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Supporting Information

Rhodium(III)-Catalyzed Tandem Annulation Reaction to Build Polycyclic Benzothiazine Derivatives

Yang Li, Xin-Yang Liu, Yan-Jun Xu* and Lin Dong*

1. **General experimental methods.**
2. **General procedure for the synthesis of compounds 3aa, 4 and 5.**
3. **Control experiments.**
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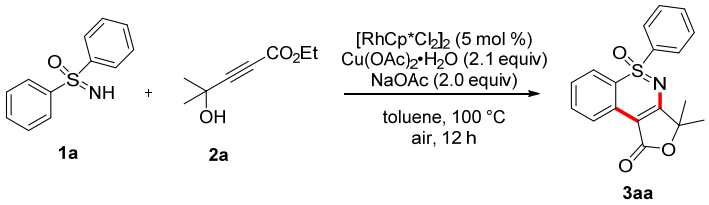
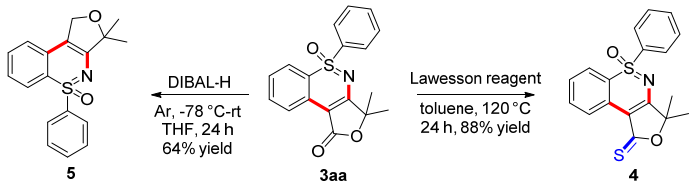
1. General methods.

NMR data were obtained for ^{1}H at 400 MHz or 600 MHz, and for ^{13}C at 100 MHz or 151 MHz. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in CDCl3 solution. ESI HRMS was recorded on a Waters SYNAPT G2 and Water XEVO G2 Q-ToF. UV detection was monitored at 220 nm. TLC was performed on glass-backed silica plates. Column chromatography was performed on silica gel (200-300 mesh), eluting with ethyl acetate and petroleum ether. These NH-sulfoximine substrates were prepared according to the literatures.[1,2,3] And these popargyl acohols were prepared according to the literatures.[4,5]

2. General procedure for the synthesis of compounds 3aa, 4 and 5.



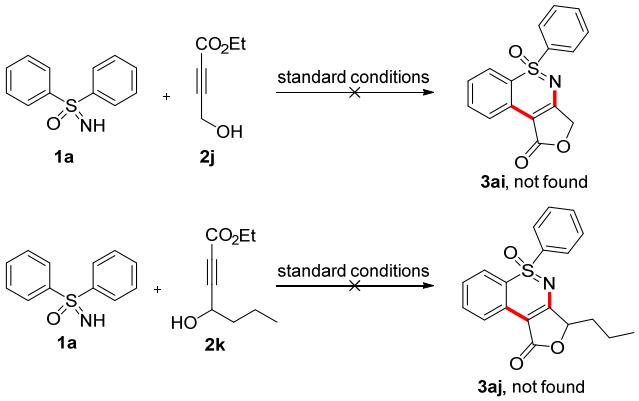
NH-Sulfoximine **1a** (0.1 mmol, 1.0 equiv), ethyl 4-hydroxy-4-methylpent-2-ynoate **2a** (0.2 mmol, 2.0 equiv), $[Cp^*RhCl_2]_2$ (0.005 mmol, 5.0 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.21 mmol, 2.1 equiv), and NaOAc (0.2 mmol, 2.0 equiv) were dissolved in 1.0 mL of toluene at 100 °C in sealing tube under air atmosphere. After stirring for 12 h, the reaction mixture was purified by flash chromatography eluting to give the product **3aa** as faint yellow oil (26.7 mg, 82%).



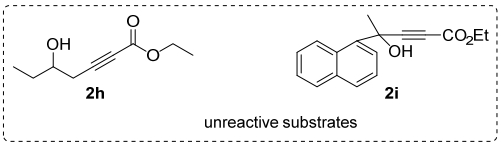
3,3-dimethyl-5-phenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazine-1(3H)-thione 5-oxide **4**: A mixture of **3aa** (32.5 mg, 0.1 mmol, 1.0 equiv), Lawesson reagent (202 mg, 0.5 mmol, 5.0 equiv) dissolved in 1 mL toluene in sealing tube was stirred vigorously at 120 °C for 24 h. After completion, the mixture was extracted with ethyl acetate and washed with brine. The combine organic layers were dried with anhydrous sodium sulfate, concentrated under vacuum and the compound **4** was obtained as oil (30 mg, yield 88%) after purification by flash column chromatography on silica gel.

3,3-dimethyl-5-phenyl-1,3-dihydrobenzo[*e*]furo[3,4-*c*][1,2]thiazine 5-oxide **5**: To a solution of **3aa** (32.5 mg, 0.1 mmol, 1.0 equiv) in 1 mL steamed THF at Ar atmosphere was added DIBAL-H (0.3 mL, 0.45 mmol, 4.5 equiv) slowly at -78 °C then cooled to room temperature and stirred for 24 h. After completion, the mixture was quenched with ethyl acetate and washed with brine. The combine organic layers were dried with anhydrous sodium sulfate, concentrated under vacuum and the compound **5** was obtained as oil (20 mg, yield 64%) after purification by flash column chromatography on silica gel.

3. Control experiments.



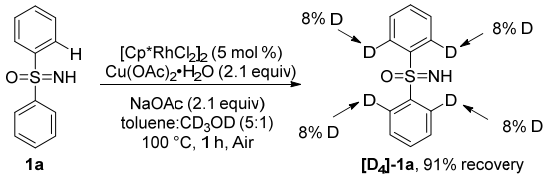
Both ethyl 4-hydroxybut-2-ynoate **2j** and ethyl 4-hydroxyhept-2-ynoate **2k** were tried as coupling partners to react with **1a** under standard conditions. But disappointedly, it turned out that the desired products **3ai** and **3aj** were not obtained while most of the starting material **1a** remained intact. In addition, other popargyl acohols (**2h** and **2i**) shown bad activity to give desired products.

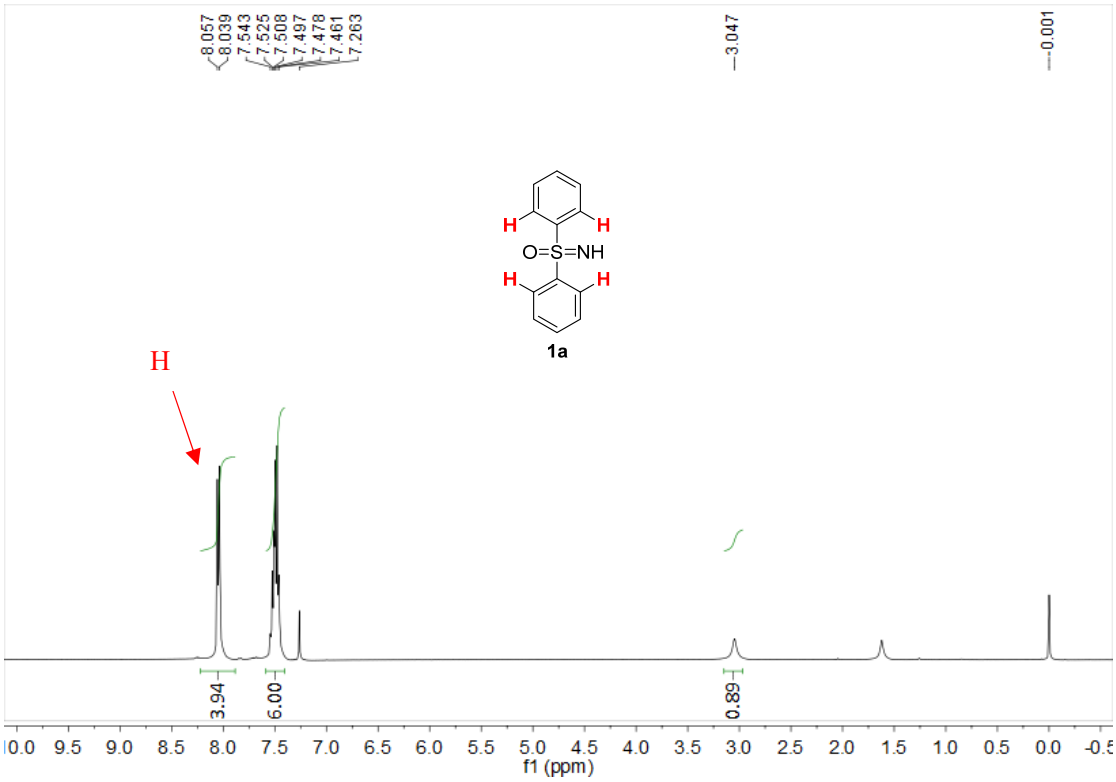


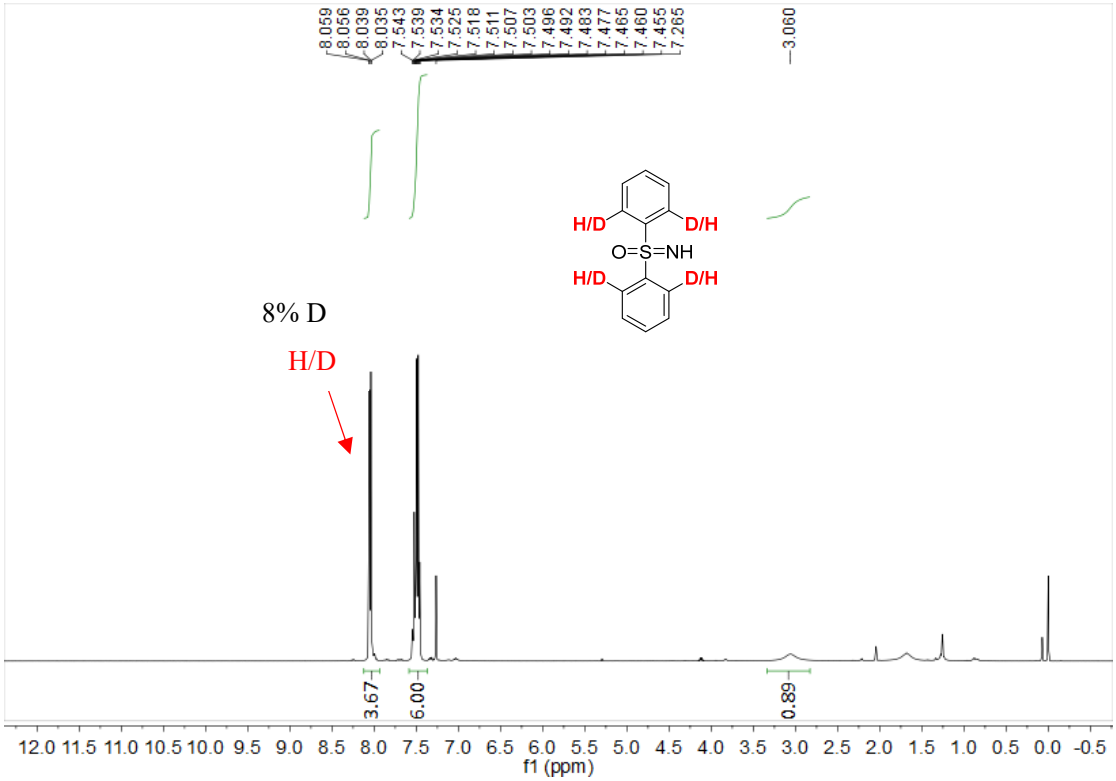
4. Characterization data.

Deuterium-labelling experiments were carried out to study the mechanism of this coupling reaction.

NH-Sulfoximine **1a** (0.05 mmol, 1.0 equiv), $[Cp^*RhCl_2]_2$ (5.0 mol %), $Cu(OAc)_2{\cdot}H_2O$ (2.1 equiv) and NaOAc (2.0 equiv) were dissolved in mixed solvents of 0.5 mL toluene and 0.1 mL CD_3OD at 100 °C in sealing tube under air atmosphere for 1h. After completion, the reaction mixture was filtered. The filtrate was concentrated in vacuo, and the reaction mixture was purified by flash chromatography eluting to give the product **[D$_4$]-1a** as a white solid (9.9 mg, 91%). The deuterium rate (8%) was obtained from ^{1}H NMR. Deuterium was observed at four *ortho*-positions, which indicated the possibility of the reaction pathway via ortho C–H activation.

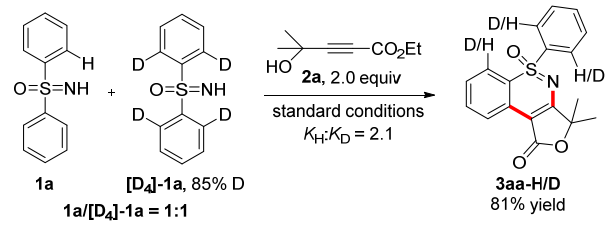






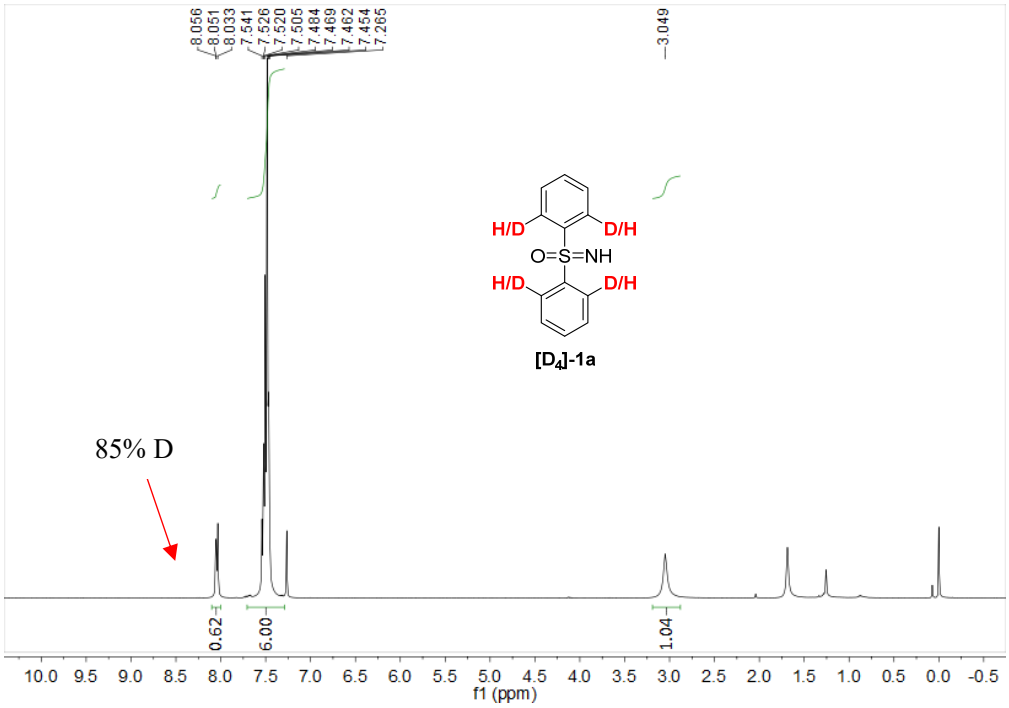
In addition, the kinetic isotope effect (KIE) study was conducted. NH-Sulfoximine **1a** (9.2 mg, 0.042 mmol), **[D_4]-1a** (9.2 mg, 0.042 mmol, 85% D), ethyl 4-hydroxy-4-methylpent-2-ynoate **2a** (26.0 mg, 0.168 mmol), [Cp*$RhCl_2$]$_2$ (2.6 mg, 5 mol %), $Cu(OAc)_2{\cdot}H_2O$ (35.2 mg, 2.1 equiv) and NaOAc (13.8 mg, 2 equiv) were stirred in toluene (0.9 mL) under air atmosphere at 100 °C for 12 h. After completion, the reaction mixture was purified by flash chromatography eluting with ethyl acetate and petroleum ether to give **3aa** + **3aa-[D]** (81%) as a yellow oil. The ratio of two products

was determined by ^{1}H NMR integration method to give kinetic isotopic effect (KIE) k_H/k_D = 2.1, thus indicating that the first C–H bond cleavage might be involved in the rate-determining step.

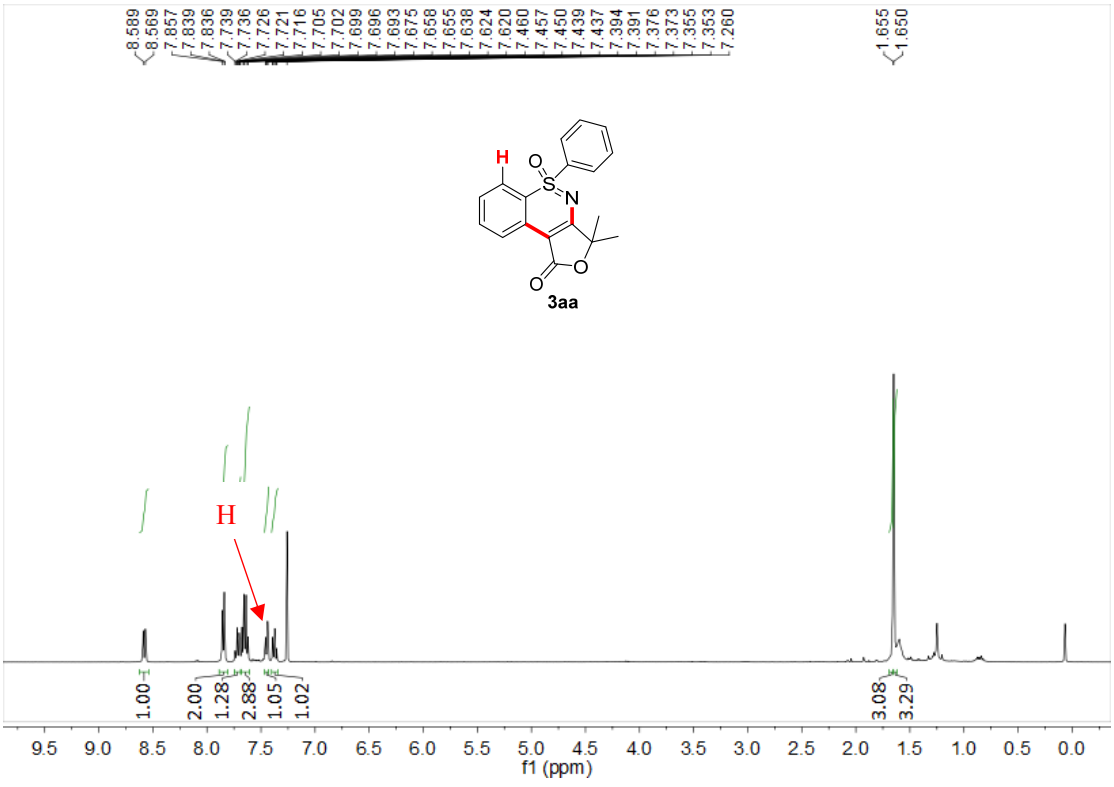


1a **[D$_4$]-1a**, 85% D
1a/[D$_4$]-1a = 1:1

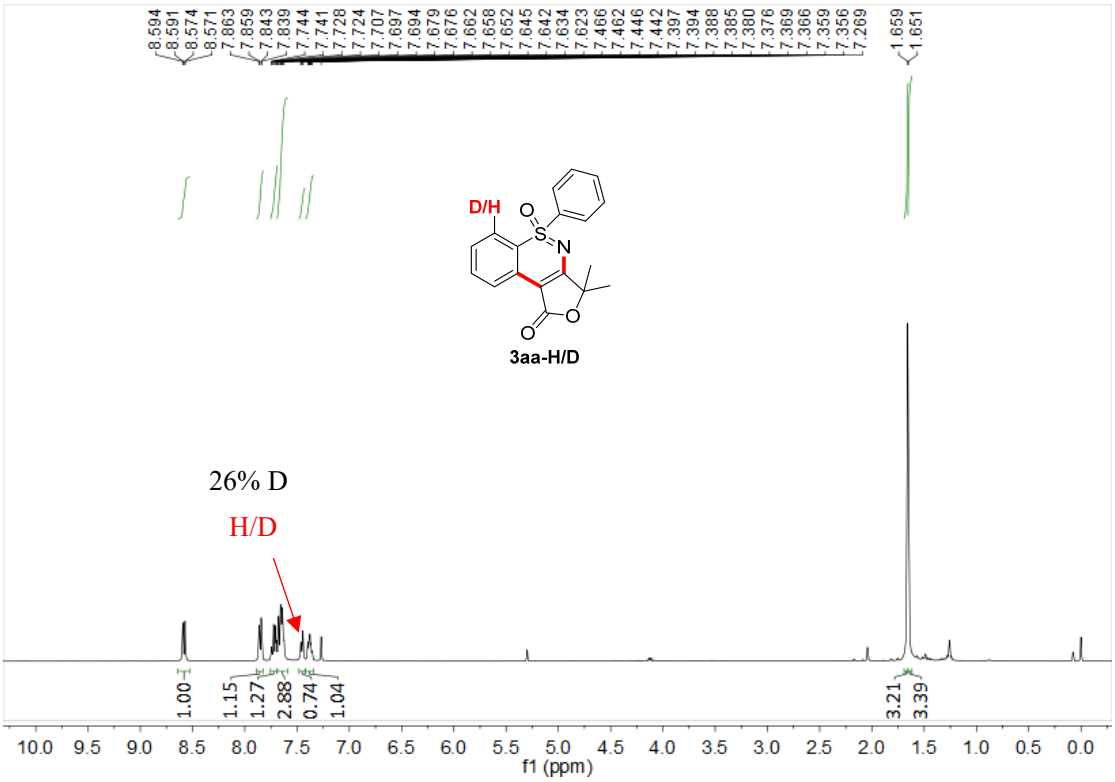
3aa-H/D
81% yield



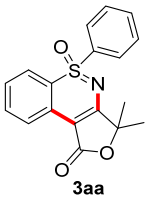
[D$_4$]-1a



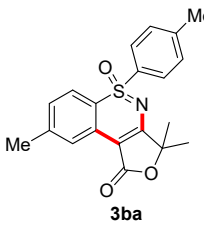
3aa



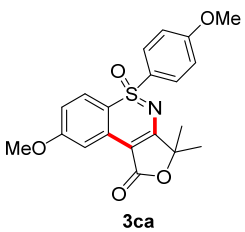
5. Characterization data.



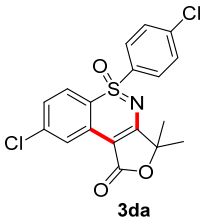
3,3-dimethyl-5-phenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3aa**). 12 h, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 8.0 Hz, 1H), 7.89-7.81 (m, 2H), 7.74-7.62 (m, 4H), 7.46-7.44 (m, 1H), 7.39-7.35 (m, 1H), 1.66 (s, 3H), 1.65 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.51, 168.7, 138.6, 133.5, 132.9, 130.3, 128.5, 127.3, 126.6, 124.7, 122.0, 118.0, 91.9, 82.3, 24.1, 23.7 ppm. ESI HRMS: calcd. for $C_{18}H_{15}NO_3S$+Na 348.0670, found 348.0676.



3,3,8-trimethyl-5-(p-tolyl)-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ba**). 12 h, 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 1H), 2.47 (s, 3H), 2.44 (s, 3H), 1.63 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.8, 169.9, 145.7, 145.2, 137.0, 131.3, 130.1, 128.8, 128.2, 125.7, 122.8, 116.6, 92.6, 83.2, 25.1, 24.8, 22.0, 21.7 ppm. ESI HRMS: calcd. for $C_{20}H_{19}NO_3S$+H 354.1164, found 354.1158.

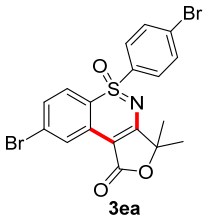


8-methoxy-5-(4-methoxyphenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ca**). 14 h, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 2.8 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 1H), 7.05 (d, *J* = 9.0 Hz, 2H), 6.88 (dd, J_1 = 2.4 Hz, J_2 = 8.8 Hz, 1H), 3.92 (s, 3H), 3.89 (s, 3H), 1.62 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 169.9, 164.2, 163.6, 133.9, 131.5, 130.3, 127.6, 117.2, 114.7, 111.6, 103.7, 92.5, 83.2, 55.9, 55.9, 25.1, 24.8 ppm. ESI HRMS: calcd. for $C_{20}H_{19}NO_5S$+H 386.1062, found 386.1058.



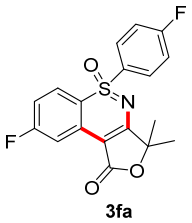
3da

8-chloro-5-(4-chlorophenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2] thiazin -1(3H)-one 5-oxide (**3da**). 12 h, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 1.6 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.39-7.32 (m, 2H), 1.64 (s, 3H), 1.63 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 169.1, 141.9, 141.3, 137.9, 132.8, 130.1, 129.6, 128.3, 127.2, 122.8, 116.7, 92.7, 83.5, 25.1, 24.7 ppm. ESI HRMS: calcd. for $C_{18}H_{13}Cl_2NO_3S$+H 394.0071, found 394.0070.



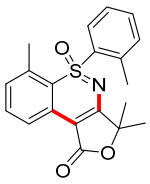
3ea

8-bromo-5-(4-bromophenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin -1(3H)-one 5-oxide (**3ea**).12 h, 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 1.6 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.46 (dd, J_1 = 1.6 Hz, J_2 = 8.4 Hz, 1H), 7.26-7.22 (m, 1H), 1.59 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 169.0, 138.4, 133.1, 132.7, 131.1, 130.6, 130.0, 129.6, 127.1, 125.9, 117.1, 92.5, 83.5, 25.1, 24.7 ppm. ESI HRMS: calcd. for $C_{18}H_{13}Br_2NO_3S$+H 481.9061, found 481.9064.



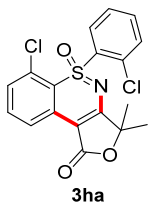
3fa

8-fluoro-5-(4-fluorophenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3fa**). 14 h, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (dd, J_1 = 2.4 Hz, J_2 = 10.0 Hz, 1H), 7.86-7.83 (m, 2H), 7.47 (dd, J_1 = 5.2 Hz, J_2 = 9.2 Hz, 1H), 7.33 (t, *J* = 8.4 Hz, 2H), 7.12-7.07 (m, 1H), 1.64 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 169.2, 167.6, 167.0, 165.0, 164.4, 135.6, 134.3 (d, *J* = 12.0 Hz), 131.2 (d, *J* = 10.0 Hz), 128.8 (d, *J* = 10.5 Hz), 117.3, 117.0, 116.5, 116.2, 115.0, 109.4, 109.2, 93.1, 83.4, 25.1, 24.7 ppm. ESI HRMS: calcd. for $C_{18}H_{13}F_2NO_3S$+H 362.0662, found 362.0658.



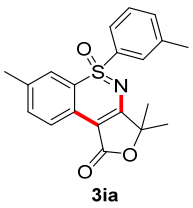
3ga

3,3,6-trimethyl-5-(o-tolyl)-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ga**). 17 h, 47% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 8.4 Hz, 1H), 8.35 (d, *J* = 7.6 Hz, 1H), 7.64-7.53 (m, 3H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 2.12 (s, 3H), 1.70 (s, 3H), 1.61 (s, 3H), 1.58 (s, 3H) ppm. ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 172.2, 168.7, 139.2, 138.9, 136.2, 135.0, 134.2, 133.5, 132.9, 130.9, 128.3, 126.9, 120.5, 116.8, 91.6, 81.8, 24.4, 24.2, 19.5, 18.1 ppm. ESI HRMS: calcd. for $C_{20}H_{19}NO_3S$+H 354.1164, found 354.1170.



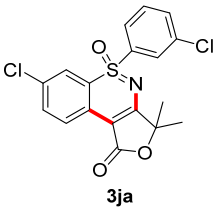
3ha

6-chloro-5-(2-chlorophenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ha**). 12 h, 26% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.4 Hz, 1H), 8.52-8.49 (m, 1H), 7.67-7.64 (m, 3H), 7.49 (d, *J* = 8.8 Hz, 1H), 7.35 (d, *J* = 7.6 Hz, 1H), 1.60 (s, 3H), 1.57 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.4, 169.6, 137.5, 135.7, 135.7, 135.2, 134.9, 132.2, 131.2, 131.0, 129.4, 127.3, 121.8, 114.9, 92.2, 83.0, 24.9, 24.7 ppm. ESI HRMS: calcd. for $C_{18}H_{13}Cl_2NO_3S$+H 394.0071, found 394.0069.



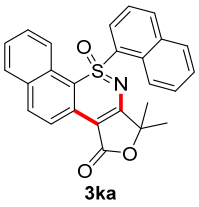
3ia

3,3,7-trimethyl-5-(m-tolyl)-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ia**). 12 h, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.0 Hz, 1H), 7.62-7.60 (m, 2H), 7.53-7.47 (m, 3H), 7.22 (s, 1H), 2.46 (s, 3H), 2.33 (s, 3H), 1.64 (s, 3H), 1.63 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 169.9, 140.0, 139.7, 137.9, 135.4, 135.2, 129.4, 128.9, 128.4, 125.5, 125.1, 123.0, 118.9, 92.9, 83.3, 25.1, 24.8, 21.5 ppm. ESI HRMS: calcd. for $C_{20}H_{19}NO_3S$+H 354.1164, found 354.1163.



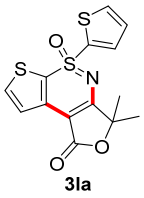
3ja

7-chloro-5-(3-chlorophenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2] thiazin -1(3H)-one 5-oxide (**3ja**). 12 h, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 8.4 Hz, 1H), 7.82 (t, *J* = 1.6 Hz, 1H), 7.73-7.70 (m, 2H), 7.66-7.59 (m, 2H), 7.40 (d, *J* = 2.0 Hz, 1H), 1.66 (s, 3H), 1.64 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 169.2, 140.8, 136.2, 135.0, 134.9, 133.2, 131.0, 129.8, 128.3, 126.5, 125.0, 125.0, 119.4, 93.3, 83.6, 25.1, 24.7 ppm. ESI HRMS: calcd. for $C_{18}H_{13}Cl_2NO_3S$+Na 415.9891, found 415.9892.



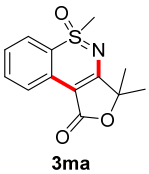
3ka

1,1-dimethyl-10-(naphthalen-1-yl)-10λ^4-furo[3,4-*c*]naphtho[2,1-*e*][1,2]thiazin-3(1H)-one 10-oxide (**3ka**). 13 h, 42 yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 8.8 Hz, 1H), 8.84 (d, *J* = 7.2 Hz, 1H), 8.19 (t, *J* = 8.0 Hz, 2H), 8.11 (d, *J* = 9.2 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.80 (t, *J* = 8.4 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.40-7.36 (m, 1H), 7.33-7.29 (m, 2H), 6.81 (d, *J* = 8.4 Hz, 1H), 1.66 (s, 3H), 1.49 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 170.0, 136.3, 135.8, 134.5, 134.3, 132.7, 130.5, 129.5, 129.5, 129.4, 128.7, 128.6, 127.6, 127.1, 126.3, 124.0, 122.9, 121.9, 120.6, 92.4, 83.0, 25.1, 24.9 ppm. ESI HRMS: calcd. for $C_{26}H_{19}NO_3S$+H 426.1164, found 426.1171.



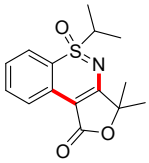
3la

3,3-dimethyl-5-(thiophen-2-yl)-5λ^4-furo[3,4-*c*]thieno[3,2-*e*][1,2]thiazin-1(3H)-one 5-oxide (**3la**). 12 h, 27% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 5.2 Hz, 1H), 7.87 (d, *J* = 5.2 Hz, 1H), 7.77 (d, *J* = 5.2 Hz, 1H), 7.65 (d, *J* = 2.8 Hz, 1H), 7.23 (t, *J* = 4.8 Hz, 1H), 1.67 (s, 3H), 1.66 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.7, 168.6, 142.4, 141.3, 137.0, 135.0, 134.4, 128.5, 122.5, 115.5, 95.8, 84.1, 25.2, 24.9 ppm. ESI HRMS: calcd. for $C_{14}H_{11}NO_3S_3$+H 337.9979, found 337.9978.



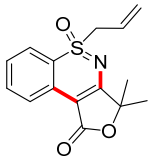
3ma

3,3,5-trimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ma**). 12 h, 59% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 3.57 (s, 3H), 1.574 (s, 3H), 1.571 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5, 169.6, 134.6, 131.4, 127.6, 124.4, 123.4, 117.8, 93.0, 83.0, 46.6, 25.0, 24.7 ppm. ESI HRMS: calcd. for $C_{13}H_{13}NO_3S$+H 264.0694, found 264.0694.



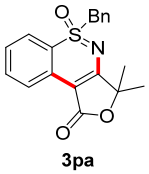
3na

5-isopropyl-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3na**). 12 h, 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 3.78-3.71 (m, 1H), 1.60 (s, 3H), 1.56 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H), 1.14 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3, 168.7, 133.8, 132.3, 126.4, 124.3, 122.1, 113.0, 91.3, 82.0, 59.2, 24.2, 23.7, 15.2, 12.3 ppm. ESI HRMS: calcd. for $C_{15}H_{17}NO_3S$+H 292.1007, found 292.1006.



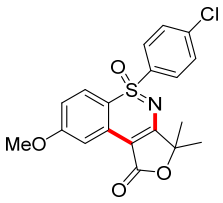
3oa

5-allyl-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3oa**). 13 h, 14% yield. ^{1}H NMR (400 MHz, $CDCL_3$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 5.53-5.45 (m, 1H), 5.33 (dd, J_1 = 10.0, J_2 = 22.0 Hz, 2H), 4.33-4.28 (m, 1H), 4.19-4.13 (m, 1H), 1.58 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174. 8, 169.6, 134.9, 132.9, 127.5, 127.3, 125.2, 123.2, 122.6, 115.3, 92.6, 83.1, 63.5, 25.2, 24.8 ppm. ESI HRMS: calcd. for $C_{15}H_{15}NO_3S$+Na 312.0670, found 312.0669.



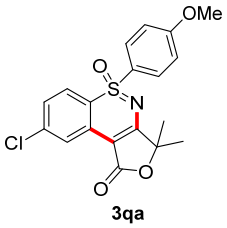
3pa

5-benzyl-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3pa**). 13 h, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.24-7.22 (m, 1H), 7.13 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 7.2 Hz, 2H), 4.79 (d, *J* = 14.0 Hz, 1H), 4.56 (d, *J* = 14.0 Hz, 1H), 1.48 (s, 3H), 1.44 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 169.4, 135.0, 133.2, 131.1, 129.7, 128.8, 127.3, 126.0, 125.7, 123.0, 114.6, 92.2, 82.9, 65.8, 25.0, 24.8 ppm. ESI HRMS: calcd. for $C_{19}H_{17}NO_3S$+H 340.1007, found 340.1010.



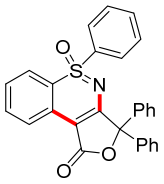
3qa'

5-(4-chlorophenyl)-8-methoxy-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2] thiazin-1(3H)-one 5-oxide (**3qa'**). 13 h, 29% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.8 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 3.94 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 169.7, 164.1, 141.1, 139.3, 134.3, 129.8, 129.2, 127.7, 117.5, 110.3, 104.1, 92.8, 83.2, 56.0, 25.1, 24.8 ppm. ESI HRMS: calcd. for $C_{19}H_{16}ClNO_3S$+H 390.0567, found 390.0564.



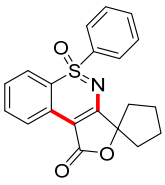
3qa

8-chloro-5-(4-methoxyphenyl)-3,3-dimethyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2] thiazin-1(3H)-one 5-oxide (**3qa**). 13 h, 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.30-7.20 (m, 2H), 7.02 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4, 169.4, 164.7, 140.6, 132.4, 130.7, 130.0, 127.9, 127.1, 122.5, 117.8, 115.0, 92.4, 83.5, 56.0, 25.1, 24.7 ppm. ESI HRMS: calcd. for $C_{19}H_{16}ClNO_3S$+H 390.0567, found 390.0565.



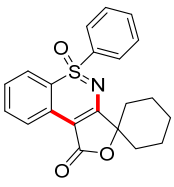
3ab

3,3,5-triphenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ab**). 14 h, 24% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (dd, J_1 = 1.1 Hz, J_2 = 8.2 Hz, 1H), 7.71-7.59 (m, 8H), 7.55-7.46 (m, 3H), 7.42-7.30 (m, 7H) ppm. ^{13}C NMR (151 MHz, $cdcl_3$) δ 166.7, 165.6, 135.7, 135.5, 135.1, 130.4, 130.0, 126.8, 125.4, 124.5, 124.3, 124.3, 124.2, 124.1, 124.0, 123.5, 122.8, 121.6, 119.3, 114.9, 90.5, 84.2 ppm. ESI HRMS: calcd. for $C_{28}H_{19}NO_3S$+H 450.1164, found 450.1159.



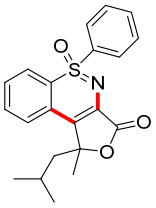
3ac

5-phenyl-1H-5λ^6-spiro[benzo[*e*]furo[3,4-*c*][1,2]thiazine-3,1'-cyclopentan]-1-one 5-oxide (**3ac**). 14 h, 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, J = 8.2 Hz, 1H), 7.89-7.81 (m, 2H), 7.73-7.61 (m, 4H), 7.45-7.43 (m, 1H), 7.38-7.34 (m, 1H), 2.29-2.26 (m, 2H), 2.04-2.01 (m, 4H), 1.91-1.87 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 169.9, 139.7, 134.4, 133.9, 131.2, 129.5, 128.4, 127.5, 125.7, 123.0, 119.1, 94.2, 93.4, 37.6, 37.0, 25.4, 25.4 ppm. ESI HRMS: calcd. for $C_{20}H_{17}NO_3S$+H 352.1007, found 352.1003.



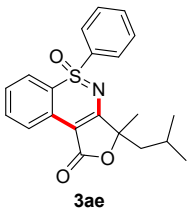
3ad

5-phenyl-1H-5λ^6-spiro[benzo[*e*]furo[3,4-*c*][1,2]thiazine-3,1'-cyclohexan]-1-one 5-oxide (**3ad**). 14 h, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, J = 8.0 Hz, 1H), 7.84-7.82 (m, 2H), 7.72-7.60 (m, 4H), 7.45-7.43 (m, 1H), 7.37-7.33 (m, 1H), 2.07-1.94 (m, 2H), 1.89-1.71 (m, 7H), 1.34-1.23 (m, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 170.1, 139.8, 134.4, 133.9, 131.5, 129.5, 128.3, 127.4, 125.8, 123.1, 119.2, 93.3, 84.9, 33.8, 33.5, 24.6, 21.9, 21.8 ppm. ESI HRMS: calcd. for $C_{21}H_{19}NO_3S$+H 366.1164, found 366.1169.



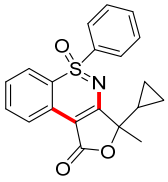
3ae'

1-isobutyl-1-methyl-5-phenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-3(1H)-one 5-oxide (**3ae'**). 12 h, 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 7.6 Hz, 2H), 7.74-7.62 (m, 4H), 7.42-7.35 (m, 2H), 1.96 (dd, J_1 = 5.8 Hz, J_2 = 14.5 Hz, 1H), 1.81 (dd, J_1 = 6.2 Hz, J_2 = 14.5 Hz, 1H), 1.76-1.68 (m, 1H), 1.61 (s, 3H), 0.96 (d, J = 6.6 Hz, 3H), 0.88 (d, J = 6.6 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 170.0, 139.3, 134.5, 134.0, 131.3, 129.5, 128.5, 127.5, 125.7, 123.1, 118.8, 94.1, 85.9, 45.3, 24.9, 24.4, 24.3, 23.9 ppm. ESI HRMS: calcd. for $C_{21}H_{21}KNO_3S$+H 406.0879, found 406.0942.



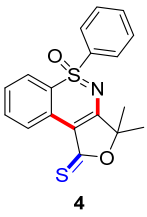
3ae

3-isobutyl-3-methyl-5-phenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3ae**). 12 h, 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 8.0 Hz, 1H), 7.86 – 7.84 (m, 2H), 7.74 – 7.62 (m, 4H), 7.43 (d, J = 7.6 Hz, 1H), 7.40 – 7.31 (m, 1H), 2.00 – 1.91 (m, 1H), 1.82 (t, J = 7.0 Hz, 1H), 1.74 (dd, J_1 = 6.6 Hz, J_2 = 13.0 Hz, 1H), 1.62 (s, 3H), 0.95 (d, J = 6.4 Hz, 3H), 0.92 (d, J = 6.4 Hz, 3H) ppm. ^{13}C NMR (151 MHz, $cdcl_3$) δ 169.1, 166.0, 135.4, 130.4, 129.9, 127.1, 125.5, 124.4, 123.5, 121.6, 119.0, 114.9, 90.0, 81.8, 42.0, 20.3, 20.1, 19.7 ppm. ESI HRMS: calcd. for $C_{21}H_{21}NO_3S$+H 368.1320, found 368.1324.



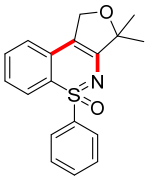
3af

3-cyclopropyl-3-methyl-5-phenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazin-1(3H)-one 5-oxide (**3af**). 12 h, 63% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (t, *J* = 8.0 Hz, 1H), 7.87-7.82 (m, 2H), 7.74-7.58 (m, 4H), 7.54-7.35 (m, 1H), 7.39-7.35 (m, 1H), 1.70 (s, 3H), 1.47-1.36 (m, 1H), 0.71-0.56 (m, 2H), 0.51-0.36 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 171.5, 168.4, 168.4, 138.3, 137.9, 132.7, 132.7, 132.3, 132.2, 130.7, 129.5, 127.8, 127.6, 126.6, 126.4, 125.8, 125.8, 124.4, 124.1, 124.0, 121.3, 117.3, 117.3, 91.5, 91.3, 81.9, 81.7, 21.8, 21.5, 16.4, 16.1, -1.1, -1.5 ppm. ESI HRMS: calcd. for $C_{20}H_{17}NO_3S$+H 352.1007, found 352.1005.



4

3,3-dimethyl-5-phenyl-5λ^4-benzo[*e*]furo[3,4-*c*][1,2]thiazine-1(3H)-thione 5-oxide (**4**). 24 h, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 7.2 Hz, 2H), 7.76-7.70 (m, 2H), 7.64 (t, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 6.8Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 1.69 (s, 3H), 1.68 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.3, 175.6, 139.4, 134.7, 134.1, 131.6, 129.7, 128.1, 128.0, 126.1, 123.4, 119.0, 105.4, 90.6, 24.6, 24.3 ppm. ESI HRMS: calcd. for $C_{18}H_{15}NO_2S_2$+H 342.0622, found 342.0618.



5

3,3-dimethyl-5-phenyl-1,3-dihydrobenzo[*e*]furo[3,4-*c*][1,2]thiazine 5-oxide (**5**). 24 h, 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.19-7.14 (m, *J* = 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 5.03 (d, *J* = 2.4 Hz, 2H), 1.461 (s, 3H), 1.455 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.2, 139.9, 133.8, 132.6, 131.8, 129.3, 129.1, 125.8, 125.8, 122.3, 119.0, 101.4, 86.5, 69.5, 26.5, 25.8 ppm. ESI HRMS: calcd. for $C_{18}H_{17}NO_2S$+Na 334.0878, found 334.0853.

Reference

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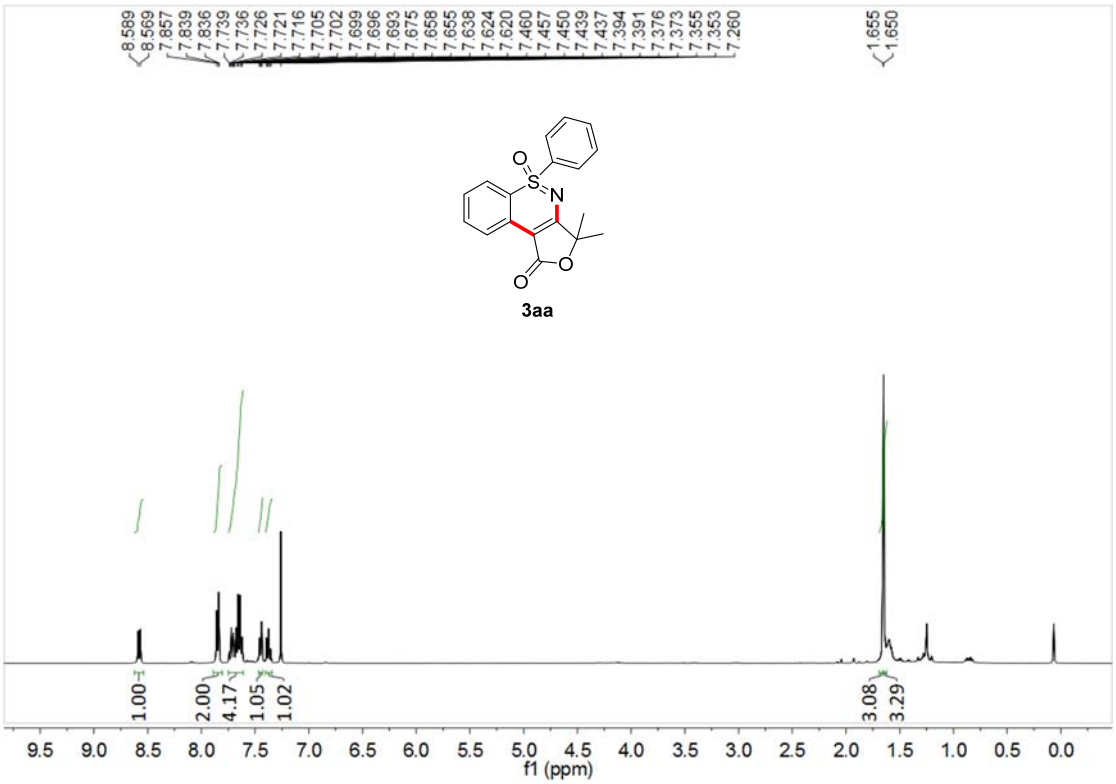
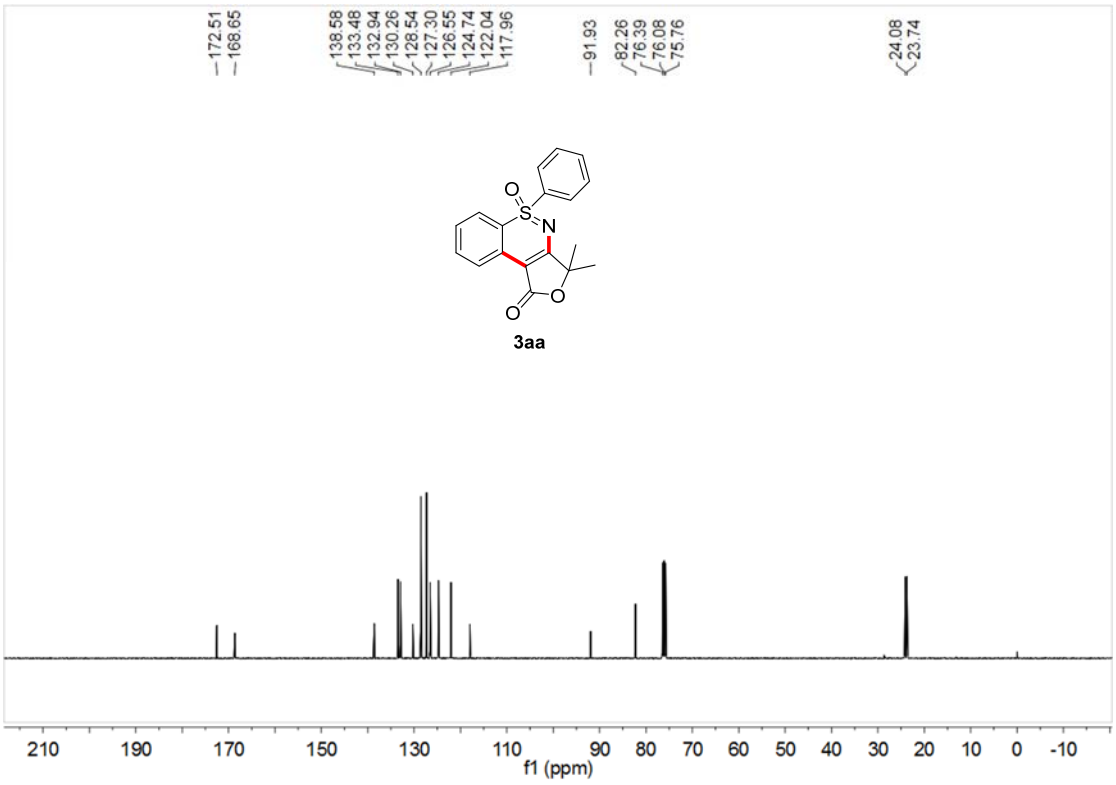
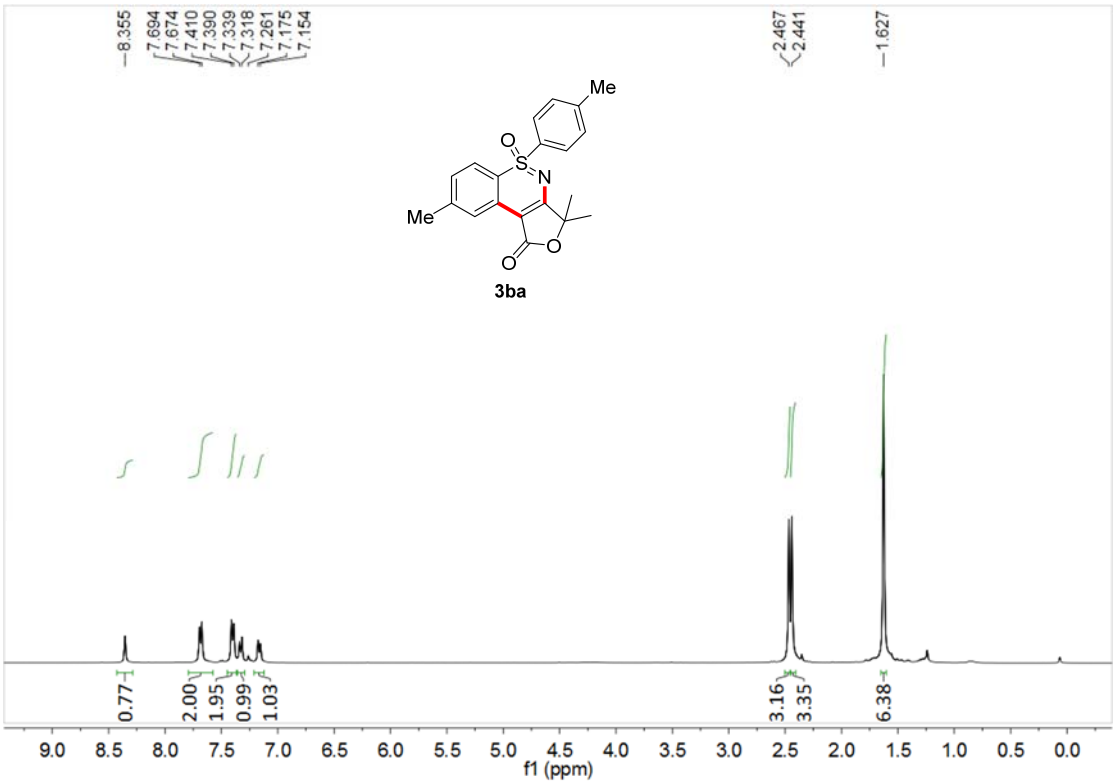
6. ^{1}H and ^{13}C NMR spectra.



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7.694
7.674
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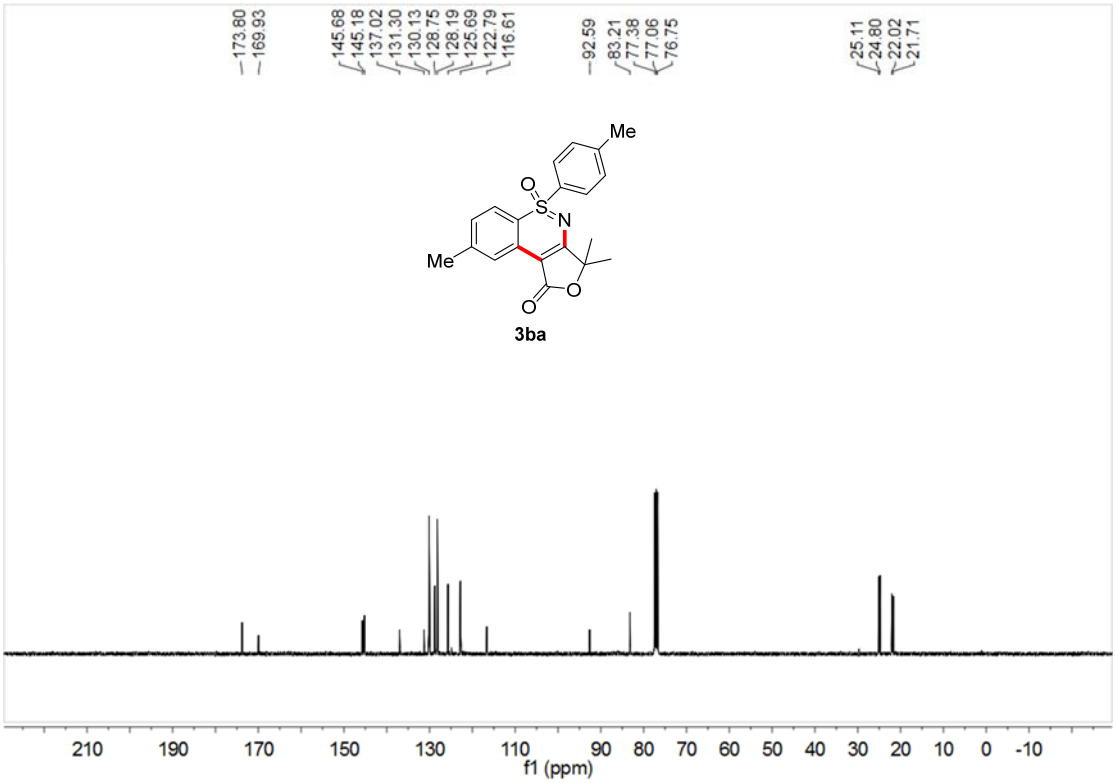
7.390
7.339
7.318
7.261
7.175
7.154
2.467
2.441
1.627
Me
O
S
N
Me
O
O
O
3ba
0.77
2.00
1.95
0.99
1.03
3.16
3.35
6.38
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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145.68
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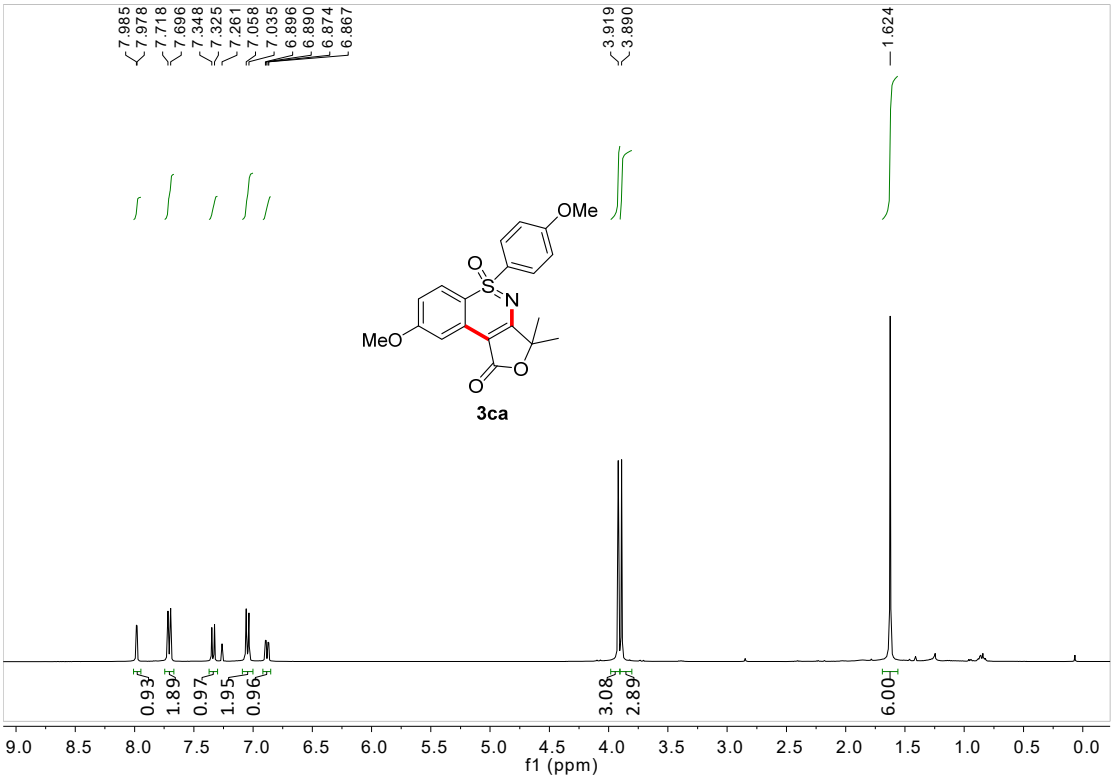
130.13
128.75
128.19
125.69
122.79
116.61
92.59
83.21
77.38
77.06
76.75
25.11
24.80
22.02
21.71
Me
O
S
N
Me
O
O
3ba
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.058
7.035
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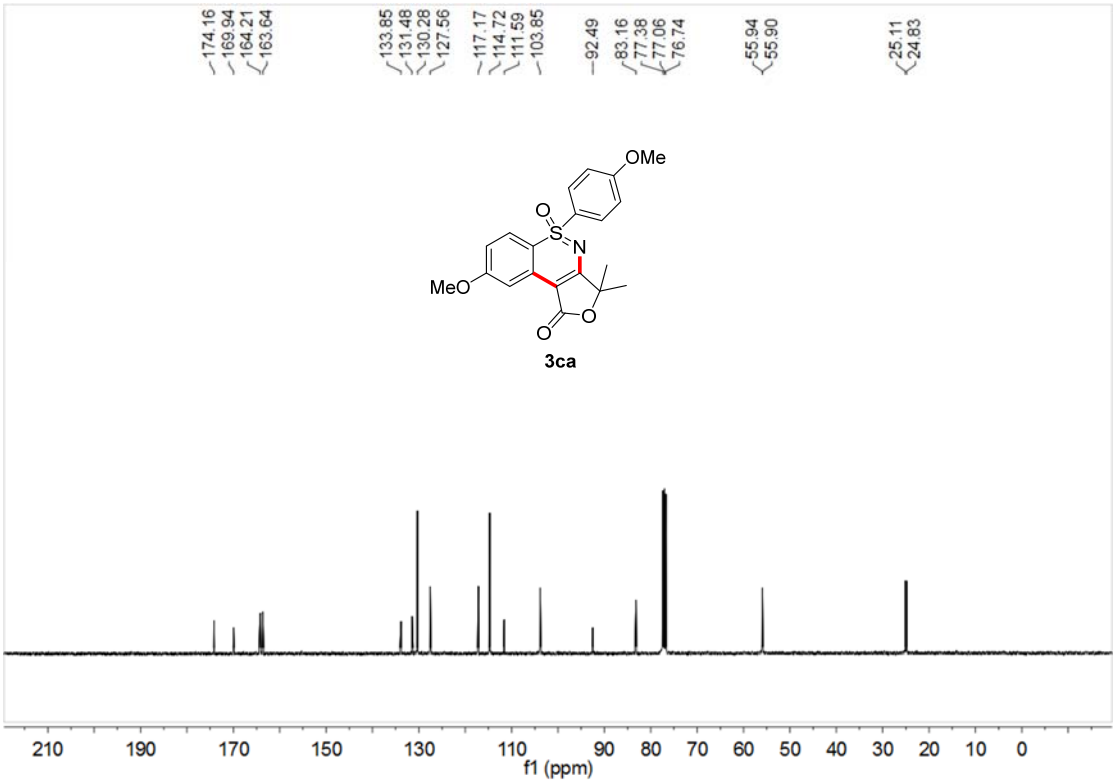
6.890
6.874
6.867
3.919
3.890
1.624
OMe
MeO
O
S
N
O
O
O
3ca
0.93
1.89
0.97
1.95
0.96
3.08
2.89
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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164.21
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130.28
127.56
117.17
114.72
111.59
103.85
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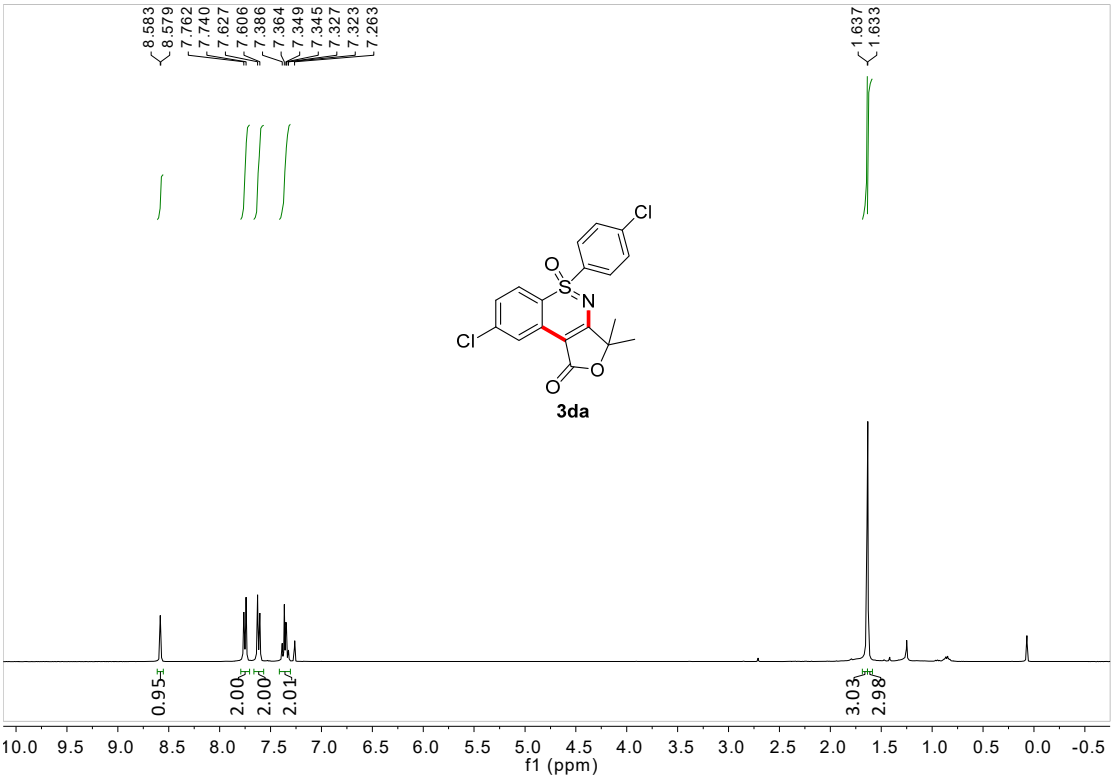
83.16
77.38
77.06
76.74
55.94
55.90
25.11
24.83
OMe
MeO
O
S
N
O
O
O
3ca
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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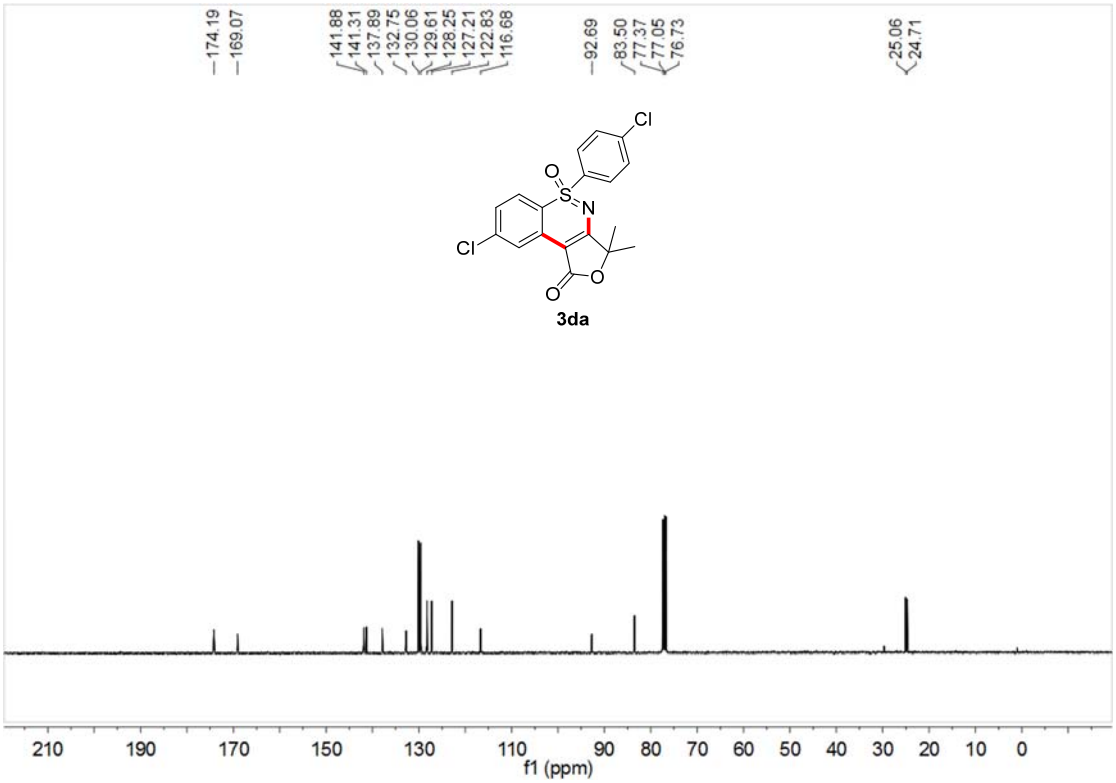
7.606
7.386
7.364
7.349
7.345
7.327
7.323
7.263
1.637
1.633
Cl
O
S
N
Cl
O
O
3da
0.95
2.00
2.00
2.01
3.03
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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169.07
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141.31
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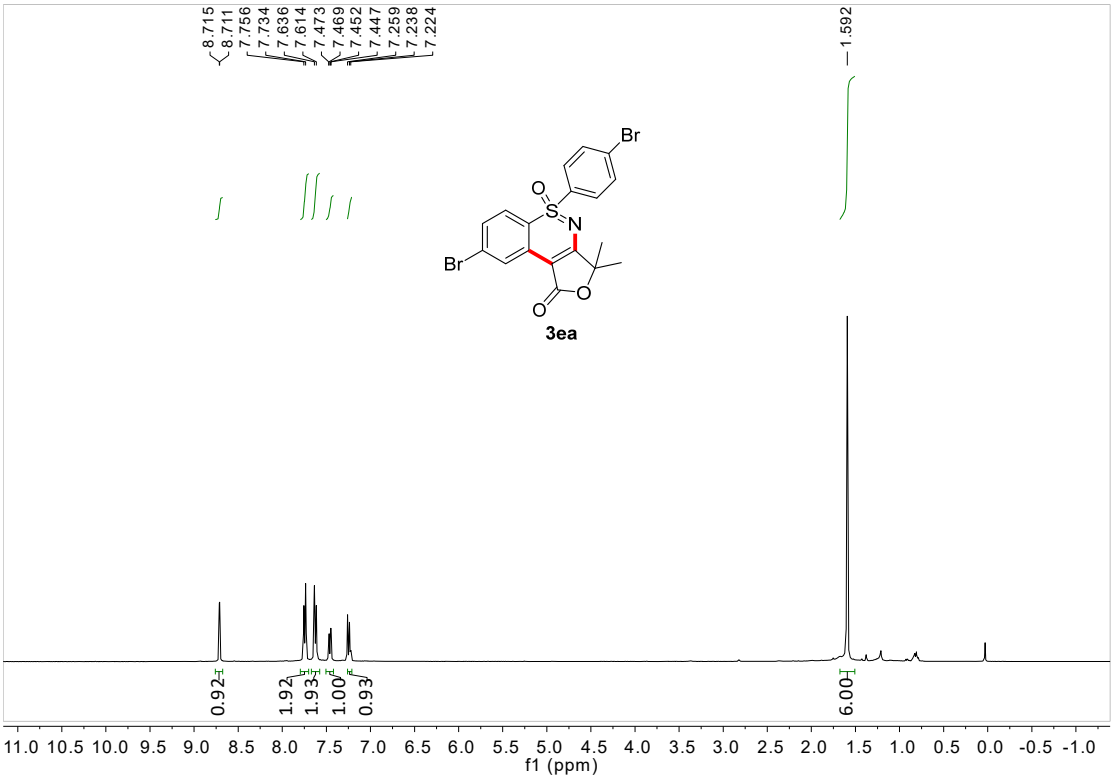
132.75
130.06
129.61
128.25
127.21
122.83
116.68
92.69
83.50
77.37
77.05
76.73
25.06
24.71
Cl
O
S
N
Cl
O
O
3da
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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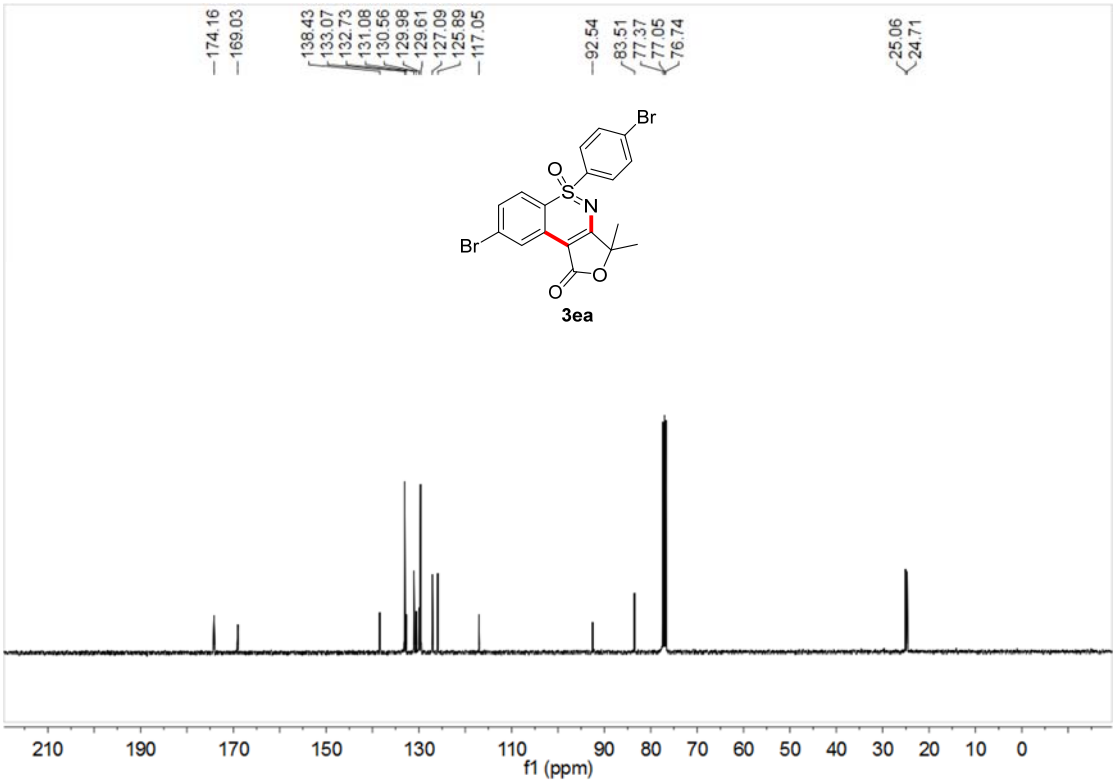
8.711
7.756
7.734
7.636
7.614
7.473
7.469
7.452
7.447
7.259
7.238
7.224
1.592
Br
O
S
N
Br
O
O
3ea
0.92
1.92
1.93
1.00
0.93
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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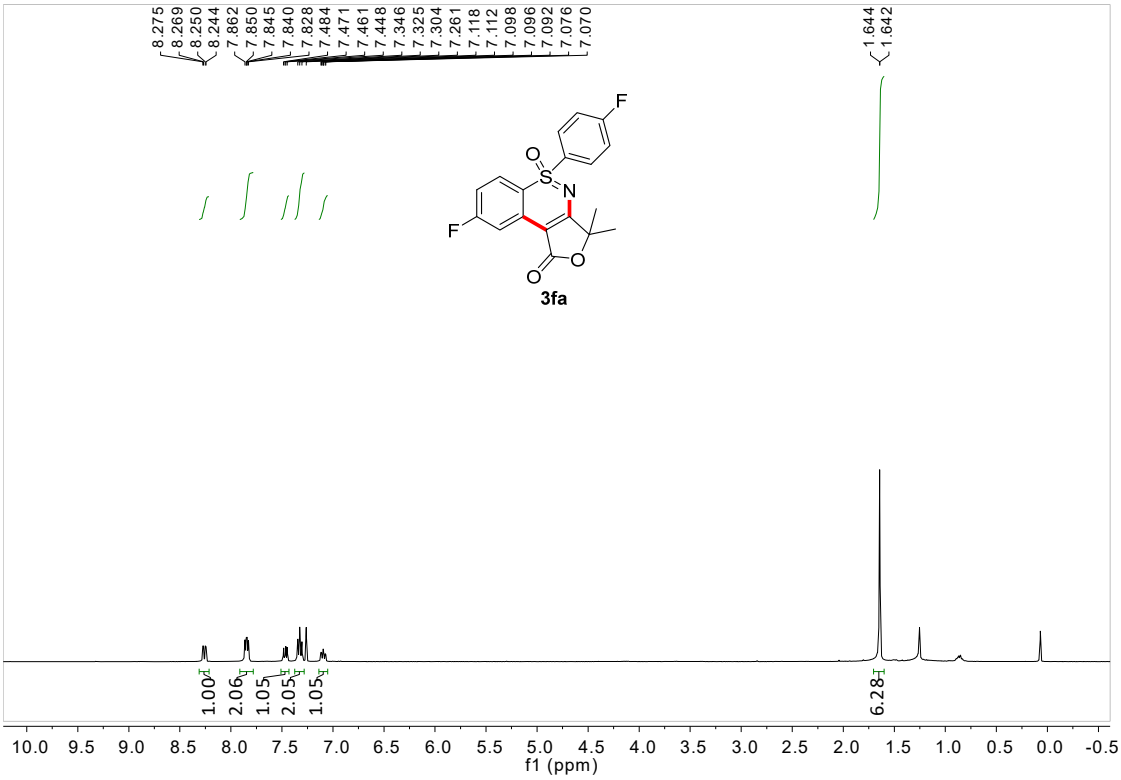
138.43
133.07
132.73
131.08
130.56
129.98
129.61
127.09
125.89
117.05
92.54
83.51
77.37
77.05
76.74
25.06
24.71
Br
O
S
N
Br
O
O
3ea
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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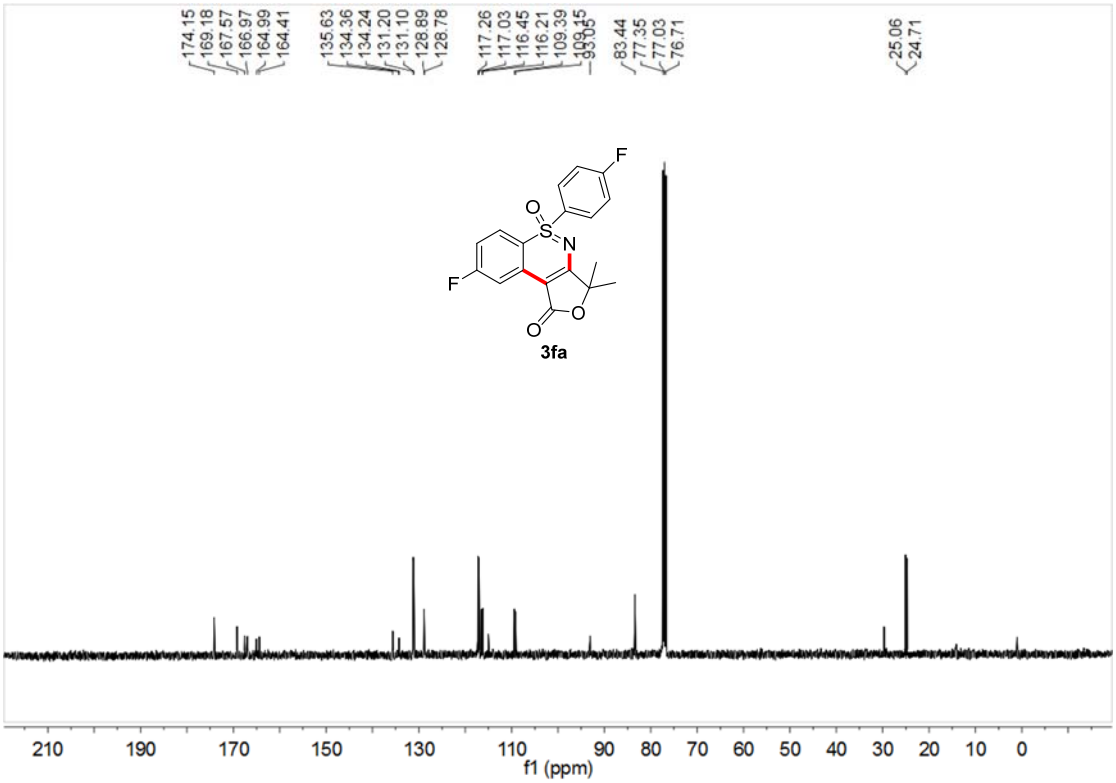
8.269
8.250
8.244
7.862
7.850
7.845
7.840
7.828
7.484
7.471
7.461
7.448
7.346
7.325
7.304
7.261
7.118
7.112
7.098
7.096
7.092
7.076
7.070
1.644
1.642
F
O
S
N
F
O
O
3fa
1.00
2.06
1.05
2.05
1.05
6.28
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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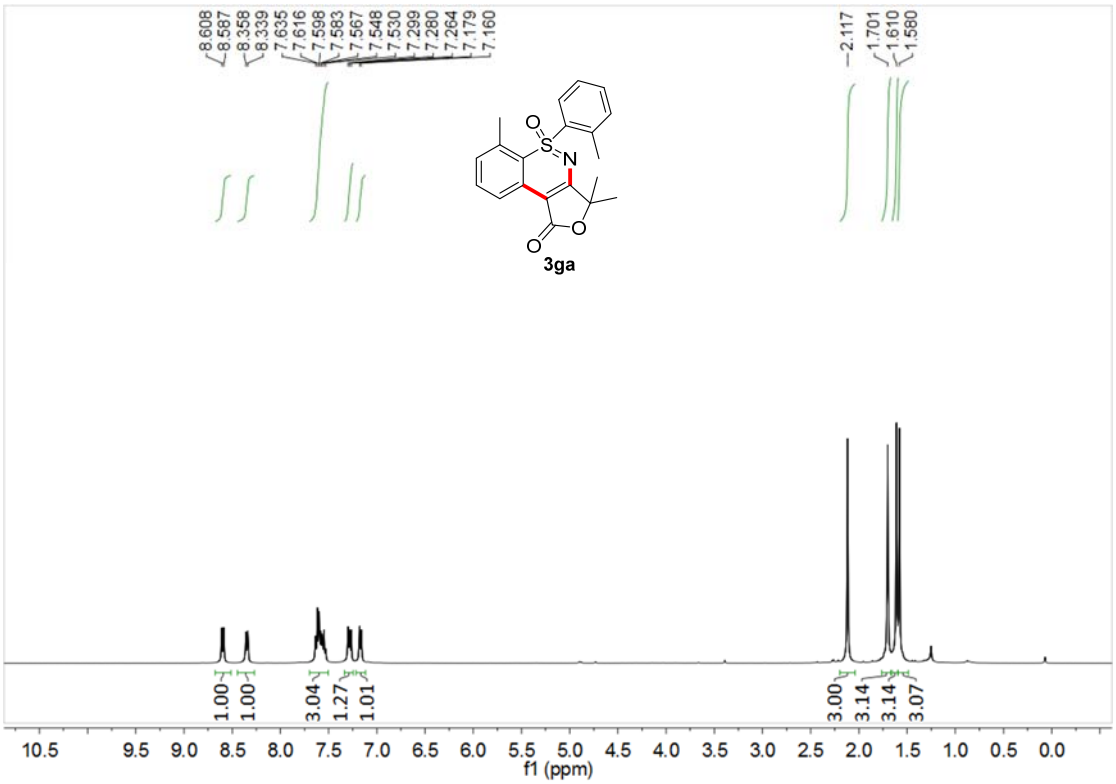
169.18
167.57
166.97
164.99
164.41
135.63
134.36
134.24
131.20
131.10
128.89
128.78
117.26
117.03
116.45
116.21
109.39
83.44
77.35
77.03
76.71
25.06
24.71
F
O
S
N
F
O
O
3fa
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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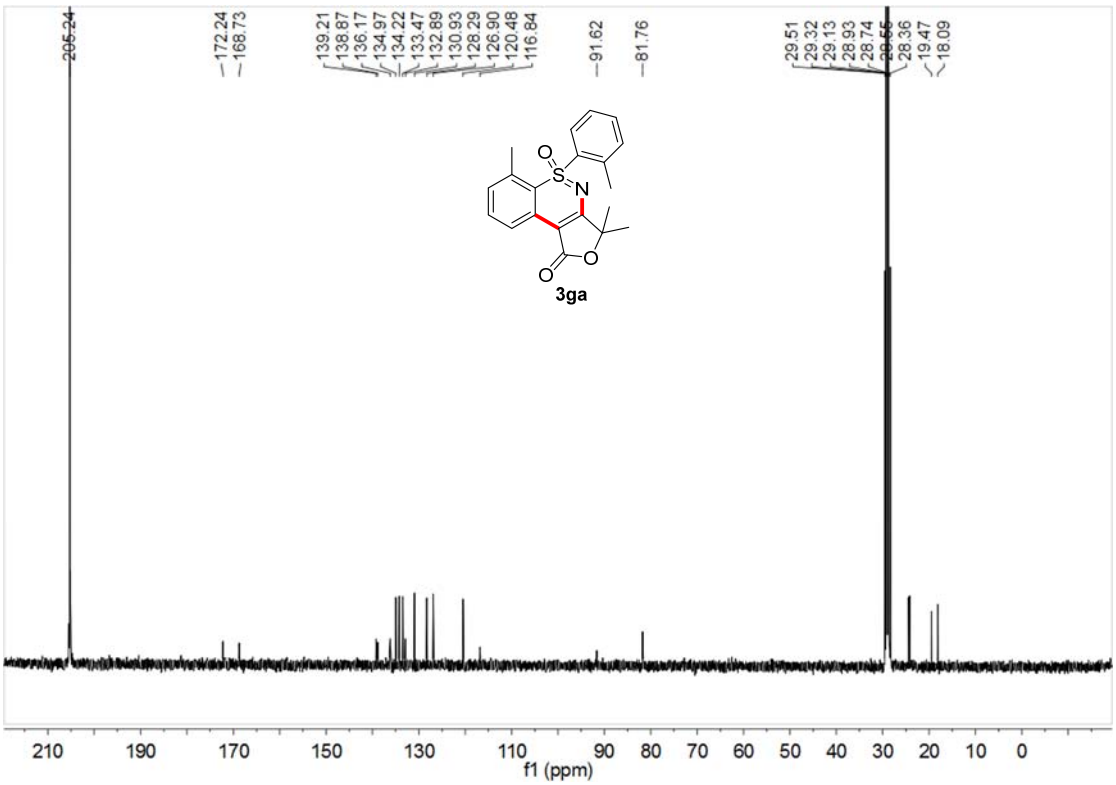
8.358
8.339
7.635
7.616
7.598
7.583
7.567
7.548
7.530
7.299
7.280
7.264
7.179
7.160
2.117
1.701
1.610
1.580
3ga
1.00
1.00
3.04
1.27
1.01
3.00
3.14
3.14
3.07
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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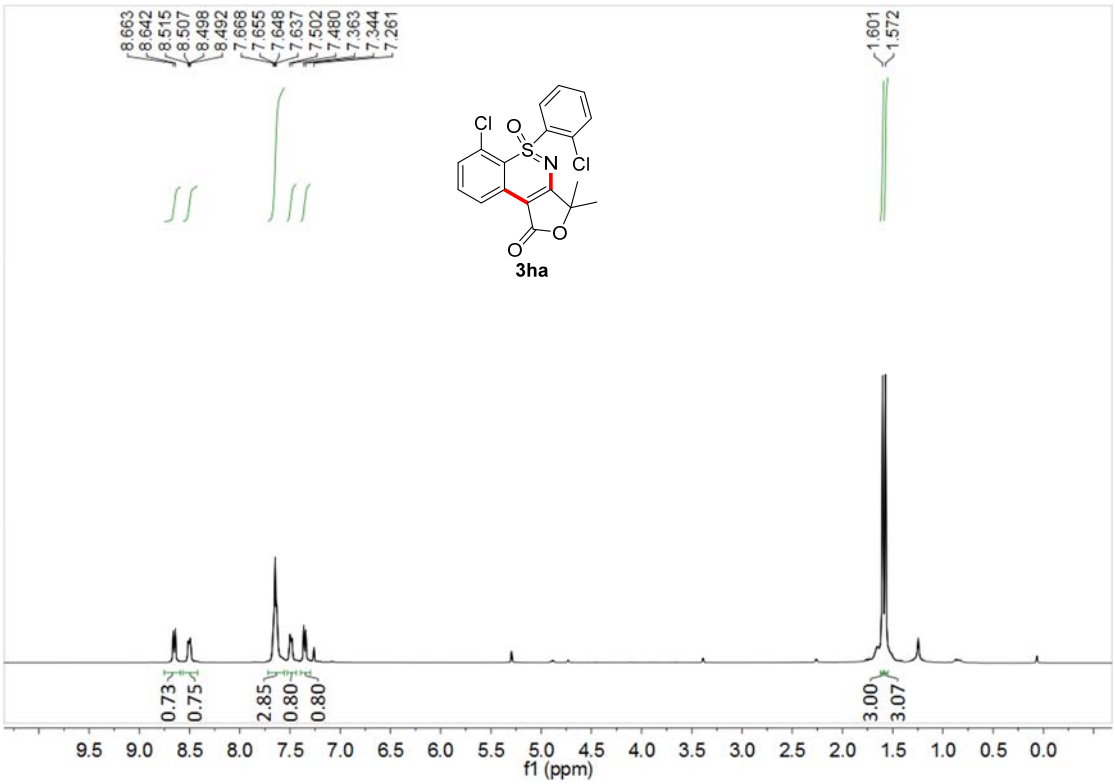
168.73
139.21
138.87
136.17
134.97
134.22
133.47
132.89
130.93
128.29
126.90
120.48
116.84
91.62
81.76
29.51
29.32
29.13
28.93
28.74
28.36
19.47
18.09
3ga
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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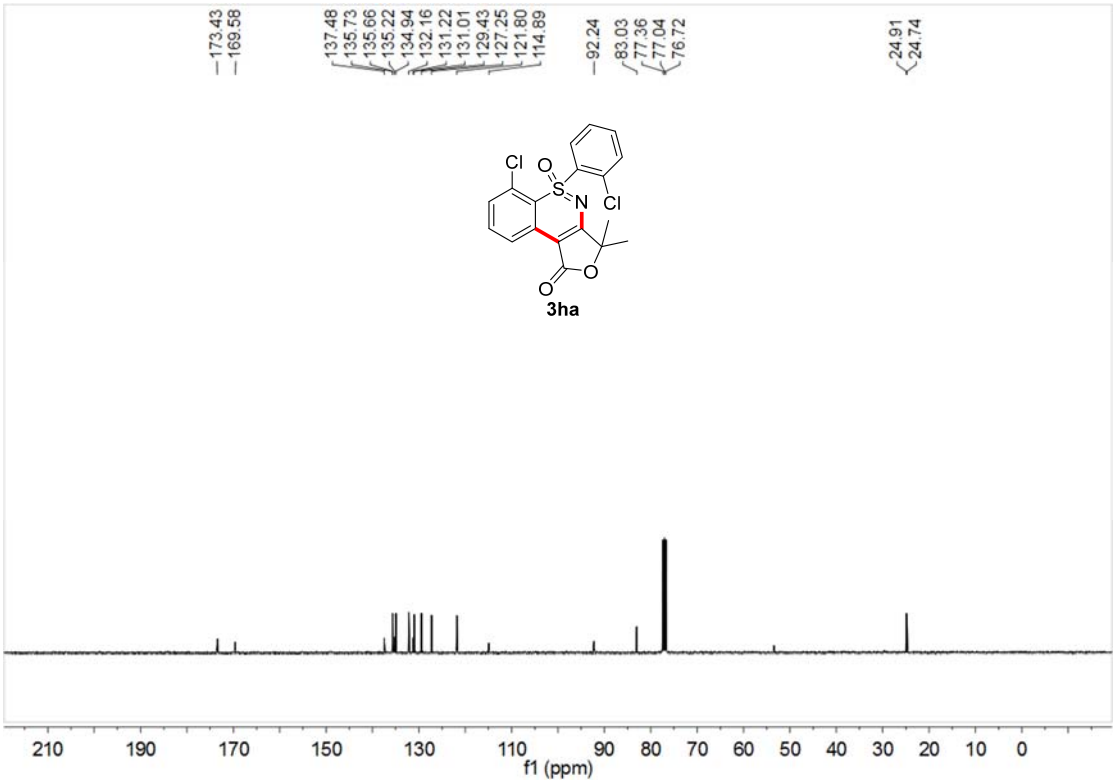
8.492
7.668
7.655
7.648
7.637
7.502
7.480
7.363
7.344
7.261
1.601
1.572
Cl
O
S
N
Cl
O
O
3ha
0.73
0.75
2.85
0.80
0.80
3.00
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.22
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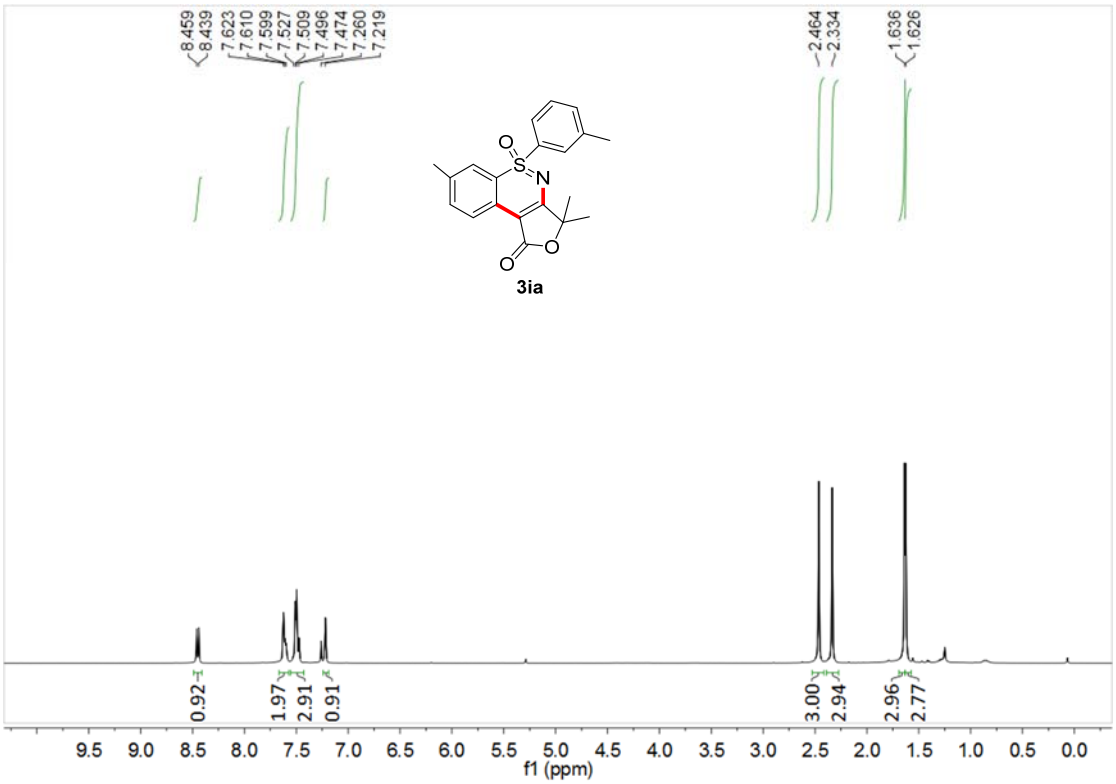
132.16
131.22
131.01
129.43
127.25
121.80
114.89
92.24
83.03
77.36
77.04
76.72
24.91
24.74
Cl
O
S
N
Cl
O
O
3ha
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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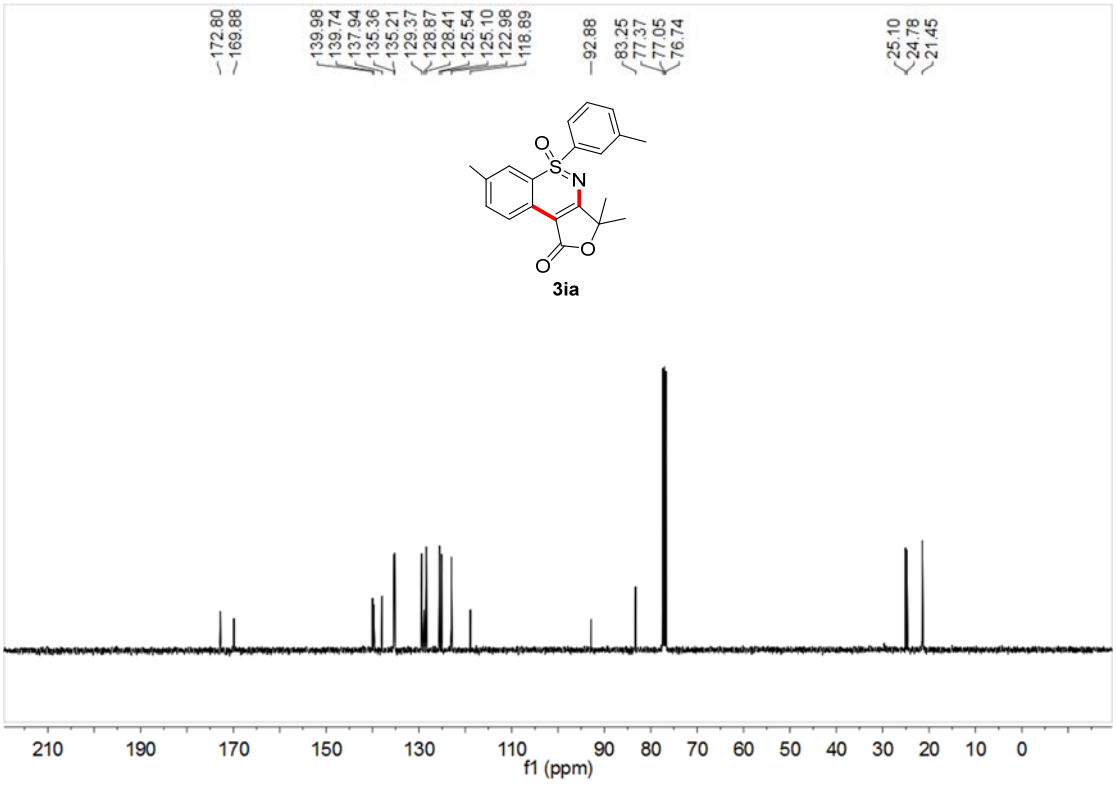
7.599
7.527
7.509
7.496
7.474
7.260
7.219
2.464
2.334
1.636
1.626
3ia
0.92
1.97
2.91
0.91
3.00
2.94
2.96
2.77
f1 (ppm)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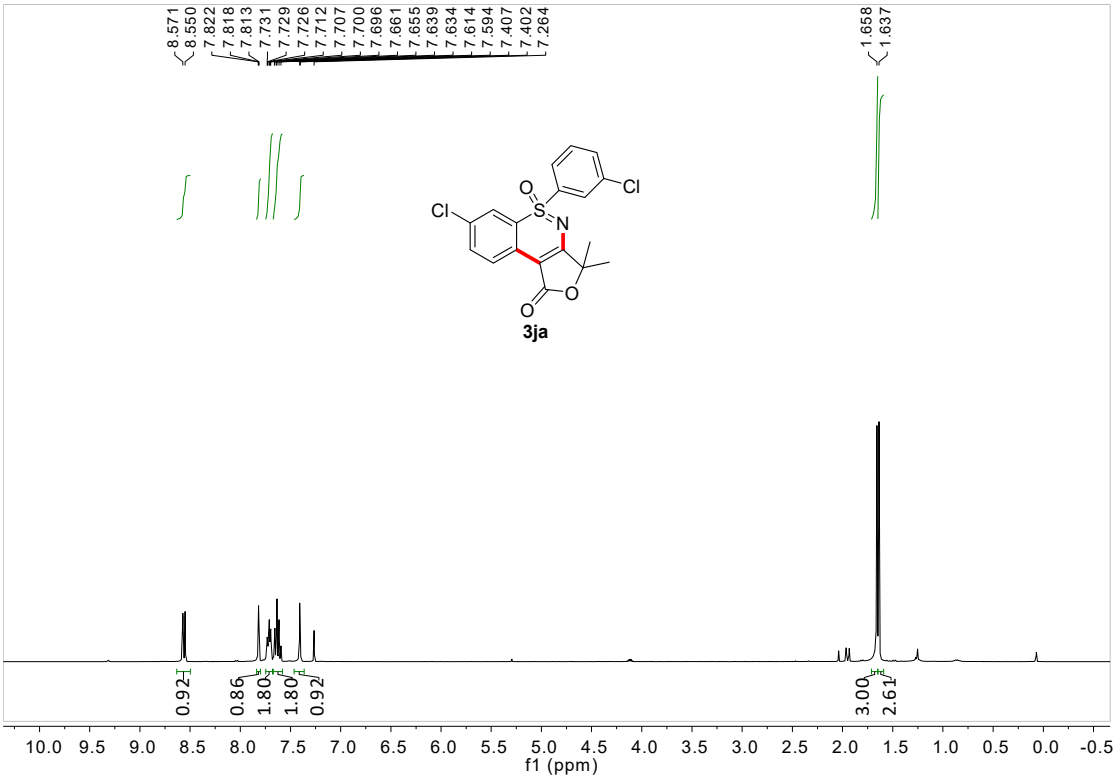
135.21
129.37
128.87
128.41
125.54
125.10
122.98
118.89
92.88
83.25
77.37
77.05
76.74
25.10
24.78
21.45
3ia
f1 (ppm)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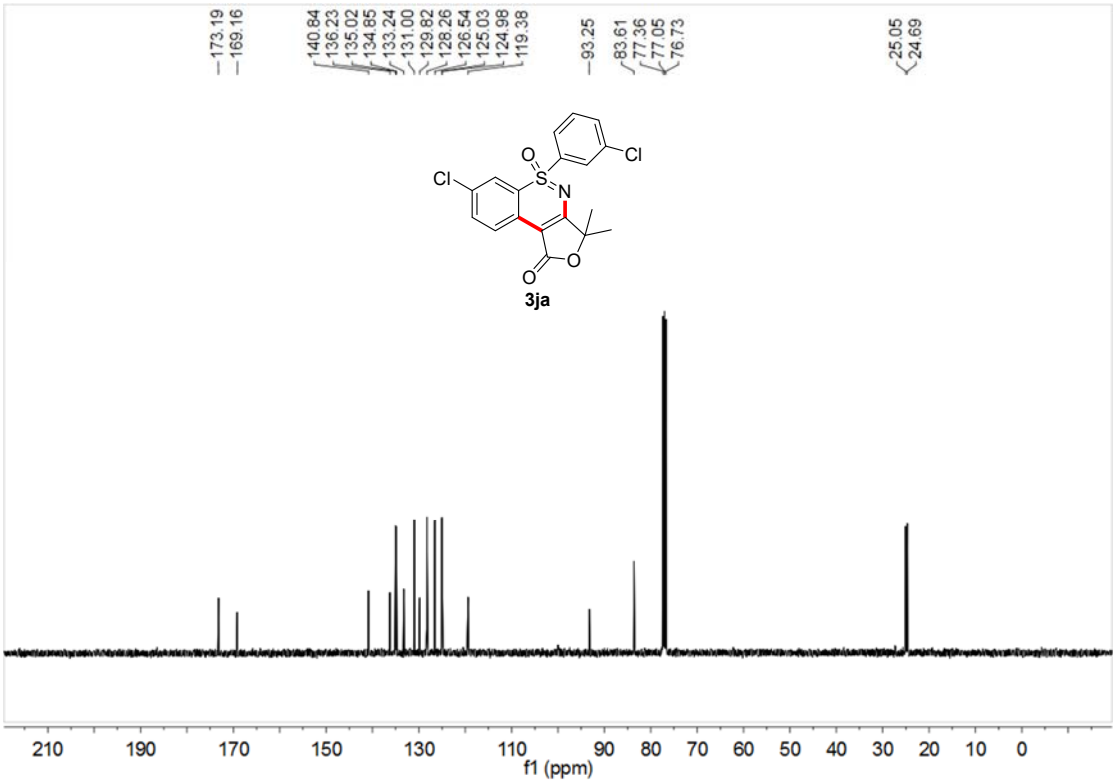
7.726
7.712
7.707
7.700
7.696
7.661
7.655
7.639
7.634
7.614
7.594
7.407
7.402
7.264
1.658
1.637
Cl
Cl
O
S
N
O
O
3ja
0.92
0.86
1.80
1.80
0.92
3.00
2.61
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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135.02
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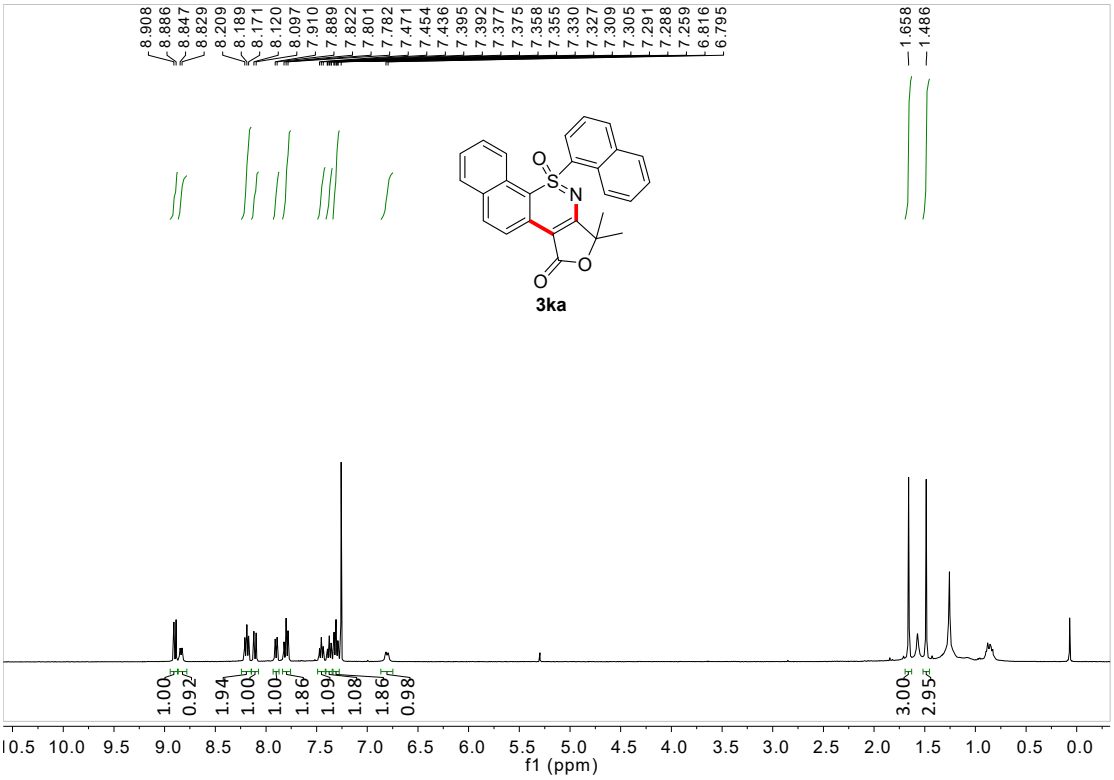
133.24
131.00
129.82
128.26
126.54
125.03
124.98
119.38
93.25
83.61
77.36
77.05
76.73
25.05
24.69
Cl
Cl
O
S
N
O
O
3ja
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.120
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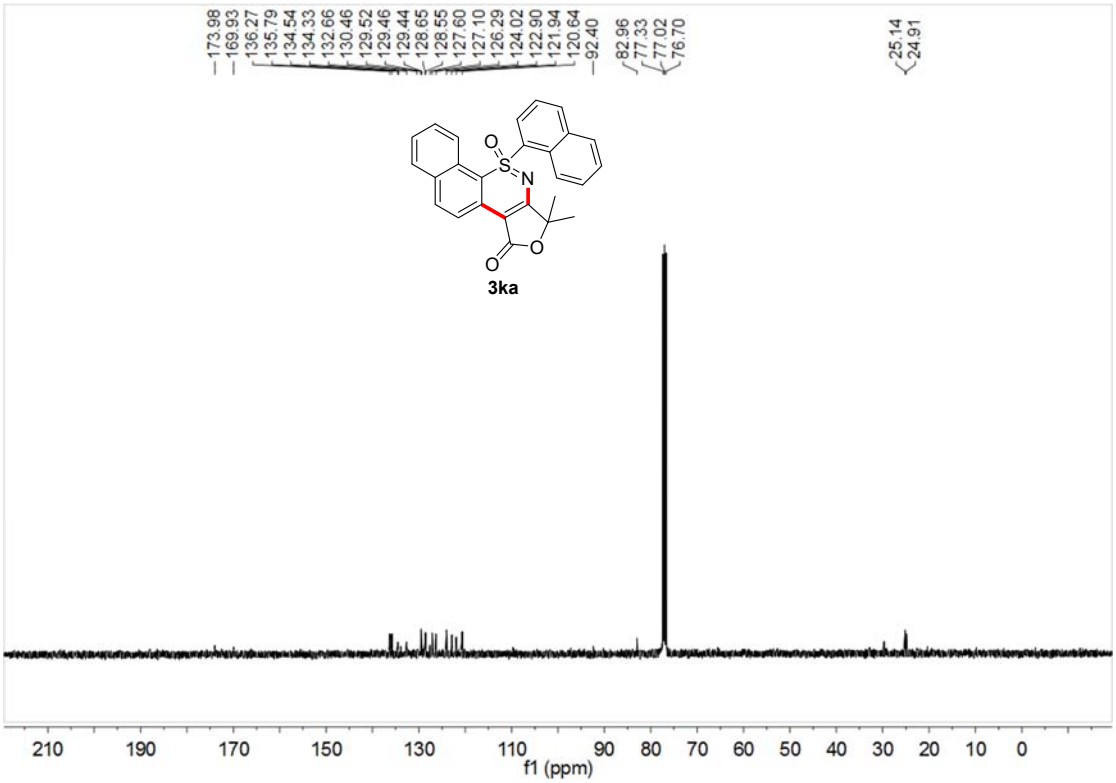
7.910
7.889
7.822
7.801
7.782
7.471
7.454
7.436
7.395
7.392
7.377
7.375
7.358
7.355
7.330
7.327
7.309
7.305
7.291
7.288
7.259
6.816
6.795
1.658
1.486
3ka
1.00
0.92
1.94
1.00
1.00
1.86
1.09
1.08
1.86
0.98
3.00
2.95
f1 (ppm)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129.46
129.44
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128.55
127.60
127.10
126.29
124.02
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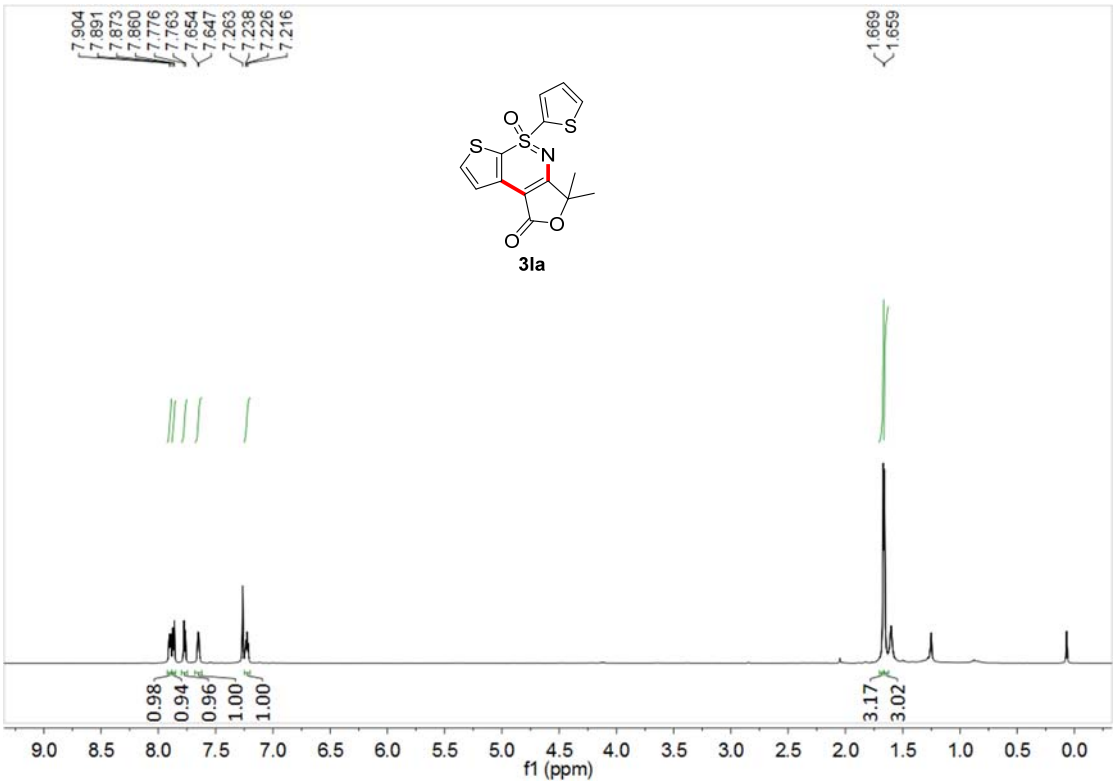
92.40
82.96
77.33
77.02
76.70
25.14
24.91
3ka
f1 (ppm)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7.763
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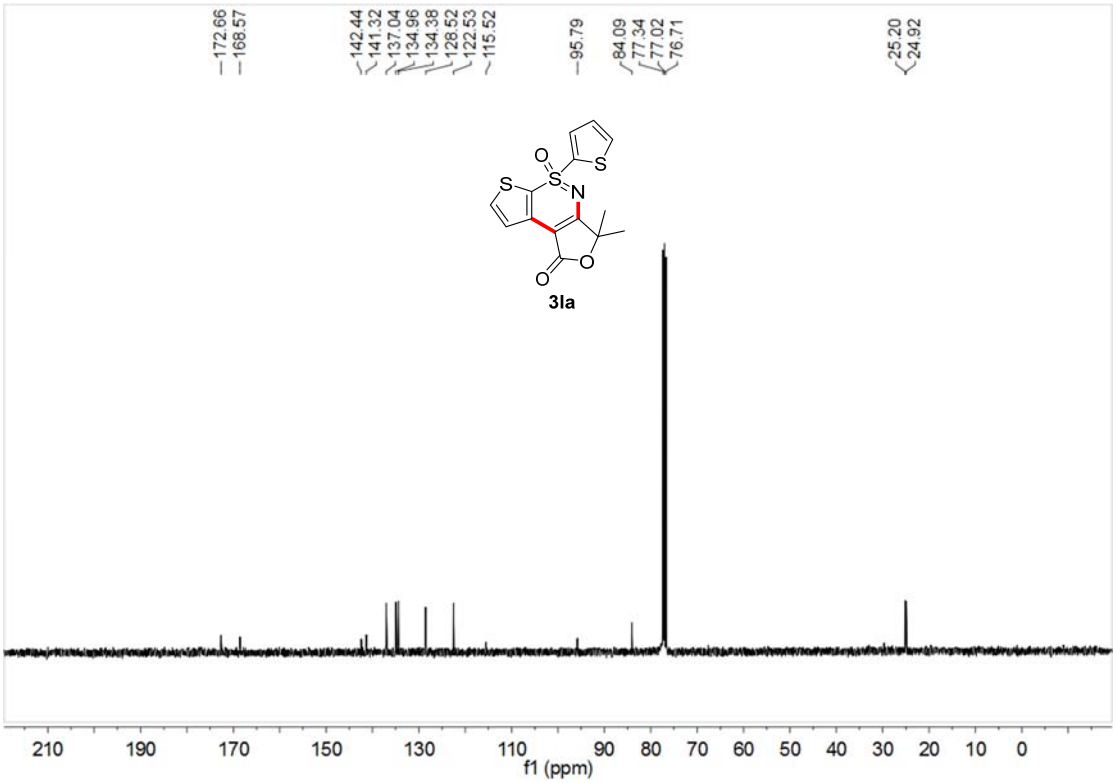
7.647
7.263
7.238
7.226
7.216
1.669
1.659
3Ia
0.98
0.94
0.96
1.00
1.00
3.17
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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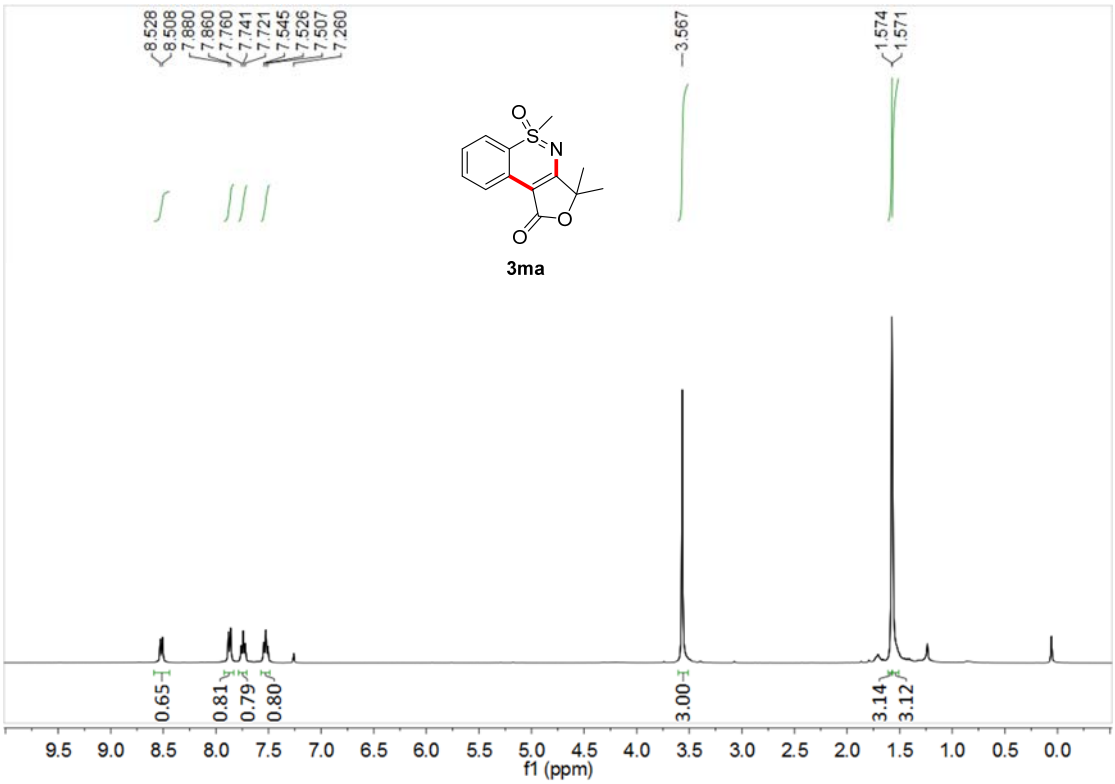
134.96
134.38
128.52
122.53
115.52
95.79
84.09
77.34
77.02
76.71
25.20
24.92
3Ia
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.721
7.545
7.526
7.507
7.260
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1.571
3ma
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0.81
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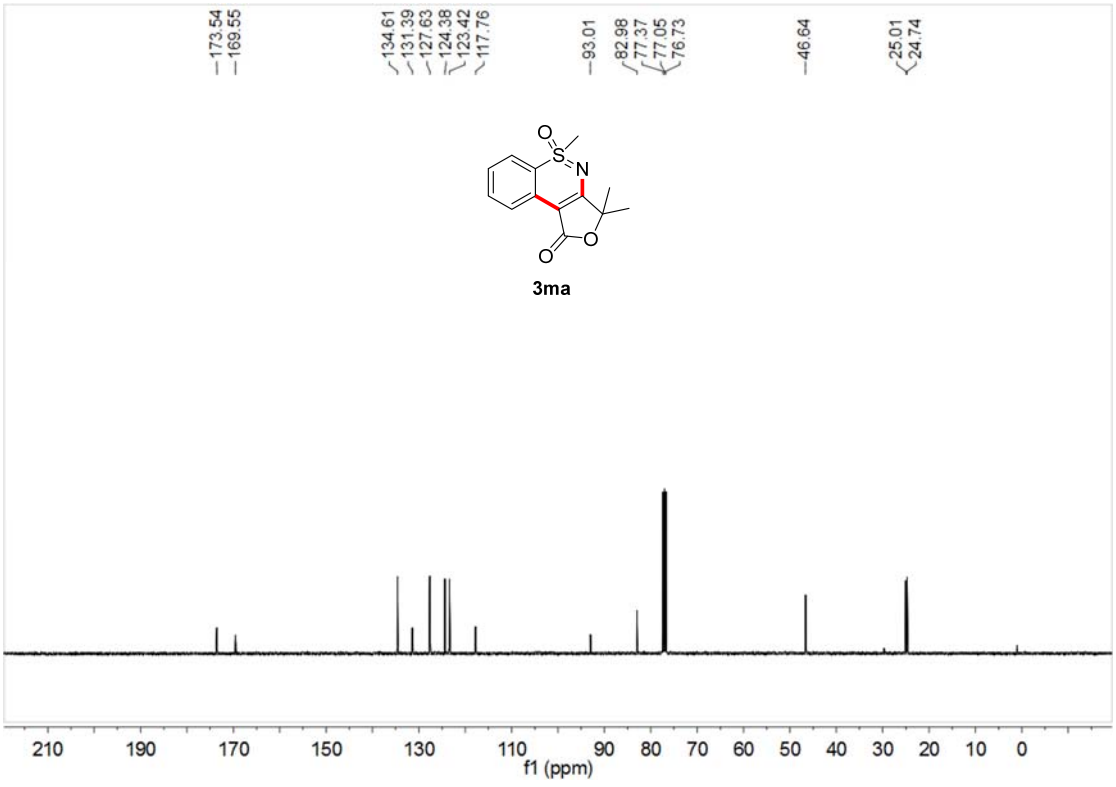
0.80
3.00
3.14
3.12
f1 (ppm)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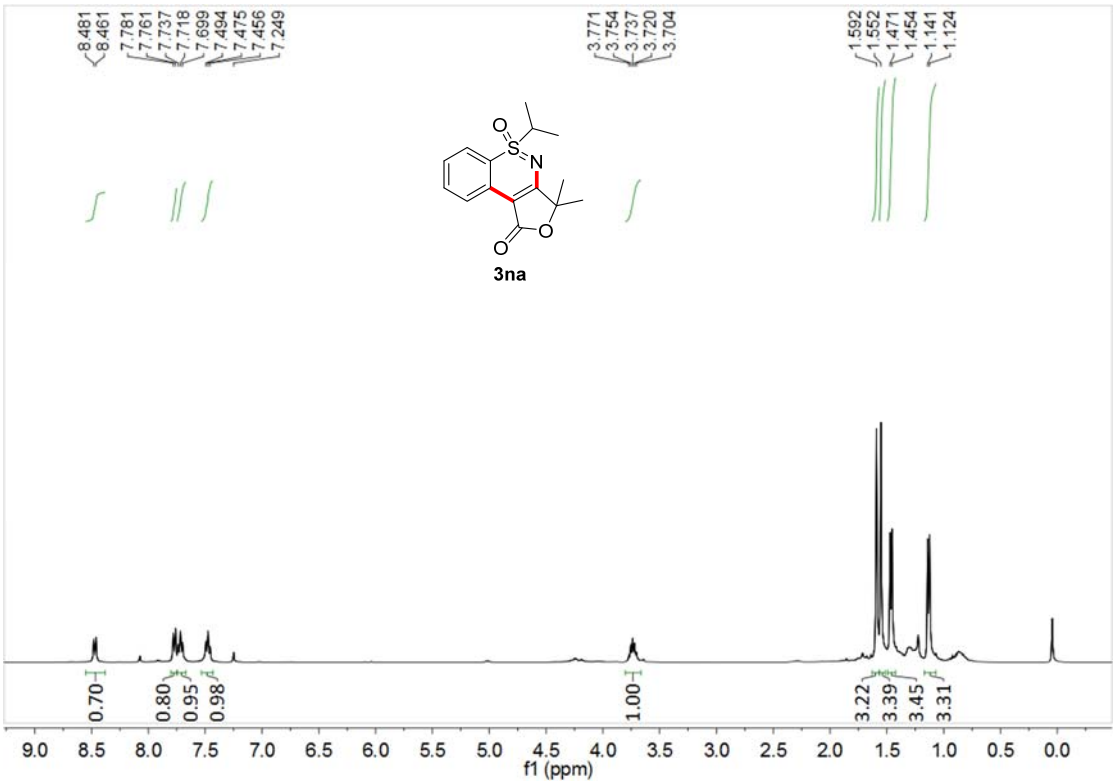
46.64
25.01
24.74
3ma
f1 (ppm)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7.456
7.249
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3.754
3.737
3.720
3.704
1.592
1.552
1.471
1.454
1.141
1.124
3na
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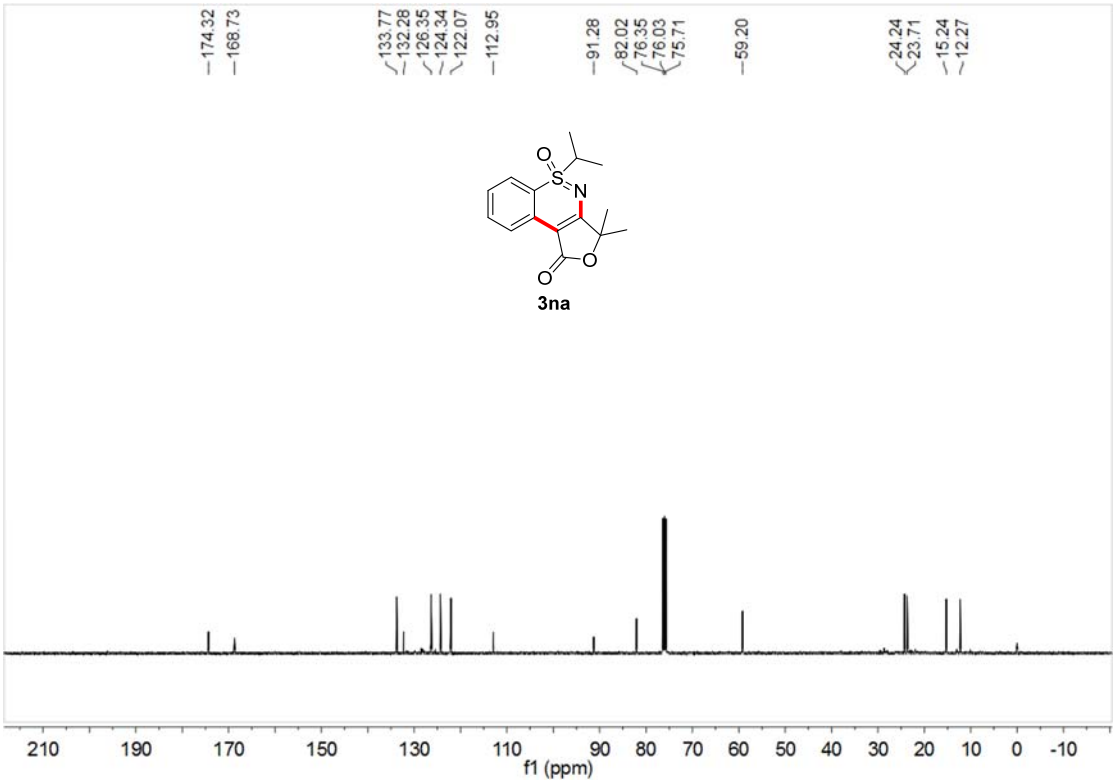
0.80
0.95
0.98
1.00
3.22
3.39
3.45
3.31
f1 (ppm)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132.28
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124.34
122.07
112.95
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82.02
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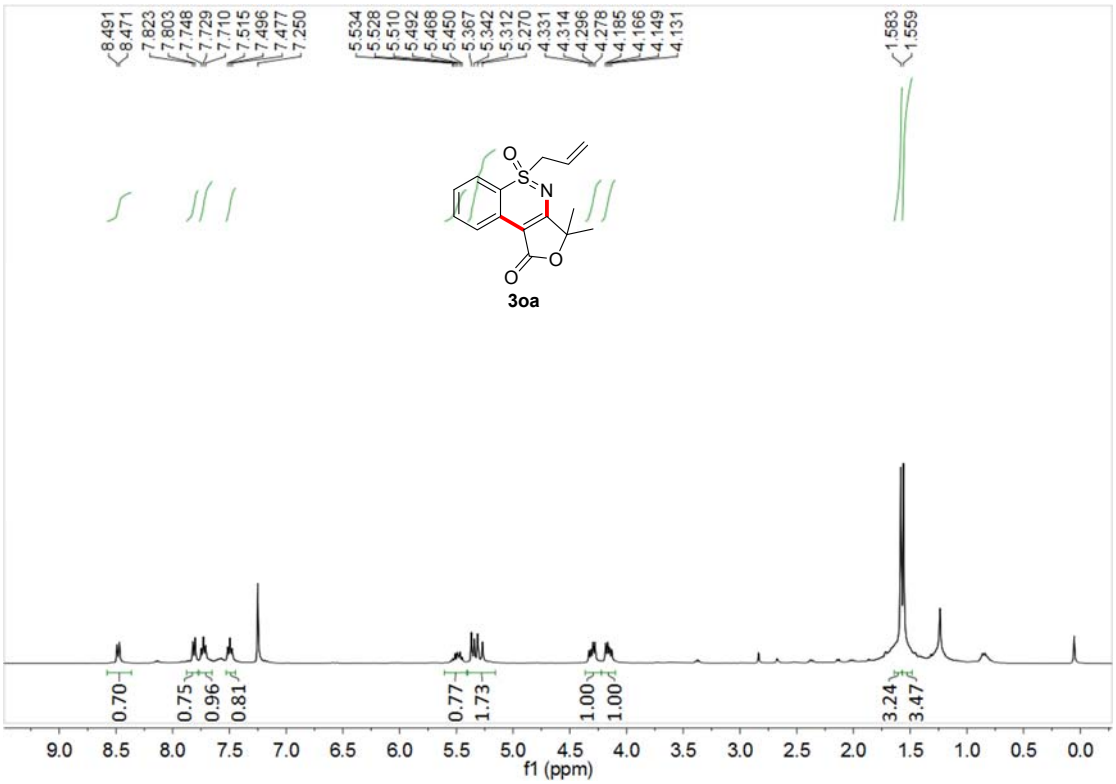
76.03
75.71
59.20
24.24
23.71
15.24
12.27
3na
f1 (ppm)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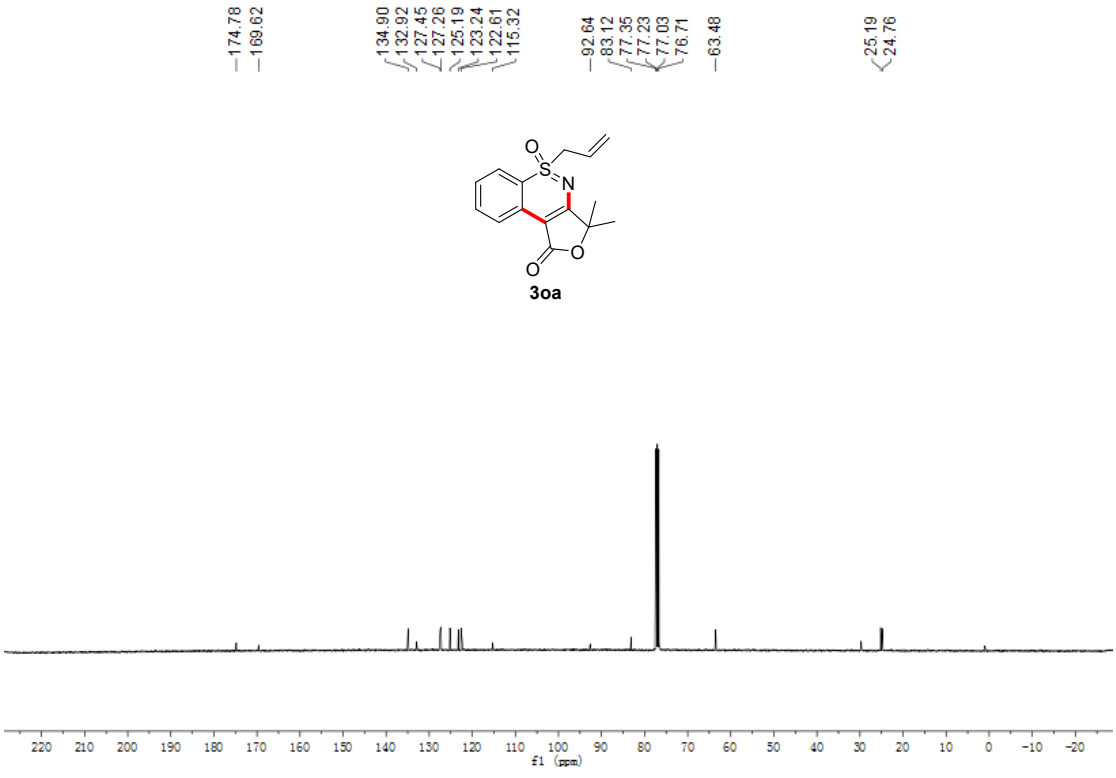
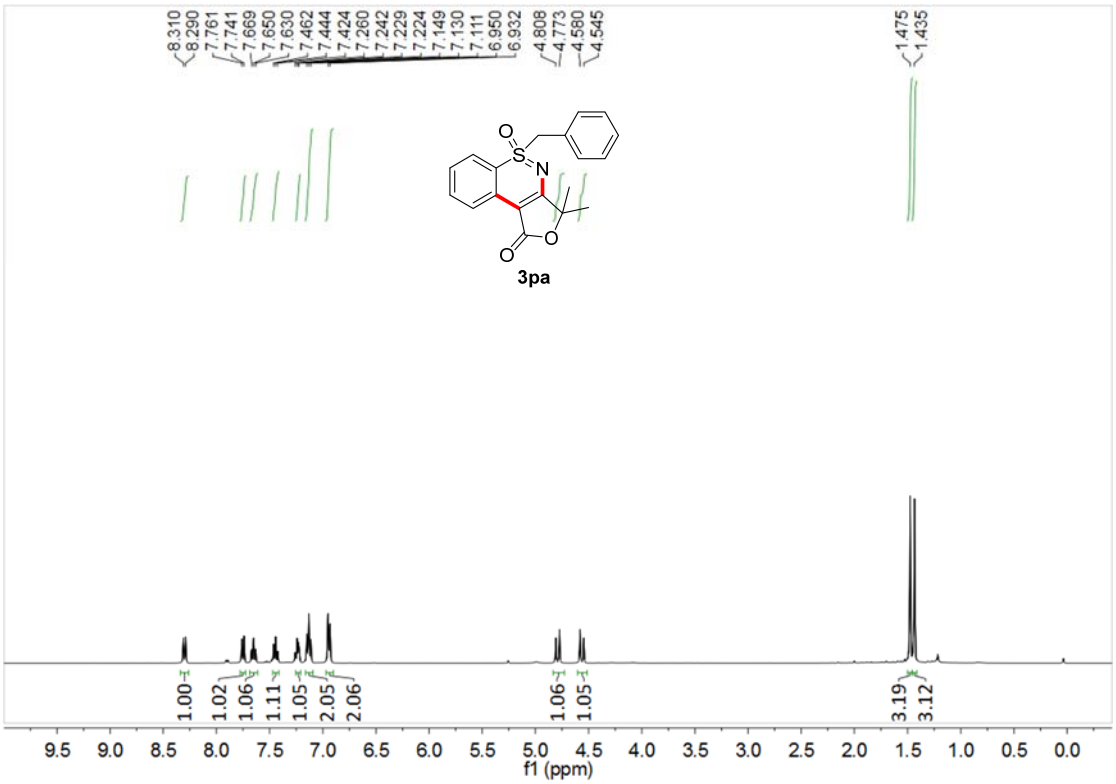
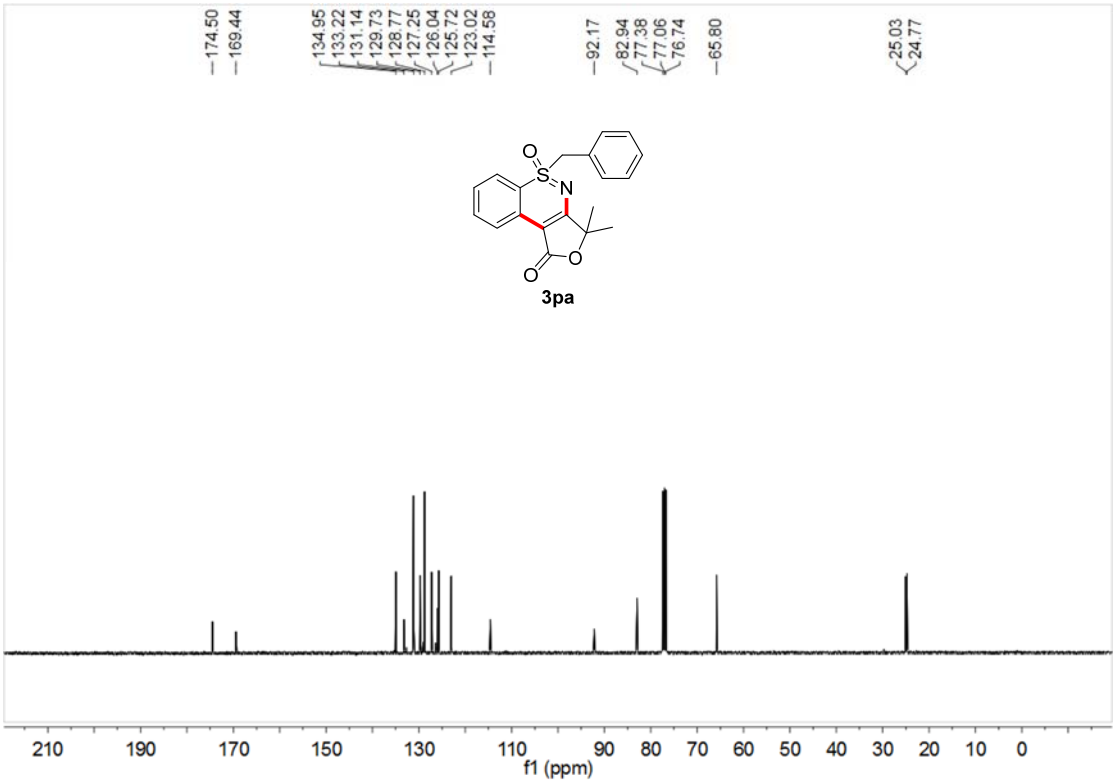
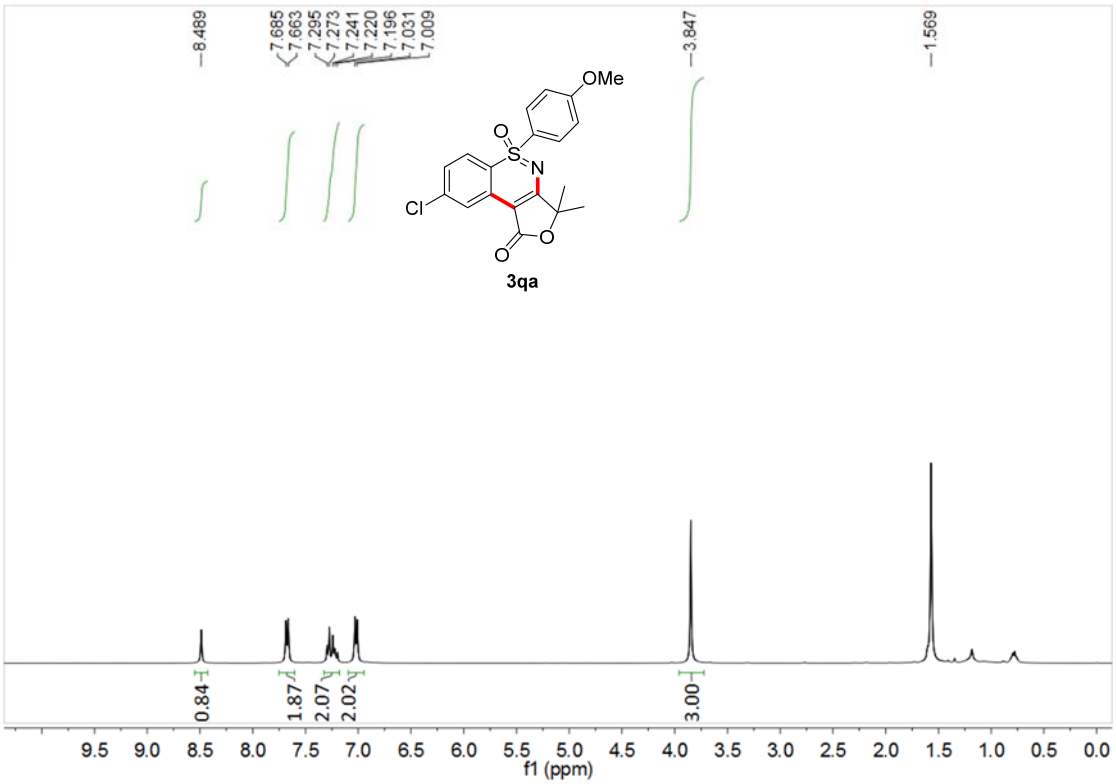
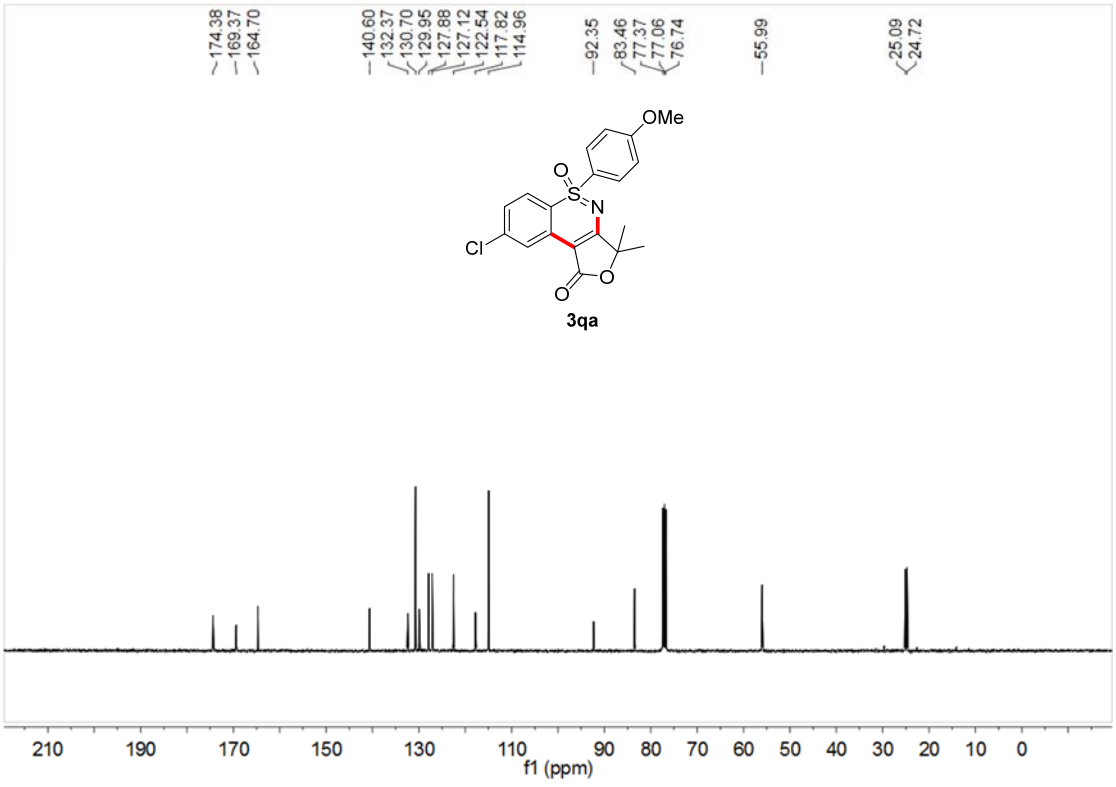
5.528
5.510
5.492
5.468
5.450
5.367
5.342
5.312
5.270
4.331
4.314
4.296
4.278
4.185
4.166
4.149
4.131
1.583
1.559
O
S
N
O
O
3oa
0.70
0.75
0.96
0.81
0.77
1.73
1.00
1.00
3.24
3.47
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

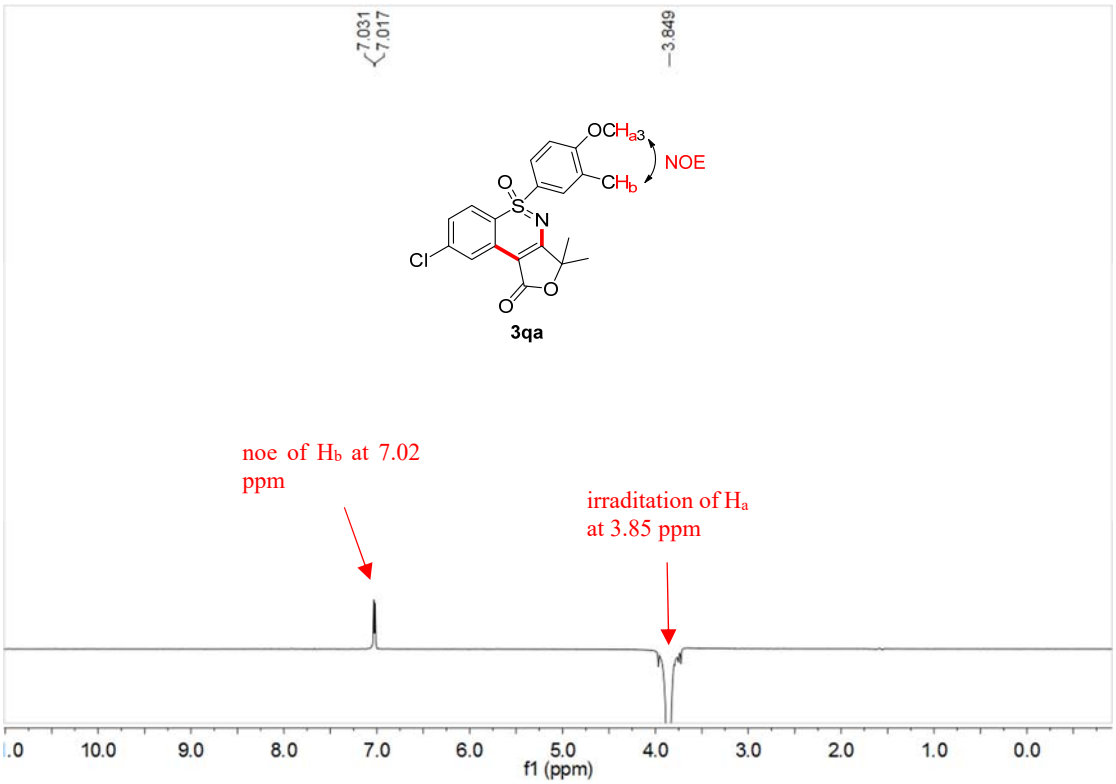

174.78
169.62
134.90
132.92
127.45
127.26
125.19
123.24
122.61
115.32
92.64
83.12
77.35
77.23
77.03
76.71
63.48
25.19
24.76
O
S
N
O
O
3oa
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

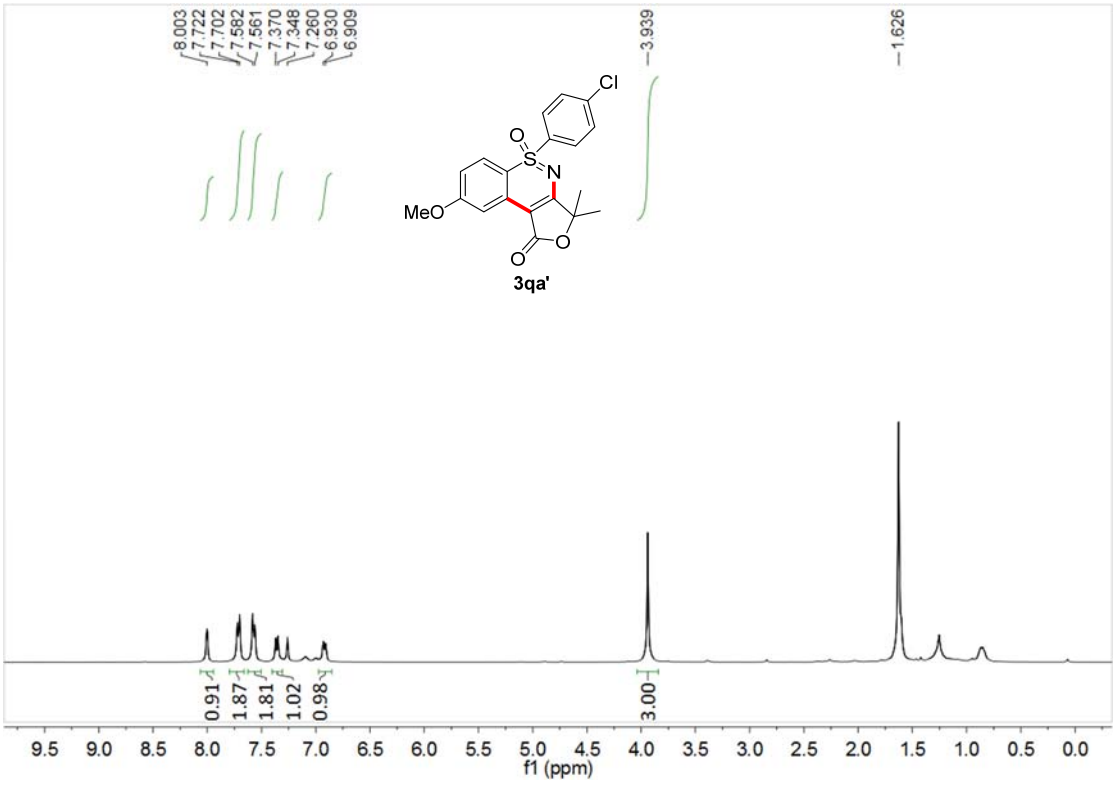

8.310
8.290
7.761
7.741
7.669
7.650
7.630
7.462
7.444
7.424
7.260
7.242
7.229
7.224
7.149
7.130
7.111
6.950
6.932
4.808
4.773
4.580
4.545
1.475
1.435
3pa
1.00
1.02
1.06
1.11
1.05
2.05
2.06
1.06
1.05
3.19
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

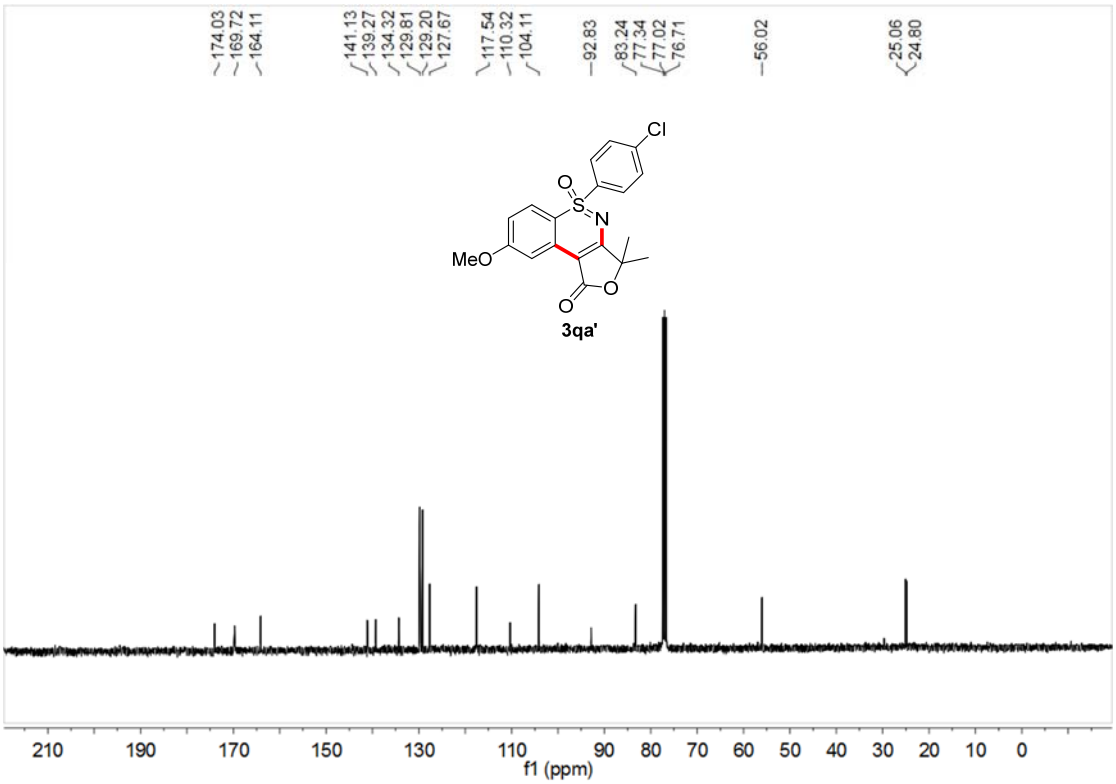

174.50
169.44
134.95
133.22
131.14
129.73
128.77
127.25
126.04
125.72
123.02
114.58
92.17
82.94
77.38
77.06
76.74
65.80
25.03
24.77
3pa
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

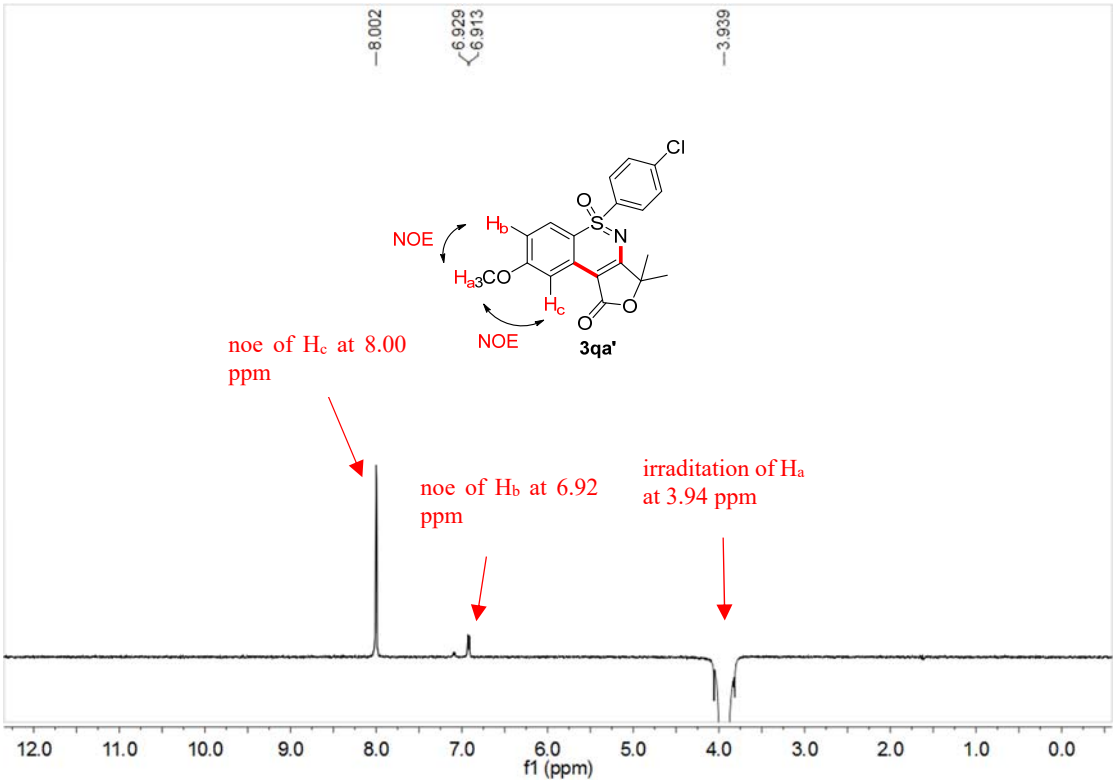

8.489
7.685
7.663
7.295
7.273
7.241
7.220
7.196
7.031
7.009
3.847
1.569
OMe
O
S
N
Cl
O
O
3qa
0.84
1.87
2.07
2.02
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

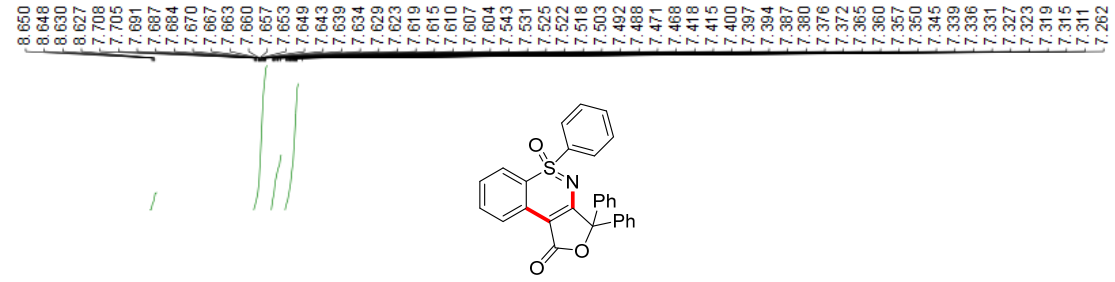

174.38
169.37
164.70
140.60
132.37
130.70
129.95
127.88
127.12
122.54
117.82
114.96
92.35
83.46
77.37
77.06
76.74
55.99
25.09
24.72
OMe
O
S
N
Cl
O
O
3qa
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.031
7.017
3.849
OCH$_{a3}$
NOE
CH$_b$
O
S
N
Cl
O
O
3qa
noe of H$_b$ at 7.02 ppm
irraditation of H$_a$ at 3.85 ppm
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

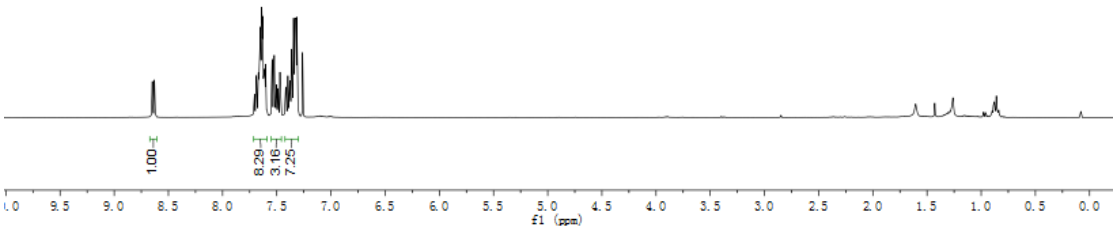

8.003
7.722
7.702
7.582
7.561
7.370
7.348
7.260
6.930
6.909
3.939
1.626
Cl
O
S
N
MeO
O
O
3qa'
0.91
1.87
1.81
1.02
0.98
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

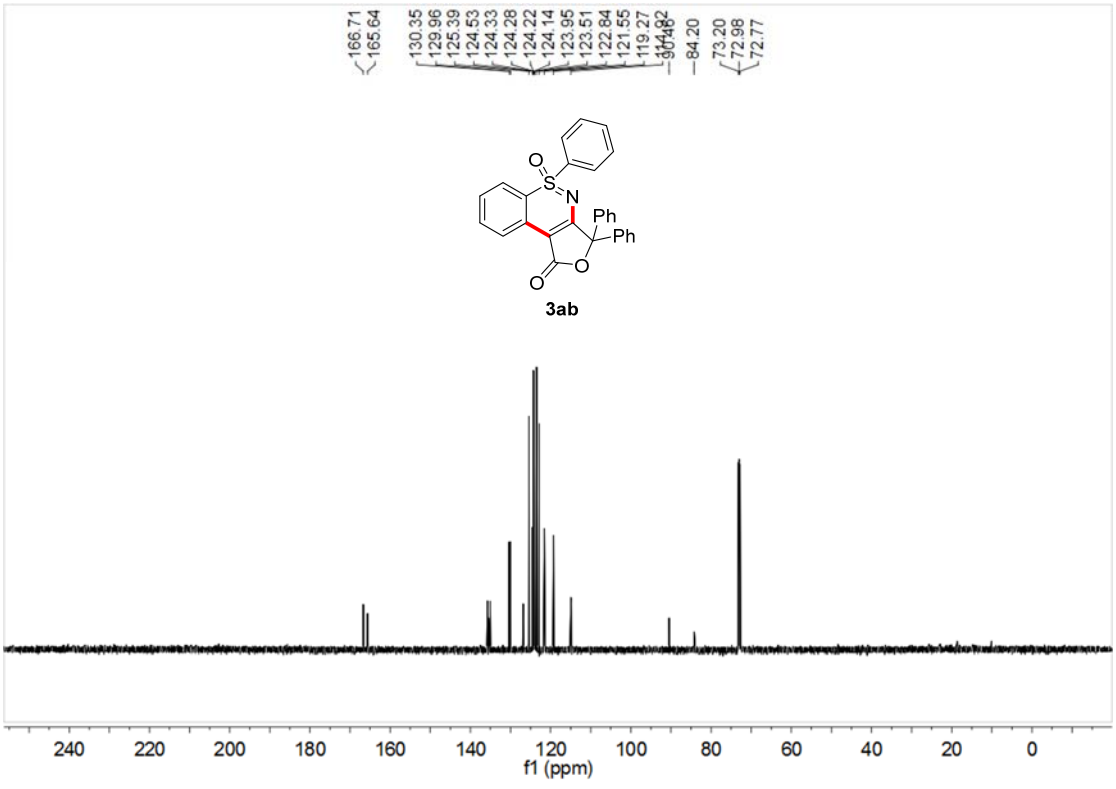

174.03
169.72
164.11
141.13
139.27
134.32
129.81
129.20
127.67
117.54
110.32
104.11
92.83
83.24
77.34
77.02
76.71
56.02
25.06
24.80
Cl
O
S
N
MeO
O
O
3qa'
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.002
6.929
6.913
3.939
Cl
O
S
N
Hb
NOE
Ha3CO
Hc
O
O
NOE
3qa'
noe of Hc at 8.00 ppm
noe of Hb at 6.92 ppm
irraditation of Ha at 3.94 ppm
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

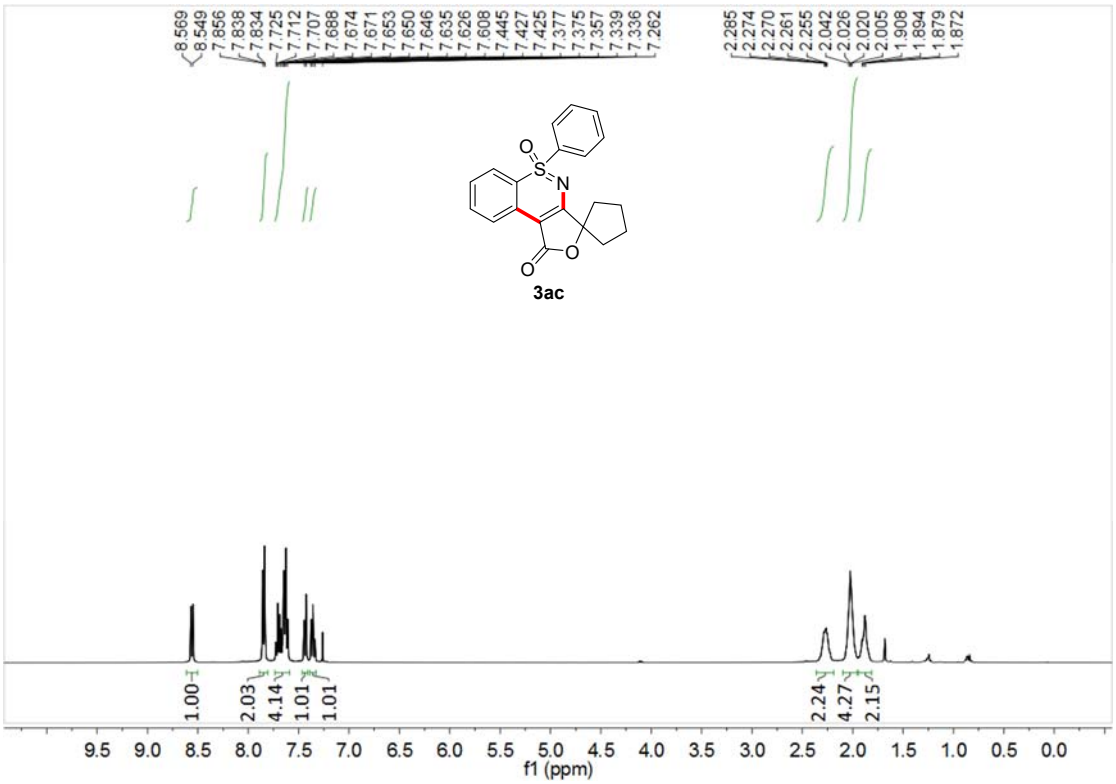

8.650
8.648
8.630
8.627
7.708
7.705
7.691
7.687
7.684
7.670
7.667
7.663
7.660
7.657
7.653
7.649
7.643
7.639
7.634
7.629
7.623
7.619
7.615
7.610
7.607
7.604
7.543
7.531
7.525
7.522
7.518
7.503
7.492
7.488
7.471
7.468
7.418
7.415
7.400
7.397
7.394
7.387
7.380
7.376
7.372
7.365
7.360
7.357
7.350
7.345
7.339
7.336
7.331
7.327
7.323
7.319
7.315
7.311
7.262
O
S
N
Ph
Ph
O
O

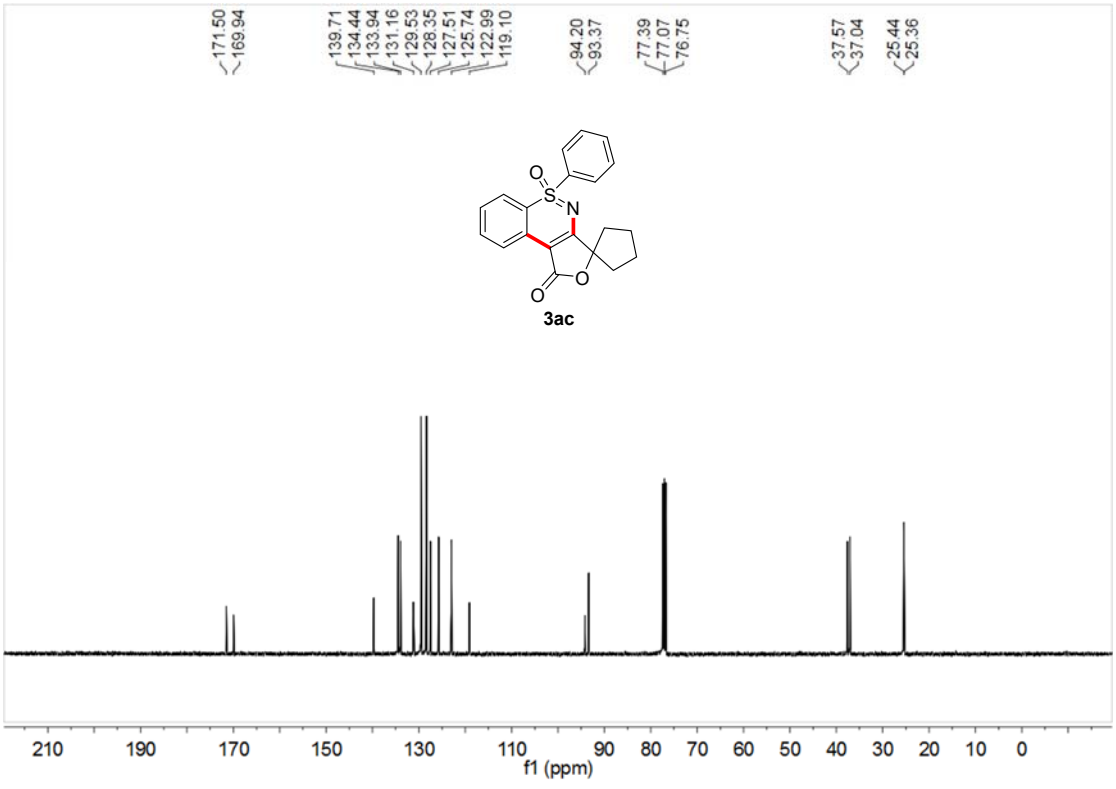
3ab

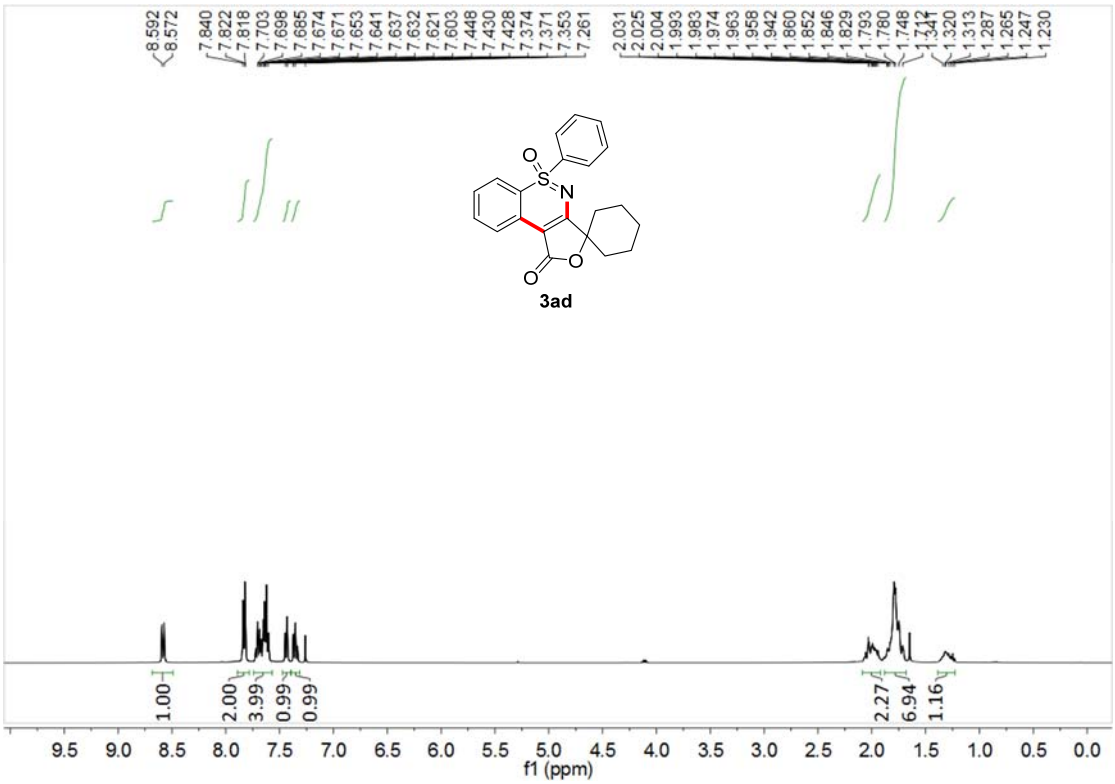

1.00
8.29
3.16
7.25
f1 (ppm)

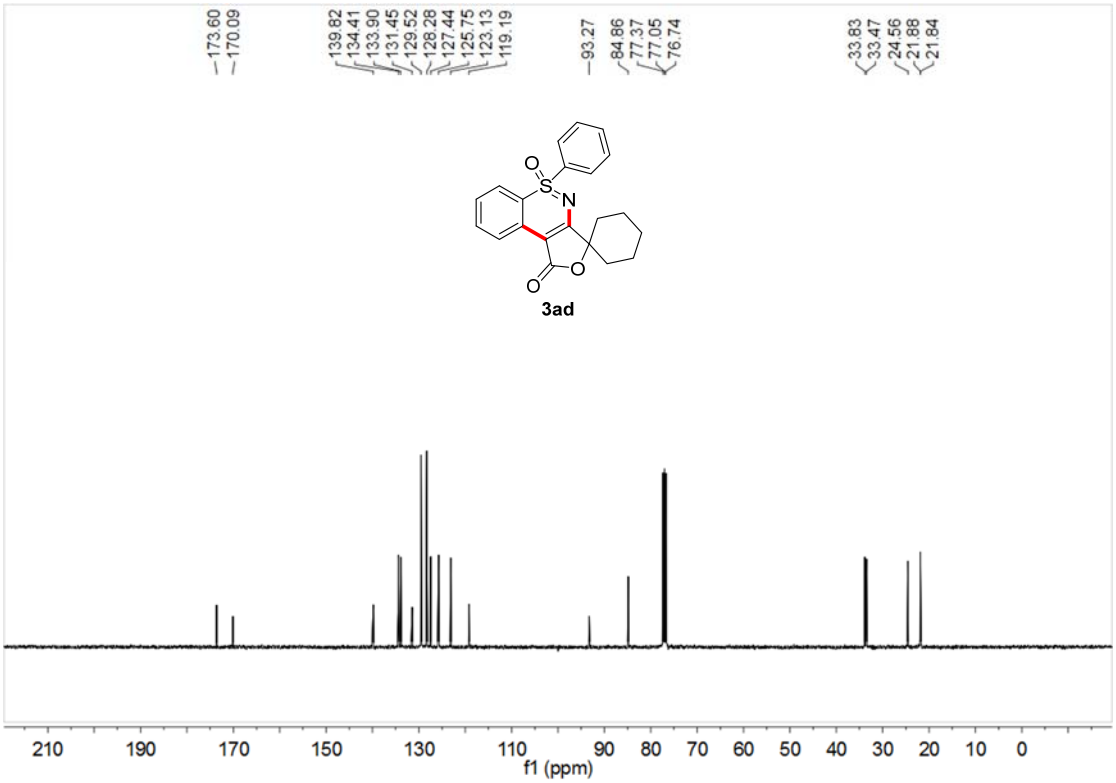

166.71
165.64
130.35
129.96
125.39
124.53
124.33
124.28
124.22
124.14
123.95
123.51
122.84
121.55
119.27
84.20
73.20
72.98
72.77
O
S
N
Ph
Ph
O
O
f1 (ppm)

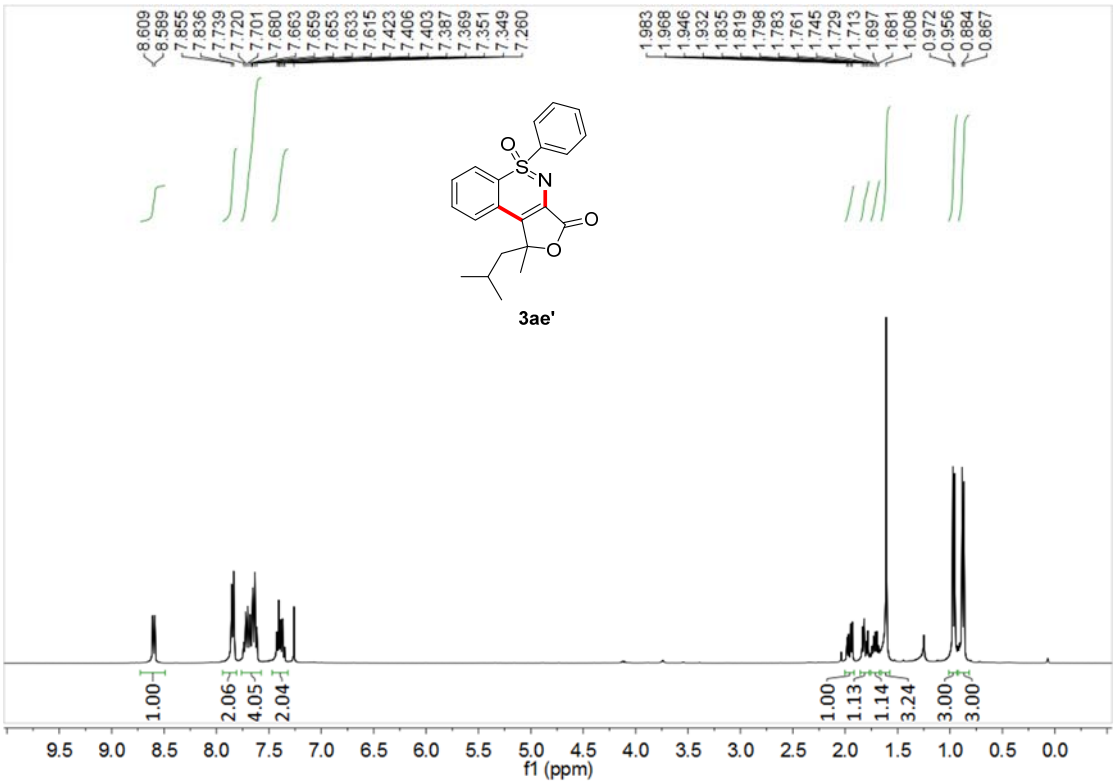
3ab

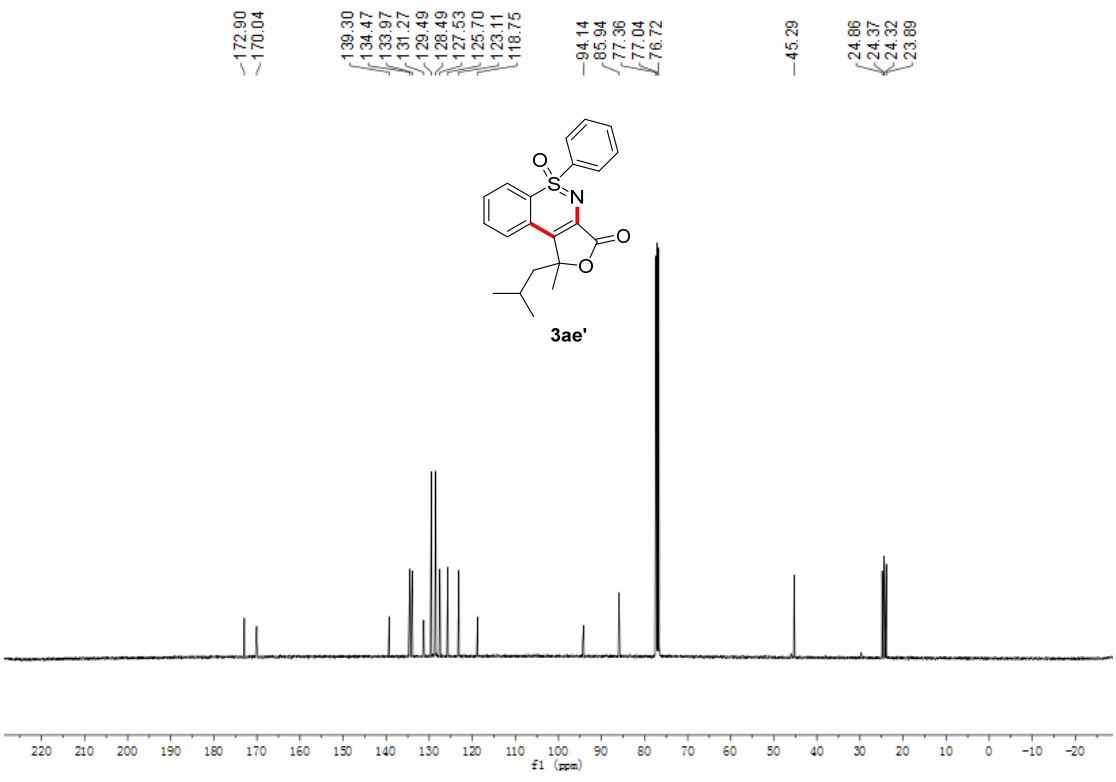

8.569
8.549
7.856
7.838
7.834
7.725
7.712
7.707
7.688
7.674
7.671
7.653
7.650
7.646
7.635
7.626
7.608
7.445
7.427
7.425
7.377
7.375
7.357
7.339
7.336
7.262
2.285
2.274
2.270
2.261
2.255
2.042
2.026
2.020
2.005
1.908
1.894
1.879
1.872
O
S
N
O
O
3ac
1.00
2.03
4.14
1.01
1.01
2.24
4.27
2.15
9.5 9.0 8.5 8.0 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)

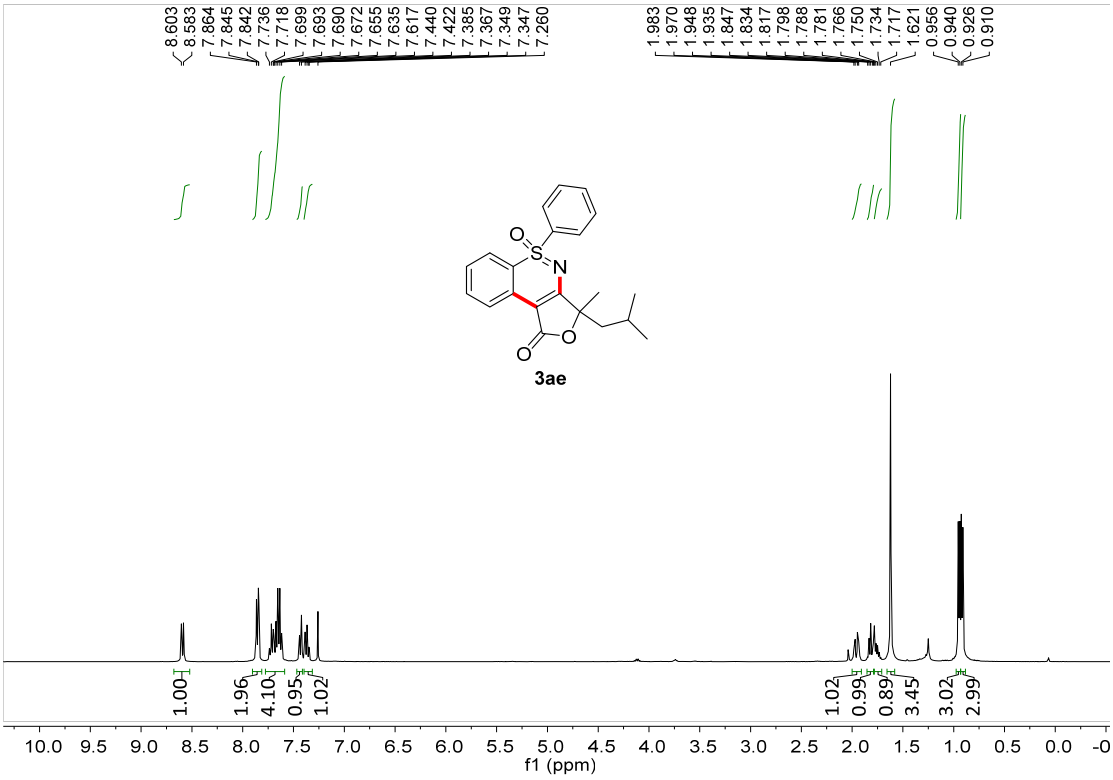

171.50
169.94
139.71
134.44
133.94
131.16
129.53
128.35
127.51
125.74
122.99
119.10
94.20
93.37
77.39
77.07
76.75
37.57
37.04
25.44
25.36
O
S
N
O
O
3ac
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

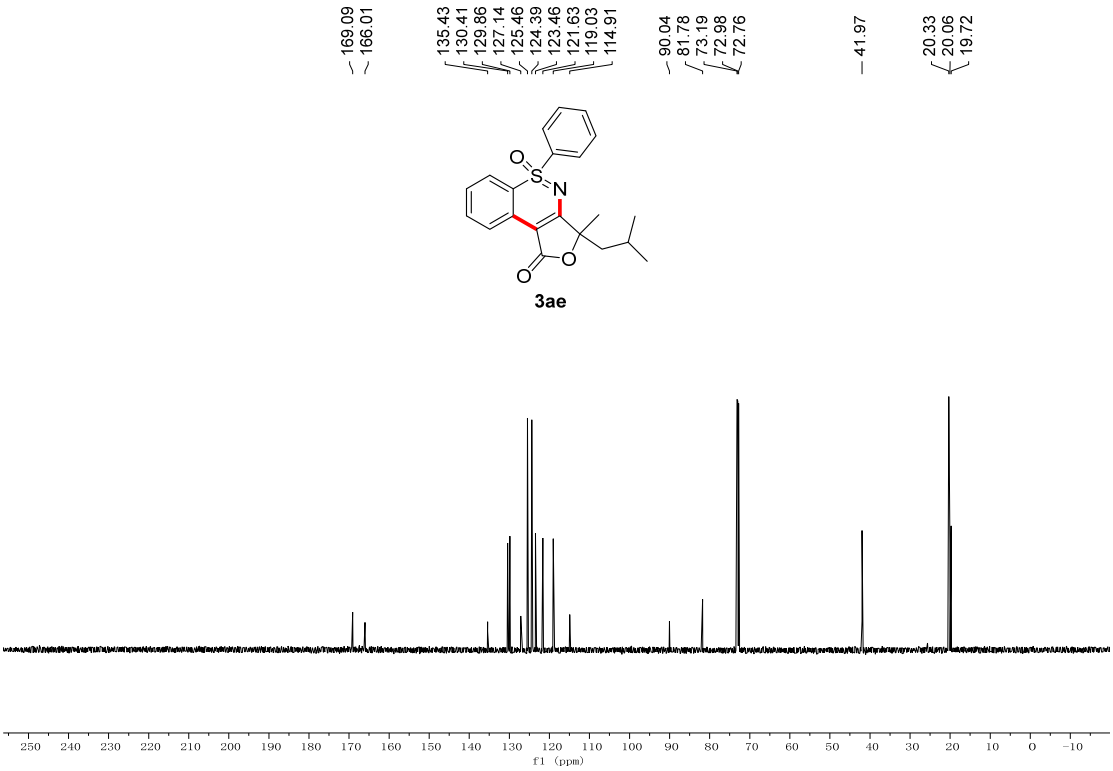

8.592
8.572
7.840
7.822
7.818
7.703
7.698
7.685
7.674
7.671
7.653
7.641
7.637
7.632
7.621
7.603
7.448
7.430
7.428
7.374
7.371
7.353
7.261
2.031
2.025
2.004
1.993
1.983
1.974
1.963
1.958
1.942
1.860
1.852
1.846
1.829
1.793
1.780
1.748
1.712
1.341
1.320
1.313
1.287
1.265
1.247
1.230
O
S
N
O
O
3ad
1.00
2.00
3.99
0.99
0.99
2.27
6.94
1.16
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)

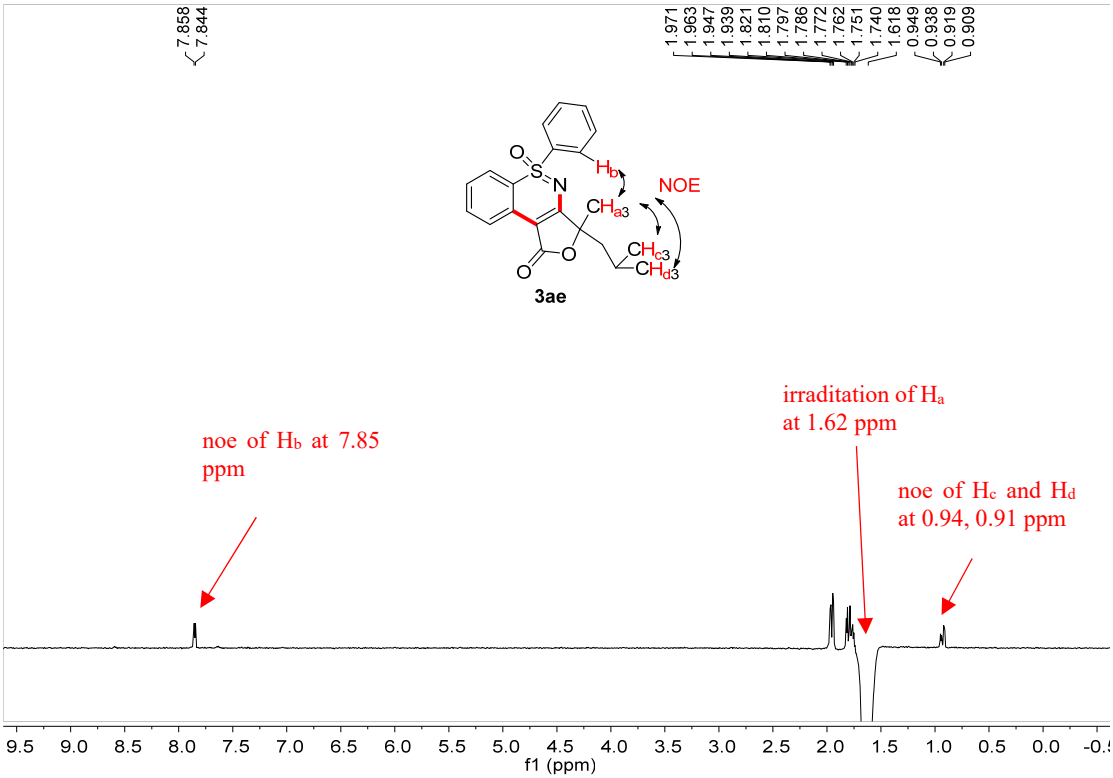

173.60
170.09
139.82
134.41
133.90
131.45
129.52
128.28
127.44
125.75
123.13
119.19
93.27
84.86
77.37
77.05
76.74
33.83
33.47
24.56
21.88
21.84
O
S
N
O
O
3ad
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

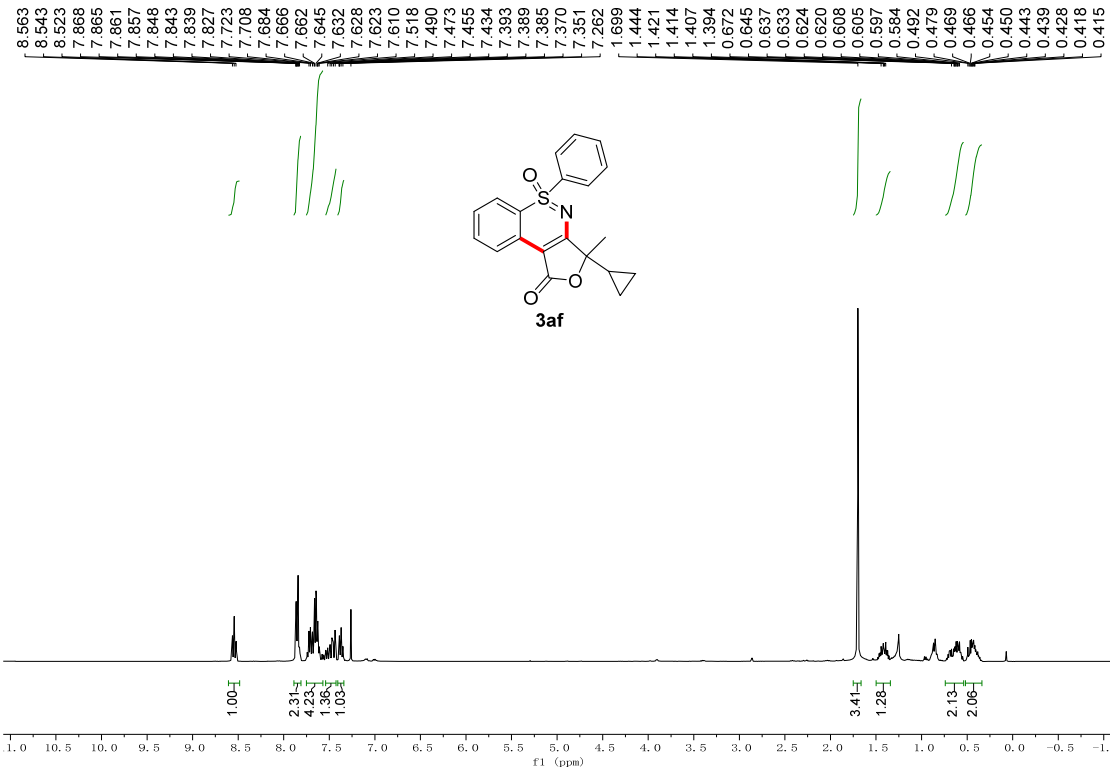

8.609
8.589
7.855
7.836
7.739
7.720
7.701
7.680
7.663
7.659
7.653
7.633
7.615
7.423
7.406
7.403
7.387
7.369
7.351
7.349
7.260
1.983
1.968
1.946
1.932
1.835
1.819
1.798
1.783
1.761
1.745
1.729
1.713
1.697
1.681
1.608
0.972
0.956
0.884
0.867
O
S
N
O
O
3ae'
1.00
2.06
4.05
2.04
1.00
1.13
1.14
3.24
3.00
3.00
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)

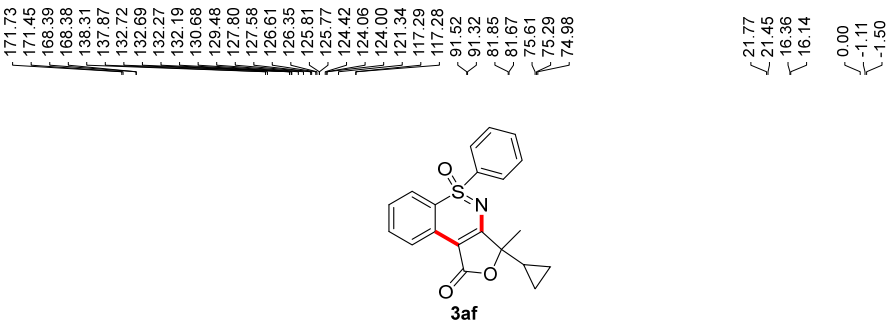

172.90
170.04
139.30
134.47
133.97
131.27
129.49
128.49
127.53
125.70
123.11
118.75
94.14
85.94
77.36
77.04
76.72
45.29
24.86
24.37
24.32
23.89
O
S
N
O
O
3ae'
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

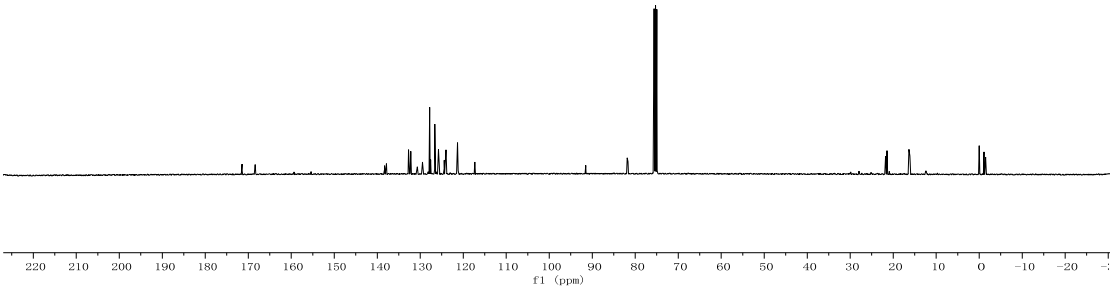

8.603
8.583
7.864
7.845
7.842
7.736
7.718
7.699
7.693
7.690
7.672
7.655
7.635
7.617
7.440
7.422
7.385
7.367
7.349
7.347
7.260
1.983
1.970
1.948
1.935
1.847
1.834
1.817
1.798
1.788
1.781
1.766
1.750
1.734
1.717
1.621
0.956
0.940
0.926
0.910
O
S
N
O
O
3ae
1.00
1.96
4.10
0.95
1.02
1.02
0.99
0.89
3.45
3.02
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

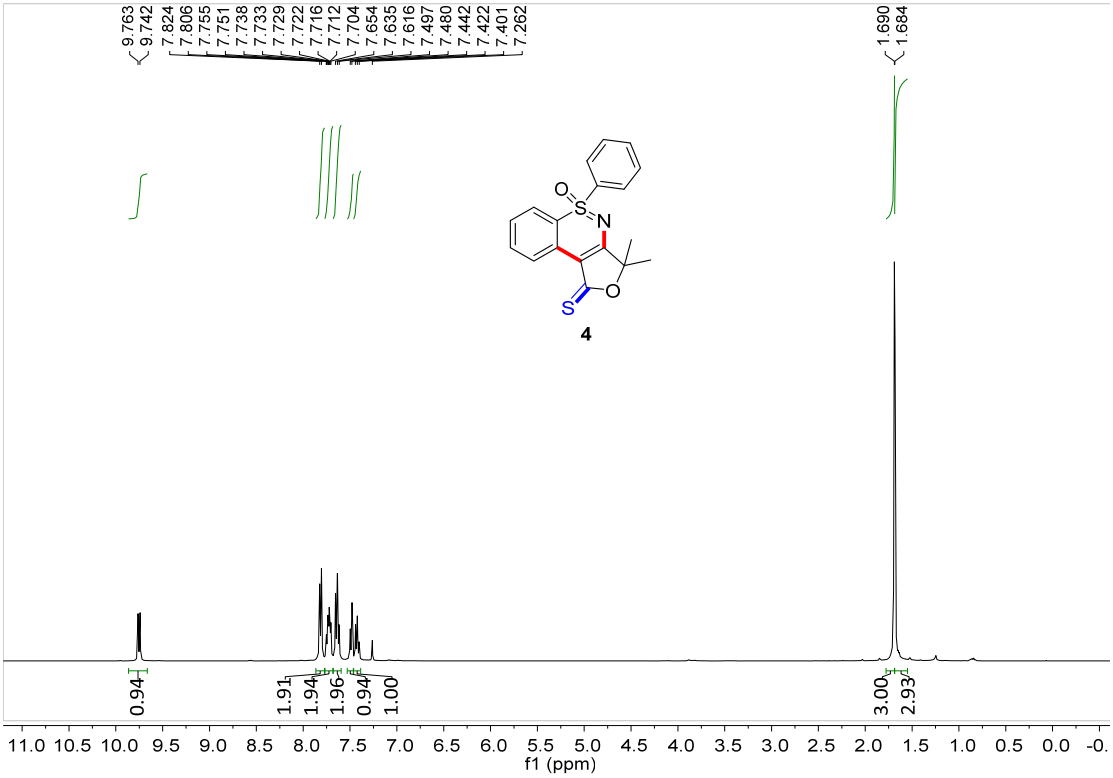

169.09
166.01
135.43
130.41
129.86
127.14
125.46
124.39
123.46
121.63
119.03
114.91
90.04
81.78
73.19
72.98
72.76
41.97
20.33
20.06
19.72
O
S
N
O
O
3ae
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

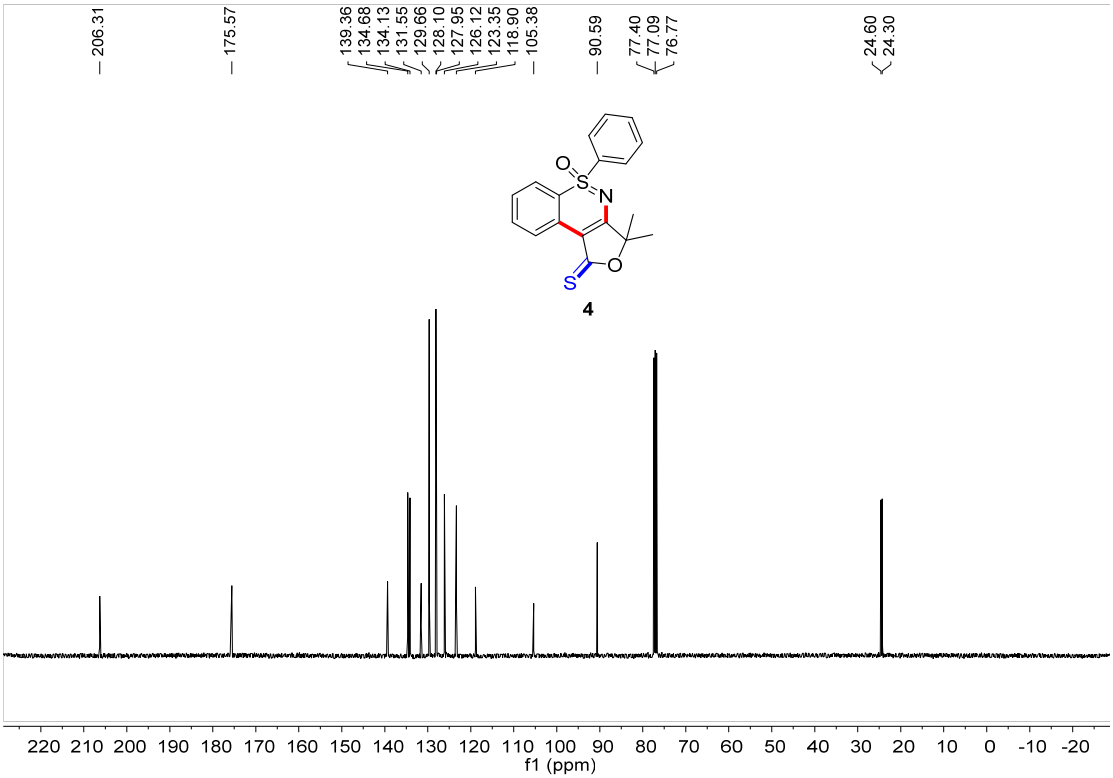

7.858
7.844
1.971
1.963
1.947
1.939
1.821
1.810
1.797
1.786
1.772
1.762
1.751
1.740
1.618
0.949
0.938
0.919
0.909
Hb
NOE
CHa3
CHc3
CHd3
3ae
irraditation of Ha
at 1.62 ppm
noe of Hb at 7.85
ppm
noe of Hc and Hd
at 0.94, 0.91 ppm
f1 (ppm)

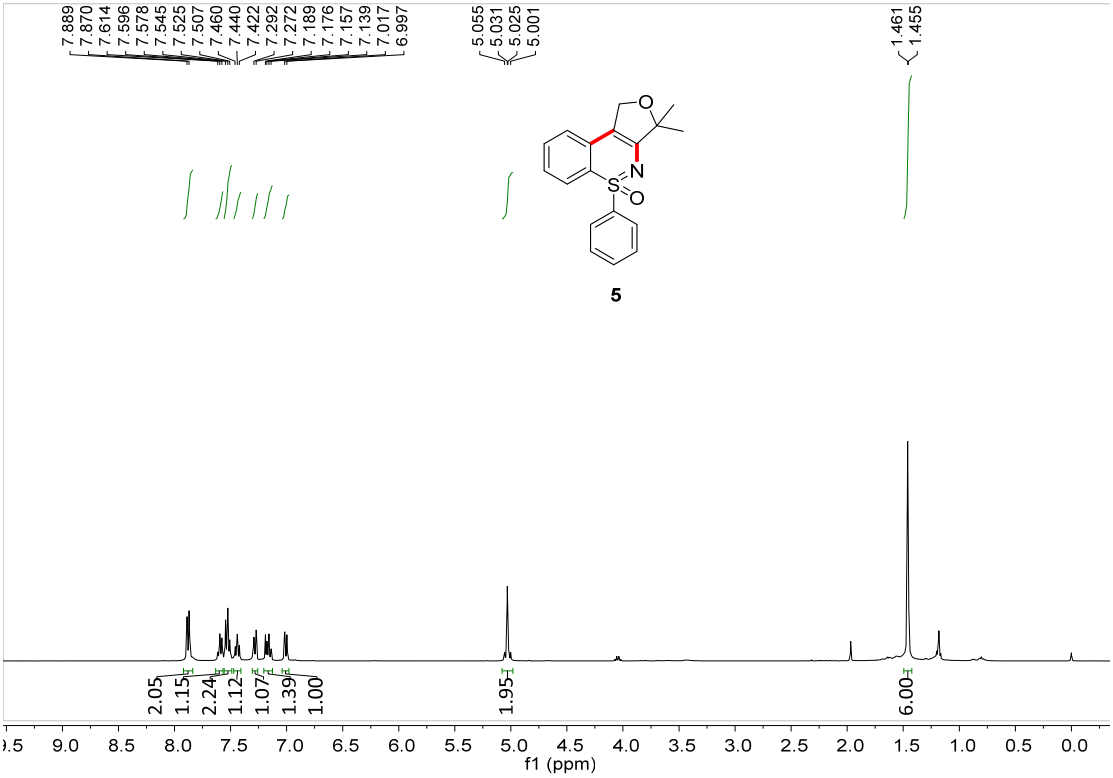

8.563
8.543
8.523
7.868
7.865
7.861
7.857
7.848
7.843
7.839
7.827
7.723
7.708
7.684
7.666
7.662
7.645
7.632
7.628
7.623
7.610
7.518
7.490
7.473
7.455
7.434
7.393
7.389
7.385
7.370
7.351
7.262
1.699
1.444
1.421
1.414
1.407
1.394
0.672
0.645
0.637
0.633
0.624
0.620
0.608
0.605
0.597
0.584
0.492
0.479
0.469
0.466
0.454
0.450
0.443
0.439
0.428
0.418
0.415
3af
1.00
2.31
4.23
1.36
1.03
3.41
1.28
2.13
2.06
f1 (ppm)

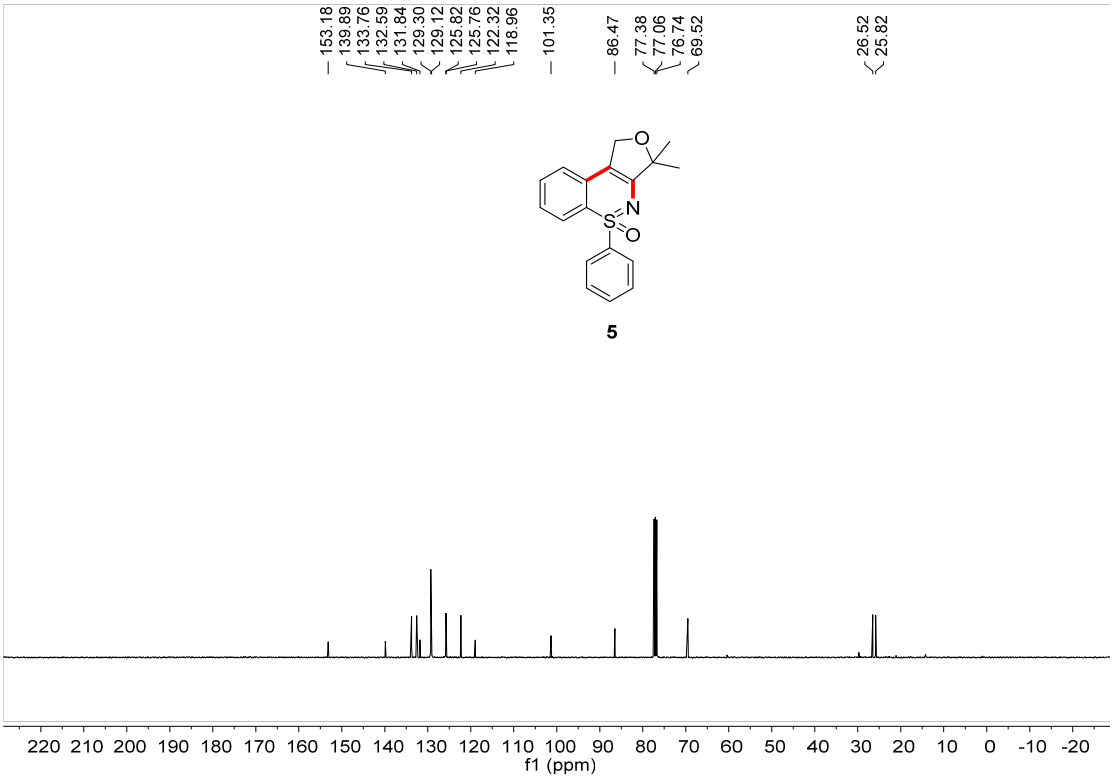

171.73
171.45
168.39
168.38
138.31
137.87
132.72
132.69
132.27
132.19
130.68
129.48
127.80
127.58
126.61
126.35
125.81
125.77
124.42
124.06
124.00
121.34
117.29
117.28
91.52
91.32
81.85
81.67
75.61
75.29
74.98
21.77
21.45
16.36
16.14
0.00
-1.11
-1.50
O
S
N
O
O
3af


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)


9.763
9.742
7.824
7.806
7.755
7.751
7.738
7.733
7.729
7.722
7.716
7.712
7.704
7.654
7.635
7.616
7.497
7.480
7.442
7.422
7.401
7.262
1.690
1.684
O
S
N
O
S
4
0.94
1.91
1.94
1.96
0.94
1.00
3.00
2.93
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


206.31
175.57
139.36
134.68
134.13
131.55
129.66
128.10
127.95
126.12
123.35
118.90
105.38
90.59
77.40
77.09
76.77
24.60
24.30
O
S
N
O
S
4
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.889
7.870
7.614
7.596
7.578
7.545
7.525
7.507
7.460
7.440
7.422
7.292
7.272
7.189
7.176
7.157
7.139
7.017
6.997
5.055
5.031
5.025
5.001
1.461
1.455
O
N
S
O
5
2.05
1.15
2.24
1.12
1.07
1.39
1.00
1.95
6.00
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)


153.18
139.89
133.76
132.59
131.84
129.30
129.12
125.82
125.76
122.32
118.96
101.35
86.47
77.38
77.06
76.74
69.52
26.52
25.82
O
N
S
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

5