Supporting Information

Cp*Ir(III)-catalyzed C–H functionalization of sulfoximines for the synthesis of 1,2-benzothiazines at room temperature

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Table of Content S-1

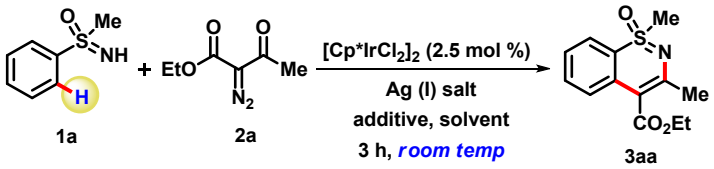
1. General Methods

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F254 plates. Visualization via TLC was achieved by the use of UV light (254 nm). Column chromatography was undertaken on silica gel (100−200 mesh) using a proper eluent system. NMR spectra were recorded in chloroform-d at 300, 400 or 500 MHz for ^{1}H NMR spectra and 75, 100 or 125 MHz for ^{13}C NMR spectra. Chemical shifts are quoted in parts per million referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, m = multiplet. Coupling constants, J, are reported in hertz. For ^{13}C NMR, chemical shifts are reported in parts per million referenced to the center of a triplet at 77.0 ppm of chloroform-d. HRMS spectra were recorded using ESI-TOF techniques. [Cp*Co(CO)I_2] was synthesized according to the literature.[1] sulfoxomines[2] and diazo compounds[3] were prepared according to the procedure described in the literature.

2. Experimental Procedure of the Optimization Study

To a screw capped vial with a spinvane triangular-shaped Teflon stirbar were added sulfoximne **1a** (15.5 mg, 0.10 mmol), diazo compound **2a** (18.7 mg, 0.12 mmol), $[Cp^*IrCl_2]_2$ (2.0 mg, 2.5 mol %), additive, and solvent (0.5 mL) under air atomosphere. The reaction mixture was stirred at room temeperature for 3 h. After indicated time, the reaction mixture was filtered through a pad of celite and the celite pad was washed with $CHCl_3$ (10 mL × 2). Solvents were removed under reduced pressure and crude yield was measured by ^1H NMR using an internal standard (1,1,2,2-tetrachloroethane).

Table S1. *Optimization of the Ir-Catalyzed C−H Functionalization of Sulfoximines*[a]



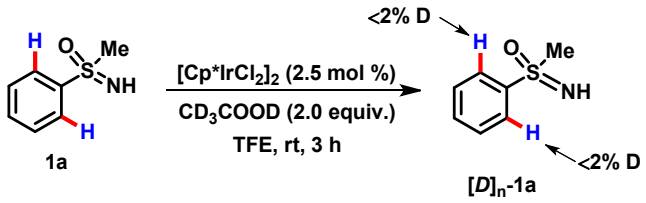
entry	Ag(I) salt (10 mol %)	Additive (equiv.)	Solvent	Yield (%)[b]
1	$AgSbF_6$	-	TFE	23
2	$AgSbF_6$	AcOH (1.0)	TFE	94
3	-	AcOH (1.0)	TFE	77
4	-	AcOH (2.0)	TFE	90
5	**-**	**PivOH (2.0)**	**TFE**	**96 (90)**
6	-	$AdCO_2H$ (2.0)	TFE	82
7	-	$PhCO_2H$ (2.0)	TFE	78
8	-	PivOH (2.0)	MeOH	81
9	-	PivOH (2.0)	1,2-DCE	18
10	-	PivOH (2.0)	1,4-Dioxane	n.d.
11	-	PivOH (2.0)	THF	n.d.
12	-	NaOAc (2.0)	TFE	12
13	-	KOAc (2.0)	TFE	15
14[c]	-	PivOH (2.0)	TFE	n.d.
15[d]	-	PivOH (2.0)	TFE	14
16[e]	-	PivOH (2.0)	TFE	12
17[f]	-	PivOH (2.0)	TFE	n.d.

[a]Reaction conditions: **1a** (0.10 mmol), **2a** (0.12 mmol), $[Cp^*IrCl_2]_2$ (2.5 mol %), $AgSbF_6$ (10 mol %) and additive in solvent (0.5 mL) at room temperature for 3 h. [b]Yields are based on crude ^1H NMR (internal standard: 1,1,2,2 tetrachloroethane). [c]Without $[Cp^*IrCl_2]_2$. [d]Using $[Cp^*RhCl_2]_2$ (2.5 mol %). [e]Using $[Ru(p\text{-Cymene})Cl_2]_2$ (2.5 mol %). [f]Using $[Cp^*Co(CO)I_2]$ (5.0 mol %). n.d. = not detected. TFE = 2,2,2-Trifluoroethanol.

3. H/D Exchange Experiment

Iridium-Catalyzed H/D Exchange in NH-Sulfoximine 1a with CD_3COOD as an additive

To a dried screw capped vial with a spinvane triangular-shaped Teflon stirbar were added **1a** (15.5 mg, 0.10 mmol), $[Cp^*IrCl_2]_2$ (2.0 mg, 2.5 mol %), CD_3COOD (2.0 equiv) and TFE (0.5 mL). The reaction mixture was stirred at room temperature for 3 h, filtered through a pad of celite and the celite pad was washed with $CHCl_3$ (10 mL × 2). The solvent was removed under reduced pressure and the extents of deuterium incorporation was measured by ^1H NMR analysis of the crude mixture.



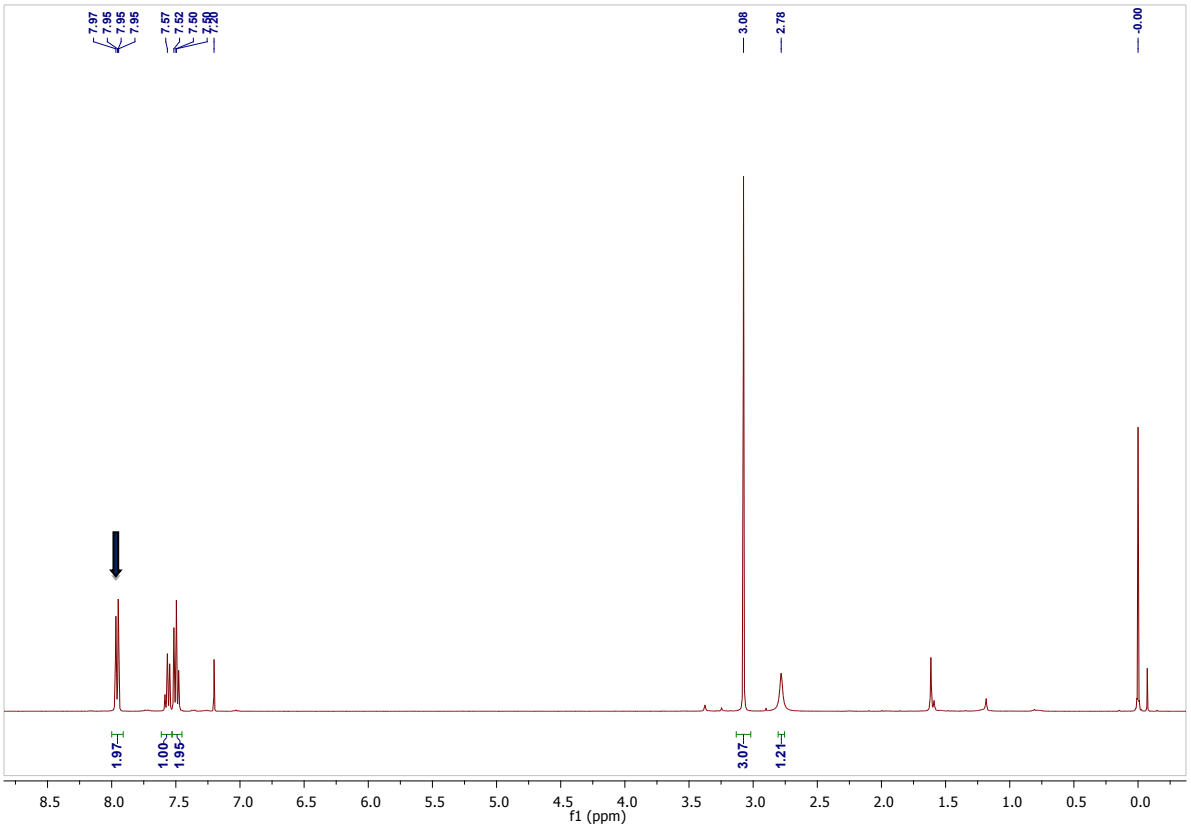
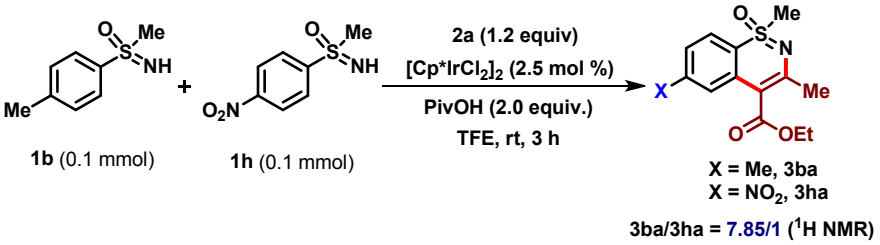


Figure S1. Crude ^1H NMR for H/D exchange experiment of **1a** with CD_3COOD in absence of **2a.**

4. Intermolecular Competitive Experiment



To a dried screw capped vial with a spinvane triangular-shaped Teflon stirbar were added **1b** (16.9 mg, 0.10 mmol), **1h** (20.0 mg, 0.10 mmol), ethyl diazoacetate **2a** (18.7 mg, 0.12 mmol), $[Cp^*IrCl_2]_2$ (2.0 mg, 2.5 mol %), PivOH (20.4 mg, 2.0 equiv.), and TFE (0.5 mL) under air atmosphere. The reaction mixture was stirred at room temperature for 3 h, filtered through a pad of celite and then the celite pad was washed with $CHCl_3$ (10 mL × 2). The combined organic layers were removed under reduced pressure. The solvent was evaporated under reduced pressure and dried under vacuo. The crude ^{1}H NMR was recorded to determine the ratio of the products **3ba** and **3ha**.

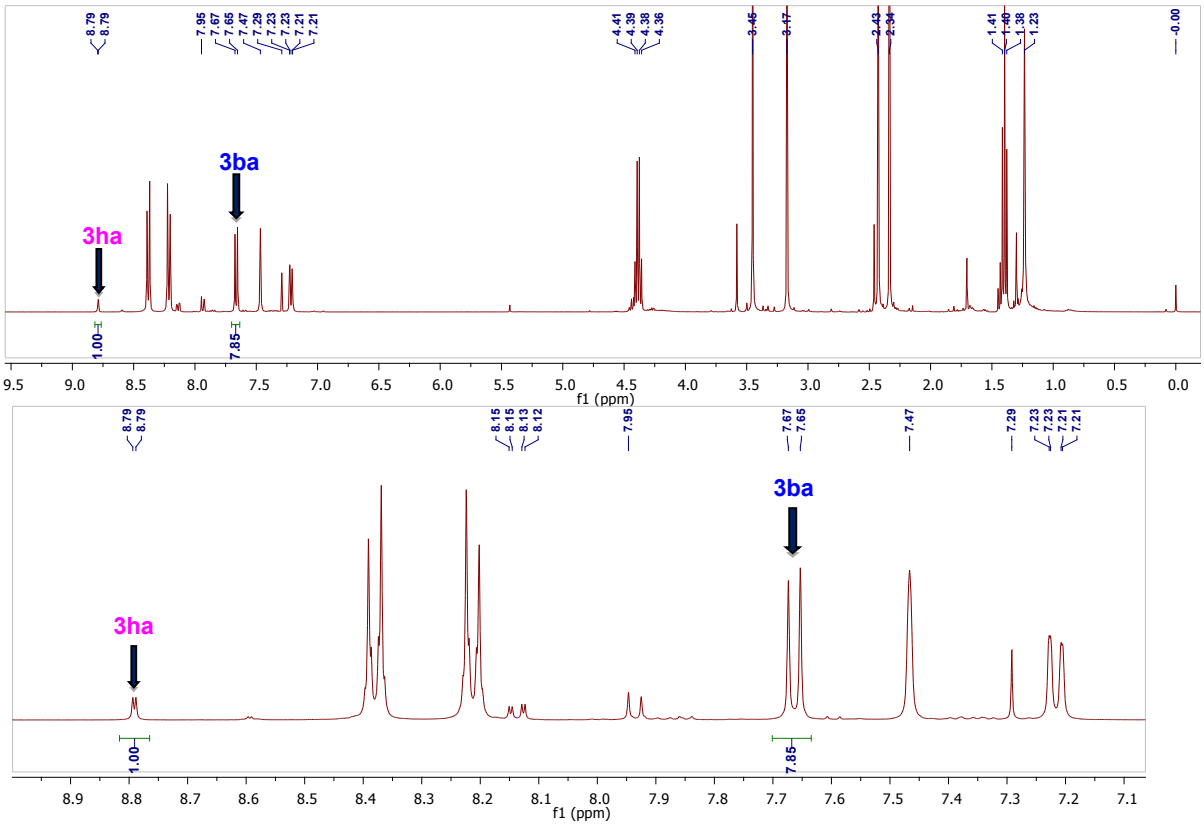
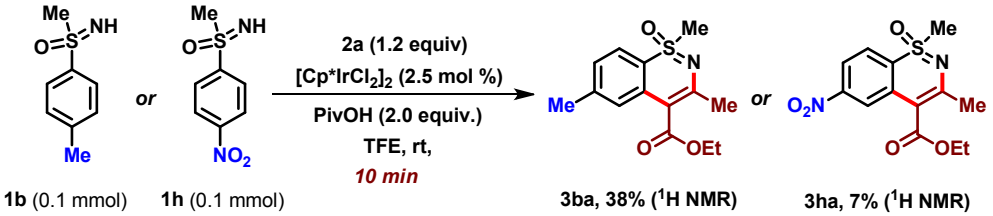


Figure S2. Crude ^{1}H NMR for intermolecular competitive experiment between **3b** and **3h**.

5. Procedure for comparing reaction rates of 3ba and 3ha

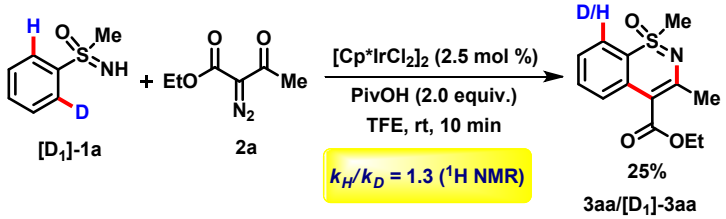


1b (0.1 mmol) **1h** (0.1 mmol) **3ba, 38% (^{1}H NMR)** **3ha, 7% (^{1}H NMR)**

RATE of 3ba: To a dried screw capped vial with a spinvane triangular-shaped Teflon stirbar were added **1b** (16.9 mg, 0.10 mmol), ethyl diazoacetate **2a** (18.7 mg, 0.12 mmol), $[Cp^*IrCl_2]_2$ (2.0 mg, 2.5 mol %), PivOH (20.4 mg, 2.0 equiv.), and TFE (0.5 mL) under air atmosphere. The reaction mixture was stirred at room temperature for 10 min, filtered through a pad of celite and then the celite pad was washed with $CHCl_3$ (10 mL × 2). The combined organic layers were removed under reduced pressure. The solvent was evaporated under reduced pressure and dried under vacuo. The crude yield of **3ba** was measured by ^{1}H NMR using an internal standard (1,1,2,2-tetrachloroethane) which was found to be 38%.

RATE of 3ha: To a dried screw capped vial with a spinvane triangular-shaped Teflon stirbar were added **1h** (20.0 mg, 0.10 mmol), ethyl diazoacetate **2a** (18.7 mg, 0.12 mmol), $[Cp^*IrCl_2]_2$ (2.0 mg, 2.5 mol %), PivOH (20.4 mg, 2.0 equiv.), and TFE (0.5 mL) under air atmosphere. The reaction mixture was stirred at room temperature for 10 min, filtered through a pad of celite and then the celite pad was washed with $CHCl_3$ (10 mL × 2). The combined organic layers were removed under reduced pressure. The solvent was evaporated under reduced pressure and dried under vacuo. The crude yield of **3ha** was measured by ^{1}H NMR using an internal standard (1,1,2,2-tetrachloroethane) which was found to be 7%.

6. Intramolecular Kinetic Isotope Effect Experiments



To a dried screw capped vial with a spinvane triangular-shaped Teflon stirbar were added **[D_1]-1a** (15.6 mg, 0.10 mmol), ethyl diazoacetate **2a** (18.7 mg, 0.12 mmol), [Cp*$IrCl_2$]$_2$ (2.0 mg, 2.5 mol %), PivOH (20.4 mg, 2.0 equiv.), and TFE (0.5 mL) under air atmosphere. The reaction mixture was stirred at room temperature for 10 min, filtered through a pad of celite and then the celite pad was washed with $CHCl_3$ (10 mL × 2). The combined organic layers were removed under reduced pressure. The residue was purified by column chromatography to afford the desired **3aa** and **[D_1]-3aa**. **KIE = 1.3**.

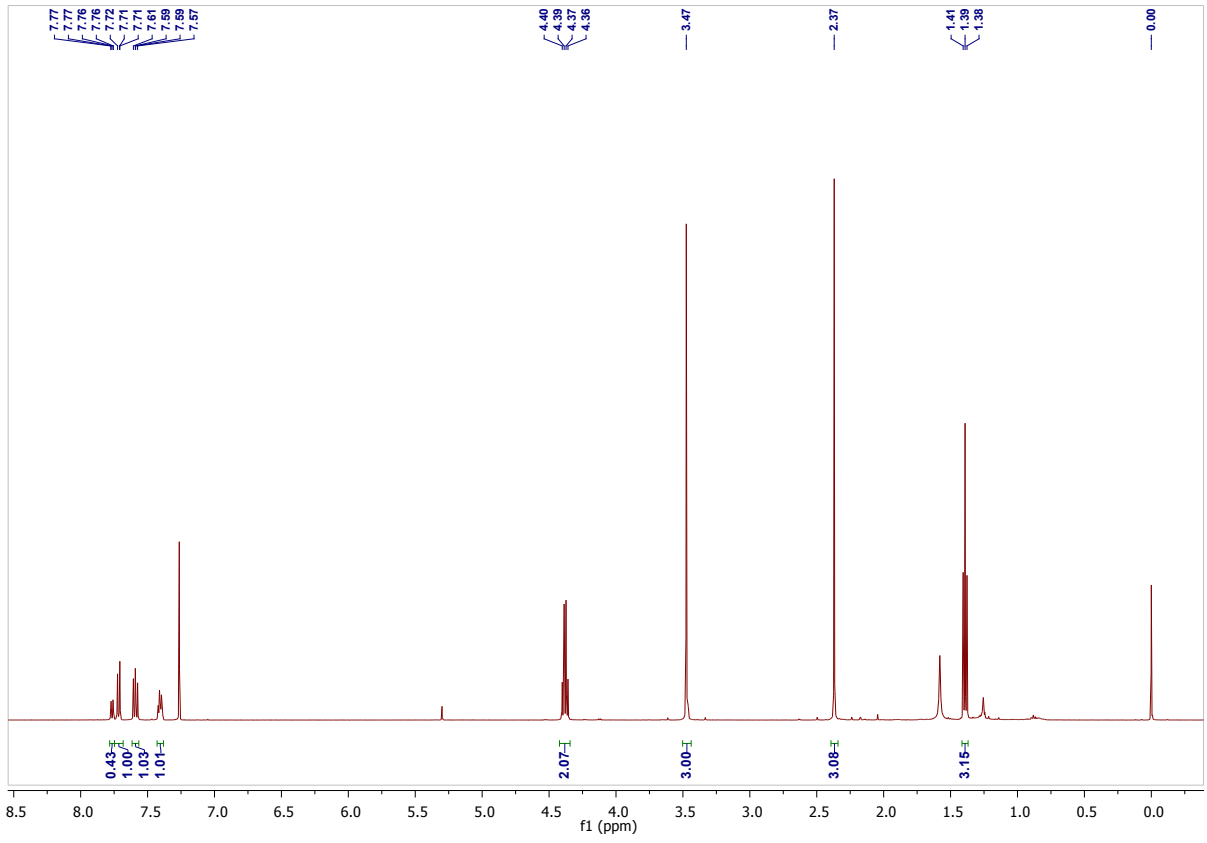


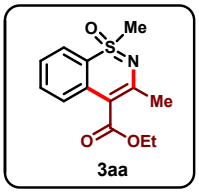
Figure S3. ^{1}H NMR for Intramolecular KIE Study.

7. General Procedure for the Ir-Catalyzed C–H Functionalization of Sulfoximines for the Synthesis of 1,2-Benzothaizines

To a screw capped seal tube vial with a Teflon stirbar were added sulfoximine **1** (0.40 mmol), diazo compound **2** (0.60 mmol, 1.2 equiv), $[Cp^*IrCl_2]_2$ (8.0 mg, 2.5 mol %), PivOH (81.6 mg, 2.0 equiv.), and TFE (2.0 mL) under air atmosphere. The reaction mixture was stirred at room temperature for 3 h, filtered through a pad of celite and then the celite pad was washed with $CHCl_3$ (10 mL × 2). The solvents were removed under reduced pressure and the residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc) to give the desired 1,2-benzothaizne derivatives.

8. Spectroscopic Data of 1,2-Benzothiazines Obtained in this Study

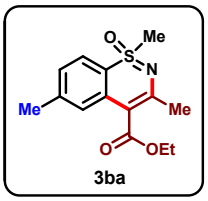
Ethyl 1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3aa).[4]



3aa

Pale yellow solid (95.0 mg, 90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.76 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.42 – 7.36 (m, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.47 (s, 3H), 2.37 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.6, 152.1, 134.1, 133.0, 126.0, 124.6, 123.4, 116.8, 105.2, 60.8, 45.1, 24.7, 14.2.

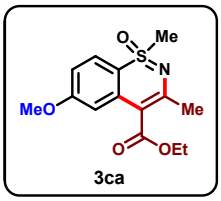
Ethyl 1,3,6-trimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ba).[4]



3ba

White solid (92.0 mg, 82%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.66 (d, *J* = 8.2 Hz, 1H), 7.47 (s, 1H), 7.21 (d, *J* = 8.2 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.44 (s, 3H), 2.42 (s, 3H), 2.34 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.8, 151.9, 143.9, 134.3, 127.4, 124.3, 123.5, 114.4, 104.9, 60.7, 45.5, 24.7, 22.1, 14.2.

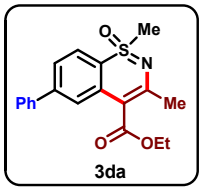
Ethyl 6-methoxy-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ca).[4]



3ca

Light yellow syrup (102.0 mg, 86%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.68 (d, *J* = 8.9 Hz, 1H), 7.21 (d, *J* = 2.4 Hz, 1H), 6.95 (dd, *J* = 8.9, 2.4 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.86 (s, 3H), 3.41 (s, 3H), 2.36 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.7, 163.0, 153.5, 136.8, 125.7, 115.1, 109.5, 106.2, 104.5, 60.6, 55.4, 45.8, 25.1, 14.2.

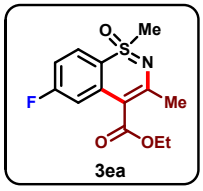
Ethyl 1,3-dimethyl-6-phenylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3da).



3da

White solid (119.0 mg, 87%); m.p. 105– 108 °C; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 (d, *J* = 1.6 Hz, 1H), 7.82 (d, *J* = 8.3 Hz, 1H), 7.63 – 7.57 (m, 3H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.44 – 7.39 (m, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.49 (s, 3H), 2.40 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.6, 152.8, 146.0, 139.8, 134.7, 128.9, 128.4, 127.4, 125.2, 124.1, 123.1, 115.4, 105.3, 60.8, 45.4, 24.9, 14.3; **HRMS (ESI)** m/z calcd. for $C_{19}H_{20}NO_3S$ $[M+H]^+$: 342.1164, found: 342.1161.

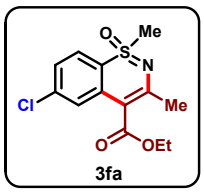
Ethyl 6-fluoro-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ea).



3ea

White solid (91.0 mg, 80%); m.p. 82– 85 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.78 (dd, *J* = 8.8, 5.5 Hz, 1H), 7.51 (dd, *J* = 11.7, 2.4 Hz, 1H), 7.11 (ddd, *J* = 8.8, 7.7, 2.5 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.45 (s, 3H), 2.39 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 165.1 (d, $J_{C\text{-}F}$ = 251.2 Hz), 154.6, 137.4 (d, $J_{C\text{-}F}$ = 11.0 Hz), 126.5 (d, $J_{C\text{-}F}$ = 10.3 Hz), 114.6 (d, $J_{C\text{-}F}$ = 24.5 Hz), 113.0, 110.5 (d, $J_{C\text{-}F}$ = 25.0 Hz), 104.6, 60.9, 45.6, 25.2, 14.2; **HRMS (ESI)** m/z calcd. for $C_{13}H_{15}FNO_3S$ $[M+H]^+$: 284.0757, found: 284.0760.

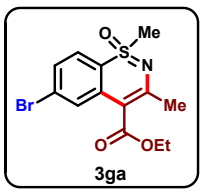
Ethyl 6-chloro-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3fa).[4]



3fa

White solid (100.0 mg, 83%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 1.9 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.35 (dd, *J* = 8.5, 1.9 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 3H), 2.38 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.1, 154.3, 139.7, 135.9, 126.4, 125.1, 124.3, 114.8, 104.4, 60.9, 45.3, 25.1, 14.2.

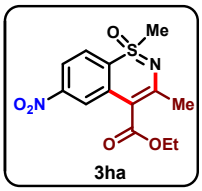
Ethyl 6-bromo-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ga).[4]



3ga

White solid (110.0 mg, 80%); **H NMR (400 MHz, $CDCl_3$)** δ 7.97 (d, *J* = 1.7 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.50 (dd, *J* = 8.5, 1.8 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 3H), 2.38 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.0, 154.3, 135.8, 129.1, 128.3, 127.3, 124.9, 115.2, 104.2, 60.9, 45.2, 25.1, 14.2.

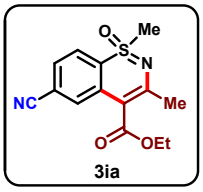
Ethyl 1,3-dimethyl-6-nitrobenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ha).[4]



3ha

Yellow solid (84.0 mg, 68%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.80 (d, *J* = 2.1 Hz, 1H), 8.15 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.92 (d, *J* = 8.7 Hz, 1H), 4.52 – 4.33 (m, 2H), 3.57 (s, 3H), 2.46 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.4, 156.3, 150.1, 135.6, 125.1, 120.9, 119.74, 119.70, 105.4, 61.2, 44.7, 25.4, 14.2.

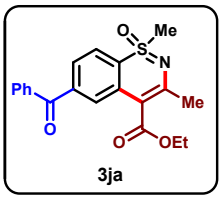
Ethyl 6-cyano-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ia).



3ia

Yellow solid (64.0 mg, 55%); m.p. 175– 178 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.23 (d, *J* = 1.1 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 1H), 7.60 (dd, *J* = 8.3, 1.4 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 3.53 (s, 3H), 2.43 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.6, 155.7, 134.7, 129.8, 127.6, 124.4, 118.7, 117.5, 116.8, 104.6, 61.2, 44.7, 25.4, 14.2; **HRMS (ESI)** m/z calcd. for $C_{14}H_{15}N_2O_3S$ $[M+H]^+$: 291.0803, found: 291.0807.

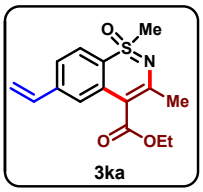
Ethyl 6-benzoyl-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ja).



3ja

Yellow Syrup (128.0 mg, 87%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 1.4 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.82 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.77 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.66 – 7.59 (m, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 4.34 – 4.23 (m, 2H), 3.56 (s, 3H), 2.41 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.4, 168.0, 153.9, 141.3, 136.4, 134.0, 133.2, 130.1, 128.5, 126.9, 126.2, 123.6, 118.5, 105.5, 60.9, 44.8, 24.9, 14.1; **HRMS (ESI)** m/z calcd. for $C_{20}H_{20}NO_4S$ $[M+H]^+$: 370.1113, found: 370.1104.

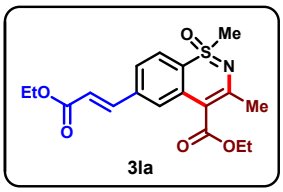
Ethyl 1,3-dimethyl-6-vinylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ka).



3ka

Pale yellow syrup (92.0 mg, 82%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.72 (d, *J* = 8.3 Hz, 1H), 7.68 (d, *J* = 1.4 Hz, 1H), 7.48 (dd, *J* = 8.4, 1.5 Hz, 1H), 6.74 (dt, *J* = 18.1, 9.1 Hz, 1H), 5.87 (d, *J* = 17.6 Hz, 1H), 5.44 (d, *J* = 10.9 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 3H), 2.37 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.6, 152.6, 142.1, 135.8, 134.7, 123.9, 123.3, 122.8, 117.6, 115.5, 105.1, 60.8, 45.4, 24.9, 14.3; **HRMS (ESI)** m/z calcd. for $C_{15}H_{18}NO_3S$ $[M+H]^+$: 292.1007, found 292.1012.

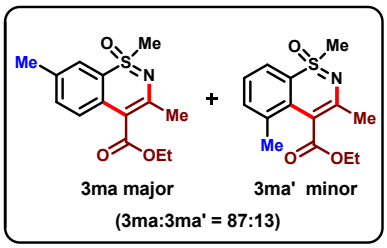
(*E*)-Ethyl 6-(3-ethoxy-3-oxoprop-1-en-1-yl)-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1 -oxide (3la).



3la

Yellow solid (125.0 mg, 86%); m.p. 97– 99 °C; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.88 (s, 1H), 7.77 (d, *J* = 8.3 Hz, 1H), 7.68 (d, *J* = 16.0 Hz, 1H), 7.54 (dd, *J* = 8.4, 1.4 Hz, 1H), 6.52 (d, *J* = 16.0 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 4.28 (q, *J* = 7.1 Hz, 2H), 3.50 (s, 3H), 2.39 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H), 1.35 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.3, 166.1, 153.5, 142.8, 138.8, 134.7, 125.1, 124.1, 121.7, 116.8, 105.0, 60.9, 60.8, 45.1, 25.0, 14.22, 14.19; **HRMS (ESI)** m/z calcd. for $C_{18}H_{22}NO_5S$ $[M+H]^+$: 364.1219, found 364.1216.

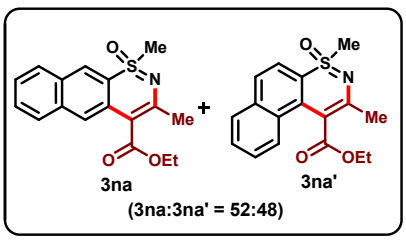
Ethyl 1,3,7-trimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ma, major).
Ethyl 1,3,5-trimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ma', minor).



3ma major 3ma' minor
(3ma:3ma' = 87:13)

White solid (91.0 mg, 81%); m.p. 114– 116 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.66 – 7.59 (m, 1.14H {major+minor}), 7.55 (s, 1H), 7.45 – 7.37 (m, 1.16H {major+minor}), 7.33 (t, *J* = 7.6 Hz, 0.17H{minor}), 4.37 (q, *J* = 7.1 Hz, 2.19H {major+minor}), 3.46 (s, 3H {major}), 3.41 (s, 0.45H {minor}), 2.43 (s, 3H {major}), 2.37 (s, 0.53H {minor}), 2.35 (s, 3H), 1.42 – 1.31 (m, 3.65H {major+minor}); **^{13}C NMR (100 MHz, $CDCl_3$, major+minor)** 170.2, 168.7, 151.2, 151.0, 136.3, 135.9, 134.5, 134.1, 132.8, 131.8, 126.2, 124.7, 122.9, 121.0, 120.1, 116.9, 106.4, 105.0, 60.9, 60.7, 45.3, 43.9, 24.7, 23.8, 21.2, 21.0, 14.2, 14.1; **HRMS (ESI)** m/z calcd. for $C_{14}H_{18}NO_3S$ $[M+H]^+$: 280.1007, found 280.1010.

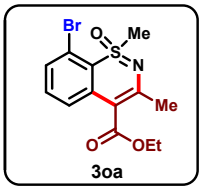
Ethyl 1,3-dimethylnaphtho[2,3-*e*][1,2]thiazine-4-carboxylate 1-oxide (3na, major).[4]
Ethyl 2,4-dimethylnaphtho[1,2-*e*][1,2]thiazine-1-carboxylate 4-oxide (3na', minor).[4]



3na 3na'
(3na:3na' = 52:48)

Yellow solid (108.0 mg, 86%); **^{1}H NMR (500 MHz, $CDCl_3$, 3na+3na')** δ 8.40 (s, 1H), 8.16 (s, 1H), 8.04 (d, *J* = 8.6 Hz, 1H), 7.95 – 7.78 (m, 4H), 7.66 (d, *J* = 8.6 Hz, 1H), 7.63 – 7.55 (m, 2H), 7.55 – 7.44 (m, 2H), 4.45 (q, *J* = 7.1 Hz, 2H), 4.33 – 4.16 (m, 2H), 3.53 (s, 3H), 3.45 (s, 3H), 1.44 (t, *J* = 7.1 Hz, 3H), 1.12 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$, 3na+3na')** δ 170.6, 168.9, 154.0, 151.1, 135.7, 135.3, 133.8, 130.9, 129.4, 129.1, 128.7, 128.5, 128.4, 128.2, 127.8, 126.7, 126.6, 126.4, 125.0, 122.7, 119.3, 118.1, 114.8, 105.8, 105.4, 60.9, 60.8, 45.3, 44.5, 25.0, 24.1, 14.3, 13.9.

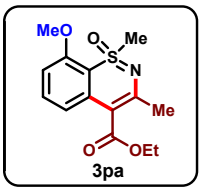
Ethyl 8-bromo-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3oa).[4]



3oa

Yellow solid (115.0 mg, 83%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.40 (t, *J* = 8.1 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.76 (s, 3H), 2.34 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.8, 150.8, 137.3, 133.2, 131.7, 124.3, 118.7, 116.9, 105.2, 61.1, 49.7, 24.3, 14.2.

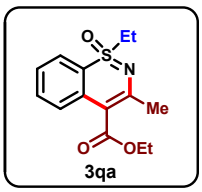
Ethyl 8-methoxy-1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3pa).



3pa

White solid (104.0 mg, 88%); m.p. 81– 83 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.50 (t, *J* = 8.3 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.02 (s, 3H), 3.64 (s, 3H), 2.33 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 169.1, 155.8, 151.1, 135.9, 133.6, 116.7, 106.9, 106.7, 104.9, 60.8, 56.2, 48.2, 24.4, 14.2; **HRMS (ESI)** m/z calcd. for $C_{14}H_{18}NO_4S$ $[M+H]^+$: 296.0957, found: 296.0959.

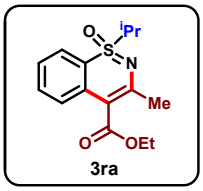
Ethyl 1-ethyl-3-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3qa).[4]



3qa

Yellow syrup (97.0 mg, 87%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.71 (t, *J* = 8.0 Hz, 2H), 7.58 (t, *J* = 7.8, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.74 – 3.63 (m, 1H), 3.56 – 3.45 (m, 1H), 2.38 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.19 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.7, 152.9, 135.5, 133.1, 125.9, 124.6, 123.8, 113.8, 104.6, 60.8, 51.0, 24.9, 14.2, 8.3.

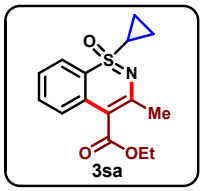
Ethyl 1-isopropyl-3-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ra).[4]



3ra

White solid (93.0 mg, 79%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 (dd, *J* = 8.4, 1.0 Hz, 2H), 7.57 (ddd, *J* = 8.4, 7.2, 1.3 Hz, 1H), 7.39 – 7.32 (m, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.79 – 3.64 (m, 1H), 2.38 (s, 3H), 1.47 (d, *J* = 6.9 Hz, 3H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.17 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.9, 153.8, 136.3, 133.2, 125.7, 124.4, 124.4, 112.9, 104.2, 60.7, 57.7, 25.1, 16.7, 14.3, 13.6.

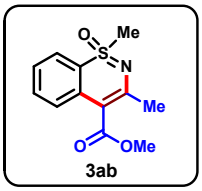
Ethyl 1-cyclopropyl-3-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3sa).[4]



3sa

Light yellow syrup (94.0 mg, 81%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.83 (dd, *J* = 8.0, 0.6 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.54 (m, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.83 – 2.75 (m, 1H), 2.38 (s, 3H), 1.81 – 1.69 (m, 1H), 1.45 – 1.30 (m, 5H), 1.28 – 1.17 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.8, 152.1, 134.4, 132.7, 125.8, 124.4, 123.6, 117.5, 105.2, 60.7, 32.6, 24.9, 14.2, 6.9, 4.9.

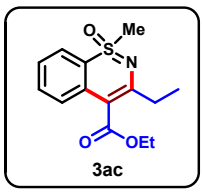
Methyl 1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ab).[4]



3ab

White solid (94.0 mg, 94%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 1H), 7.59 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.44 – 7.37 (m, 1H), 3.89 (s, 3H), 3.47 (s, 3H), 2.36 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 169.1, 152.7, 134.2, 133.1, 126.1, 124.7, 123.4, 116.8, 104.9, 51.7, 45.1, 24.9.

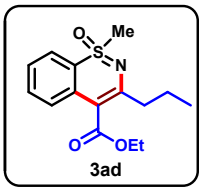
Ethyl 3-ethyl-1-methylbenzo[e][1,2]thiazine-4-carboxylate 1-oxide (3ac).



3ac

White solid (98.0 mg, 88%); m.p. 100– 103 °C; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.77 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.42 – 7.37 (m, 1H), 4.44 – 4.32 (m, 2H), 3.47 (s, 3H), 2.70 – 2.42 (m, 2H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.28 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.8, 156.4, 134.2, 133.0, 126.1, 124.6, 123.5, 116.9, 104.8, 60.9, 45.2, 30.9, 14.2, 13.1; **HRMS (ESI)** m/z calcd. for $C_{14}H_{18}NO_3S$ $[M+H]^+$: 280.1007, found: 280.1013.

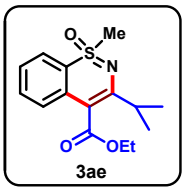
Ethyl 1-methyl-3-propylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ad).



3ad

White solid (105.0 mg, 90%); m.p. 112– 115 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.76 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.67 – 7.53 (m, 2H), 7.40 (ddd, *J* = 8.1, 7.0, 1.3 Hz, 1H), 4.45 – 4.30 (m, 2H), 3.47 (s, 3H), 2.72 – 2.43 (m, 2H), 1.87 – 1.65 (m, 2H), 1.39 (t, *J* = 7.1 Hz, 3H), 0.97 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.8, 154.9, 134.1, 133.0, 126.1, 124.6, 123.5, 117.0, 105.5, 60.9, 45.2, 39.3, 22.0, 14.2, 13.9; **HRMS (ESI)** m/z calcd. for $C_{15}H_{20}NO_3S$ $[M+H]^+$: 294.1164, found: 294.1169.

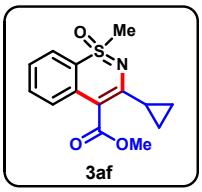
Ethyl 3-isopropyl-1-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ae).



3ae

White solid (104.0 mg, 89%); m.p. 95– 97 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 – 7.71 (m, 1H), 7.61 – 7.52 (m, 2H), 7.38 (ddd, *J* = 8.2, 6.5, 1.8 Hz, 1H), 4.37 (q, *J* = 7.2 Hz, 2H), 3.45 (s, 3H), 3.08 – 2.95 (m, 1H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.23 (d, *J* = 4.3 Hz, 3H), 1.22 (d, *J* = 4.3 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 169.1, 158.7, 134.2, 132.9, 126.1, 124.4, 123.6, 117.0, 104.3, 60.9, 45.2, 34.1, 21.4, 20.7, 14.2; **HRMS (ESI)** m/z calcd. for $C_{15}H_{20}NO_3S$ $[M+H]^+$: 294.1164, found: 294.1165.

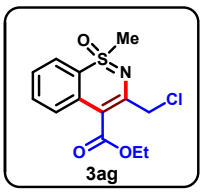
Methyl 3-cyclopropyl-1-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3af).



3af

Light orange syrup (93.0 mg, 80%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.72 (dd, *J* = 8.1, 0.6 Hz, 1H), 7.63 – 7.51 (m, 2H), 7.35 (ddd, *J* = 8.1, 6.7, 1.6 Hz, 1H), 3.92 (s, 3H), 3.38 (s, 3H), 2.28 – 2.17 (m, 1H), 1.23 – 1.17 (m, 1H), 1.15 – 1.08 (m, 1H), 0.92 – 0.78 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 169.5, 156.5, 134.4, 133.0, 125.7, 124.4, 123.4, 117.1, 104.8, 51.9, 45.0, 15.6, 9.2, 7.7; **HRMS (ESI)** m/z calcd. for $C_{14}H_{16}NO_3S$ $[M+H]^+$: 278.0851, found: 278.0855.

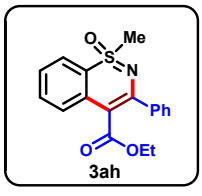
Ethyl 3-(chloromethyl)-1-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ag).



3ag

Yellow syrup (99.0 mg, 83%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.85 – 7.79 (m, 1H), 7.68 – 7.62 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 4.58 (d, *J* = 11.1 Hz, 1H), 4.47 (d, *J* = 11.1 Hz, 1H), 4.42 (q, *J* = 7.2 Hz, 2H), 3.53 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.2, 149.1, 133.4, 133.2, 127.6, 125.7, 123.4, 118.3, 106.9, 61.4, 46.1, 44.9, 14.1; **HRMS (ESI)** m/z calcd. for $C_{13}H_{15}NO_3SCl$ $[M+H]^+$: 300.0461, found: 300.0463.

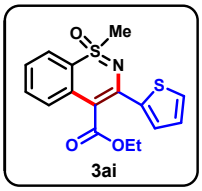
Ethyl 1-methyl-3-phenylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ah).[4]



3ah

Yellow solid (120.0 mg, 92%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.84 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.67 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.52 – 7.46 (m, 1H), 7.44 – 7.36 (m, 3H), 4.03 – 3.95 (m, 1H), 3.94 – 3.86 (m, 1H), 3.61 (s, 3H), 0.81 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.9, 153.0, 140.5, 133.9, 133.3, 128.9, 128.3, 128.1, 126.7, 124.9, 123.4, 117.3, 105.7, 60.9, 45.1, 13.3.

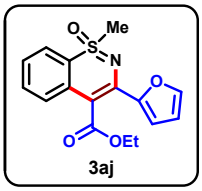
Ethyl 1-methyl-3-(thiophen-2-yl)benzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ai).



3ai

Pale yellow solid (73.0 mg, 55%); m.p. 133– 136 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (t, *J* = 7.6 Hz, 2H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 5.2 Hz, 1H), 7.34 (d, *J* = 3.6 Hz, 1H), 7.03 (t, *J* = 4.2 Hz, 1H), 4.33 – 4.06 (m, 2H), 3.58 (s, 3H), 1.12 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 169.0, 143.4, 142.7, 133.6, 133.3, 128.3, 127.6, 127.1, 126.8, 124.6, 123.4, 117.8, 105.4, 61.5, 44.8, 13.7; **HRMS (ESI)** m/z calcd. for $C_{16}H_{16}NO_3S_2$ $[M+H]^+$: 334.0572, found: 334.0572.

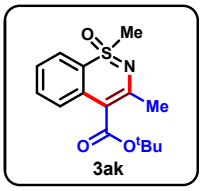
Ethyl 3-(furan-2-yl)-1-methylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3aj).[4]



3aj

Yellow solid (100.0 mg, 79%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.82 – 7.76 (m, 2H), 7.66 – 7.59 (m, 1H), 7.47 (dd, *J* = 1.7, 0.8 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 6.97 (dd, *J* = 3.4, 0.7 Hz, 1H), 6.50 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.33 (q, *J* = 7.2 Hz, 2H), 3.57 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.7, 152.2, 143.8, 138.5, 133.4, 133.2, 126.8, 124.6, 123.4, 118.2, 112.6, 111.8, 104.5, 61.3, 44.8, 14.1.

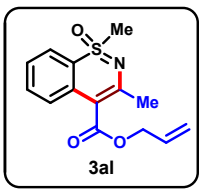
***tert*-Butyl 1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3ak).**



3ak

White solid (110.0 mg, 94%); m.p. 120– 123 °C; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.75 (d, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 3.48 (s, 3H), 2.35 (s, 3H), 1.60 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 168.0, 150.2, 134.2, 133.0, 125.9, 124.3, 123.5, 116.8, 106.9, 81.4, 45.4, 28.2, 24.4; **HRMS (ESI)** m/z calcd. for $C_{15}H_{20}NO_3S$ $[M+H]^+$: 294.1164, found: 294.1165.

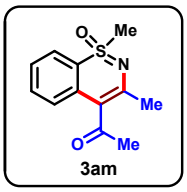
Allyl 1,3-dimethylbenzo[*e*][1,2]thiazine-4-carboxylate 1-oxide (3al).



3al

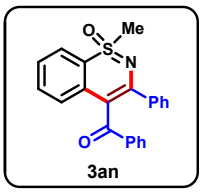
Pale yellow syrup (100.0 mg, 90%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.58 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 1H), 7.40 (td, *J* = 7.7, 0.9 Hz, 1H), 6.13 – 5.98 (m, 1H), 5.41 (ddd, *J* = 17.2, 2.8, 1.4 Hz, 1H), 5.30 (dd, *J* = 10.4, 1.2 Hz, 1H), 4.81 (dt, *J* = 5.9, 1.2 Hz, 2H), 3.47 (s, 3H), 2.38 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.2, 152.7, 134.2, 133.1, 131.9, 126.1, 124.7, 123.4, 118.9, 116.8, 104.8, 65.6, 45.2, 24.9; **HRMS (ESI)** m/z calcd. for $C_{14}H_{16}NO_3S$ $[M+H]^+$: 278.0851, found: 278.0856.

1-(1,3-Dimethyl-1-oxidobenzo[*e*][1,2]thiazin-4-yl)ethanone (3am).



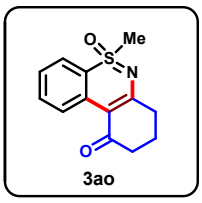
Light brown solid (64.0 mg, 68%); m.p. 111– 113 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.59 (ddd, *J* = 8.4, 7.4, 1.3 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 3.52 (s, 3H), 2.51 (s, 3H), 2.27 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 204.4, 147.9, 133.4, 133.0, 126.2, 124.0, 123.6, 117.3, 114.3, 45.0, 32.9, 23.9; **HRMS (ESI)** m/z calcd. for $C_{12}H_{13}NO_2S$ $[M+H]^+$: 236.0745, found: 236.0749.

(1-Methyl-1-oxido-3-phenylbenzo[*e*][1,2]thiazin-4-yl)(phenyl)methanone (3an).



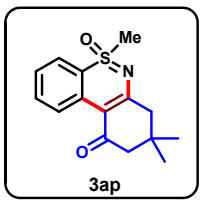
White solid (71.0 mg, 49%); m.p. 195– 196 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.63 – 7.57 (m, 1H), 7.54 – 7.46 (m, 3H), 7.33 – 7.27 (m, 1H), 7.21 – 7.09 (m, 5H), 3.71 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 197.8, 150.5, 139.3, 139.2, 134.2, 133.2, 132.6, 129.5, 129.5, 129.1, 128.0, 127.9, 126.8, 125.1, 123.3, 117.8, 111.3, 44.8; **HRMS (ESI)** m/z calcd. for $C_{22}H_{18}NO_2S$ $[M+H]^+$: 360.1058, found: 360.1056.

5-Methyl-8,9-dihydrodibenzo[*c*,*e*][1,2]thiazin-10(7*H*)-one 5-oxide (3ao).[4]



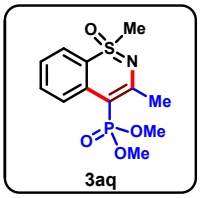
White solid (75.0 mg, 76%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.10 (d, *J* = 8.2 Hz, 1H), 7.79 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.69 (ddd, *J* = 8.6, 7.2, 1.5 Hz, 1H), 7.50 – 7.42 (m, 1H), 3.41 (s, 3H), 2.88 – 2.73 (m, 2H), 2.63 – 2.55 (m, 2H), 2.09 – 1.95 (m, 2H).; **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.2, 166.2, 134.2, 133.9, 127.4, 126.8, 123.2, 118.6, 108.5, 44.8, 39.4, 35.2, 20.8.

5,8,8-Trimethyl-8,9-dihydrodibenzo[*c*,*e*][1,2]thiazin-10(7*H*)-one 5-oxide (3ap).



White solid (68.0 mg, 62%); m.p. 98– 102 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.22 (dd, *J* = 8.6, 0.7 Hz, 1H), 7.79 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.69 (ddd, *J* = 8.6, 7.2, 1.5 Hz, 1H), 7.46 (ddd, *J* = 8.2, 7.3, 1.1 Hz, 1H), 3.42 (s, 3H), 2.71, 2.65 (ABq, *J* = 17.7 Hz, 2H), 2.48, 2.44 (ABq, *J* = 16.7 Hz, 2H), 1.10 (s, 6H).; **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.3, 164.6, 134.0, 133.9, 127.0, 126.7, 123.2, 118.3, 107.1, 53.1, 48.7, 44.9, 31.5, 28.4, 27.7; **HRMS (ESI)** m/z calcd. for $C_{15}H_{18}NO_2S$ $[M+H]^+$: 276.1058, found: 276.1061.

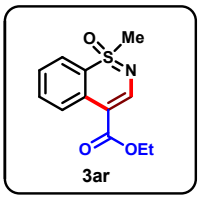
Dimethyl (1,3-dimethyl-1-oxidobenzo[*e*][1,2]thiazin-4-yl)phosphonate (3aq).[4]



3aq

Yellow syrup (98.0 mg, 81%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.27 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.68 – 7.58 (m, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 3.75 (d, *J* = 11.4 Hz, 3H), 3.72 (d, *J* = 11.4 Hz, 3H), 3.43 (s, 3H), 2.64 (d, *J* = 1.8 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 162.7 (d, $J_{C\text{-}P}$ = 19.2 Hz), 136.0 (d, $J_{C\text{-}P}$ = 14.7 Hz), 132.8, 126.6, 126.1, 122.7, 117.3 (d, $J_{C\text{-}P}$ = 11.2 Hz), 94.9 (d, $J_{C\text{-}P}$ = 200.3 Hz), 51.93 (d, $J_{C\text{-}P}$ = 2.2 Hz), 51.88 (d, $J_{C\text{-}P}$ = 2.1 Hz), 43.4, 26.8.

Ethyl 1-methylbenzo[e][1,2]thiazine-4-carboxylate 1-oxide (3ar).[4]



3ar

Light yellow solid (70.0 mg, 70%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.81 (d, *J* = 8.4 Hz, 1H), 8.27 (s, 1H), 7.82 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.69 (ddd, *J* = 8.6, 7.2, 1.4 Hz, 1H), 7.51 – 7.44 (m, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 166.3, 150.0, 134.1, 133.7, 126.8, 125.8, 123.9, 117.6, 102.6, 60.1, 45.8, 14.4.

9. References

(1) (a) B. Sun, T. Yoshino, S. Matsunaga and M. Kanai, *Adv. Synth. Catal.,* 2014, **356**, 1491; (b) S. A. Frith and J. Spencer, *Inorganic Syntheses.,*1990, **28**, 273.

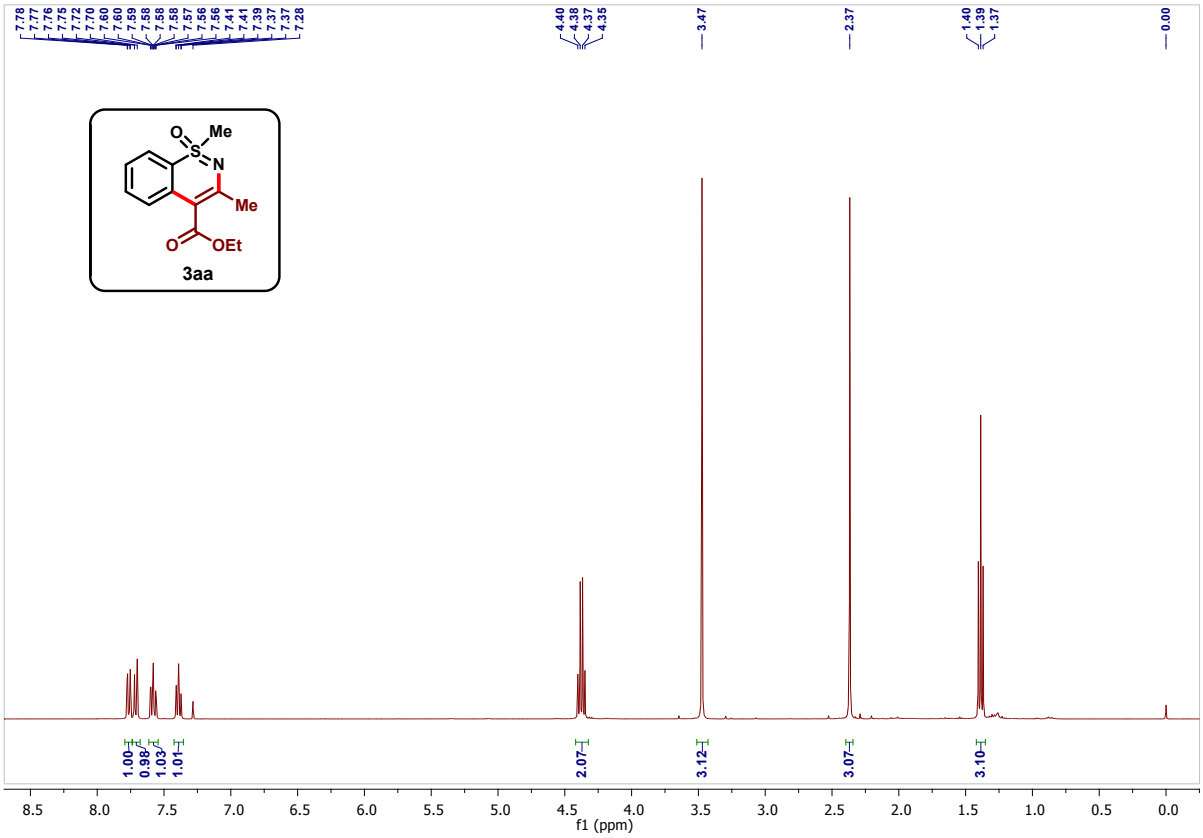
(2) (a) M. Zenola, R. Doran, L. Degennaro, R. Luisi and J. A. Bull, *Angew. Chem., Int. Ed.,* 2016, **55**, 7203; (b) A. Tota, M. Zenzola, S. J. Chawner, S. St. John-Campbell, C. Carlucci, G. Romanazzi, L. Degennaro and J. A. Bull, *Chem. Commun.*, 2017, **53**, 348.

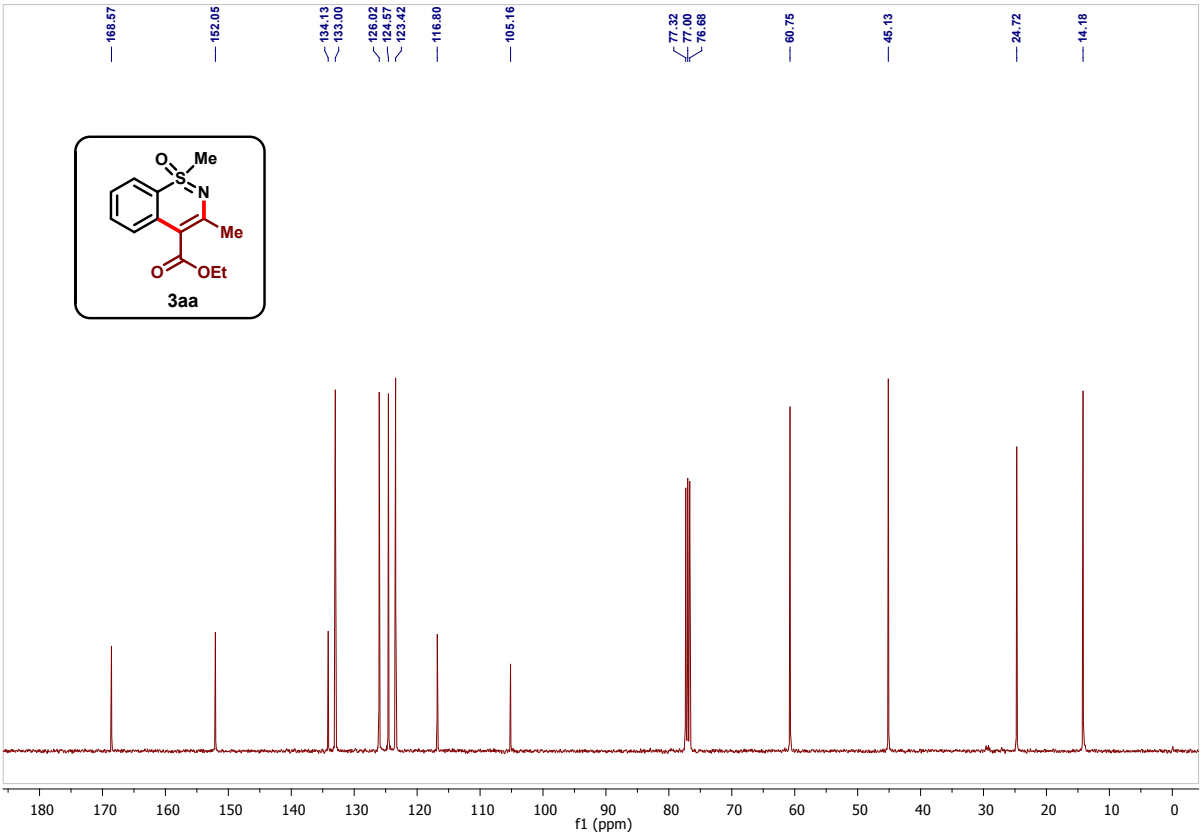
(3) (a) P. Meffre, S. Hermann, P. Durand, G. Reginato and A. Riu, *Tetrahedron,* 2002, **58**, 5159; (b) A. M. P. Koskinen and L.Muñoz, *J. Chem. Soc., Chem. Commun.,* 1990, 652.

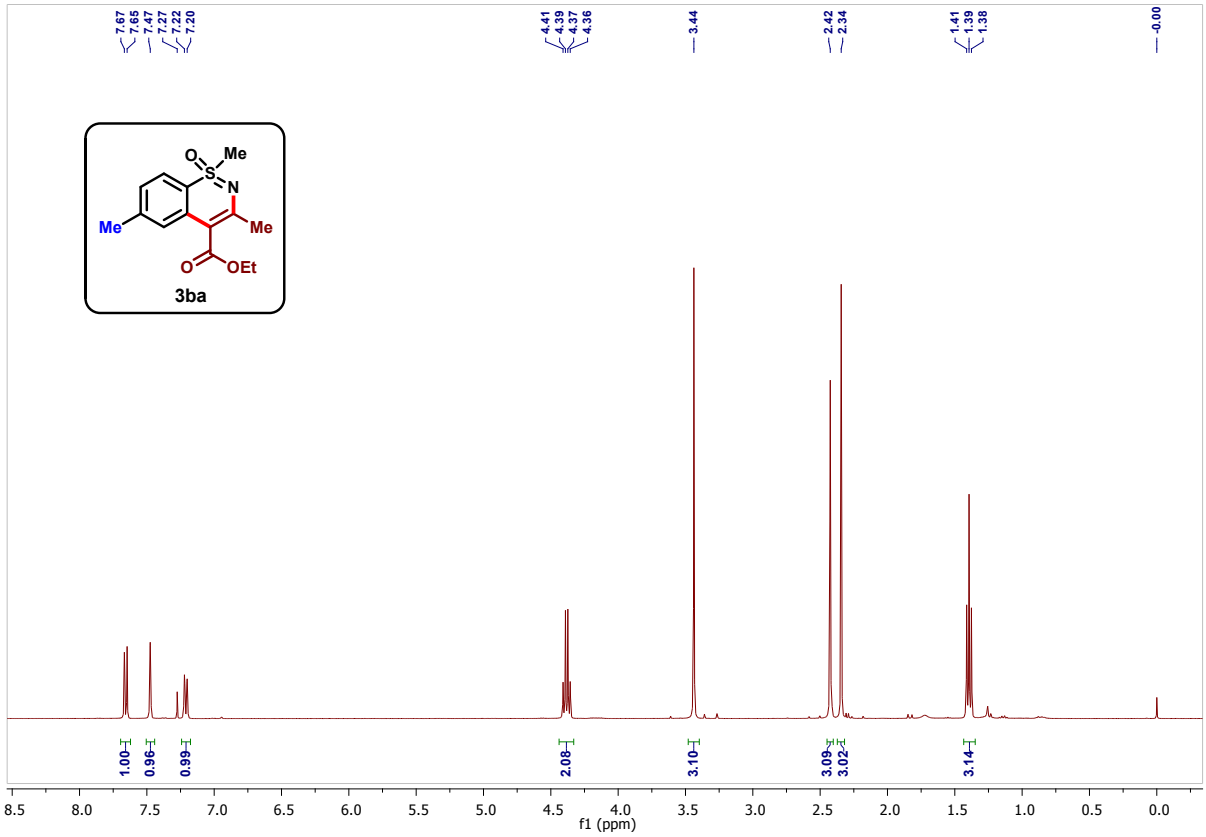
(4) Y. Cheng and C. Bolm, *Angew. Chem., Int. Ed.,* 2015, **54**, 12349.

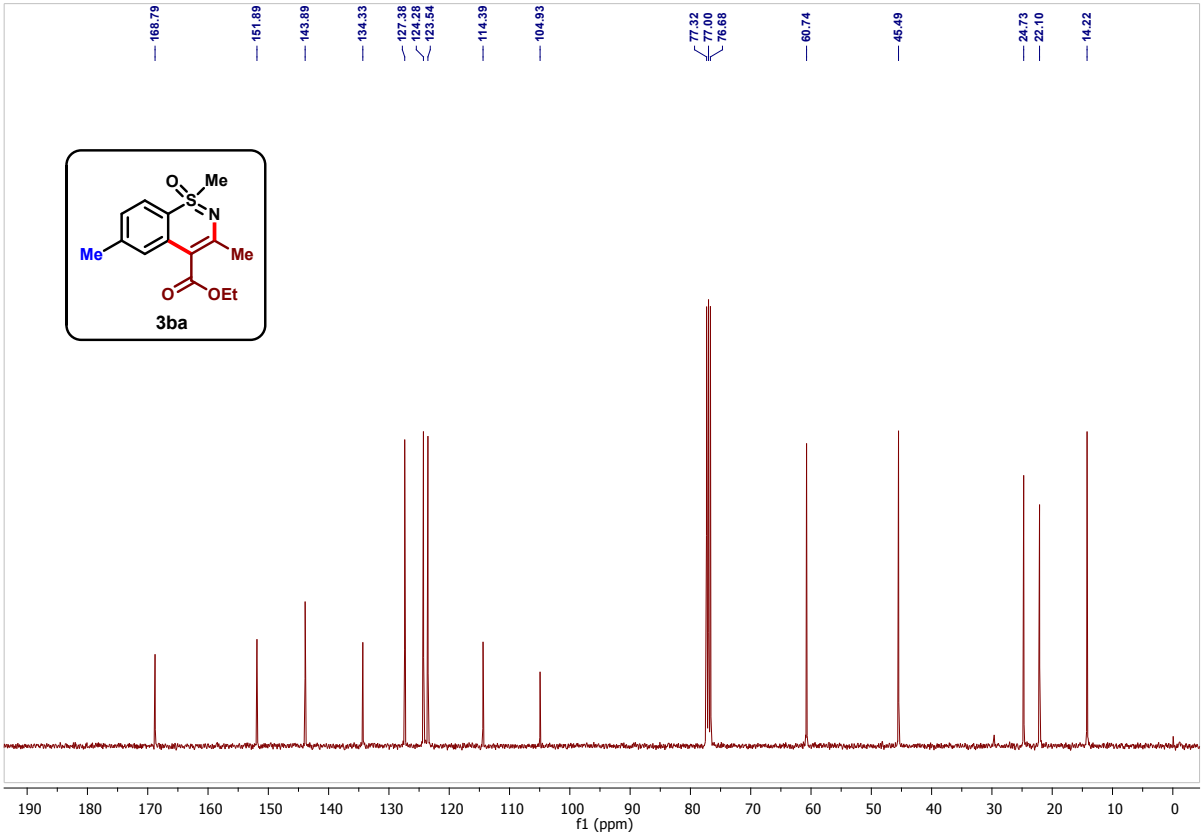
Appendix I

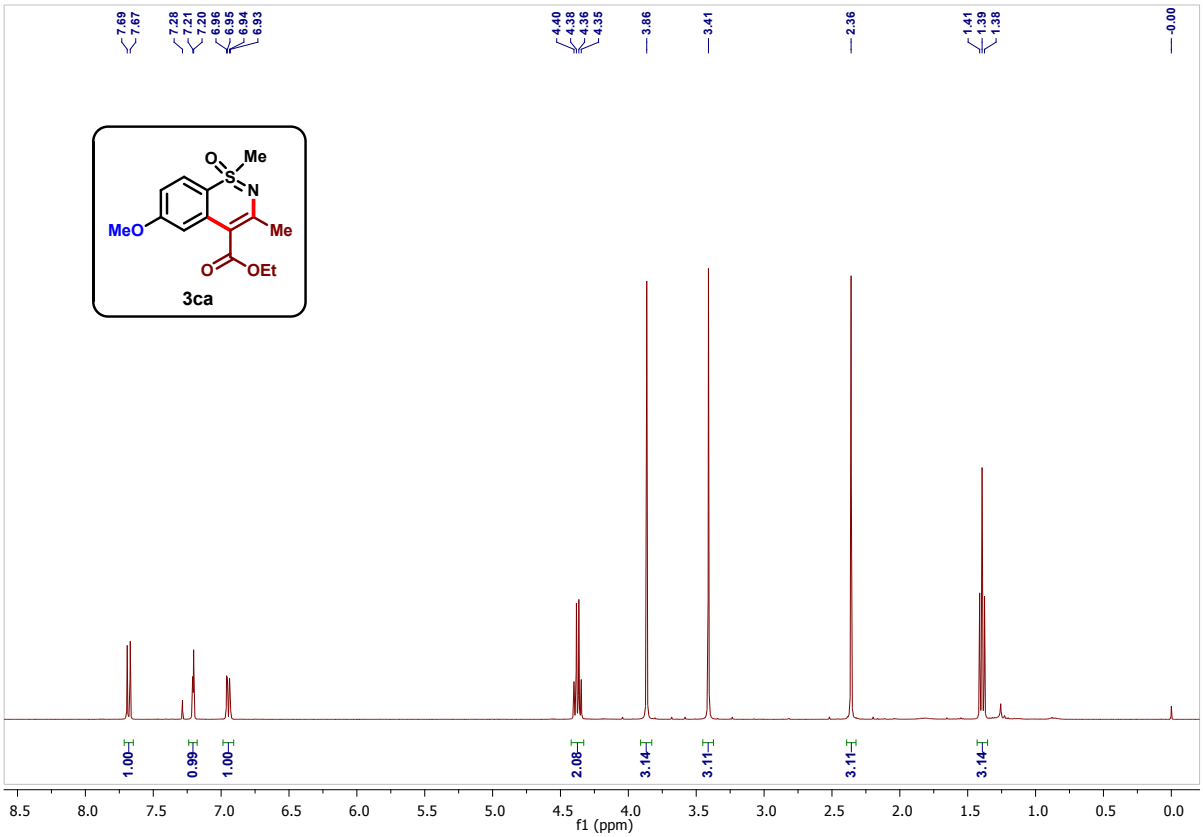
Spectral Copies of ^{1}H and ^{13}C NMR of Compounds Obtained in this study

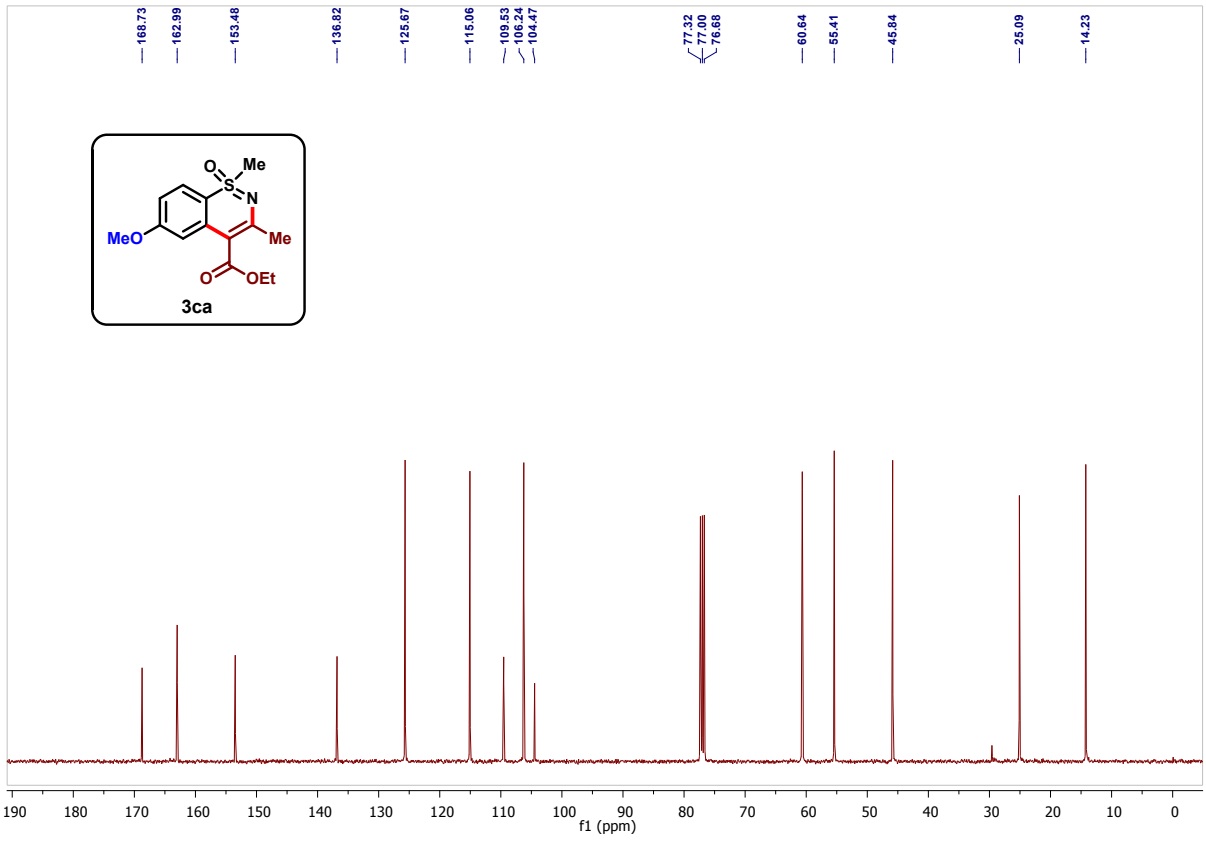

7.78
7.77
7.76
7.75
7.72
7.70
7.60
7.60
7.59
7.58
7.58
7.58
7.57
7.56
7.56
7.41
7.41
7.39
7.37
7.37
7.28
4.40
4.38
4.37
4.35
3.47
2.37
1.40
1.39
1.37
0.00
O
Me
S
N
Me
O
OEt
3aa
1.00
0.98
1.03
1.01
2.07
3.12
3.07
3.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


168.57
152.05
134.13
133.00
126.02
124.57
123.42
116.80
105.16
77.32
77.00
76.68
60.75
45.13
24.72
14.18
O
Me
S
N
Me
O
OEt
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.67
7.65
7.47
7.27
7.22
7.20
4.41
4.39
4.37
4.36
3.44
2.42
2.34
1.41
1.39
1.38
0.00
Me
O
S
N
Me
Me
O
OEt
3ba
1.00
0.96
0.99
2.08
3.10
3.09
3.02
3.14
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)


168.79
151.89
143.89
134.33
127.38
124.28
123.54
114.39
104.93
77.32
77.00
76.68
60.74
45.49
24.73
22.10
14.22
Me
O
S
N
Me
Me
O
OEt
3ba
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.69
7.67
7.28
7.21
7.20
6.96
6.95
6.94
6.93
4.40
4.38
4.36
4.35
3.86
3.41
2.36
1.41
1.39
1.38
0.00
O
Me
S
N
MeO
Me
O
OEt
3ca
1.00
0.99
1.00
2.08
3.14
3.11
3.11
3.14
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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162.99
153.48
136.82
125.67
115.06
109.53
106.24
104.47
77.32
77.00
76.68
60.64
55.41
45.84
25.09
14.23
O
Me
S
N
MeO
Me
O
OEt
3ca
190
180
170
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130
120
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90
80
70
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50
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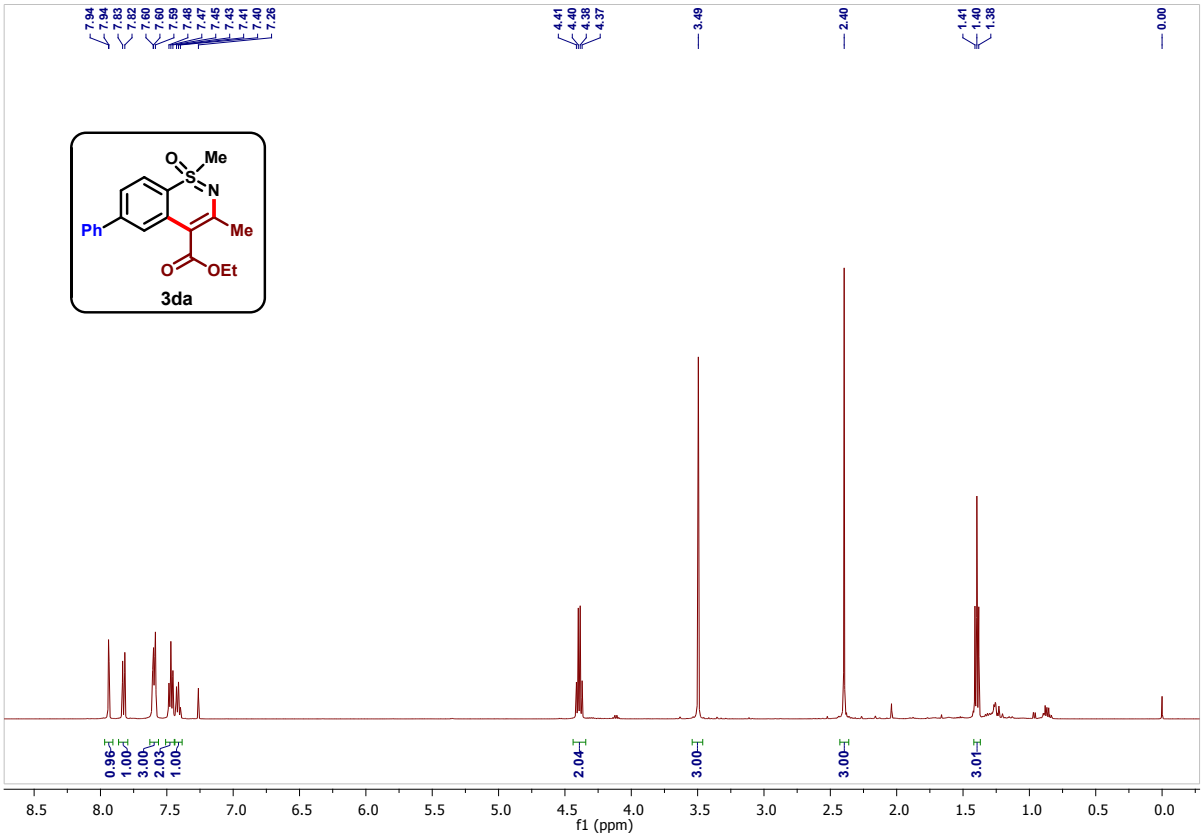
10
0
f1 (ppm)


7.94
7.94
7.83
7.82
7.60
7.60
7.59
7.48
7.47
7.45
7.43
7.41
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7.26
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3.49
2.40
1.41
1.40
1.38
0.00
Me
O
S
N
Ph
Me
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OEt
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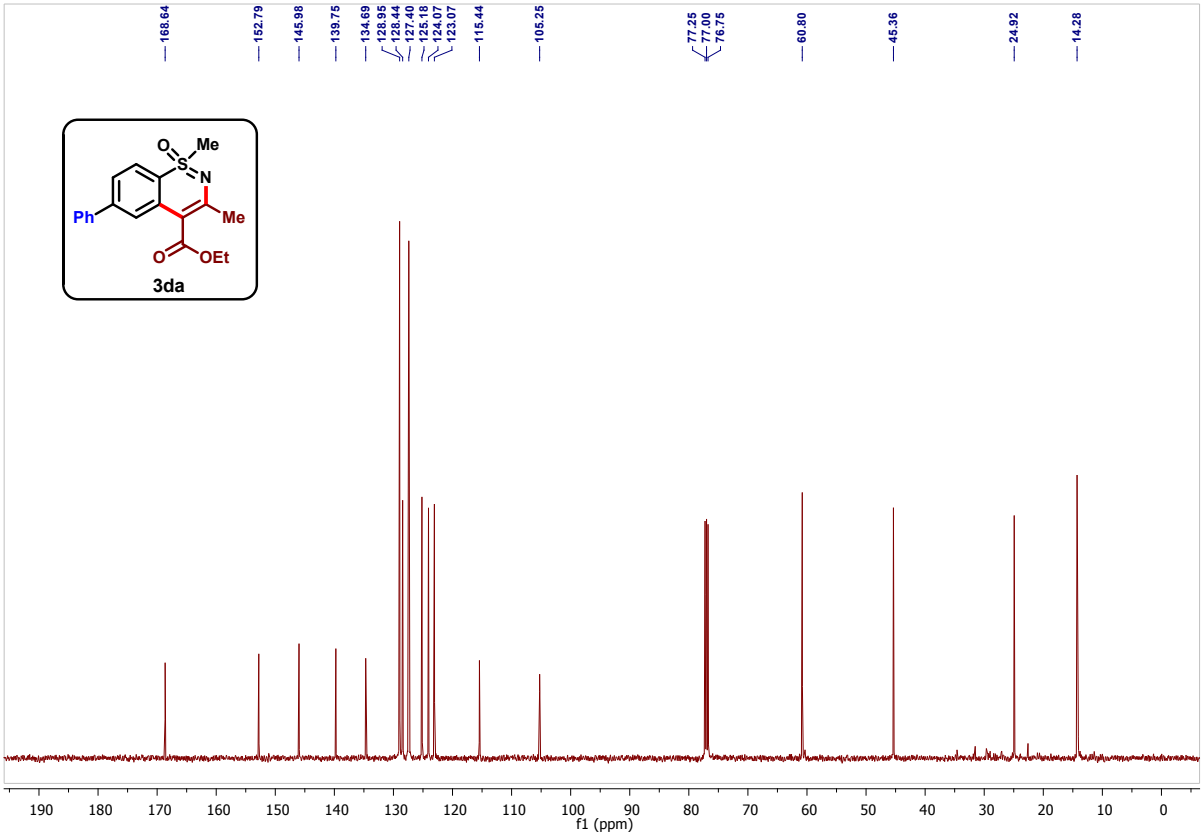
3.00
3.00
3.01
f1 (ppm)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77.25
77.00
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60.80
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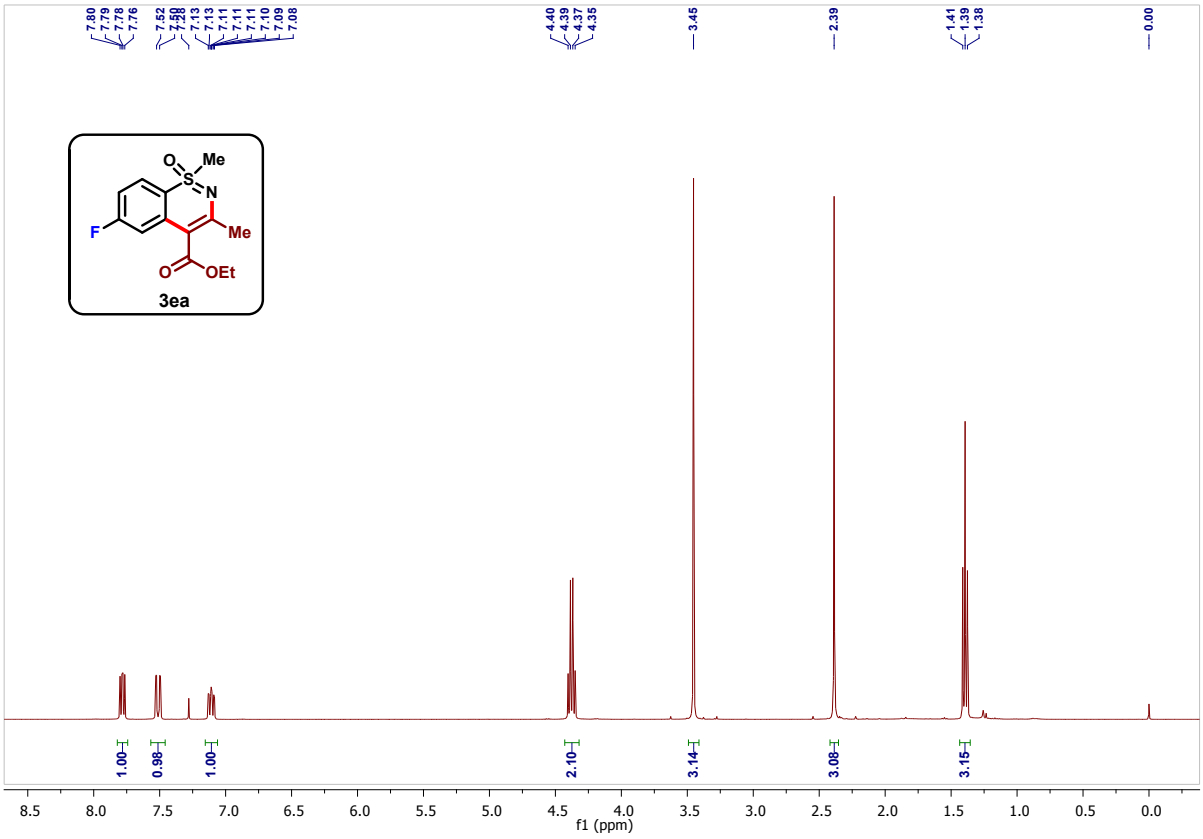
24.92
14.28
Me
O
S
N
Ph
Me
O
OEt
3da
f1 (ppm)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7.50
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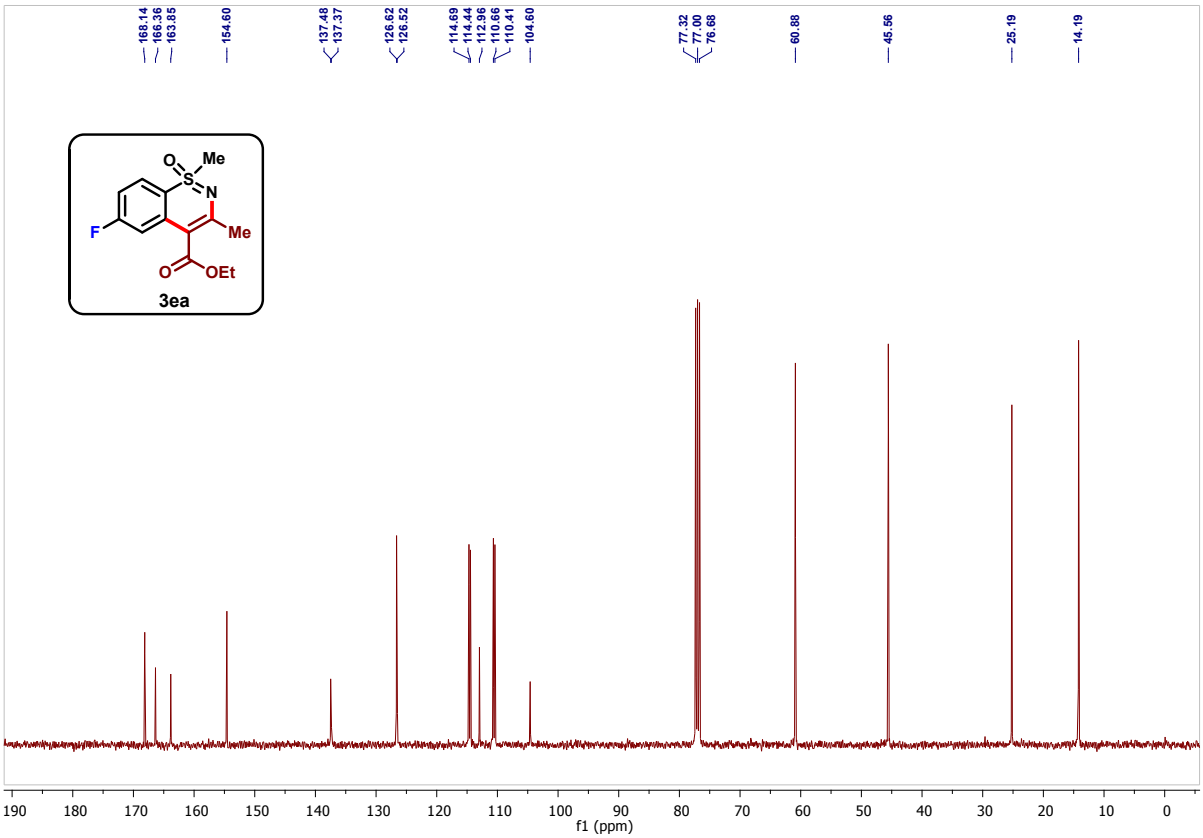
7.13
7.11
7.11
7.10
7.09
7.08
4.40
4.39
4.37
4.35
3.45
2.39
1.41
1.39
1.38
0.00
Me
O
S
N
F
Me
O
OEt
3ea
1.00
0.98
1.00
2.10
3.14
3.08
3.15
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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126.52
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114.44
112.96
110.66
110.41
104.60
77.32
77.00
76.68
60.88
45.56
25.19
14.19
Me
O
S
N
F
Me
O
OEt
3ea
190
180
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90
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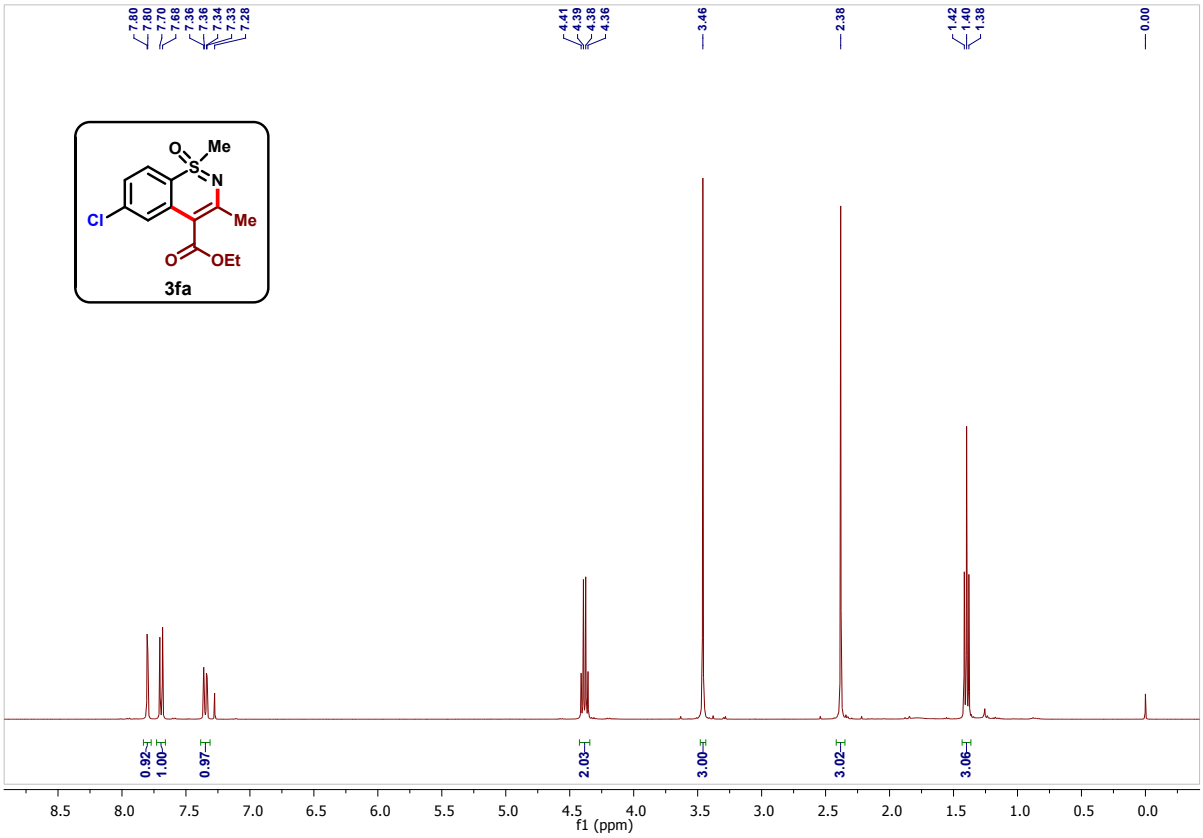
f1 (ppm)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4.39
4.38
4.36
3.46
2.38
1.42
1.40
1.38
0.00
Me
O
S
N
Cl
Me
O
OEt
3fa
0.92
1.00
0.97
2.03
3.00
3.02
3.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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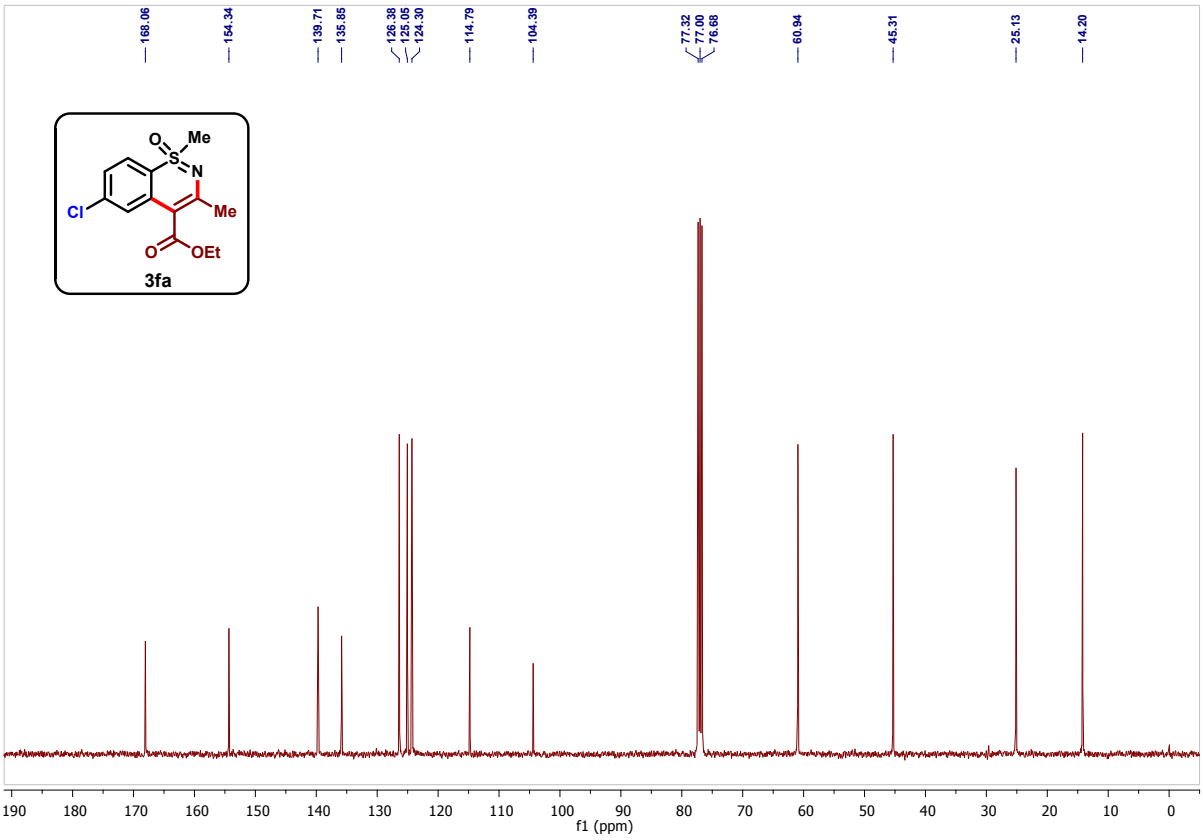
f1 (ppm)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25.13
14.20
Me
O
S
N
Cl
Me
O
OEt
3fa
190
180
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10
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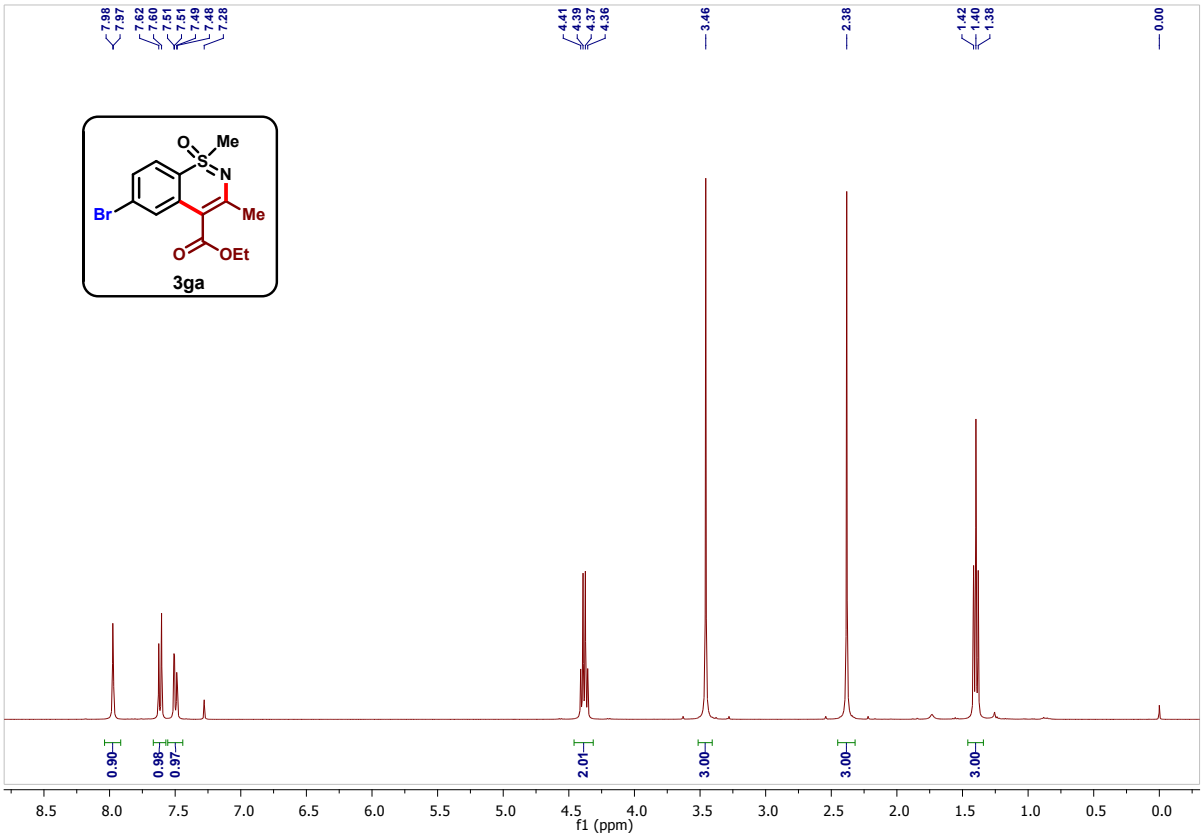
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7.49
7.48
7.28
4.41
4.39
4.37
4.36
3.46
2.38
1.42
1.40
1.38
0.00
O
Me
S
N
Br
Me
O
OEt
3ga
0.90
0.98
0.97
2.01
3.00
3.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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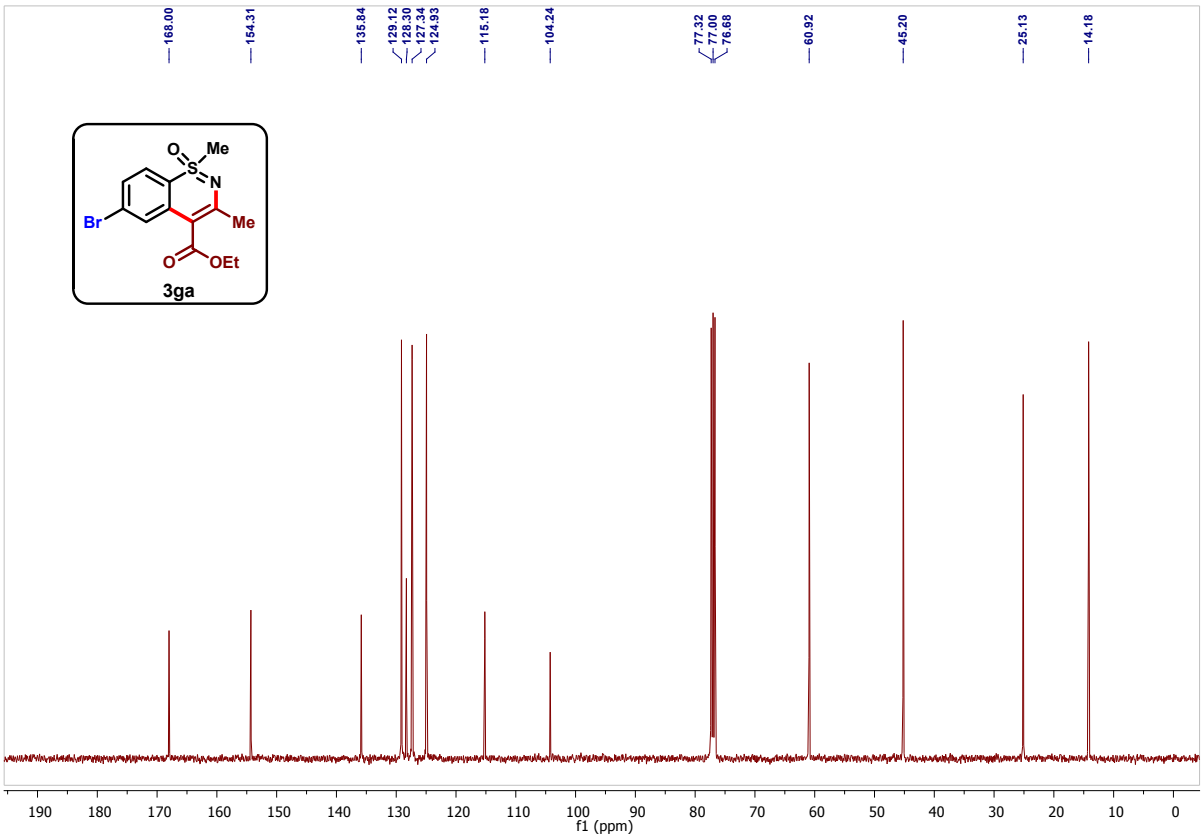
0.0
f1 (ppm)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76.68
60.92
45.20
25.13
14.18
O
Me
S
N
Br
Me
O
OEt
3ga
190
180
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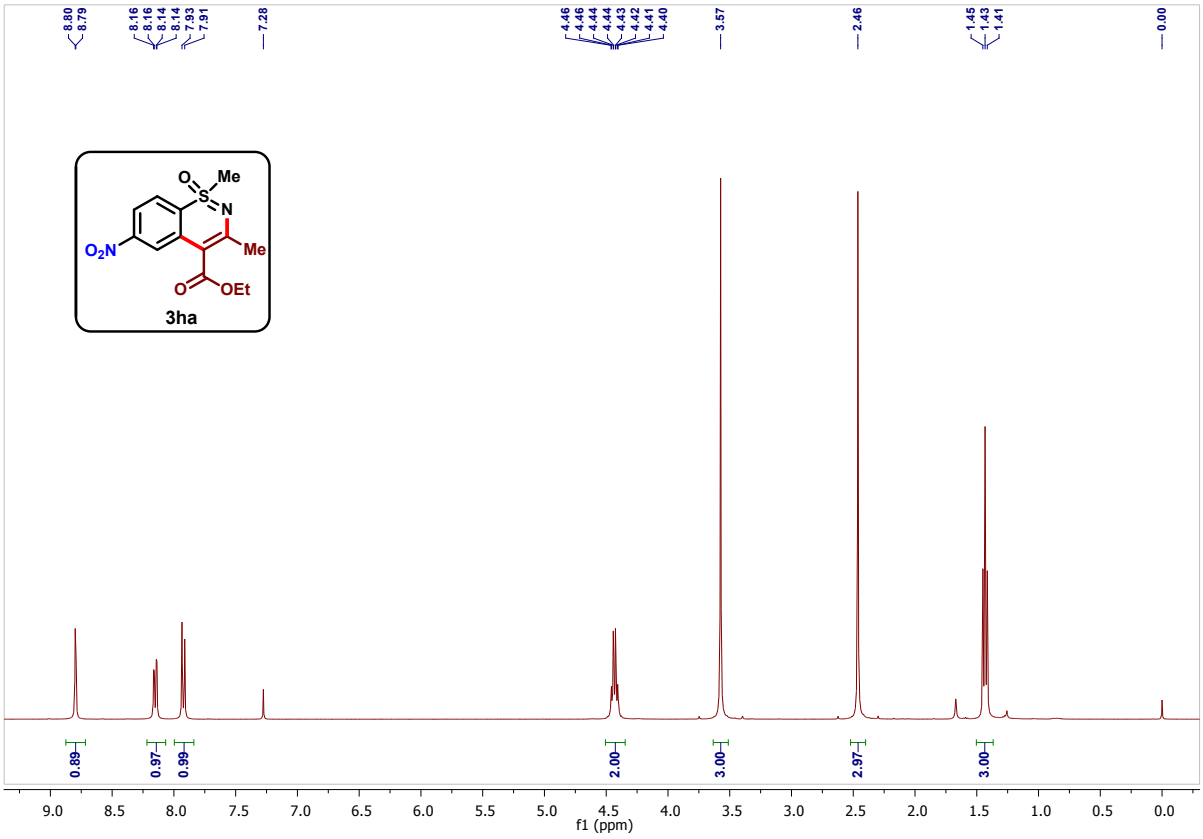
f1 (ppm)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7.91
7.28
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4.46
4.44
4.44
4.43
4.42
4.41
4.40
3.57
2.46
1.45
1.43
1.41
0.00
Me
O
S
N
O2N
Me
O
OEt
3ha
0.89
0.97
0.99
2.00
3.00
2.97
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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1.0
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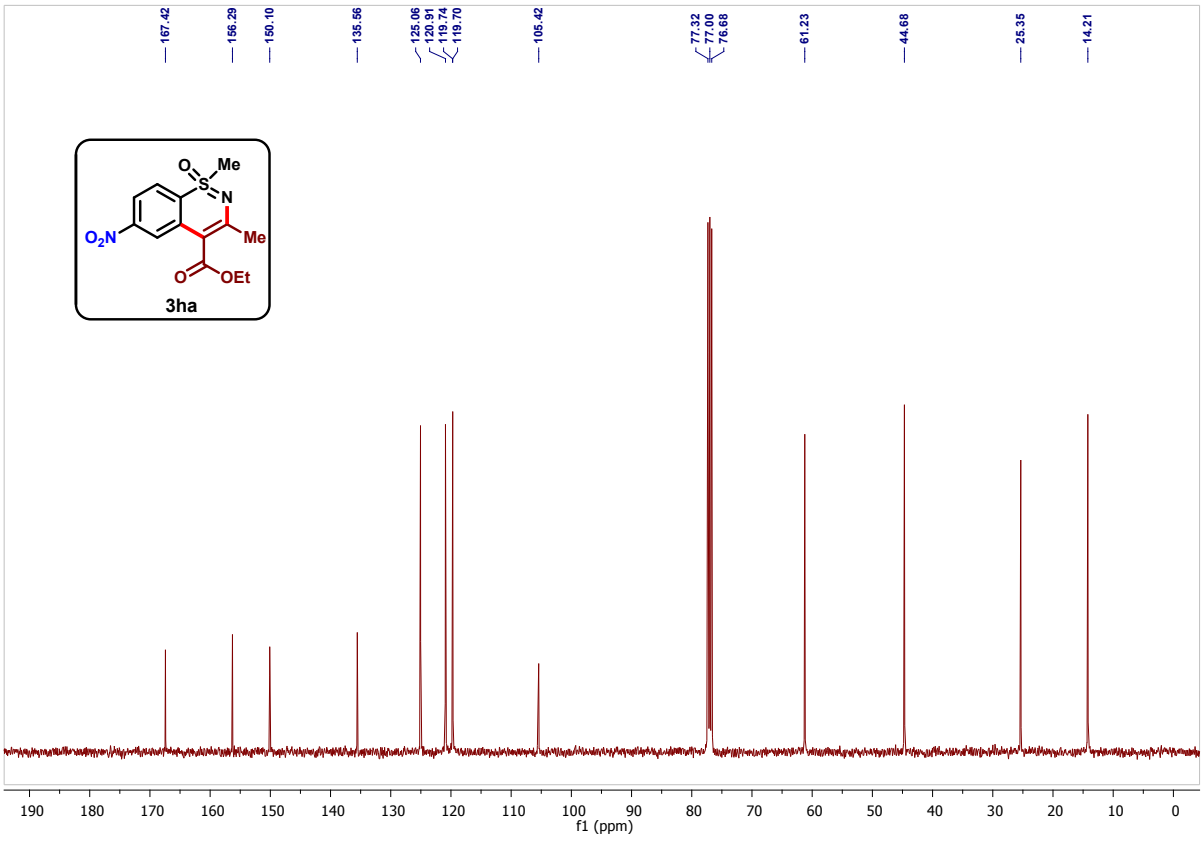
0.0
f1 (ppm)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150.10
135.56
125.06
120.91
119.74
119.70
105.42
77.32
77.00
76.68
61.23
44.68
25.35
14.21
Me
O
S
N
O2N
Me
O
OEt
3ha
190
180
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160
150
140
130
120
110
100
90
80
70
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50
40
30
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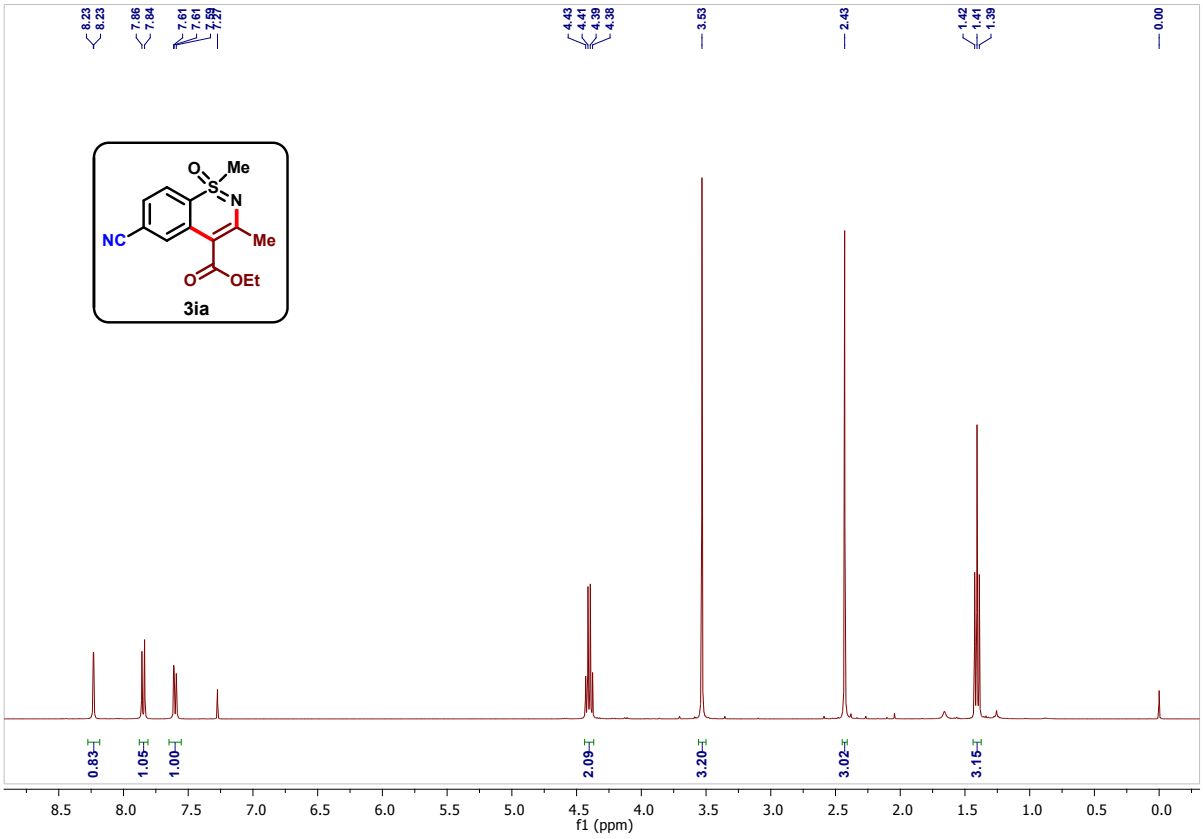
10
0
f1 (ppm)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7.61
7.59
7.57
4.43
4.41
4.39
4.38
3.53
2.43
1.42
1.41
1.39
0.00
Me
O
S
N
NC
Me
O
OEt
3ia
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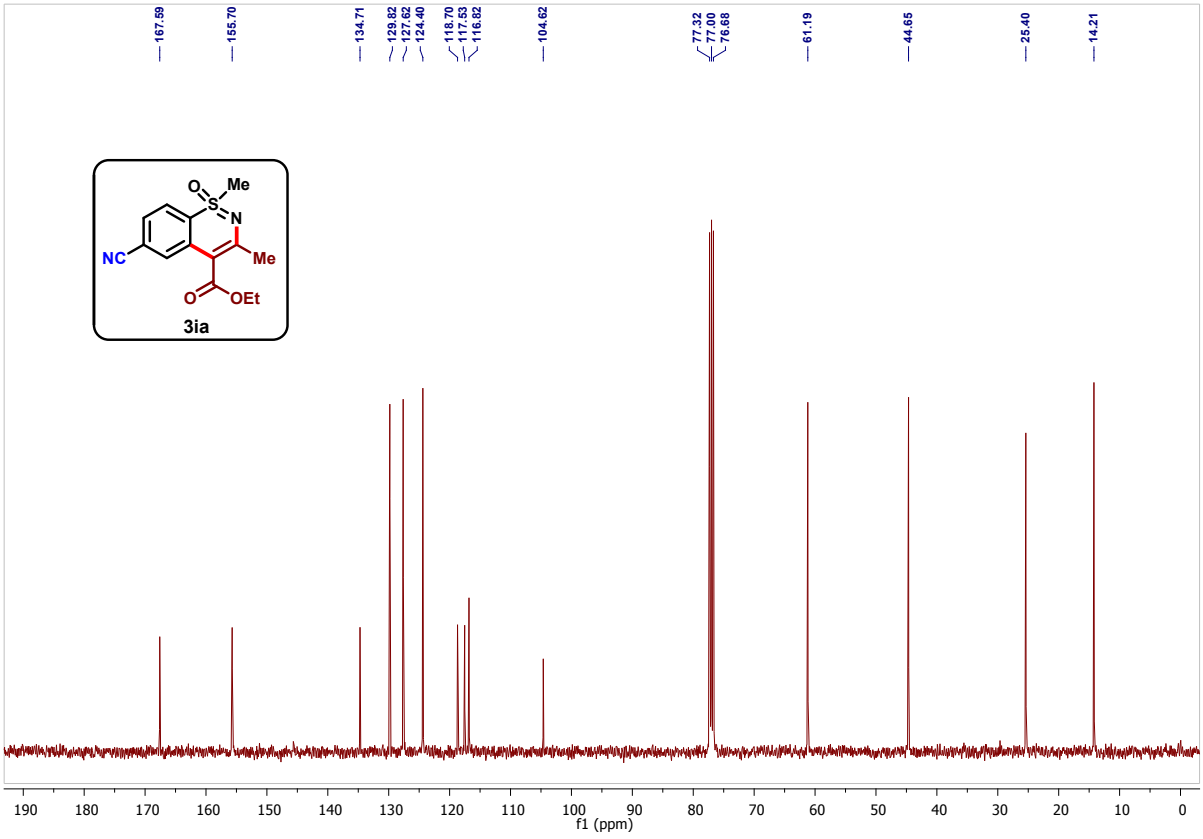
1.05
1.00
2.09
3.20
3.02
3.15
f1 (ppm)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116.82
104.62
77.32
77.00
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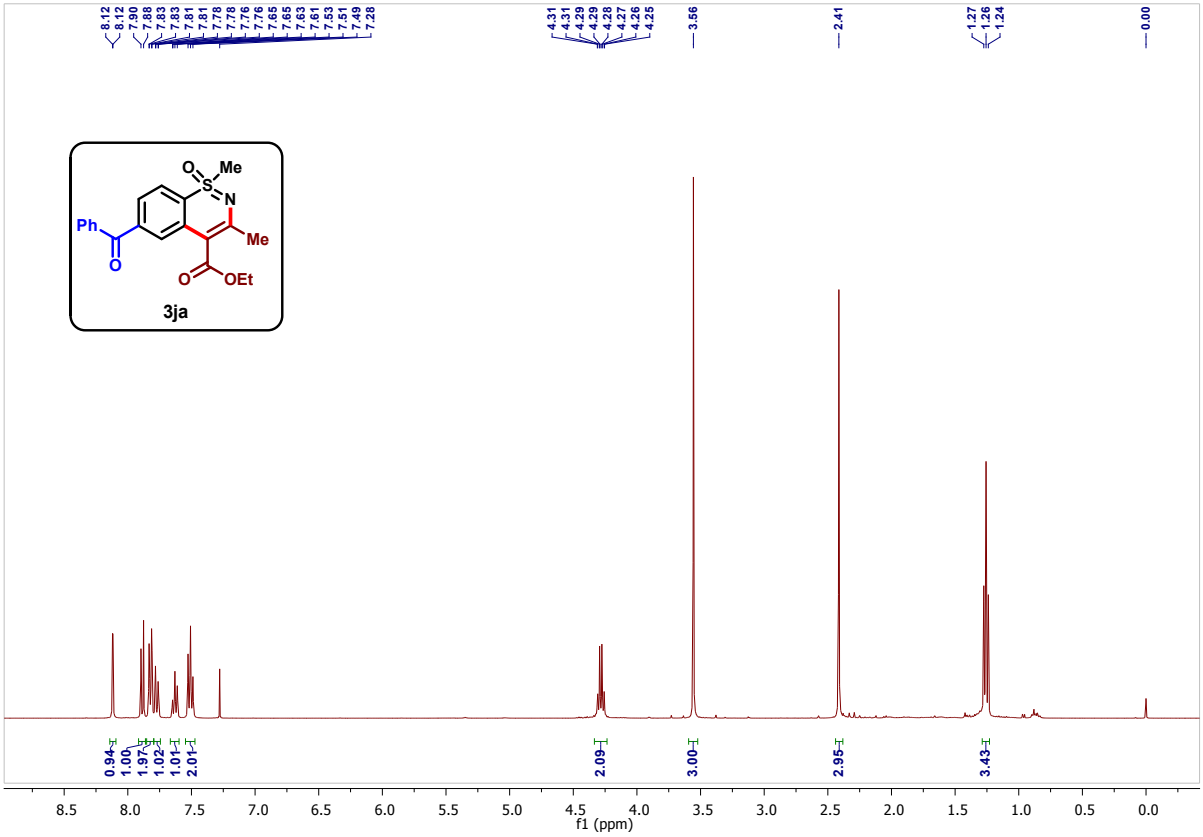
25.40
14.21
Me
O
S
N
NC
Me
O
OEt
3ia
f1 (ppm)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7.76
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7.65
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7.53
7.51
7.49
7.28
4.31
4.31
4.29
4.29
4.28
4.27
4.26
4.25
3.56
2.41
1.27
1.26
1.24
0.00
Me
O
S
N
Ph
O
Me
O
OEt
3ja
0.94
1.00
1.97
1.02
1.01
2.01
2.09
3.00
2.95
3.43
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
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2.0
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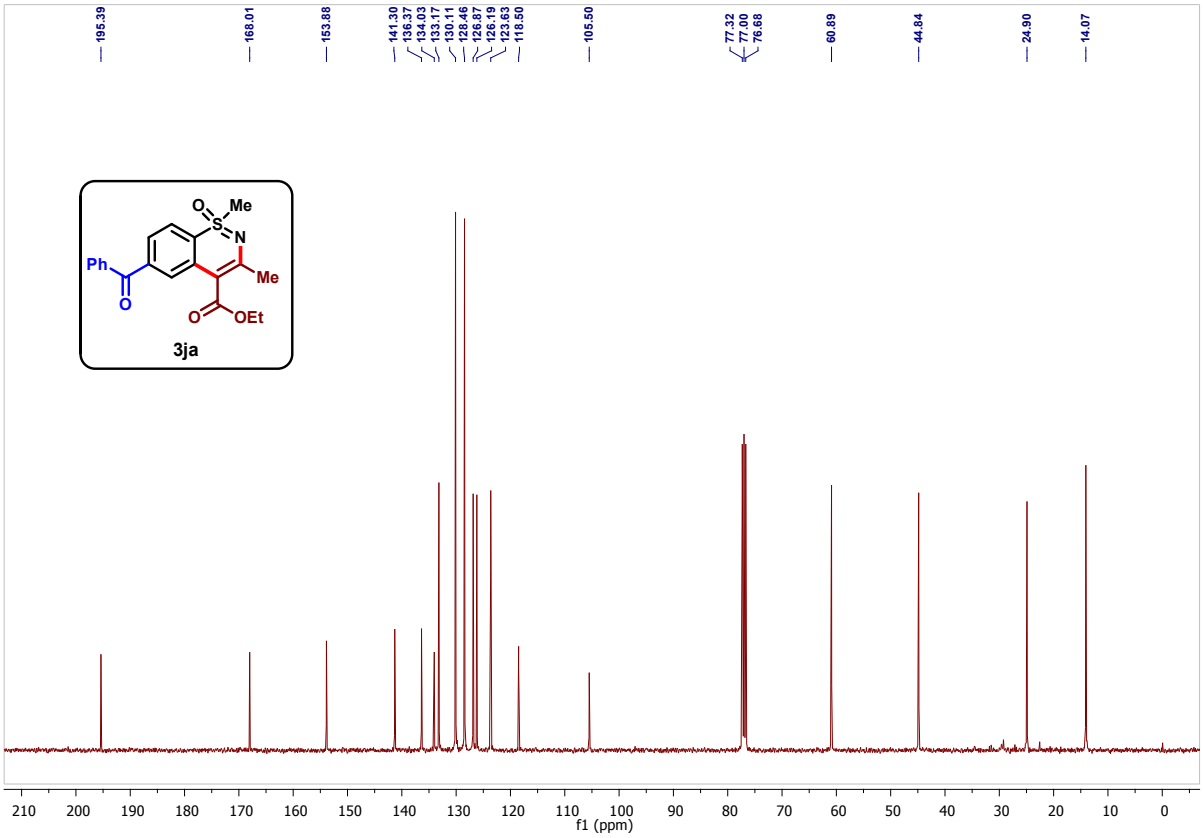
0.0
f1 (ppm)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123.63
118.50
105.50
77.32
77.00
76.68
60.89
44.84
24.90
14.07
Me
O
S
N
Ph
O
Me
O
OEt
3ja
210
200
190
180
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50
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30
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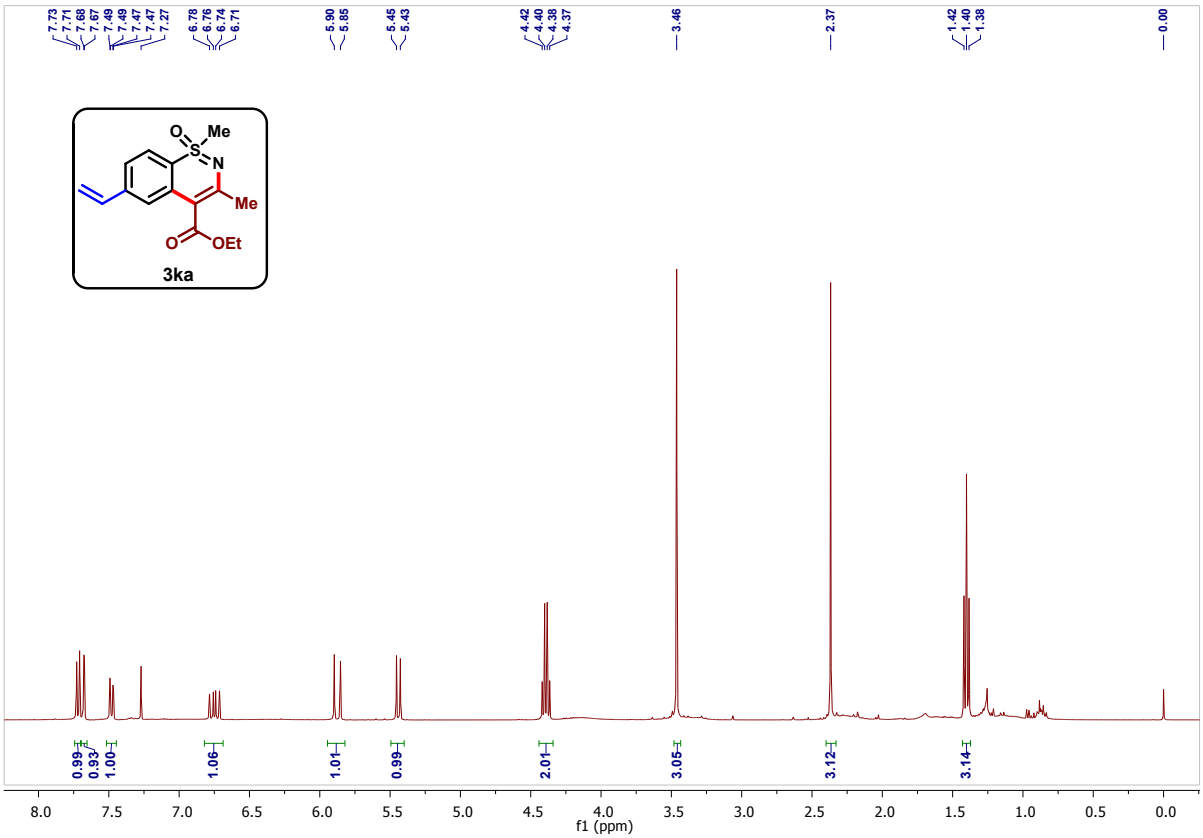
f1 (ppm)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6.71
5.90
5.85
5.45
5.43
4.42
4.40
4.38
4.37
3.46
2.37
1.42
1.40
1.38
0.00
O
Me
S
N
Me
O
OEt
3ka
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0.93
1.00
1.06
1.01
0.99
2.01
3.05
3.12
3.14
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
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2.0
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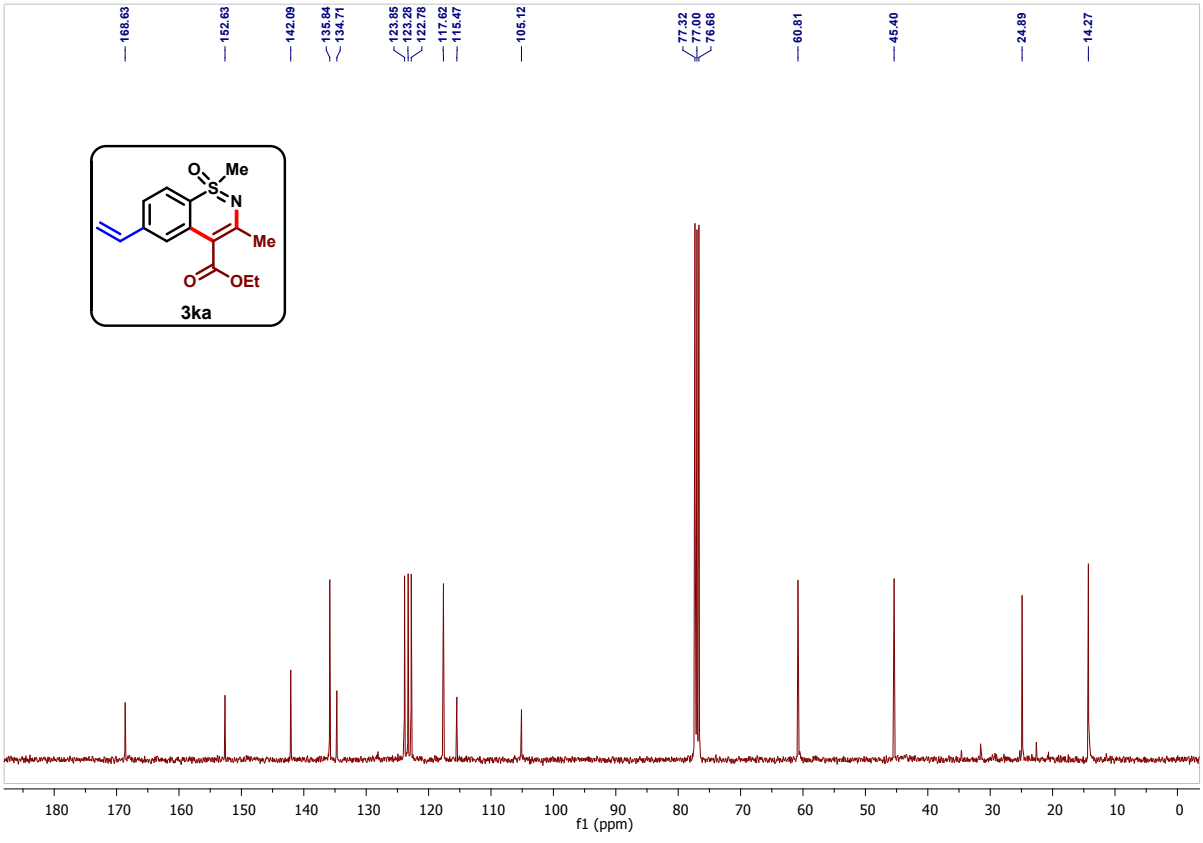
0.0
f1 (ppm)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123.85
123.28
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115.47
105.12
77.32
77.00
76.68
60.81
45.40
24.89
14.27
O
Me
S
N
Me
O
OEt
3ka
180
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150
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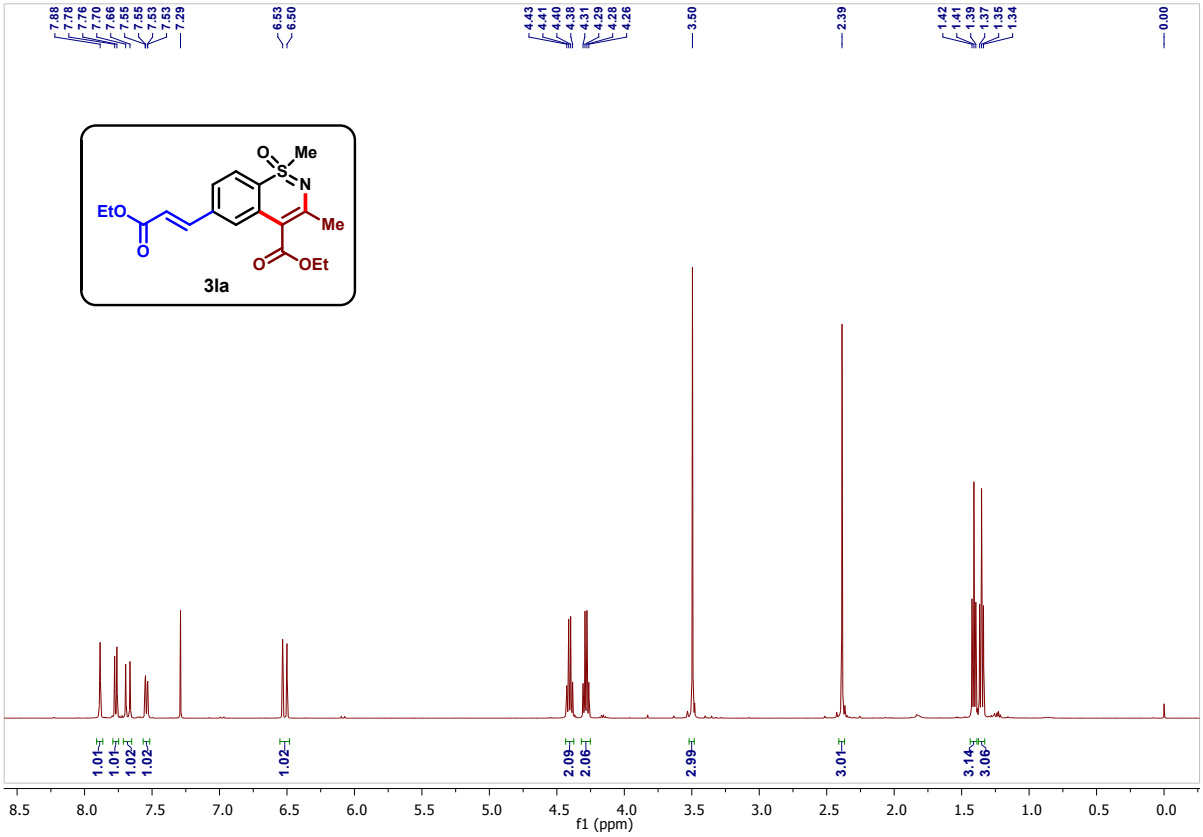
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.31
4.29
4.28
4.26
3.50
2.39
1.42
1.41
1.39
1.37
1.35
1.34
0.00
O
Me
S
N
EtO
Me
O
O
OEt
3la
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1.01
1.02
1.02
1.02
2.09
2.06
2.99
3.01
3.14
3.06
8.5
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7.0
6.5
6.0
5.5
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4.5
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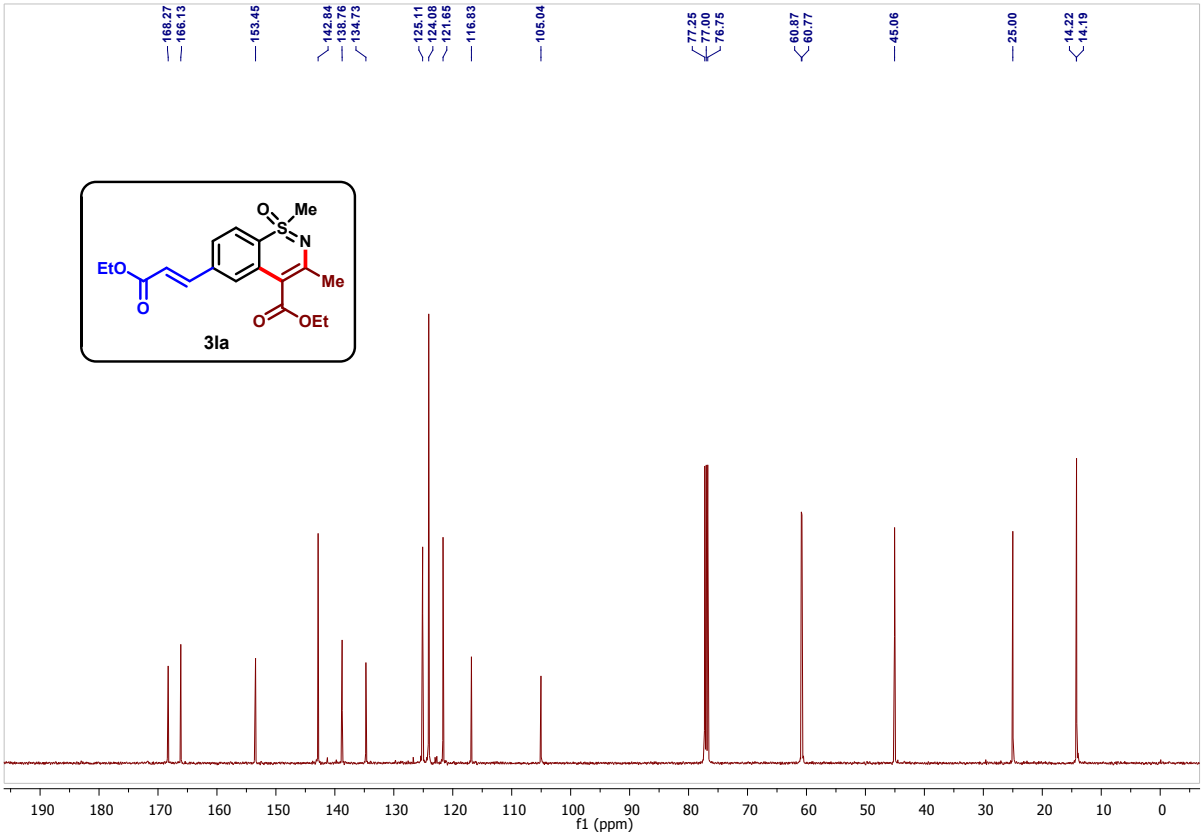
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.00
76.75
60.87
60.77
45.06
25.00
14.22
14.19
O
Me
S
N
EtO
Me
O
O
OEt
3la
190
180
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130
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110
100
90
80
70
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50
40
30
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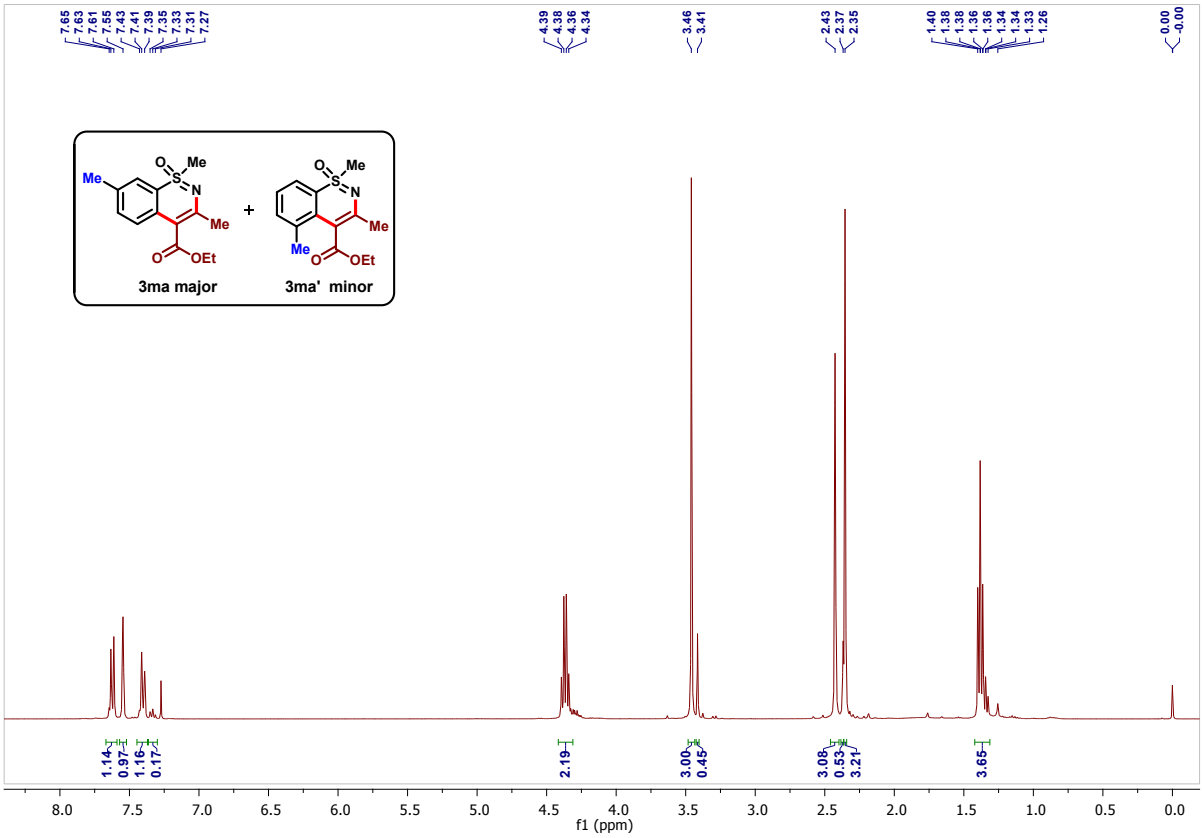
10
0
f1 (ppm)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7.27
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4.38
4.36
4.34
3.46
3.41
2.43
2.37
2.35
1.40
1.38
1.38
1.36
1.36
1.34
1.34
1.33
1.26
0.00
-0.00
3ma major
3ma' minor
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0.97
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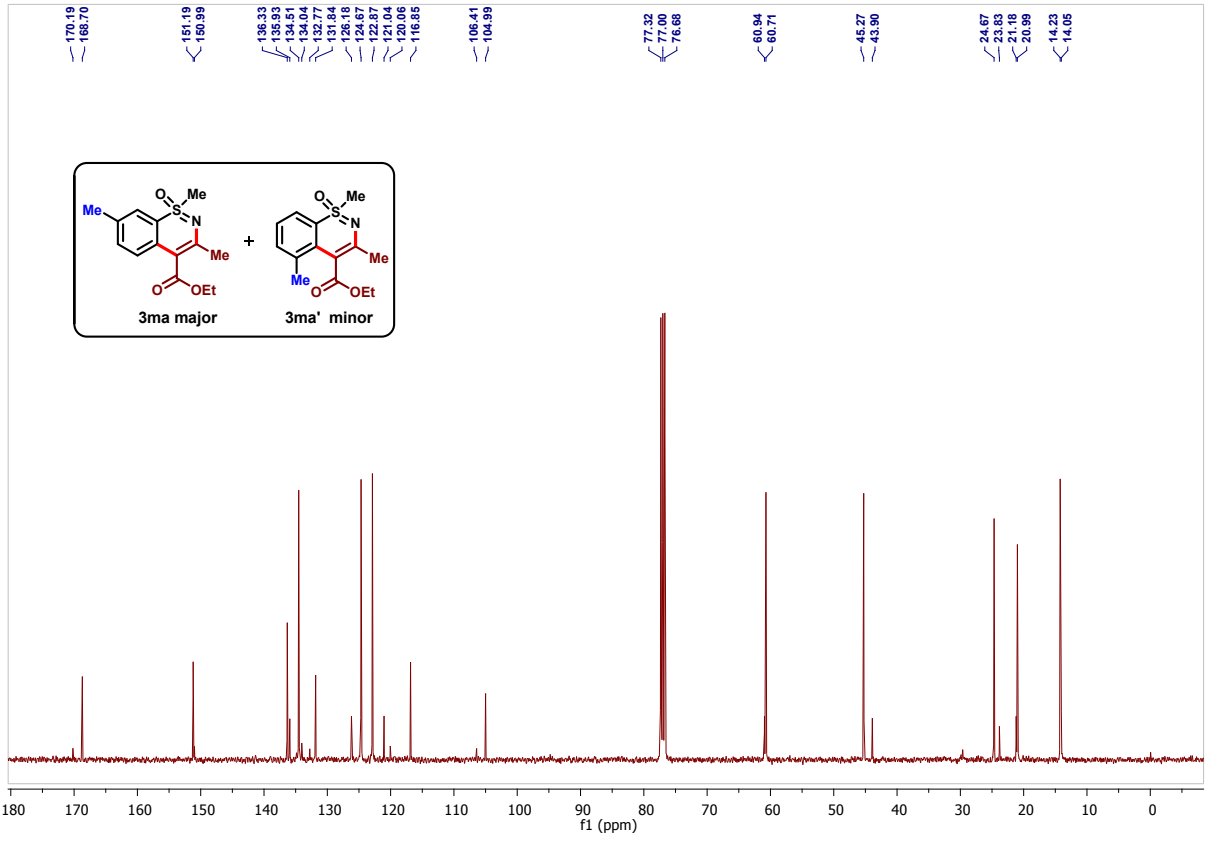
0.17
2.19
3.00
0.45
3.08
0.53
3.21
3.65
f1 (ppm)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135.93
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134.04
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131.84
126.18
124.67
122.87
121.04
120.06
116.85
106.41
104.99
77.32
77.00
76.68
60.94
60.71
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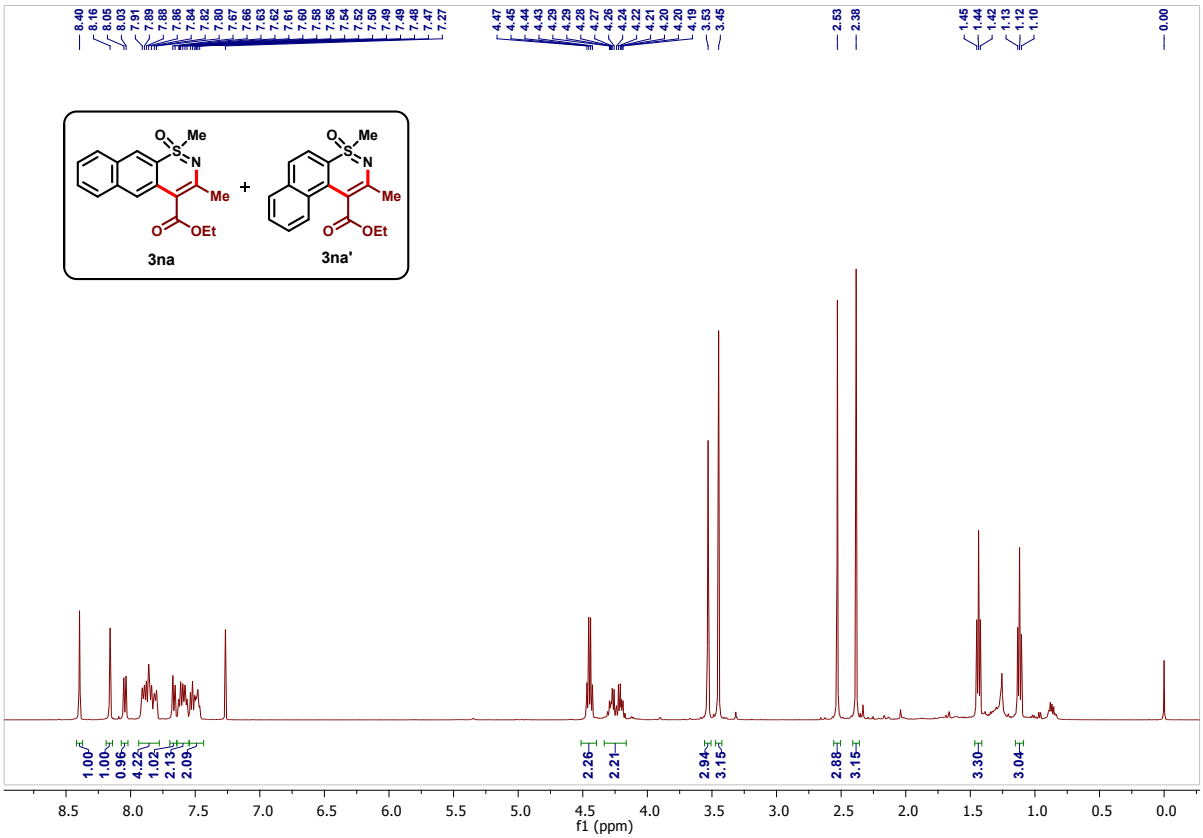
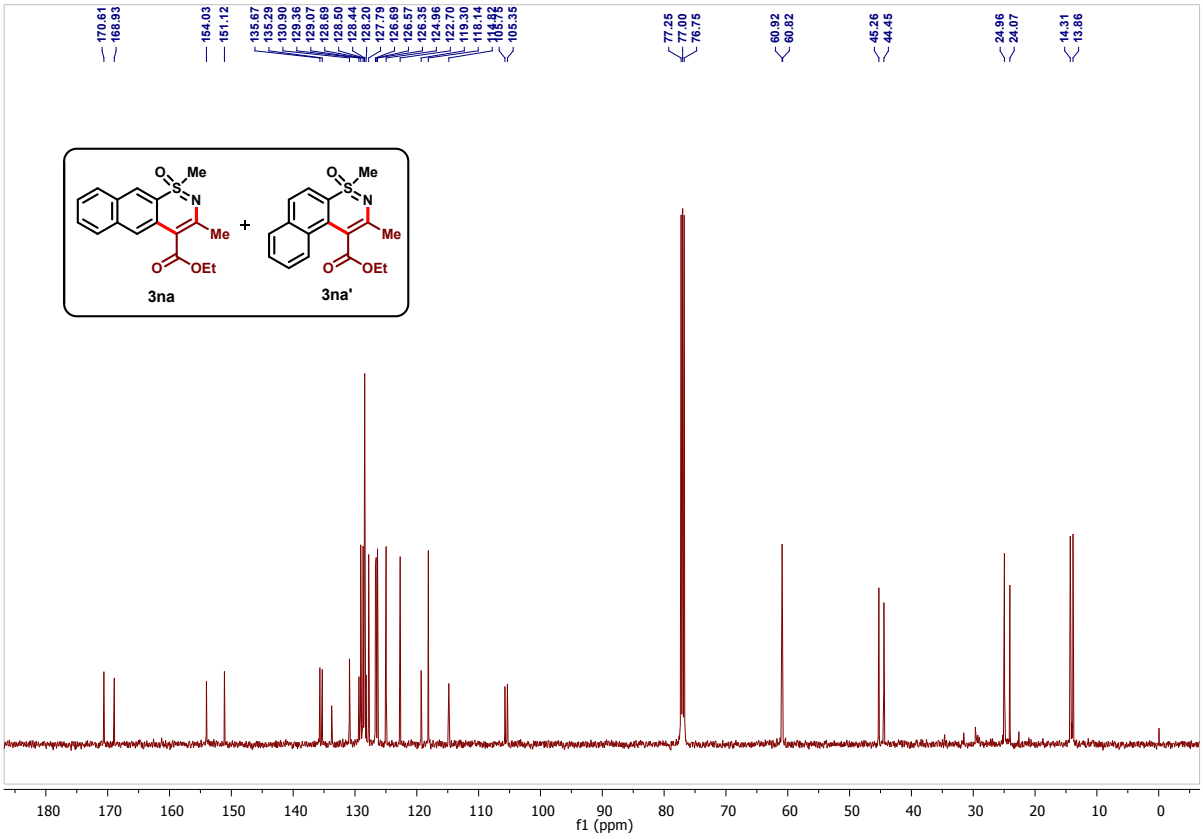
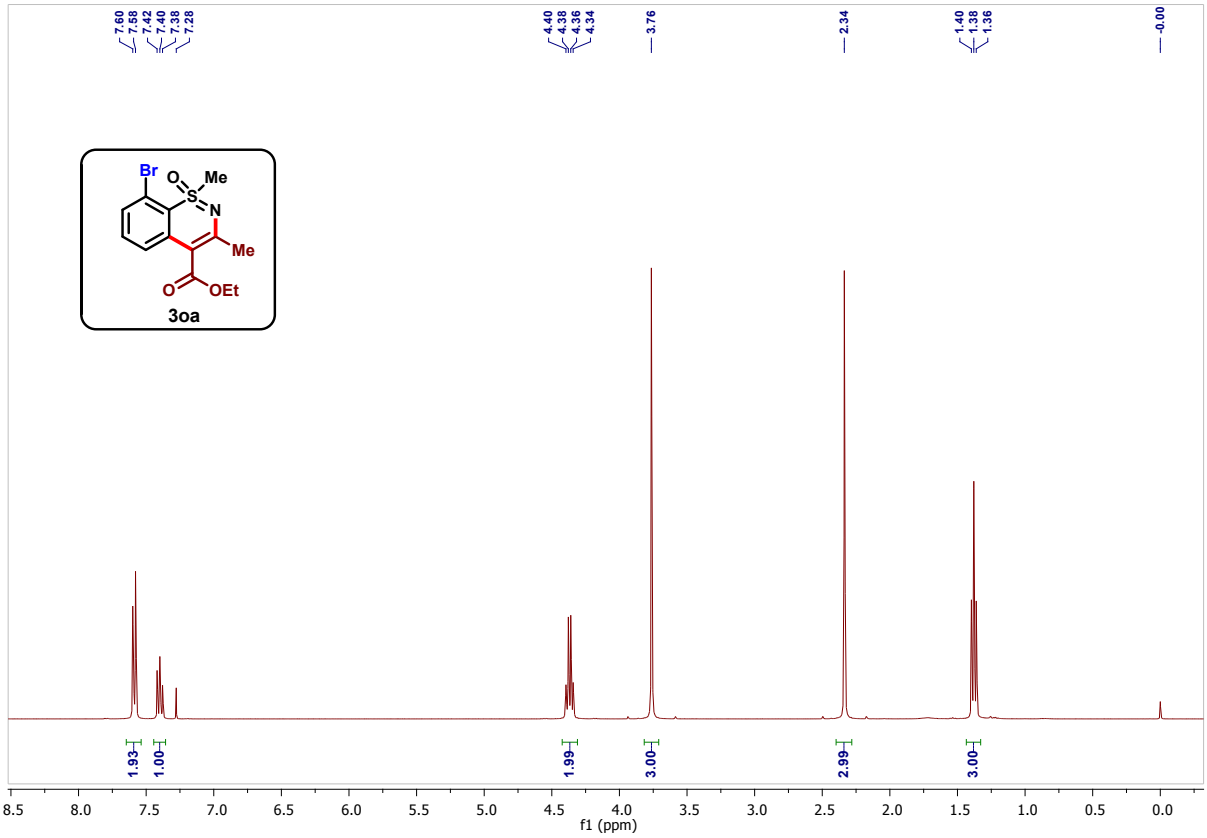
24.67
23.83
21.18
20.99
14.23
14.05
3ma major
3ma' minor
f1 (ppm)


3na
3na'
f1 (ppm)


3na
3na'
f1 (ppm)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4.38
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4.34
3.76
2.34
1.40
1.38
1.36
-0.00
Br
O
Me
S
N
Me
O
OEt
3oa
1.93
1.00
1.99
3.00
2.99
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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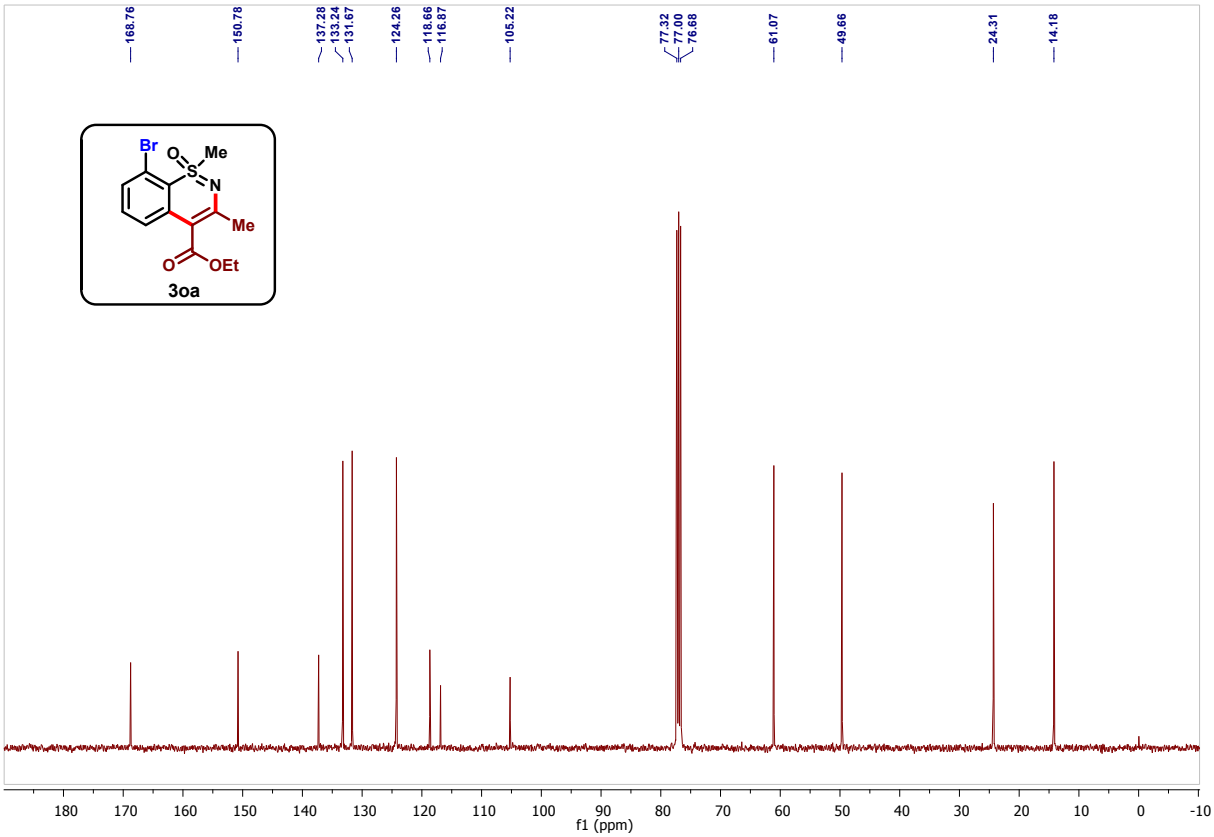
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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116.87
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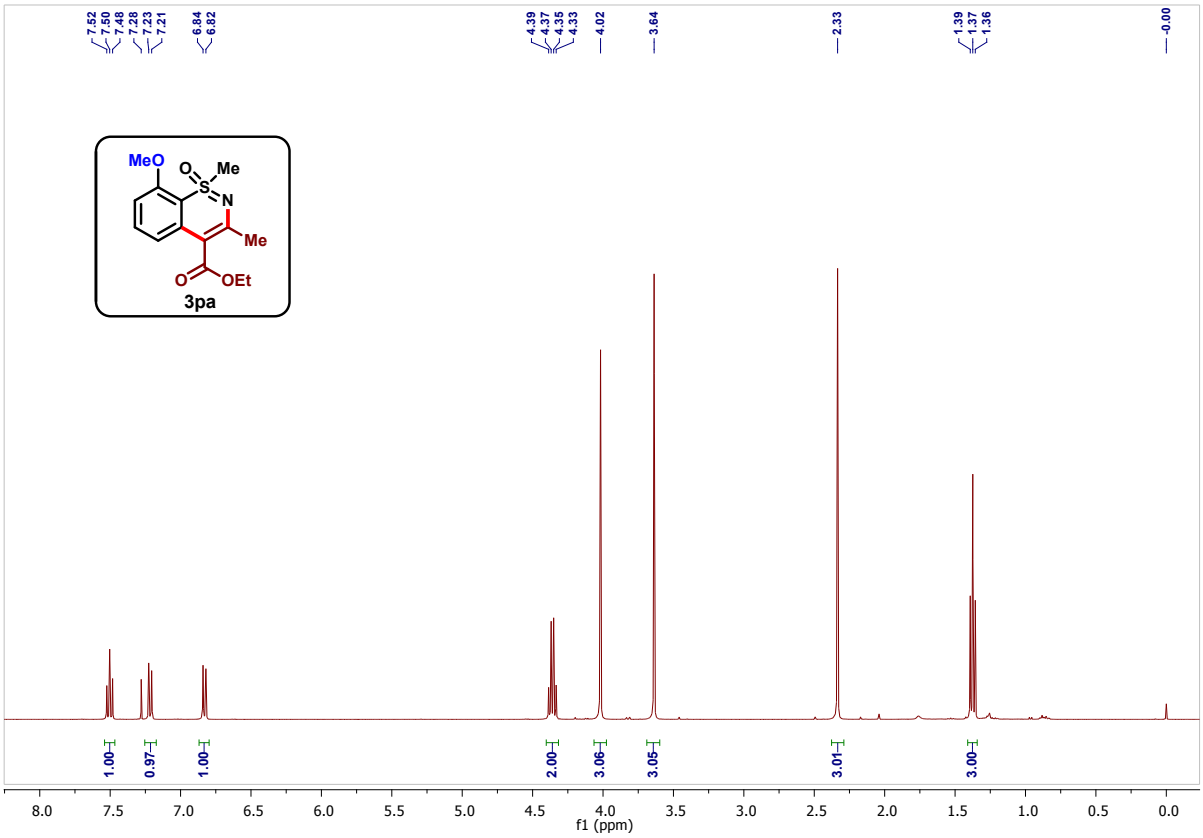
77.32
77.00
76.68
61.07
49.66
24.31
14.18
Br
O
Me
S
N
Me
O
OEt
3oa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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6.82
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4.37
4.35
4.33
4.02
3.64
2.33
1.39
1.37
1.36
-0.00
MeO
O
Me
S
N
Me
O
OEt
3pa
1.00
0.97
1.00
2.00
3.06
3.05
3.01
3.00
8.0
7.5
7.0
6.5
6.0
5.5
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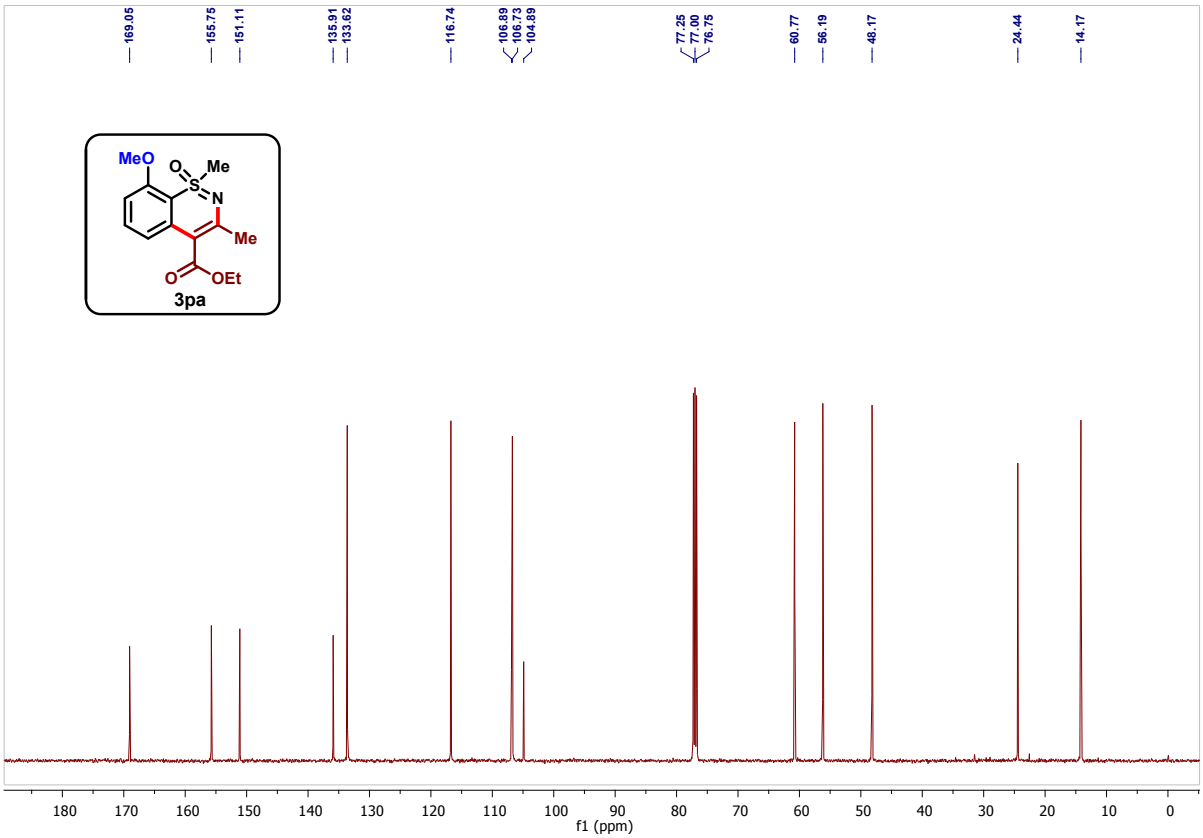
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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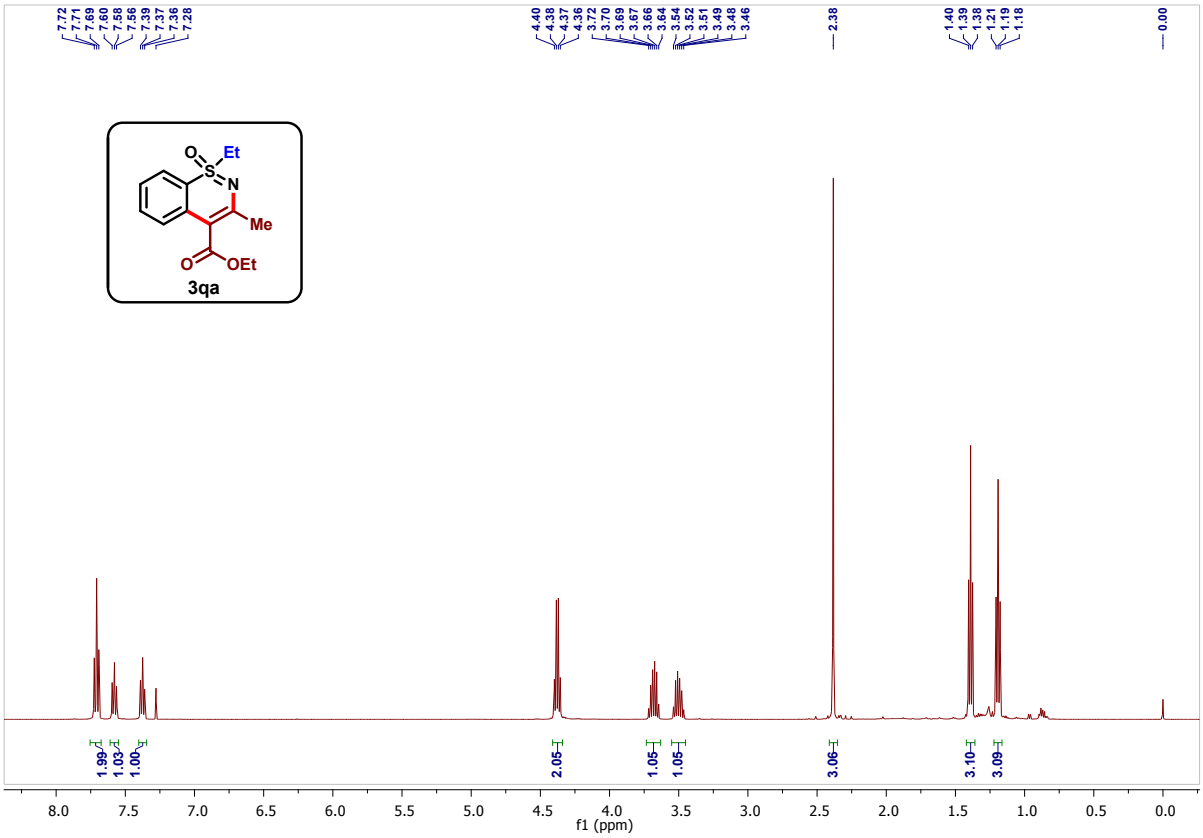
77.00
76.75
60.77
56.19
48.17
24.44
14.17
MeO
O
Me
S
N
Me
O
OEt
3pa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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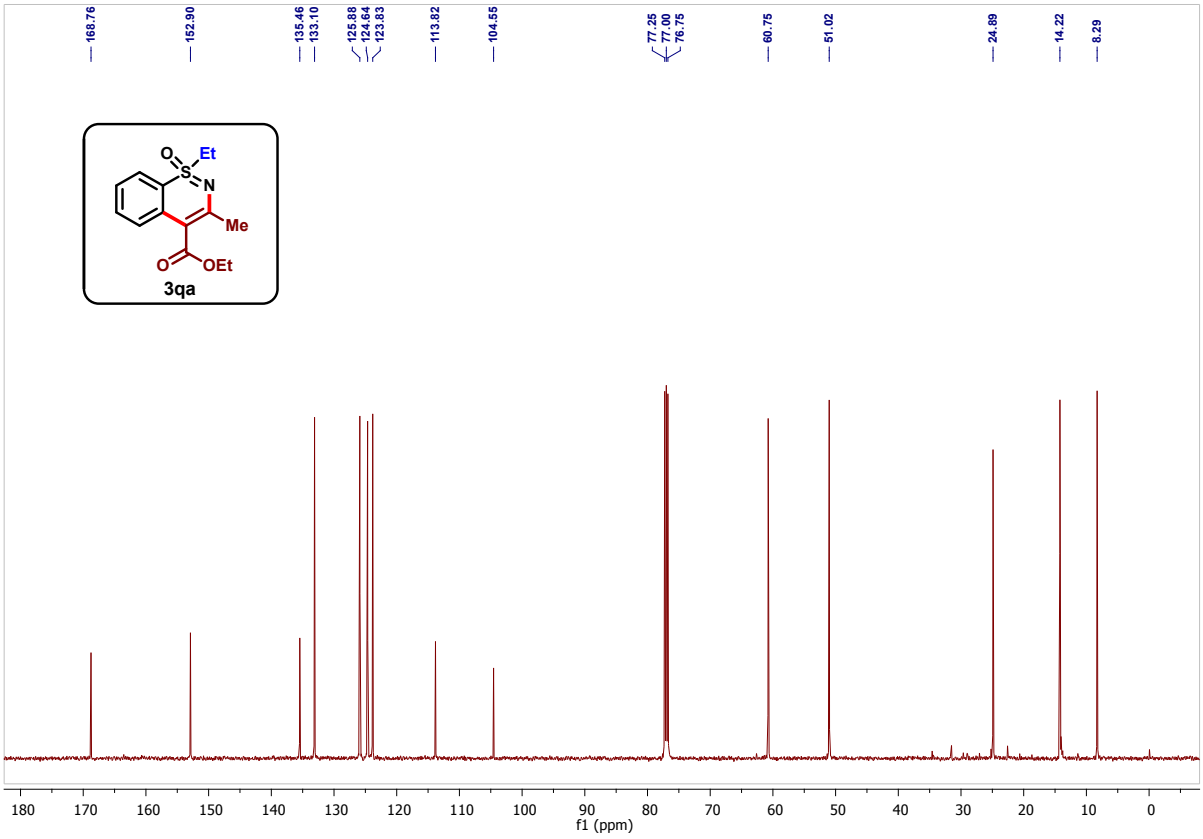
3.54
3.52
3.51
3.49
3.48
3.46
2.38
1.40
1.39
1.38
1.21
1.19
1.18
0.00
Et
N
Me
O
OEt
3qa
1.99
1.03
1.00
2.05
1.05
1.05
3.06
3.10
3.09
f1 (ppm)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77.25
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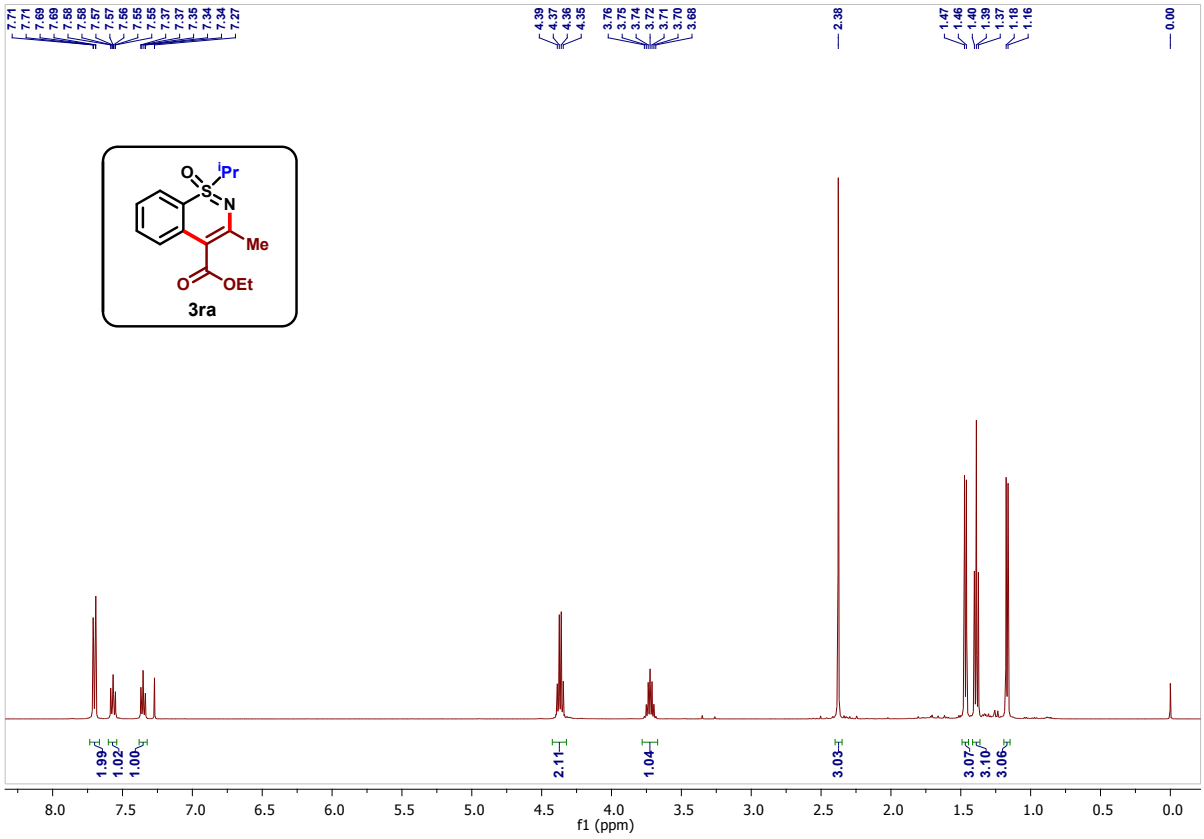
24.89
14.22
8.29
Et
N
Me
O
OEt
3qa
f1 (ppm)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4.39
4.37
4.36
4.35
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3.75
3.74
3.72
3.71
3.70
3.68
2.38
1.47
1.46
1.40
1.39
1.37
1.18
1.16
0.00
iPr
O
S
N
Me
O
OEt
3ra
1.99
1.02
1.00
2.11
1.04
3.03
3.07
3.10
3.06
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
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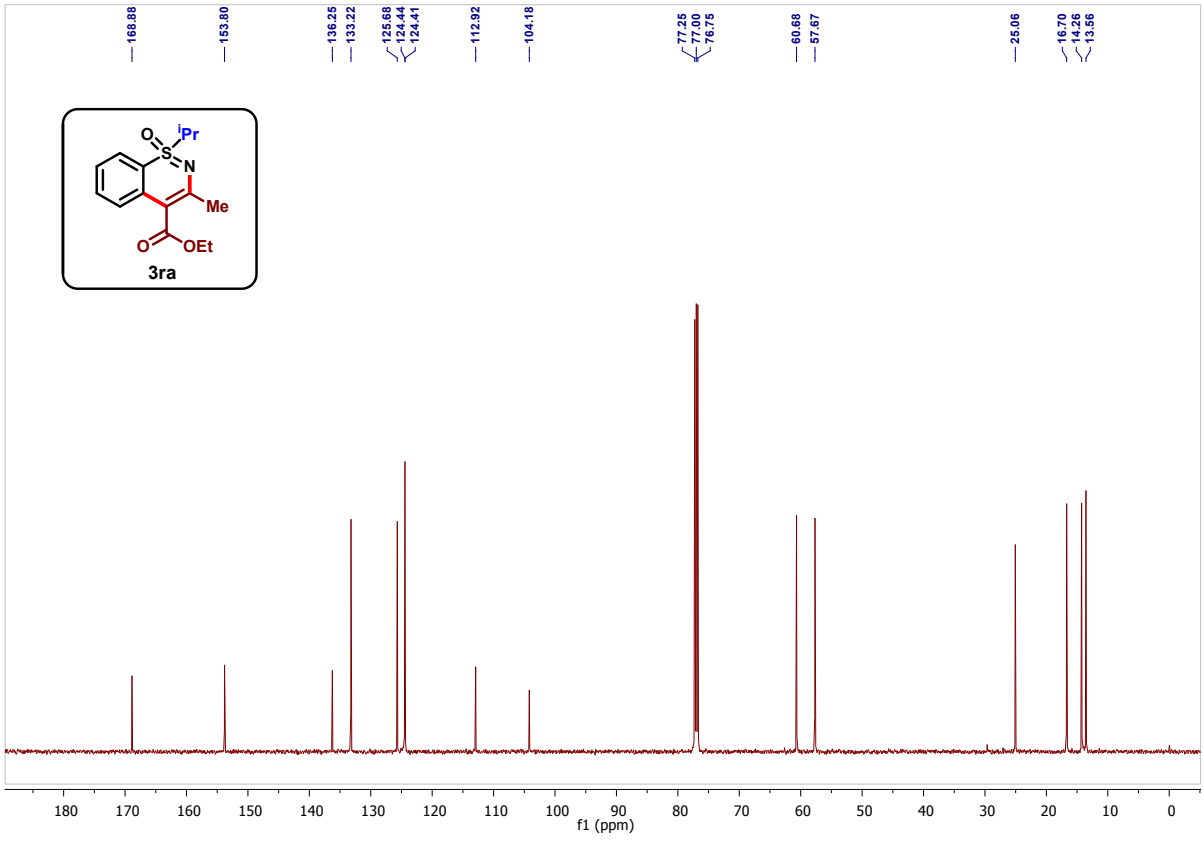
0.0
f1 (ppm)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60.68
57.67
25.06
16.70
14.26
13.56
iPr
O
S
N
Me
O
OEt
3ra
180
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130
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110
100
90
80
70
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50
40
30
20
10
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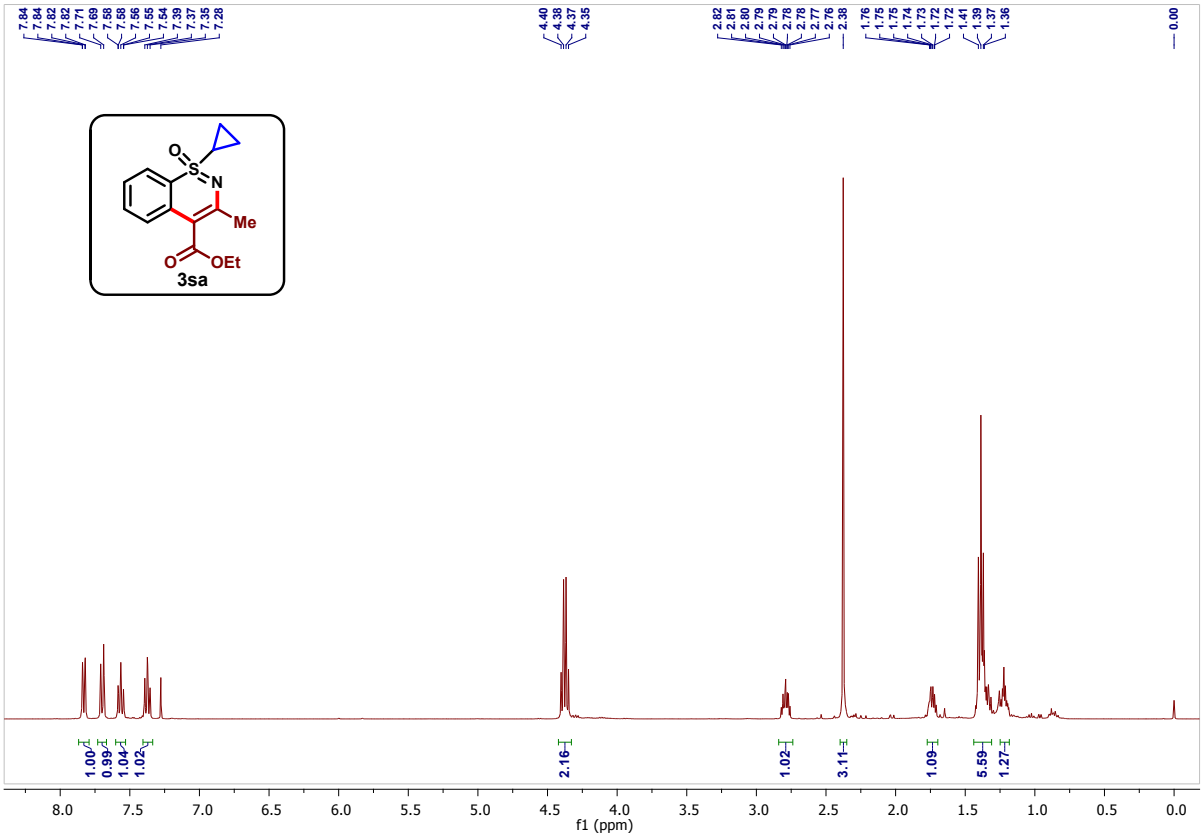
f1 (ppm)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7.37
7.35
7.28
4.40
4.38
4.37
4.35
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2.80
2.79
2.79
2.78
2.78
2.77
2.76
2.38
1.76
1.75
1.75
1.74
1.73
1.72
1.72
1.41
1.39
1.37
1.36
0.00
Me
OEt
3sa
1.00
0.99
1.04
1.02
2.16
1.02
3.11
1.09
5.59
1.27
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
1.5
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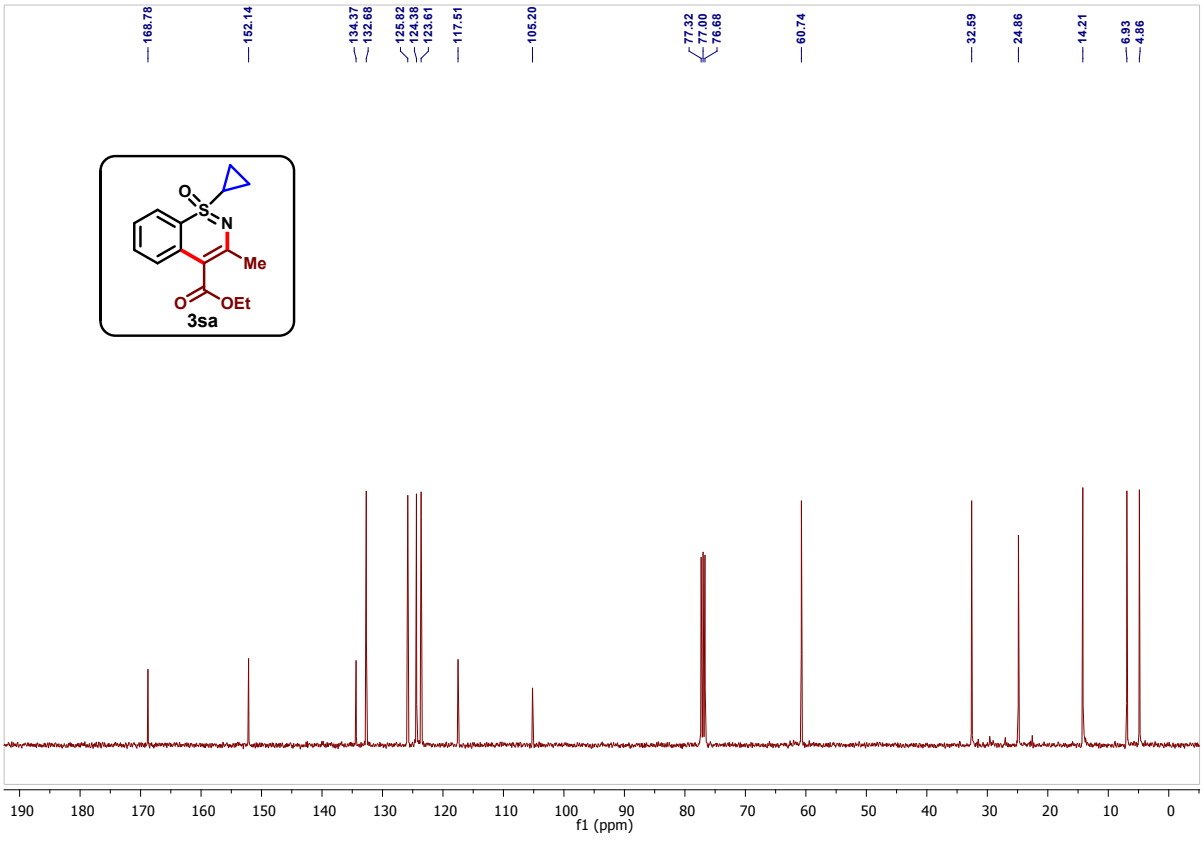
f1 (ppm)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77.32
77.00
76.68
60.74
32.59
24.86
14.21
6.93
4.86
Me
OEt
3sa
190
180
170
160
150
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130
120
110
100
90
80
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50
40
30
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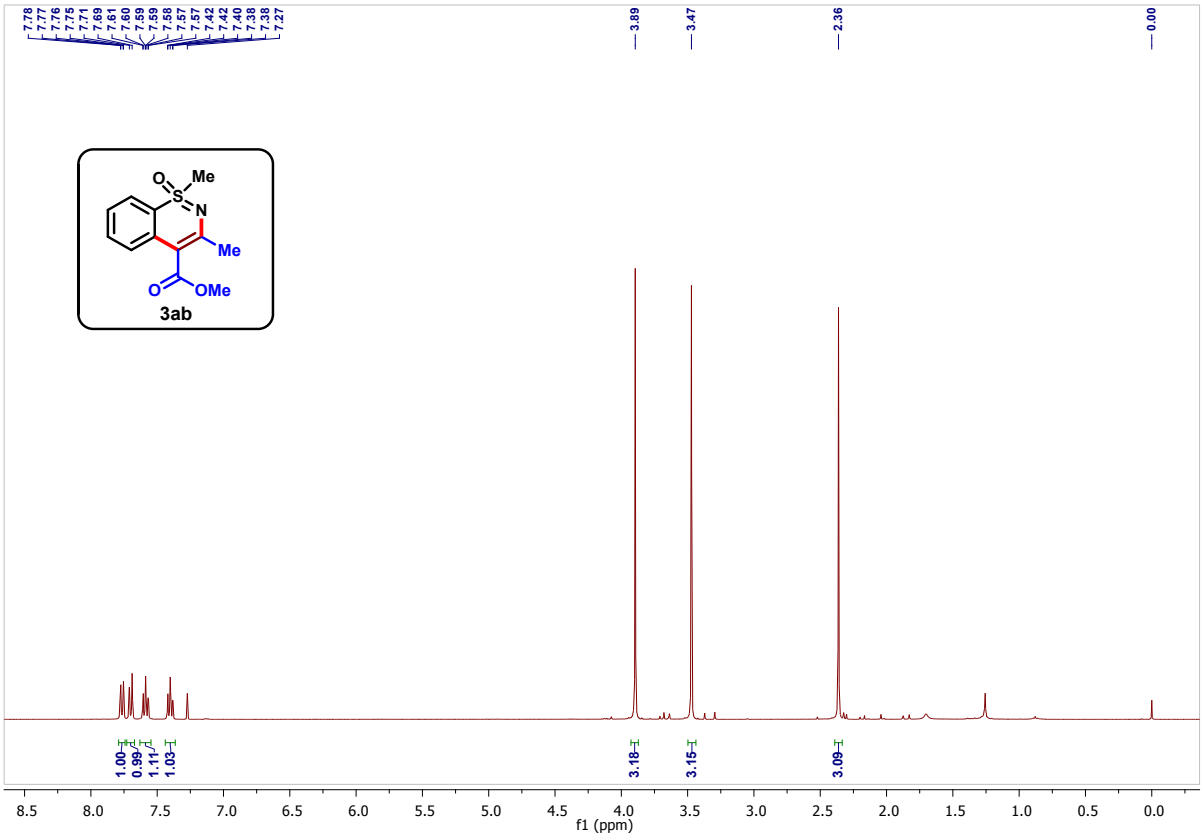
10
0
f1 (ppm)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7.57
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7.42
7.40
7.38
7.38
7.27
3.89
3.47
2.36
0.00
Me
O
S
N
Me
O
OMe
3ab
1.00
0.99
1.11
1.03
3.18
3.15
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
1.5
1.0
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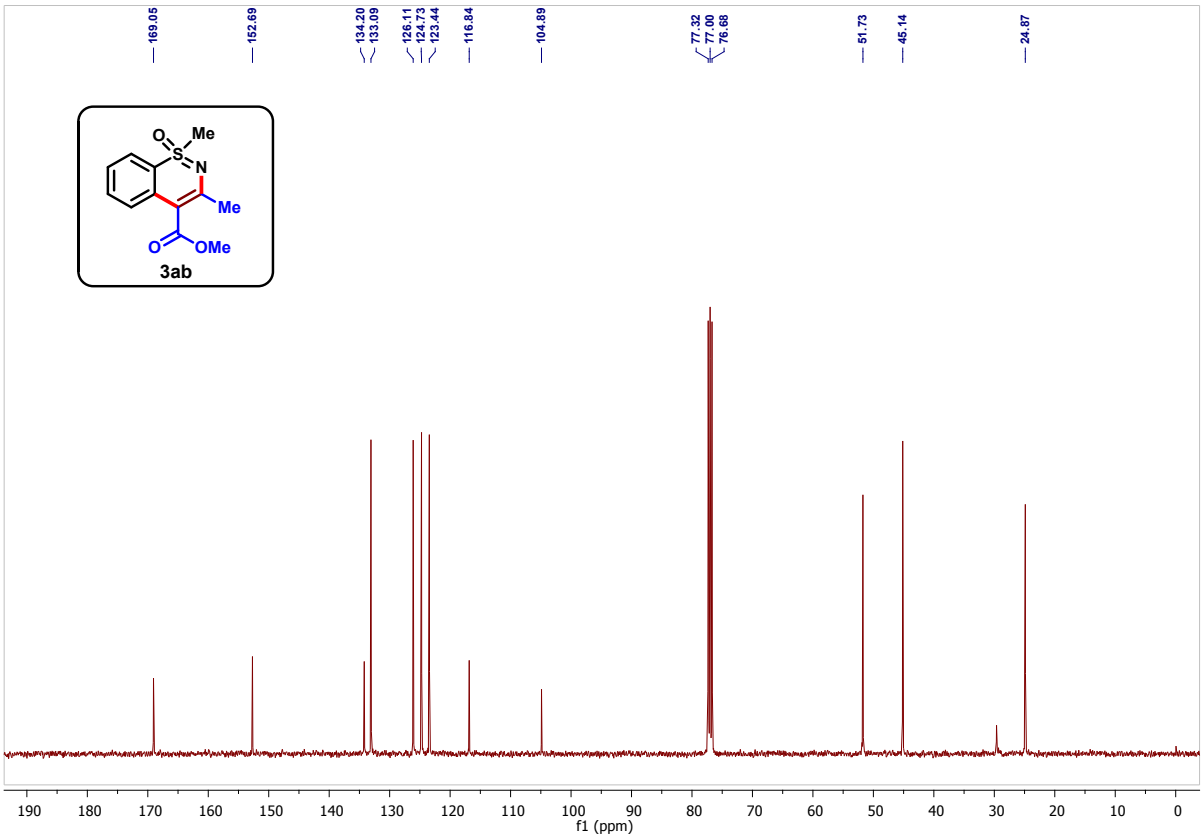
0.0
f1 (ppm)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123.44
116.84
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77.32
77.00
76.68
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45.14
24.87
Me
O
S
N
Me
O
OMe
3ab
190
180
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130
120
110
100
90
80
70
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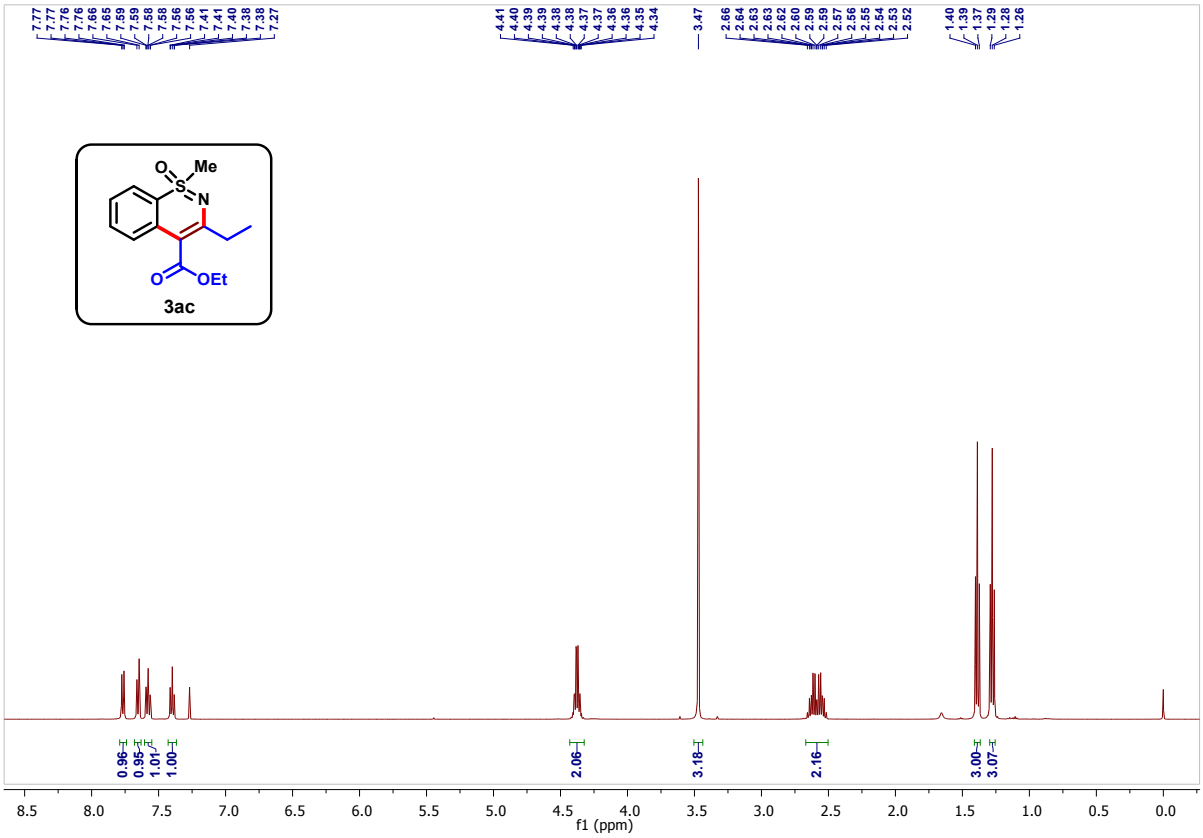
50
40
30
20
10
0
f1 (ppm)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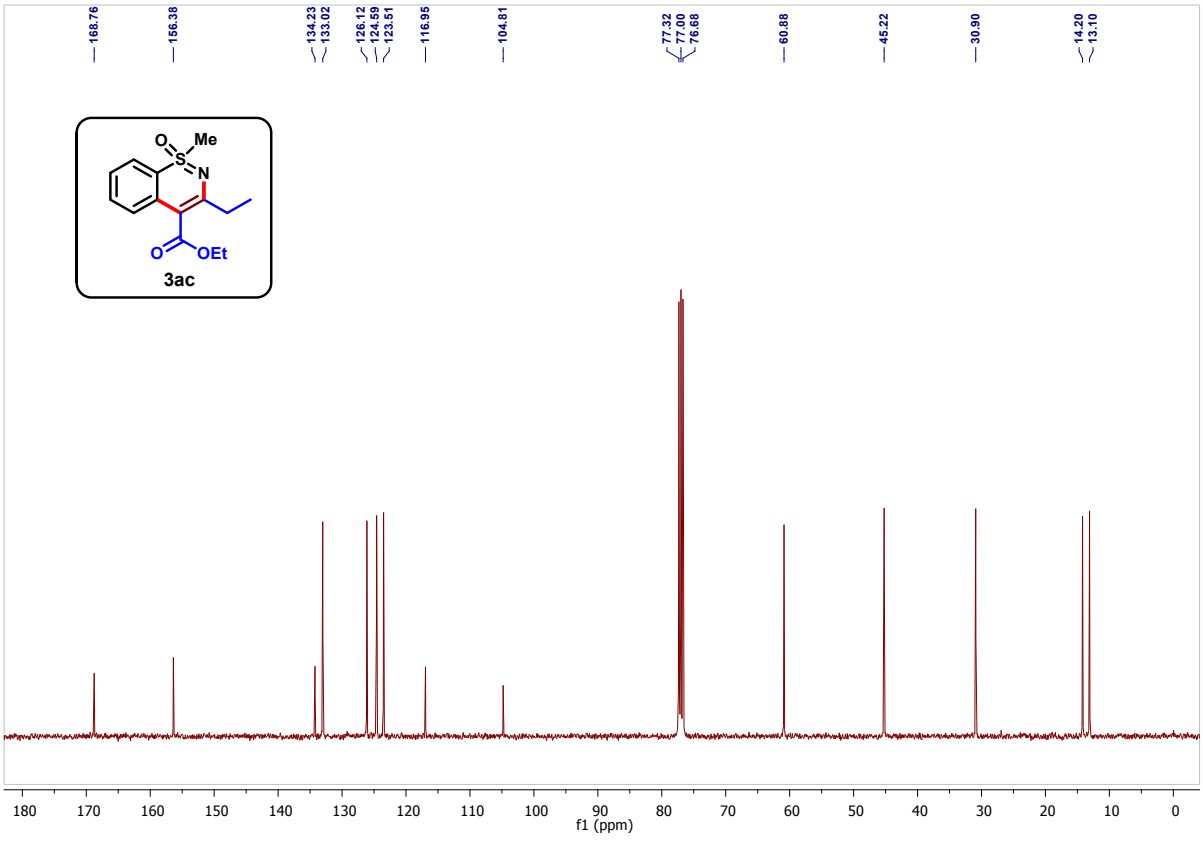
4.41 4.40 4.39 4.39 4.38 4.38 4.37 4.37 4.36 4.36 4.35 4.34
3.47
2.66 2.64 2.63 2.63 2.62 2.60 2.59 2.59 2.57 2.56 2.55 2.54 2.53 2.52
1.40 1.39 1.37 1.29 1.28 1.26
O
Me
S
N
O
OEt
3ac
0.96 0.95 1.01 1.00
2.06
3.18
2.16
3.00 3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.59
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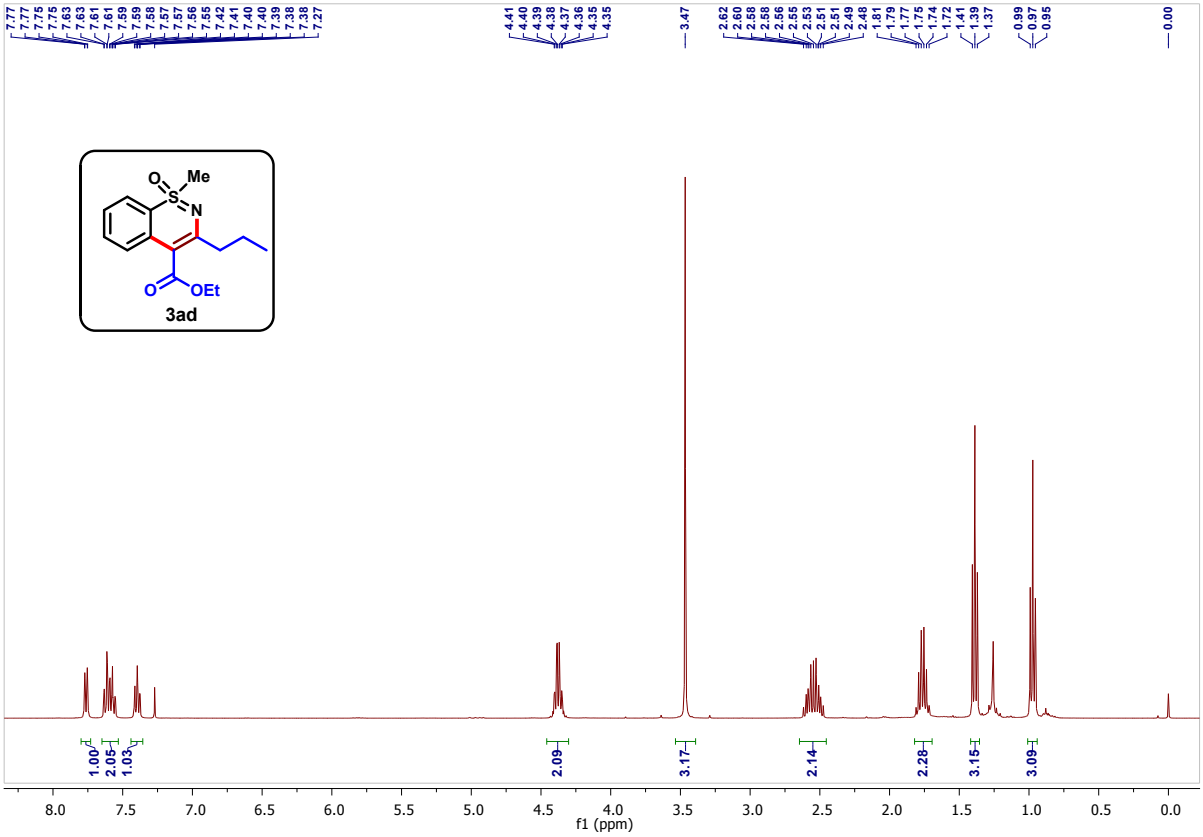
77.32
77.00
76.68
60.88
45.22
30.90
14.20
13.10
O
Me
S
N
O
OEt
3ac
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.58
7.57
7.57
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7.40
7.40
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7.38
7.27
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4.40
4.39
4.38
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4.36
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2.53
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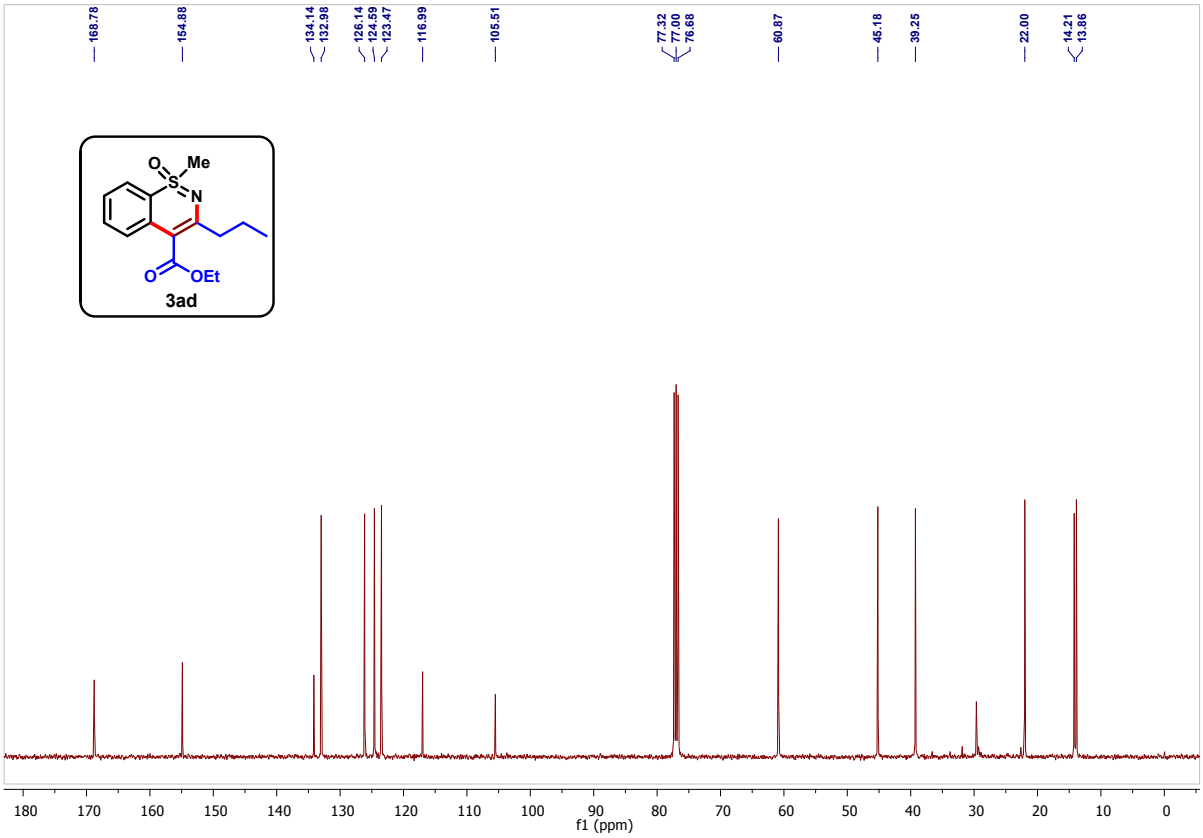
2.51
2.49
2.48
1.81
1.79
1.77
1.75
1.74
1.72
1.41
1.39
1.37
0.99
0.97
0.95
0.00
Me
O
S
N
O
OEt
3ad
1.00
2.05
1.03
2.09
3.17
2.14
2.28
3.15
3.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.00
76.68
60.87
45.18
39.25
22.00
14.21
13.86
Me
O
S
N
O
OEt
3ad
180
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150
140
130
120
110
100
90
80
70
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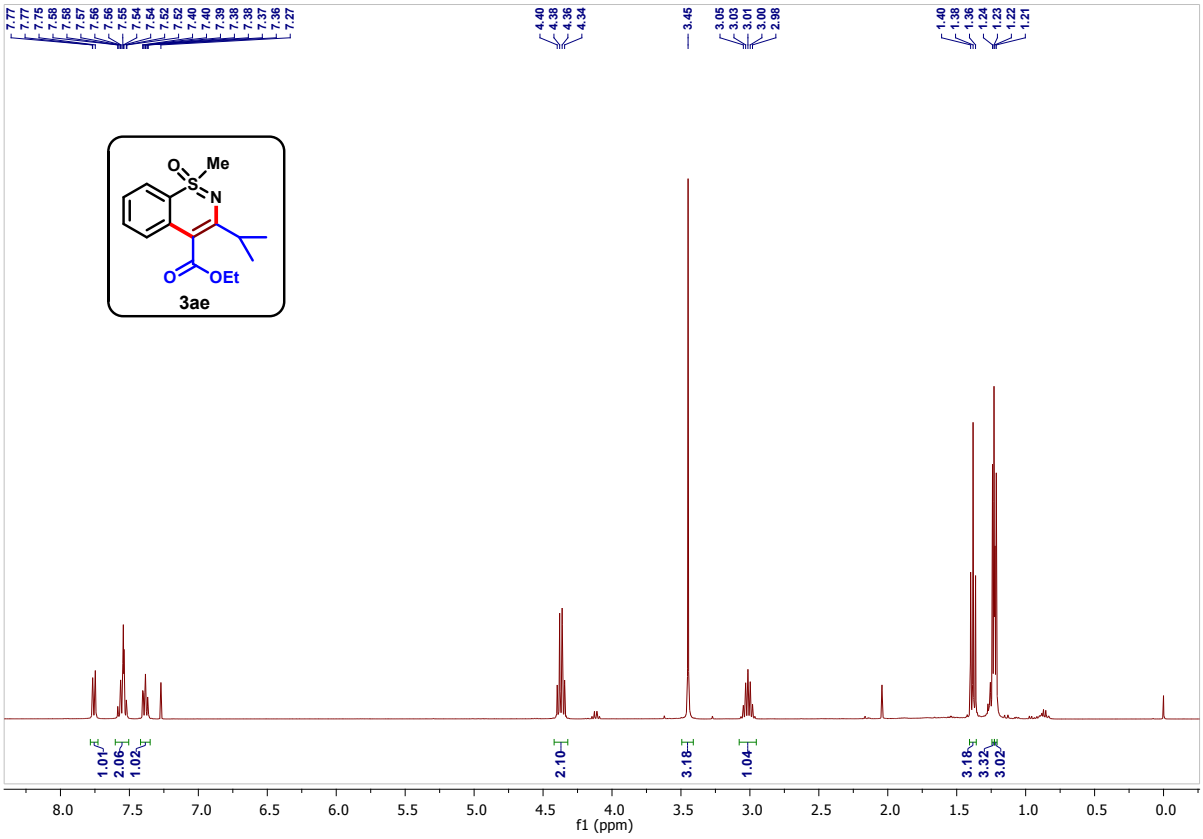
50
40
30
20
10
0
f1 (ppm)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4.40 4.38 4.36 4.34
3.45
3.05 3.03 3.01 3.00 2.98
1.40 1.38 1.36 1.24 1.23 1.22 1.21
Me
O
S
N
O
OEt
3ae
1.01 2.06 1.02 2.10 3.18 1.04 3.18 3.32 3.02
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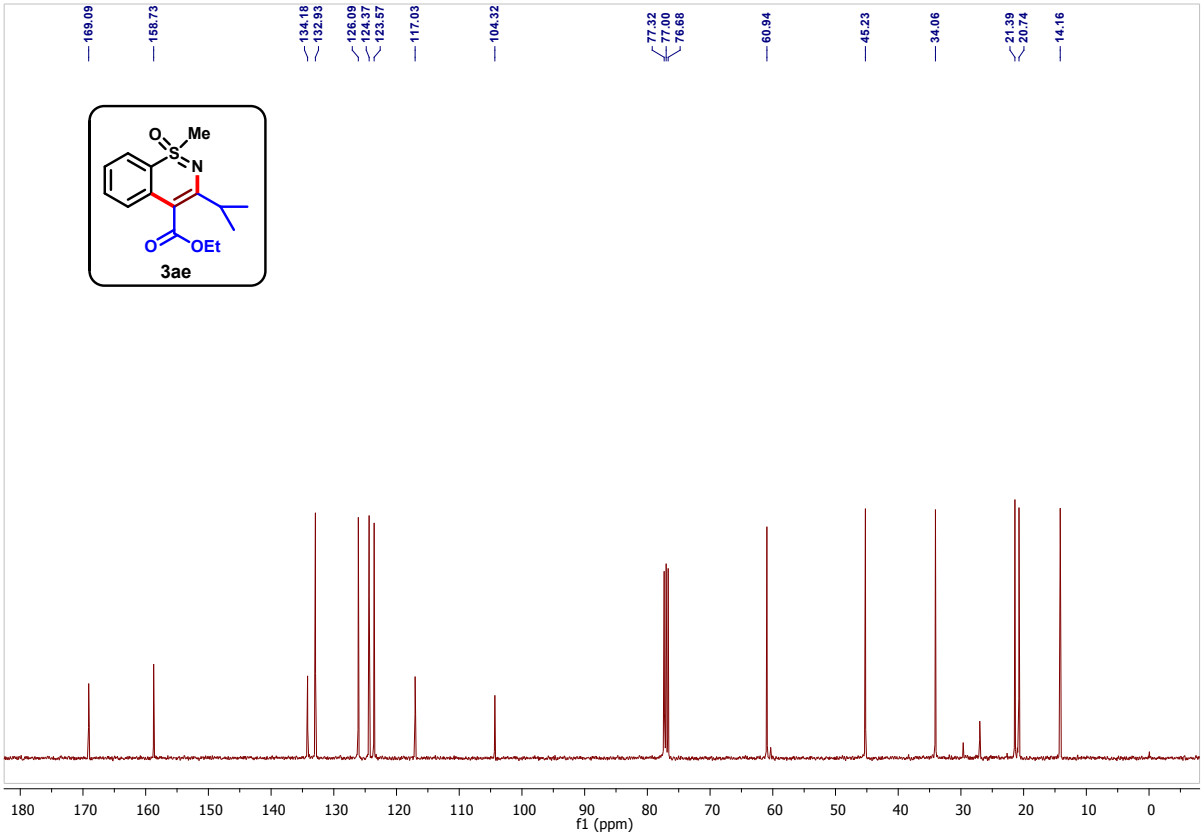
f1 (ppm)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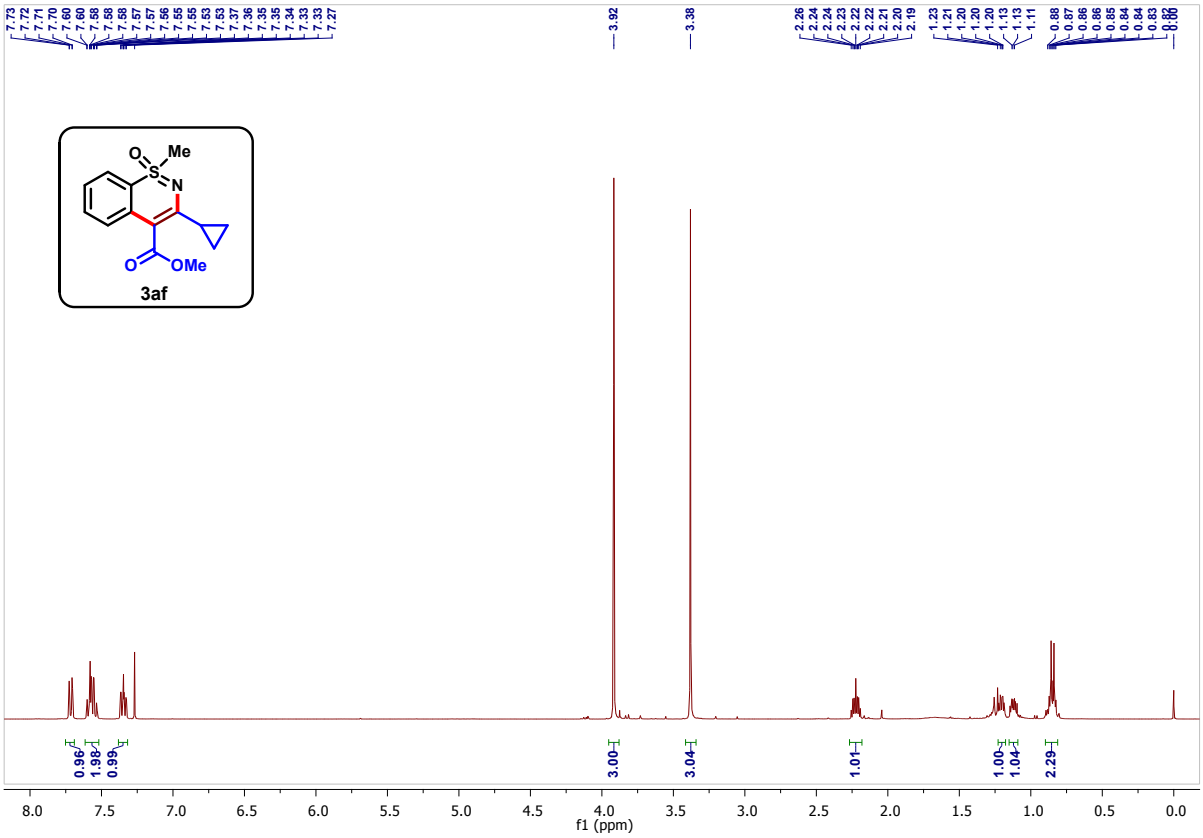
Me
O
S
N
O
OEt
3ae
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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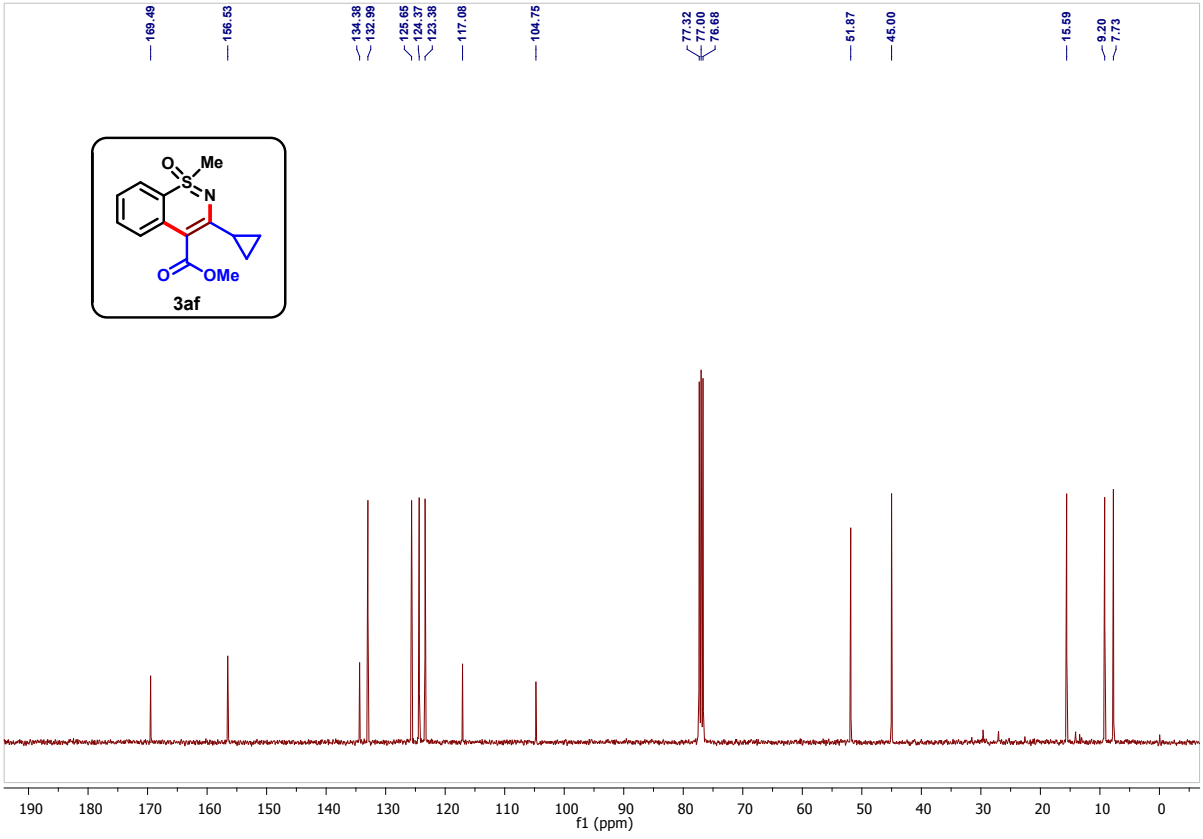
f1 (ppm)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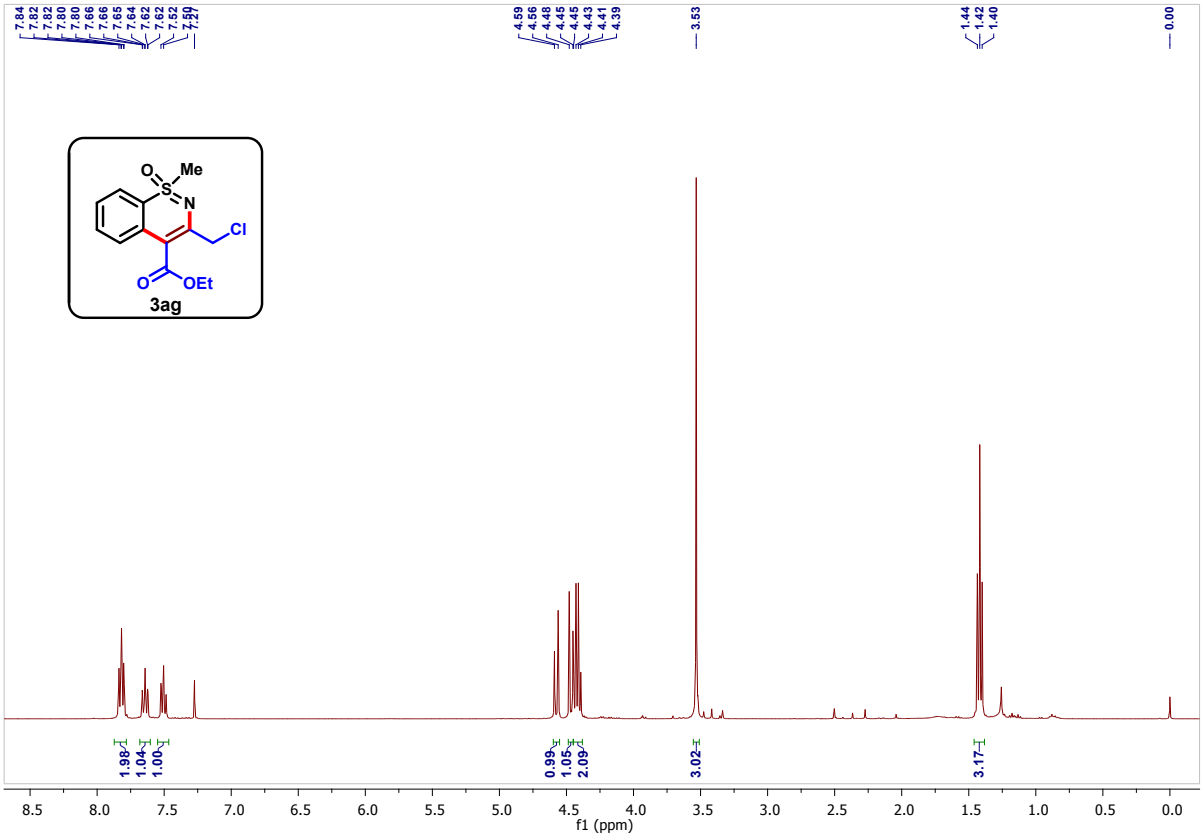
f1 (ppm)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4.56
4.48
4.45
4.45
4.43
4.41
4.39
3.53
1.44
1.42
1.40
0.00
Me
O
S
N
Cl
O
OEt
3ag
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1.04
1.00
0.99
1.05
2.09
3.02
3.17
8.5
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7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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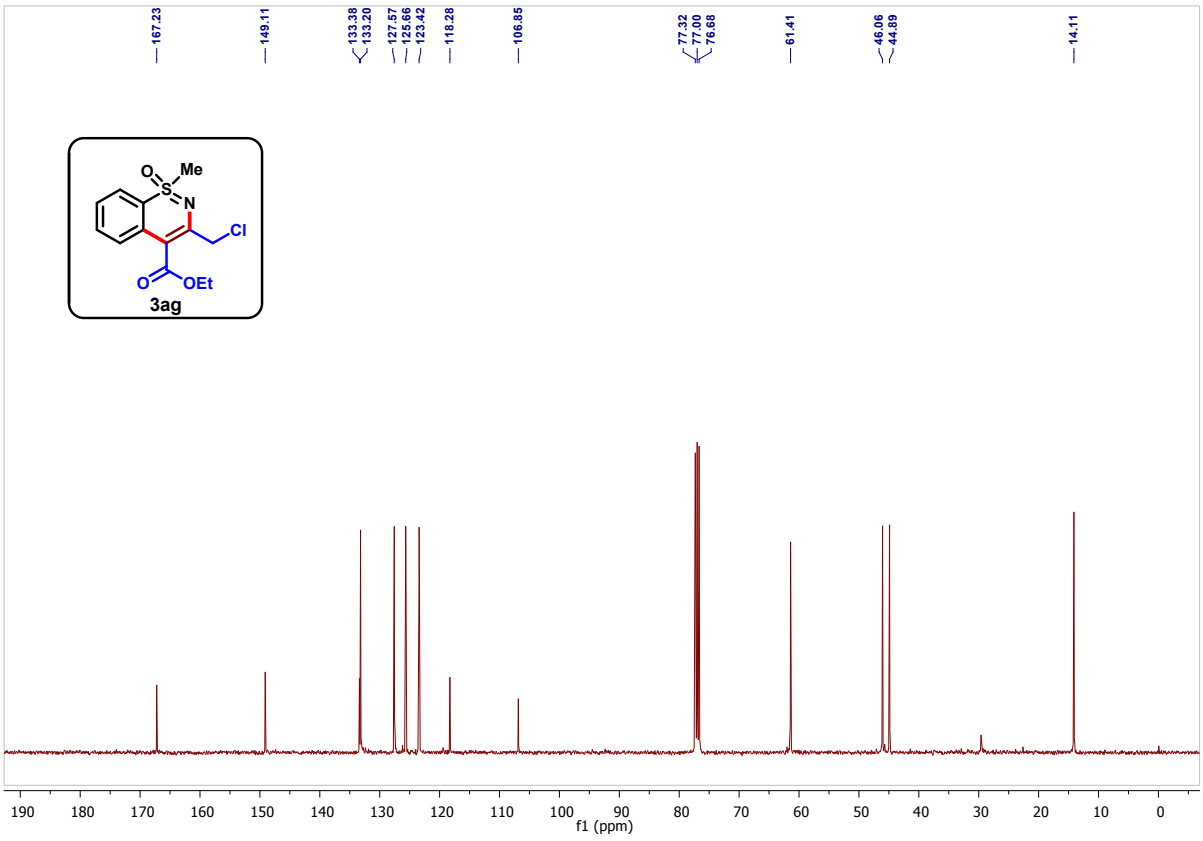
0.0
f1 (ppm)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77.32
77.00
76.68
61.41
46.06
44.89
14.11
Me
O
S
N
Cl
O
OEt
3ag
190
180
170
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130
120
110
100
90
80
70
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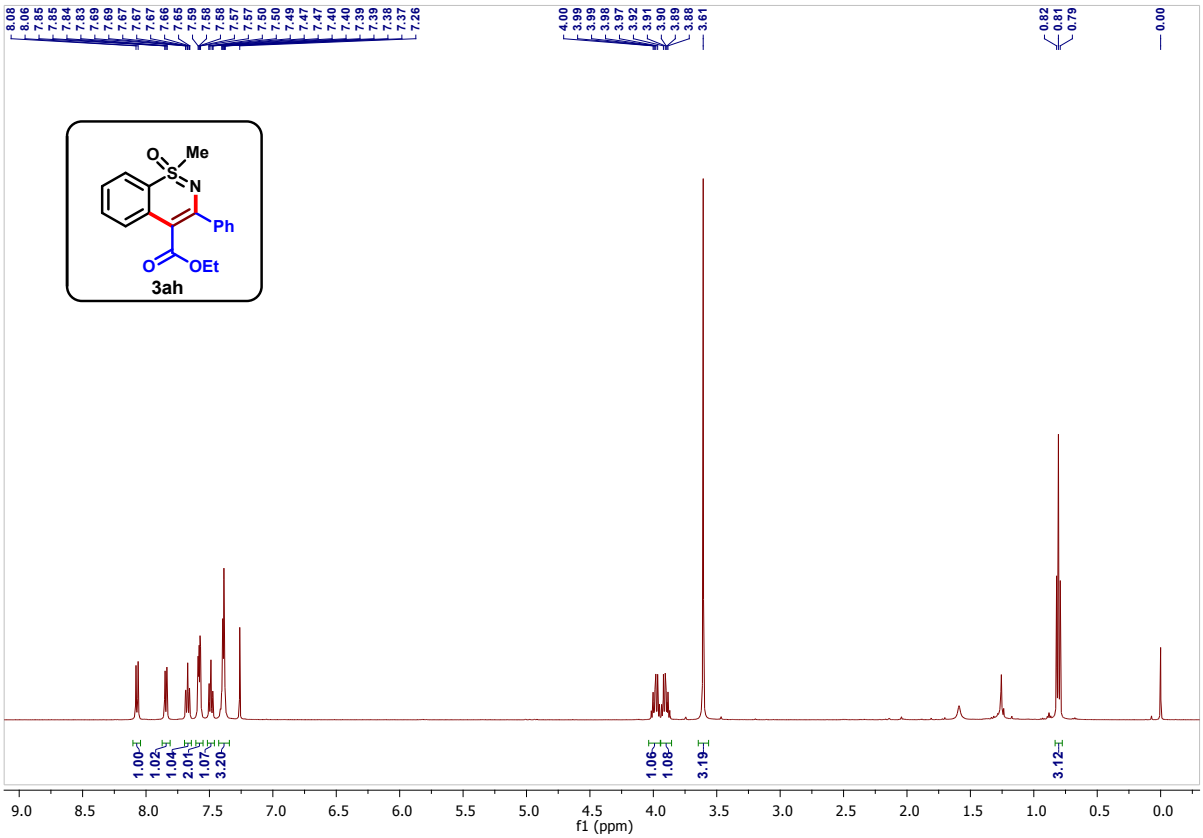
50
40
30
20
10
0
f1 (ppm)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7.39
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3.99
3.99
3.98
3.97
3.92
3.91
3.90
3.89
3.88
3.61
0.82
0.81
0.79
0.00
Me
O
S
N
Ph
O
OEt
3ah
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1.02
1.04
2.01
1.07
3.20
1.06
1.08
3.19
3.12
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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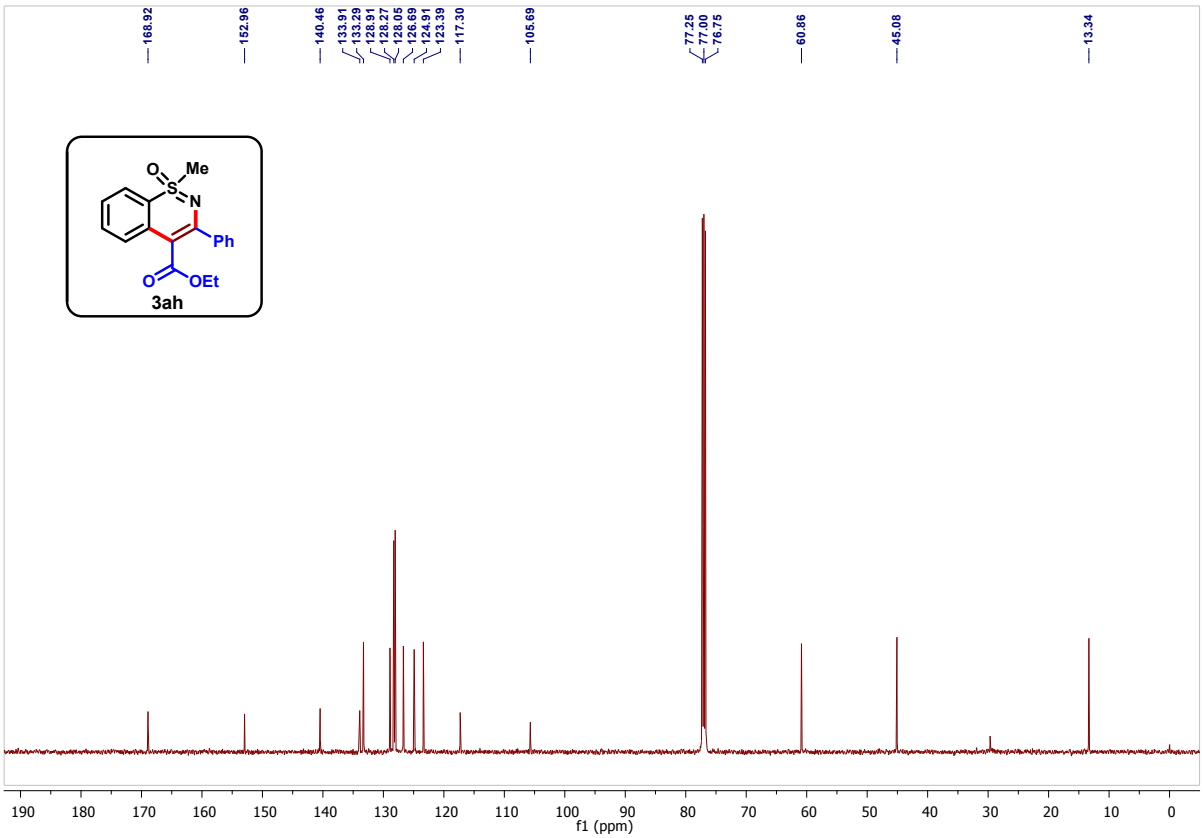
0.0
f1 (ppm)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124.91
123.39
117.30
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77.25
77.00
76.75
60.86
45.08
13.34
Me
O
S
N
Ph
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OEt
3ah
190
180
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90
80
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50
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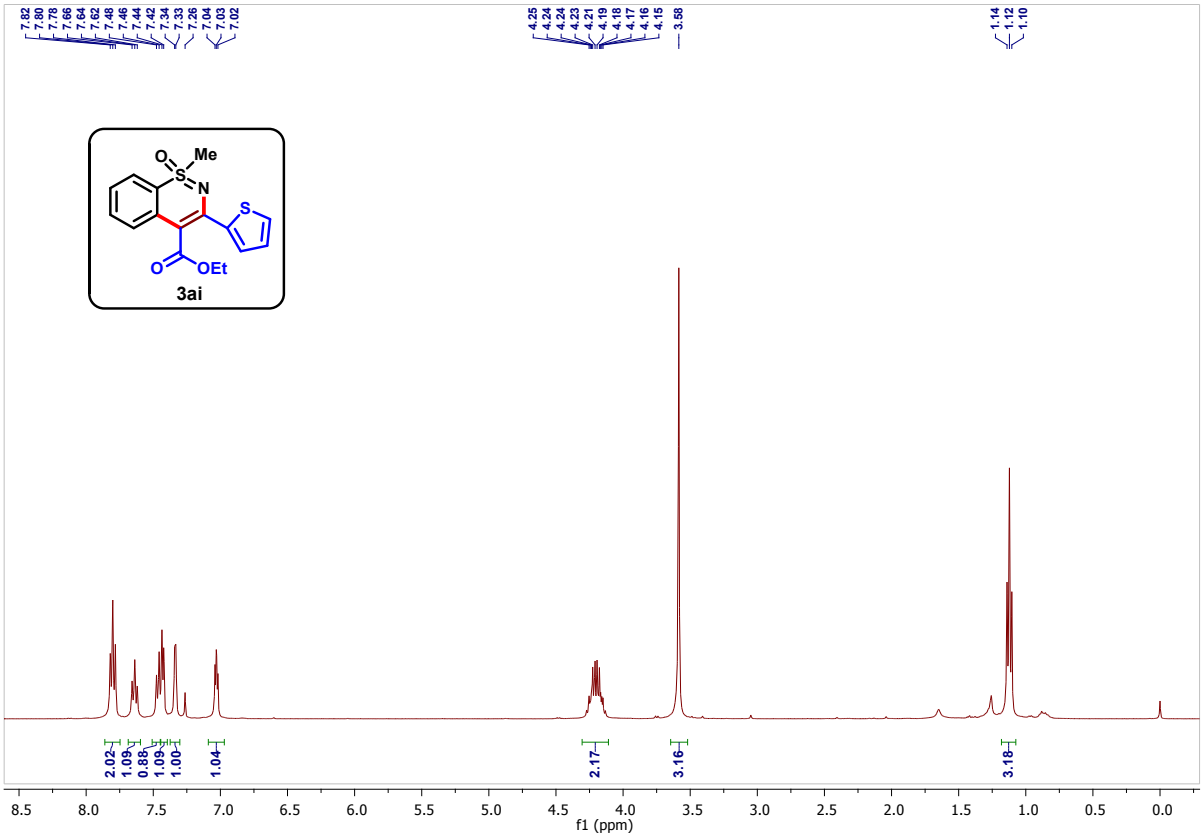
f1 (ppm)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7.04
7.03
7.02
4.25
4.24
4.24
4.23
4.21
4.19
4.18
4.17
4.16
4.15
3.58
1.14
1.12
1.10
Me
O
S
N
S
O
OEt
3ai
2.02
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1.09
1.00
1.04
2.17
3.16
3.18
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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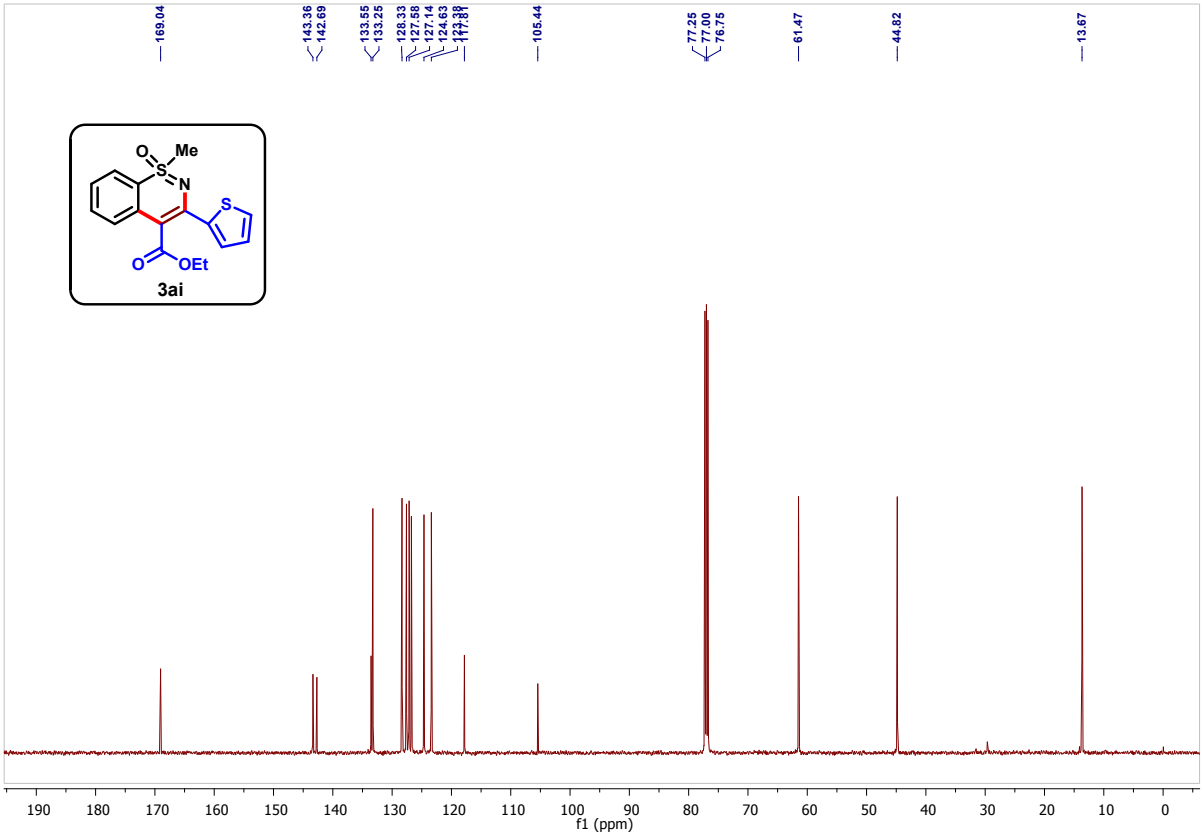
0.0
f1 (ppm)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127.14
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123.38
117.81
105.44
77.25
77.00
76.75
61.47
44.82
13.67
Me
O
S
N
S
O
OEt
3ai
190
180
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130
120
110
100
90
80
70
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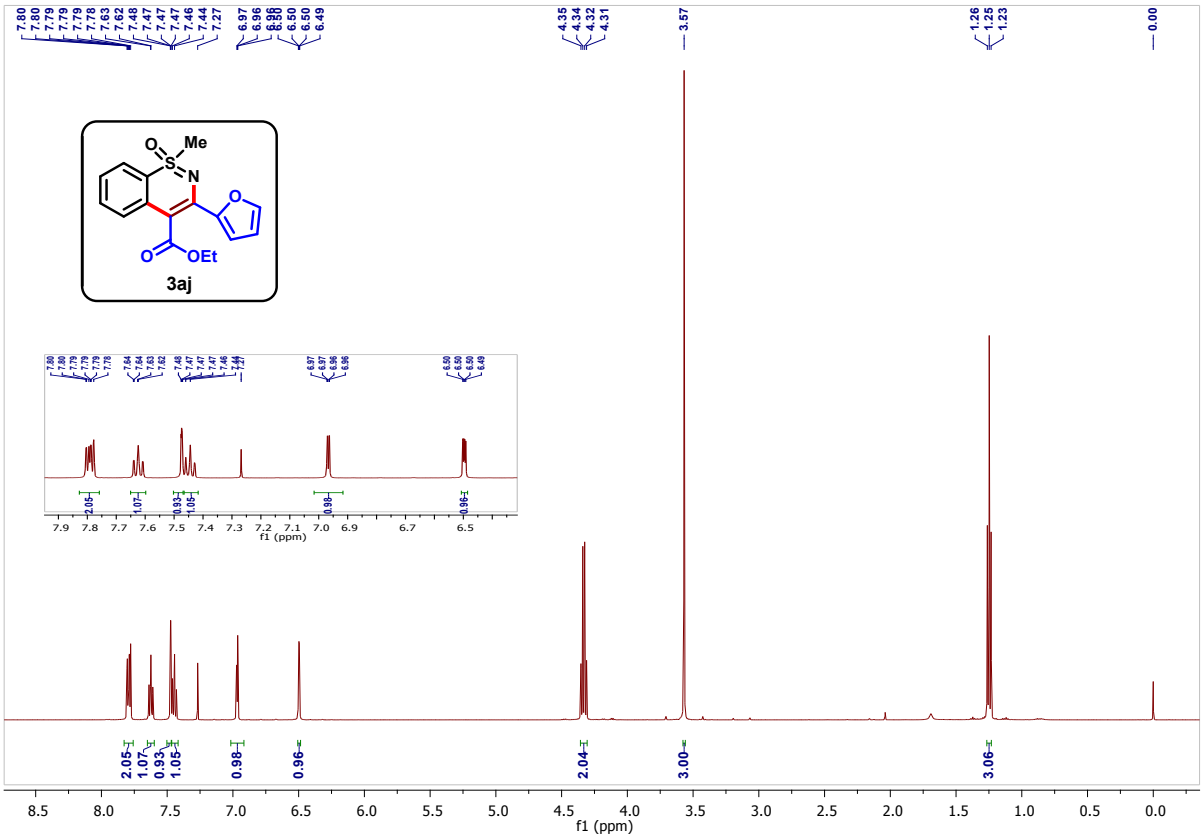
50
40
30
20
10
0
f1 (ppm)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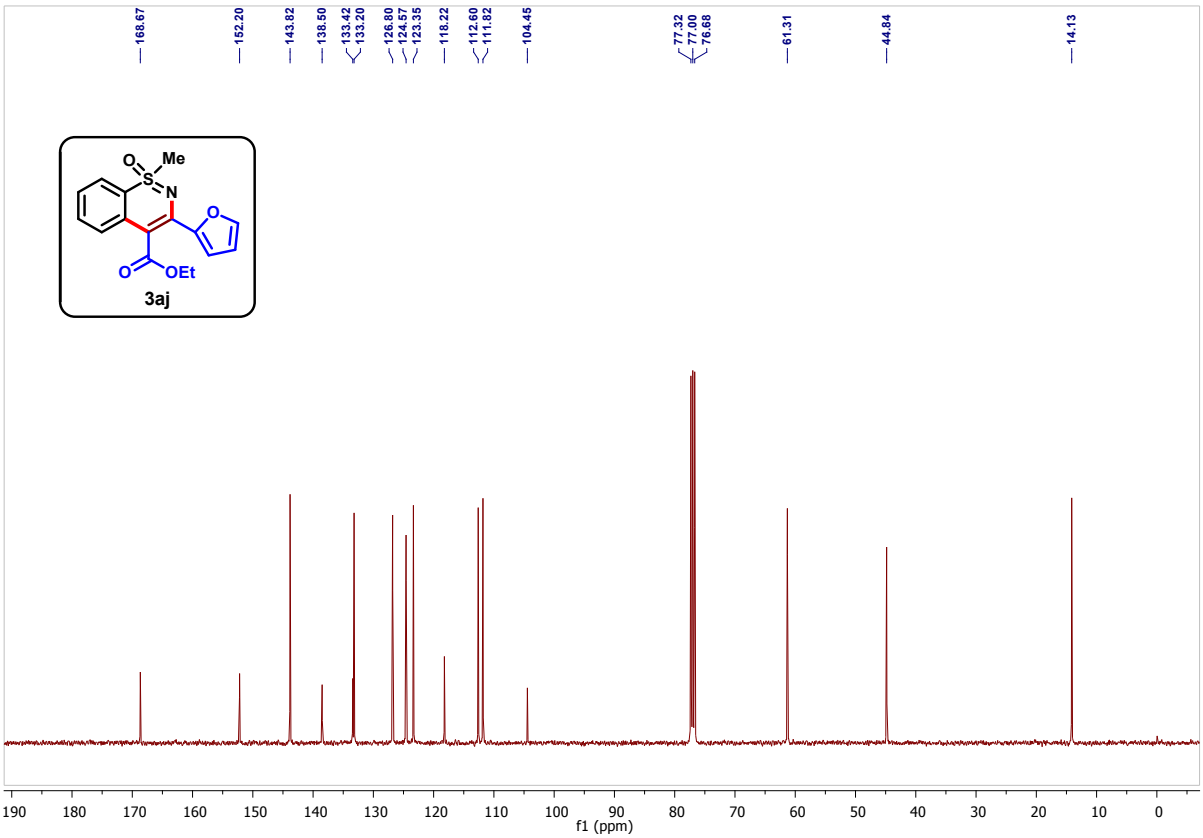
f1 (ppm)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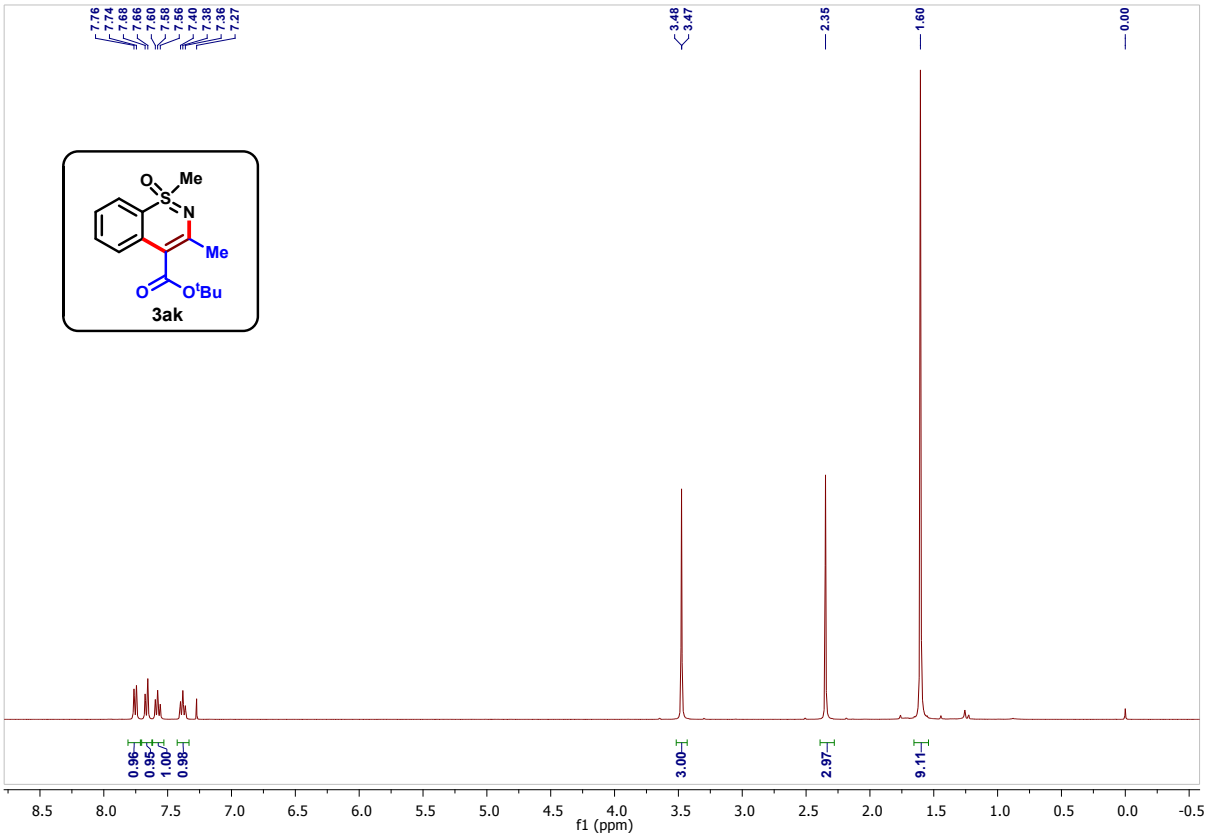
f1 (ppm)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3.47
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N
Me
O
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0.95
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0.98
3.00
2.97
9.11
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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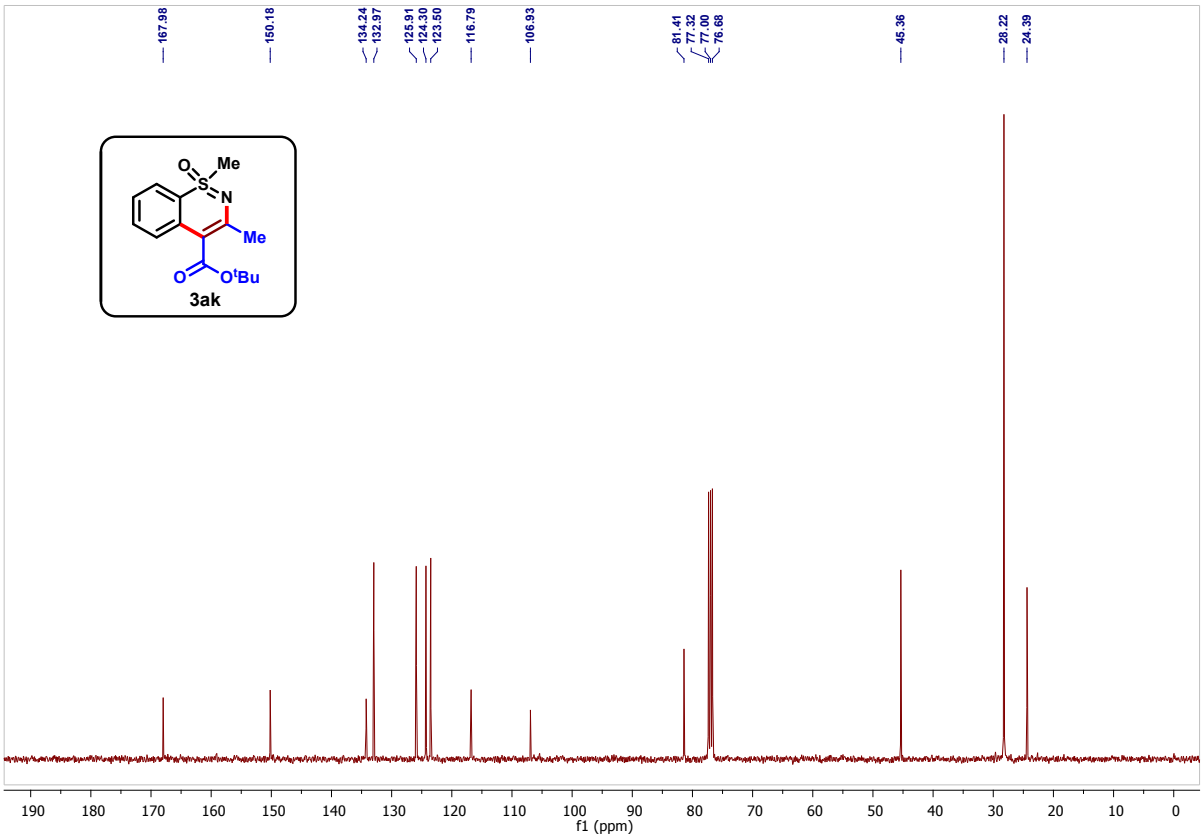
0.5
0.0
-0.5
f1 (ppm)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116.79
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81.41
77.32
77.00
76.68
45.36
28.22
24.39
Me
S
O
N
Me
O
O
tBu
3ak
190
180
170
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150
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130
120
110
100
90
80
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50
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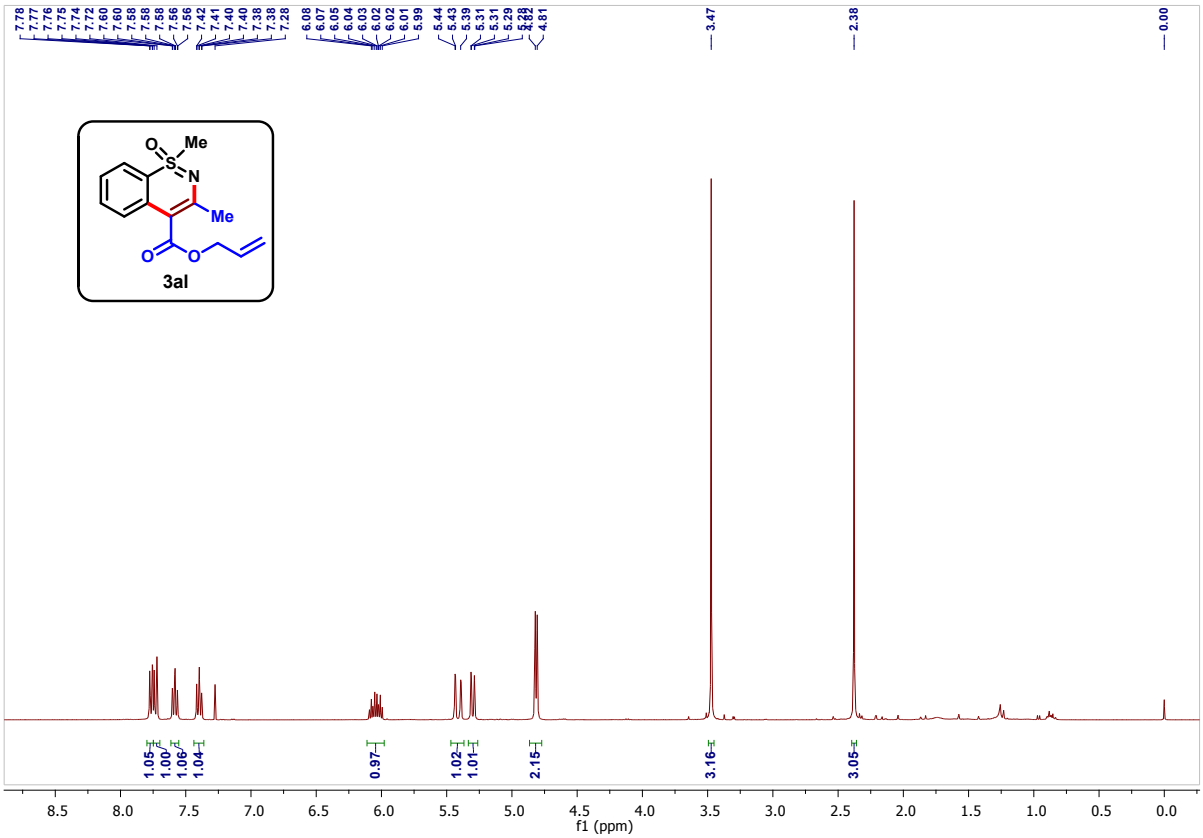
f1 (ppm)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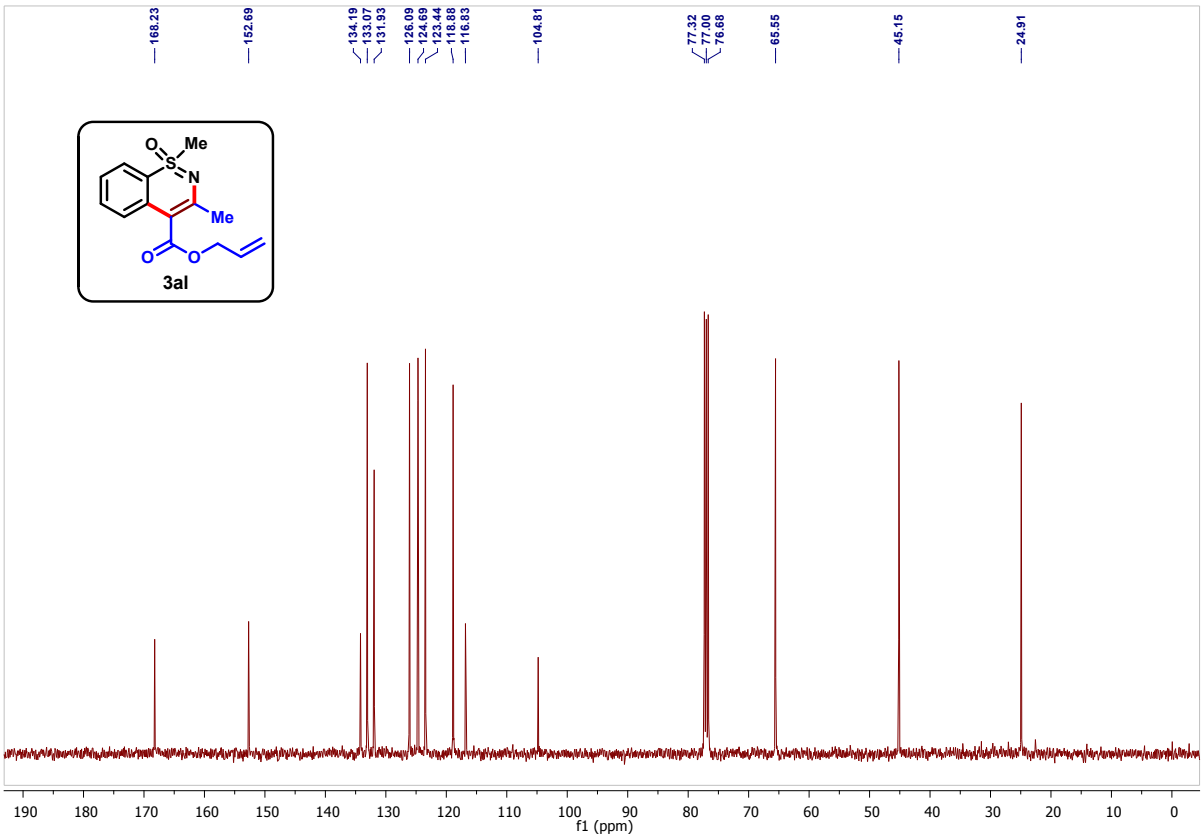
6.08 6.07 6.05 6.04 6.03 6.02 6.02 6.01 6.01 5.99
5.44 5.43 5.39 5.31 5.31 5.29 5.28 5.28 4.61
3.47
2.38
0.00
O
Me
S
N
Me
O
O
3al
1.05 1.00 1.06 1.04 0.97 1.02 1.01 2.15 3.16 3.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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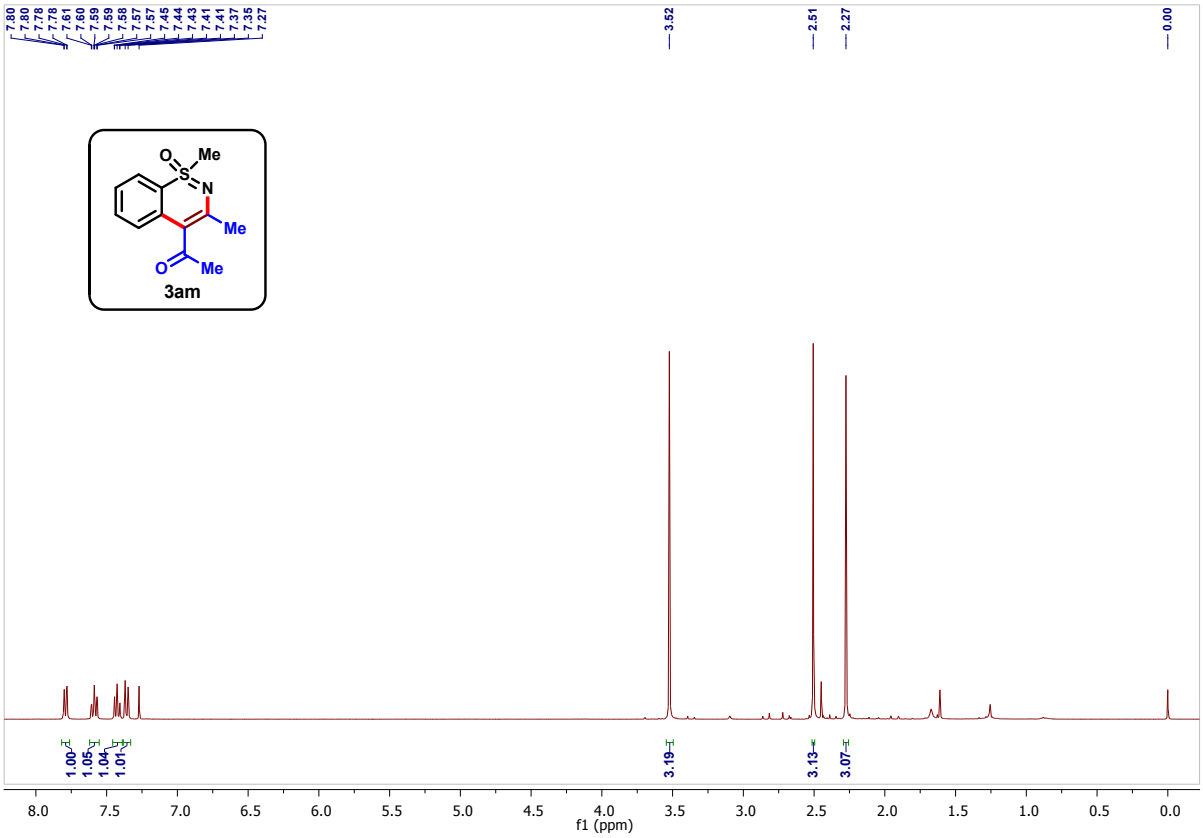
152.69
134.19 133.07 131.93
126.09 124.69 123.44 118.88 116.83
104.81
77.32 77.00 76.68
65.55
45.15
24.91
O
Me
S
N
Me
O
O
3al
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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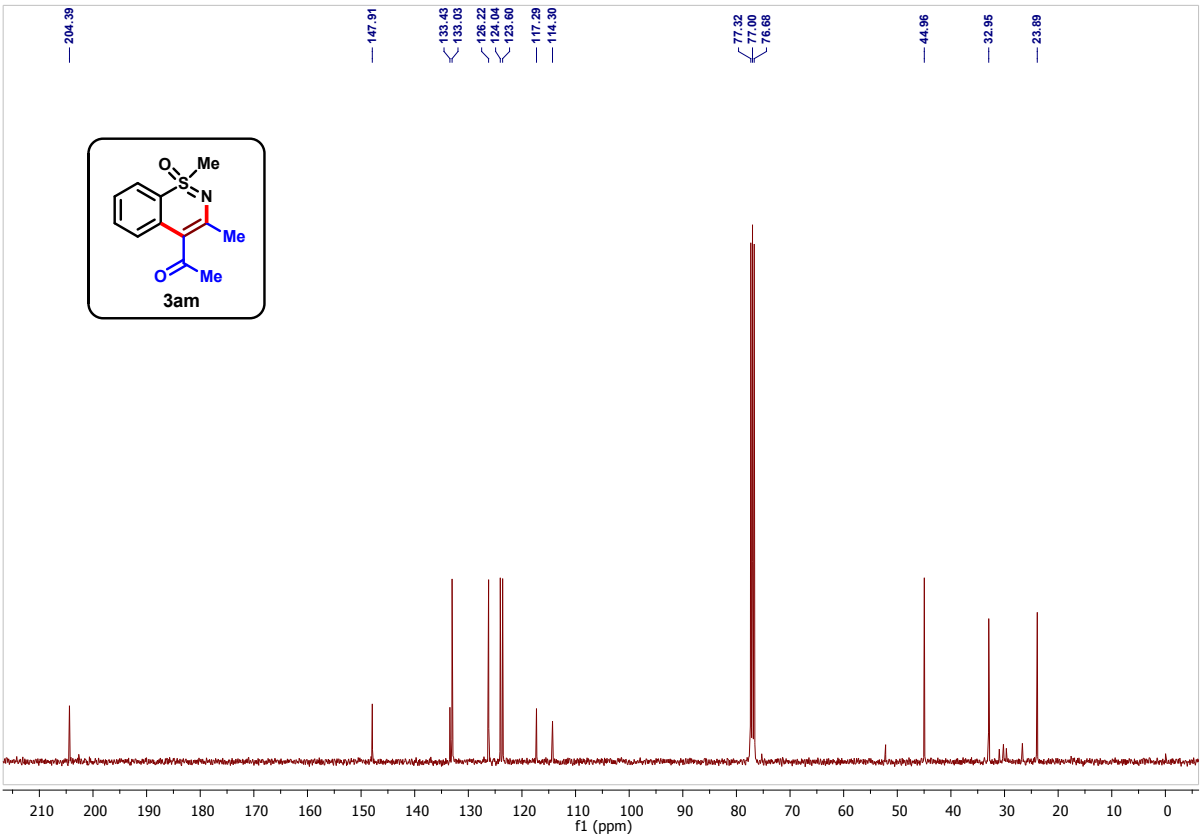
7.80
7.78
7.78
7.61
7.60
7.59
7.59
7.58
7.57
7.57
7.45
7.44
7.43
7.41
7.41
7.37
7.35
7.27
3.52
2.51
2.27
0.00
O
Me
S
N
Me
O
Me
3am
1.00
1.05
1.04
1.01
3.19
3.13
3.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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147.91
133.43
133.03
126.22
124.04
123.60
117.29
114.30
77.32
77.00
76.68
44.96
32.95
23.89
O
Me
S
N
Me
O
Me
3am
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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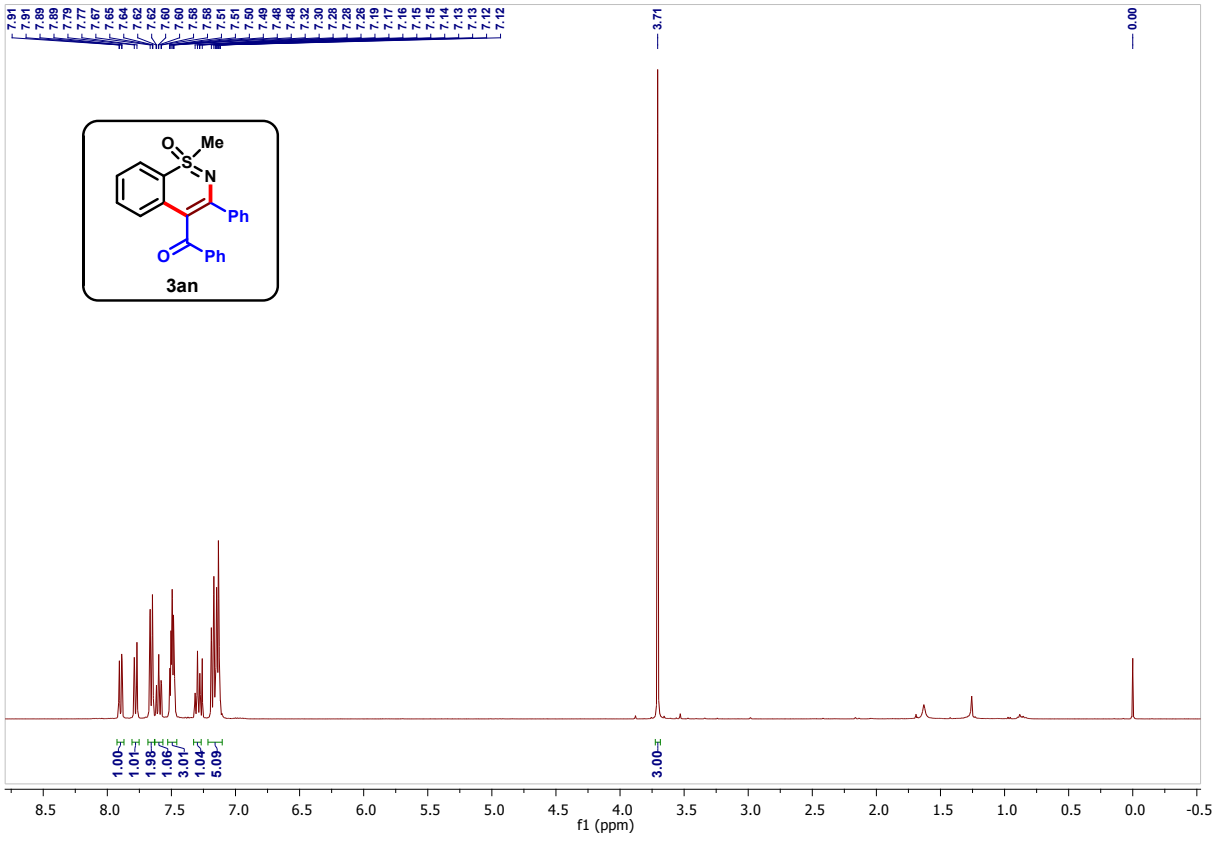
50
40
30
20
10
0
f1 (ppm)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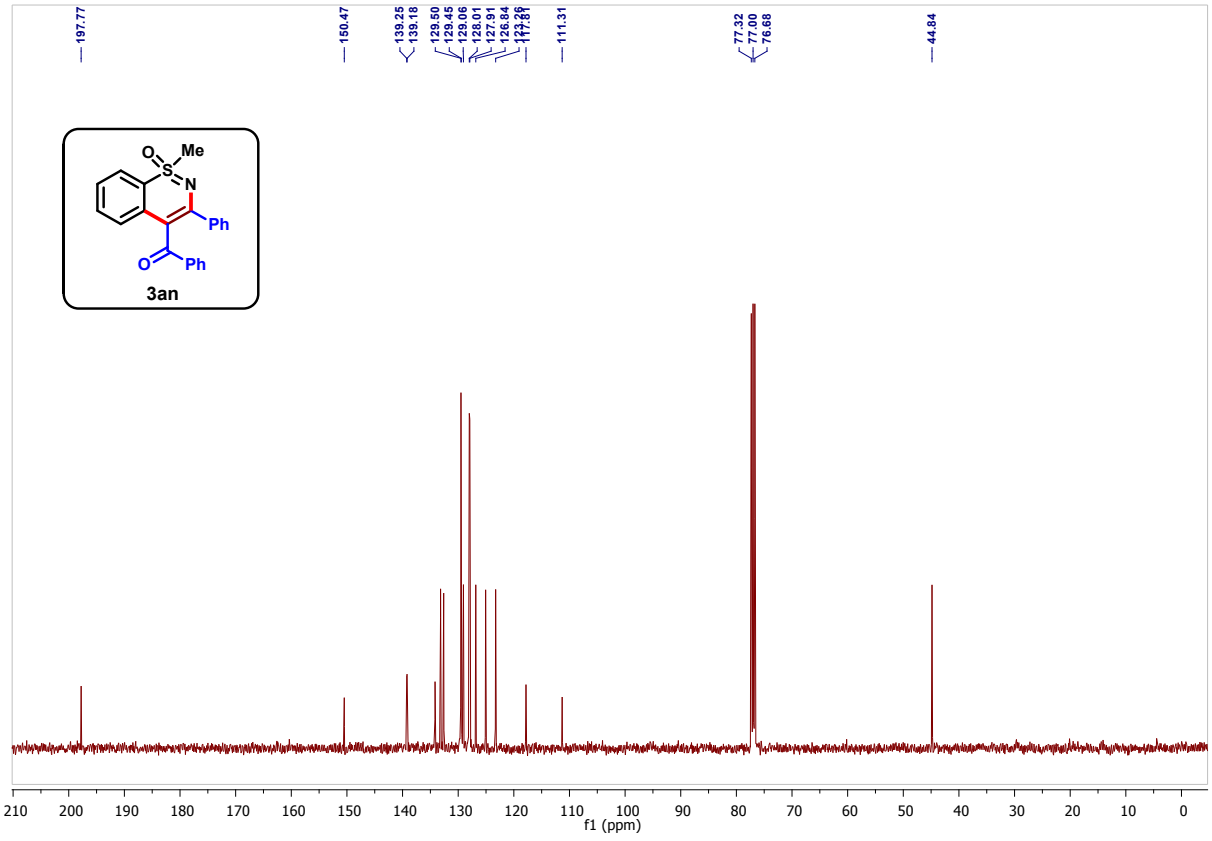
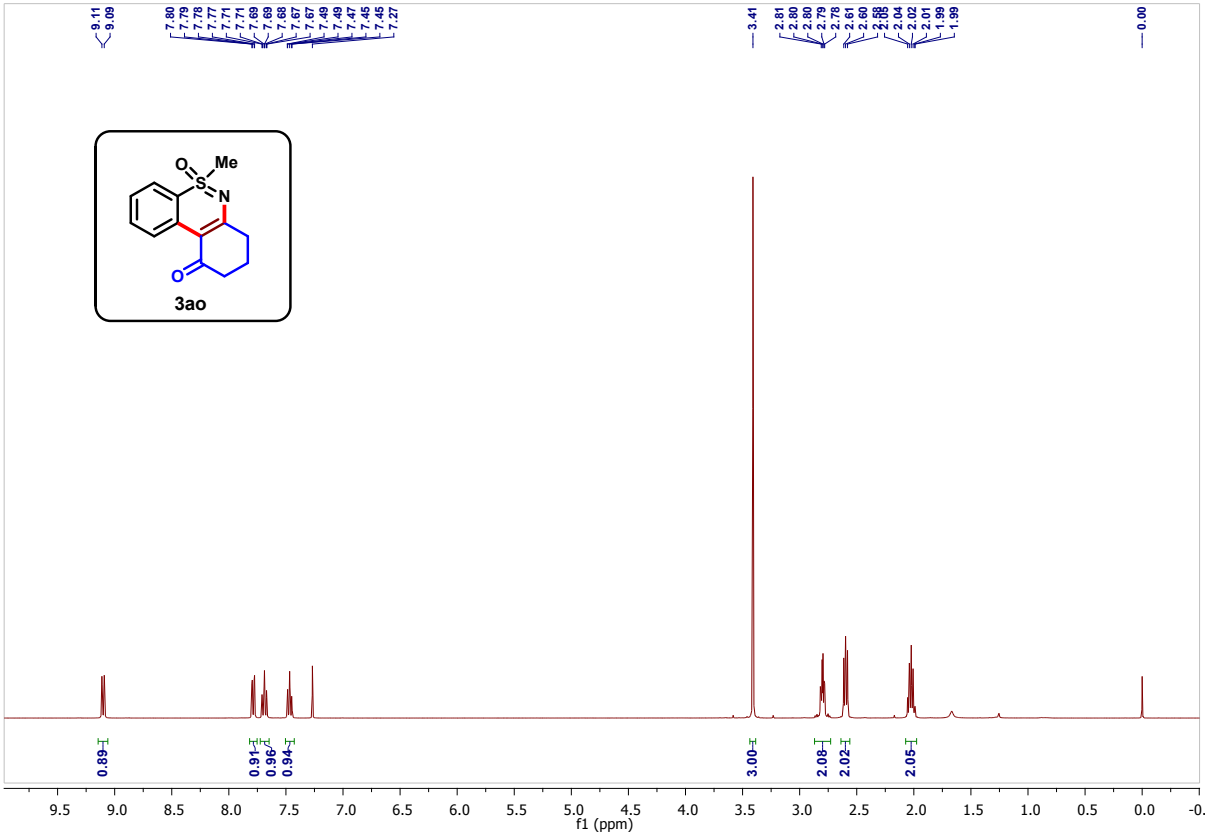
f1 (ppm)


3an
f1 (ppm)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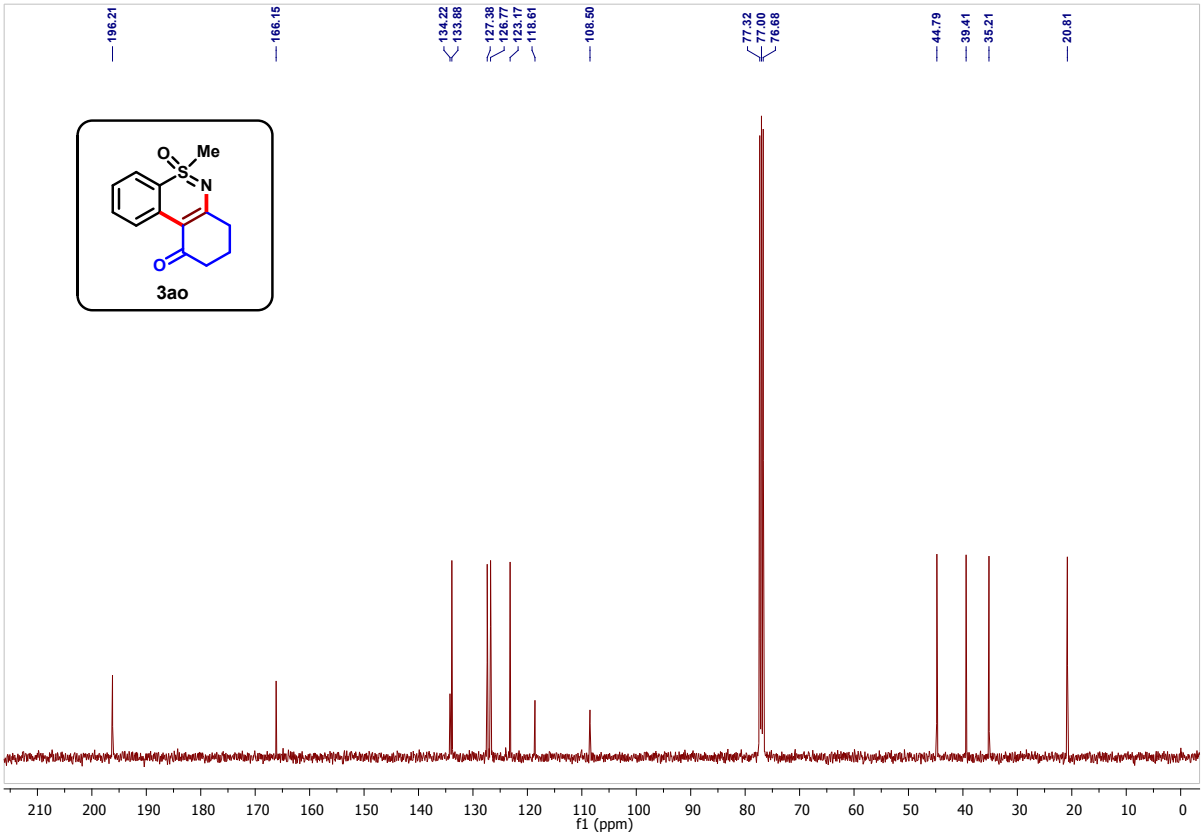
9.09
7.80
7.79
7.78
7.77
7.71
7.69
7.68
7.67
7.49
7.47
7.45
7.27
3.41
2.81
2.80
2.79
2.78
2.61
2.60
2.04
2.02
2.01
1.99
1.99
0.00
Me
O
S
N
O
3ao
0.89
0.91
0.96
0.94
3.00
2.08
2.02
2.05
f1 (ppm)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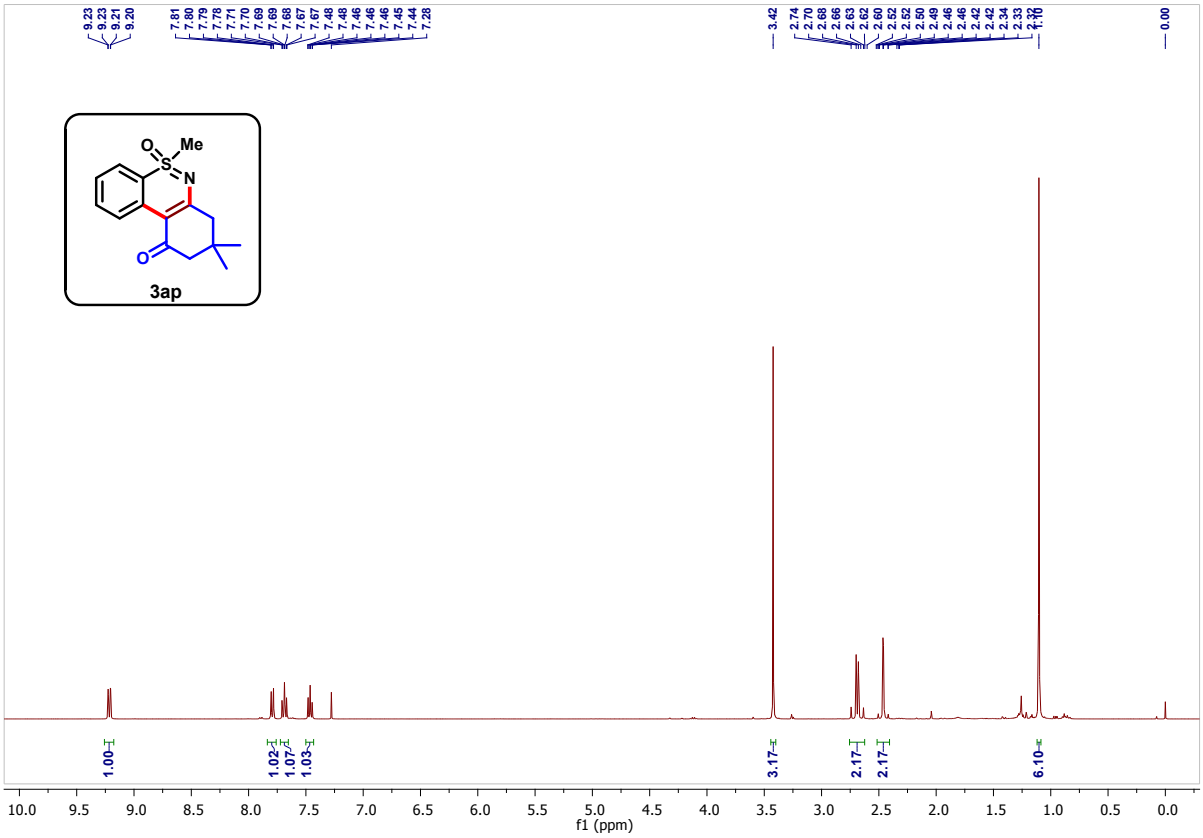
166.15
134.22
133.88
127.38
126.77
123.17
118.61
108.50
77.32
77.00
76.68
44.79
39.41
35.21
20.81
Me
O
S
N
O
3ao
f1 (ppm)


9.23
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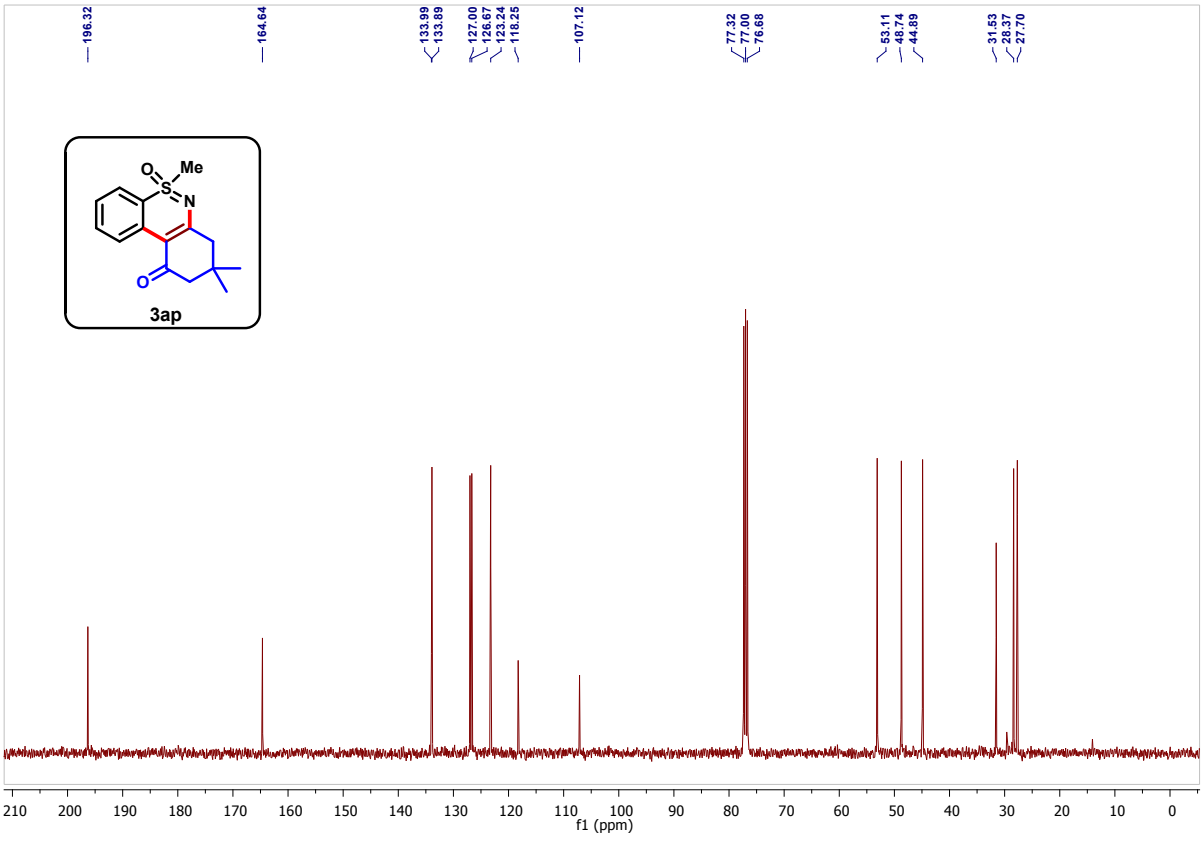
9.21
9.20
7.81
7.80
7.79
7.78
7.71
7.70
7.69
7.69
7.68
7.67
7.67
7.48
7.48
7.46
7.46
7.46
7.45
7.44
7.28
3.42
2.74
2.70
2.68
2.66
2.63
2.62
2.60
2.52
2.52
2.50
2.49
2.46
2.42
2.42
2.34
2.33
2.32
1.10
0.00
Me
O
S
N
O
3ap
1.00
1.02
1.07
1.03
3.17
2.17
2.17
6.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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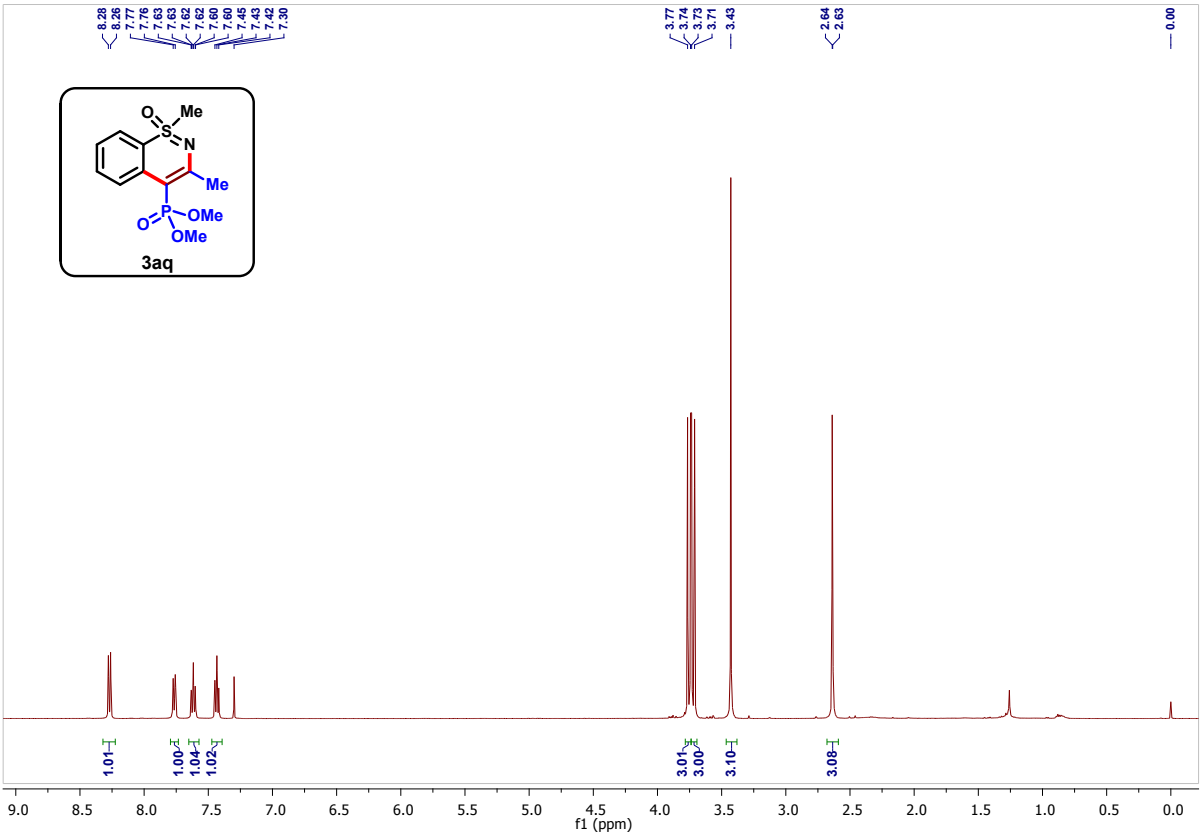
127.00
126.67
123.24
118.25
107.12
77.32
77.00
76.68
53.11
48.74
44.89
31.53
28.37
27.70
Me
O
S
N
O
3ap
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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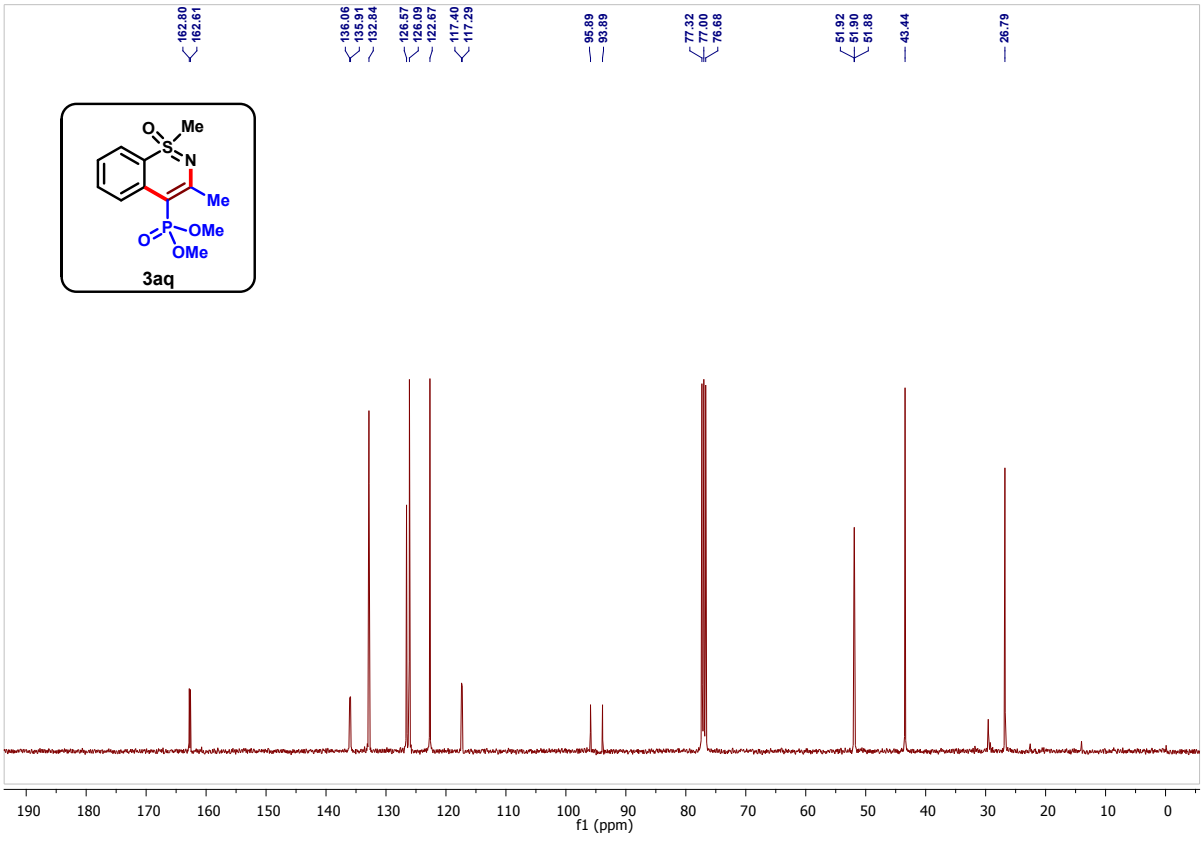
8.26
7.77
7.76
7.63
7.63
7.62
7.62
7.60
7.60
7.45
7.43
7.42
7.30
3.77
3.74
3.73
3.71
3.43
2.64
2.63
0.00
Me
O
S
N
Me
P
O
OMe
OMe
3aq
1.01
1.00
1.04
1.02
3.01
3.00
3.10
3.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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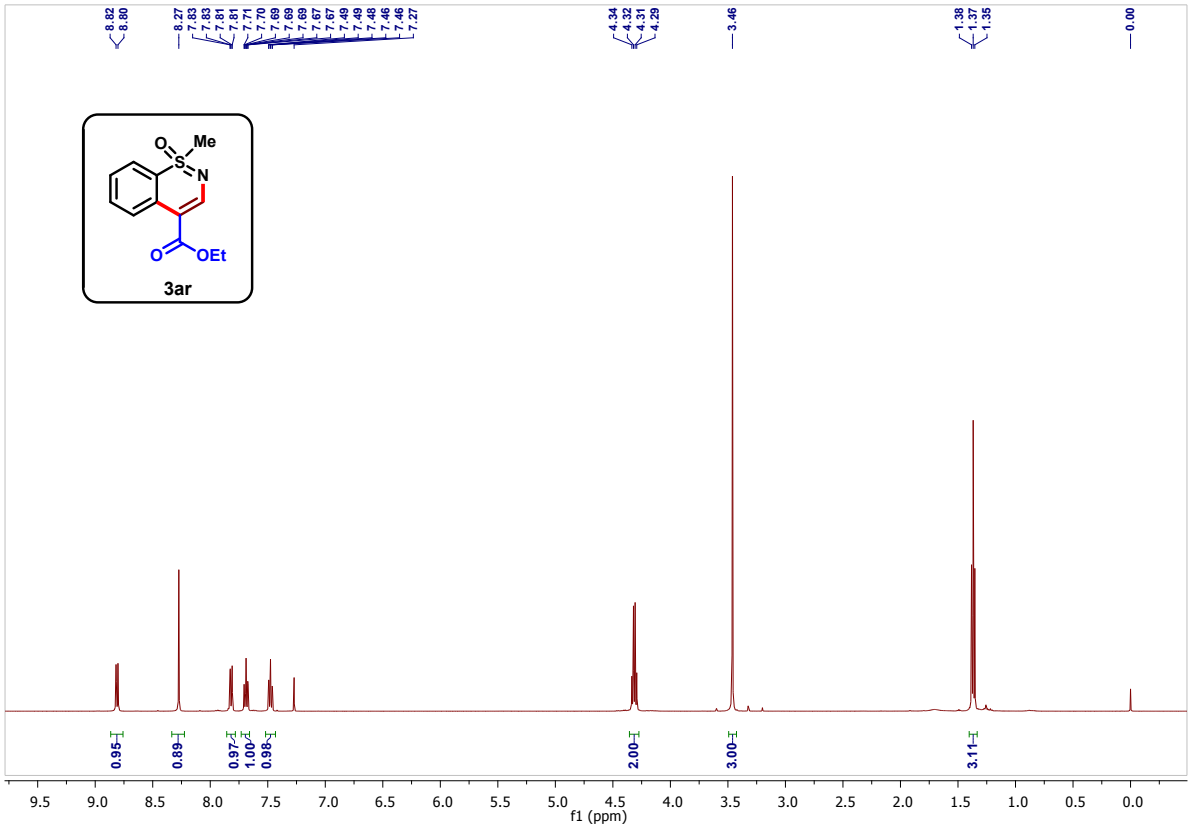
162.61
136.06
135.91
132.84
126.57
126.09
122.67
117.40
117.29
95.89
93.89
77.32
77.00
76.68
51.92
51.90
51.88
43.44
26.79
Me
O
S
N
Me
P
O
OMe
OMe
3aq
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.81
7.81
7.71
7.70
7.69
7.69
7.69
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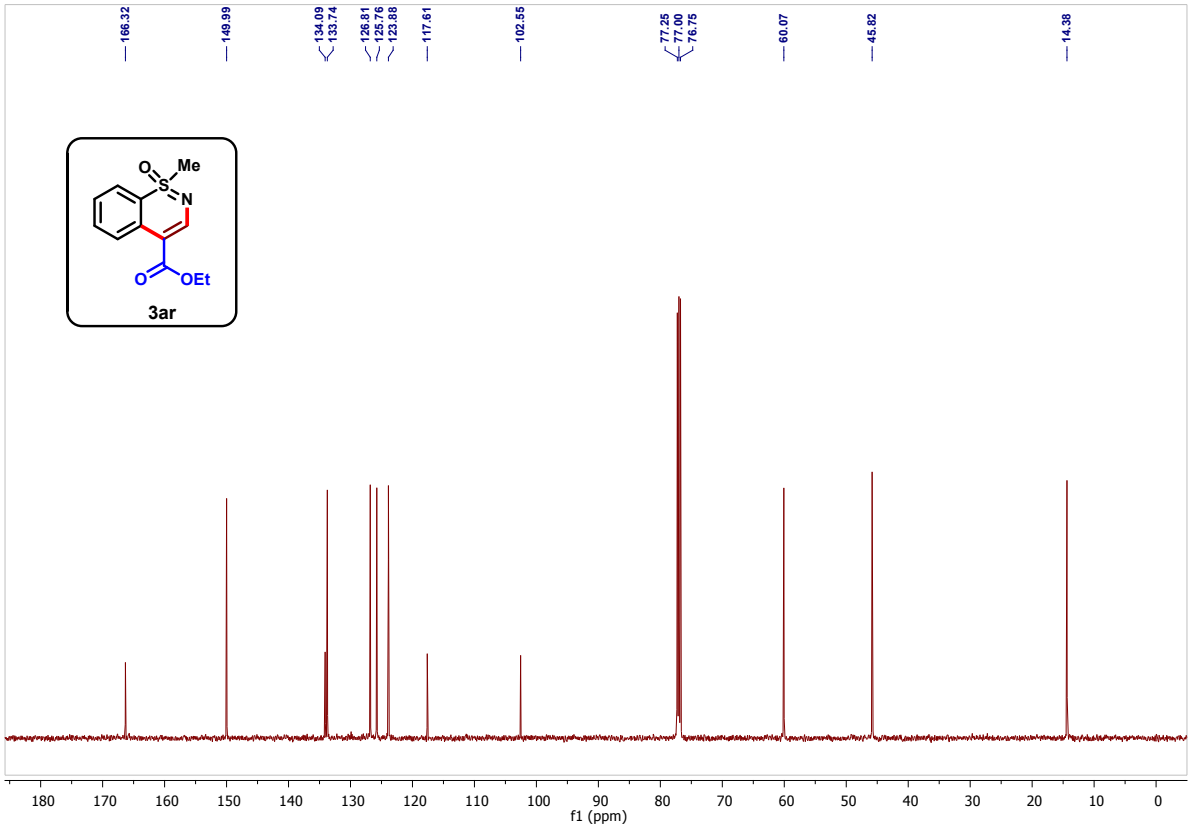
7.67
7.49
7.49
7.48
7.46
7.46
7.27
4.34
4.32
4.31
4.29
3.46
1.38
1.37
1.35
0.00
Me
O
S
N
O
OEt
3ar
0.95
0.89
0.97
1.00
0.98
2.00
3.00
3.11
f1 (ppm)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134.09
133.74
126.81
125.76
123.88
117.61
102.55
77.25
77.00
76.75
60.07
45.82
14.38
Me
O
S
N
O
OEt
3ar
f1 (ppm)