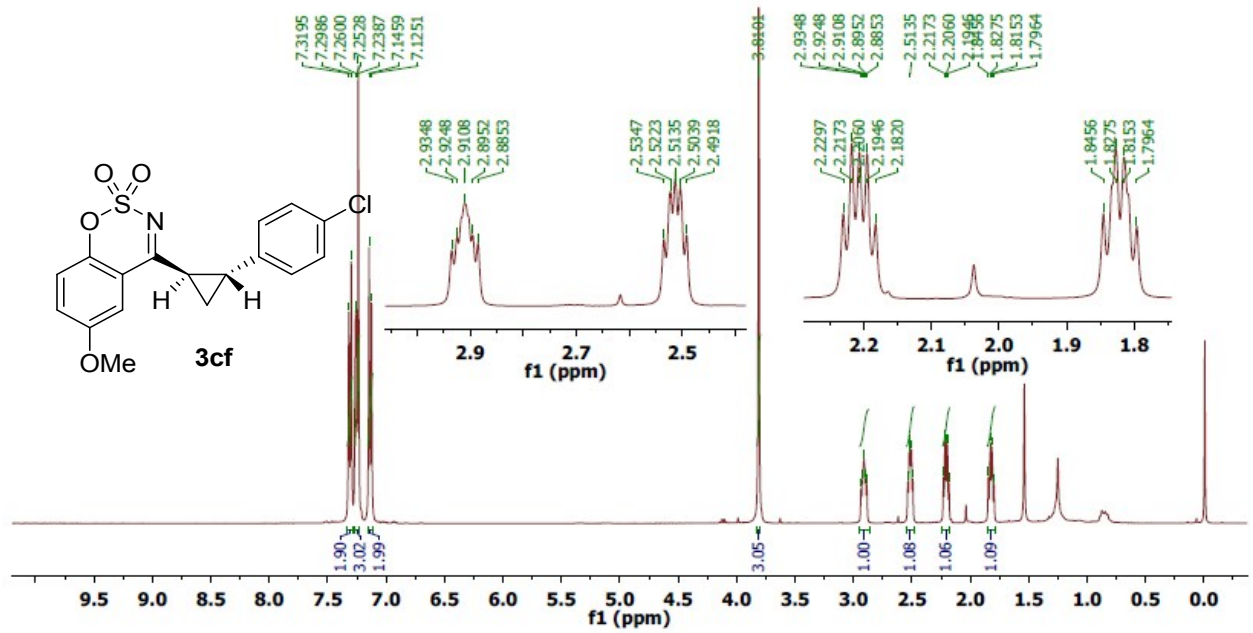
25.5344
20.9672
20.7908
f1 (ppm)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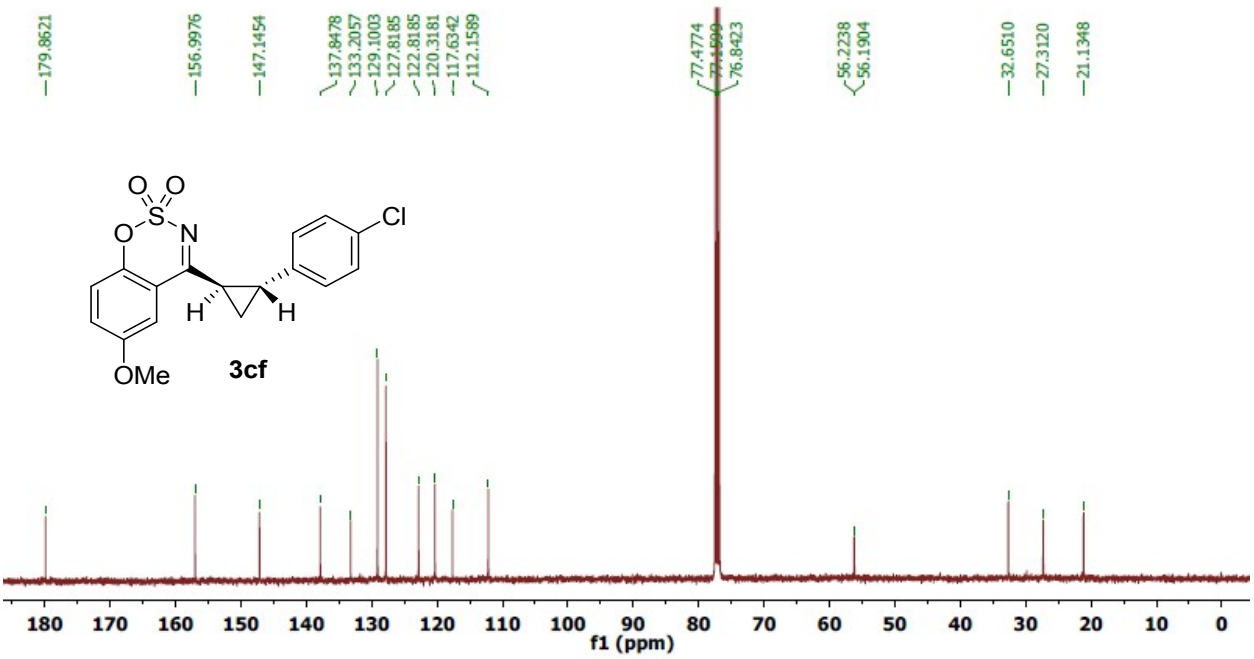
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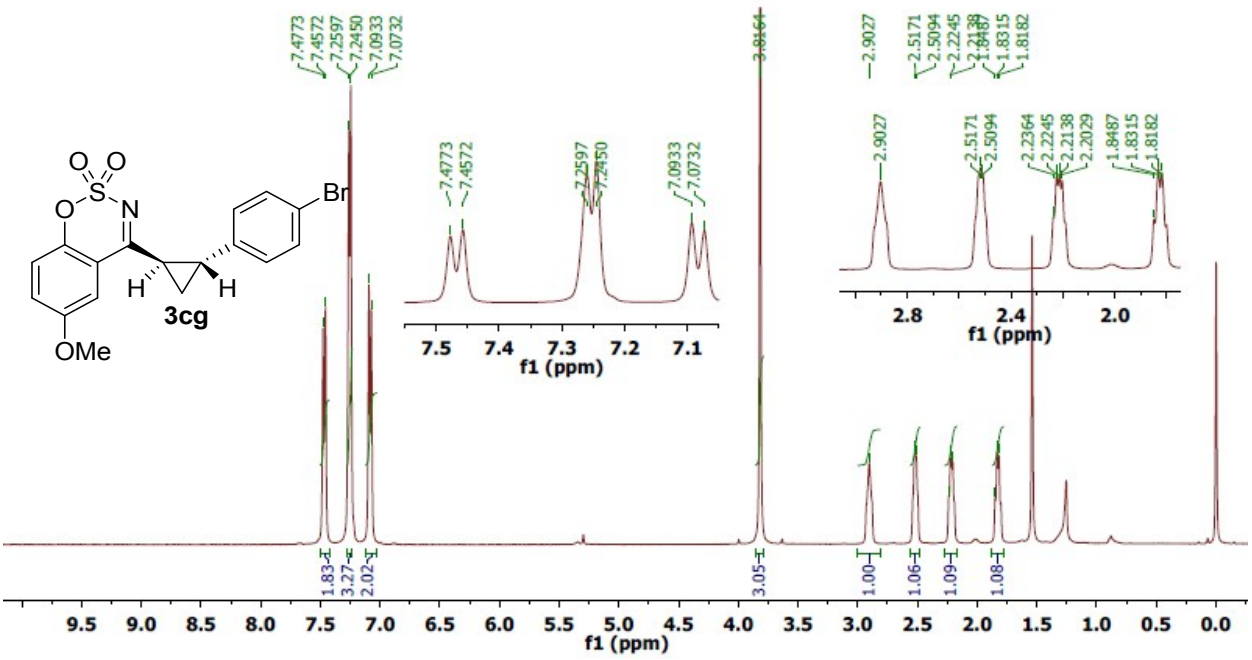
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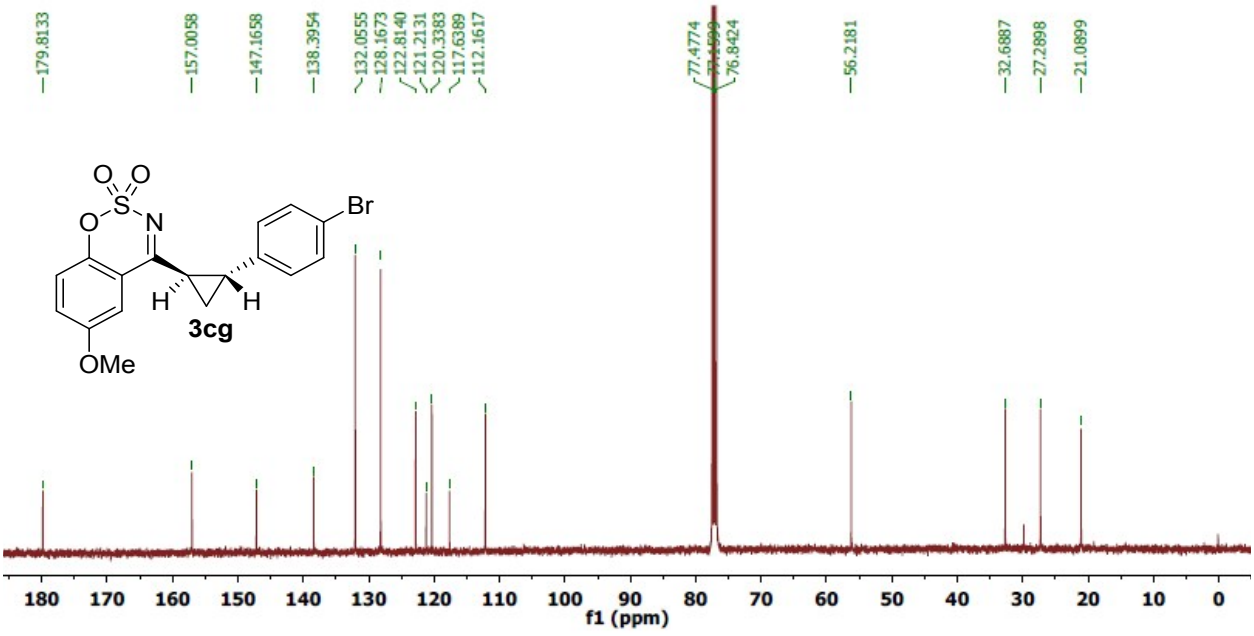
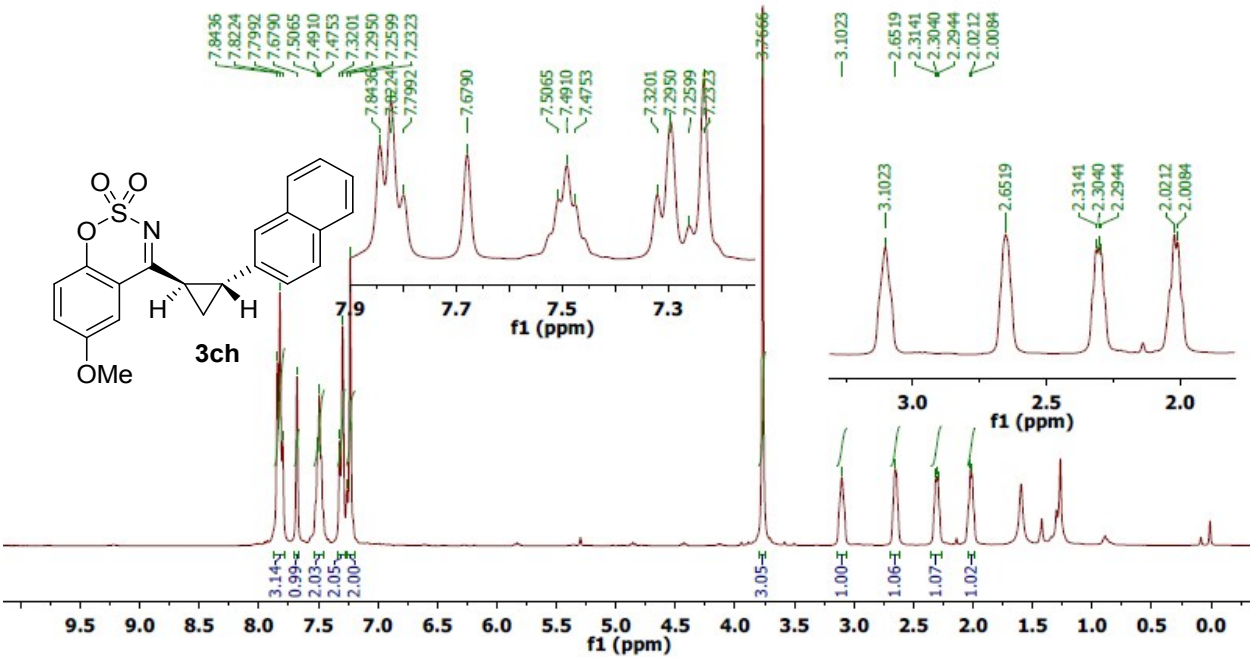
OMe
Br
f1 (ppm)


3cg
OMe
Br
f1 (ppm)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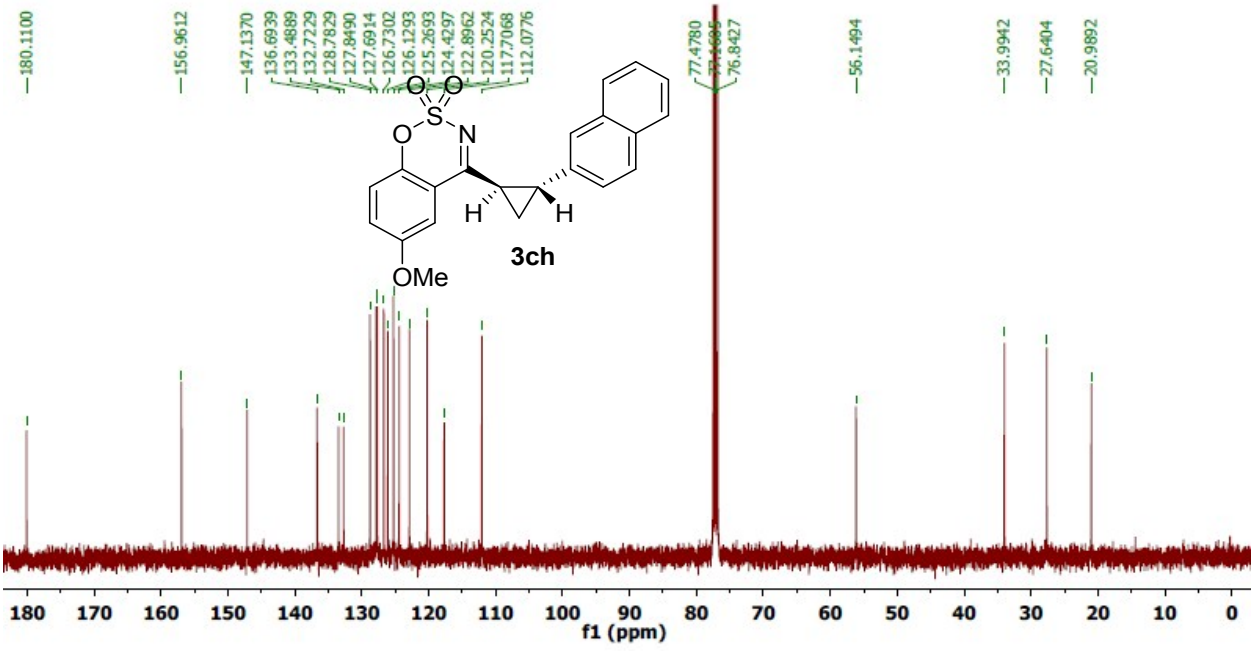
OMe
f1 (ppm)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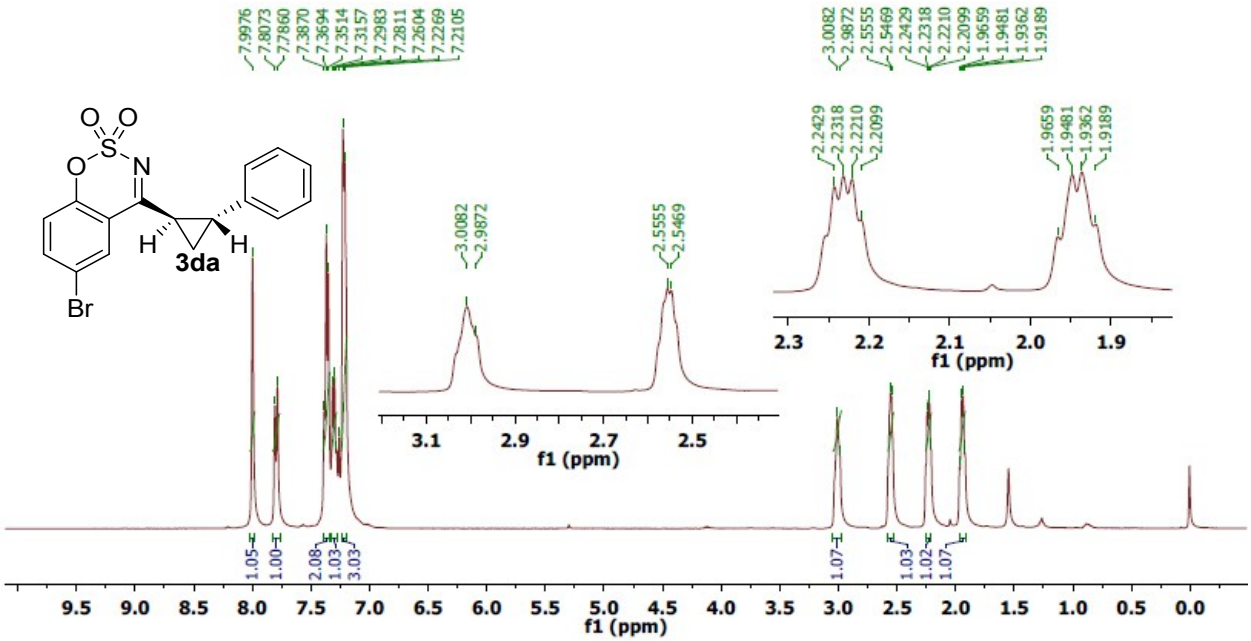
OMe
f1 (ppm)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7.3694
7.3514
7.3157
7.2983
7.2811
7.2604
7.2269
7.2105
3.0082
2.9872
2.5555
2.5469
2.2429
2.2318
2.2210
2.2099
1.9659
1.9481
1.9362
1.9189
O
O
S
O
N
H
H
3da
Br
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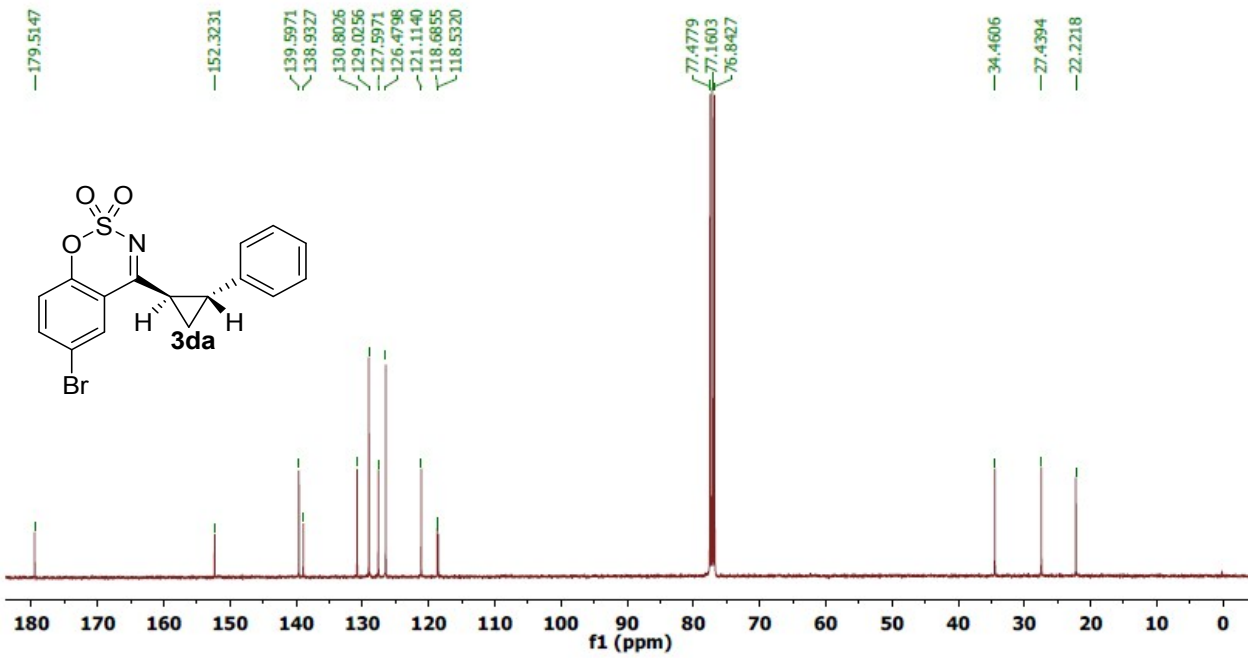
1.00
2.08
1.03
3.03
1.07
1.03
1.02
1.07
f1 (ppm)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138.9327
130.8026
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127.5971
126.4798
121.1140
118.6855
118.5320
77.4779
77.1603
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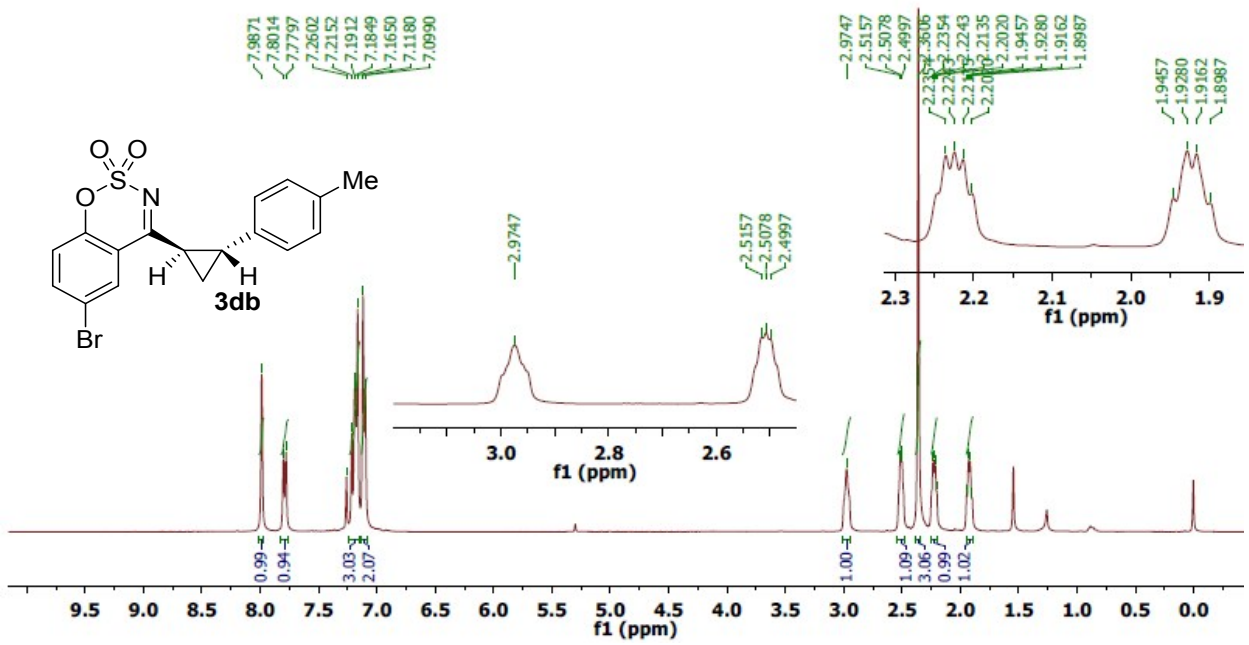
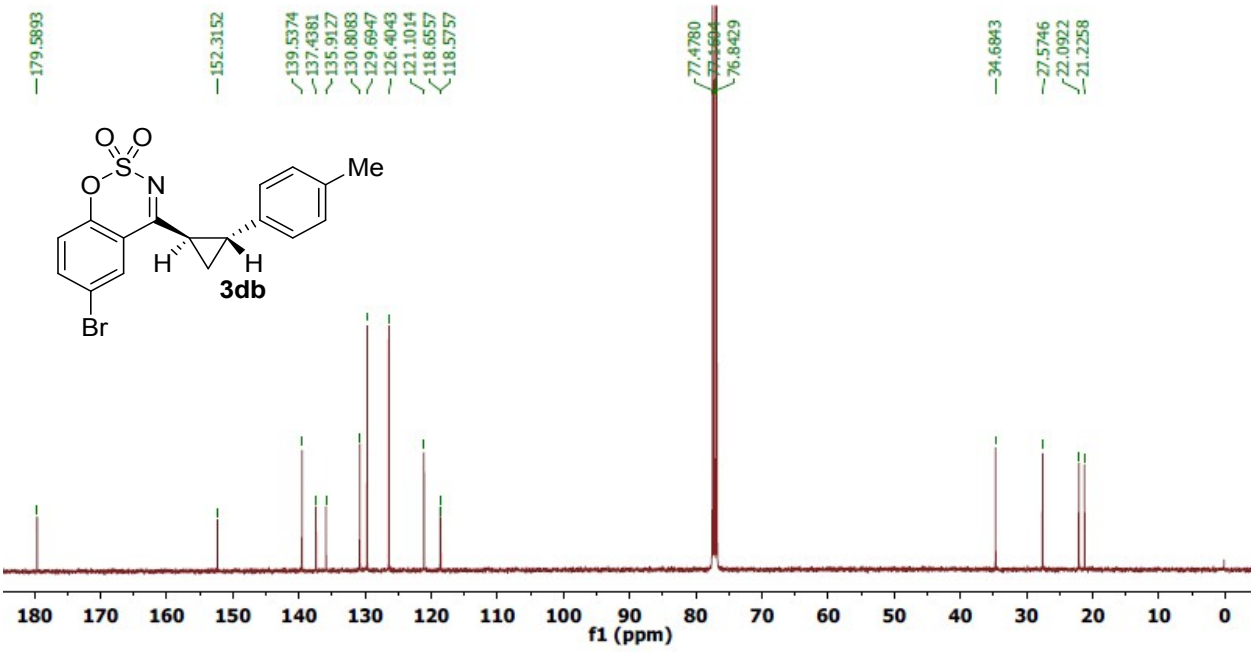
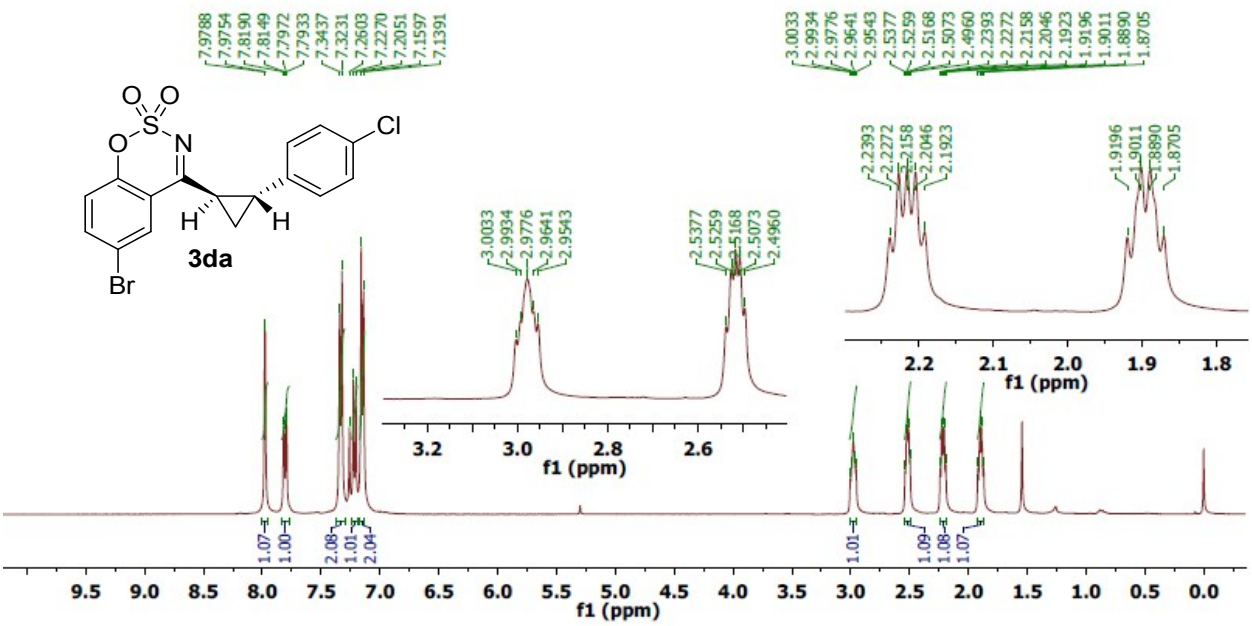
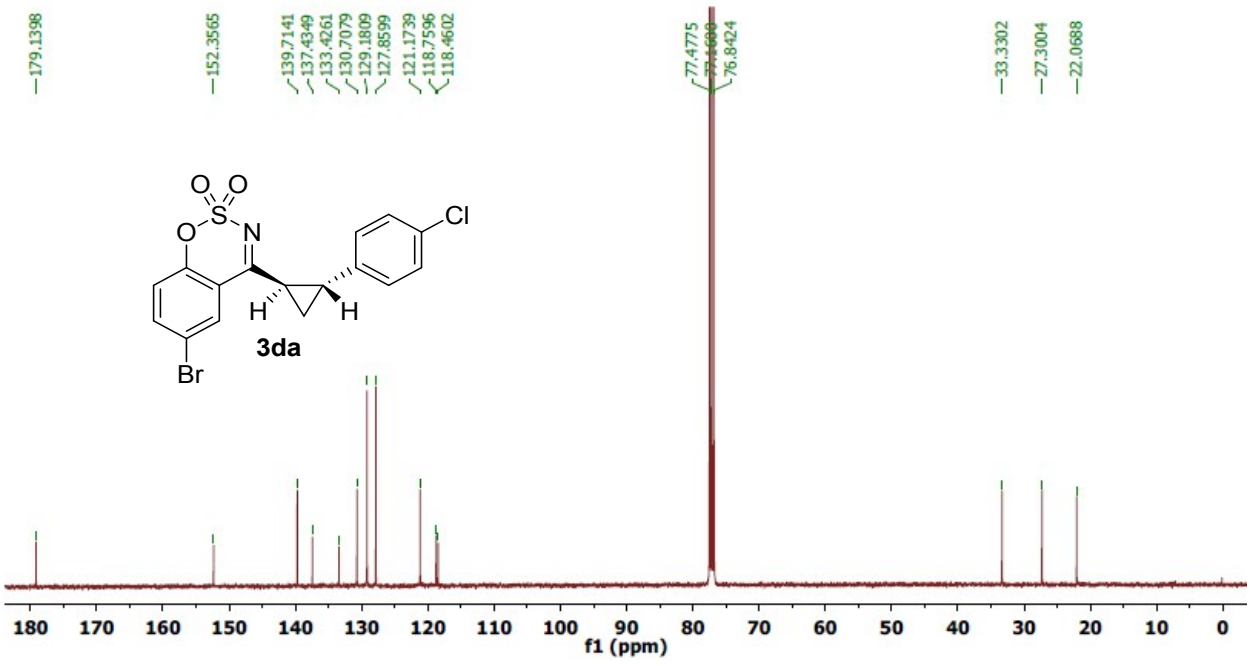
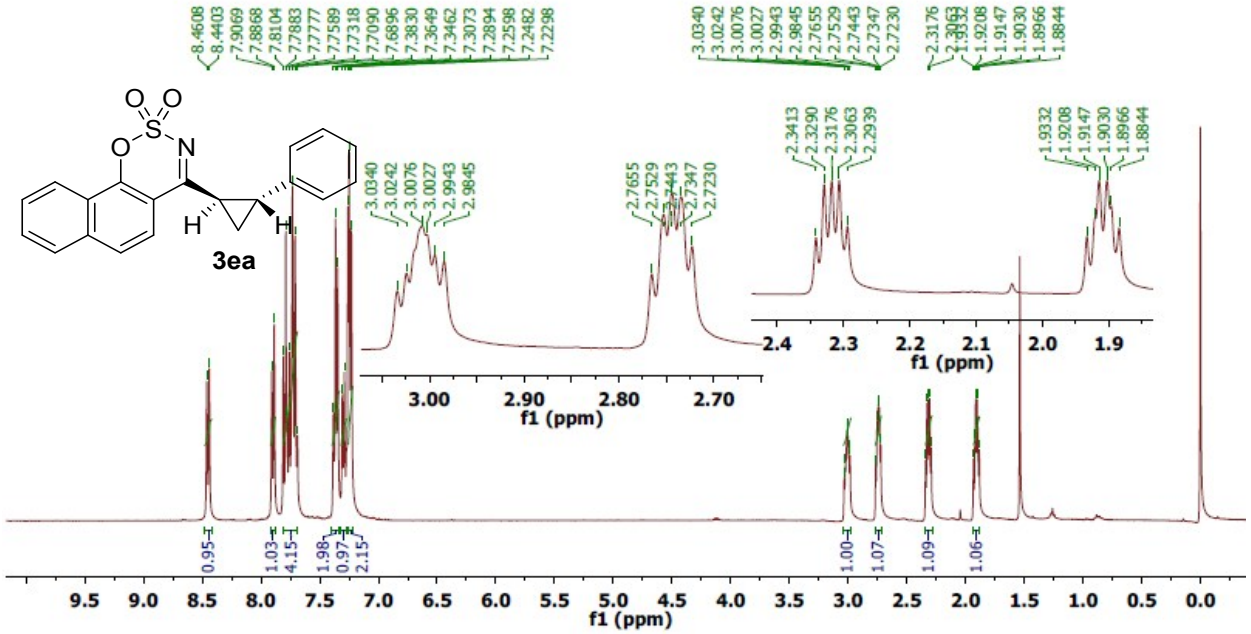
27.4394
22.2218
O
O
S
O
N
H
H
3da
Br
f1 (ppm)


3db
Br
Me
f1 (ppm)


3db
Br
Me
f1 (ppm)


3da
Br
Cl
f1 (ppm)


3da
Br
Cl
f1 (ppm)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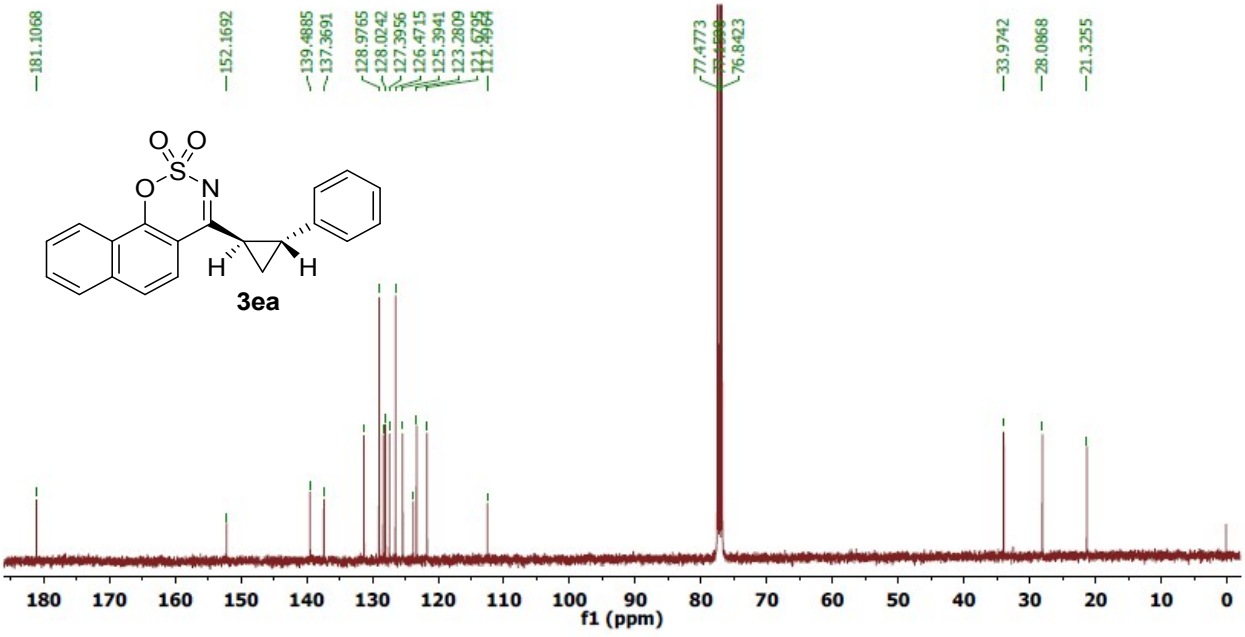
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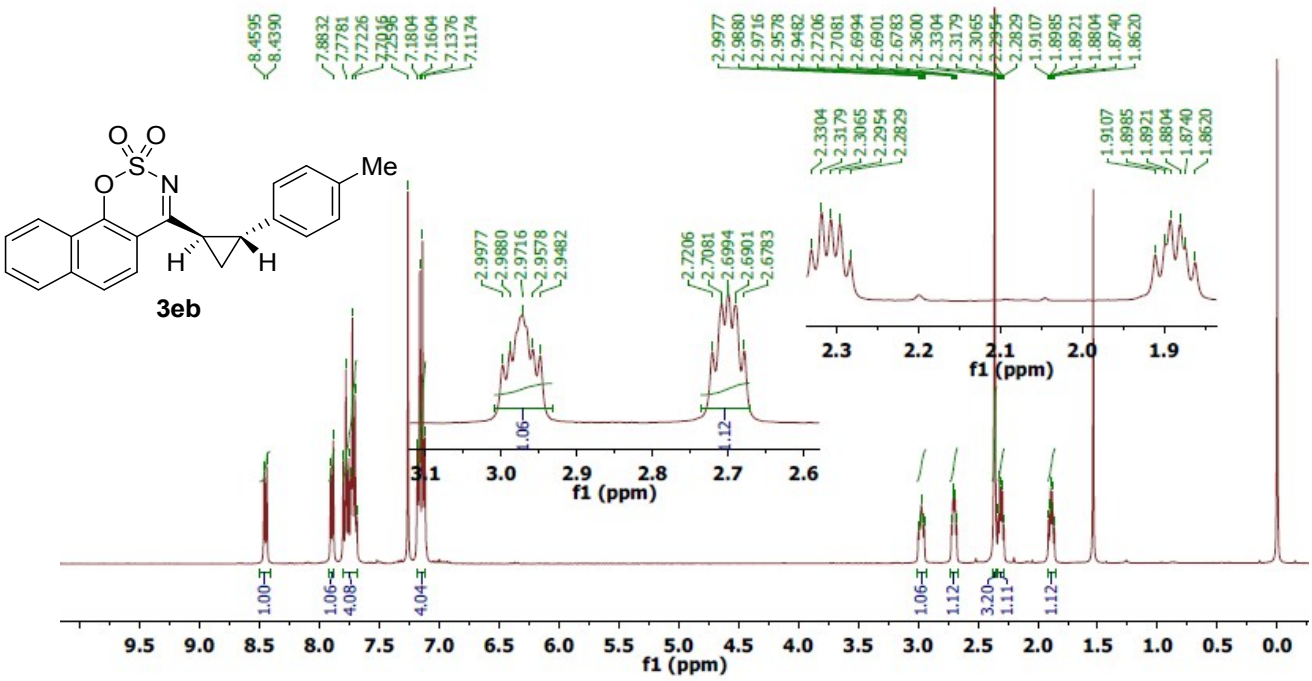
f1 (ppm)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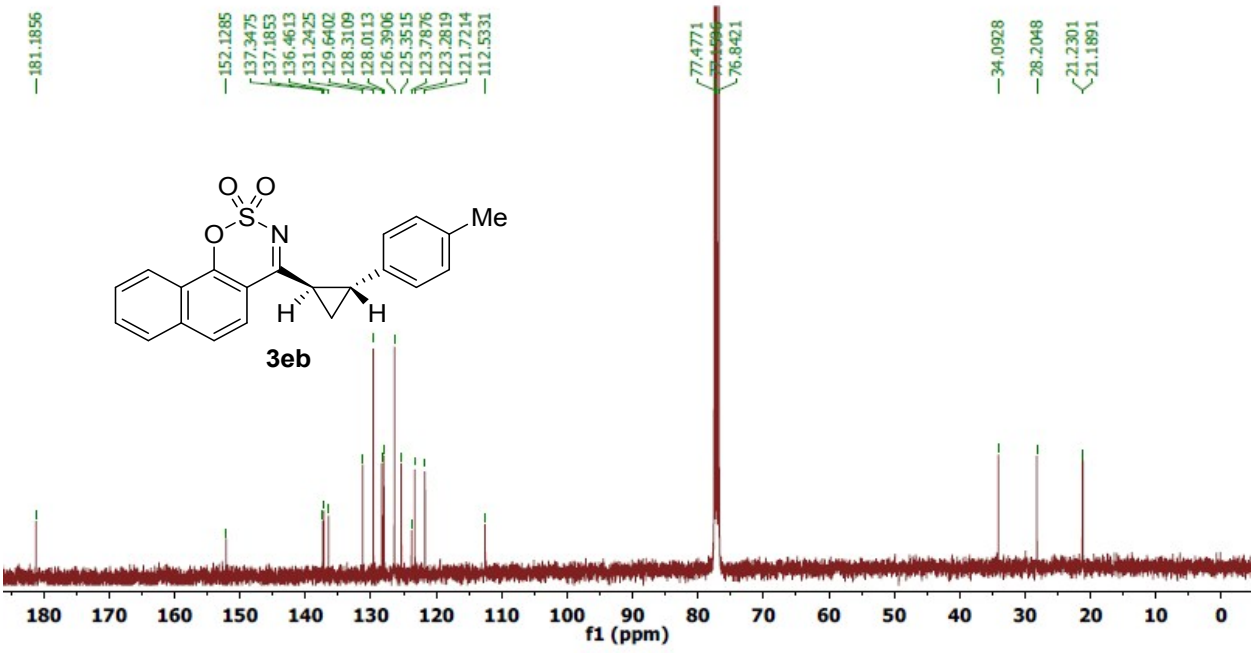
f1 (ppm)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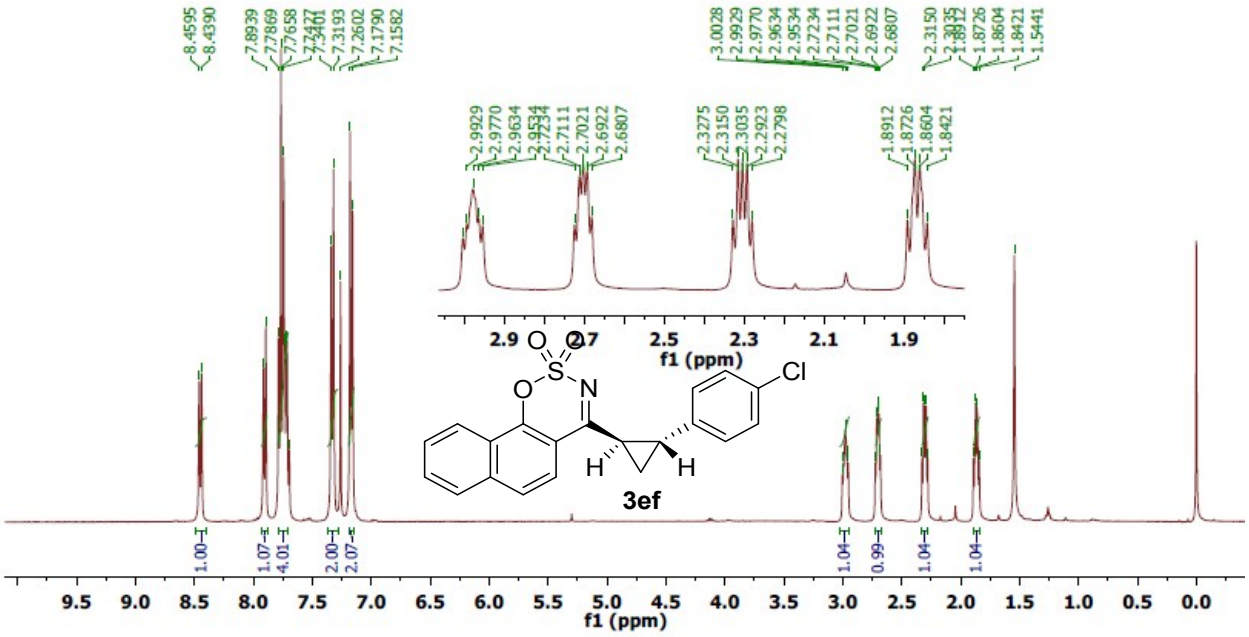
f1 (ppm)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2.9770
2.9634
2.9534
2.7234
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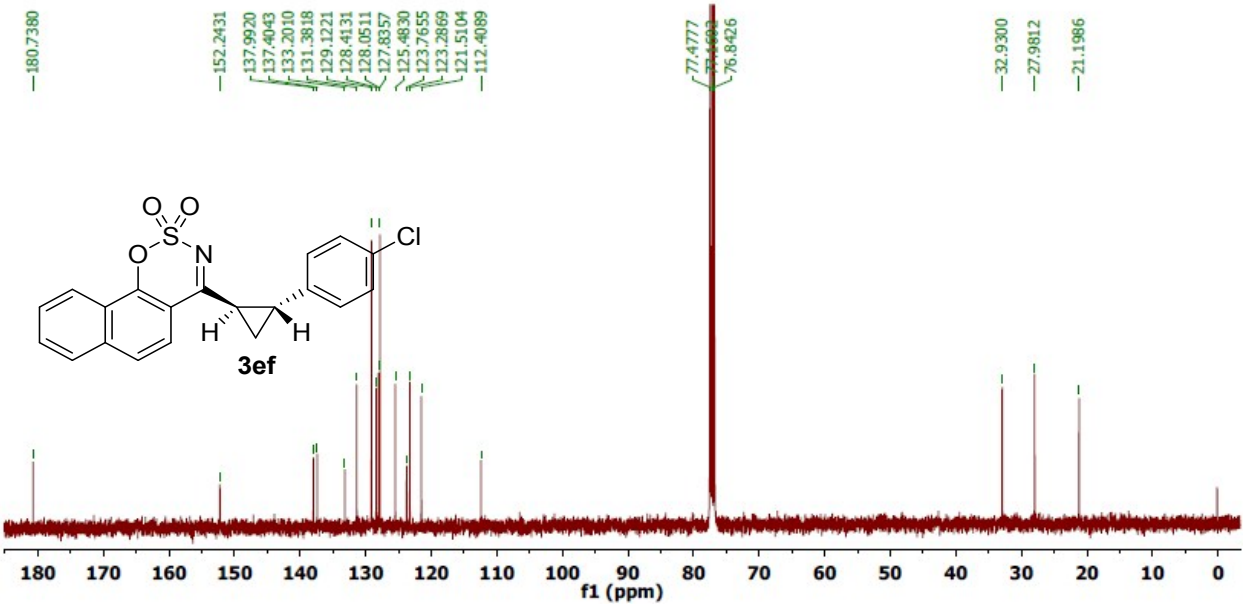
2.7021
2.6922
2.6807
2.3150
2.3035
1.8912
1.8726
1.8604
1.8421
1.5441
1.00
1.07
4.01
2.00
2.07
1.04
0.99
1.04
1.04
f1 (ppm)
O
O
S
O
N
Cl
H
H
3ef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125.4830
123.7655
123.2869
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112.4089
77.4777
77.1603
76.8426
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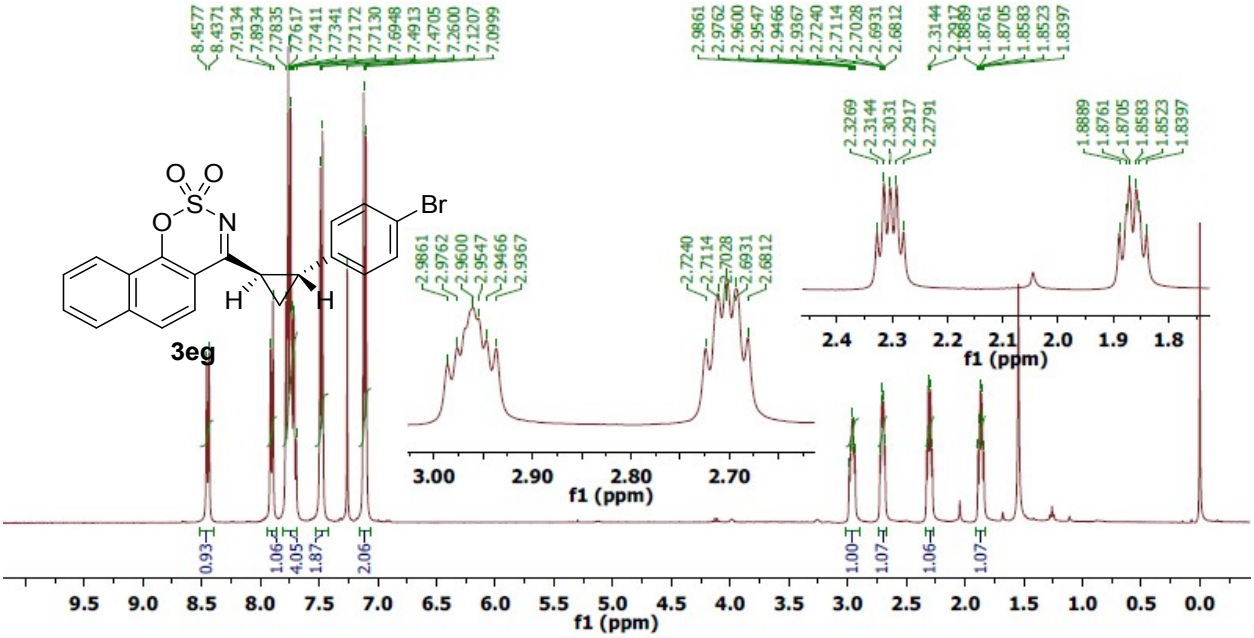
27.9812
21.1986
O
O
S
O
N
Cl
H
H
3ef
f1 (ppm)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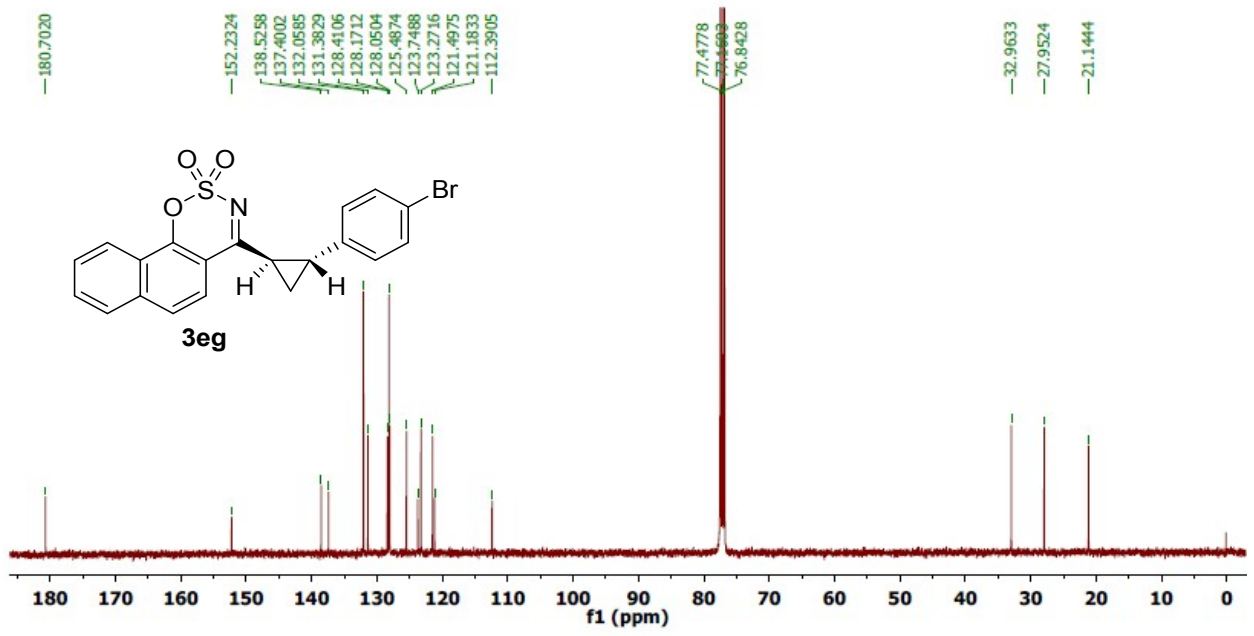
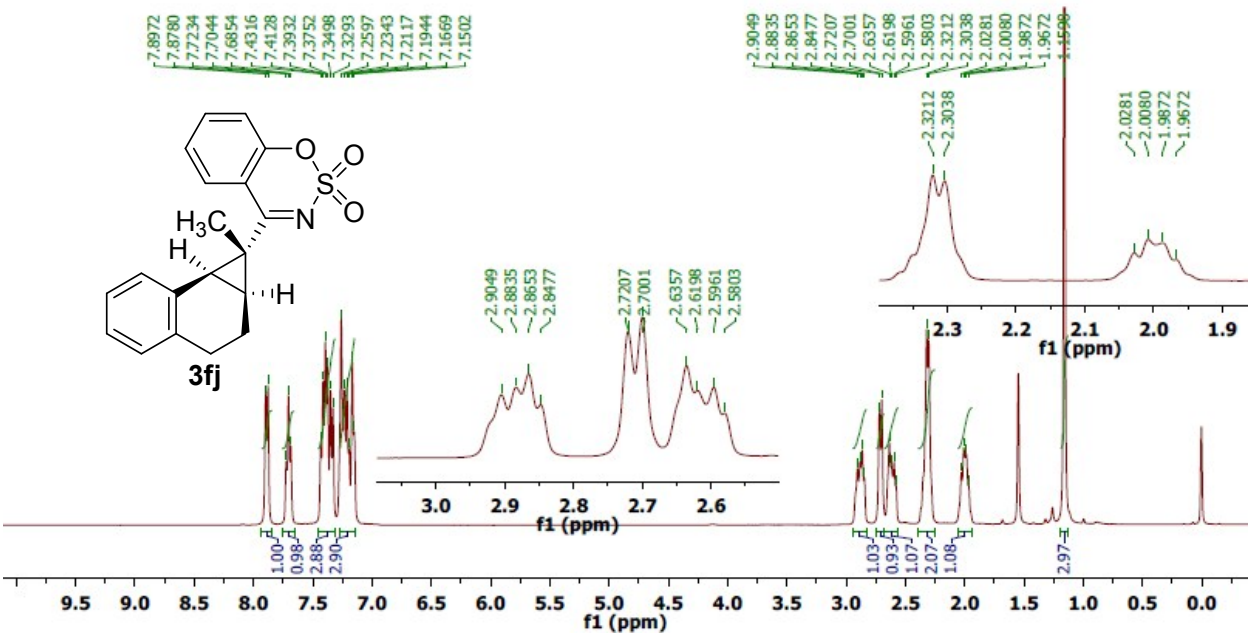
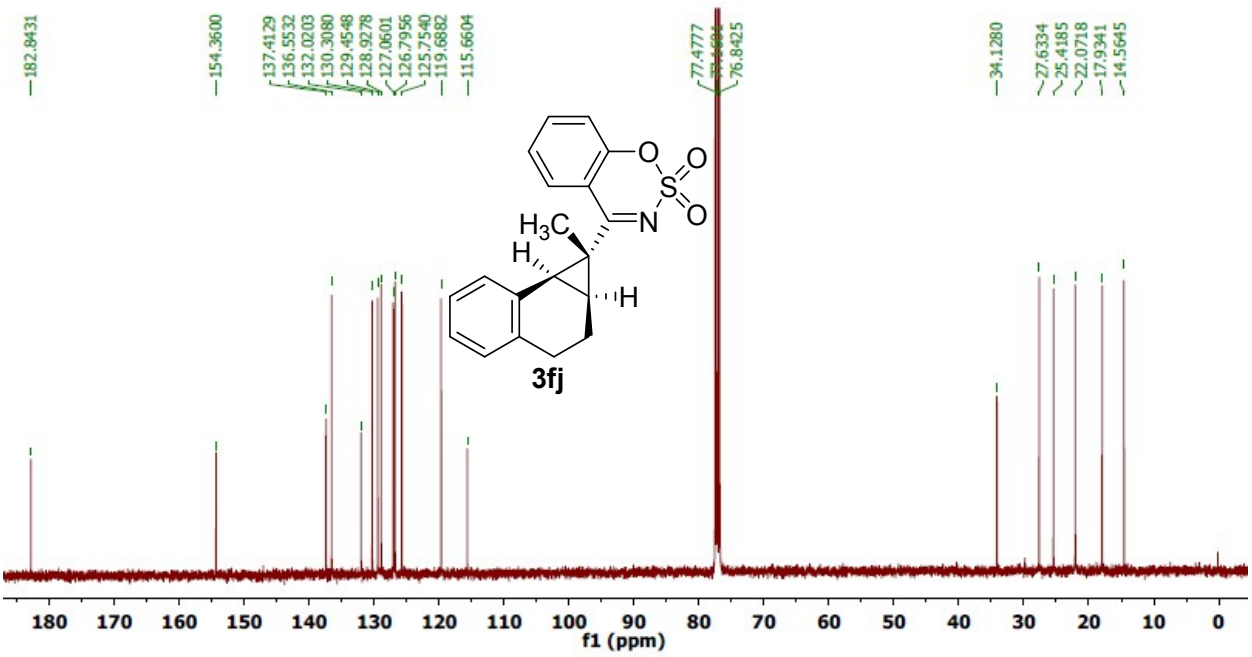
f1 (ppm)


3eg
f1 (ppm)


3fj
f1 (ppm)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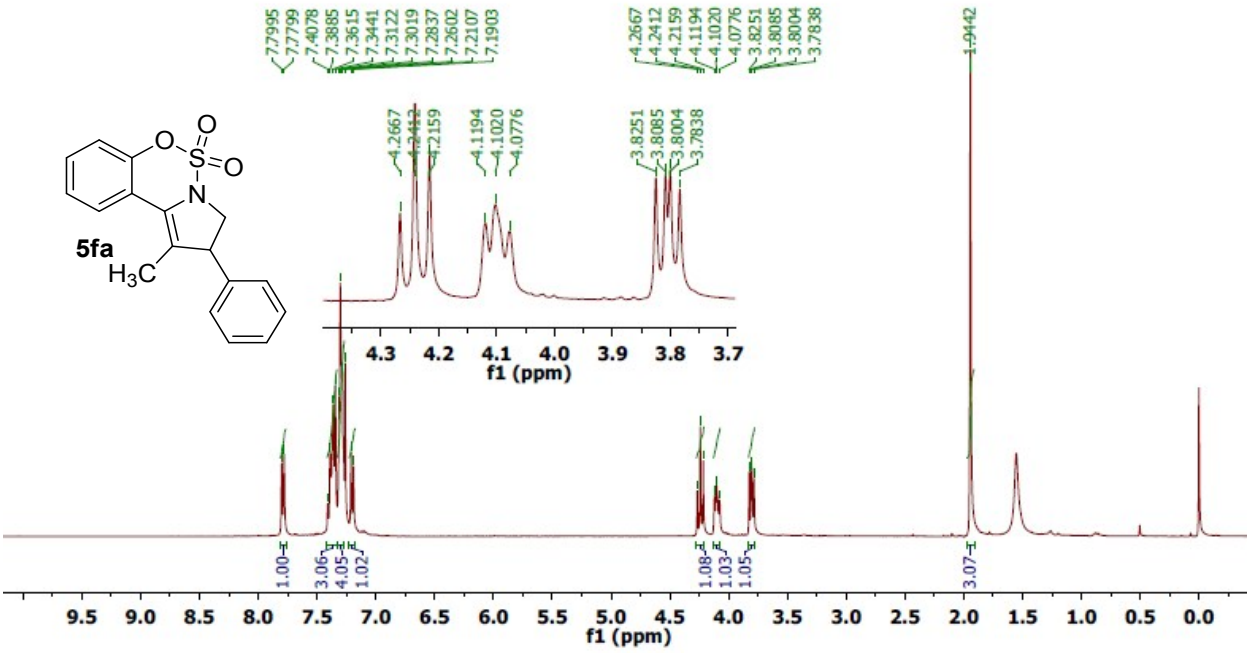
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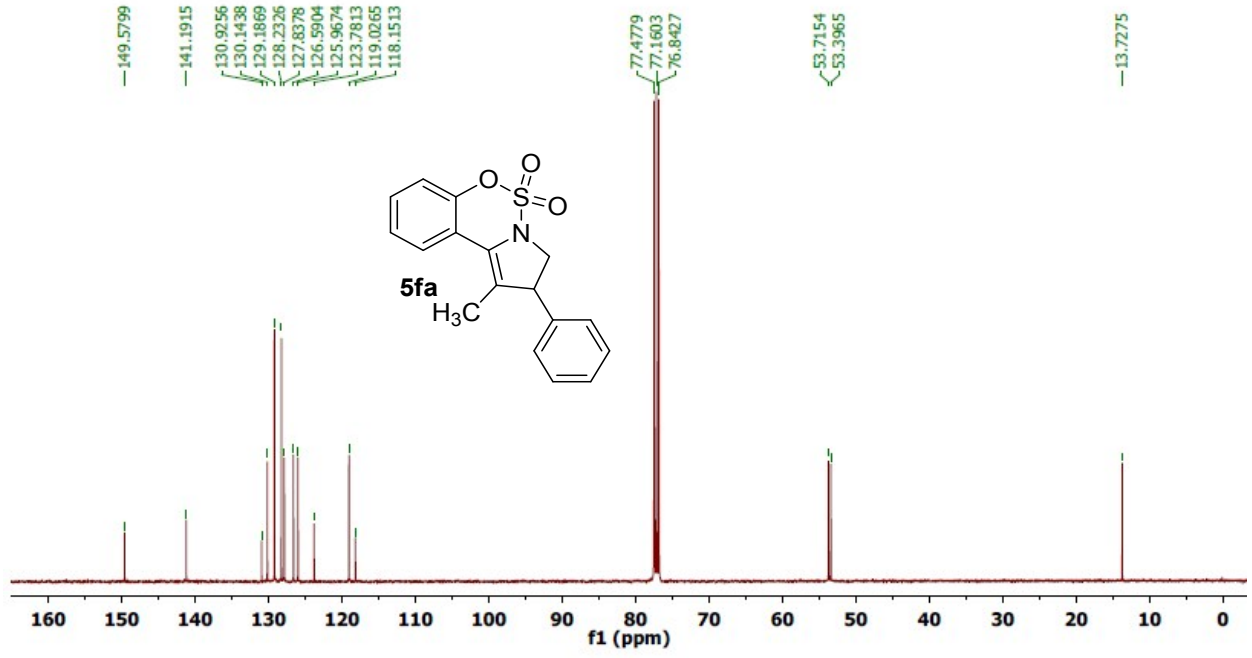
7.2602
7.2107
7.1903
4.2667
4.2412
4.2159
4.1194
4.1020
4.0776
3.8251
3.8085
3.8004
3.7838
1.9442
5fa
H3C
4.3 4.2 4.1 4.0 3.9 3.8 3.7
f1 (ppm)
1.00
3.06
4.05
1.02
1.08
1.03
1.05
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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118.1513
77.4779
77.1603
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53.3965
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5fa
H3C
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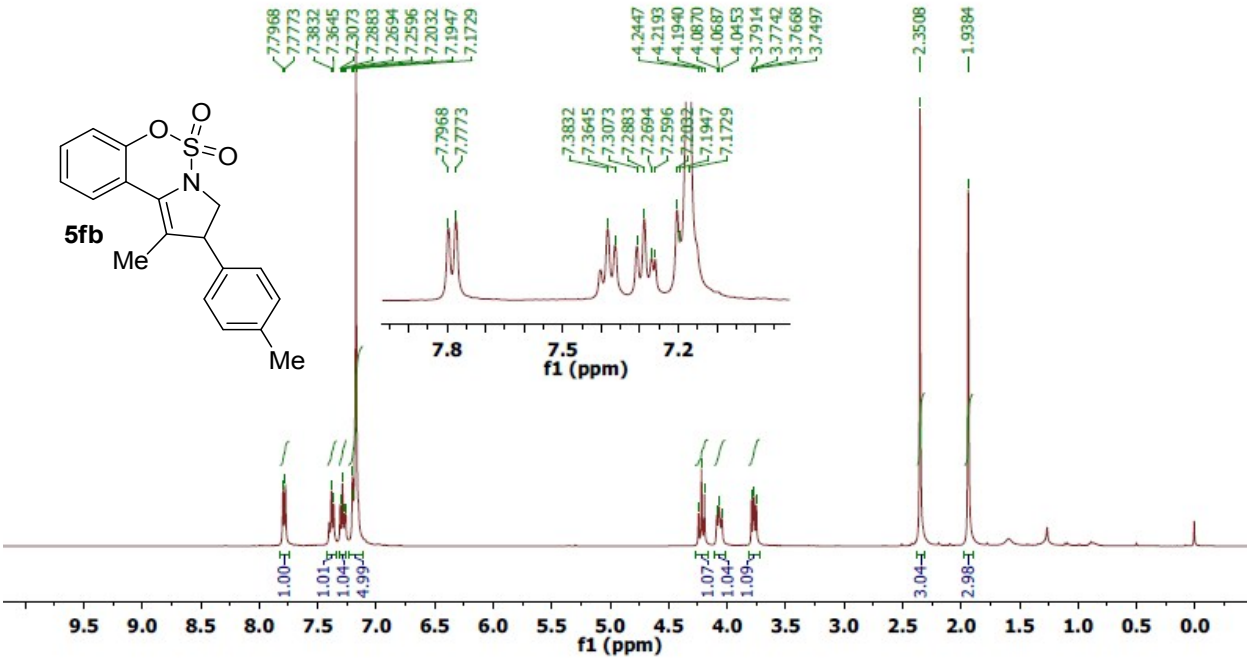
f1 (ppm)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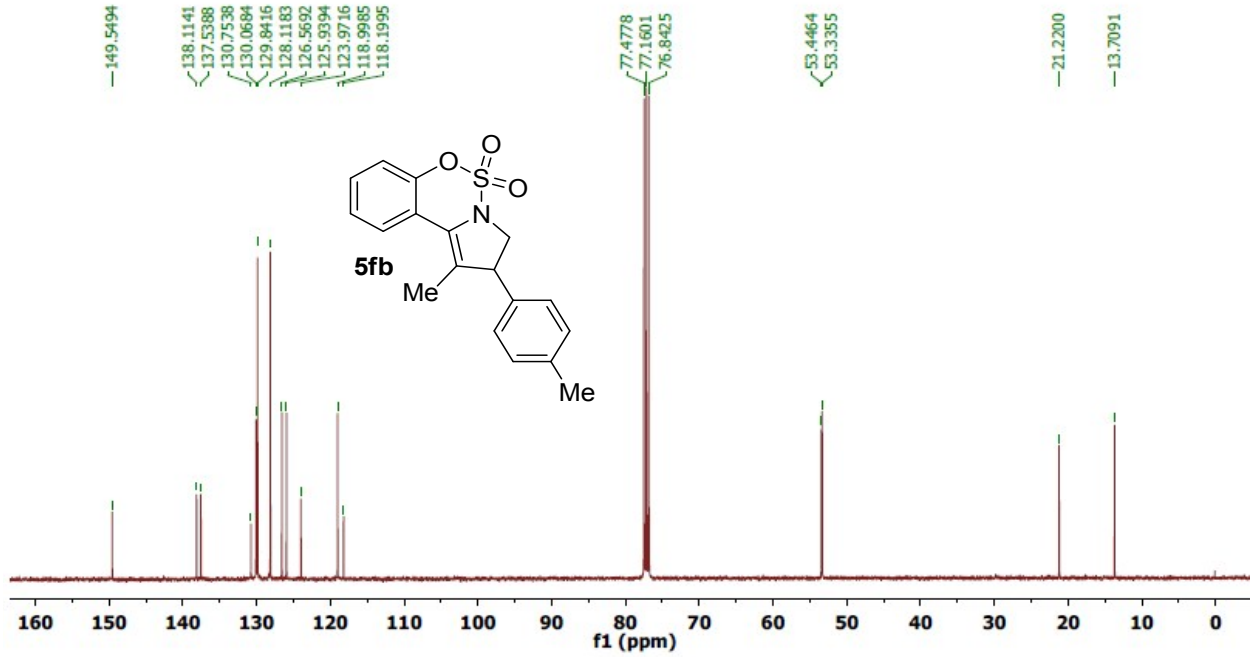
7.1729
4.2447
4.2193
4.1940
4.0870
4.0687
4.0453
3.7914
3.7742
3.7668
3.7497
2.3508
1.9384
5fb
Me
Me
7.8
7.5
7.2
f1 (ppm)
1.00
1.01
1.04
4.99
1.07
1.04
1.09
3.04
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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118.9985
118.1995
77.4778
77.1601
76.8425
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21.2200
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5fb
Me
Me
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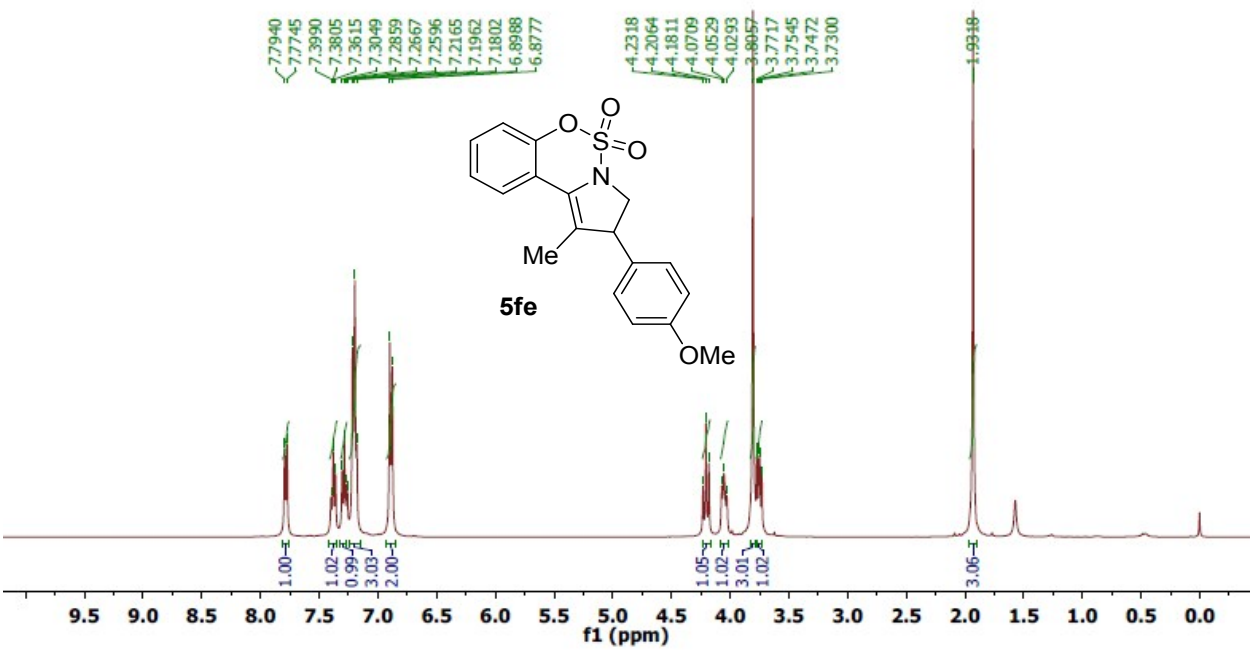
f1 (ppm)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6.8988
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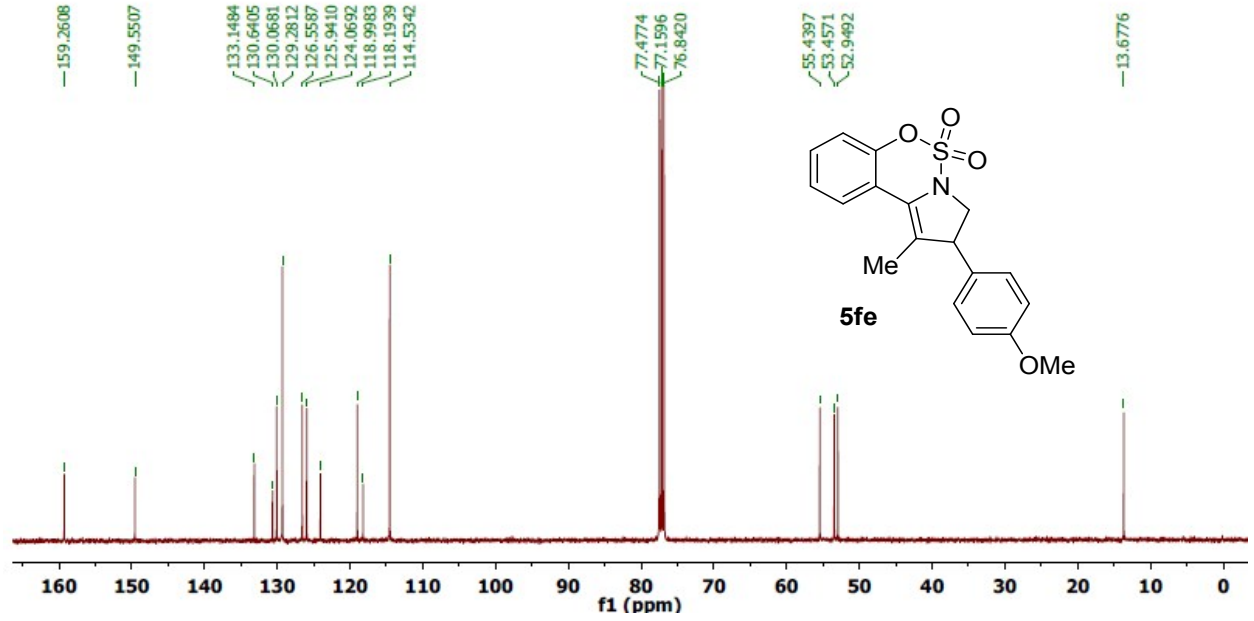
3.7545
3.7472
3.7300
1.9318
1.00
1.02
0.99
3.03
2.00
1.05
1.02
3.01
1.02
3.06
O
S
O
N
Me
OMe
5fe
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.9410
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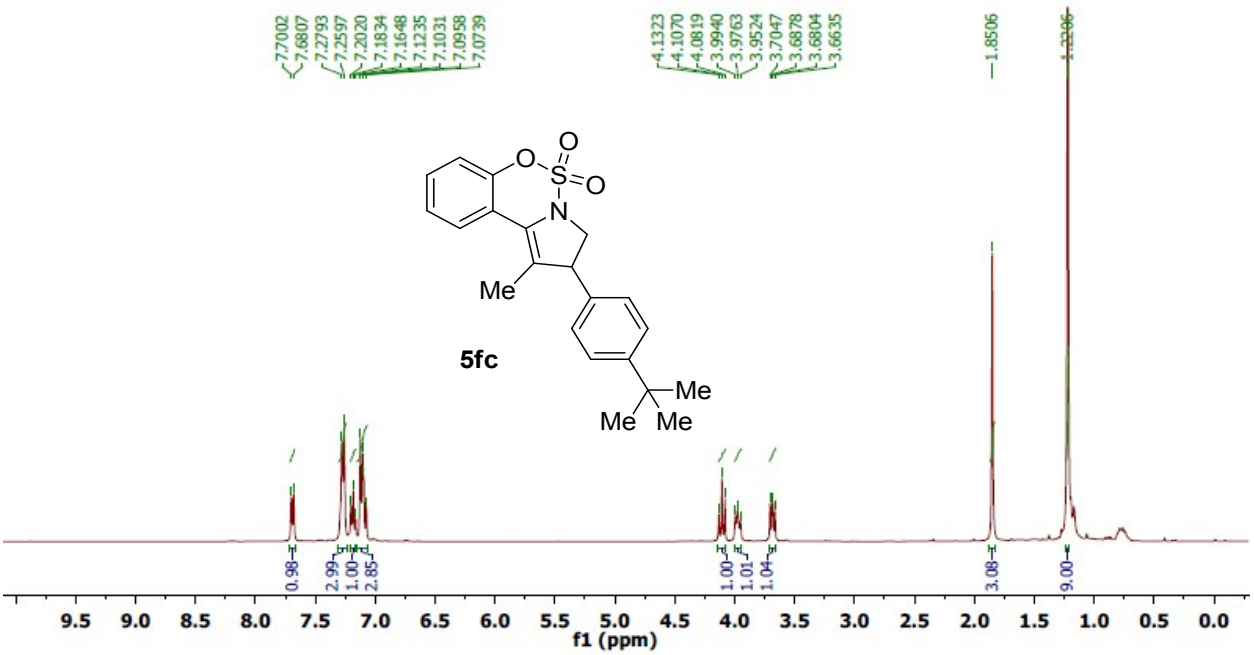
118.1939
114.5342
77.4774
77.1596
76.8420
55.4397
53.4571
52.9492
13.6776
O
S
O
N
Me
OMe
5fe
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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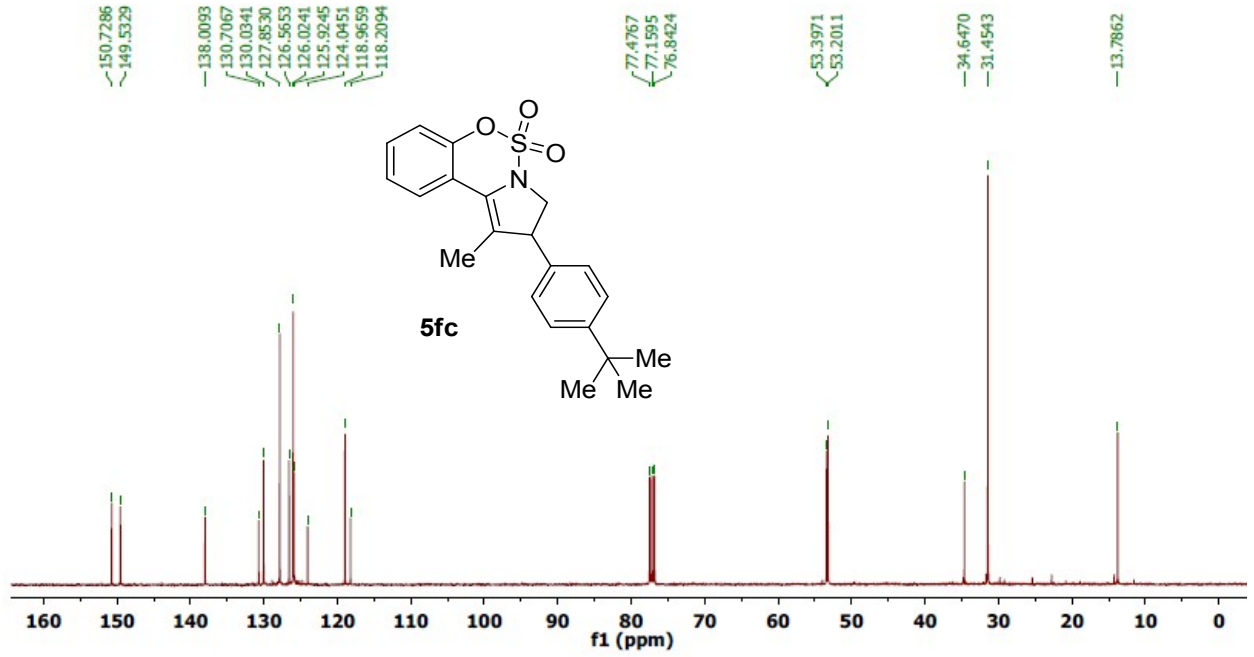
7.1031
7.0958
7.0739
4.1323
4.1070
4.0819
3.9940
3.9763
3.9524
3.7047
3.6878
3.6804
3.6635
1.8506
1.3286
O
O
S
O
N
Me
5fc
Me
Me Me
0.98
2.99
1.00
2.85
1.00
1.01
1.04
3.08
9.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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118.2094
77.4767
77.1595
76.8424
53.3971
53.2011
34.6470
31.4543
13.7862
O
O
S
O
N
Me
5fc
Me
Me Me
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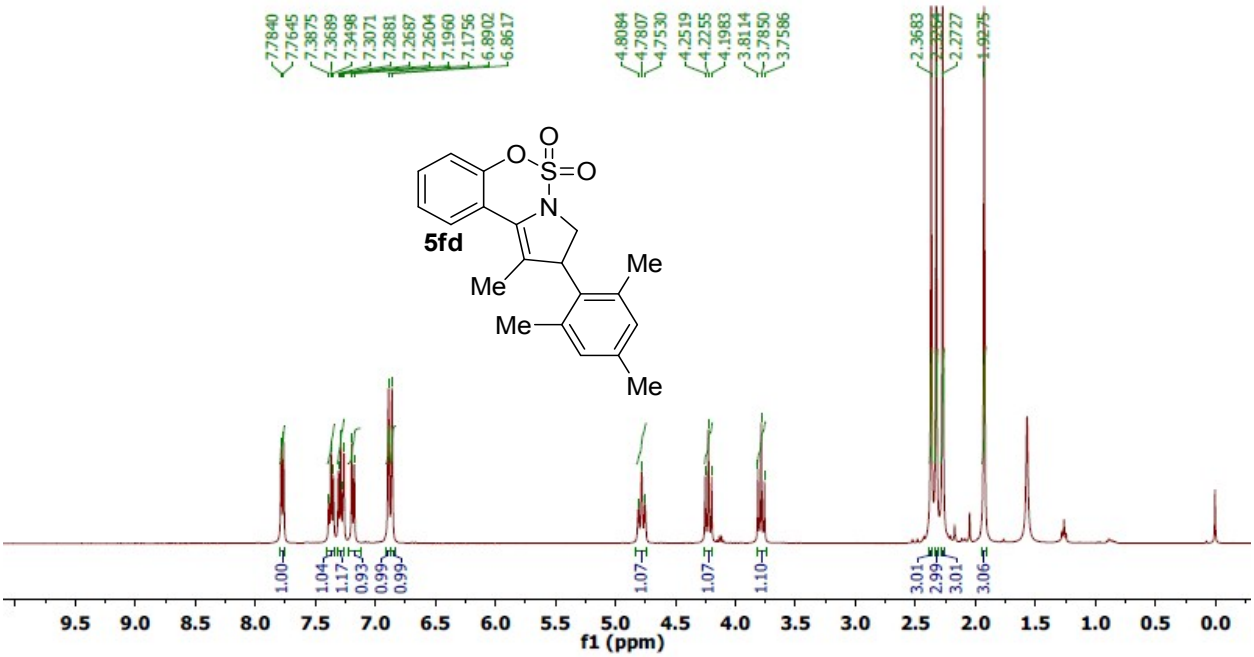
f1 (ppm)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6.8617
4.8084
4.7807
4.7530
4.2519
4.2255
4.1983
3.8114
3.7850
3.7586
2.3683
2.2727
1.9275
5fd
Me
Me
Me
Me
1.00
1.04
1.17
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0.99
1.07
1.07
1.10
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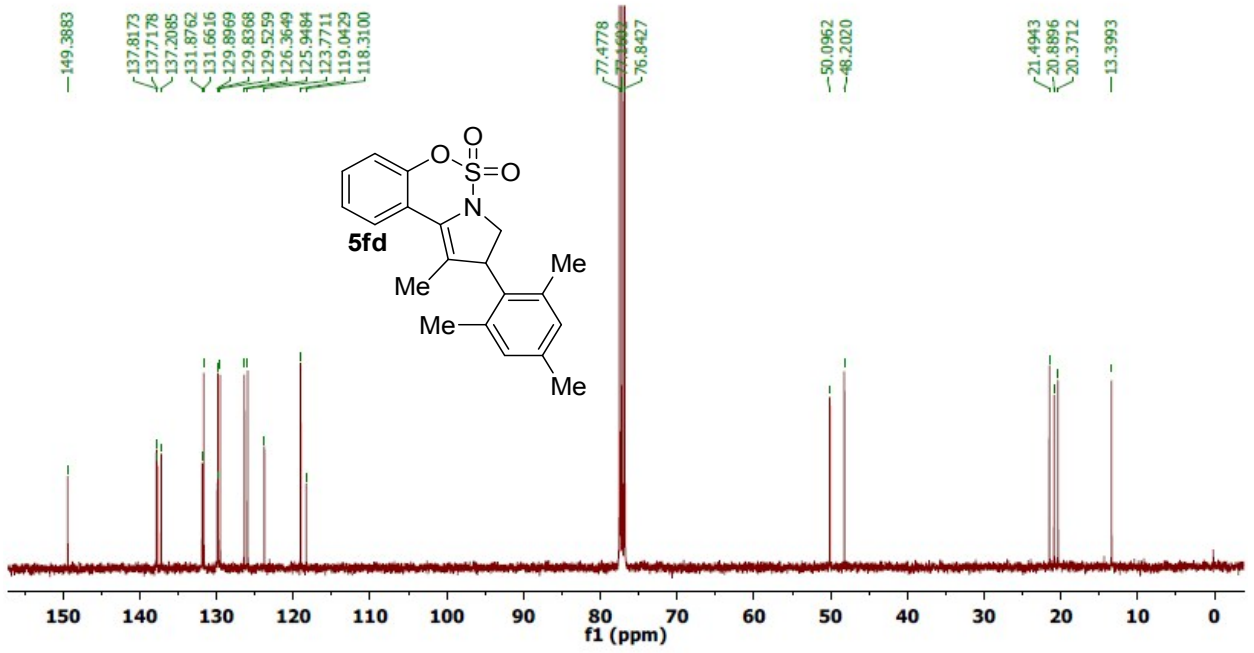
2.99
3.01
3.06
f1 (ppm)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123.7711
119.0429
118.3100
77.4778
76.8427
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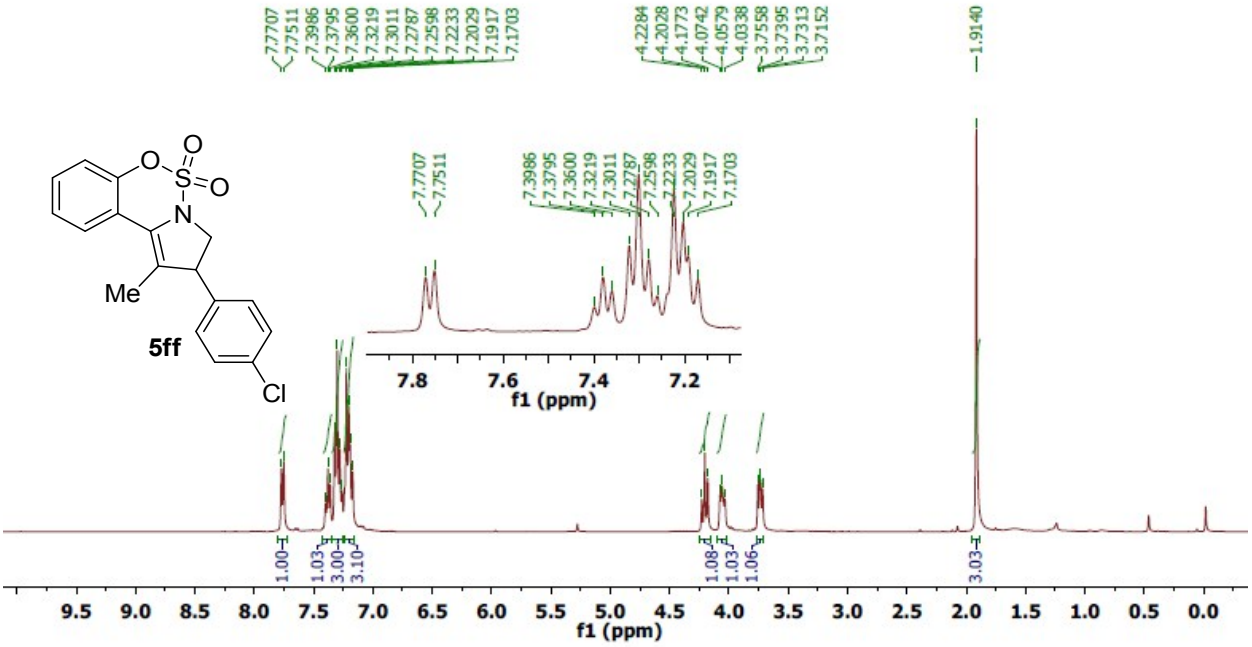
20.3712
13.3993
5fd
Me
Me
Me
Me
f1 (ppm)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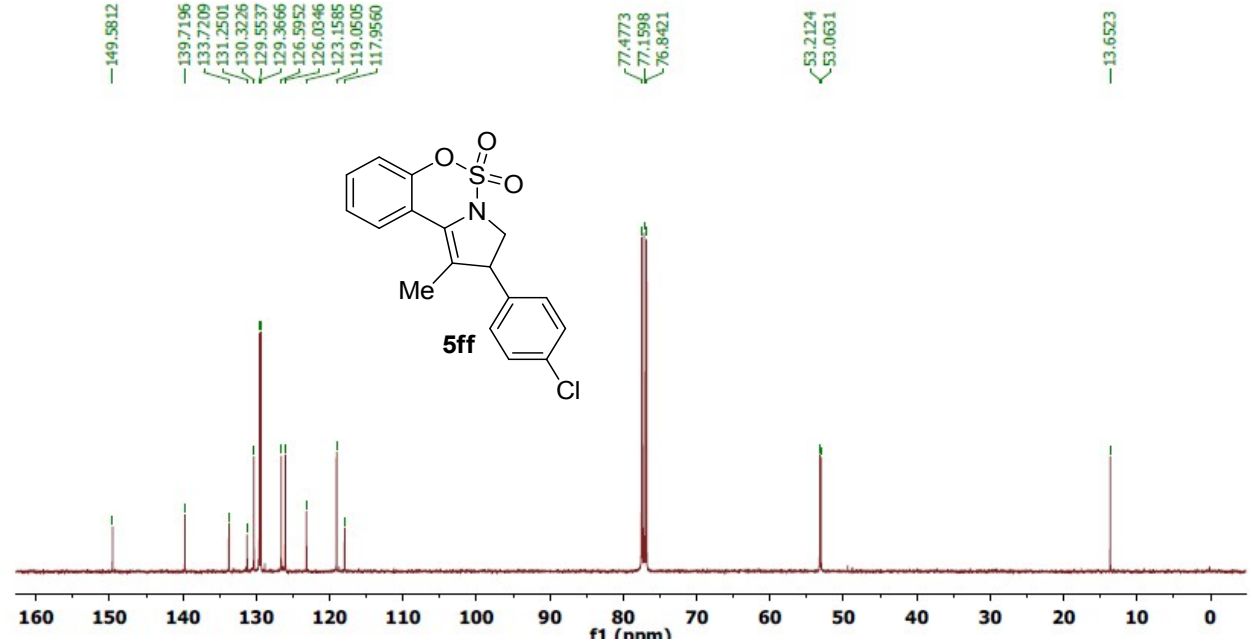
7.2029
7.1917
7.1703
4.2284
4.2028
4.1773
4.0742
4.0579
4.0338
3.7558
3.7395
3.7313
3.7152
1.9140
O
S
O
N
Me
Cl
5ff
7.8
7.6
7.4
7.2
f1 (ppm)
1.00
1.03
3.00
3.10
1.08
1.03
1.06
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.4773
77.1598
76.8421
53.2124
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S
O
N
Me
Cl
5ff
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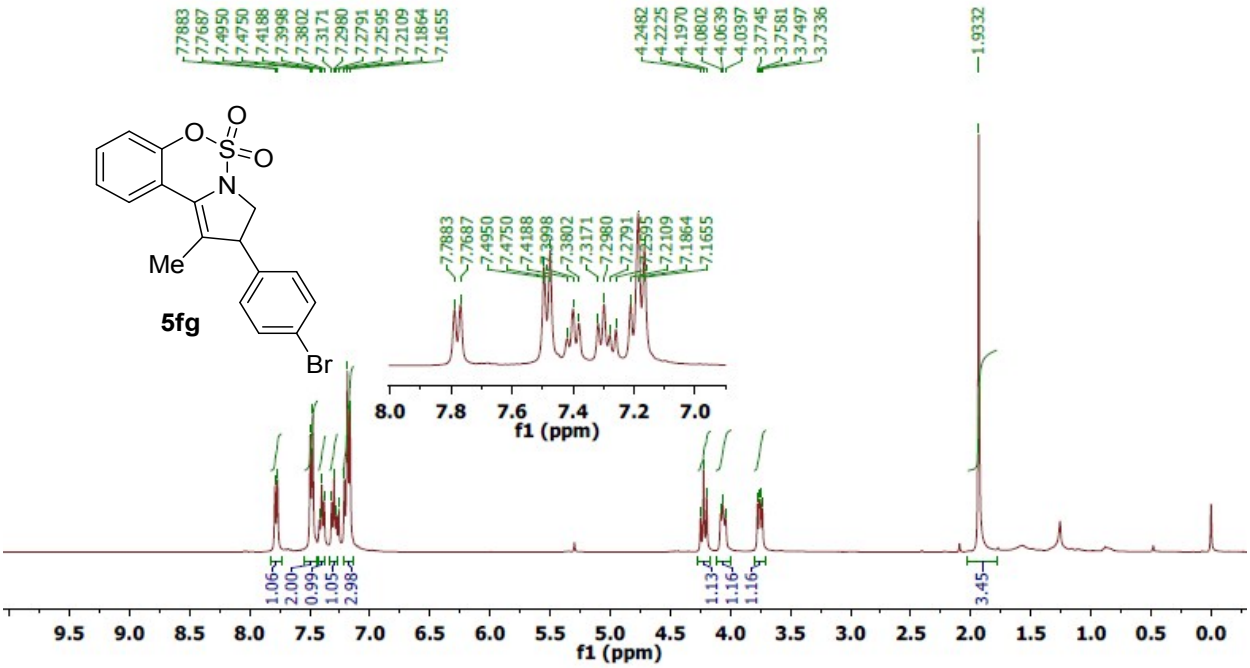
f1 (ppm)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7.2109
7.1864
7.1655
4.2482
4.2225
4.1970
4.0802
4.0639
4.0397
3.7745
3.7581
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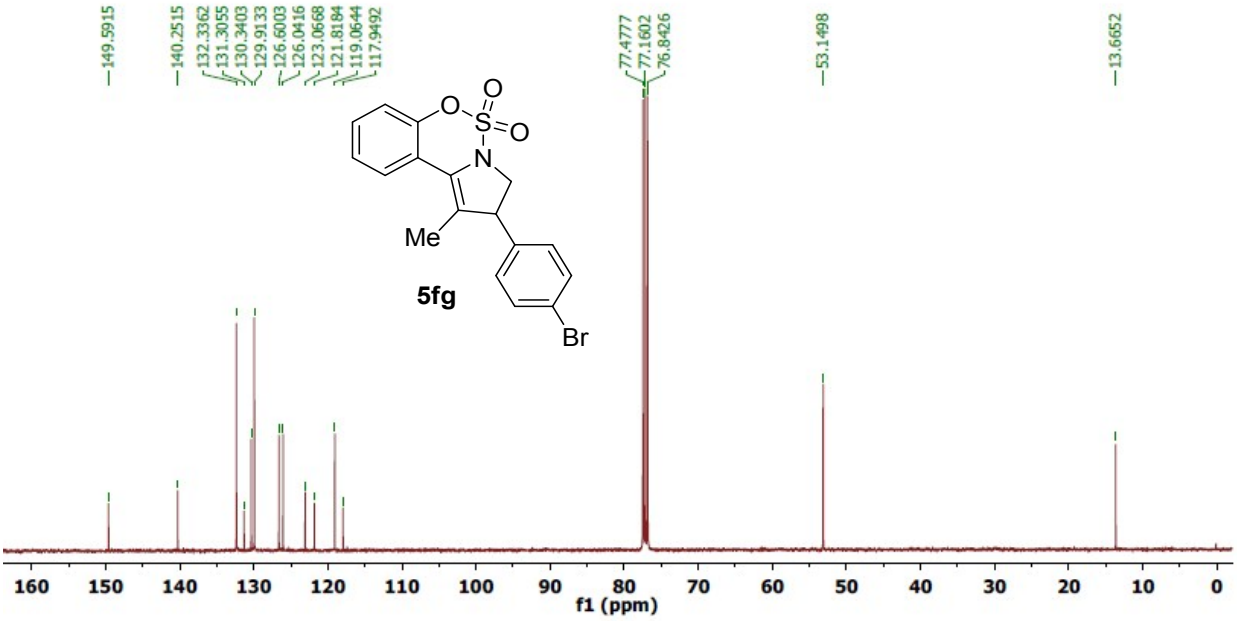
3.7336
1.9332
Me
5fg
Br
8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
1.06
2.00
0.99
1.05
2.98
1.13
1.16
1.16
3.45
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.8184
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117.9492
77.4777
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53.1498
13.6652
Me
5fg
Br
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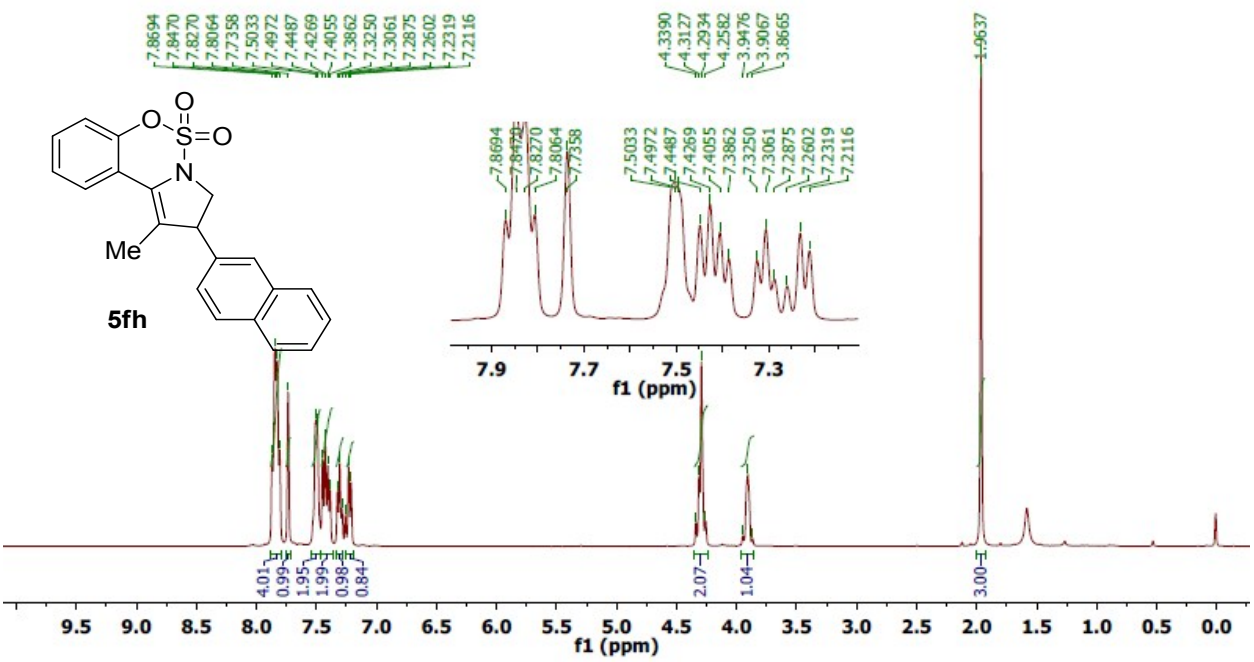
f1 (ppm)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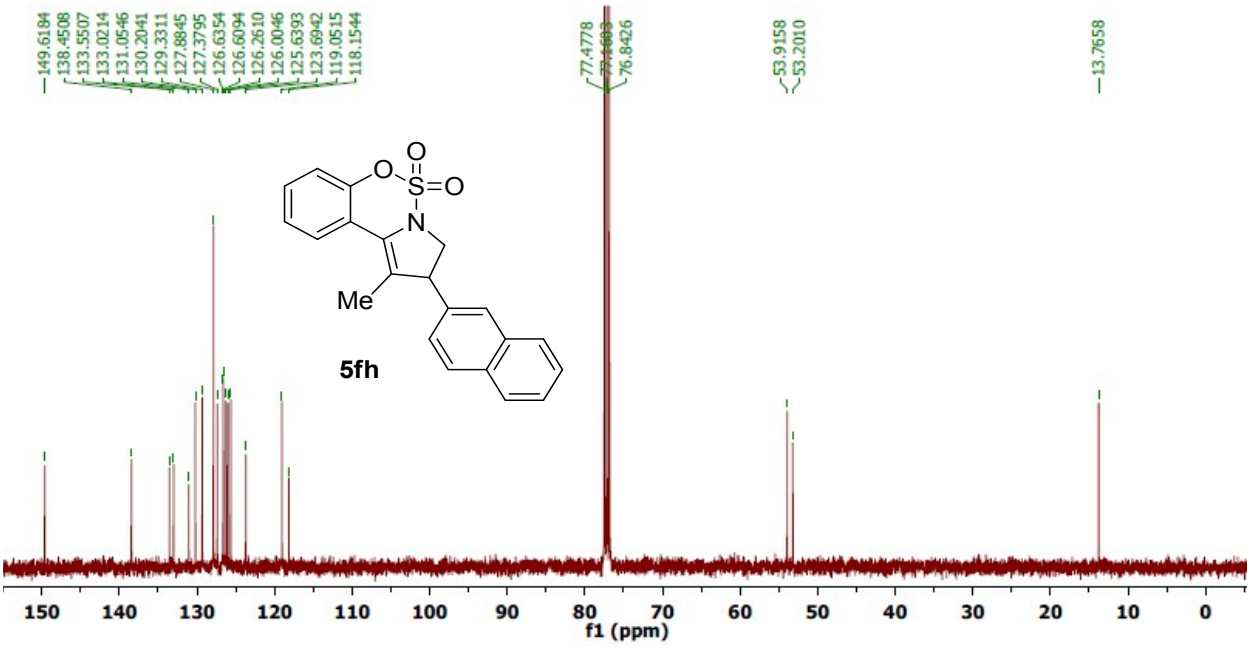
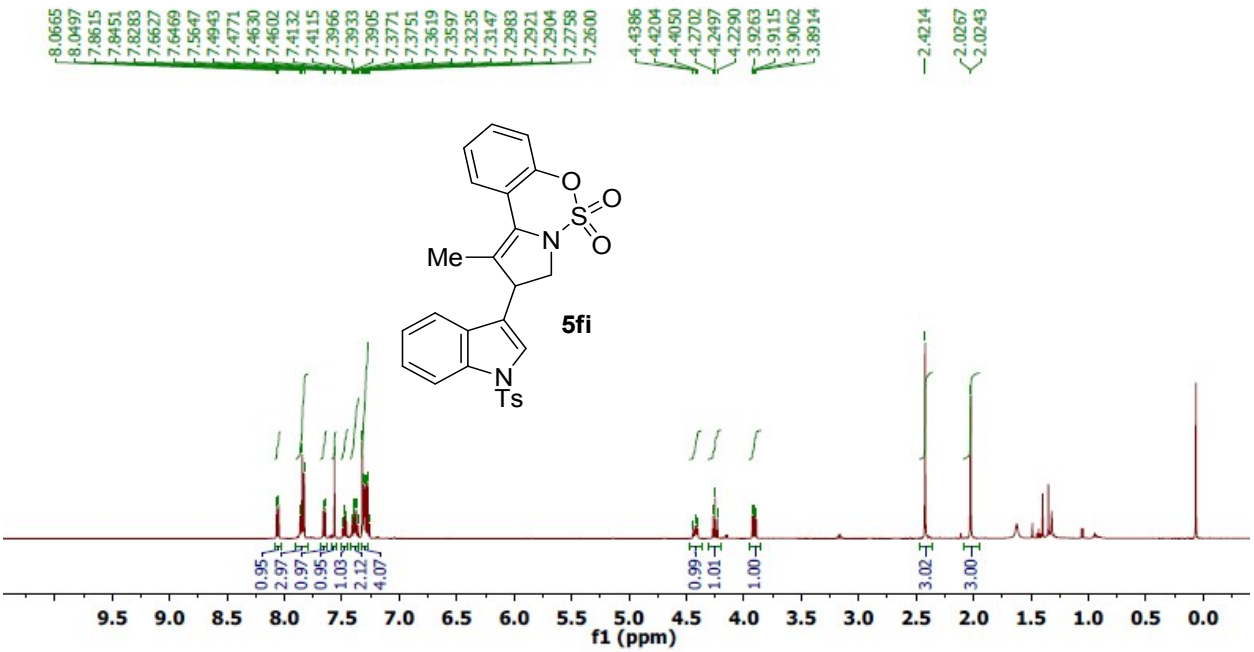

5fh
f1 (ppm)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7.4602
7.4132
7.4115
7.3966
7.3933
7.3905
7.3771
7.3751
7.3619
7.3597
7.3235
7.3147
7.2983
7.2921
7.2904
7.2758
7.2600
4.4386
4.4204
4.4050
4.2702
4.2497
4.2290
3.9263
3.9115
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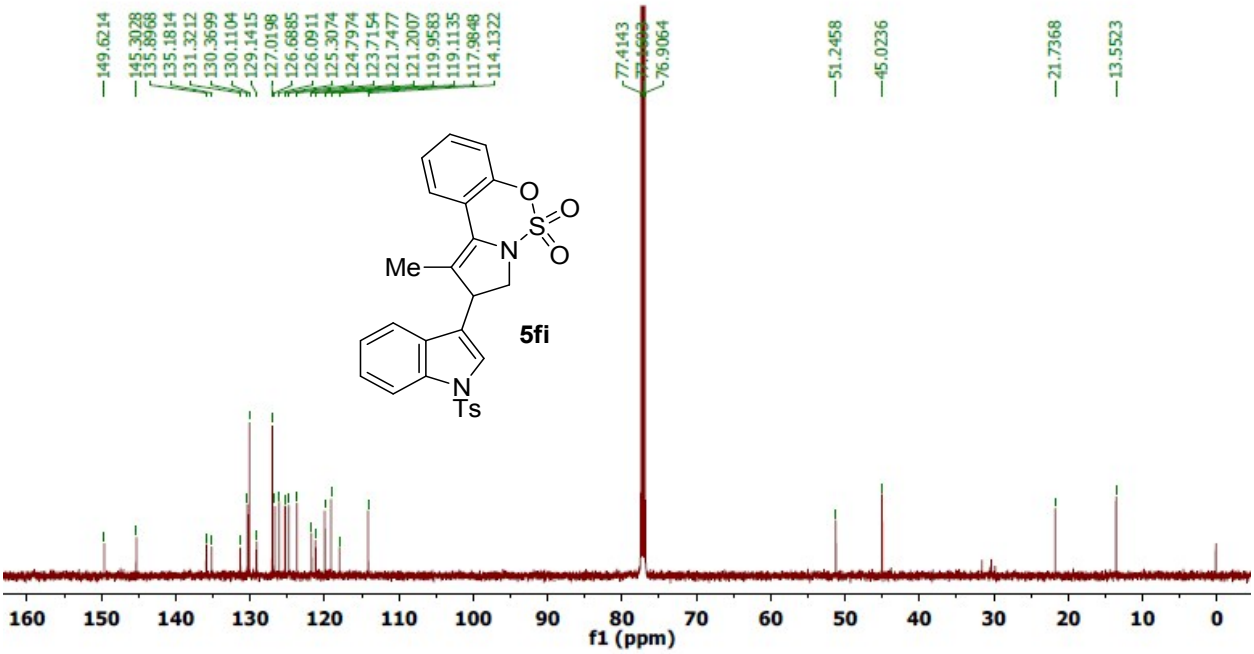
2.4214
2.0267
2.0043
O
S
O
O
N
Me
5fi
N
Ts
0.95
2.97
0.97
0.95
1.03
2.12
4.07
0.99
1.01
1.00
3.02
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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119.1135
117.9848
114.1322
77.4143
77.1603
76.9064
51.2458
45.0236
21.7368
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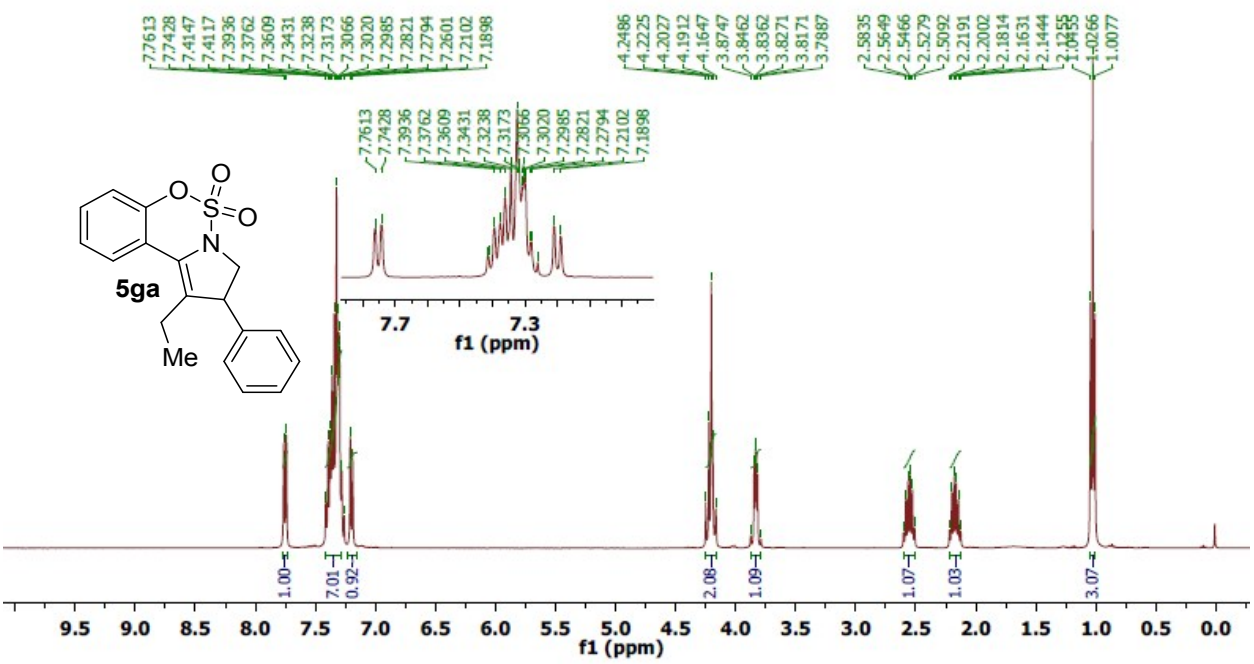
O
O
N
Me
5fi
N
Ts
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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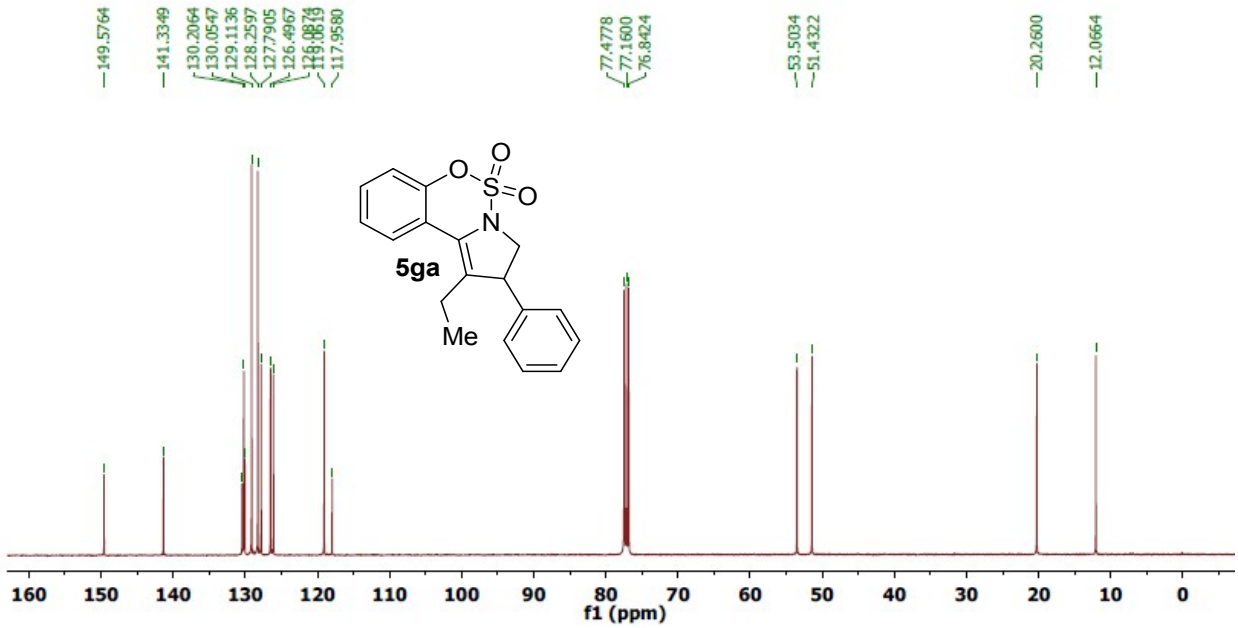
5ga
Me
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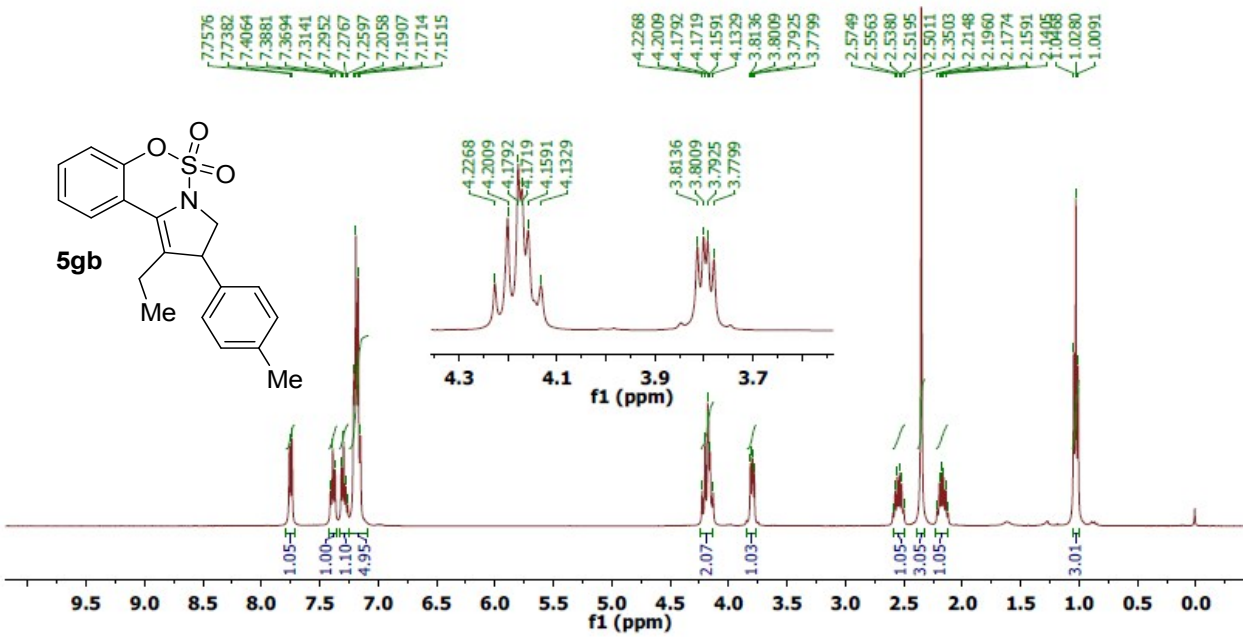
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Me
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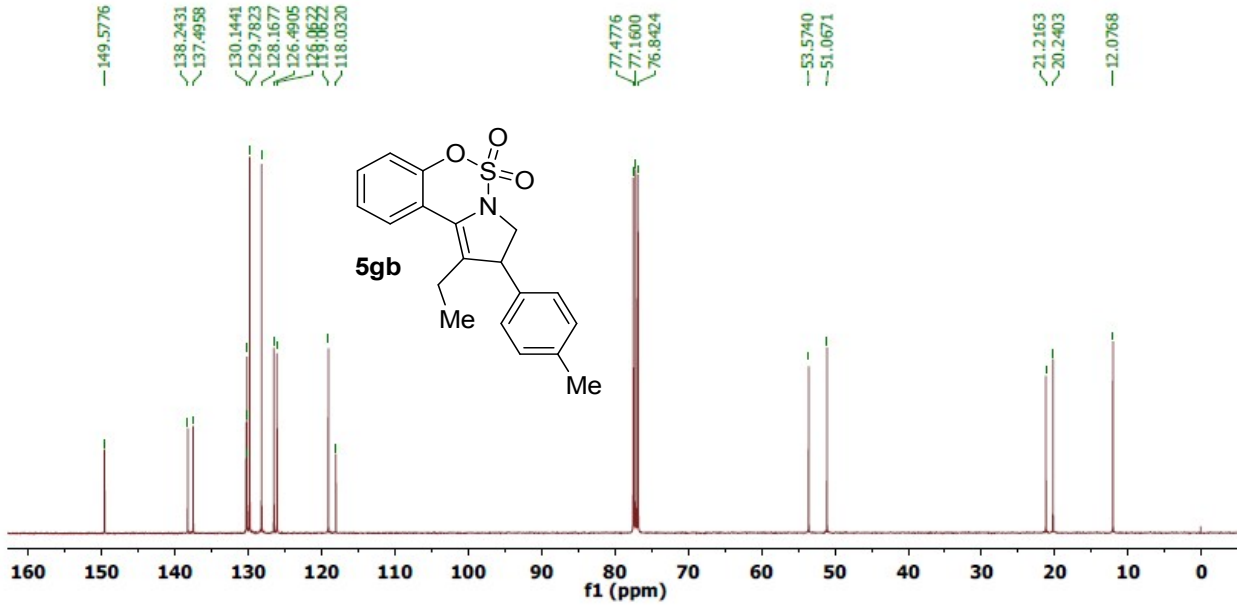
f1 (ppm)
f1 (ppm)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Me
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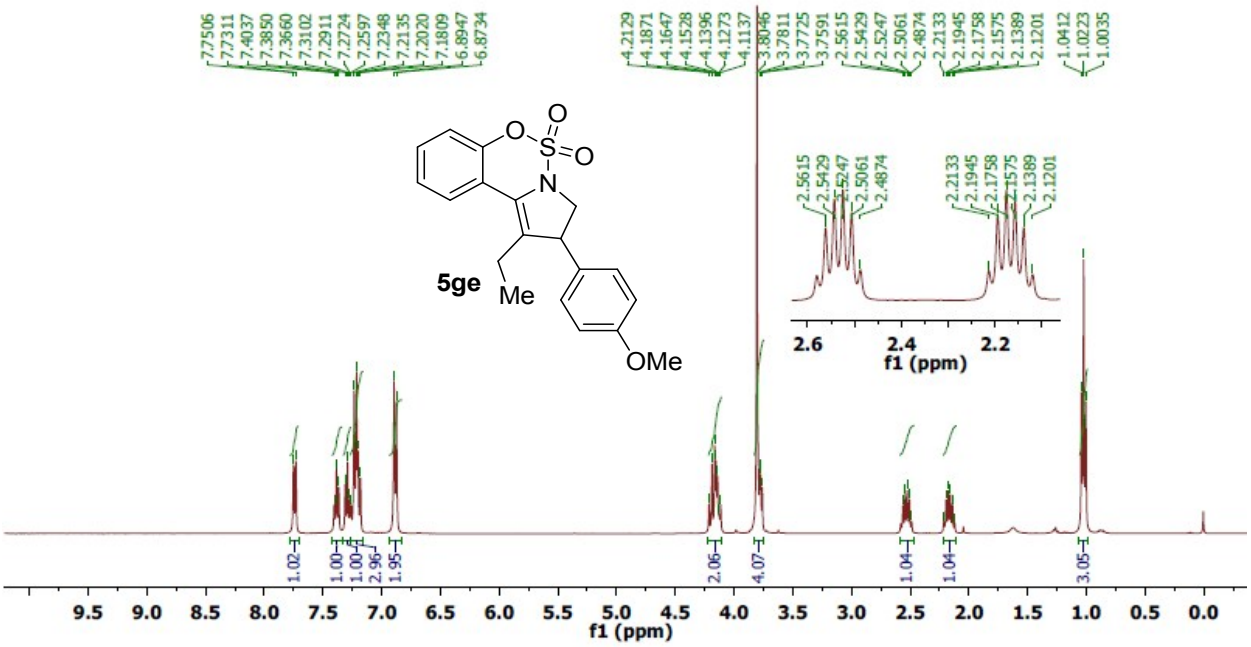
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7.2020
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6.8947
6.8734
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4.1647
4.1528
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4.1273
4.1137
3.8046
3.7811
3.7725
3.7591
2.5615
2.5429
2.5247
2.5061
2.4874
2.2133
2.1945
2.1758
2.1575
2.1389
2.1201
1.0412
1.0223
1.0035
5ge
Me
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1.00
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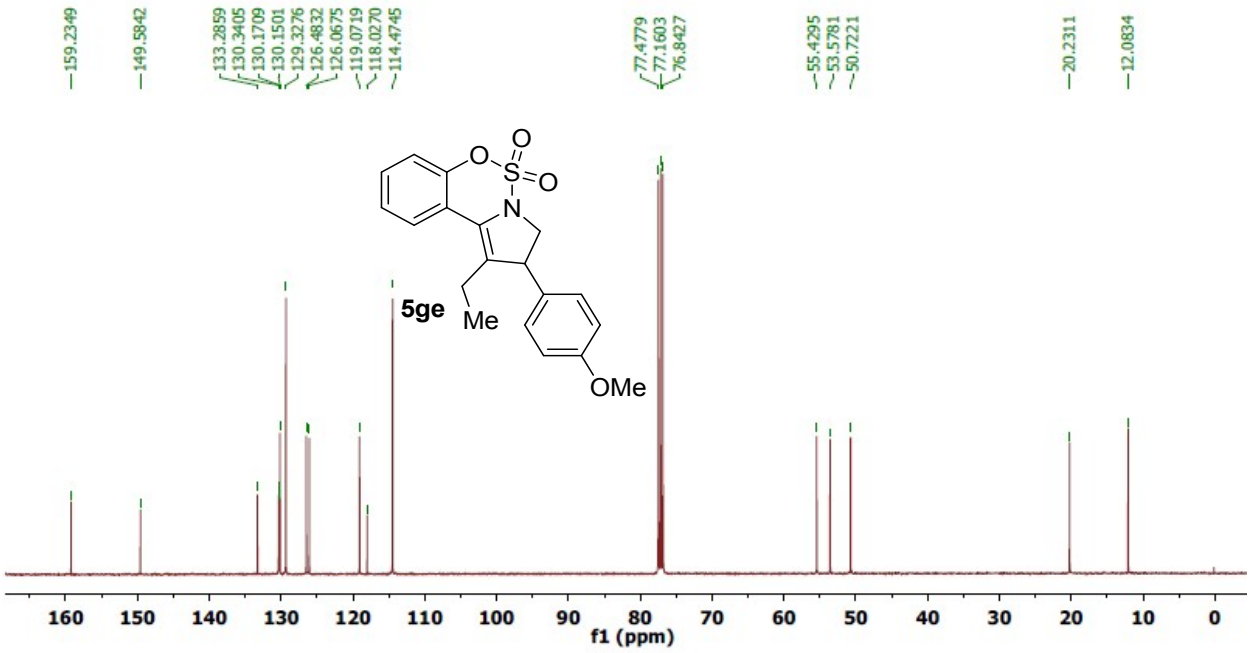
1.95
2.06
4.07
1.04
1.04
3.05
f1 (ppm)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77.4779
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12.0834
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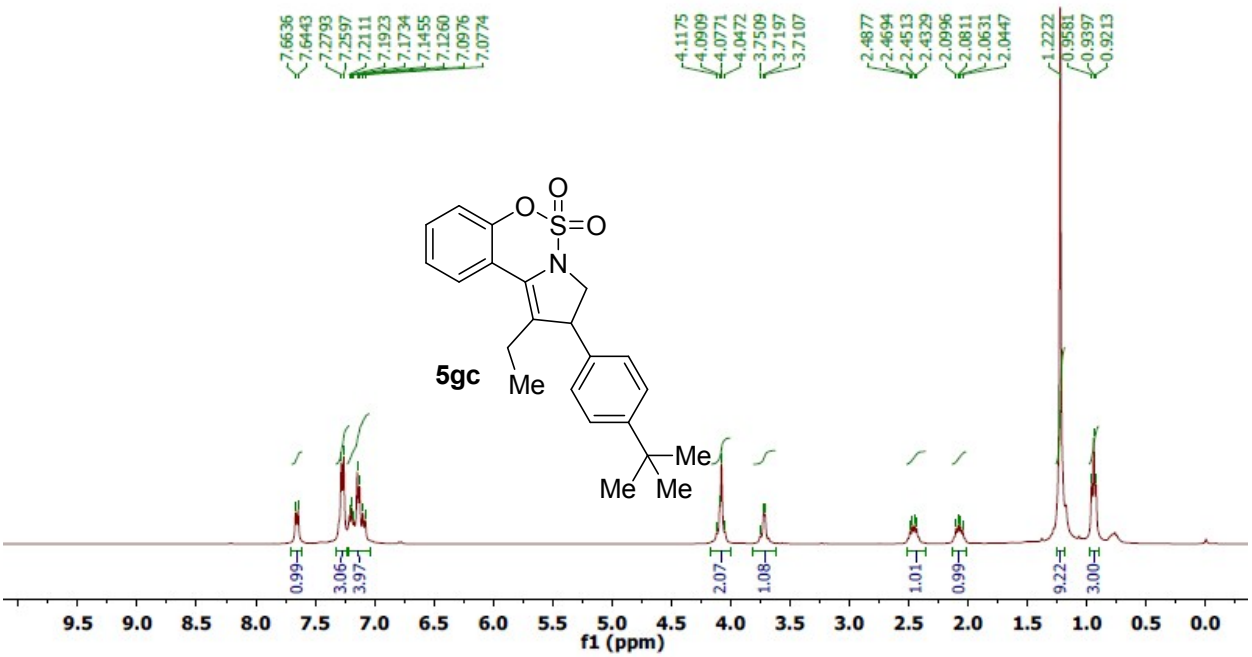
Me
OMe
f1 (ppm)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2.4329
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2.0811
2.0631
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0.9397
0.9213
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O
S=O
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Me
Me
Me
Me
0.99
3.06
3.97
2.07
1.08
1.01
0.99
9.22
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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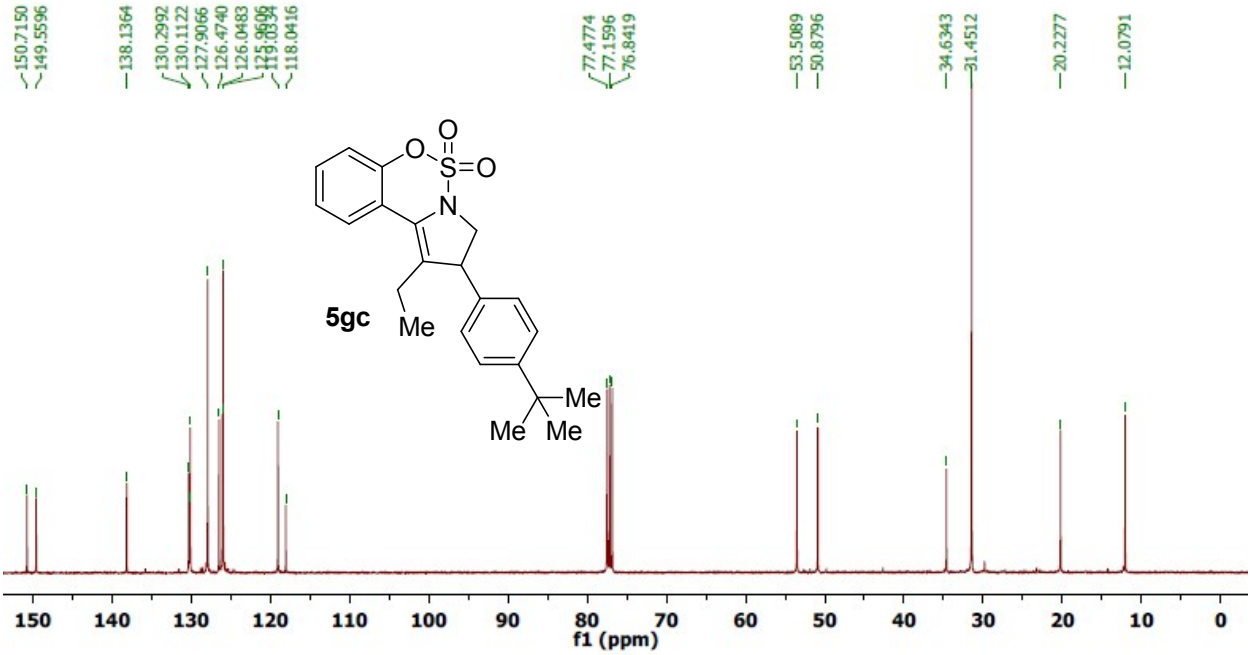
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53.5089
50.8796
34.6343
31.4512
20.2277
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S=O
N
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Me
Me
Me
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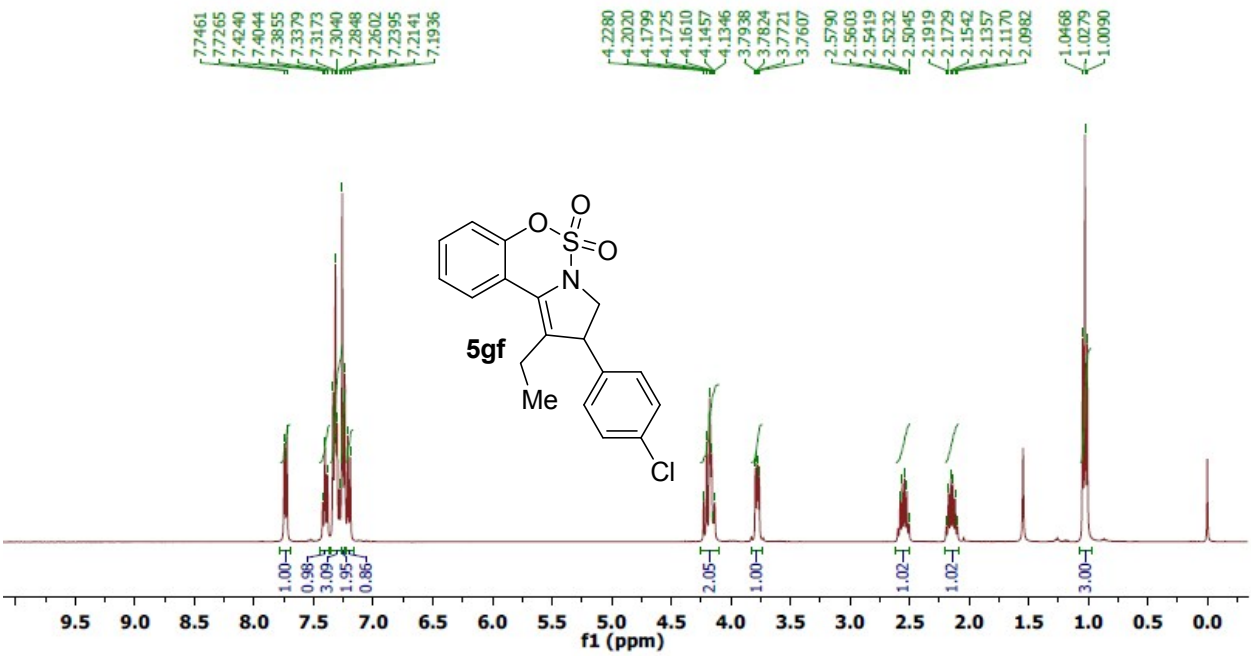
f1 (ppm)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5gf
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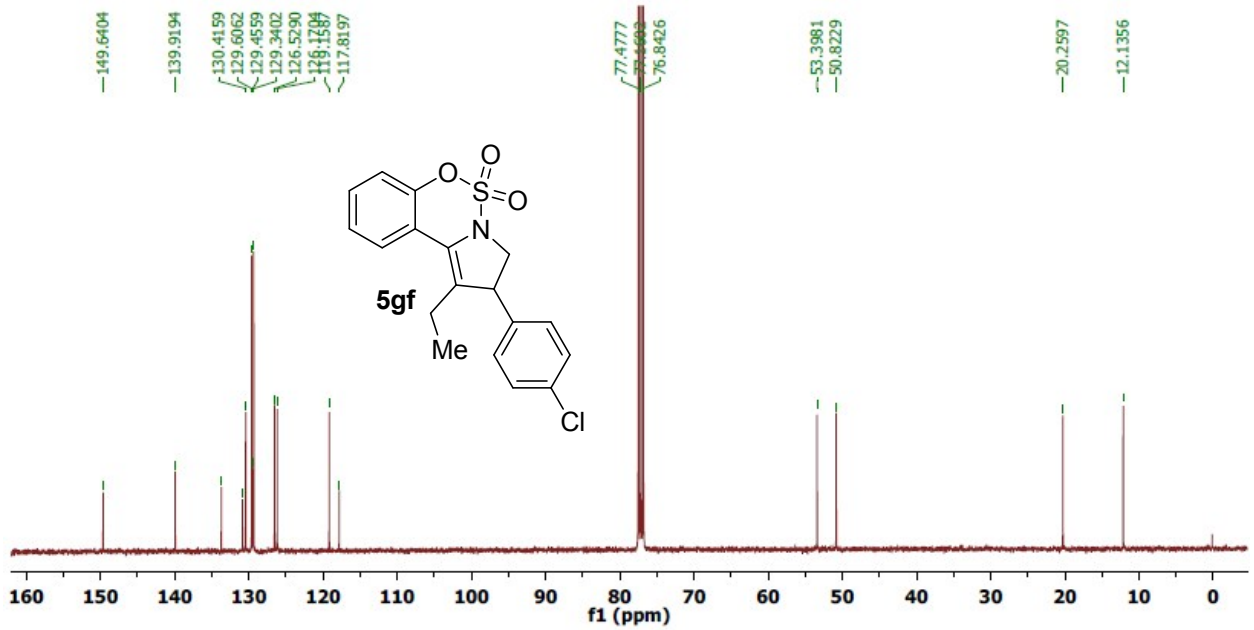
3.00
f1 (ppm)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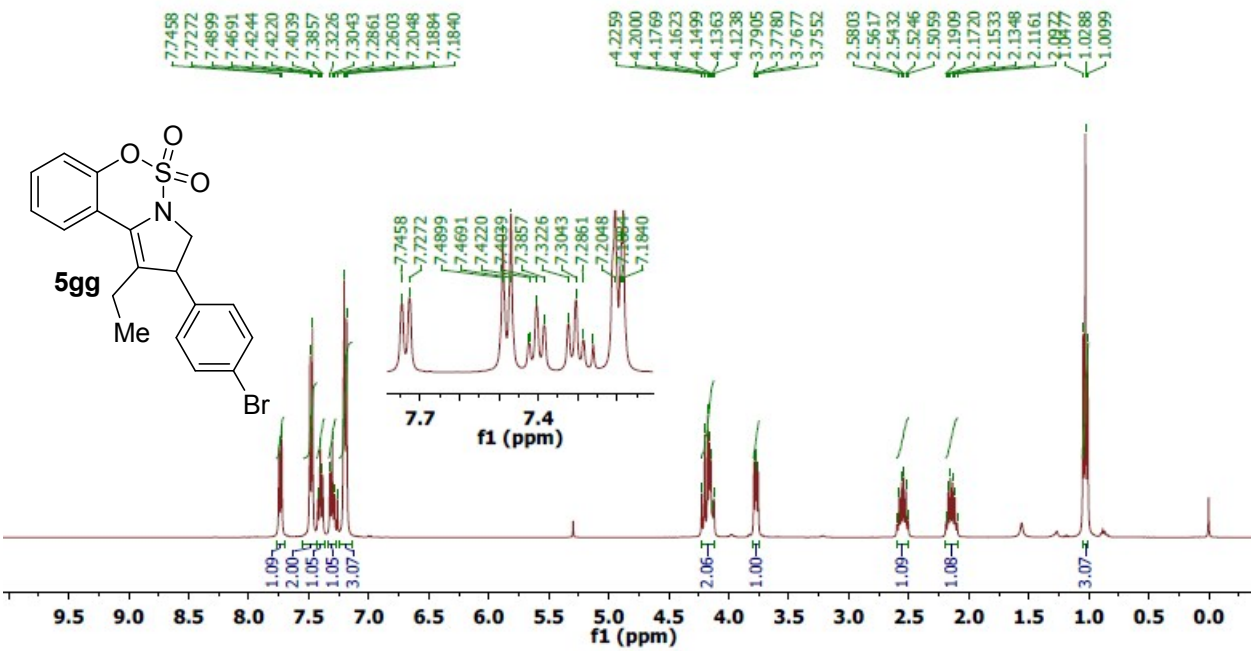
Me
Cl
f1 (ppm)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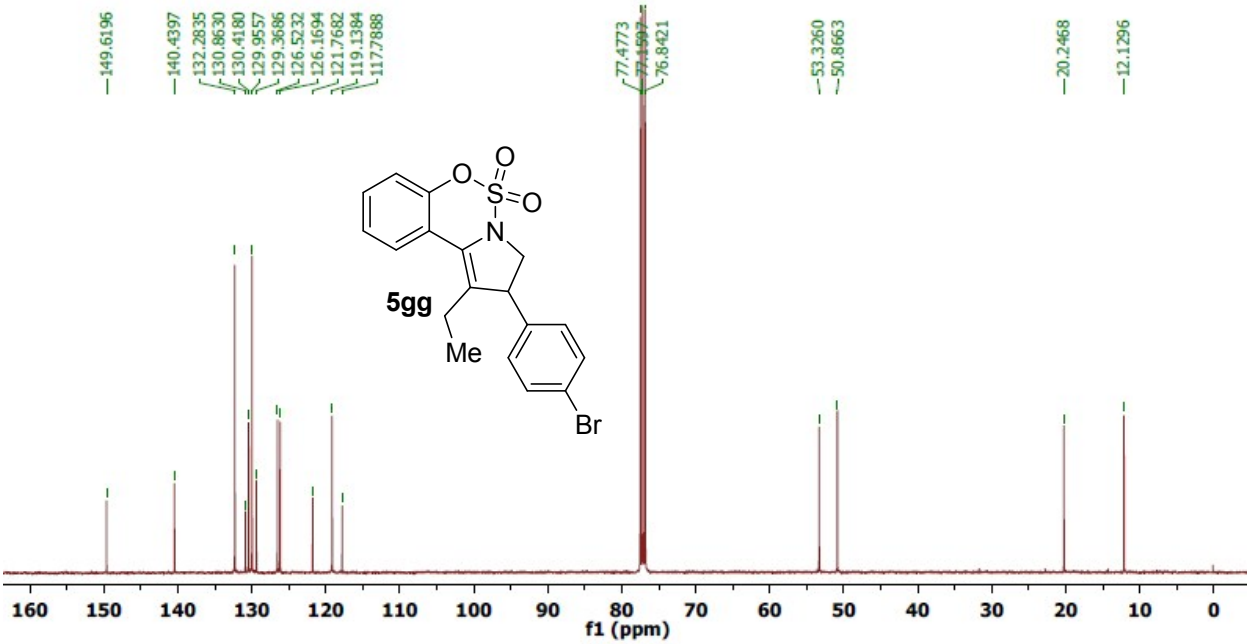
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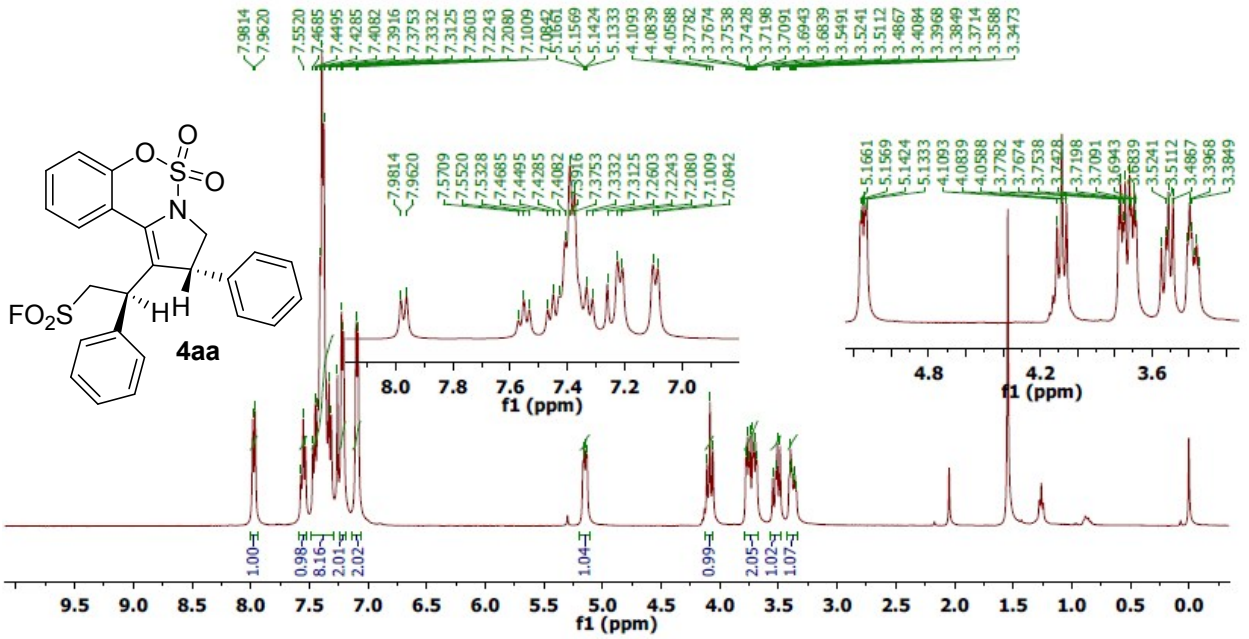
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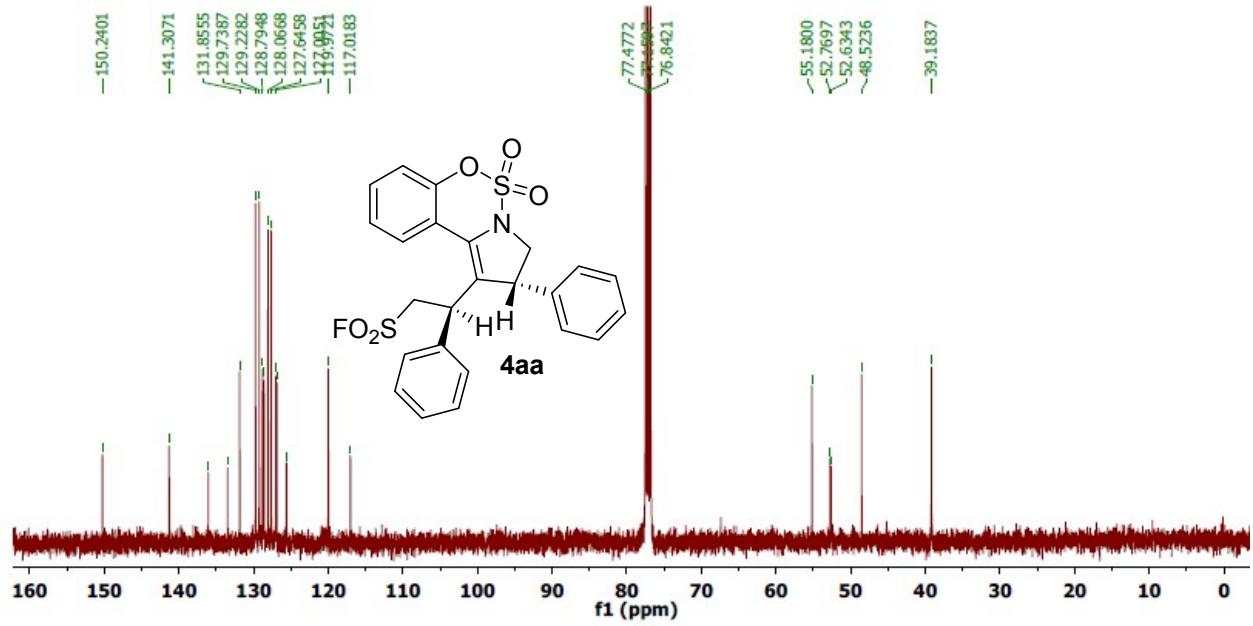
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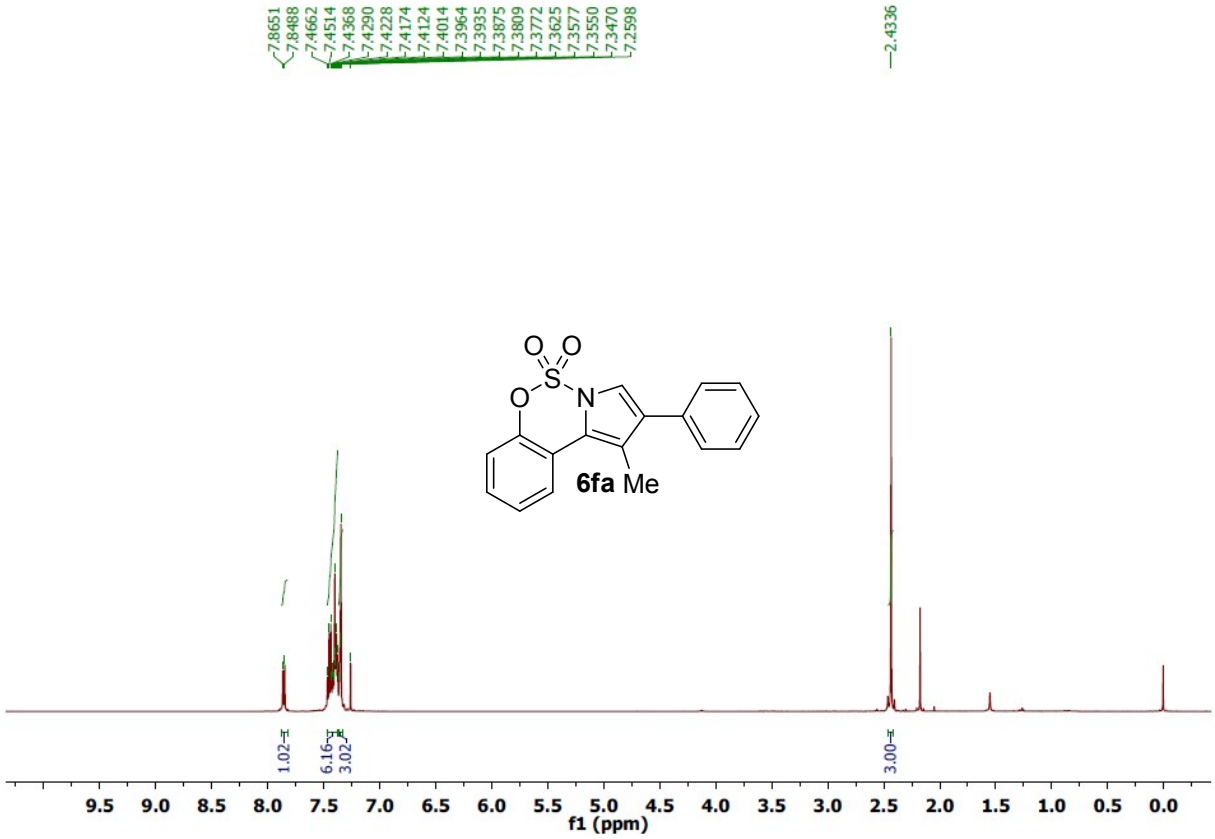
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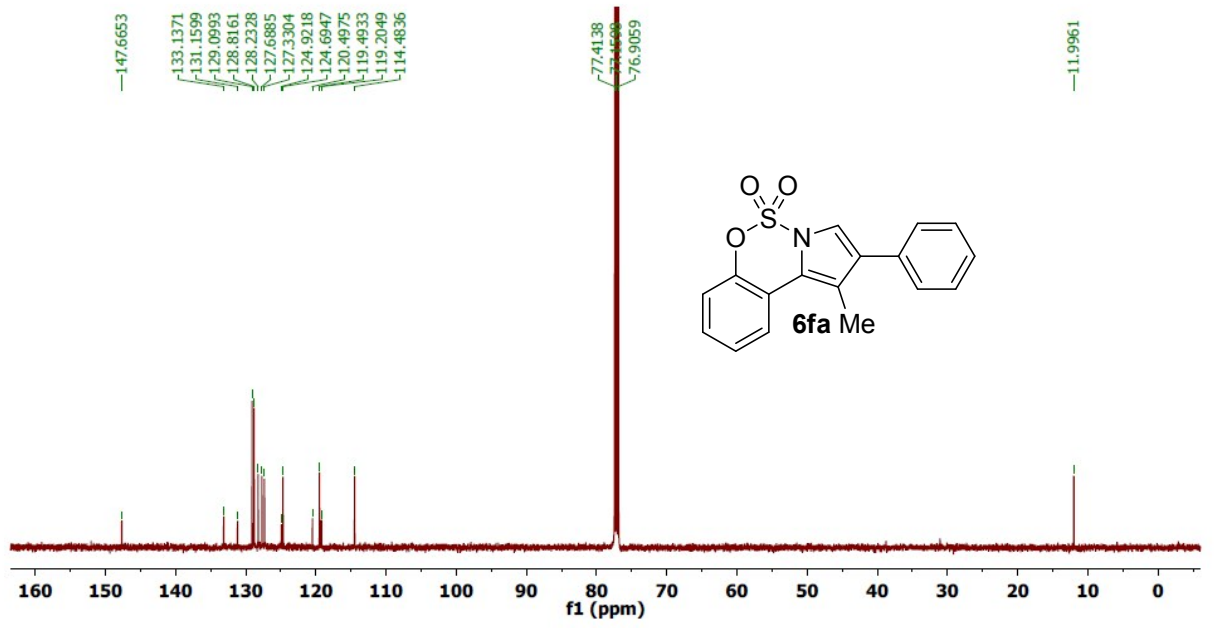
f1 (ppm)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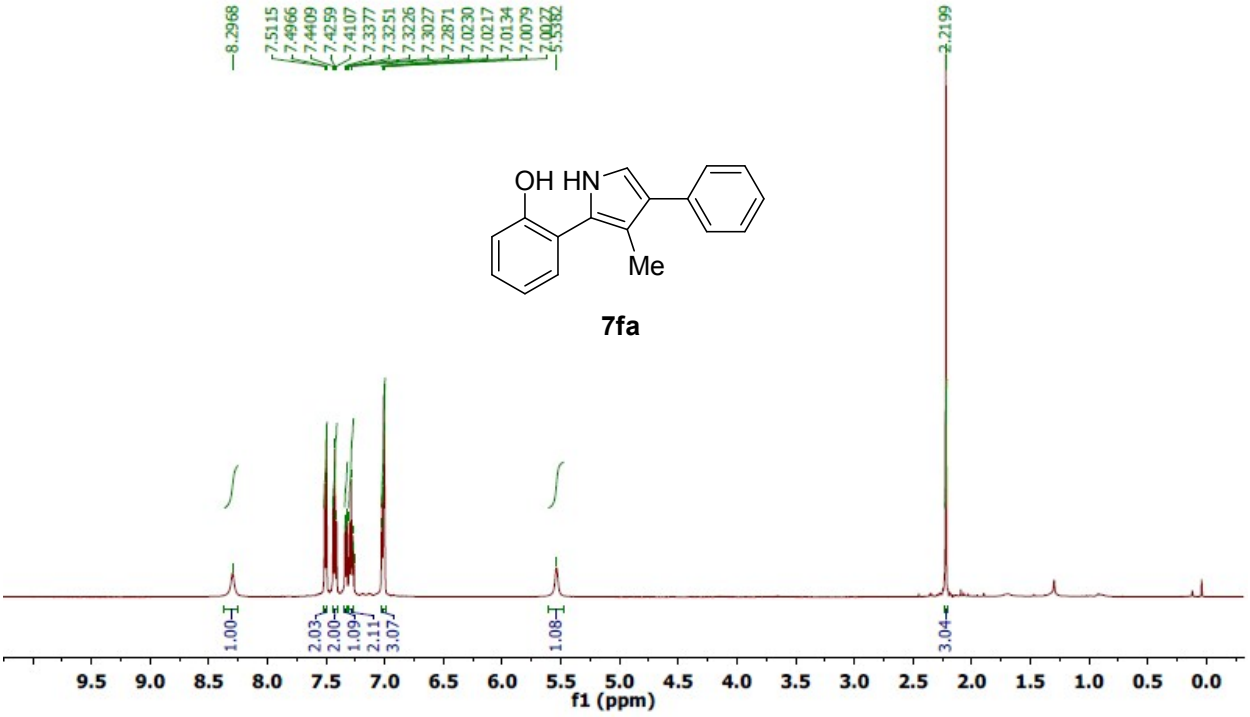
6fa Me
f1 (ppm)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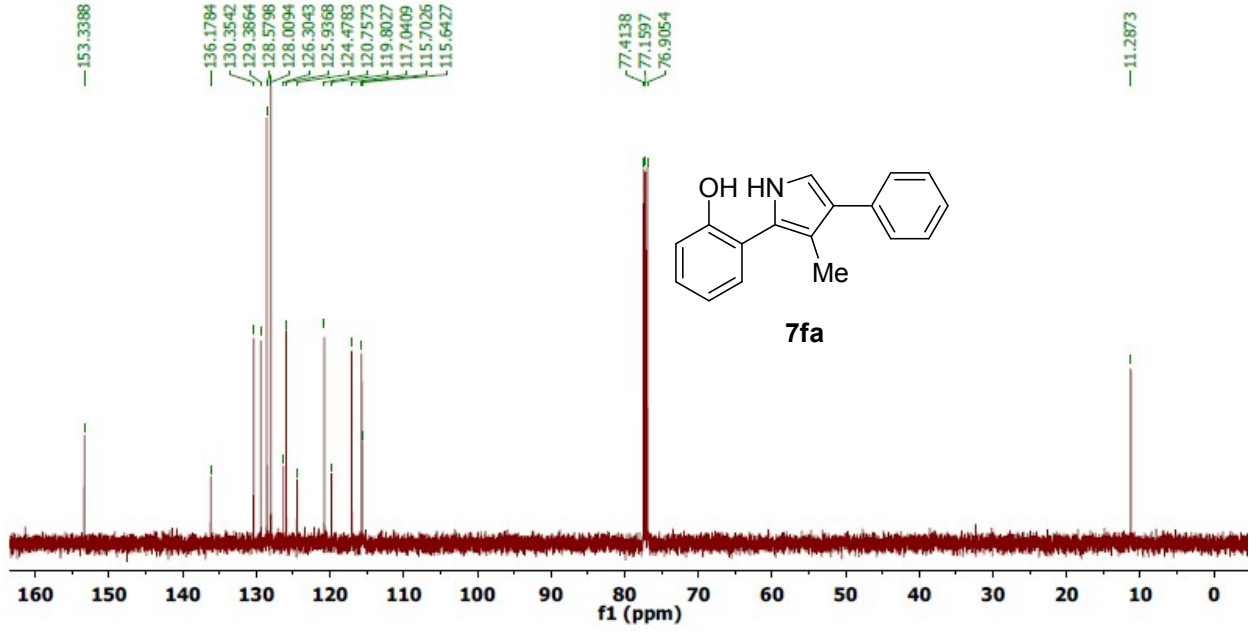
7.0217
7.0134
7.0079
5.3382
2.2199
OH HN
Me
1.00
2.03
2.00
1.09
2.11
3.07
1.08
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

7fa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117.0409
115.7026
115.6427
77.4138
77.1597
76.9054
11.2873
OH HN
Me
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

7fa