Supplementary Information

Brønsted Base-Catalyzed Assembly of Sulfochromeno[4,3-*b*]Pyrrolidines via Tandem [3+2] Cycloaddition-SuFEx Click Reaction of Ethenesulfonyl Fluorides and *o*-Hydroxyaryl Azomethines

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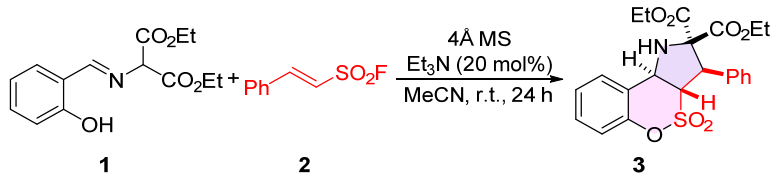
Table of Contents

1. General information.

Unless otherwise indicated, all reactions were conducted under air atmosphere in oven-dried glassware with magnetic stirring bar. All other chemicals were obtained from commercial supplies and used as received without any further purification. *β*-aryl-substituted ethenesulfonyl fluoride[1], *o*-hydroxy aromatic aldimine[2], glycine esters adlmines[3], fluorinated phenoxo-imine[4] and arylideneaminoacetonitriles[5] were prepared according to literature procedures. Column chromatograph was performed with silica gel (200~300 mesh) and analytical TLC on silica gel 60-F_{254}. ^{1}H, ^{13}C, ^{19}F NMR spectras were recorded on a Bruker AVANCE III spectrometer (400 MHz, 100 MHz and 376 MHz, respectively), Chemical shifts are reported parts per million (ppm) referenced to Chloroform-*d* (δ 7.26 ppm), tetramethylsilane (TMS, δ 0.00 ppm) for ^{1}H, ^{13}C and ^{19}F NMR. High-resolution mass spectra (HRMS) were obtained on a Q Exactive mass spectrometry and a LTQ Orbitrap XL mass spectrometry equipped with an APCI source from Thermo Scientific. X-Ray diffraction study for product **3a, 3af, 3am, 4a** and **9a** were carried out on Bruker D8 VENTURE photon II diffractometer with Iμs 3.0 microfocus X-ray source using APEX III program. Melting points were recorded on INESA SGW X-4. Infrared absorption spectrum (IR) was recorded on Bruker vertex 70V using potassium bromide (KBr) as tabletting.

2. Synthesis of products.

2.1 Synthesis of sulfochromeno[4,3-*b*]pyrrolidines (3).



1 **2** **3**

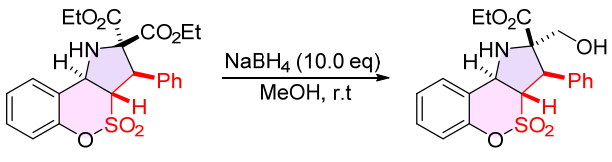
To a 10 mL reaction tube equipped with a magnetic stir bar was taken the *o*-hydroxyaryl azomethines **1** (0.20 mmol), *β*-arylethenesulfonyl fluorides **2** (0.20 mmol), 4Å MS (200 mg), MeCN (2.0 mL) and Et_3N (0.04 mmol) were added in turn to the reaction tube. The reaction mixture was stirred at ambient temperature for 24 h. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 7 : 1 (v / v)) on silica gel to give the desired product **3**.

2.2 Gram-Scale Reaction for the sulfochromeno[4,3-*b*]pyrrolidines (3a, 3w).

1a or 1w, 3.0 mmol **2a**, 3.0 mmol **3a or 3w**

To a 50 mL reaction tube equipped with a magnetic stir bar was taken the *o*-hydroxyaryl azomethines **1a/1w** (3.0 mmol), *β*-phenylethenesulfonyl fluoride **2a** (3.0 mmol), 4Å MS (3.0 g), MeCN (10.0 mL) and Et_3N (0.6 mmol) were added in turn to the reaction tube. The reaction mixture was stirred at ambient temperature for 48 h. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 7 : 1 (v / v)) on silica gel to give the desired product **3a**/**3w**.

2.4 Procedure for compound 4a.

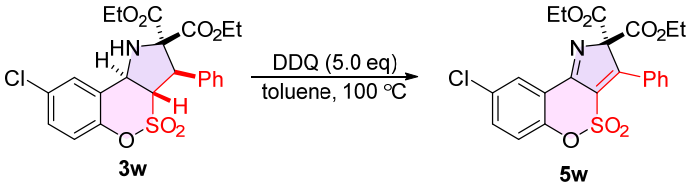


3a **4a**

To a 10 mL reaction tube equipped with a magnetic stir bar was taken the **3a** (89.0 mg, 0.2 mmol) and MeOH (2.0 mL), and $NaBH_4$ (75.6 mg, 2.0 mmol) were added in

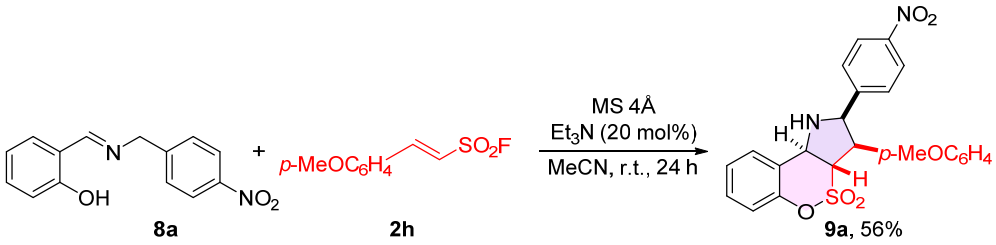
portions to the reaction tube. The reaction mixture was stirred 4 h until the complete consumption of **3a**. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 1 : 1 (v / v)) on silica gel to give the desired product **4a** (White solid, 75%, 60.5 mg).

2.3 Procedure for compound 5w.



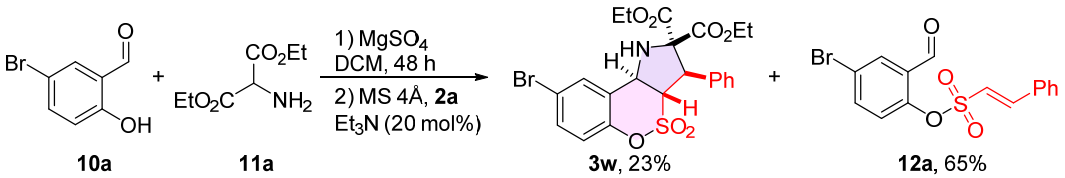
To a 10 mL reaction tube equipped with a magnetic stir bar was taken the **3w** (96.0 mg, 0.2 mmol) and DDQ (227.0 mg, 1.0 mmol), 2.0 mL of toluene was added to the tube and heated to 100 ℃ in a heating block. The reaction mixture was stirred 24 h until the complete consumption of **3w**. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 5 : 1 (v / v)) on silica gel to give the desired product **5w** (Red solid, 70%, 66.6 mg).

2.5 Procedure for compound 9a.



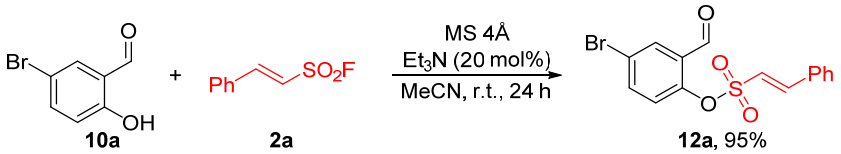
To a 10 mL reaction tube equipped with a magnetic stir bar was taken the *o*-hydroxyaryl azomethine **8a** (0.20 mmol), *β*-aryl ethenesulfonyl fluoride **2h** (0.20 mmol), 4Å MS (200 mg), MeCN (2.0 mL) and Et_3N (0.04 mmol) were added in turn to the reaction tube. The reaction mixture was stirred at ambient temperature for 24 h. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / dichloromethane = 1 : 2 (v / v)) on silica gel to give the desired product **9a**.

2.6 Procedure for “one pot” experiment.



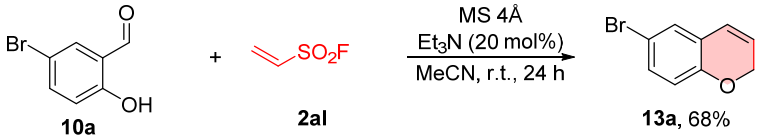
To a solution of salicylaldehyde **10a** (0.4 mmol, 2.0 equiv.) in DCM (2 mL), was added the diethyl aminomalonate **11a** (0.4 mmol, 2.0 equiv.) and $MgSO_4$ (2.0 mmol, 10.0 equiv.). The *β*-phenylethenesulfonyl fluoride **2a** (0.2 mmol, 1.0 equiv.), 4Å MS (200 mg) and Et_3N (0.04 mmol) were added after the resulting mixture was stirred 48 h at RT. After the full conversion of the *β*-phenylethenesulfonyl fluoride **2a** the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (Petroleum ether / ethyl acetate = 10 : 1 to 5 : 1 (v / v)) to furnish the corresponding products.

2.7 Procedure for compound 12a.



To a 10 mL reaction tube equipped with a magnetic stir bar was taken the salicylaldehyde **10a** (0.20 mmol), *β*-phenylethenesulfonyl fluoride **2a** (0.20 mmol), 4Å MS (200 mg), MeCN (2.0 mL) and Et_3N (0.04 mmol) were added in turn to the reaction tube. The reaction mixture was stirred at ambient temperature for 24 h. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 10 : 1 (v / v)) on silica gel to give the desired product **12a**.

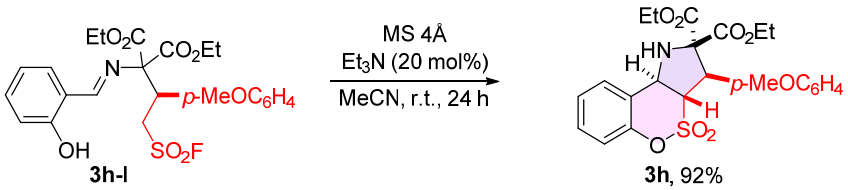
2.8 Procedure for compound 13a.



To a 10 mL reaction tube equipped with a magnetic stir bar was taken the salicylaldehyde **10a** (0.20 mmol), 4Å MS (200 mg), MeCN (2.0 mL) and Et_3N (0.04 mmol) were added in turn to the reaction tube, then ethenesulfonyl fluoride **2al** (0.20 mmol, 18 *μ*L) is added dropwise. The reaction mixture was stirred at ambient

temperature for 24 h. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 30 : 1 (v / v)) on silica gel to give the desired product **13a**.

2.9 Procedure for intermediates to compound 3h.



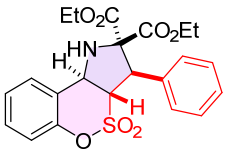
To a 10 mL reaction tube equipped with a magnetic stir bar was taken the compound **3h-I** (0.10 mmol), 4Å MS (100 mg), MeCN (1.0 mL) and Et_3N (0.02 mmol) were added in turn to the reaction tube. The reaction mixture was stirred at ambient temperature for 24 h. When the reaction was finished (monitored by TLC). The crude products were purified by column chromatography (Petroleum ether / ethyl acetate = 7 : 1 (v / v)) on silica gel to give the desired product **3h**.

2.10 Procedure for ^{19}F NMR experiments.

To a 10 mL reaction tube equipped with a magnetic stir bar was taken MeCN (2.0 mL) at 0 ℃, *o*-hydroxyaryl azomethine **1a** (0.20 mmol), *β*-arylethenesulfonyl fluoride **2h** (0.20 mmol), 4Å MS (200 mg) and Et_3N (0.04 mmol) were added in turn to the reaction tube. The reaction mixture was stirred at 0 ℃ for 5 min, aspirate 0.5 mL of the reaction solution for NMR analysis. When the reaction was stirring for 30 min, aspirate 0.5 mL of the reaction solution for NMR analysis. The reaction mixture was stirred at ambient temperature. When the reaction was finished (monitored by TLC, about 24 h), aspirate 0.5 mL of the reaction solution for NMR analysis.

3. Characterization data of products.

diethyl 3-phenyl-1, 3, 3a, 9b-tetrahydro-2H-benzo [5, 6] [1,2] oxathiino [4, 3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3a)



3a, 95%

White solid, 84.6 mg, 95% yield, m.p. 182.1 – 182.4 °C.

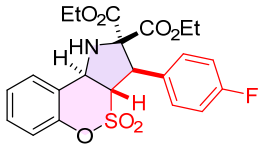
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.54 (m, 1H), 7.45 – 7.37 (m, 1H), 7.36 – 7.27 (m, 6H), 7.14 (dd, *J* = 8.4, 0.8 Hz, 1H), 5.00 (d, *J* = 12.4 Hz, 1H), 4.59 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.39 (m, 1H), 4.35 – 4.24 (m, 1H), 3.87 – 3.77 (m, 2H), 3.65 (s, 1H), 3.39 – 3.29 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 168.8, 150.7, 133.9, 130.2, 128.7, 128.6, 128.4, 125.9, 125.8, 123.7, 118.2, 64.7, 62.9, 62.9, 60.7, 51.5, 14.1, 13.3.

IR (KBr, thin film): 3630, 2925, 2360, 2345, 1729, 1700, 1653, 1373, 1163, 764 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{22}H_{24}NO_7S$ $[M+H]^+$: 466.1268, found 466.1272.

diethyl 3-(4-fluorophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3b)



3b, 93%

White solid, 86.2 mg, 93% yield, m.p. 201.1 – 201.4 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.36 – 7.31 (m, 2H), 7.30 – 7.25 (m, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 7.02 (t, *J* = 8.6 Hz, 2H), 4.97 (d, *J* = 12.4 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.37 (m, 1H), 4.34 – 4.22 (m, 1H), 3.91 – 3.81 (m, 1H), 3.76 (t, *J* = 12.0 Hz, 1H), 3.60 – 3.00 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.80 (t, *J* = 7.2 Hz, 3H).

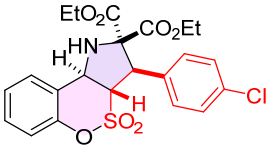
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 168.7, 162.8 (d, *J* = 246.0 Hz), 150.7, 130.3, 130.2, 129.6 (d, *J* = 3.0 Hz), 125.9, 125.81, 123.6, 118.2, 115.6 (d, *J* = 21.0 Hz), 64.6, 62.9, 60.6, 50.7, 14.1, 13.4.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -113.33.

IR (KBr,thin film): 3649, 3546, 2361, 2342, 1734, 1700, 1653, 1457, 1395, 668 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{22}H_{23}FNO_7S$ $[M+H]^+$: 464.1174, found 464.1180.

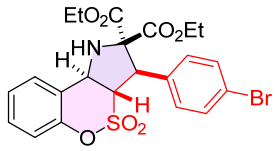
diethyl 3-(4-chlorophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3c)



3c, 96%

White solid, 92.1 mg, 96% yield, m.p. 220.1 – 220.4 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.34 – 7.25 (m, 5H), 7.13 (d, *J* = 8.4 Hz, 1H), 4.95 (d, *J* = 12.4 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.37 (m, 1H), 4.34 – 4.22 (m, 1H), 3.90 – 3.80 (m, 1H), 3.76 (t, *J* = 12.0 Hz, 1H), 3.59 – 3.26 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.80 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.6, 150.6, 134.5, 132.4, 130.3, 129.8, 128.8, 125.9, 125.8, 123.5, 118.2, 64.4, 63.0, 60.7, 50.8, 14.0, 13.4.
IR (KBr, thin film): 3732, 2359, 2342, 1700, 1683, 1653, 1558, 1521, 677, 668 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{23}ClNO_7S$ $[M+H]^+$: 480.0878, found 480.0882.

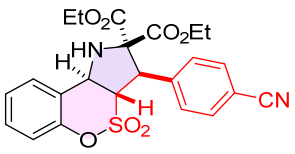
diethyl 3-(4-bromophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-b] pyrrole-2,2-dicarboxylate 4,4-dioxide (3d)



3d, 84%

White solid, 88.1 mg, 84% yield, m.p. 177.6 – 178.2 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.2 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.31 – 7.20 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 1H), 4.93 (d, *J* = 12.0 Hz, 1H), 4.57 (d, *J* = 11.2 Hz, 1H), 4.48 – 4.36 (m, 1H), 4.34 – 4.22 (m, 1H), 3.90 – 3.80 (m, 1H), 3.76 (t, *J* = 12.0 Hz, 1H), 3.51 – 2.89 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.80 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.6, 133.0, 131.8, 130.3, 130.1, 125.9, 125.8, 123.5, 122.6, 118.2, 64.3, 63.0, 60.7, 50.8, 14.0.
IR (KBr,thin film): 2984, 2908, 2359, 1729, 1418, 1386, 1303, 1211, 1162, 862 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{24}BrNO_7S$ $[M+H]^+$: 524.0373, found 524.0378.

diethyl 3-(4-cyanophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3e)

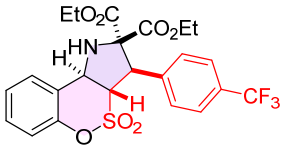


3e, 97%

White solid, 91.2 mg, 97% yield, m.p. 260.1 – 260.5 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.38 (m, 1H), 7.33 – 7.27 (m, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 5.01 (d, *J* = 12.4 Hz, 1H), 4.59 (d, *J* = 11.6 Hz, 1H), 4.50 – 4.39 (m, 1H), 4.35 – 4.22 (m, 1H), 3.91 – 3.74 (m, 2H), 3.65 (s, 1H), 3.46 – 3.33 (m, 1H), 1.37 – 1.29 (m, 3H), 0.79 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.2, 168.3, 150.6, 139.4, 132.3, 130.4, 129.4, 126.0, 125.8, 123.2, 118.2, 112.4, 64.1, 63.2, 60.8, 51.1, 14.0, 13.4.

IR (KBr, thin film): 3676, 3630, 2368, 2344, 1734, 1700, 1653, 1559, 1419, 760 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{23}N_2O_7S$ $[M+H]^+$: 471.1221, found 471.1224.

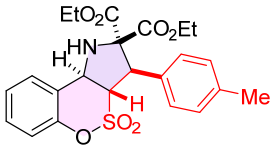
diethyl 3-(4-(trifluoromethyl)phenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3f)



3f, 92%

White solid, 94.4 mg, 92% yield, m.p. 186.2 – 186.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.54 (m, 3H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.25 (m, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 5.04 (d, *J* = 12.0 Hz, 1H), 4.60 (d, *J* = 11.6 Hz, 1H), 4.50 – 4.39 (m, 1H), 4.35 – 4.23 (m, 1H), 3.88 – 3.76 (m, 2H), 3.74 – 3.45 (m, 1H), 3.44 – 3.32 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.72 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.5, 150.7, 138.1, 130.9 (q, *J* = 33.0 Hz), 130.4, 129.00, 126.0, 125.9, 125.6 (q, *J* = 4.0 Hz), 124.0 (q, *J* = 271.0 Hz), 123.4, 118.3, 64.3, 63.1, 63.1, 60.8, 51.1, 14.1, 13.2.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.82.
IR (KBr,thin film): 3823, 3662, 2922, 2391, 1730, 1692, 1125, 1052, 1033, 781 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{23}F_3NO_7S$ $[M+H]^+$: 514.1142, found 514.1148.

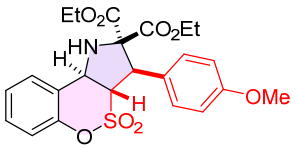
diethyl 3-(p-tolyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3g)



3g, 95%

White solid, 87.3 mg, 95% yield, m.p. 208.6 – 209.1 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.12 (d, *J* = 7.6 Hz, 3H), 4.95 (d, *J* = 12.0 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.37 (m, 1H), 4.33 – 4.21 (m, 1H), 3.88 – 3.74 (m, 2H), 3.65 – 3.15 (m, 2H), 2.31 (s, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 0.74 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 168.8, 150.7, 138.2, 130.7, 130.1, 129.3, 128.2, 125.8, 125.7, 123.7, 118.1, 64.7, 62.8, 60.6, 51.1, 21.1, 14.0, 13.2.
IR (KBr,thin film): 3641, 2391, 2349, 1728, 1532, 1386, 1370, 1213, 1162, 772 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_7S$ $[M+H]^+$: 460.1425, found 460.1431.

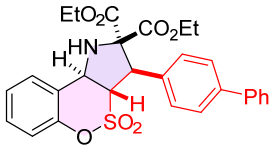
diethyl -3-(4- methoxyphenyl)-1, 3, 3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino [4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide (3h)



3h, 97%

White solid, 92.2 mg, 97% yield, m.p. 207.2 – 207.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.44 (m, 1H), 7.36 – 7.27 (m, 1H), 7.22 – 7.14 (m, 3H), 7.10 – 7.02 (m, 1H), 6.81 – 6.72 (m, 2H), 4.87 (d, *J* = 12.4 Hz, 1H), 4.49 (d, *J* = 11.6 Hz, 1H), 4.40 – 4.30 (m, 1H), 4.25 – 4.15 (m, 1H), 3.83 – 3.74 (m, 1H), 3.73 – 3.65 (m, 4H), 3.57 – 3.03 (m, 2H), 1.24 (t, *J* = 7.2 Hz, 3H), 0.72 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.6, 168.9, 159.7, 150.7, 130.2, 129.5, 125.8, 125.8, 125.7, 123.7, 118.2, 114.1, 64.7, 62.9, 62.8, 60.6, 55.4, 50.9, 14.1, 13.4.
IR (KBr, thin film): 3685, 3642, 2350, 1730, 1694, 1454, 1213, 1164, 1045, 832 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_8S$ $[M+H]^+$: 476.1374, found 476.1381.

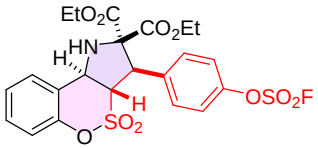
diethyl3-([1,1'-biphenyl]-4-yl)-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3i)



3i, 93%

White solid, 97.0 mg, 93% yield, m.p. 201.3 – 201.7 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.52 (m, 5H), 7.45 – 7.32 (m, 6H), 7.30 – 7.23 (m, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 5.05 (d, *J* = 12.4 Hz, 1H), 4.61 (d, *J* = 11.6 Hz, 1H), 4.50 – 4.39 (m, 1H), 4.35 – 4.24 (m, 1H), 3.88 – 3.76 (m, 2H), 3.68 – 3.31 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.72 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 168.8, 150.7, 141.4, 140.5, 132.9, 132.9, 130.2, 128.9, 128.8, 127.6, 127.3, 127.1, 125.8, 125.8, 123.6, 118.2, 76.8, 64.6, 62.9, 62.9, 60.8, 51.2, 14.1, 13.3.
IR (KBr,thin film): 3704, 3452, 2360, 2342, 1729, 1487, 1454, 1386, 1163, 776 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{28}H_{28}NO_7S$ $[M+H]^+$: 522.1581, found 522.1585.

diethyl 3-(4-((fluorosulfonyl)oxy)phenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3j)

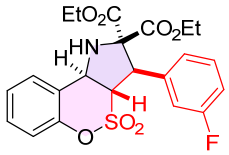


3j, 87%

White solid, 94.5 mg, 87% yield, m.p. 230.5 – 231.1 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.36 – 7.27 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 1H), 5.02 (d, *J* = 12.4 Hz, 1H), 4.59 (d, *J* = 11.2 Hz, 1H), 4.49 – 4.39 (m, 1H), 4.34 – 4.24 (m, 1H), 3.91 – 3.82 (m, 1H), 3.82 – 3.74 (m, 1H), 3.68 – 3.20 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.79 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.5, 150.6, 149.9, 135.0, 130.6, 130.4, 126.0, 125.8, 123.3, 121.3, 118.2, 77.6, 64.2, 63.2, 63.1, 60.8, 50.7, 14.0, 13.3.
^{19}F NMR (376 MHz, Chloroform-*d*) δ 43.25.
IR (KBr,thin film): 3672, 3504, 2363, 2334, 1772, 1733, 1653, 1558, 1213, 919 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{23}FNO_{10}S_2$ $[M+H]^+$: 544.0742, found 544.0749.

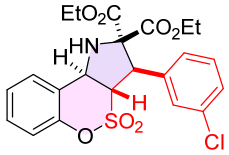
diethyl 3-(3-fluorophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3k)



3k, 90%

White solid, 83.4 mg, 90% yield, m.p. 165.2 – 165.9 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.16 – 7.07 (m, 3H), 7.05 – 6.96 (m, 1H), 4.97 (d, *J* = 12.0 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.39 (m, 1H), 4.34 – 4.24 (m, 1H), 3.91 – 3.81 (m, 1H), 3.76 (t, *J* = 12.0 Hz, 1H), 3.65 – 2.93 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.79 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.6, 162.8 (d, *J* = 245.0 Hz), 150.7, 136.4 (d, *J* = 7.0 Hz), 130.3, 130.3 (d, *J* = 8.0 Hz), 125.9, 125.8, 123.9 (d, *J* = 3.0 Hz), 123.5, 118.2, 115.9 (d, *J* = 23.0 Hz), 115.5 (d, *J* = 21.0 Hz), 64.6, 63.0, 63.0, 60.7, 51.0, 51.0, 14.1, 13.4.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -112.26.
IR (KBr,thin film): 3657, 2992, 2380, 2320, 1729, 1590, 1551, 1455, 1157, 896 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{23}FNO_7S$ $[M+H]^+$: 464.1174, found 464.1178.

diethyl 3-(3-chlorophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3l)

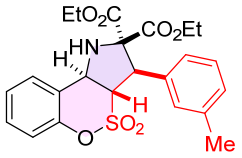


3l, 90%

White solid, 86.3 mg, 90% yield, m.p. 177.3 – 178.1 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.31 – 7.24 (m, 3H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 4.95 (d, *J* = 12.0 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.39 (m, 1H), 4.34 – 4.24 (m, 1H), 3.91 – 3.81 (m, 1H), 3.76 (t, *J* = 12.0 Hz, 1H), 3.65 – 2.99 (m, 2H), 1.33 (t, *J* = 7.2 Hz,

3H), 0.80 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.5, 150.6, 136.0, 134.6, 130.3, 130.0, 128.9, 128.7, 126.4, 125.9, 125.8, 123.5, 118.2, 64.5, 63.1, 63.0, 60.7, 51.0, 14.1, 13.3.
IR (KBr, thin film): 3637, 2391, 1729, 1405, 1300, 1200, 1162, 1033, 832, 765 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{23}ClNO_7S$ $[M+H]^+$: 480.0878, found 480.0883.

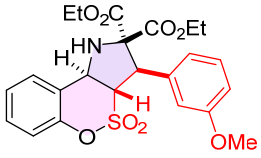
diethyl 3-(m-tolyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3m)



3m, 96%

White solid, 88.2 mg, 96% yield, m.p. 150.3 – 151.0 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 7.2 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.31 – 7.24 (m, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.16 – 7.04 (m, 4H), 4.96 (d, *J* = 12.4 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.37 (m, 1H), 4.34 – 4.23 (m, 1H), 3.86 – 3.74 (m, 2H), 3.41 – 3.32 (m, 1H), 2.32 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 168.7, 150.7, 138.3, 133.9, 130.2, 129.3, 129.2, 128.6, 125.8, 125.8, 125.2, 123.7, 118.1, 64.9, 62.9, 62.8, 60.7, 51.4, 21.4, 14.1, 13.3.
IR (KBr, thin film): 3647, 3200, 2952, 2385, 2316, 1728, 1668, 1162, 902, 772 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_7S$ $[M+H]^+$: 460.1425, found 460.1433.

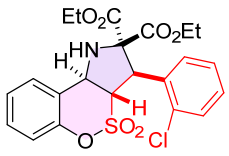
diethyl 3-(3-methoxyphenyl)-1, 3, 3a,9b-tetrahydro-2H-benzo[5, 6][1, 2]oxathiino [4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide(3n)



3n, 98%

White solid, 93.1 mg, 98% yield, m.p. 195.2 – 195.4 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.34(m, 1H), 7.31 – 7.18 (m, 2H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.93 – 6.79 (m, 3H), 4.97 (d, *J* = 12.0 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.48 – 4.37 (m, 1H), 4.34 – 4.21 (m, 1H), 3.89 – 3.73 (m, 5H), 3.66 (s, 1H), 3.46 – 3.35 (m, 1H), 1.36 – 1.29 (m, 3H), 0.77 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.7, 159.8, 150.7, 135.4, 135.4, 130.2, 129.7, 125.8, 123.6, 120.3, 118.1, 114.2, 64.8, 62.9, 60.7, 55.4, 51.4, 14.1, 13.3.
IR (KBr, thin film): 3686, 3642, 2355, 1728, 1694, 1454, 1214, 1164, 1045, 762 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_8S$ $[M+H]^+$: 476.1374, found 476.1381.

diethyl 3-(2-chlorophenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3o)



3o, 98%

White solid, 94.1 mg, 98% yield, m.p. 219.5 – 219.9 °C.

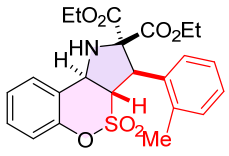
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 7.6 Hz, 1H), 7.47 – 7.36 (m, 2H), 7.30 – 7.19 (m, 3H), 7.16 – 7.07 (m, 2H), 5.67 (d, *J* = 11.6 Hz, 1H), 4.68 (d, *J* = 11.6 Hz, 1H), 4.48 – 4.36 (m, 1H), 4.36 – 4.25 (m, 1H), 3.93 – 3.83 (m, 1H), 3.80 – 3.51 (m, 2H), 3.45 – 3.30 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.81 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.6, 168.1, 150.8, 136.0, 133.5, 130.3, 130.3, 129.6, 127.6, 127.0, 125.9, 125.8, 123.6, 118.2, 66.9, 63.0, 62.7, 60.4, 47.1, 14.1, 13.4.

IR (KBr,thin film): 3676, 3195, 2360, 2341, 1700, 1559, 1539, 1506, 1037, 768 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{22}H_{23}ClNO_7S$ $[M+H]^+$: 480.0878, found 480.0884.

diethyl 3-(o-tolyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3p)



3p, 98%

White solid, 90.0 mg, 98% yield, m.p. 200.2 – 200.6 °C.

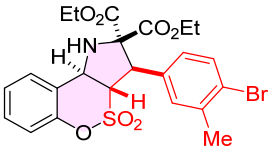
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 7.2 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.06 (m, 4H), 6.96 (d, *J* = 7.6 Hz, 1H), 5.37 (d, *J* = 11.6 Hz, 1H), 4.56 (d, *J* = 11.6 Hz, 1H), 4.48 – 4.37 (m, 1H), 4.31 – 4.21 (m, 1H), 3.88 – 3.77 (m, 1H), 3.75 – 3.41 (m, 2H), 3.38 – 3.26 (m, 1H), 2.54 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H), 0.74 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.2, 150.8, 138.3, 133.8, 131.0, 130.2, 128.2, 126.3, 125.9, 125.8, 125.7, 123.9, 118.2, 68.0, 63.0, 62.7, 60.4, 46.6, 20.3, 14.1, 13.3.

IR (KBr,thin film): 3620, 3400, 2945, 2394, 1725, 1638, 1546, 1508, 1163, 805 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_7S$ $[M+H]^+$: 460.1425, found 460.1429.

diethyl 3-(4-bromo-3-methylphenyl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3q)

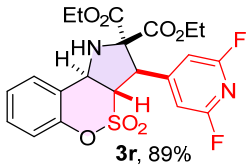


3q, 90%

White solid, 96.9 mg, 90% yield, m.p. 207.1 – 207.8 °C.

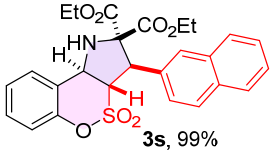
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.2 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.22 (s, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 4.91 (d, *J* = 12.4 Hz, 1H), 4.56 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.37 (m, 1H), 4.35 – 4.23 (m, 1H), 3.90 – 3.80 (m, 1H), 3.80 – 3.52 (m, 2H), 3.49 – 3.40 (m, 1H), 2.37 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.78 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.6, 150.7, 138.3, 133.2, 132.6, 131.1, 130.3, 127.1, 125.9, 125.8, 125.1, 123.6, 118.2, 64.6, 63.0, 60.7, 50.9, 23.0, 14.1, 13.3.
IR (KBr,thin film): 3683, 3557, 2399, 1726, 1530, 1513, 1386, 1162, 1033, 950 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{25}BrNO_7S$ $[M+H]^+$: 538.0530, found 538.0534.

diethyl 3-(2,6-difluoropyridin-4-yl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3r)



White solid, 85.8 mg, 89% yield, 198.2 – 198.4 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 6.88 (s, 2H), 4.95 (d, *J* = 12.0 Hz, 1H), 4.58 (d, *J* = 11.2 Hz, 1H), 4.50 – 4.41 (m, 1H), 4.37 – 4.27 (m, 1H), 4.01 – 3.91 (m, 1H), 3.79 – 3.59 (m, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.0, 168.0, 162.0 (dd, *J* = 246.0, 16.0 Hz), 153.5 (t, *J* = 8.0 Hz), 150.5, 130.5, 126.2, 125.8, 123.0, 118.3, 106.3 (dd, *J* = 27.0, 14.0 Hz), 63.7, 63.5, 63.4, 60.9, 50.25, 50.22, 50.2, 14.0, 13.5.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -67.05.
IR (KBr,thin film): 3632, 2951, 2350, 1729, 1626, 1432, 1372, 1164, 1032, 761 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{21}H_{21}F_2N_2O_7S$ $[M+H]^+$: 483.1032, found 483.1035.

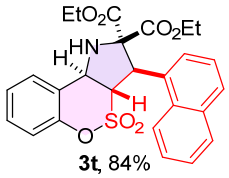
diethyl 3-(naphthalen-2-yl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3s)



White solid, 98.1 mg, 99% yield, m.p. 221.5 – 221.7 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.74 (m, 4H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.51 – 7.36 (m, 4H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 5.17 (d, *J* = 12.0 Hz, 1H), 4.65 (d, *J* = 11.6 Hz, 1H), 4.52 – 4.39 (m, 1H), 4.36 – 4.24 (m, 1H), 3.94 (t, *J* = 12.0 Hz, 1H), 3.84 – 3.46 (m, 2H), 3.21 – 3.09 (m, 1H), 1.33 (t, *J* = 7.2 Hz, 3H), 0.46 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.6, 168.8, 150.8, 133.2, 133.2, 131.3, 130.2, 128.4, 128.1, 127.8, 127.6, 126.6, 126.5, 125.9, 125.8, 123.7, 118.2, 64.9, 62.8, 60.8, 51.6, 14.1, 13.1.

IR (KBr, thin film): 3451, 2970, 2363, 2344, 1719, 1685, 1654, 1559, 1165, 768 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{26}H_{26}NO_7S$ $[M+H]^+$: 496.1424, found 496.1431.

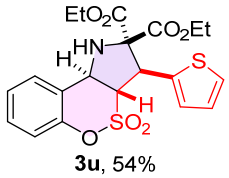
diethyl 3-(naphthalen-1-yl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3t)



3t, 84%

White solid, 84.2 mg, 84% yield, m.p. 253.1 – 253.6 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.53 (d, *J* = 8.8 Hz, 1H), 7.82 (dd, *J* = 21.2, 8.0 Hz, 2H), 7.66 – 7.57 (m, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.40 – 7.35 (m, 2H), 7.32 – 7.24 (m, 2H), 7.15 (d, *J* = 8.4 Hz, 1H), 5.97 (d, *J* = 11.6 Hz, 1H), 4.72 (d, *J* = 11.6 Hz, 1H), 4.49 – 4.38 (m, 1H), 4.35 – 4.23 (m, 1H), 3.96 (t, *J* = 11.6 Hz, 1H), 3.83 – 3.23 (m, 2H), 2.98 – 2.87 (m, 1H), 1.28 (t, *J* = 7.2 Hz, 3H), 0.24 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.2, 150.9, 134.0, 132.9, 131.6, 130.3, 129.2, 128.7, 127.0, 126.2, 126.0, 125.8, 124.9, 124.0, 124.0, 123.6, 118.3, 78.2, 67.2, 63.1, 62.4, 60.6, 45.9, 14.1, 12.7.
IR (KBr,thin film): 3851, 3839, 3283, 2360, 2337, 1748, 1717, 1374, 1162, 764 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{26}H_{26}NO_7S$ $[M+H]^+$: 496.1424, found 496.1430.

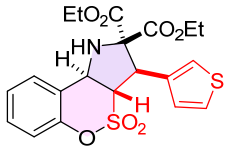
diethyl 3-(thiophen-2-yl)-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3u)



3u, 54%

White solid, 48.7 mg, 54% yield, m.p. 176.3 – 176.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.24 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.04 (d, *J* = 3.6 Hz, 1H), 6.99 – 6.93 (m, 1H), 5.17 (d, *J* = 12.0 Hz, 1H), 4.59 (d, *J* = 11.6 Hz, 1H), 4.50 – 4.39 (m, 1H), 4.38 – 4.28 (m, 1H), 3.98 – 3.86 (m, 1H), 3.76 (t, *J* = 12.0 Hz, 1H), 3.64 – 3.54 (m, 1H), 3.38 (s, 1H), 1.35 (t, *J* = 7.2 Hz, 3H), 0.89 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.7, 150.6, 136.0, 130.2, 127.1, 127.0, 126.0, 125.9, 125.7, 123.8, 118.2, 66.0, 63.2, 60.6, 47.3, 14.1, 13.5.
IR (KBr, thin film): 3637, 3585, 2360, 2342, 1702, 1457, 1223, 1185, 1092, 784 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{20}H_{22}NO_7S_2$ $[M+H]^+$: 452.0832, found 452.0837.

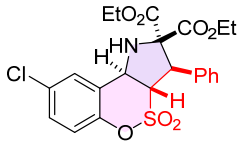
diethyl 3-(thiophen-3-yl)-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide(3v)



3v, 95%

White solid, 85.6 mg, 95% yield, m.p. 168.2 – 168.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.31 – 7.27 (m, 3H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.09 – 7.03 (m, 1H), 5.02 (d, *J* = 12.4 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.45 – 4.38 (m, 1H), 4.36 – 4.25 (m, 1H), 3.95 – 3.85 (m, 1H), 3.80 – 3.71 (m, 1H), 3.62 (s, 1H), 3.54 – 3.45 (m, 1H), 1.34 (t, *J* = 7.2 Hz, 3H), 0.89 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.6, 169.0, 150.6, 134.3, 130.1, 127.6, 125.8, 124.0, 123.8, 118.2, 65.1, 62.9, 60.6, 47.2, 14.1, 13.5.
IR (KBr, thin film): 3676, 3363, 2371, 2345, 1830, 1700, 1684, 1653, 1160, 847 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{20}H_{22}NO_7S_2$ $[M+H]^+$: 452.0832, found 452.0835.

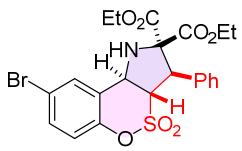
diethyl 8-chloro-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide(3w)



3w, 94%

White solid, 90.1 mg, 94% yield, m.p. 219.5 – 219.9 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J*=1.2, 1H), 7.38 – 7.29 (m, 6H), 7.08 (d, *J* = 8.8 Hz, 1H), 4.97 (d, *J* = 12.4 Hz, 1H), 4.60 – 4.51 (m, 1H), 4.49 – 4.38 (m, 1H), 4.32 – 4.22 (m, 1H), 3.87 – 3.77 (m, 2H), 3.63 (d, *J* = 12.4 Hz, 1H), 3.39 – 3.29 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.6, 149.1, 133.6, 131.3, 130.2, 128.8, 128.4, 126.0, 125.2, 119.6, 64.3, 63.0, 62.9, 60.4, 51.4, 14.1, 13.3.
IR (KBr, thin film): 3685, 3664, 2359, 1726, 1712, 1514, 1371, 1211, 1165, 802 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{23}ClNO_7S$ $[M+H]^+$: 480.0878, found 480.0885.

diethyl 8-bromo-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3x)

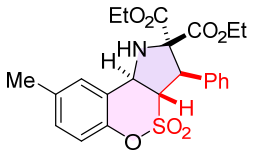


3x, 95%

White solid, 99.4 mg, 95% yield, m.p. 268.1 – 268.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 – 7.60 (m, 1H), 7.43 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.24 (s, 5H), 6.94 (d, *J* = 8.4 Hz, 1H), 4.90 (d, *J* = 12.0 Hz, 1H), 4.55 – 4.43 (m,

1H), 4.41– 4.29 (m, 1H), 4.26 – 4.14 (m, 1H), 3.80 – 3.68 (m, 2H), 3.56 (d, *J* = 11.6 Hz, 1H), 3.32 – 3.19 (m, 1H), 1.24 (t, *J* = 7.2 Hz, 3H), 0.66 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.6, 149.7, 133.6, 133.2, 128.9, 128.8, 128.6, 128.4, 125.5, 119.9, 118.7, 64.3, 63.0, 62.9, 60.4, 51.4, 14.1, 13.3.
IR (KBr, thin film): 3729, 3612, 2361, 2341, 1774, 1733, 1652, 1557, 1205, 668 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{23}BrNO_7S$ $[M+H]^+$: 524.0373, found 524.0375.

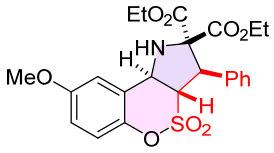
diethyl 8-methyl-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide (3y)



3y, 95%

White solid, 87.2 mg, 95% yield, m.p. 170.6 – 171.2 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.36 (m, 1H), 7.35 – 7.28 (m, 5H), 7.22 – 7.14 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 4.98 (d, *J* = 12.0 Hz, 1H), 4.59 – 4.50 (m, 1H), 4.48 – 4.38 (m, 1H), 4.34 – 4.23 (m, 1H), 3.86 – 3.73 (m, 2H), 3.64 (s, 1H), 3.39 – 3.27 (m, 1H), 2.37 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.6, 168.8, 148.7, 135.8, 134.0, 130.6, 128.7, 128.5, 126.1, 123.3, 117.9, 64.8, 62.9, 62.9, 60.8, 51.5, 20.9, 14.1, 13.3.
IR (KBr,thin film): 3774, 3642, 2396, 2282, 1726, 1713, 1653, 1547, 1203, 717 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_7S$ $[M+H]^+$: 460.1425, found 460.1433.

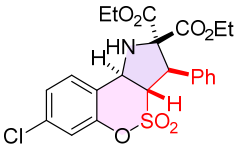
diethyl 8-methoxy-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino [4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide(3z)



3z, 90%

White solid, 85.5 mg, 90% yield, m.p. 187.2 – 187.6 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.27 (m, 5H), 7.07 (d, *J* = 9.2 Hz, 2H), 6.90 (dd, *J* = 8.8, 2.8 Hz, 1H), 4.98 (d, *J* = 12.4 Hz, 1H), 4.55 (d, *J* = 11.4 Hz, 1H), 4.49 – 4.39 (m, 1H), 4.33 – 4.24 (m, 1H), 3.86 – 3.73 (m, 5H), 3.65 (s, 1H), 3.40 – 3.27 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.79 – 0.66 (m, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 168.8, 157.4, 144.3, 134.0, 128.7, 128.6, 128.4, 124.8, 119.3, 115.7, 64.7, 62.9, 60.9, 56.1, 51.5, 14.1, 13.3.
IR (KBr, thin film): 3847, 3642, 2392, 1725, 1711, 1691, 1658, 1584, 1162, 815 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{26}NO_8S$ $[M+H]^+$: 476.1374, found 476.1374.

diethyl 7-chloro-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide (3aa)



3aa, 89%

White solid, 87.2 mg, 91% yield, m.p. 174.5 – 174.8 °C.

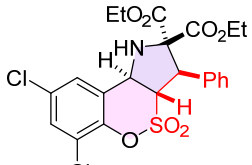
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.48 (m, 1H), 7.34 – 7.26 (m, 6H), 7.16 (d, *J* = 2.0 Hz, 1H), 4.98 (d, *J* = 12.4 Hz, 1H), 4.53 (t, *J* = 12.0 Hz, 1H), 4.48 – 4.38 (m, 1H), 4.33 – 4.22 (m, 1H), 3.86 – 3.75 (m, 2H), 3.61 (d, *J* = 12.4 Hz, 1H), 3.41 – 3.24 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 0.73 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.7, 150.9, 135.6, 133.7, 128.8, 128.7, 128.4, 126.9, 126.0, 122.0, 118.6, 64.6, 63.0, 60.4, 51.4, 14.1, 13.3.

IR (KBr, thin film): 3855, 3677, 3415, 3273, 2360, 1718, 1701, 1685, 1170, 920 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{22}H_{23}ClNO_7S$ $[M+H]^+$: 480.0884, found 480.0883.

diethyl 6,8-dichloro-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide(3ab)



3ab, 91%

White solid, 93.5 mg, 91% yield, m.p. 168.7 – 168.2 °C.

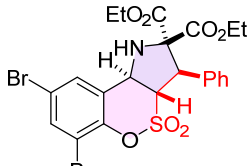
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.45 (m, 2H), 7.32 (s, 5H), 4.97 (d, *J* = 12.4 Hz, 1H), 4.58 (t, *J* = 10.8 Hz, 1H), 4.48 – 4.38 (m, 1H), 4.33 – 4.23 (m, 1H), 3.92 – 3.76 (m, 2H), 3.63 (d, *J* = 10.0 Hz, 1H), 3.41– 3.29 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.74 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.2, 168.5, 145.3, 133.3, 131.3, 130.6, 128.8, 128.8, 128.4, 126.7, 124.5, 124.3, 64.4, 63.1, 63.0, 60.6, 51.4, 27.0, 14.1, 13.3.

IR (KBr, thin film): 3578, 3555, 1753, 1712, 1630, 1468, 1376, 1215, 1034, 912 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{22}H_{22}Cl_2NO_7S$ $[M+H]^+$: 514.0494, found 514.0495.

diethyl 6,8-dibromo-3-phenyl-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide(3ac)



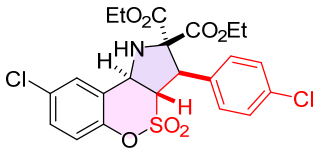
3ac, 93%

White solid, 111.6 mg, 93% yield, m.p. 219.5 – 220.1 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 1.6 Hz, 1H), 7.67 (s, 1H), 7.32 (s, 5H), 4.96 (d, *J* = 12.4 Hz, 1H), 4.68 – 4.52 (m, 1H), 4.49 – 4.38 (m, 1H), 4.33 – 4.22 (m, 1H), 3.93 – 3.76 (m, 2H), 3.63 (d, *J* = 10.0 Hz, 1H), 3.40 – 3.30 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.74 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.2, 168.5, 146.9, 136.3, 133.3, 128.8, 128.8, 128.4, 127.8, 127.0, 118.8, 113.1, 64.5, 63.0, 60.5, 51.3, 14.1, 13.3.
IR (KBr, thin film): 3731, 3395, 2360, 1713, 1656, 1436, 1250, 1210, 1166, 852 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{22}Br_2NO_7S$ $[M+H]^+$: 601.9484, found 601.9484.

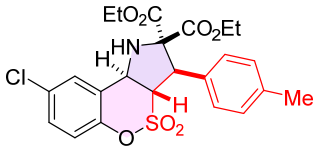
diethyl 8-chloro-3-(4-chlorophenyl)-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxa-thiino [4,3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide (3ad)



3ad, 93%

White solid, 95.6 mg, 93% yield, m.p. 192.4 – 192.9 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.54 (m, 1H), 7.36 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.34 – 7.26 (m, 4H), 7.08 (d, *J* = 8.8 Hz, 1H), 4.92 (d, *J* = 12.4 Hz, 1H), 4.54 (d, *J* = 10.0 Hz, 1H), 4.48 – 4.38 (m, 1H), 4.33 – 4.23 (m, 1H), 3.92 – 3.82 (m, 1H), 3.81 – 3.72 (m, 1H), 3.61 (s, 1H), 3.51 – 3.41 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.81 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 168.5, 149.0, 134.7, 132.1, 131.4, 130.3, 129.8, 128.9, 126.0, 125.0, 119.6, 64.0, 63.1, 60.4, 50.8, 14.1, 13.4.
IR (KBr, thin film): 3660, 3281, 2394, 2282, 1723, 1654, 1542, 1207, 1168, 815 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{22}H_{22}Cl_2NO_7S$ $[M+H]^+$: 514.0489, found 514.0490.

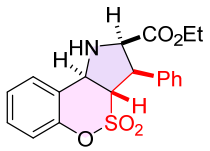
diethyl 8-chloro-3-(p-tolyl)-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxa-thiino[4, 3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide (3ae)



3ae, 99%

White solid, 97.6 mg, 99% yield, m.p. 254.2 – 254.6 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.55 (m, 1H), 7.39 – 7.33 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.8 Hz, 1H), 4.93 (d, *J* = 12.4 Hz, 1H), 4.54 (d, *J* = 10.8 Hz, 1H), 4.48 – 4.38 (m, 1H), 4.33 – 4.22 (m, 1H), 3.88 – 3.74 (m, 2H), 3.61 (s, 1H), 3.45 – 3.34 (m, 1H), 2.31 (s, 3H), 1.36 – 1.27 (m, 3H), 0.75 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 168.7, 149.1, 138.5, 131.3, 130.5, 130.2, 129.4, 128.3, 126.0, 125.3, 64.4, 60.4, 51.2, 21.2, 14.1, 13.3.
IR (KBr, thin film): 3802, 3650, 2362, 2342, 1733, 1684, 1558, 1507, 1165, 901 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{25}ClNO_7S$ $[M+H]^+$: 494.1035, found 494.1044.

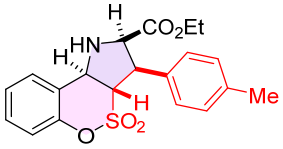
ethyl 3-phenyl-2,3,3a,9b-tetrahydro-1H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2-carboxylate 4,4-dioxide (3af)



3af, 80%

White solid, 59.7 mg, 80% yield, m.p. 254.3 – 254.7 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.35 – 7.27 (m, 4H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 1H), 4.60 (d, *J* = 11.2 Hz, 1H), 4.47 (d, *J* = 10.0 Hz, 1H), 4.24 (t, *J* = 10.8 Hz, 1H), 3.82 – 3.62 (m, 2H), 3.49 – 3.37 (m, 1H), 2.90 (s, 1H), 0.74 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.2, 150.8, 134.8, 130.2, 128.9, 128.4, 128.0, 125.8, 124.0, 118.2, 65.8, 65.3, 62.0, 61.8, 50.0, 13.5.
IR (KBr, thin film): 3849, 3730, 3267, 2359, 1716, 1558, 1540, 1455, 1274, 970 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{19}H_{20}NO_5S$ $[M+H]^+$: 374.1057, found 374.1061.

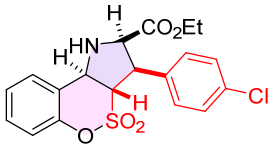
ethyl 3-(p-tolyl)-2,3,3a,9b-tetrahydro-1H-benzo[5,6][1,2]oxathiino[4,3-*b*] pyrrole -2-carboxylate 4,4-dioxide (3ag)



3ag, 75%

White solid, 58.0 mg, 75% yield, m.p. 196.7 – 197.2 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.31 – 7.25 (m, 1H), 7.16 – 7.06 (m, 5H), 4.58 (d, *J* = 11.2 Hz, 1H), 4.44 (d, *J* = 10.0 Hz, 1H), 4.26 – 4.16 (m, 1H), 3.81 – 3.71 (m, 1H), 3.66 (t, *J* = 11.6 Hz, 1H), 3.52 – 3.41 (m, 1H), 2.91 (s, 1H), 2.31 (s, 3H), 0.75 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.3, 138.1, 131.6, 130.1, 129.5, 127.9, 125.8, 125.8, 124.0, 118.1, 65.8, 65.3, 61.9, 49.6, 21.2, 13.4.
IR (KBr,thin film): 3778, 3652, 2394, 1762, 1726, 1725, 1653, 1547, 1203, 1015 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{20}H_{22}NO_5S$ $[M+H]^+$: 388.1213, found 388.1215.

ethyl 3-(4-chlorophenyl)-2,3,3a,9b-tetrahydro-1H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole-2-carboxylate 4,4-dioxide (3ah)

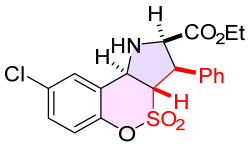


3ah, 78%

White solid, 63.5 mg, 78% yield, m.p. 196.0 – 196.4 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.33 – 7.26 (m, 3H), 7.20 – 7.11 (m, 3H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.45 (d, *J* = 10.4

Hz, 1H), 4.18 (s, 1H), 3.83 – 3.73 (m, 1H), 3.63 (t, *J* = 11.6 Hz, 1H), 3.54 – 3.44 (m, 1H), 2.92 (s, 1H), 0.80 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.0, 150.8, 134.4, 133.4, 130.2, 129.4, 129.0, 125.9, 125.9, 123.8, 118.1, 65.6, 65.2, 62.0, 49.2, 13.6.
IR (KBr, thin film): 3849, 3730, 2359, 1830, 1732, 1716, 1653, 1568, 1212, 760 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{19}H_{19}ClNO_5S$ $[M+H]^+$: 408.0673, found 408.0675.

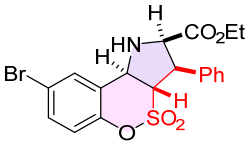
ethyl 8-chloro-3-phenyl-2,3,3a,9b-tetrahydro-1H-benzo[5,6][1,2]oxathiino[4,3-*b*] pyrrole-2-carboxylate 4,4-dioxide (3ai)



3ai, 82%

White solid, 66.7 mg, 82% yield, m.p. 203.1 – 203.5 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.52 (m, 1H), 7.39 – 7.26 (m, 4H), 7.24 – 7.17 (m, 2H), 7.08 (d, *J* = 8.8 Hz, 1H), 4.57 (d, *J* = 11.6 Hz, 1H), 4.45 (d, *J* = 10.4 Hz, 1H), 4.29 – 4.17 (m, 1H), 3.81 – 3.61 (m, 2H), 3.48 – 3.36 (m, 1H), 2.90 (s, 1H), 0.78 – 0.69 (m, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.1, 149.2, 134.4, 131.3, 130.1, 128.9, 128.5, 128.0, 126.0, 125.6, 119.5, 65.7, 64.9, 61.8, 49.9, 13.5.
IR (KBr, thin film): 3850, 3731, 2924, 2361, 1713, 1587, 1470, 1212, 1165, 795 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{19}H_{19}ClNO_5S$ $[M+H]^+$: 408.0673, found 408.0671.

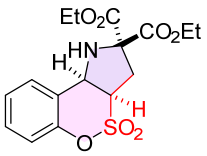
ethyl 8-bromo-3-phenyl-2,3,3a,9b-tetrahydro-1H-benzo[5,6][1,2]oxathiino[4,3-*b*] pyrrole-2-carboxylate 4,4-dioxide (3aj)



3aj, 82%

White solid, 74.0 mg, 82% yield, m.p. 212.2 – 212.7 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.64 (m, 1H), 7.51 (dd, *J* = 9.6, 2.4 Hz, 1H), 7.37 – 7.27 (m, 3H), 7.23 – 7.14 (m, 2H), 7.02 (d, *J* = 8.8 Hz, 1H), 4.67 – 4.51 (m, 1H), 4.49 – 4.37 (m, 1H), 4.28 – 4.17 (m, 1H), 3.83 – 3.59 (m, 2H), 3.50 – 3.35 (m, 1H), 3.00 – 2.78 (m, 1H), 0.74 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.1, 149.8, 134.4, 133.1, 129.0, 128.9, 128.5, 128.0, 126.0, 119.9, 118.7, 65.7, 64.9, 61.9, 61.7, 49.9, 13.5.
IR (KBr, thin film): 3792, 3685, 3395, 1723, 1693, 1639, 1615, 1384, 1164, 712 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{19}H_{19}BrNO_5S$ $[M+H]^+$: 452.0167, found 452.0167.

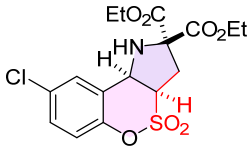
diethyl 1, 3, 3a, 9b-tetrahydro-2H-benzo[5, 6][1, 2]oxathiino[4, 3-*b*]pyrrole-2,2-dicarboxylate 4,4-dioxide (3am)



3am, 62%

White solid, 45.8 mg, 62% yield, m.p. 115.3 – 116.0 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 7.2 Hz, 1H), 7.39 – 7.31 (m, 1H), 7.29 – 7.23 (m, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 4.88 (d, *J* = 7.6 Hz, 1H), 4.37 – 4.24 (m, 2H), 4.24 – 4.15 (m, 2H), 4.15 – 4.07 (m, 1H), 3.52 (s, 1H), 3.17 (dd, *J* = 14.8, 8.4 Hz, 1H), 2.98 (dd, *J* = 15.2, 6.4 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 168.7, 150.0, 130.4, 130.3, 126.5, 123.0, 119.5, 72.0, 62.9, 62.7, 60.9, 58.8, 34.7, 14.1, 14.0.
IR (KBr, thin film): 3687, 3397, 1730, 1697, 1625, 1615, 1384, 1164, 1128, 712 cm^{-1}.
HRMS (APCI) m/z: Calcd for $C_{16}H_{20}NO_7S$ $[M+H]^+$: 370.0955; Found: 370.0958.

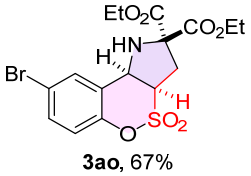
diethyl 8-chloro-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole -2,2-dicarboxylate 4,4-dioxide (3an)



3an, 70%

White solid, 56.4 mg, 70% yield, m.p. 116.7 – 117.2 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 2.4 Hz, 1H), 7.32 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 4.90 – 4.82 (m, 1H), 4.34 – 4.24 (m, 2H), 4.24 – 4.16 (m, 2H), 4.09 (dd, *J* = 15.6, 7.2 Hz, 1H), 3.57 (d, *J* = 8.8 Hz, 1H), 3.13 (dd, *J* = 14.8, 8.8 Hz, 1H), 3.03 – 2.93 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.2, 168.5, 148.4, 131.9, 130.4, 130.2, 124.9, 120.9, 71.9, 63.0, 62.8, 60.5, 58.4, 34.5, 14.1, 14.0.
IR (KBr, thin film): 3837, 3650, 2995, 2361, 1734, 1700, 1559, 1473, 1163, 848 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{16}H_{19}ClNO_7S$ $[M+H]^+$: 404.0571, found 404.0570.

diethyl 8-bromo-1,3,3a,9b-tetrahydro-2H-benzo[5,6][1,2]oxathiino[4,3-*b*]pyrrole -2,2-dicarboxylate 4,4-dioxide (3ao)

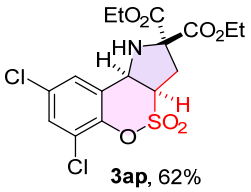


3ao, 67%

White solid, 60.0 mg, 67% yield, m.p. 121.8 – 122.3 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 2.0 Hz, 1H), 7.50 – 7.42 (m, 1H), 6.99 (d, *J* = 8.8 Hz, 1H), 4.89 – 4.82 (m, 1H), 4.35 – 4.24 (m, 2H), 4.24 – 4.16 (m, 2H), 4.09 (q, *J* = 7.6 Hz, 1H), 3.57 (d, *J* = 8.8 Hz, 1H), 3.18 – 3.08 (m, 1H), 2.98 (dd, *J* = 14.8, 6.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.2, 168.5, 149.0, 133.3, 133.2, 125.2, 121.2, 119.4, 71.9, 63.0, 62.8, 60.5, 58.5, 34.5, 14.1, 14.0.
IR (KBr, thin film): 3673, 3649, 2394, 1733, 1557, 1475, 1376, 1163, 1114, 795 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{16}H_{19}BrNO_7S$ $[M+H]^+$: 448.0066, found 448.0067.

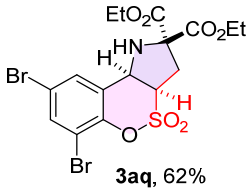
diethyl 6, 8-dichloro-1, 3, 3a, 9b-tetrahydro-2H-benzo[5, 6][1, 2]oxathiino[4, 3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3ap)



3ap, 62%

White solid, 54.2 mg, 62% yield, m.p. 125.3 – 125.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 2.0 Hz, 1H), 7.60 (d, *J* = 2.0 Hz, 1H), 4.88 (t, *J* = 8.0 Hz, 1H), 4.36 – 4.25 (m, 2H), 4.25 – 4.19 (m, 2H), 4.12 (q, *J* = 7.6 Hz, 1H), 3.55 (d, *J* = 8.4 Hz, 1H), 3.12 (dd, *J* = 14.8, 8.4 Hz, 1H), 3.03 – 2.93 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.26 – 1.22 (m, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.2, 168.4, 146.2, 136.3, 132.1, 127.0, 119.5, 114.3, 71.8, 63.1, 62.9, 60.6, 58.8, 34.5, 14.1, 14.0.
IR (KBr, thin film): 3854, 3638, 2392, 1734, 1446, 1383, 1278, 1156, 1045, 791 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{16}H_{18}Cl_2NO_7S$ $[M+H]^+$: 438.0181, found 438.0180.

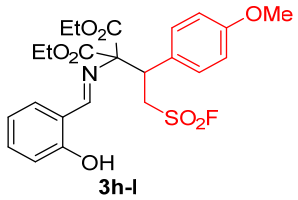
diethyl 6, 8-dibromo-1, 3, 3a, 9b-tetrahydro-2H-benzo[5, 6][1, 2]oxathiino[4, 3-*b*] pyrrole-2,2-dicarboxylate 4,4-dioxide (3aq)



3aq, 62%

White solid, 65.0 mg, 62% yield, m.p. 140.7 – 141.2 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 2.4 Hz, 1H), 7.60 (d, *J* = 2.0 Hz, 1H), 4.88 (t, *J* = 6.8 Hz, 1H), 4.38 – 4.17 (m, 4H), 4.16 – 4.06 (m, 1H), 3.55 (d, *J* = 6.4 Hz, 1H), 3.19 – 3.07 (m, 1H), 2.97 (dd, *J* = 15.2, 7.2 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.2, 168.4, 146.3, 136.3, 132.1, 127.0, 119.5, 114.4, 71.8, 63.1, 62.9, 60.7, 58.8, 34.5, 14.1, 14.0.
IR (KBr, thin film): 3731, 3626, 2985, 2360, 1732, 1556, 1537, 1188, 1158, 832 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{16}H_{18}Br_2NO_7S$ $[M+H]^+$: 525.9171, found 525.9164.

diethyl-2-(2-(fluorosulfonyl)-1-(4-methoxyphenyl)ethyl)-2-((2-hydroxybenzy lidene)amino)malonate (3h-I)



3h-I

White solid, 39.6 mg, 40% yield, m.p. 160.7 – 161.2 °C.

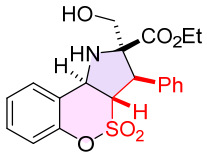
^{1}H NMR (400 MHz, Chloroform-*d*) δ 12.43 (s, 1H), 8.49 (s, 1H), 7.47 – 7.22 (m, 2H), 7.19 – 7.11 (m, 2H), 6.99 – 6.83 (m, 2H), 6.82 – 6.68 (m, 2H), 4.35 – 4.13 (m, 4H), 4.08 – 3.86 (m, 3H), 3.69 (s, 3H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.12 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.2, 167.3, 166.4, 161.1, 159.9, 134.3, 133.3, 130.5, 126.6, 119.5, 118.8, 117.5, 114.3, 63.4, 62.9, 55.3, 45.7, 14.1, 14.0.

^{19}F NMR (376 MHz, Chloroform-*d*) δ 59.89.

HRMS (ESI) m/z calcd for $C_{23}H_{27}FNO_8S$ $[M+H]^+$: 496.1436, found 496.1440.

ethyl - 2 -(hydroxymethyl)- 3-phenyl-2, 3, 3a, 9b- tetrahydro- 1H- benzo [5,6] [1,2] oxathiino[4,3-*b*]pyrrole-2-carboxylate 4,4-dioxide (4a)



4a, 75%

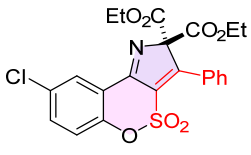
White solid, 60.5 mg, 75% yield, m.p. 183.4 – 183.9 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.48 (m, 1H), 7.38 – 7.31 (m, 1H), 7.30 – 7.22 (m, 4H), 7.15 – 7.10 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 4.53 (d, *J* = 9.6 Hz, 1H), 4.02 (d, *J* = 11.2 Hz, 1H), 3.79 – 3.70 (m, 4H), 3.52 – 3.23 (m, 2H), 2.61 (s, 1H), 1.54 (s, 1H), 0.67 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.6, 150.8, 134.3, 130.3, 129.0, 128.6, 127.9, 125.9, 125.8, 123.6, 118.3, 65.3, 65.2, 62.6, 60.3, 52.6, 13.4.

HRMS (ESI) m/z calcd for $C_{20}H_{22}NO_6S$ $[M+H]^+$: 404.1162, found 404.1168.

diethyl 3-phenyl- 2H- benzo [5,6] [1,2] oxathiino [4,3-*b*] pyrrole-2, 2-dicarboxylate 4,4-dioxide (5w)



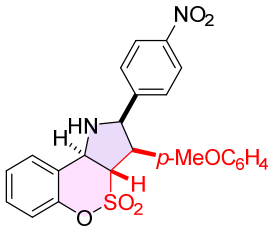
5w, 70%

Red solid, 61.7 mg, 70% yield, m.p. 163.3 – 163.8 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 2.2 Hz, 1H), 7.57 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.45 – 7.36 (m, 3H), 7.28 – 7.24 (m, 1H), 4.63 (q, *J* = 7.2 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 1.50 (t, *J* = 7.2 Hz, 3H), 1.05 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 159.8, 150.4, 148.5, 134.0, 130.1, 129.4, 129.1, 129.0, 128.2, 128.0, 127.2, 123.6, 121.9, 119.3, 119.1, 116.7, 67.3, 62.0, 13.8, 13.7.
HRMS (ESI) m/z calcd for $C_{22}H_{20}NO_7S$ $[M+H]^+$: 442.0955, found 442.0958.

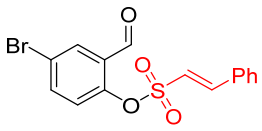
3-(4-methoxyphenyl)-2-(4-nitrophenyl)-2, 3, 3a, 9b-tetrahydro-1H-benzo[5, 6][1, 2] oxathiino[4,3-*b*]pyrrole 4,4-dioxide (9a)



9a, 56%

White solid, 50.7 mg, 90% yield, m.p. 235.2 – 235.8 °C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.87 (m, 2H), 7.54 – 7.49 (m, 1H), 7.46 – 7.39 (m, 1H), 7.39 – 7.31 (m, 1H), 7.19 (d, *J* = 8.8 Hz, 3H), 6.73 (d, *J* = 8.4 Hz, 2H), 6.58 (d, *J* = 8.8 Hz, 2H), 5.16 (d, *J* = 9.6 Hz, 1H), 4.97 (d, *J* = 11.2 Hz, 1H), 4.41 (dd, *J* = 11.6, 10.0 Hz, 1H), 3.75 (t, *J* = 11.6 Hz, 1H), 3.67 (s, 3H), 2.96 (s, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 159.2, 150.7, 148.1, 147.0, 129.7, 129.6, 128.8, 127.3, 126.1, 126.0, 124.9, 122.9, 118.3, 114.0, 64.7, 63.6, 59.1, 55.2, 49.7.
IR (KBr, thin film): 3612, 2820, 1734, 1653, 1541, 1344, 1254, 1156, 1031, 756 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{23}H_{21}N_2O_6S$ $[M+H]^+$: 453.1115, found 453.1112.

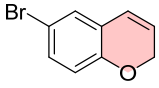
4-bromo-2-formylphenyl-2-phenylethene-1-sulfonate (12a)(known compound) [6]



12a, 95%

White solid, 69.7 mg, 95% yield.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.26 (s, 1H), 8.03 (d, *J* = 2.8 Hz, 1H), 7.72 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.60 (d, *J* = 15.6 Hz, 1H), 7.53 – 7.47 (m, 3H), 7.47 – 7.41 (m, 2H), 7.30 (d, *J* = 8.8 Hz, 1H), 6.93 (d, *J* = 15.6 Hz, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.6, 149.6, 148.1, 138.2, 132.5, 132.2, 131.2, 130.7, 129.5, 129.0, 125.7, 121.5, 119.5.

6-bromo-2H-chromene (13a) (known compound) [7]



13a, 68%

Colorless liquid, 28.7 mg, 68% yield.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.17 (dd, J = 8.6, 2.2 Hz, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.64 (d, *J* = 8.8 Hz, 1H), 6.34 (d, *J* = 9.6 Hz, 1H), 5.80 (dt, *J* = 9.8, 3.4 Hz, 1H), 4.81 (s, 2H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 153.2, 131.7, 129.1, 124.3, 123.7, 123.3, 117.6, 113.4, 65.8.

4. Single-crystal X-ray structure analysis.

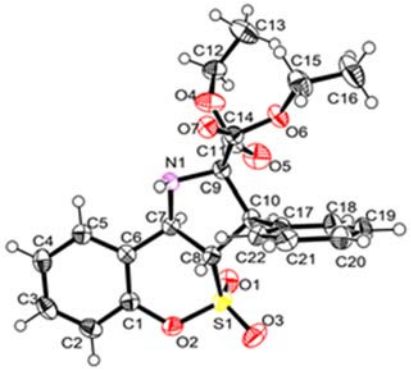


Figure S1. Crystal structure of **3a** at 30% probability level.

Table S1. Crystal data and structure refinement for **3a**.

Identification code	**3a**	
Empirical formula	$C_{22}H_{23}NO_7S$	
Formula weight	445.47	
Temperature	173.15 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.6166(3) Å	α = 73.3600(10)°.
	b = 10.0879(3) Å	β = 77.3780(10)°.
	c = 11.7837(4) Å	γ = 84.3940(10)°.
Volume	1068.06(6) $Å^3$	
Z	2	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	1.735 mm^{-1}	
F(000)	468	
Crystal size	0.25 x 0.23 x 0.21 mm^3	
Theta range for data collection	4.578 to 72.225°.	
Index ranges	-10<=h<=11, -12<=k<=12, -14<=l<=14	
Reflections collected	25182	
Independent reflections	4164 [R(int) = 0.0298]	
Completeness to theta = 67.679°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6429	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4164 / 10 / 305	

Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0893
R indices (all data)	R1 = 0.0365, wR2 = 0.0899
Extinction coefficient	n/a
Largest diff. peak and hole	0.363 and -0.437 e.$Å^{-3}$

The CCDC number of product **3a** is 2218888.

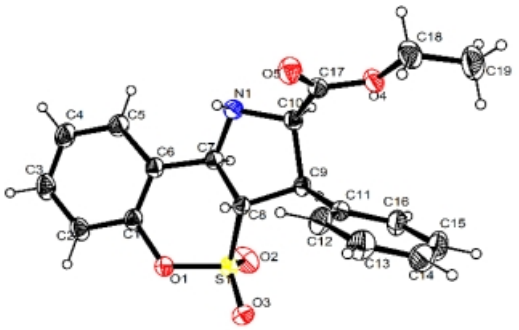


Figure S23. Crystal structure of **3af** at 30% probability level.

Table S2. Crystal data and structure refinement for **3af**.

Identification code	**3af**	
Empirical formula	$C_{19}H_{19}NO_5S$	
Formula weight	373.41	
Temperature	298.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 12.3087(3) Å	α = 90°.
	b = 18.9005(5) Å	β = 102.4740(10)°.
	c = 16.1113(4) Å	γ = 90°.
Volume	3659.66(16) $Å^3$	
Z	8	
Density (calculated)	1.355 Mg/m^3	
Absorption coefficient	0.206 mm^{-1}	
F(000)	1568	
Crystal size	0.25 x 0.23 x 0.22 mm^3	
Theta range for data collection	2.514 to 26.737°.	
Index ranges	-15<=h<=15, -23<=k<=23, -20<=l<=20	
Reflections collected	22145	
Independent reflections	3884 [R(int) = 0.0375]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6685	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3884 / 7 / 227	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1182	
R indices (all data)	R1 = 0.0572, wR2 = 0.1279	

Extinction coefficient	n/a
Largest diff. peak and hole	0.358 and -0.248 e.Å^{-3}

The CCDC number of product **3af** is 2347754.

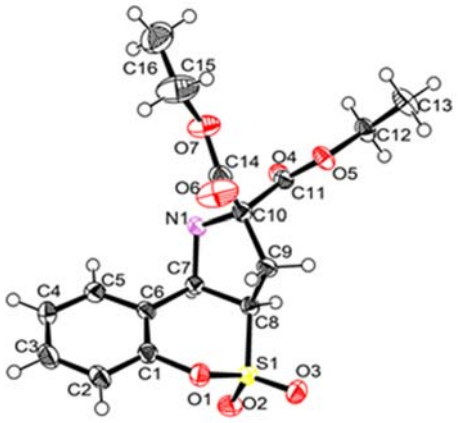


Figure S3. Crystal structure of **3am** at 30% probability level.

Table S3. Crystal data and structure refinement for **3am**.

Identification code	**3am**	
Empirical formula	$C_{16}H_{18}NO_7S$	
Formula weight	368.37	
Temperature	173.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 6.9700(2) Å	α = 90°.
	b = 20.0713(4) Å	β = 91.7350(10)°.
	c = 12.4232(3) Å	γ = 90°.
Volume	1737.17(7) $Å^3$	
Z	4	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	0.224 mm^{-1}	
F(000)	772	
Crystal size	0.24 x 0.17 x 0.11 mm^3	
Theta range for data collection	2.610 to 26.748°.	
Index ranges	-8<=h<=7, -25<=k<=25, -15<=l<=15	
Reflections collected	21863	
Independent reflections	7359 [R(int) = 0.0336]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7359 / 1 / 456	
Goodness-of-fit on F^2	1.027	

Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0913
R indices (all data)	R1 = 0.0413, wR2 = 0.0956
Absolute structure parameter	0.49(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.507 and -0.377 e.Å^{-3}

The CCDC number of product **3am** is 2218887.

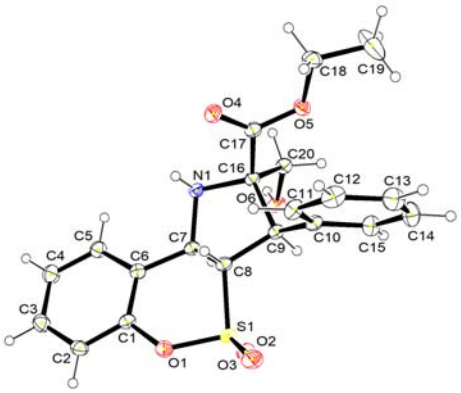


Figure S4. Crystal structure of **4a** at 30% probability level.

Table S4. Crystal data and structure refinement for **4a**.

Identification code	**4a**	
Empirical formula	$C_{20}H_{21}NO_6S$	
Formula weight	403.44	
Temperature	173.0 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 10.0053(2) Å	α = 90°.
	b = 13.4636(3) Å	β = 107.2020(10)°.
	c = 15.1329(3) Å	γ = 90°.
Volume	1947.33(7) $Å^3$	
Z	4	
Density (calculated)	1.376 Mg/m^3	
Absorption coefficient	1.803 mm^{-1}	
F(000)	848	
Crystal size	0.17 x 0.16 x 0.14 mm^3	
Theta range for data collection	4.488 to 72.138°.	
Index ranges	-12<=h<=12, -15<=k<=16, -15<=l<=18	
Reflections collected	14602	
Independent reflections	3807 [R(int) = 0.0457]	
Completeness to theta = 67.679°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6674	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3807 / 0 / 258	
Goodness-of-fit on F^2	1.036	

Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.0968
R indices (all data)	R1 = 0.0552, wR2 = 0.1051
Extinction coefficient	n/a
Largest diff. peak and hole	0.272 and -0.437 e.Å^{-3}

The CCDC number of product **4a** is 2378446.

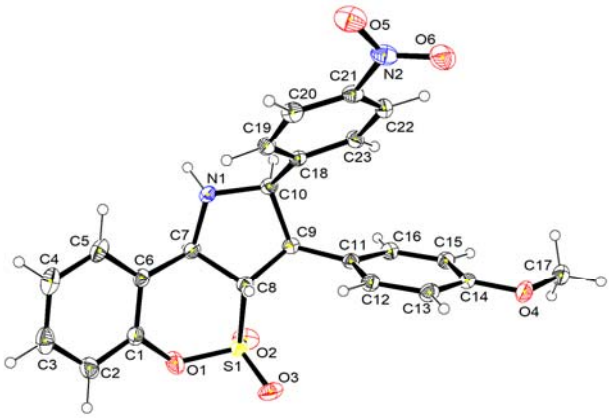


Figure S5. Crystal structure of **9a** at 30% probability level.

Table S5. Crystal data and structure refinement for **9a**.

Identification code	**9a**	
Empirical formula	$C_{23}H_{20}N_2O_6S$	
Formula weight	452.47	
Temperature	173.0 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 7.3391(6) Å	α = 90°.
	b = 27.293(2) Å	β = 105.174(3)°.
	c = 10.5772(9) Å	γ = 90°.
Volume	2044.8(3) $Å^3$	
Z	4	
Density (calculated)	1.470 Mg/m^3	
Absorption coefficient	1.804 mm^{-1}	
F(000)	944	
Crystal size	0.22 x 0.21 x 0.2 mm^3	
Theta range for data collection	4.624 to 71.984°.	
Index ranges	-9<=h<=8, -33<=k<=31, -12<=l<=13	
Reflections collected	15630	
Independent reflections	3926 [R(int) = 0.0434]	
Completeness to theta = 67.679°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6662	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3926 / 1 / 293	
Goodness-of-fit on F^2	1.044	

Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.0988
R indices (all data)	R1 = 0.0515, wR2 = 0.1053
Extinction coefficient	n/a
Largest diff. peak and hole	0.516 and -0.384 e.Å^{-3}

The CCDC number of product **9a** is 2353272.

5. Computational details

We performed the DFT calculation on the template reaction and the structures **1a, 2a, 2am, 3a** and **3am** are not simplified. All theoretical calculations were performed with Gaussian 16[9]. All structures were completely optimized by using the M062X-D3[10] method and the def2-SVP[11] basis set in solvent of MeCN, which employs the integral equation formalism polarizable continuum model (IEFPCM)[12]. Frequency calculations were carried out at the same level to confirm all the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency), and provided the thermal relative Gibbs free energy correction. For all transition states (TSs), intrinsic reaction coordinate (IRC)[13] calculations were employed to verify the TS led to its relevant intermediates. The single-point energies (SPE) by using a higher computational level of the M062X-D3 method and the ma-def2-TZVPP basis set in solvent of MeCN, which employs the integral equation formalism polarizable continuum model (SMD)[14]. All thermodynamic data were corrected by Shermo[15] software at 298.15 K, 1.0 atm. Images of the 3D structures of molecules were generated using CYLview[16].

Figure S6. Potential energy surfaces of **TS1** and **TS2**

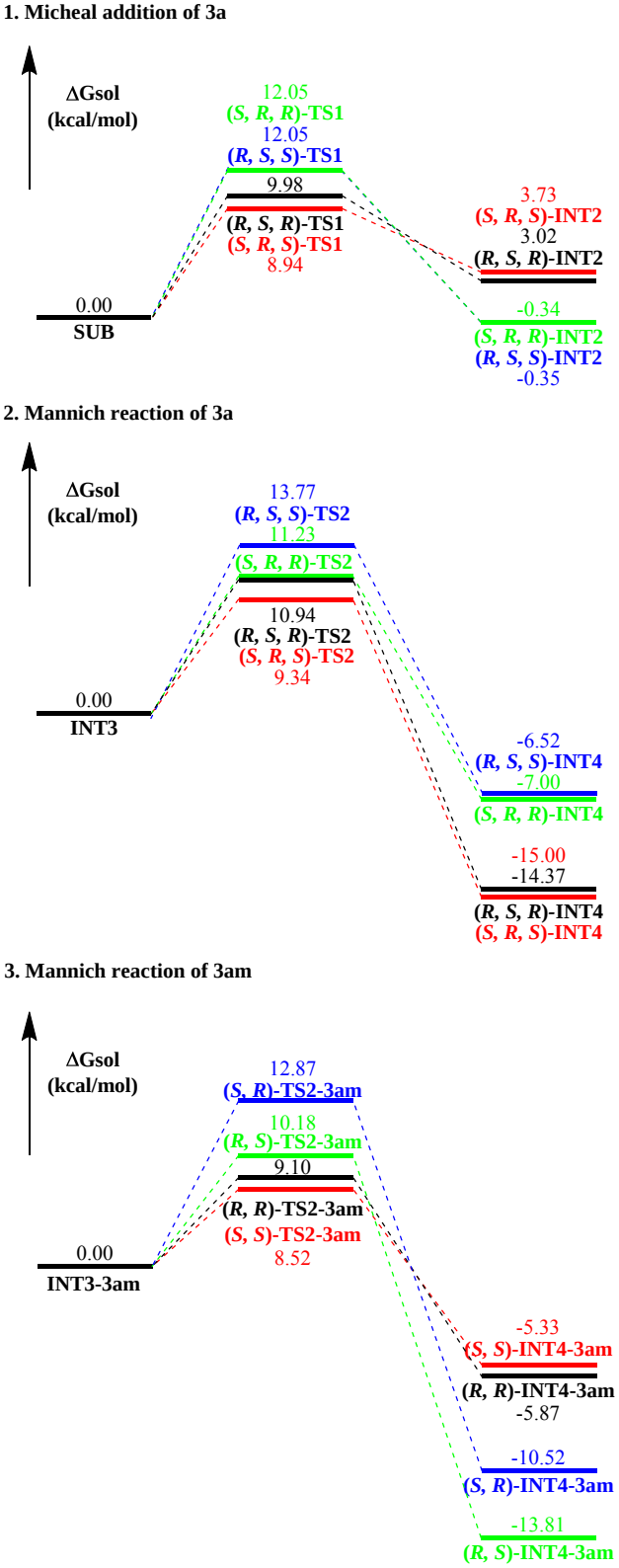


Table S6. Configuration of **TS1**, **TS2** and **TS2-3am**

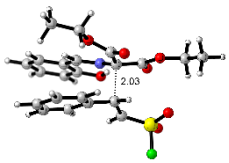
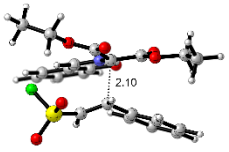
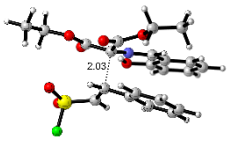
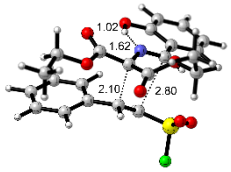
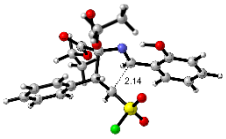
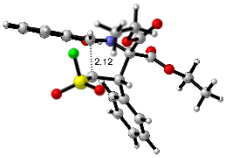
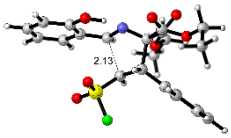
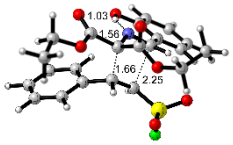
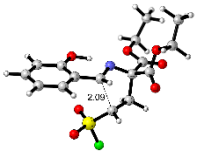
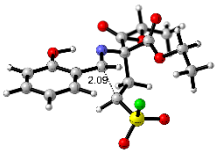
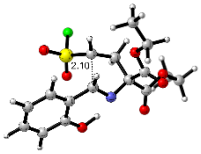
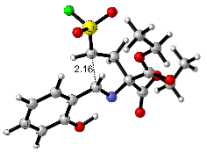
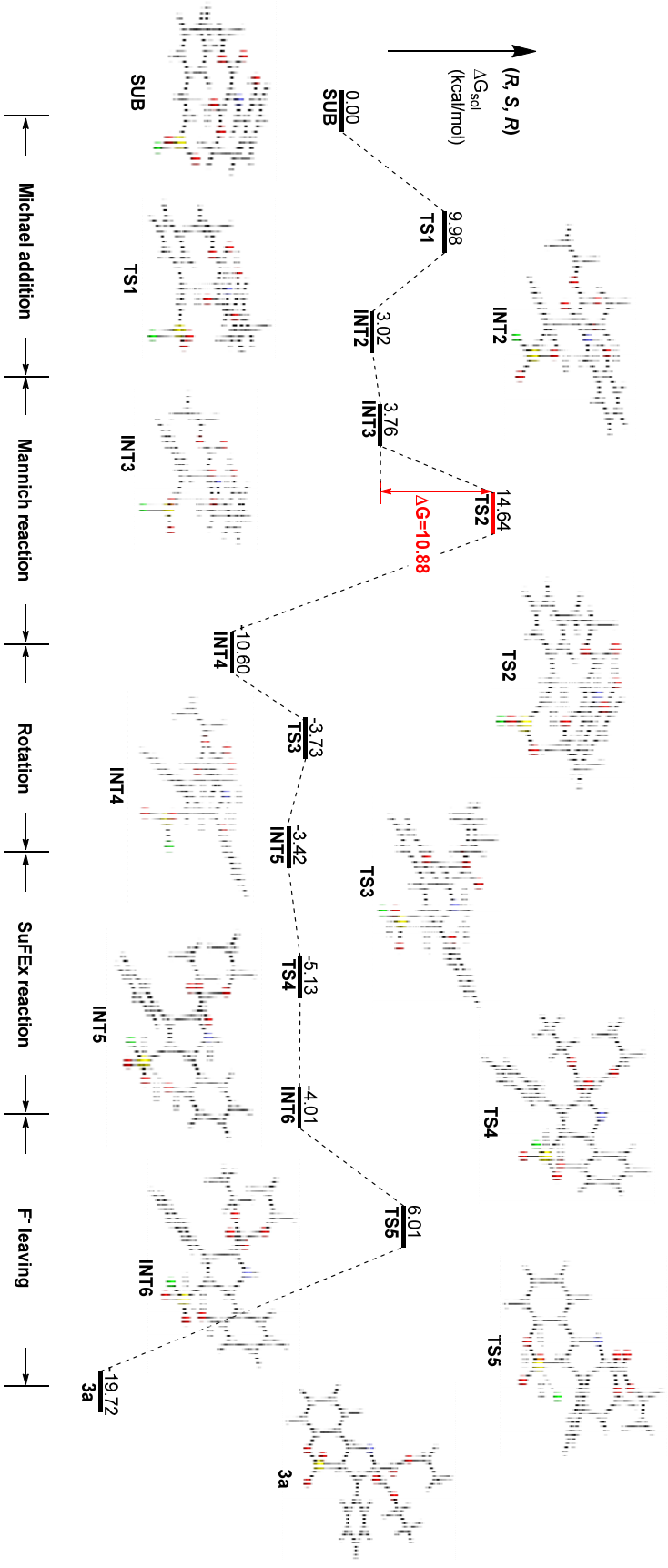
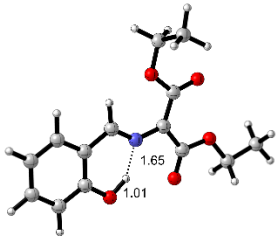
			
(*R*, *S*, *S*)-TS1	**(*S*, *R*, *S*)-TS1**	**(*S*, *R*, *R*)-TS1**	**(*R*, *S*, *R*)-TS1**
			
(*R*, *S*, *S*)-TS2	**(*S*, *R*, *S*)-TS2**	**(*S*, *R*, *R*)-TS2**	**(*R*, *S*, *R*)-TS2**
			
(*S*, *S*)-TS2-3am	**(*R*, *S*)-TS2-3am**	**(*R*, *R*)-TS2-3am**	**(*S*, *R*)-TS2-3am**

Figure S7. DFT calculations for the (*R, S, R*) reaction pathway, and the free energy profile obtained at $SMD_{(MeCN)}$/M062X-D3/ma-def2-TZVPP//def2-SVP level



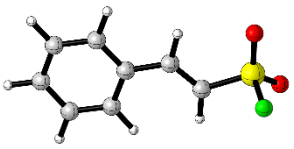
1a-



Charge = -1 Multiplicity = 1

C	-2.99385	-1.19949	0.07683
C	-4.32589	-1.63358	0.14256
H	-4.50836	-2.70464	0.24636
C	-5.37835	-0.72359	0.07673
H	-6.40657	-1.08638	0.12998
C	-5.12169	0.64404	-0.05642
H	-5.94303	1.35971	-0.10826
C	-3.80125	1.08202	-0.12149
H	-3.58277	2.14843	-0.22508
C	-2.7206	0.19004	-0.05792
C	-1.34287	0.69162	-0.12947
H	-1.21207	1.77516	-0.23172
C	1.00224	-0.02239	-0.10488
C	1.7378	1.21936	-0.22675
C	1.49807	3.57775	-0.41583
H	0.72379	4.22317	-0.85147
C	1.94226	4.10315	0.93653
H	2.33763	5.12379	0.83695
H	2.73051	3.46127	1.35082
C	1.65521	-1.31876	-0.00073
C	3.6533	-2.55749	0.07581
H	3.31941	-3.2154	-0.74122
H	3.35994	-3.04577	1.01802
C	5.1442	-2.31198	0.01842
H	5.68911	-3.26225	0.09606
H	5.46007	-1.6599	0.84438
H	5.4191	-1.82814	-0.92897
N	-0.36325	-0.14146	-0.07001
O	-2.01184	-2.10098	0.14224
O	0.8971	2.29319	-0.31145
O	2.9446	1.38872	-0.26168
O	3.00441	-1.29841	-0.03089
O	1.06056	-2.383	0.10783
H	2.34778	3.52807	-1.11018
H	1.09581	4.12585	1.63734
H	-1.13772	-1.59316	0.07821

2a



Charge = 0 Multiplicity = 1

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C	-4.29008	-0.22321	0.02094
C	-3.77094	1.07083	0.01415
C	-2.39139	1.26422	-0.00682
C	-1.51825	0.16619	-0.02099
C	-2.05181	-1.13385	-0.01449
C	-0.07705	0.42709	-0.04067
C	0.89474	-0.49551	-0.06098
S	2.54948	0.02714	-0.1257
O	2.65902	1.46246	-0.1613
O	3.31376	-0.80734	-1.01409
F	3.02664	-0.3971	1.34506
H	-3.83467	-2.33642	0.01168
H	-5.36983	-0.37802	0.03736
H	-4.44063	1.93138	0.02502
H	-1.98041	2.27558	-0.01211
H	-1.39026	-2.0013	-0.02604
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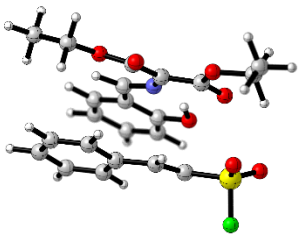
H	0.77587	-1.57941	-0.0724

(*R*, *S*, *S*)-INT1

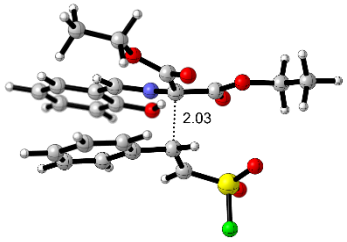


Charge = -1 Multiplicity = 1

C	-1.91525	-2.25846	-1.36681
C	-2.70166	-3.41773	-1.42623
H	-2.19151	-4.37611	-1.53726
C	-4.09018	-3.34256	-1.34336
H	-4.68186	-4.25853	-1.3932
C	-4.72288	-2.10454	-1.19585
H	-5.80966	-2.0427	-1.12825
C	-3.94642	-0.95027	-1.13202
H	-4.42299	0.02553	-1.00259
C	-2.5476	-0.99453	-1.21736

C	-1.76091	0.23583	-1.08713
H	-2.30769	1.15727	-0.85126
C	0.52605	1.09292	-1.0447
C	0.34812	2.47418	-0.63909
C	-1.2648	4.16096	-0.25295
H	-0.70421	4.90653	-0.83751
C	-2.75859	4.35216	-0.389
H	-3.04854	5.35243	-0.04039
H	-3.2979	3.60239	0.20778
C	1.83133	0.5111	-1.29335
C	4.14662	0.8248	-1.5905
H	4.14751	0.57758	-2.66481
H	4.31853	-0.10477	-1.03431
C	5.18779	1.87075	-1.26263
H	6.1881	1.51135	-1.53902
H	5.18093	2.08852	-0.18537
H	4.98941	2.80461	-1.80671
N	-0.48085	0.17926	-1.21002
O	-0.58393	-2.37034	-1.43609
O	-0.95307	2.85828	-0.7215
O	1.18937	3.2604	-0.23817
O	2.87576	1.35996	-1.23598
O	2.0078	-0.67329	-1.55839
H	-0.93439	4.26279	0.79339
H	-3.06622	4.2457	-1.43859
H	-0.20434	-1.42803	-1.40425
C	-2.98754	-0.17827	2.23701
C	-3.1692	1.18814	2.46299
C	-2.07267	2.05172	2.43351
C	-0.79901	1.55128	2.17468
C	-0.60845	0.18202	1.93773
C	-1.7162	-0.67835	1.97476
C	0.74447	-0.30088	1.64793
C	1.05083	-1.52281	1.18728
S	2.7202	-1.94967	1.00331
O	3.5905	-0.80268	1.1126
O	2.92823	-2.9788	0.02037
F	2.93671	-2.72353	2.40692
H	-3.8419	-0.85622	2.25822
H	-4.16694	1.57998	2.66758
H	-2.21217	3.11895	2.61424
H	0.06115	2.22456	2.13487
H	-1.585	-1.74786	1.79817
H	1.56321	0.40296	1.82918
H	0.35846	-2.3082	0.88282

(*R, S, S*)-TS1



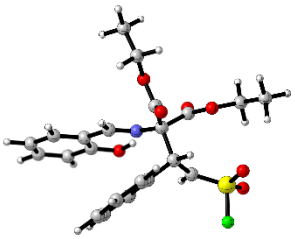
Charge = -1 Multiplicity = 1

Imaginary frequency = -367.7035 cm^{-1}

C	-2.33123	-2.54586	-0.97105
C	-3.26314	-3.59672	-0.94909
H	-2.88729	-4.61636	-1.04525
C	-4.62116	-3.33654	-0.80653
H	-5.32597	-4.17002	-0.79313
C	-5.09048	-2.02322	-0.67829
H	-6.15617	-1.82469	-0.56306
C	-4.17576	-0.97735	-0.69742
H	-4.51639	0.05629	-0.59239
C	-2.80027	-1.21041	-0.84753
C	-1.86125	-0.08653	-0.82369
H	-2.28015	0.91053	-0.64126
C	0.49298	0.52524	-0.86355
C	0.41615	2.00925	-0.98571
C	-1.04822	3.8516	-1.19785
H	-0.56811	4.31029	-2.07533
C	-2.54168	4.07813	-1.18257
H	-2.75823	5.15457	-1.18236
H	-2.98491	3.63251	-0.28015
C	1.69426	-0.15883	-1.43094
C	3.92668	-0.00944	-2.13455
H	3.75829	-0.36373	-3.16368
H	4.12404	-0.87875	-1.49631
C	5.04454	1.00321	-2.06075
H	5.97757	0.56234	-2.43608
H	5.19901	1.31509	-1.01878
H	4.81077	1.89171	-2.66334
N	-0.61162	-0.31018	-1.0024
O	-1.03648	-2.82814	-1.09979
O	-0.82607	2.44043	-1.23502
O	1.3356	2.7736	-0.80596
O	2.73612	0.63089	-1.6704
O	1.72732	-1.35747	-1.60696

H	-0.56379	4.2633	-0.30079
H	-3.01328	3.62747	-2.06663
H	-0.53636	-1.94806	-1.11329
C	-2.57083	0.88456	2.54704
C	-2.57568	2.26823	2.71884
C	-1.43547	3.00716	2.39327
C	-0.30765	2.36647	1.88627
C	-0.29511	0.97558	1.69034
C	-1.43959	0.24379	2.04093
C	0.90736	0.31757	1.11093
C	1.16137	-1.04189	1.41386
S	2.70883	-1.6304	1.38634
O	3.66868	-0.69358	0.81598
O	2.80413	-3.04665	1.07959
F	3.18731	-1.63522	2.9678
H	-3.45252	0.29601	2.80615
H	-3.46021	2.76961	3.1147
H	-1.42369	4.08899	2.53797
H	0.58067	2.94638	1.62892
H	-1.4533	-0.83974	1.91601
H	1.78898	0.96658	1.07106
H	0.40571	-1.79233	1.63092

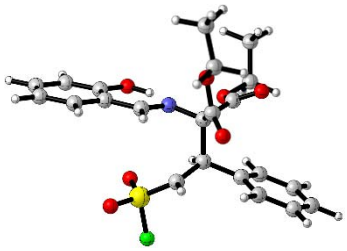
(*R*, *S*, *S*)-INT2



Charge = -1 Multiplicity = 1

C	-3.22773	-0.4491	-1.92919
C	-4.43485	-0.89601	-2.48995
H	-4.40013	-1.38401	-3.46458
C	-5.63309	-0.71509	-1.81144
H	-6.56033	-1.06854	-2.266
C	-5.66763	-0.08982	-0.55715
H	-6.61317	0.04448	-0.03226
C	-4.47926	0.35101	0.00691
H	-4.47741	0.83452	0.98677
C	-3.25491	0.18545	-0.66
C	-2.01184	0.61993	-0.03059
H	-2.09182	1.0273	0.99283
C	0.36122	0.74223	0.01221
C	0.30697	1.80408	1.12384
C	-0.36838	4.00862	1.60653
H	0.6468	4.28015	1.92931
C	-1.06831	5.14568	0.90381
H	-1.15714	6.00258	1.58393
H	-2.07617	4.84397	0.58866
C	1.34857	1.25252	-1.04932
C	3.62913	1.71676	-1.35585
H	3.41028	2.52715	-2.06568
H	3.74008	0.77954	-1.92415
C	4.84213	2.00162	-0.50588
H	5.72154	2.14066	-1.14862
H	5.01899	1.15222	0.16574
H	4.69573	2.91532	0.08653
N	-0.89473	0.49642	-0.63597
O	-2.08967	-0.63789	-2.59473
O	-0.27197	2.9147	0.68105
O	0.75398	1.67756	2.23163
O	2.50706	1.55394	-0.47831
O	1.11501	1.35122	-2.22161
H	-0.92052	3.66521	2.49311
H	-0.50129	5.46039	0.01763
H	-1.35464	-0.22442	-2.04635
C	-1.95121	-2.86479	1.57637
C	-1.92876	-2.7432	2.96775
C	-0.96224	-1.93996	3.57116
C	-0.02874	-1.25556	2.78929
C	-0.04011	-1.36935	1.39464
C	-1.01169	-2.18869	0.80103
C	0.96932	-0.61584	0.54272
C	1.54579	-1.38457	-0.60912
S	3.09861	-1.83936	-0.61768
O	3.9556	-1.08079	0.29815
O	3.6125	-2.16579	-1.94866
F	3.24527	-3.35955	0.09375
H	-2.70372	-3.48999	1.09241
H	-2.66089	-3.27528	3.5774
H	-0.93224	-1.8433	4.65791
H	0.71619	-0.61388	3.26194
H	-1.03996	-2.28188	-0.28719
H	1.80286	-0.30663	1.18681
H	0.9484	-1.79411	-1.42193

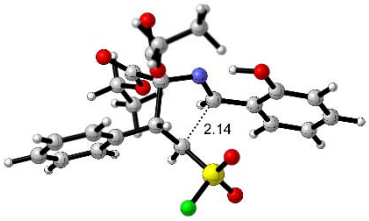
(*R*, *S*, *S*)-INT3



Charge = -1 Multiplicity = 1

C	3.37408	0.58021	1.33375
C	4.70425	0.47241	1.76994
H	4.91114	0.61426	2.83137
C	5.71988	0.18807	0.86539
H	6.74689	0.10753	1.22642
C	5.44414	0.00025	-0.49561
H	6.24703	-0.22803	-1.19636
C	4.13167	0.10551	-0.93562
H	3.8879	-0.04601	-1.98999
C	3.0888	0.39864	-0.04421
C	1.71256	0.46248	-0.52434
H	1.55059	0.24728	-1.59228
C	-0.60743	0.59201	-0.16703
C	-0.82898	1.04894	-1.61734
C	-0.46909	2.82652	-3.11469
H	-1.54259	2.88502	-3.34553
C	0.18657	4.18589	-3.10625
H	0.08563	4.6534	-4.09424
H	1.25534	4.09837	-2.86888
C	-1.52576	1.45131	0.69946
C	-2.05654	2.07464	2.91063
H	-1.89044	1.57554	3.8722
H	-3.10246	1.93157	2.60625
C	-1.69084	3.54259	2.97386
H	-2.30302	4.04412	3.73536
H	-1.87249	4.02793	2.00605
H	-0.63262	3.66321	3.24255
N	0.75101	0.74501	0.27165
O	2.41725	0.85163	2.21766
O	-0.31574	2.25911	-1.80729
O	-1.38151	0.41865	-2.47813
O	-1.21269	1.37065	1.98504
O	-2.45933	2.07336	0.26075
H	-0.00754	2.14826	-3.84695
H	-0.28723	4.83849	-2.36082
H	1.54754	0.86694	1.71334
C	-4.59457	-1.72069	-1.02633
C	-5.27461	-1.59402	0.18652
C	-4.56236	-1.27041	1.34041
C	-3.18288	-1.06954	1.27463
C	-2.49148	-1.17911	0.06052
C	-3.21662	-1.51712	-1.08845
C	-0.98637	-0.9486	0.04302
C	-0.1895	-1.81058	-0.87211
S	0.99534	-2.75882	-0.29388
O	1.49368	-2.36045	1.02441
O	1.95275	-3.19586	-1.30833
F	0.34418	-4.25691	0.11425
H	-5.14225	-1.98314	-1.93327
H	-6.35287	-1.75513	0.23206
H	-5.07805	-1.1821	2.29823
H	-2.62805	-0.82941	2.18523
H	-2.69307	-1.61239	-2.03888
H	-0.62805	-1.1297	1.06615
H	-0.41631	-1.95081	-1.92561

(*R*, *S*, *S*)-TS2



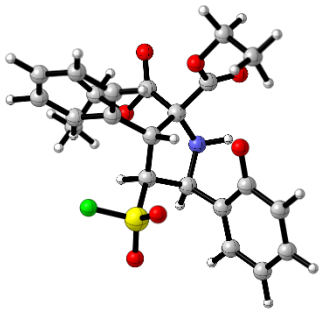
Charge = -1 Multiplicity = 1

Imaginary frequency = -231.6978 cm^{-1}

C	3.43672	0.7184	-0.52797
C	4.82468	0.70398	-0.30481
H	5.32425	1.65653	-0.12155
C	5.53243	-0.4926	-0.32236
H	6.61009	-0.47883	-0.14705
C	4.87992	-1.70736	-0.56256
H	5.43798	-2.6439	-0.57382
C	3.50632	-1.69946	-0.78191
H	2.97152	-2.637	-0.95678
C	2.76935	-0.51005	-0.7714
C	1.30261	-0.5423	-0.95926
H	0.92572	-1.48158	-1.37614
C	-0.70248	0.6393	-0.87603
C	-1.65451	-0.16274	-1.7679
C	-2.06862	-2.27817	-2.71757

H	-2.25352	-1.85635	-3.71591
C	-1.39528	-3.62789	-2.78412
H	-2.03279	-4.33627	-3.32888
H	-1.21954	-4.02394	-1.77406
C	-1.0811	2.12482	-0.9776
C	-1.03792	4.19103	0.16639
H	-1.30975	4.48051	1.18802
H	-1.83396	4.50483	-0.52103
C	0.30558	4.76208	-0.23819
H	0.2739	5.85938	-0.20359
H	0.56138	4.45344	-1.26102
H	1.09237	4.41107	0.44327
N	0.68537	0.62153	-1.16239
O	2.78065	1.87431	-0.52836
O	-1.1997	-1.39402	-1.99865
O	-2.72602	0.2224	-2.15528
O	-0.98361	2.75815	0.19104
O	-1.31839	2.68325	-2.01483
H	-3.0334	-2.32049	-2.18993
H	-0.43063	-3.55511	-3.30448
H	1.80301	1.62354	-0.74652
C	-4.15886	-1.86702	0.96677
C	-4.98969	-0.87355	1.48661
C	-4.46333	0.39093	1.74976
C	-3.11955	0.65993	1.48872
C	-2.27578	-0.32849	0.96581
C	-2.81486	-1.5969	0.71139
C	-0.84141	0.0198	0.63038
C	0.16767	-1.06953	0.77397
S	1.24974	-0.91589	2.04585
O	1.77903	0.42999	2.17978
O	2.14122	-2.05493	2.15587
F	0.33864	-1.05231	3.41545
H	-4.55732	-2.86213	0.76137
H	-6.04044	-1.08597	1.68935
H	-5.10136	1.17447	2.16203
H	-2.71095	1.65227	1.6897
H	-2.18021	-2.38746	0.30629
H	-0.53253	0.86494	1.2556
H	-0.12196	-2.11611	0.66384

(*R*, *S*, *S*)-INT4

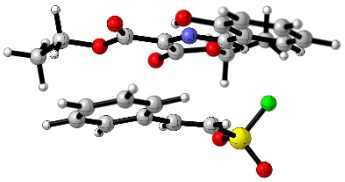


Charge = -1 Multiplicity = 1

C	-2.91686	0.82203	0.10264
C	-4.28473	1.0661	-0.26412
H	-4.49048	2.00872	-0.77795
C	-5.30616	0.16672	-0.00468
H	-6.32544	0.41053	-0.31776
C	-5.05208	-1.04448	0.65457
H	-5.85423	-1.75165	0.86771
C	-3.73955	-1.31187	1.04188
H	-3.51389	-2.24708	1.56448
C	-2.68549	-0.43264	0.78275
C	-1.29649	-0.81908	1.2524
H	-1.41154	-1.66461	1.94837
C	0.50578	0.77913	1.04555
C	1.87922	0.55133	1.68805
C	3.28642	-1.05389	2.67293
H	3.52003	-0.38977	3.51706
C	3.21725	-2.50284	3.09025
H	4.18225	-2.81514	3.50978
H	2.98871	-3.14742	2.22989
C	0.34664	2.29231	0.87313
C	0.72471	4.11988	-0.56885
H	1.59613	4.36641	-1.18784
H	0.77915	4.68813	0.36815
C	-0.57995	4.36846	-1.29726
H	-0.72587	5.44587	-1.45496
H	-1.41373	3.95422	-0.71543
H	-0.57467	3.86889	-2.27642
N	-0.5487	0.26269	1.90464
O	-1.99192	1.65652	-0.15942
O	2.0034	-0.68913	2.14615
O	2.75266	1.37814	1.74683
O	0.85858	2.72461	-0.26801
O	-0.11753	2.9954	1.73206
H	4.04338	-0.88117	1.89237
H	2.44055	-2.64855	3.8528

H	-1.17209	1.03045	2.14247
C	3.81363	-1.30691	-1.53388
C	4.05803	-0.45201	-2.60851
C	3.11714	0.52411	-2.93661
C	1.9486	0.65035	-2.1867
C	1.69723	-0.19181	-1.0963
C	2.64178	-1.1804	-0.78834
C	0.41845	-0.00595	-0.30751
C	-0.29071	-1.27479	0.15847
S	-1.10595	-2.14813	-1.15844
O	-1.67924	-1.27851	-2.15192
O	-1.82347	-3.29049	-0.65258
F	0.20576	-2.76637	-1.86005
H	4.5348	-2.08423	-1.2761
H	4.97369	-0.55237	-3.19325
H	3.29155	1.1909	-3.78252
H	1.21578	1.41794	-2.43949
H	2.46377	-1.87398	0.03462
H	-0.30317	0.56679	-0.90291
H	0.40249	-2.01907	0.57563

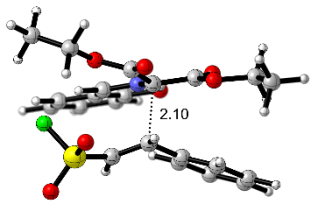
(*S*, *R*, *S*)-INT1



Charge = -1 Multiplicity = 1

C	1.6565	2.9549	-0.94979
C	2.46694	4.08797	-0.78539
H	1.99	5.06831	-0.83636
C	3.83564	3.96037	-0.56148
H	4.4451	4.85722	-0.43583
C	4.42644	2.6947	-0.49403
H	5.49715	2.59205	-0.31393
C	3.62899	1.56567	-0.65893
H	4.0704	0.56649	-0.6039
C	2.24837	1.66307	-0.89154
C	1.44338	0.44784	-1.0445
H	1.96888	-0.51078	-0.99171
C	-0.84052	-0.36687	-1.23904
C	-0.67124	-1.81046	-1.25303
C	0.90879	-3.54625	-1.59966
H	0.16928	-3.98109	-2.28753
C	2.3141	-3.67996	-2.14383
H	2.5529	-4.73962	-2.30825
H	3.04405	-3.26323	-1.43788
C	-2.15	0.27648	-1.28067
C	-4.49001	0.05361	-1.20776
H	-4.64081	0.48055	-2.21224
H	-4.54021	0.88708	-0.49179
C	-5.51467	-1.01361	-0.89662
H	-6.5289	-0.59696	-0.95746
H	-5.36071	-1.40972	0.11719
H	-5.43527	-1.84668	-1.60865
N	0.16687	0.55165	-1.20572
O	0.34691	3.11359	-1.15445
O	0.63009	-2.15972	-1.4341
O	-1.52707	-2.6713	-1.14726
O	-3.20558	-0.55061	-1.1391
O	-2.31696	1.47787	-1.41609
H	0.79873	-4.05391	-0.63047
H	2.4086	-3.14996	-3.10201
H	-0.06351	2.18755	-1.21207
C	-1.59366	2.97396	1.6415
C	-2.9623	2.82248	1.87017
C	-3.51157	1.5449	1.99516
C	-2.69273	0.42365	1.89757
C	-1.31219	0.56917	1.68935
C	-0.77058	1.85607	1.55237
C	-0.48129	-0.63419	1.62121
C	0.86069	-0.64305	1.72519
S	1.67883	-2.15836	1.8554
O	0.79992	-3.27408	1.60365
O	2.56858	-2.16488	2.98947
F	2.67831	-2.10138	0.59428
H	-1.16473	3.96921	1.51825
H	-3.6042	3.70193	1.94183
H	-4.58242	1.42262	2.1664
H	-3.11872	-0.57811	1.9838
H	0.29613	1.98296	1.35534
H	-1.00479	-1.59162	1.53535
H	1.50726	0.22076	1.88278

(*S*, *R*, *S*)-TS1

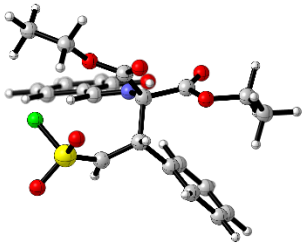


Charge = -1 Multiplicity = 1

Imaginary frequency = -322.9305 cm^{-1}

C	-2.19296	-2.70825	-0.89209
C	-3.13677	-3.74363	-0.79499
H	-2.7987	-4.76366	-0.98376
C	-4.45956	-3.46851	-0.4662
H	-5.17525	-4.28986	-0.39676
C	-4.87799	-2.15451	-0.22348
H	-5.91545	-1.94287	0.03629
C	-3.95042	-1.12373	-0.31818
H	-4.25178	-0.0901	-0.12826
C	-2.60948	-1.37094	-0.65028
C	-1.65623	-0.26002	-0.71996
H	-2.03257	0.74223	-0.49741
C	0.66152	0.3261	-0.96958
C	0.60105	1.79054	-1.22584
C	-0.85153	3.61746	-1.56336
H	-0.18488	3.98525	-2.35665
C	-2.30663	3.84765	-1.89772
H	-2.48984	4.92053	-2.04481
H	-2.94496	3.49103	-1.07894
C	1.89175	-0.40506	-1.38508
C	4.23159	-0.38907	-1.55865
H	4.20665	-0.70563	-2.61212
H	4.28828	-1.29894	-0.94237
C	5.378	0.55461	-1.28185
H	6.33167	0.06815	-1.52527
H	5.39587	0.84378	-0.22183
H	5.28461	1.46532	-1.8889
N	-0.43417	-0.50786	-1.0461
O	-0.93148	-3.0034	-1.20415
O	-0.65538	2.20954	-1.41345
O	1.54021	2.55233	-1.23487
O	3.01899	0.29845	-1.25078
O	1.89591	-1.56336	-1.74121
H	-0.56029	4.10318	-0.62095
H	-2.581	3.3189	-2.82113
H	-0.42074	-2.12589	-1.23245
C	1.41466	-3.25381	1.64343
C	2.79814	-3.31237	1.82224
C	3.54939	-2.13694	1.78524
C	2.92127	-0.91251	1.5607
C	1.53311	-0.84448	1.37987
C	0.78498	-2.03014	1.42858
C	0.88808	0.46611	1.116
C	-0.36488	0.70229	1.70524
S	-0.90334	2.26181	1.98496
O	0.05572	3.2673	1.5617
O	-1.58237	2.39903	3.25861
F	-2.15778	2.50826	0.94731
H	0.82042	-4.16881	1.66435
H	3.28906	-4.27201	1.99107
H	4.63079	-2.17228	1.92902
H	3.51004	0.00631	1.52154
H	-0.29545	-1.99717	1.27475
H	1.5749	1.31419	1.03422
H	-0.98409	-0.06362	2.16699

(*S*, *R*, *S*)-INT2

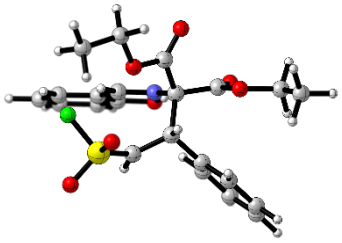


Charge = -1 Multiplicity = 1

C	-2.61519	-2.67826	-0.60117
C	-3.65019	-3.61956	-0.48092
H	-3.47202	-4.63082	-0.84866
C	-4.86367	-3.26046	0.09311
H	-5.65478	-4.00794	0.17694
C	-5.08362	-1.95869	0.5631
H	-6.03877	-1.68671	1.01215
C	-4.06525	-1.02206	0.44782
H	-4.20731	-0.00005	0.80829
C	-2.82947	-1.35787	-0.1265
C	-1.77441	-0.3482	-0.22188
H	-1.99383	0.64824	0.17508
C	0.49839	0.18238	-0.81088
C	0.29153	1.57172	-1.45093
C	-1.25115	3.3136	-1.77597

H	-0.80115	3.53254	-2.75442
C	-2.75005	3.48799	-1.78024
H	-3.00149	4.5228	-2.0484
H	-3.15019	3.27259	-0.78141
C	1.55849	-0.58281	-1.62569
C	3.84883	-0.76747	-2.09359
H	3.67505	-0.90463	-3.17049
H	3.85959	-1.76488	-1.62718
C	5.11559	0.00361	-1.81274
H	5.97828	-0.53217	-2.22951
H	5.26377	0.11745	-0.73015
H	5.06934	1.00154	-2.26904
N	-0.6535	-0.66343	-0.7579
O	-1.45843	-3.04355	-1.15229
O	-0.97282	1.94627	-1.44028
O	1.19315	2.24826	-1.87055
O	2.75652	-0.02694	-1.53873
O	1.34052	-1.60558	-2.22222
H	-0.76169	3.93632	-1.01346
H	-3.21898	2.81587	-2.51215
H	-0.87289	-2.21615	-1.17965
C	2.21716	-3.07984	1.62059
C	3.47474	-2.8348	2.16887
C	3.96203	-1.52657	2.21027
C	3.19332	-0.47931	1.70689
C	1.92798	-0.71372	1.15345
C	1.44652	-2.02802	1.11786
C	1.12061	0.47152	0.64517
C	0.15212	0.88921	1.70145
S	-0.34898	2.42392	1.8678
O	0.44352	3.37479	1.08477
O	-0.77183	2.78227	3.21737
F	-1.85699	2.63202	1.09849
H	1.82725	-4.0983	1.57935
H	4.07486	-3.65801	2.55954
H	4.94706	-1.3216	2.63314
H	3.57924	0.5426	1.73657
H	0.47341	-2.24193	0.6732
H	1.82875	1.29066	0.45826
H	-0.32333	0.1771	2.37308

(*S*, *R*, *S*)-INT3

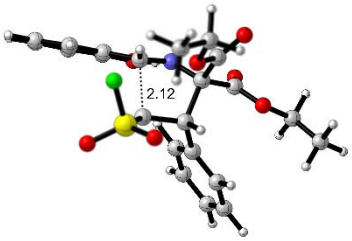


Charge = -1 Multiplicity = 1

C	-2.82002	-2.56273	-0.63317
C	-3.96322	-3.36301	-0.48051
H	-3.85822	-4.44141	-0.60528
C	-5.18917	-2.78463	-0.17449
H	-6.06533	-3.42527	-0.05871
C	-5.31461	-1.39843	-0.0096
H	-6.27972	-0.95598	0.23664
C	-4.18987	-0.59935	-0.16145
H	-4.25121	0.48347	-0.02648
C	-2.94136	-1.15793	-0.47669
C	-1.77223	-0.29227	-0.60886
H	-1.92066	0.78527	-0.45329
C	0.56075	0.00511	-0.8621
C	0.40509	1.23461	-1.76688
C	-0.35652	3.44341	-1.95097
H	-0.87712	3.16451	-2.87797
C	-1.12692	4.45509	-1.13885
H	-1.16007	5.40565	-1.6882
H	-0.64098	4.59925	-0.166
C	1.70056	-0.81555	-1.47212
C	4.02756	-0.83572	-1.78974
H	3.9358	-1.1858	-2.8279
H	4.10323	-1.72223	-1.14078
C	5.19644	0.10088	-1.60464
H	6.12898	-0.40973	-1.87788
H	5.26908	0.42355	-0.55701
H	5.08529	0.9893	-2.24081
N	-0.62643	-0.8005	-0.88359
O	-1.6511	-3.13799	-0.91659
O	-0.17145	2.25497	-1.16127
O	0.74046	1.23639	-2.92507
O	2.83573	-0.12665	-1.43457
O	1.60731	-1.94005	-1.88417
H	0.64042	3.81401	-2.23172
H	-2.15075	4.10986	-0.95247
H	-0.97113	-2.39837	-1.00901
C	2.16879	-2.99186	1.93127

C	3.44749	-2.68351	2.39731
C	3.92158	-1.37526	2.28926
C	3.12062	-0.38575	1.71883
C	1.83643	-0.68386	1.25088
C	1.369	-1.99982	1.36349
C	0.96305	0.40538	0.64615
C	-0.17302	0.67356	1.57266
S	-0.73245	2.14908	1.94873
O	0.18839	3.24532	1.64883
O	-1.47321	2.17815	3.20806
F	-2.0218	2.55549	0.91872
H	1.79033	-4.01262	2.00745
H	4.07278	-3.4599	2.84081
H	4.92123	-1.12336	2.64782
H	3.49766	0.6359	1.62956
H	0.37627	-2.25401	0.98344
H	1.56685	1.31855	0.55515
H	-0.74394	-0.13316	2.02918

(*S*, *R*, *S*)-TS2

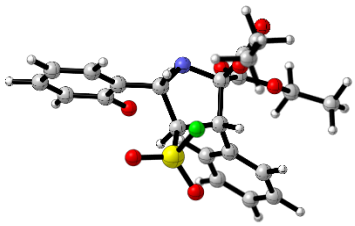


Charge = -1 Multiplicity = 1

Imaginary frequency = -314.1367 cm^{-1}

C	-2.50231	-2.36614	-1.12626
C	-3.60721	-3.22908	-1.03577
H	-3.46176	-4.27871	-1.29572
C	-4.8462	-2.75068	-0.62234
H	-5.69057	-3.43968	-0.55741
C	-5.01829	-1.40228	-0.28889
H	-5.98988	-1.03327	0.04073
C	-3.9298	-0.54052	-0.38136
H	-4.02728	0.5137	-0.10871
C	-2.67438	-0.99756	-0.79979
C	-1.5226	-0.07248	-0.8429
H	-1.78709	0.99045	-0.85129
C	0.73943	0.23109	-0.99517
C	0.71775	1.65773	-1.55719
C	-0.1081	3.84484	-1.29671
H	-0.44671	3.82489	-2.34213
C	-1.05964	4.59736	-0.39854
H	-1.05618	5.66042	-0.67385
H	-0.75554	4.48821	0.65059
C	2.0224	-0.4286	-1.48667
C	4.36092	-0.36068	-1.26929
H	4.52464	-0.50343	-2.34723
H	4.33518	-1.35621	-0.79878
C	5.40906	0.52966	-0.64709
H	6.4047	0.09018	-0.79101
H	5.22877	0.64036	0.43101
H	5.39655	1.52528	-1.11083
N	-0.39146	-0.52129	-1.38052
O	-1.31898	-2.84387	-1.51791
O	-0.00828	2.49253	-0.82272
O	1.25186	1.97271	-2.59134
O	3.08578	0.25698	-1.07211
O	2.08904	-1.45633	-2.10531
H	0.90162	4.28101	-1.28503
H	-2.08018	4.20707	-0.49609
H	-0.68602	-2.02105	-1.55584
C	1.95686	-3.25796	1.44904
C	3.12159	-2.9973	2.17274
C	3.50462	-1.67585	2.40652
C	2.72666	-0.62574	1.91834
C	1.55544	-0.87617	1.19451
C	1.17883	-2.20653	0.96438
C	0.73049	0.26803	0.64599
C	-0.69581	0.1919	1.08808
S	-1.34448	1.48777	1.95811
O	-0.42321	2.57527	2.24187
O	-2.26259	1.04027	2.98982
F	-2.3866	2.20504	0.90238
H	1.65172	-4.28805	1.25704
H	3.7285	-3.82075	2.55247
H	4.41383	-1.46012	2.97061
H	3.03326	0.40776	2.09607
H	0.28127	-2.41798	0.37792
H	1.18755	1.2158	0.95511
H	-1.04232	-0.72511	1.56653

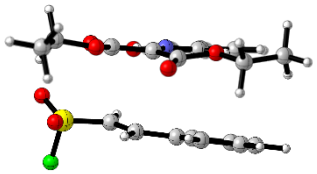
(*S*, *R*, *S*)-INT4



Charge = -1 Multiplicity = 1

C	-2.58758	-2.03768	-1.0003
C	-3.77061	-2.80847	-1.23764
H	-3.641	-3.8837	-1.38539
C	-5.03357	-2.23247	-1.28052
H	-5.90359	-2.86884	-1.46566
C	-5.21164	-0.85566	-1.09115
H	-6.20526	-0.4075	-1.12325
C	-4.07941	-0.07107	-0.85859
H	-4.18795	1.00684	-0.70087
C	-2.80264	-0.62444	-0.81284
C	-1.59576	0.22867	-0.54311
H	-1.88821	1.28747	-0.4654
C	0.6959	0.50355	-1.00676
C	0.83922	1.99564	-1.32705
C	0.12621	4.16033	-0.73408
H	-0.31098	4.30252	-1.73265
C	-0.69972	4.80955	0.34916
H	-0.74907	5.89238	0.17573
H	-0.25312	4.63048	1.33617
C	1.85191	-0.23728	-1.66732
C	4.17683	-0.54883	-1.54867
H	4.26016	-0.65923	-2.63893
H	4.02425	-1.55002	-1.11394
C	5.37216	0.15158	-0.95064
H	6.2823	-0.42621	-1.1576
H	5.25612	0.24427	0.13786
H	5.48952	1.15479	-1.38214
N	-0.57063	0.08622	-1.58071
O	-1.41669	-2.54967	-0.95655
O	0.18155	2.75245	-0.46064
O	1.40507	2.42041	-2.29976
O	3.01447	0.23678	-1.25023
O	1.71903	-1.17417	-2.40838
H	1.15471	4.54744	-0.76126
H	-1.72108	4.40642	0.35206
H	-0.50459	-0.91891	-1.78351
C	2.33279	-3.19206	1.0115
C	3.44584	-2.85169	1.78147
C	3.63449	-1.52558	2.17345
C	2.71667	-0.54805	1.79077
C	1.60224	-0.8814	1.01455
C	1.41195	-2.21546	0.62807
C	0.65152	0.20287	0.55337
C	-0.82997	-0.16762	0.7539
S	-1.4879	0.54336	2.23062
O	-0.59685	0.3485	3.34761
O	-2.90116	0.30228	2.36416
F	-1.35709	2.10423	1.8591
H	2.17745	-4.22791	0.70519
H	4.16263	-3.61857	2.07927
H	4.49936	-1.25032	2.77942
H	2.87053	0.49111	2.09079
H	0.53932	-2.48588	0.0231
H	0.89294	1.12902	1.08959
H	-0.95422	-1.25021	0.90958

(*S*, *R*, *R*)-INT1

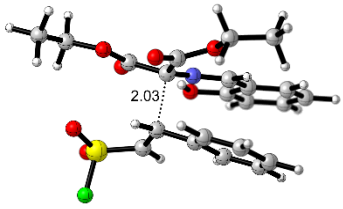


Charge = -1 Multiplicity = 1

C	1.91522	-2.25858	-1.36705
C	2.70163	-3.41784	-1.42654
H	2.19147	-4.37621	-1.53771
C	4.09014	-3.34269	-1.34358
H	4.68182	-4.25866	-1.39347
C	4.72283	-2.10469	-1.19589
H	5.80962	-2.04286	-1.12822
C	3.94638	-0.95042	-1.13199
H	4.42295	0.02537	-1.00242
C	2.54756	-0.99466	-1.21741
C	1.76087	0.23568	-1.08714
H	2.30766	1.15714	-0.85134
C	-0.52608	1.09279	-1.04467
C	-0.34813	2.47409	-0.6392
C	1.26481	4.16089	-0.25326
H	0.9344	4.26285	0.79306
C	2.75861	4.35204	-0.38933
H	3.04858	5.35236	-0.04088

H	3.06623	4.2454	-1.43891
C	-1.83137	0.51096	-1.29325
C	-4.14663	0.82465	-1.59054
H	-4.31885	-0.10458	-1.03387
H	-4.14728	0.57683	-2.66471
C	-5.18774	1.87092	-1.26349
H	-6.18803	1.51147	-1.53987
H	-4.98913	2.80444	-1.80808
H	-5.18106	2.08932	-0.18637
N	0.48081	0.17911	-1.20999
O	0.58391	-2.37043	-1.43642
O	0.95306	2.85816	-0.72164
O	-1.18938	3.26036	-0.23838
O	-2.87579	1.35982	-1.23596
O	-2.00785	-0.67345	-1.55819
H	0.70424	4.90639	-0.83791
H	3.2979	3.60236	0.20757
H	0.20433	-1.42812	-1.4044
C	2.98754	-0.17782	2.23741
C	3.16907	1.18862	2.4633
C	2.07247	2.05211	2.43361
C	0.79888	1.55154	2.17469
C	0.60845	0.18225	1.93786
C	1.71627	-0.67803	1.97508
C	-0.74442	-0.30079	1.64804
C	-1.05073	-1.52276	1.18748
S	-2.7201	-1.9497	1.00357
O	-2.92814	-2.97896	0.02077
O	-3.5904	-0.8027	1.11274
F	-2.93655	-2.72338	2.40729
H	3.84195	-0.8557	2.25878
H	4.16676	1.58056	2.66796
H	2.21187	3.11938	2.61426
H	-0.06133	2.22476	2.13476
H	1.58517	-1.74757	1.79861
H	-1.56321	0.40302	1.82921
H	-0.35833	-2.30817	0.88311

(*S*, *R*, *R*)-TS1



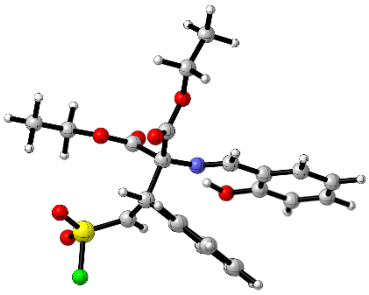
Charge = -1 Multiplicity = 1

Imaginary frequency = -367.6950 cm^{-1}

C	2.33143	-2.54572	-0.97126
C	3.2634	-3.59653	-0.9494
H	2.88762	-4.61617	-1.04582
C	4.62139	-3.33631	-0.80661
H	5.32625	-4.16975	-0.7933
C	5.09062	-2.02299	-0.67804
H	6.15629	-1.82442	-0.56263
C	4.17585	-0.97716	-0.69707
H	4.51641	0.05647	-0.59178
C	2.80039	-1.21027	-0.8474
C	1.8613	-0.08645	-0.82347
H	2.28014	0.91061	-0.64081
C	-0.49291	0.52527	-0.86352
C	-0.41609	2.00929	-0.98563
C	1.04821	3.85167	-1.19777
H	0.56396	4.26334	-0.30059
C	2.54166	4.07828	-1.18281
H	2.75815	5.15473	-1.18259
H	3.01309	3.62769	-2.067
C	-1.69417	-0.15878	-1.43101
C	-3.92661	-0.00936	-2.13458
H	-4.12387	-0.8788	-1.49649
H	-3.7583	-0.36342	-3.1638
C	-5.04451	1.00322	-2.06044
H	-5.97756	0.56239	-2.4358
H	-4.81085	1.89187	-2.66284
H	-5.19889	1.31483	-1.01838
N	0.61171	-0.31011	-1.00237
O	1.03672	-2.82804	-1.10021
O	0.82612	2.44049	-1.23491
O	-1.33555	2.77363	-0.80589
O	-2.73604	0.63094	-1.67041
O	-1.72719	-1.35741	-1.60711
H	0.5679	4.31035	-2.07514
H	2.98513	3.63264	-0.28052
H	0.53655	-1.94799	-1.1136
C	2.5707	0.88399	2.54737
C	2.57574	2.26767	2.71914
C	1.43567	3.00676	2.39346
C	0.3078	2.36622	1.88636
C	0.29507	0.97533	1.69045
C	1.43942	0.24338	2.04116

C	-0.90744	0.31748	1.11095
C	-1.16161	-1.04197	1.41378
S	-2.70914	-1.63031	1.38614
O	-2.80458	-3.04652	1.07922
O	-3.66886	-0.69334	0.81586
F	-3.18765	-1.63528	2.96758
H	3.45228	0.29531	2.80657
H	3.4603	2.76892	3.11509
H	1.42404	4.08859	2.53813
H	-0.58041	2.94626	1.62893
H	1.45299	-0.84016	1.91624
H	-1.78899	0.96659	1.07107
H	-0.40604	-1.79252	1.63076

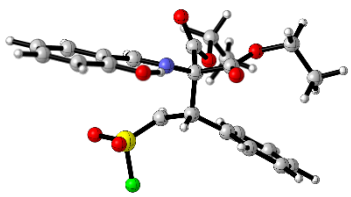
(*S*, *R*, *R*)-INT2



Charge = -1 Multiplicity = 1

C	3.22771	-0.44869	-1.92941
C	4.43482	-0.89545	-2.49031
H	4.40012	-1.383	-3.46516
C	5.63304	-0.71494	-1.81165
H	6.56027	-1.06828	-2.26632
C	5.66757	-0.09025	-0.55708
H	6.6131	0.04372	-0.03208
C	4.47921	0.35044	0.00712
H	4.47736	0.83352	0.98718
C	3.25489	0.1853	-0.65994
C	2.01182	0.61964	-0.03042
H	2.09178	1.02663	0.99315
C	-0.36121	0.74219	0.01228
C	-0.30695	1.80399	1.12397
C	0.36856	4.00845	1.60682
H	0.92061	3.66495	2.49342
C	1.06863	5.14548	0.9042
H	1.15746	6.00235	1.58435
H	0.5017	5.46026	0.01799
C	-1.34856	1.25255	-1.04923
C	-3.62911	1.7168	-1.3558
H	-3.74009	0.77955	-1.92407
H	-3.4102	2.52715	-2.06565
C	-4.84211	2.00175	-0.50587
H	-5.72151	2.14075	-1.14863
H	-4.69571	2.91549	0.08647
H	-5.01901	1.1524	0.16582
N	0.89474	0.49645	-0.63591
O	2.08968	-0.63708	-2.5951
O	0.27214	2.91458	0.68128
O	-0.75406	1.67747	2.23172
O	-2.50706	1.55394	-0.47824
O	-1.11497	1.35129	-2.22151
H	-0.64662	4.28004	1.92954
H	2.07649	4.84371	0.58912
H	1.35464	-0.22381	-2.04657
C	1.95114	-2.86498	1.57628
C	1.92873	-2.74339	2.96766
C	0.96226	-1.94012	3.5711
C	0.02876	-1.25568	2.78926
C	0.04009	-1.36947	1.39461
C	1.01162	-2.18884	0.80097
C	-0.96933	-0.6159	0.54273
C	-1.54581	-1.38456	-0.60916
S	-3.09866	-1.83923	-0.61777
O	-3.61257	-2.16553	-1.94878
O	-3.95561	-1.08065	0.2981
F	-3.24546	-3.35946	0.09354
H	2.70361	-3.49021	1.0923
H	2.66087	-3.27549	3.57729
H	0.93229	-1.84346	4.65785
H	-0.71615	-0.61399	3.26193
H	1.03985	-2.28204	-0.28725
H	-1.80286	-0.30671	1.18683
H	-0.94844	-1.79402	-1.42202

(*S*, *R*, *R*)-INT3

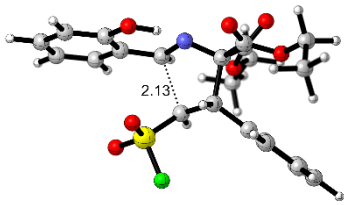


Charge = -1 Multiplicity = 1

C	3.76127	1.49517	-0.7419

C	5.11186	1.64669	-1.09508
H	5.34984	2.25001	-1.97201
C	6.10841	1.03779	-0.34223
H	7.15186	1.16858	-0.63504
C	5.79241	0.2602	0.77964
H	6.58047	-0.21744	1.36162
C	4.45919	0.10472	1.13516
H	4.18511	-0.50423	2.0002
C	3.43411	0.71294	0.39584
C	2.03827	0.50676	0.77453
H	1.84492	-0.15813	1.62748
C	-0.28284	0.76267	0.34728
C	-0.61742	0.61722	1.84033
C	-2.1069	-0.27086	3.42107
H	-2.39601	0.72998	3.77425
C	-3.26375	-1.24012	3.45632
H	-3.65023	-1.31705	4.48091
H	-2.94491	-2.24044	3.13182
C	-1.09429	1.93206	-0.22966
C	-3.01845	3.27773	0.0812
H	-2.3869	4.11582	-0.24214
H	-3.56269	3.56751	0.98716
C	-3.96034	2.83618	-1.01748
H	-4.67963	3.63903	-1.22963
H	-4.51392	1.93673	-0.71241
H	-3.4053	2.60773	-1.93625
N	1.10038	1.07655	0.11819
O	2.82368	2.0856	-1.47969
O	-1.66643	-0.15763	2.0621
O	-0.00417	1.17446	2.71344
O	-2.165	2.20215	0.50536
O	-0.78982	2.51649	-1.23485
H	-1.26291	-0.61101	4.0376
H	-4.07622	-0.89829	2.80052
H	1.93495	1.85623	-1.06361
C	-4.28146	-1.58608	-0.72531
C	-4.65275	-0.99482	-1.93554
C	-3.70807	-0.27247	-2.66146
C	-2.40844	-0.13232	-2.17158
C	-2.02622	-0.71065	-0.9546
C	-2.97997	-1.45153	-0.24552
C	-0.58171	-0.56544	-0.49127
C	0.01761	-1.73696	0.21115
S	1.25029	-2.55936	-0.45519
O	1.94216	-3.44055	0.48272
O	2.04241	-1.78189	-1.41038
F	0.63263	-3.71831	-1.50694
H	-5.00945	-2.16567	-0.15447
H	-5.67025	-1.10749	-2.31342
H	-3.97987	0.1856	-3.61419
H	-1.67258	0.43557	-2.74604
H	-2.69505	-1.92989	0.69035
H	0.0097	-0.38792	-1.40045
H	-0.45759	-2.2389	1.05105

(*S, R, R*)-TS2



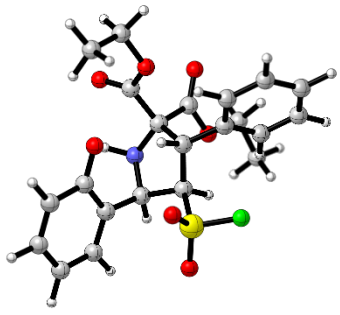
Charge = -1 Multiplicity = 1

Imaginary frequency = -236.7922 cm^{-1}

C	-3.41527	1.5448	-0.09349
C	-4.76816	1.73189	0.24274
H	-5.0602	2.69088	0.67361
C	-5.69896	0.72164	0.02953
H	-6.74314	0.89132	0.30014
C	-5.3128	-0.50359	-0.52661
H	-6.04554	-1.29412	-0.69031
C	-3.97681	-0.69595	-0.86269
H	-3.64675	-1.64908	-1.28477
C	-3.01965	0.30401	-0.65926
C	-1.59851	0.05638	-0.98113
H	-1.42802	-0.80576	-1.63913
C	0.5885	0.78261	-0.82163
C	1.12167	0.09976	-2.08435
C	1.11933	-1.89137	-3.34851
H	2.21529	-1.9042	-3.44298
C	0.53941	-3.28169	-3.24484
H	0.7794	-3.85264	-4.15116
H	-0.55338	-3.23829	-3.1396
C	1.39052	2.06091	-0.56795
C	3.5647	2.97048	-0.42371
H	3.12618	3.83827	-0.934
H	4.50013	2.69681	-0.92572
C	3.79049	3.25902	1.0461

H	4.45856	4.12473	1.15246
H	4.2554	2.39826	1.54515
H	2.83935	3.49282	1.54351
N	-0.78177	1.10834	-0.95984
O	-2.54651	2.52881	0.1051
O	0.77691	-1.18525	-2.14885
O	1.68358	0.67376	-2.98171
O	2.7003	1.84359	-0.61851
O	0.89732	3.12579	-0.30225
H	0.71716	-1.33776	-4.2085
H	0.95419	-3.81748	-2.37977
H	-1.6397	2.17183	-0.25273
C	3.71655	-2.44009	0.59067
C	4.51976	-1.79301	1.53026
C	4.05436	-0.62814	2.14045
C	2.80311	-0.11537	1.80126
C	1.993	-0.7447	0.84781
C	2.46449	-1.92424	0.25563
C	0.64617	-0.13758	0.51757
C	-0.51593	-1.07619	0.46892
S	-1.50045	-1.12274	1.82695
O	-2.55151	-2.11615	1.71208
O	-1.80954	0.19663	2.34966
F	-0.56128	-1.7481	3.03106
H	4.06344	-3.35967	0.11615
H	5.49795	-2.19936	1.79188
H	4.66539	-0.11655	2.88651
H	2.44339	0.79651	2.28447
H	1.84427	-2.44905	-0.47022
H	0.42414	0.61119	1.29336
H	-0.3767	-2.08541	0.07495

(*S*, *R*, *R*)-INT4

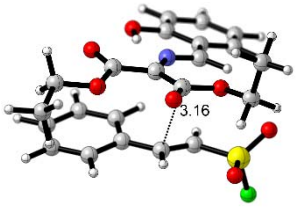


Charge = -1 Multiplicity = 1

C	2.91691	0.82208	0.10247
C	4.28477	1.06605	-0.26435
H	4.49055	2.00856	-0.77839
C	5.30618	0.1667	-0.00473
H	6.32546	0.41043	-0.31788
C	5.05209	-1.04435	0.65477
H	5.85422	-1.75149	0.86804
C	3.73955	-1.31162	1.04218
H	3.51388	-2.24672	1.56498
C	2.68553	-0.43241	0.78288
C	1.29649	-0.81873	1.2525
H	1.41144	-1.66414	1.94863
C	-0.50593	0.77933	1.04539
C	-1.87939	0.55136	1.68778
C	-3.2862	-1.05399	2.67308
H	-4.04313	-0.88142	1.89247
C	-3.21673	-2.50293	3.09037
H	-4.18168	-2.81549	3.50981
H	-2.44005	-2.64849	3.85296
C	-0.34704	2.29252	0.87287
C	-0.72528	4.11991	-0.56919
H	-0.78057	4.68831	0.36767
H	-1.59628	4.36617	-1.18889
C	0.57989	4.36866	-1.29665
H	0.72564	5.44608	-1.45443
H	0.57544	3.86892	-2.27572
H	1.41333	3.9547	-0.71413
N	0.5486	0.26309	1.90453
O	1.99194	1.65647	-0.15978
O	-2.00322	-0.68893	2.14641
O	-2.75316	1.37788	1.74593
O	-0.85917	2.72466	-0.26824
O	0.11709	2.99576	1.7317
H	-3.52001	-0.38994	3.51721
H	-2.98796	-3.14742	2.23
H	1.1719	1.03098	2.14217
C	-3.81348	-1.30766	-1.53349
C	-4.05817	-0.45293	-2.6082
C	-3.11753	0.52333	-2.93652
C	-1.94892	0.64992	-2.18676
C	-1.69726	-0.19207	-1.09629
C	-2.64157	-1.18082	-0.78811
C	-0.41846	-0.00588	-0.30761
C	0.29087	-1.27459	0.15848
S	1.10631	-2.14792	-1.15832
O	1.82381	-3.29022	-0.65234

O	1.67966	-1.27831	-2.15178
F	-0.20529	-2.76627	-1.86005
H	-4.53446	-2.0851	-1.27555
H	-4.97388	-0.55356	-3.19283
H	-3.29217	1.18999	-3.78249
H	-1.21628	1.41761	-2.43974
H	-2.46333	-1.87428	0.0349
H	0.30306	0.56691	-0.90311
H	-0.40226	-2.01895	0.57561

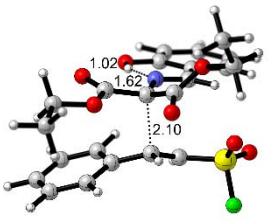
(*R, S, R*)-SUB



Charge = -1 Multiplicity = 1

C	2.06674	-2.67332	-1.04769
C	3.0247	-3.69117	-0.928
H	2.68202	-4.72513	-0.99643
C	4.3684	-3.38654	-0.7254
H	5.0949	-4.19629	-0.63534
C	4.78613	-2.05509	-0.63388
H	5.83706	-1.81437	-0.46967
C	3.8418	-1.03929	-0.75387
H	4.14552	0.00854	-0.67777
C	2.48211	-1.31554	-0.96628
C	1.5197	-0.21412	-1.06962
H	1.91823	0.80265	-0.99025
C	0.88186	0.71295	1.67247
H	1.64548	-0.06526	1.68572
C	-0.86433	0.27759	-1.21885
C	-0.45085	0.5397	1.69121
H	-1.08832	1.42933	1.70321
C	-0.9133	1.72685	-1.20503
C	0.44137	3.68018	-1.32723
H	1.41356	3.94494	-0.89222
H	0.25369	-2.14024	-1.26037
C	0.36236	4.06352	-2.79225
H	0.50479	5.14701	-2.90896
H	-0.62077	3.79656	-3.20271
C	-2.06512	-0.55514	-1.25232
C	-4.40605	-0.69702	-1.06967
H	-4.2751	-1.57766	-0.42425
H	-4.56632	-1.06656	-2.09544
C	-5.55406	0.17059	-0.60631
H	-6.49572	-0.39334	-0.64325
H	-5.65303	1.05848	-1.24592
H	-5.389	0.5057	0.42768
C	-1.13032	-0.75585	1.73929
C	-2.5107	-0.78201	1.99369
H	-3.04486	0.15881	2.14185
C	-3.1928	-1.99344	2.05682
H	-4.26474	-2.00373	2.26164
C	-2.50544	-3.19153	1.85255
H	-3.04	-4.1418	1.8961
C	-1.13646	-3.17237	1.58051
H	-0.60039	-4.10395	1.39475
C	-0.4497	-1.96396	1.52482
H	0.61742	-1.95893	1.29288
N	0.26584	-0.48498	-1.2115
O	0.48895	3.32297	1.64904
O	0.78617	-3.00255	-1.23157
O	2.67889	2.43423	0.7875
O	0.33906	2.26912	-1.15774
O	-1.89229	2.45118	-1.24753
O	-3.22552	0.09401	-1.03327
O	-2.05119	-1.76237	-1.42876
S	1.52316	2.31815	1.6434
H	-0.34617	4.17302	-0.74424
H	1.14111	3.54648	-3.37035
F	2.14785	2.37307	3.12758

(*R, S, R*)-TS1



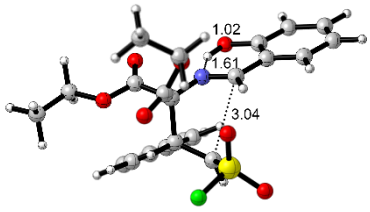
Charge = -1 Multiplicity = 1

Imaginary frequency = -283.7705 cm^{-1}

C	2.67788	-2.02995	-1.37125
C	3.79125	-2.87549	-1.48758
H	3.62938	-3.8895	-1.85614
C	5.06006	-2.42626	-1.13551
H	5.91228	-3.10147	-1.23268
C	5.25063	-1.12466	-0.65736

H	6.24569	-0.77902	-0.37614
C	4.15259	-0.27951	-0.54217
H	4.27145	0.73519	-0.15485
C	2.86382	-0.70445	-0.89695
C	1.72148	0.19588	-0.73471
H	1.92889	1.2073	-0.36484
C	0.52178	-0.02587	1.7841
H	1.06033	-0.94703	1.9967
C	-0.63273	0.44715	-0.79637
C	-0.78153	0.03782	1.26115
H	-1.36284	0.94801	1.43413
C	-0.74645	1.94308	-0.7495
C	0.36305	3.97131	-1.21915
H	1.42555	4.21071	-1.35397
H	0.81817	-1.7204	-1.57453
C	-0.49148	4.66394	-2.26175
H	-0.35867	5.75232	-2.19074
H	-1.55243	4.43032	-2.1042
C	-1.79939	-0.28712	-1.36363
C	-4.1347	-0.42839	-1.53391
H	-4.0864	-1.4456	-1.11696
H	-4.12233	-0.5175	-2.63064
C	-5.34833	0.32401	-1.04257
H	-6.26392	-0.1859	-1.36999
H	-5.35716	1.34806	-1.44018
H	-5.35162	0.37555	0.05517
C	-1.5719	-1.21895	1.26529
C	-2.93184	-1.19196	1.60034
H	-3.39851	-0.23943	1.86014
C	-3.68564	-2.3654	1.60607
H	-4.74286	-2.32871	1.87517
C	-3.09033	-3.58086	1.26566
H	-3.67931	-4.49934	1.26689
C	-1.73851	-3.6141	0.91586
H	-1.27083	-4.55828	0.63192
C	-0.98468	-2.44319	0.9136
H	0.0588	-2.46694	0.5911
N	0.54576	-0.19043	-1.10292
O	0.83562	2.54739	1.56699
O	1.46841	-2.4901	-1.70149
O	2.77203	1.15133	2.35584
O	0.28968	2.5487	-1.34099
O	-1.66172	2.55424	-0.25212
O	-2.97623	0.29231	-1.11272
O	-1.71107	-1.34354	-1.94863
S	1.34101	1.35599	2.23209
H	0.06483	4.24657	-0.19951
H	-0.20164	4.34502	-3.27253
F	0.90361	1.63471	3.78676

(*R*, *S*, *R*)-INT2

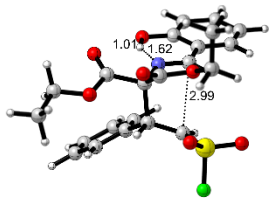


Charge = -1 Multiplicity = 1

C	3.18563	-1.53211	-1.15783
C	4.46282	-2.09697	-1.31316
H	4.53238	-3.10588	-1.72174
C	5.59764	-1.38129	-0.95305
H	6.57975	-1.83982	-1.08296
C	5.49851	-0.08563	-0.42762
H	6.39466	0.46748	-0.14666
C	4.24074	0.48005	-0.26896
H	4.13397	1.48667	0.14279
C	3.07746	-0.21962	-0.62544
C	1.76377	0.39241	-0.427
H	1.72482	1.39768	0.01335
C	0.0159	0.37831	2.05703
H	0.18483	-0.22775	2.94607
C	-0.60689	0.19573	-0.47587
C	-0.98387	-0.11399	1.04708
H	-1.96893	0.36567	1.15455
C	-0.93127	1.67896	-0.75851
C	-0.22918	3.63491	-1.84865
H	0.75716	3.96878	-2.19217
H	1.30511	-1.64465	-1.33578
C	-1.2965	3.9021	-2.88973
H	-1.34471	4.9786	-3.10327
H	-2.27926	3.574	-2.52726
C	-1.55743	-0.65379	-1.34549
C	-3.80409	-1.12332	-1.83645
H	-3.68078	-2.16037	-1.48857
H	-3.60088	-1.1058	-2.91655
C	-5.16697	-0.56741	-1.5035
H	-5.94257	-1.15931	-2.00643
H	-5.25045	0.47528	-1.83819

H	-5.34821	-0.60364	-0.42065
C	-1.17463	-1.61115	1.21292
C	-2.46211	-2.15302	1.29079
H	-3.32452	-1.48236	1.27433
C	-2.65262	-3.53334	1.38249
H	-3.66438	-3.93779	1.44469
C	-1.55294	-4.39032	1.39644
H	-1.69859	-5.46956	1.46443
C	-0.26338	-3.85852	1.32784
H	0.60278	-4.5224	1.34034
C	-0.07519	-2.4803	1.24052
H	0.93351	-2.06651	1.18616
N	0.71369	-0.24969	-0.77814
O	0.52993	2.79985	1.2068
O	2.11259	-2.23601	-1.50817
O	1.15872	2.14713	3.53935
O	-0.07345	2.22971	-1.60482
O	-1.89417	2.23574	-0.3047
O	-2.82695	-0.31095	-1.17282
O	-1.19859	-1.55051	-2.06021
S	0.29081	1.95207	2.38306
H	-0.45801	4.1186	-0.89017
H	-1.06448	3.3735	-3.82449
F	-1.12768	2.66051	2.92662

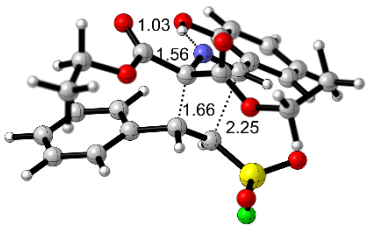
(*R*, *S*, *R*)-INT3



Charge = -1 Multiplicity = 1

C	3.53115	-1.13044	-0.74539
C	4.87734	-1.52467	-0.65899
H	5.13805	-2.5345	-0.97832
C	5.8394	-0.6449	-0.18028
H	6.87919	-0.97236	-0.12329
C	5.49411	0.65055	0.22936
H	6.256	1.33354	0.60478
C	4.16669	1.04792	0.15077
H	3.86966	2.0508	0.46737
C	3.17309	0.18073	-0.33118
C	1.77823	0.62232	-0.37491
H	1.54865	1.62005	0.01362
C	-0.52755	0.02095	-0.77812
C	-1.03721	1.35647	-1.3478
C	-0.68188	3.68975	-1.36423
H	-0.19376	4.33287	-0.62172
H	1.73668	-1.51011	-1.20452
C	-0.29216	4.05689	-2.78021
H	-0.58595	5.0946	-2.98884
H	-0.79909	3.40073	-3.5002
C	-1.16206	-1.13192	-1.57333
C	-3.15187	-2.29351	-2.01829
H	-2.75754	-3.2192	-1.57073
H	-2.91352	-2.31332	-3.09112
C	-4.63126	-2.12575	-1.76922
H	-5.18252	-2.95463	-2.23179
H	-4.989	-1.18202	-2.20219
H	-4.8497	-2.12181	-0.69253
N	0.8868	-0.17605	-0.83316
O	2.62876	-1.99075	-1.20742
O	-0.23922	2.36531	-1.03459
O	-2.03906	1.47114	-2.00456
O	-2.47761	-1.18312	-1.417
O	-0.53731	-1.93861	-2.21169
H	-1.76592	3.73479	-1.20745
H	0.7939	3.9688	-2.92021
C	0.5709	-3.42936	1.8506
C	-0.54004	-4.27026	1.9341
C	-1.80802	-3.76074	1.65721
C	-1.95873	-2.42338	1.2872
C	-0.85148	-1.57184	1.18996
C	0.41669	-2.09224	1.48728
C	-1.03806	-0.12699	0.75688
C	-0.38275	0.84153	1.67361
S	-1.06983	2.27787	1.98012
O	-2.17242	2.59534	1.06727
O	-0.13699	3.33538	2.36599
F	-1.93489	2.16454	3.41361
H	1.56733	-3.81559	2.07185
H	-0.41749	-5.31631	2.21909
H	-2.68636	-4.40458	1.7287
H	-2.95251	-2.02896	1.06499
H	1.29706	-1.4492	1.43611
H	-2.11534	0.07604	0.69302
H	0.52948	0.63186	2.22692

(*R*, *S*, *R*)-TS2

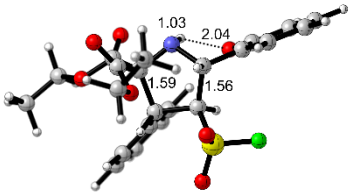


Charge = -1 Multiplicity = 1

Imaginary frequency = -254.0264 cm^{-1}

C	2.49319	-2.30901	-1.20834
C	3.59326	-3.18121	-1.17118
H	3.44546	-4.20937	-1.50488
C	4.831	-2.7377	-0.71725
H	5.6724	-3.43302	-0.6951
C	5.00534	-1.41645	-0.28877
H	5.97602	-1.0761	0.07291
C	3.92187	-0.54489	-0.329
H	4.01619	0.48633	0.02132
C	2.66651	-0.96671	-0.78621
C	1.52783	-0.03117	-0.7856
H	1.79909	1.025	-0.67515
C	-0.73847	0.31211	-0.91438
C	-0.63727	1.77264	-1.36866
C	0.33824	3.87369	-0.80576
H	0.41338	4.36826	0.16998
H	0.67811	-1.94309	-1.61343
C	1.64387	3.94029	-1.56993
H	1.90015	4.98627	-1.78639
H	1.56242	3.39859	-2.52268
C	-2.01844	-0.2747	-1.48719
C	-4.36111	-0.08983	-1.40731
H	-4.42531	-1.10743	-0.99175
H	-4.45489	-0.16763	-2.50011
C	-5.39919	0.83003	-0.81169
H	-6.40513	0.45855	-1.0465
H	-5.29744	1.84455	-1.22009
H	-5.29156	0.87802	0.28057
N	0.38685	-0.43807	-1.30964
O	1.31114	-2.75551	-1.64021
O	0.01836	2.51489	-0.487
O	-1.03795	2.17572	-2.43119
O	-3.07039	0.44084	-1.0916
O	-2.10047	-1.27397	-2.14944
H	-0.4935	4.30798	-1.37578
H	2.44918	3.49631	-0.96843
C	-1.85589	-3.4054	1.2416
C	-3.10074	-3.25553	1.85519
C	-3.58904	-1.97448	2.11473
C	-2.83565	-0.85441	1.76151
C	-1.58442	-0.99332	1.14917
C	-1.10337	-2.28457	0.89177
C	-0.79152	0.22784	0.74381
C	0.60426	0.21125	1.24656
S	1.21882	1.59617	1.98895
O	0.23647	2.61718	2.31263
O	2.49292	2.05844	1.45081
F	1.68399	1.01252	3.44621
H	-1.46805	-4.40327	1.02943
H	-3.68785	-4.13356	2.12893
H	-4.56114	-1.84473	2.5939
H	-3.22375	0.14753	1.95968
H	-0.1437	-2.41202	0.3862
H	-1.32401	1.12732	1.07652
H	1.03668	-0.69095	1.67878

(*R*, *S*, *R*)-INT4

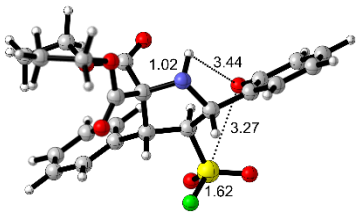


Charge = -1 Multiplicity = 1

C	2.49295	-1.90311	-1.29959
C	3.68131	-2.63357	-1.62321
H	3.5556	-3.67146	-1.94213
C	4.94588	-2.06514	-1.5377
H	5.81993	-2.66976	-1.79585
C	5.12154	-0.73712	-1.1275
H	6.11644	-0.29593	-1.06029
C	3.98377	0.00814	-0.80738
H	4.08808	1.04752	-0.47824
C	2.7058	-0.53889	-0.88728
C	1.5006	0.26635	-0.49753
H	1.80616	1.30093	-0.2824
C	-0.76779	0.68576	-0.83279
C	-0.76914	2.22004	-0.82852
C	0.12554	4.10444	0.30069
H	0.18374	4.34743	1.36752

H	0.3369	-0.68179	-1.8418
C	1.43879	4.36902	-0.40475
H	1.68062	5.43932	-0.35793
H	1.37586	4.07451	-1.46176
C	-1.99434	0.19356	-1.5845
C	-4.33867	0.10283	-1.47725
H	-4.27548	-0.98248	-1.29999
H	-4.45222	0.26464	-2.55842
C	-5.4496	0.74282	-0.68184
H	-6.41526	0.31944	-0.9871
H	-5.47399	1.82746	-0.85283
H	-5.30945	0.55588	0.39166
N	0.44818	0.28596	-1.51448
O	1.3207	-2.40713	-1.36614
O	-0.18251	2.7035	0.2593
O	-1.17567	2.8868	-1.74245
O	-3.1003	0.68898	-1.05083
O	-1.96321	-0.59779	-2.48786
H	-0.70364	4.66064	-0.15496
H	2.24821	3.80499	0.07899
C	-2.35364	-3.35981	0.39382
C	-3.4975	-3.17965	1.17242
C	-3.7212	-1.95143	1.79632
C	-2.80612	-0.91197	1.63455
C	-1.65905	-1.0851	0.85194
C	-1.43496	-2.32114	0.23086
C	-0.72491	0.08608	0.63411
C	0.77063	-0.27977	0.7658
S	1.43934	0.36867	2.27778
O	0.61788	0.0009	3.4047
O	1.93886	1.71519	2.14772
F	2.7469	-0.55711	2.3775
H	-2.17205	-4.31923	-0.0936
H	-4.21146	-3.99546	1.29633
H	-4.61008	-1.80125	2.41141
H	-2.98695	0.05189	2.11629
H	-0.5367	-2.46901	-0.37919
H	-1.00755	0.87441	1.34124
H	0.90948	-1.36669	0.8429

(*R*, *S*, *R*)-TS3



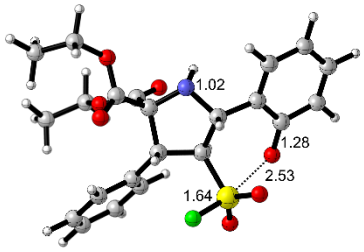
Charge = -1 Multiplicity = 1

Imaginary frequency = -41.9997 cm^{-1}

C	-3.52639	0.22212	1.24084
C	-4.7905	0.67287	1.7606
H	-5.14994	0.16475	2.65945
C	-5.53411	1.68735	1.17953
H	-6.48679	1.97802	1.6317
C	-5.08541	2.33833	0.02181
H	-5.66879	3.13309	-0.44409
C	-3.86651	1.92995	-0.51962
H	-3.49106	2.41661	-1.42646
C	-3.09123	0.91635	0.0468
C	-1.76242	0.63156	-0.60641
H	-1.88054	0.69714	-1.70364
C	-1.07699	-0.70317	-0.27788
H	-1.19973	-0.88634	0.80047
C	0.5848	0.97953	-0.22427
C	0.36349	-0.48564	-0.73309
H	0.38485	-0.41834	-1.82921
C	1.53116	1.74303	-1.15561
C	2.70359	3.77856	-1.38931
H	2.46811	4.8046	-1.08528
H	-0.93471	1.9127	0.75376
C	4.12301	3.39747	-1.02334
H	4.83134	4.06697	-1.52953
H	4.33782	2.36579	-1.33343
C	1.19667	0.94406	1.17875
C	3.19636	0.55269	2.36496
H	2.6432	-0.22554	2.91041
H	3.17624	1.47242	2.96722
C	4.59869	0.11432	2.0225
H	5.15834	-0.09144	2.94417
H	5.12629	0.89681	1.46052
H	4.56866	-0.80203	1.41608
C	1.39135	-1.50288	-0.29697
C	2.46184	-1.79979	-1.14644
H	2.51632	-1.30951	-2.12034
C	3.45565	-2.69522	-0.75102

H	4.28337	-2.9186	-1.42592
C	3.39163	-3.30177	0.50349
H	4.16782	-4.00239	0.8151
C	2.32652	-3.01035	1.35765
H	2.26597	-3.48349	2.33899
C	1.33081	-2.1198	0.9588
H	0.50149	-1.90777	1.63718
N	-0.72993	1.6092	-0.19759
O	-3.281	-1.93445	-1.19611
O	-2.87928	-0.72128	1.79662
O	-1.37137	-3.34297	-0.404
O	1.76239	2.95872	-0.6797
O	1.98508	1.31295	-2.18363
O	2.50877	0.80587	1.12952
O	0.54331	0.98271	2.18849
S	-1.86972	-2.12137	-0.98312
H	2.52176	3.67225	-2.46659
H	4.27569	3.48208	0.06128
F	-1.22954	-2.06334	-2.46656

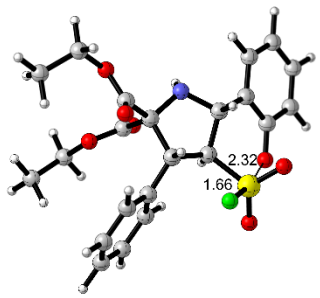
(*R*, *S*, *R*)-INT5



Charge = -1 Multiplicity = 1

C	-3.77516	0.0882	0.79658
C	-4.98292	0.57536	1.39724
H	-5.55879	-0.14355	1.98553
C	-5.42164	1.88246	1.24932
H	-6.35396	2.19144	1.73015
C	-4.68915	2.80607	0.492
H	-5.03249	3.83373	0.36861
C	-3.50309	2.37285	-0.10152
H	-2.90855	3.07437	-0.69494
C	-3.03441	1.06441	0.03941
C	-1.72927	0.70241	-0.62617
H	-1.85791	0.69211	-1.72489
C	-1.0944	-0.63879	-0.23009
H	-1.17848	-0.79911	0.84873
C	0.62432	0.99167	-0.25038
C	0.3502	-0.47771	-0.70279
H	0.36593	-0.4489	-1.79959
C	1.62284	1.68227	-1.18277
C	2.88305	3.65938	-1.45875
H	2.68612	4.70286	-1.18853
H	-0.86506	2.06847	0.62324
C	4.28155	3.23237	-1.06419
H	5.02233	3.853	-1.58598
H	4.45503	2.18223	-1.33583
C	1.19127	0.97603	1.17083
C	3.13541	0.53049	2.42814
H	2.5333	-0.21357	2.96941
H	3.13542	1.46163	3.01292
C	4.52796	0.02749	2.13863
H	5.05005	-0.18191	3.08128
H	5.10471	0.77582	1.57838
H	4.47796	-0.89924	1.54952
C	1.34389	-1.51731	-0.2395
C	2.43127	-1.83552	-1.06126
H	2.52289	-1.34052	-2.0298
C	3.3904	-2.75779	-0.64669
H	4.23071	-2.99642	-1.30057
C	3.27659	-3.37453	0.60042
H	4.02613	-4.09714	0.9267
C	2.19576	-3.06448	1.4255
H	2.09452	-3.54452	2.40011
C	1.23357	-2.14391	1.0073
H	0.39351	-1.92038	1.66777
N	-0.6646	1.6726	-0.29434
O	-3.09312	-1.71428	-1.75557
O	-3.396	-1.1234	0.93238
O	-1.91786	-3.22401	-0.08768
O	1.90113	2.8999	-0.73715
O	2.071	1.20444	-2.19197
O	2.49804	0.78797	1.16691
O	0.5083	1.06074	2.15826
S	-1.96055	-2.05448	-0.92808
H	2.70925	3.52772	-2.53456
H	4.42808	3.34873	0.01831
F	-0.84222	-2.42032	-2.06947

(*R*, *S*, *R*)-TS4

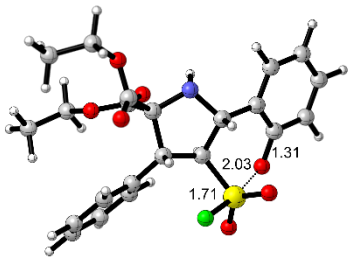


Charge = -1 Multiplicity = 1

Imaginary frequency = -65.1767 cm^{-1}

C	-3.78265	0.10291	0.7044
C	-4.99003	0.54988	1.32227
H	-5.59036	-0.20653	1.83299
C	-5.39688	1.87619	1.28631
H	-6.33122	2.16263	1.77617
C	-4.62854	2.84534	0.62994
H	-4.94687	3.88777	0.59597
C	-3.44055	2.44324	0.01913
H	-2.81982	3.18116	-0.49737
C	-3.00651	1.11595	0.05044
C	-1.70589	0.75195	-0.6179
H	-1.83715	0.73905	-1.71612
C	-1.10445	-0.60218	-0.21788
H	-1.18199	-0.75087	0.86349
C	0.64813	0.99214	-0.25074
C	0.34025	-0.47456	-0.69494
H	0.35253	-0.45395	-1.79153
C	1.65549	1.65857	-1.19111
C	2.95863	3.60585	-1.47888
H	2.78635	4.65464	-1.21241
H	-0.81332	2.09423	0.635
C	4.34816	3.14853	-1.08651
H	5.10149	3.74842	-1.61456
H	4.49591	2.09296	-1.35243
C	1.22289	0.9712	1.16716
C	3.16212	0.48975	2.41765
H	2.54944	-0.24338	2.962
H	3.17904	1.42189	3.00059
C	4.54546	-0.03657	2.1255
H	5.06638	-0.25256	3.06732
H	5.13301	0.70111	1.56238
H	4.47891	-0.96359	1.53856
C	1.31485	-1.5303	-0.22833
C	2.39928	-1.86658	-1.04689
H	2.50103	-1.37357	-2.0154
C	3.34203	-2.80445	-0.63015
H	4.17985	-3.05697	-1.28207
C	3.21529	-3.41925	0.61679
H	3.95202	-4.15409	0.94498
C	2.13761	-3.09128	1.43884
H	2.02585	-3.56959	2.41319
C	1.19159	-2.1549	1.0181
H	0.35372	-1.91832	1.67673
N	-0.62658	1.70266	-0.2876
O	-3.09678	-1.62132	-1.82767
O	-3.42235	-1.13113	0.75093
O	-2.04358	-3.17851	-0.09143
O	1.96195	2.87172	-0.75135
O	2.08914	1.16782	-2.20039
O	2.52515	0.75506	1.15779
O	0.54728	1.07555	2.15796
S	-2.04306	-1.98342	-0.90248
H	2.77879	3.47385	-2.55365
H	4.50131	3.26784	-0.00525
F	-0.87601	-2.40089	-2.00684

(*R*, *S*, *R*)-INT6

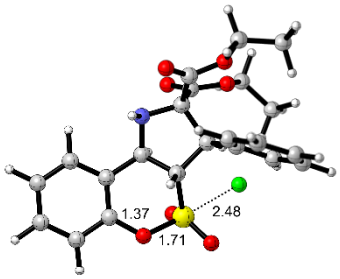


Charge = -1 Multiplicity = 1

C	3.7665	-0.11719	0.62212
C	4.99305	-0.48472	1.22756
H	5.60238	0.31657	1.64985
C	5.40643	-1.80998	1.29007
H	6.35796	-2.05245	1.76867
C	4.61939	-2.82915	0.74437
H	4.94285	-3.86959	0.78885
C	3.4097	-2.48923	0.14044
H	2.77648	-3.26847	-0.29165
C	2.97281	-1.16377	0.07743
C	1.663	-0.82194	-0.57661
H	1.785	-0.82822	-1.67552
C	1.10471	0.55122	-0.19183

H	1.16113	0.68534	0.89427
C	-0.68513	-0.99794	-0.22273
C	-0.33231	0.4575	-0.68619
H	-0.32711	0.42554	-1.78184
C	-1.68885	-1.65951	-1.16985
C	-3.03457	-3.57982	-1.44402
H	-2.89079	-4.62791	-1.15843
H	0.74085	-2.09077	0.72739
C	-4.41864	-3.08435	-1.07929
H	-5.1782	-3.67462	-1.60925
H	-4.53791	-2.02982	-1.36319
C	-1.28592	-0.93853	1.18273
C	-3.23172	-0.38432	2.39028
H	-2.61212	0.34837	2.92742
H	-3.27598	-1.30271	2.99328
C	-4.59967	0.16319	2.06643
H	-5.12819	0.41303	2.99558
H	-5.19537	-0.57554	1.51334
H	-4.50545	1.07388	1.45819
C	-1.28778	1.54175	-0.24853
C	-2.36906	1.87245	-1.07394
H	-2.48094	1.35344	-2.02767
C	-3.29489	2.83784	-0.68336
H	-4.12977	3.08543	-1.34105
C	-3.1554	3.48657	0.54508
H	-3.87896	4.24293	0.85314
C	-2.08101	3.16484	1.37364
H	-1.95809	3.67035	2.33286
C	-1.15149	2.20084	0.97834
H	-0.31319	1.97352	1.63942
N	0.57333	-1.74418	-0.21718
O	3.14256	1.45342	-1.85748
O	3.39251	1.13857	0.60815
O	2.17993	3.12425	-0.12765
O	-2.0318	-2.8572	-0.71367
O	-2.09371	-1.17826	-2.19544
O	-2.58176	-0.68992	1.14626
O	-0.63176	-1.04263	2.1882
S	2.17398	1.85945	-0.84389
H	-2.83653	-3.4696	-2.51803
H	-4.59013	-3.18325	0.00128
F	0.97246	2.3069	-1.96823

(*R*, *S*, *R*)-TS5



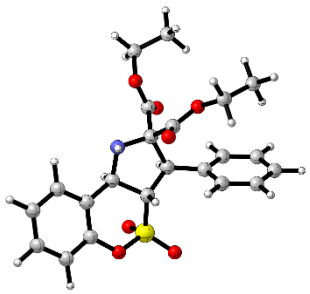
Charge = -1 Multiplicity = 1

Imaginary frequency = -87.6252 cm^{-1}

C	3.614530	-0.251681	-0.481302
C	4.997200	-0.151399	-0.310462
H	5.541157	0.579128	-0.909901
C	5.645643	-0.962542	0.616816
H	6.725008	-0.871950	0.746899
C	4.921220	-1.884888	1.374047
H	5.427480	-2.520379	2.101157
C	3.543993	-1.991282	1.192787
H	2.959365	-2.708561	1.771644
C	2.874109	-1.181654	0.272194
C	1.396537	-1.303298	0.038064
H	1.220918	-2.065059	-0.742617
C	0.778221	0.003460	-0.483407
H	1.142427	0.870257	0.088686
C	-0.783867	-1.363232	0.757205
C	-0.720274	-0.199636	-0.337320
H	-1.048022	-0.589492	-1.312339
C	-1.356403	-2.587423	0.006119
C	-2.982288	-3.124843	-1.654937
H	-3.885677	-3.641472	-1.301818
H	0.801340	-1.075573	1.987681
C	-3.257695	-2.217880	-2.836177
H	-3.571649	-2.818688	-3.701451
H	-2.353320	-1.636630	-3.084528
C	-1.620444	-0.989415	1.978993
C	-3.737431	-0.195839	2.658787
H	-3.145857	0.561146	3.192412
H	-4.059317	-0.955437	3.385903
C	-4.895801	0.418332	1.909840
H	-5.574253	0.918041	2.613708
H	-5.459644	-0.351562	1.366009
H	-4.520999	1.160460	1.189364
C	-1.483699	1.082359	-0.105076
C	-2.253110	1.574179	-1.166608
H	-2.195209	1.017767	-2.106766

C	-2.981078	2.755951	-1.021147
H	-3.579629	3.130963	-1.853565
C	-2.938827	3.464285	0.180792
H	-3.511672	4.385953	0.296320
C	-2.144623	2.997765	1.230600
H	-2.090329	3.556431	2.166717
C	-1.413276	1.818923	1.084683
H	-0.789133	1.472769	1.912851
N	0.575756	-1.659134	1.180629
O	1.842048	-0.931792	-2.828103
O	3.037588	0.628722	-1.359255
O	1.281802	1.558909	-2.717624
O	-2.508995	-2.300479	-0.577297
O	-0.770390	-3.630877	-0.102933
O	-2.893275	-0.826685	1.684662
O	-1.138858	-0.803602	3.068188
S	1.539482	0.282610	-2.098281
H	-2.217881	-3.878663	-1.881062
H	-4.067360	-1.513818	-2.594269
F	-0.706786	-0.269787	-2.992041

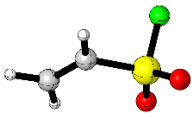
3a



Charge = 0 Multiplicity = 1

C	3.9621	0.11111	0.25872
C	5.27426	-0.04521	0.69704
H	5.92403	0.82939	0.72675
C	5.71744	-1.30315	1.09647
H	6.74384	-1.42405	1.44438
C	4.85443	-2.39915	1.05386
H	5.20039	-3.38406	1.3678
C	3.54732	-2.23277	0.60332
H	2.86442	-3.08254	0.55417
C	3.07919	-0.97823	0.2028
C	1.69544	-0.78316	-0.34357
H	1.73674	-0.92618	-1.43822
C	1.15275	0.62921	-0.10348
H	1.20033	0.88734	0.96531
C	-0.62042	-0.94532	-0.0643
C	-0.2688	0.49324	-0.62633
H	-0.22415	0.37883	-1.7192
C	-1.48678	-1.71668	-1.06637
C	-2.72446	-3.70604	-1.34244
H	-2.56363	-4.72879	-0.98426
H	0.7599	-1.72405	1.2047
C	-4.15088	-3.24962	-1.11874
H	-4.84115	-3.90643	-1.66479
H	-4.28976	-2.222	-1.48116
C	-1.40141	-0.79217	1.24385
C	-3.50906	-0.23473	2.13877
H	-2.9849	0.54801	2.7056
H	-3.61592	-1.11603	2.78715
C	-4.82927	0.24832	1.59247
H	-5.48861	0.53598	2.42155
H	-5.32345	-0.54112	1.01036
H	-4.67221	1.12367	0.94679
C	-1.24525	1.59772	-0.30159
C	-2.24434	1.91145	-1.22958
H	-2.27681	1.36909	-2.17654
C	-3.19366	2.89158	-0.94508
H	-3.96499	3.12798	-1.67951
C	-3.15854	3.56612	0.27608
H	-3.90111	4.33305	0.50096
C	-2.16685	3.25739	1.20751
H	-2.12967	3.78218	2.16321
C	-1.21332	2.28055	0.9199
H	-0.44785	2.05406	1.66483
N	0.64521	-1.63741	0.19279
O	2.4355	1.3458	-2.28336
O	3.58677	1.41409	-0.05439
O	1.96768	3.14868	-0.60003
O	-1.81228	-2.90127	-0.57617
O	-1.82145	-1.29818	-2.14304
O	-2.68373	-0.59946	1.01788
O	-0.87426	-0.78689	2.3256
S	2.2386	1.76852	-0.91287
H	-2.44111	-3.64643	-2.40114
H	-4.40349	-3.28737	-0.05029

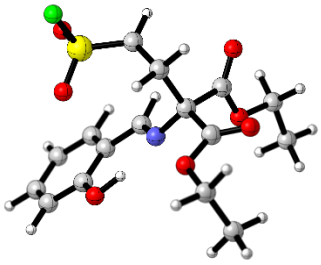
2am



Charge = 0 Multiplicity = 1

C	-2.26308	0.04458	-0.00579
C	-1.17049	-0.70942	-0.04091
S	0.39574	0.0654	-0.12876
O	0.27917	1.49901	-0.11057
O	1.24618	-0.61193	-1.06936
F	0.96049	-0.34101	1.31307
H	-2.19569	1.13465	-0.00389
H	-1.13165	-1.79989	-0.05304
H	-3.25025	-0.41969	0.0191

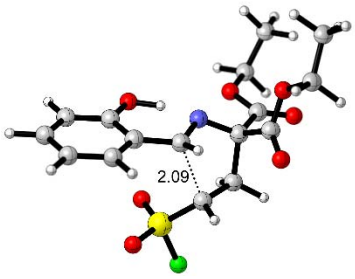
(*S*, *S*)-INT3-3am



Charge = -1 Multiplicity = 1

C	-1.97137	1.72825	-1.29201
C	-3.12167	2.42631	-1.69425
H	-3.28173	2.58229	-2.76182
C	-4.02478	2.89874	-0.74994
H	-4.91202	3.43916	-1.08523
C	-3.8144	2.68792	0.61924
H	-4.53091	3.05751	1.35266
C	-2.68036	1.99732	1.02562
H	-2.49688	1.81198	2.08686
C	-1.74891	1.51683	0.09357
C	-0.58443	0.7591	0.54227
H	-0.50703	0.56323	1.62333
C	1.29163	-0.58601	0.12174
C	1.88119	-0.31396	1.51415
C	2.78174	1.34727	2.91312
H	3.70985	0.77238	3.04437
C	3.03384	2.83467	2.8716
H	3.49431	3.16004	3.81339
H	2.09193	3.38298	2.73581
C	2.47119	-0.57434	-0.84643
C	3.11642	-0.44028	-3.11092
H	2.58883	-0.68689	-4.03906
H	3.82372	-1.24579	-2.8738
C	3.81428	0.90019	-3.20547
H	4.54557	0.88008	-4.02466
H	4.34519	1.1265	-2.27141
H	3.08734	1.69859	-3.40697
N	0.29094	0.34657	-0.29541
O	-1.11905	1.28938	-2.21319
O	2.18628	0.96922	1.66462
O	2.06554	-1.15022	2.35733
O	2.09101	-0.41738	-2.10485
O	3.60962	-0.76119	-0.49468
H	2.09767	1.06505	3.72644
H	3.71129	3.08871	2.0454
H	-0.38815	0.8001	-1.72292
C	0.67412	-2.0389	0.09426
C	-0.50218	-2.18345	0.98805
S	-2.00841	-2.20186	0.38123
O	-2.11925	-1.61353	-0.95485
O	-3.05477	-1.93359	1.36651
F	-2.41377	-3.79314	-0.00117
H	0.40427	-2.2292	-0.95361
H	-0.42486	-2.42084	2.04618
H	1.49069	-2.72327	0.36908

(*S*, *S*)-TS2-3am



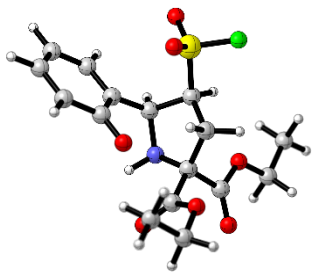
Charge = -1 Multiplicity = 1

Imaginary frequency = -273.41 cm^{-1}

C	2.0433	1.00891	1.72574
C	3.22468	1.41757	2.37111
H	3.35107	1.15132	3.42178
C	4.19504	2.14126	1.68709
H	5.10296	2.44673	2.21128
C	4.01846	2.48085	0.341
H	4.7816	3.04734	-0.19331
C	2.8536	2.07853	-0.30524
H	2.69964	2.31851	-1.36091

C	1.86183	1.35011	0.359
C	0.65022	0.89227	-0.3581
H	0.45626	1.43587	-1.29793
C	-1.25339	-0.35346	-0.38062
C	-1.9561	0.50255	-1.4403
C	-3.58202	2.17093	-1.77689
H	-4.02379	1.59356	-2.60188
C	-4.62912	2.89602	-0.96674
H	-5.17447	3.60083	-1.60767
H	-4.1622	3.45843	-0.14708
C	-2.31625	-1.07247	0.43372
C	-2.95915	-1.85992	2.55784
H	-2.38201	-2.14182	3.44586
H	-3.28356	-2.76967	2.0356
C	-4.13846	-0.9798	2.91771
H	-4.80646	-1.51519	3.60585
H	-4.70802	-0.71146	2.01807
H	-3.79513	-0.06009	3.41053
N	-0.35135	0.41655	0.38958
O	1.1211	0.33721	2.40414
O	-2.89905	1.26742	-0.89978
O	-1.64316	0.55368	-2.60335
O	-2.0275	-1.15566	1.72439
O	-3.28569	-1.57727	-0.07842
H	-2.84515	2.86146	-2.2125
H	-5.34803	2.1839	-0.53952
H	0.34099	0.18848	1.72907
C	-0.37345	-1.45756	-1.11718
C	0.90034	-0.81078	-1.5495
S	2.32981	-1.51796	-1.01217
O	2.28312	-1.87545	0.39346
O	3.50808	-0.8689	-1.55304
F	2.37856	-2.9973	-1.73669
H	-0.1833	-2.24426	-0.37326
H	1.00815	-0.48927	-2.58738
H	-0.94553	-1.88558	-1.94967

(*S*, *S*)-INT4-3am

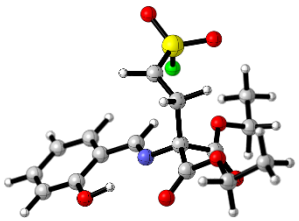


Charge = -1 Multiplicity = 1

C	2.14542	1.13497	-0.45887
C	3.49403	1.63017	-0.52055
H	3.67445	2.6079	-0.06613
C	4.53152	0.92122	-1.10455
H	5.53654	1.35312	-1.11083
C	4.31148	-0.33544	-1.68658
H	5.12425	-0.89378	-2.15201
C	3.01313	-0.84494	-1.66189
H	2.81095	-1.82147	-2.11437
C	1.94808	-0.159	-1.07451
C	0.57864	-0.80725	-1.09575
H	0.63561	-1.66401	-1.78503
C	-1.33031	0.47708	-0.34764
C	-2.76805	-0.00278	-0.58346
C	-4.12572	-1.9158	-0.809
H	-4.459	-1.59856	-1.80761
C	-3.97328	-3.41417	-0.7097
H	-4.93825	-3.9001	-0.90355
H	-3.63329	-3.70254	0.29419
C	-1.38898	1.99948	-0.23881
C	-1.74781	3.80125	1.2306
H	-2.41315	3.92271	2.09372
H	-2.20263	4.28662	0.35742
C	-0.35862	4.34017	1.50306
H	-0.39243	5.43261	1.61444
H	0.3136	4.06743	0.67907
H	0.04794	3.9054	2.4268
N	-0.52497	0.07604	-1.4992
O	1.21096	1.79318	0.0962
O	-2.84366	-1.32862	-0.5495
O	-3.71128	0.71561	-0.79445
O	-1.69418	2.38817	0.9929
O	-1.26841	2.7349	-1.18219
H	-4.84543	-1.52341	-0.07643
H	-3.24486	-3.77832	-1.44667
H	-0.16871	0.91616	-1.95033

C	-0.72827	-0.21078	0.89602
C	0.05127	-1.35214	0.26078
S	1.35798	-1.9744	1.28611
O	2.0648	-0.95627	2.01767
O	2.05908	-3.05159	0.63444
F	0.41716	-2.68696	2.38641
H	-0.03582	0.49033	1.37121
H	-0.58335	-2.23339	0.09393
H	-1.48722	-0.56116	1.60562

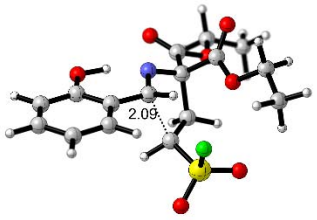
(*R, S*)-INT3-3am



Charge = -1 Multiplicity = 1

C	3.00931	-2.19139	-0.05533
C	4.35491	-2.59315	-0.0719
H	4.57727	-3.64301	-0.26684
C	5.36721	-1.66758	0.15118
H	6.40638	-2.00124	0.13107
C	5.07467	-0.31902	0.39717
H	5.87695	0.39924	0.56546
C	3.74705	0.08584	0.42154
H	3.48253	1.13099	0.6021
C	2.70622	-0.82986	0.20263
C	1.32028	-0.36766	0.23771
H	1.15004	0.688	0.48608
C	-1.00061	-0.72726	-0.066
C	-1.40424	-0.05626	1.25191
C	-1.33084	1.91633	2.52192
H	-0.98015	1.33329	3.38546
C	-0.69879	3.28462	2.45287
H	-1.02846	3.87865	3.31594
H	-0.9911	3.78071	1.51921
C	-1.89636	-1.9614	-0.19724
C	-4.12785	-2.65931	-0.45399
H	-4.04957	-3.29306	0.44128
H	-3.87282	-3.28036	-1.32479
C	-5.49346	-2.03003	-0.58595
H	-6.25785	-2.81365	-0.66697
H	-5.54391	-1.39924	-1.48361
H	-5.71945	-1.41075	0.29242
N	0.36295	-1.18298	-0.01326
O	2.05366	-3.09133	-0.27753
O	-0.99749	1.19705	1.32328
O	-1.99727	-0.62788	2.13273
O	-3.16669	-1.6027	-0.34749
O	-1.51686	-3.10161	-0.19818
H	-2.42771	1.97223	2.5848
H	0.39552	3.20949	2.46384
H	1.17172	-2.60572	-0.23762
C	-1.26905	0.21231	-1.32054
C	-0.18096	1.11479	-1.77879
S	-0.03643	2.67109	-1.34504
O	-1.26912	3.28044	-0.84461
O	0.81334	3.44621	-2.24748
F	0.93915	2.80754	0.04778
H	-2.18288	0.78233	-1.10384
H	0.67656	0.74969	-2.34096
H	-1.51479	-0.46932	-2.14865

(*R, S*)-TS2-3am



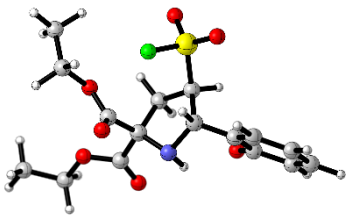
Charge = -1 Multiplicity = 1

Imaginary frequency = -348.50 cm^{-1}

C	-2.60917	-2.34489	-0.18841
C	-3.92266	-2.83793	-0.09031
H	-4.05724	-3.90173	0.11203
C	-5.0127	-1.98802	-0.24472
H	-6.02285	-2.3942	-0.1623
C	-4.82764	-0.62445	-0.50114
H	-5.68515	0.03939	-0.61467
C	-3.5312	-0.12912	-0.60564
H	-3.3528	0.93444	-0.78542
C	-2.41855	-0.96584	-0.4616
C	-1.05046	-0.40668	-0.52787
H	-0.98408	0.57106	-1.01882
C	1.19156	-0.67227	-0.17027
C	1.70326	0.31403	-1.22454
C	1.53248	2.504	-2.07327

H	1.36875	2.09434	-3.0801
C	0.7207	3.75151	-1.8207
H	1.08346	4.56237	-2.46626
H	0.80939	4.05145	-0.7683
C	2.2729	-1.72605	0.02942
C	4.51509	-2.03096	0.68107
H	4.72645	-2.59724	-0.23765
H	4.2275	-2.75471	1.4576
C	5.68867	-1.18133	1.10504
H	6.55981	-1.81984	1.30104
H	5.45152	-0.62371	2.0211
H	5.95124	-0.46463	0.31536
N	-0.03467	-1.27164	-0.54948
O	-1.57727	-3.17003	-0.03339
O	1.14768	1.51511	-1.10709
O	2.47463	0.01915	-2.10362
O	3.40791	-1.15794	0.43493
O	2.13241	-2.91224	-0.10114
H	2.61183	2.68454	-1.96167
H	-0.34129	3.5752	-2.03209
H	-0.72912	-2.58399	-0.18724
C	0.91917	0.06987	1.22812
C	-0.51554	0.47641	1.28966
S	-0.87986	2.1269	1.39837
O	0.26602	3.0158	1.49034
O	-2.04299	2.37125	2.2321
F	-1.4734	2.51067	-0.08929
H	1.61077	0.91275	1.34692
H	-1.18517	-0.04713	1.9726
H	1.13548	-0.6619	2.01796

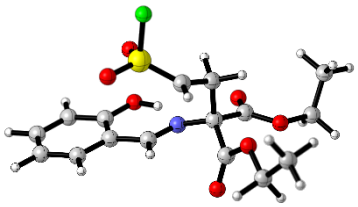
(*R, S*)-INT4-3am



Charge = -1 Multiplicity = 1

C	-3.10329	-1.48819	0.53059
C	-4.47236	-1.91097	0.50427
H	-4.78864	-2.6248	1.26945
C	-5.37203	-1.44325	-0.44547
H	-6.40572	-1.80015	-0.42012
C	-4.98332	-0.52617	-1.43112
H	-5.69536	-0.16225	-2.17257
C	-3.65528	-0.08891	-1.43733
H	-3.32269	0.63154	-2.19178
C	-2.73609	-0.54452	-0.49779
C	-1.31218	-0.07264	-0.48897
H	-1.16176	0.66785	-1.29113
C	0.88073	-0.74479	-0.05663
C	1.64733	0.20867	-0.98632
C	3.14564	2.02529	-1.04194
H	2.4429	2.46605	-1.76226
C	3.64514	3.04433	-0.04617
H	4.17498	3.8516	-0.56821
H	4.33374	2.58216	0.67394
C	1.72778	-1.98279	0.24163
C	3.89771	-2.8914	0.31113
H	3.5947	-3.74771	-0.30758
H	3.76402	-3.17391	1.3648
C	5.30621	-2.43953	0.01409
H	6.00899	-3.25511	0.22749
H	5.57368	-1.57553	0.63698
H	5.40785	-2.15841	-1.04262
N	-0.35557	-1.16904	-0.68308
O	-2.25089	-1.89391	1.38721
O	2.45781	1.00776	-0.30657
O	1.51564	0.23349	-2.18
O	3.01778	-1.7917	0.02379
O	1.24948	-3.00789	0.64828
H	3.96417	1.55653	-1.60851
H	2.79649	3.47562	0.50254
H	-0.70764	-1.9418	-0.10821
C	0.44815	-0.0507	1.26396
C	-0.89381	0.57615	0.88323
S	-0.84701	2.34587	0.77683
O	-0.16699	2.95251	1.89404
O	-2.10508	2.86469	0.30425
F	0.17068	2.52342	-0.47102
H	1.1861	0.64872	1.67143
H	-1.65865	0.39331	1.64998
H	0.23376	-0.83801	1.99678

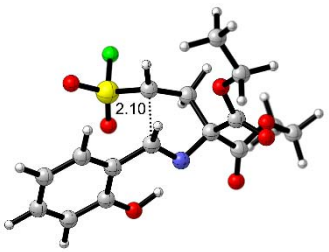
(*R, R*)-INT3-3am



Charge = -1 Multiplicity = 1

C	2.96789	-1.74412	-0.10417
C	4.33587	-2.06074	-0.07985
H	4.66501	-2.87071	0.57231
C	5.23648	-1.35218	-0.86583
H	6.29549	-1.6148	-0.83044
C	4.80562	-0.30824	-1.69502
H	5.52006	0.24602	-2.30355
C	3.45441	0.01098	-1.72522
H	3.09318	0.82725	-2.35569
C	2.52344	-0.69325	-0.94796
C	1.11435	-0.30973	-0.96568
H	0.84256	0.55282	-1.59061
C	-1.07388	-0.46489	-0.1002
C	-1.6881	0.10678	-1.38837
C	-3.22957	1.62913	-2.29456
H	-3.77527	0.81902	-2.79997
C	-4.15313	2.71685	-1.80274
H	-4.69102	3.15954	-2.65098
H	-3.58381	3.50944	-1.29863
C	-1.94107	-1.62092	0.40496
C	-4.16492	-2.39842	0.60622
H	-3.73792	-3.40443	0.50279
H	-5.03698	-2.30892	-0.05118
C	-4.51599	-2.08949	2.04641
H	-5.28249	-2.79198	2.40031
H	-4.91123	-1.06846	2.13585
H	-3.63122	-2.18884	2.68917
N	0.25613	-0.95781	-0.27239
O	2.12431	-2.43368	0.65834
O	-2.55586	1.08006	-1.15486
O	-1.4191	-0.29816	-2.48957
O	-3.22119	-1.44485	0.09235
O	-1.52021	-2.53847	1.05617
H	-2.47497	2.01105	-2.99694
H	-4.88902	2.30877	-1.09695
H	1.20731	-2.04181	0.50727
C	-1.05629	0.62116	1.05026
C	-0.24526	1.81078	0.68821
S	1.22937	2.04722	1.32669
O	2.075	2.9591	0.55773
O	1.82679	0.84495	1.91005
F	1.06707	2.96788	2.72859
H	-0.63839	0.11052	1.92902
H	-0.62969	2.6378	0.09514
H	-2.10519	0.87216	1.26478

(*R*, *R*)-TS2-3am



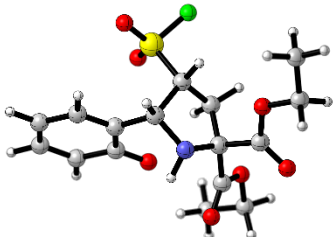
Charge = -1 Multiplicity = 1

Imaginary frequency = -274.83 cm^{-1}

C	2.48761	-1.07038	-1.4942
C	3.82735	-1.41734	-1.74734
H	4.03423	-2.42507	-2.11131
C	4.85065	-0.49875	-1.54206
H	5.88223	-0.79287	-1.74632
C	4.5714	0.79284	-1.08103
H	5.37594	1.51108	-0.92098
C	3.24896	1.14288	-0.82664
H	3.00667	2.14156	-0.45258
C	2.20089	0.23784	-1.02276
C	0.80599	0.62002	-0.70525
H	0.64905	1.70756	-0.63909
C	-1.38219	0.00545	-0.45001
C	-2.02109	1.34326	-0.83741
C	-2.06424	3.66295	-0.4255
H	-3.1632	3.68071	-0.39922
C	-1.45551	4.63967	0.55123
H	-1.77812	5.66012	0.30707
H	-0.35855	4.60059	0.50531
C	-2.38231	-1.09644	-0.77631
C	-4.55576	-1.87628	-0.26351
H	-4.59913	-2.20087	-1.31161
H	-5.48699	-1.35557	-0.01205
C	-4.30415	-3.04595	0.66581
H	-5.13137	-3.765	0.59389

H	-4.23172	-2.70183	1.70668
H	-3.37267	-3.55998	0.39384
N	-0.15858	-0.20228	-1.12917
O	1.52448	-1.95593	-1.71867
O	-1.62188	2.34822	-0.06198
O	-2.7433	1.48851	-1.79132
O	-3.53023	-0.88393	-0.13058
O	-2.16719	-2.05546	-1.46718
H	-1.75303	3.86279	-1.46088
H	-1.77297	4.40982	1.57728
H	0.63866	-1.45817	-1.49416
C	-1.04321	-0.05681	1.10908
C	0.29572	0.56722	1.32713
S	1.46967	-0.40028	2.04447
O	2.70518	0.31591	2.29525
O	1.51103	-1.73734	1.48154
F	0.91831	-0.69403	3.57056
H	-1.02707	-1.12336	1.37603
H	0.35465	1.58462	1.71915
H	-1.8416	0.42957	1.68268

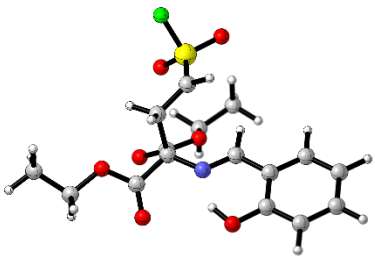
(*R, R*)-INT4-3am



Charge = -1 Multiplicity = 1

C	-2.14541	1.13487	-0.45897
C	-3.49408	1.62993	-0.52054
H	-3.67456	2.60765	-0.06613
C	-4.53155	0.92086	-1.10443
H	-5.53661	1.35266	-1.11064
C	-4.31144	-0.33579	-1.68646
H	-5.12418	-0.89422	-2.15181
C	-3.01303	-0.84516	-1.66186
H	-2.8108	-1.8217	-2.11432
C	-1.948	-0.15911	-1.07457
C	-0.57853	-0.80728	-1.09581
H	-0.63544	-1.66403	-1.7851
C	1.33032	0.47715	-0.34764
C	2.76809	-0.00267	-0.58338
C	4.12584	-1.91562	-0.80889
H	4.84547	-1.52321	-0.07625
C	3.97345	-3.41401	-0.70963
H	4.93846	-3.89989	-0.90337
H	3.24513	-3.77818	-1.44668
C	1.38893	1.99955	-0.23878
C	1.7474	3.80132	1.2307
H	2.20244	4.28673	0.35766
H	2.41248	3.92283	2.09401
C	0.35807	4.34009	1.50276
H	0.39174	5.43252	1.61429
H	-0.04873	3.90518	2.42634
H	-0.3139	4.06733	0.67857
N	0.52504	0.07608	-1.49923
O	-1.21095	1.79319	0.09598
O	2.84373	-1.32851	-0.5495
O	3.71133	0.71575	-0.79424
O	1.69398	2.38823	0.99297
O	1.26838	2.73498	-1.18215
H	4.45919	-1.59836	-1.80746
H	3.63336	-3.7024	0.29422
H	0.16874	0.91618	-1.95038
C	0.72824	-0.2107	0.89599
C	-0.05116	-1.35215	0.26074
S	-1.35788	-1.9744	1.28606
O	-2.05892	-3.05168	0.6345
O	-2.06475	-0.95619	2.01749
F	-0.41706	-2.68681	2.38647
H	0.03564	0.49038	1.371
H	0.58352	-2.23335	0.09391
H	1.48712	-0.56095	1.60572

(*S, R*)-INT3-3am

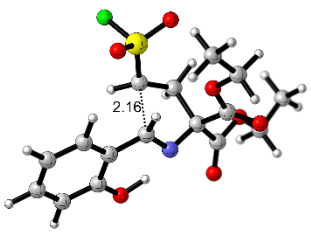


Charge = -1 Multiplicity = 1

C	-3.63888	-1.31474	-0.24527
C	-5.03428	-1.42147	-0.36707
H	-5.46757	-2.41818	-0.45927
C	-5.82976	-0.28253	-0.3694

H	-6.91179	-0.389	-0.46682
C	-5.26391	0.99371	-0.24759
H	-5.89586	1.88171	-0.24904
C	-3.8858	1.10808	-0.12367
H	-3.41901	2.09133	-0.02506
C	-3.05761	-0.02517	-0.12336
C	-1.60805	0.13164	0.01376
H	-1.21957	1.147	0.14797
C	0.58184	-0.87452	0.05
C	1.16165	-0.17907	1.29303
C	1.06118	1.73964	2.65015
H	2.13901	1.81227	2.46189
C	0.3858	3.08642	2.55577
H	0.78839	3.76071	3.32346
H	-0.69862	2.99335	2.70911
C	1.03152	-2.34297	0.15301
C	2.80958	-3.84801	-0.1351
H	2.17529	-4.53874	-0.70899
H	2.7534	-4.14593	0.92201
C	4.23053	-3.82376	-0.64343
H	4.67308	-4.82464	-0.55804
H	4.83796	-3.12175	-0.05672
H	4.25959	-3.51822	-1.69797
N	-0.85346	-0.90257	-0.02135
O	-2.89784	-2.41947	-0.2418
O	0.49295	0.90644	1.62892
O	2.13075	-0.58966	1.88039
O	2.27672	-2.52423	-0.26158
O	0.33075	-3.2319	0.5616
H	0.90124	1.25296	3.62385
H	0.57178	3.52024	1.56338
H	-1.93607	-2.12568	-0.14616
C	1.21447	-0.20979	-1.23915
C	0.75207	1.17377	-1.52816
S	1.60253	2.45374	-1.02223
O	2.55837	2.13678	0.04474
O	0.84032	3.70224	-0.94944
F	2.6981	2.90122	-2.22022
H	2.30304	-0.26268	-1.1055
H	-0.08335	1.40747	-2.18369
H	0.96166	-0.88407	-2.07111

(*S*, *R*)-TS2-3am



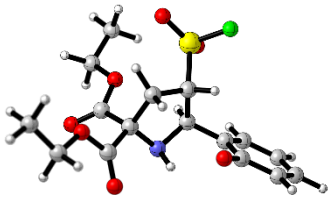
Charge = -1 Multiplicity = 1

Imaginary frequency = -282.75 cm^{-1}

C	-2.52846	-2.4123	0.12851
C	-3.81567	-2.95842	-0.0214
H	-3.89744	-4.02087	-0.2564
C	-4.94563	-2.16121	0.12624
H	-5.93442	-2.60798	0.00389
C	-4.82704	-0.79932	0.42724
H	-5.71596	-0.17728	0.53642
C	-3.55725	-0.25119	0.58211
H	-3.42814	0.8139	0.7904
C	-2.40428	-1.03317	0.44184
C	-1.06702	-0.41524	0.56384
H	-1.06583	0.56568	1.05217
C	1.20694	-0.6218	0.21407
C	1.70434	0.37347	1.265
C	1.2767	2.48933	2.24164
H	2.21579	2.97386	1.93492
C	0.12214	3.46298	2.27125
H	0.35182	4.29302	2.95249
H	-0.79196	2.96456	2.62342
C	2.29458	-1.67269	0.02949
C	4.51905	-1.98997	-0.67059
H	4.22403	-2.76676	-1.39113
H	4.76223	-2.4925	0.27695
C	5.66836	-1.15324	-1.17862
H	6.54455	-1.79054	-1.35513
H	5.93862	-0.38299	-0.44384
H	5.40013	-0.65963	-2.12243
N	-0.0181	-1.23074	0.57057
O	-1.45885	-3.1899	-0.0146
O	0.96411	1.47462	1.28005
O	2.6131	0.16662	2.03068
O	3.40537	-1.11846	-0.45257
O	2.17599	-2.8506	0.23845
H	1.44812	2.01201	3.21644
H	-0.06208	3.85719	1.26391
H	-0.64407	-2.57092	0.17659

C	0.9487	0.11943	-1.20508
C	-0.46779	0.55846	-1.26731
S	-0.7942	2.21294	-1.22112
O	0.37721	3.05729	-1.06074
O	-1.9854	2.54524	-0.45392
F	-1.2947	2.54916	-2.74829
H	1.66243	0.94499	-1.31901
H	-1.18644	0.04984	-1.91112
H	1.16652	-0.6292	-1.97818

(*S*, *R*)-INT4-3am



Charge = -1 Multiplicity = 1

C	2.51769	-2.06784	0.26507
C	3.80198	-2.70308	0.2466
H	3.91834	-3.60979	0.84617
C	4.86428	-2.19973	-0.49428
H	5.82392	-2.72436	-0.47236
C	4.73203	-1.03686	-1.2647
H	5.57116	-0.64647	-1.84151
C	3.49255	-0.38917	-1.27349
H	3.35887	0.5253	-1.8605
C	2.41366	-0.87545	-0.54219
C	1.08643	-0.17442	-0.52623
H	1.13666	0.72407	-1.1556
C	-1.21784	-0.59228	-0.3309
C	-1.81718	0.5463	-1.15614
C	-1.65699	2.83569	-1.67891
H	-2.72761	2.97434	-1.47237
C	-0.83971	4.03889	-1.279
H	-1.20968	4.92237	-1.8158
H	0.21958	3.89053	-1.52292
C	-2.23659	-1.7201	-0.25969
C	-4.39354	-2.28378	0.49143
H	-4.0021	-3.12896	1.07542
H	-4.66488	-2.66197	-0.50456
C	-5.55356	-1.60546	1.17791
H	-6.37552	-2.32065	1.31053
H	-5.91797	-0.76153	0.57711
H	-5.25339	-1.23153	2.16591
N	-0.00591	-1.03353	-1.00077
O	1.52277	-2.4969	0.93713
O	-1.20367	1.70175	-0.91598
O	-2.69641	0.40868	-1.96435
O	-3.3474	-1.31346	0.33797
O	-2.04007	-2.84189	-0.64273
H	-1.55165	2.59554	-2.74622
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H	0.19148	-1.97159	-0.63866
C	-0.7995	-0.146	1.0948
C	0.66275	0.26108	0.92193
S	0.94443	2.02018	1.19279
O	-0.18995	2.70273	1.76802
O	1.70684	2.6318	0.13075
F	1.99344	1.89559	2.40901
H	-1.43971	0.63924	1.51307
H	1.3017	-0.22604	1.66557
H	-0.82477	-1.02136	1.75511

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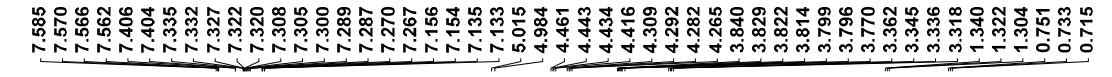
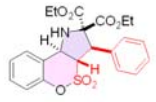
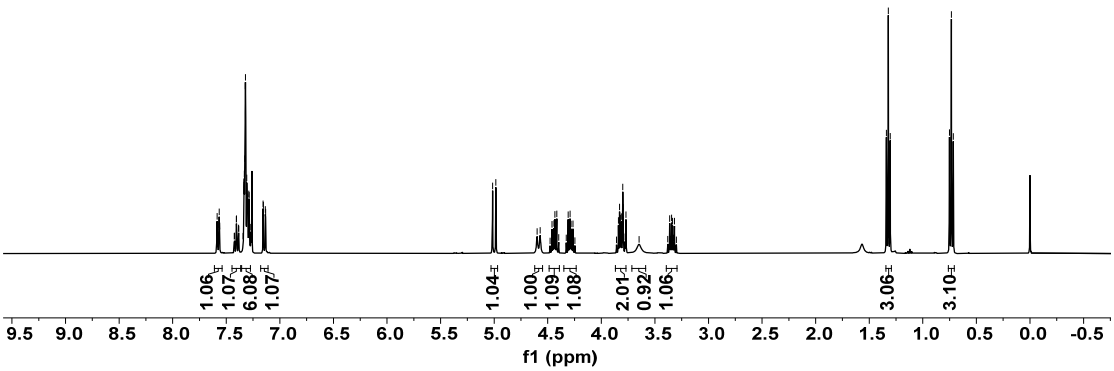
7. Copies of NMR spectra.

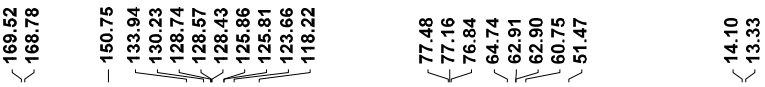


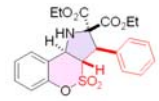


3a

^{1}H NMR (400 MHz, Chloroform-*d*)

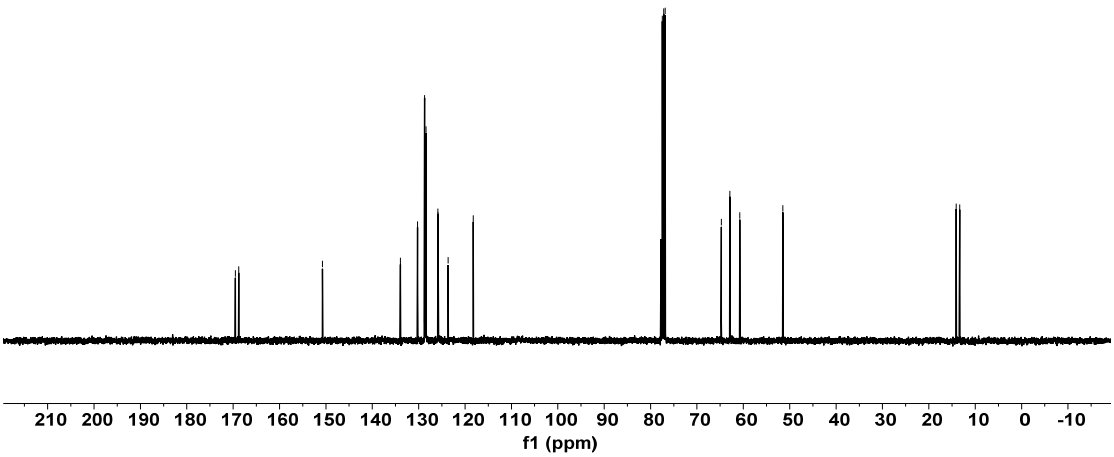


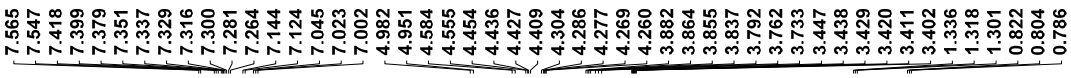


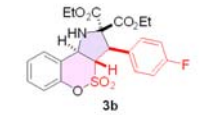


3a

^{13}C NMR (100 MHz, Chloroform-*d*)

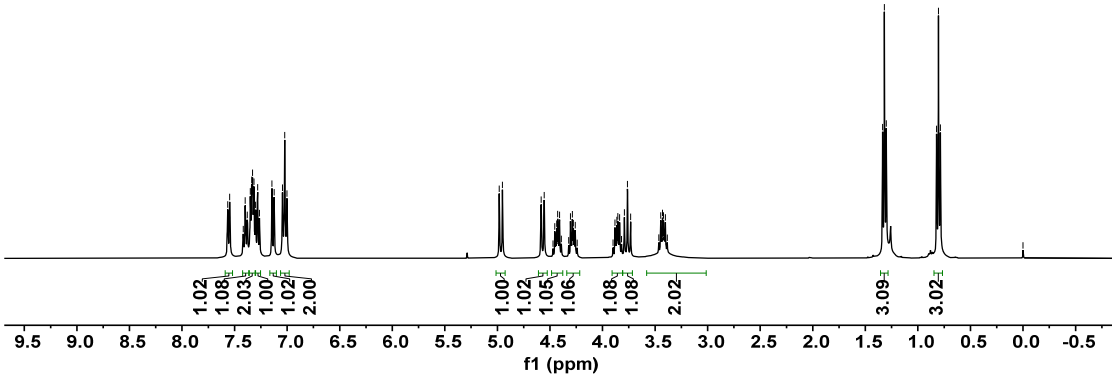


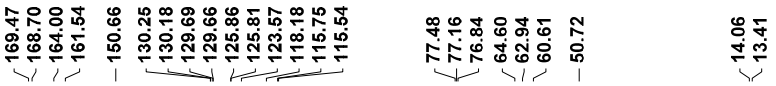


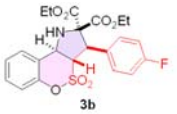


3b

^{1}H NMR (400 MHz, Chloroform-*d*)

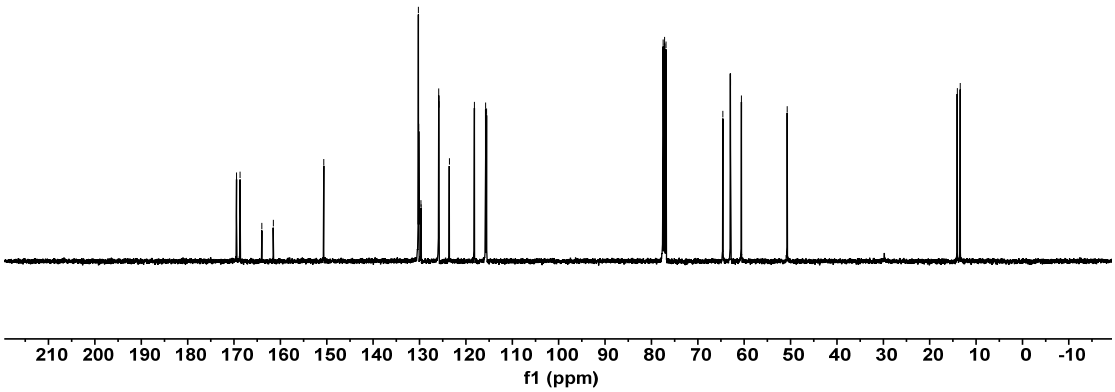


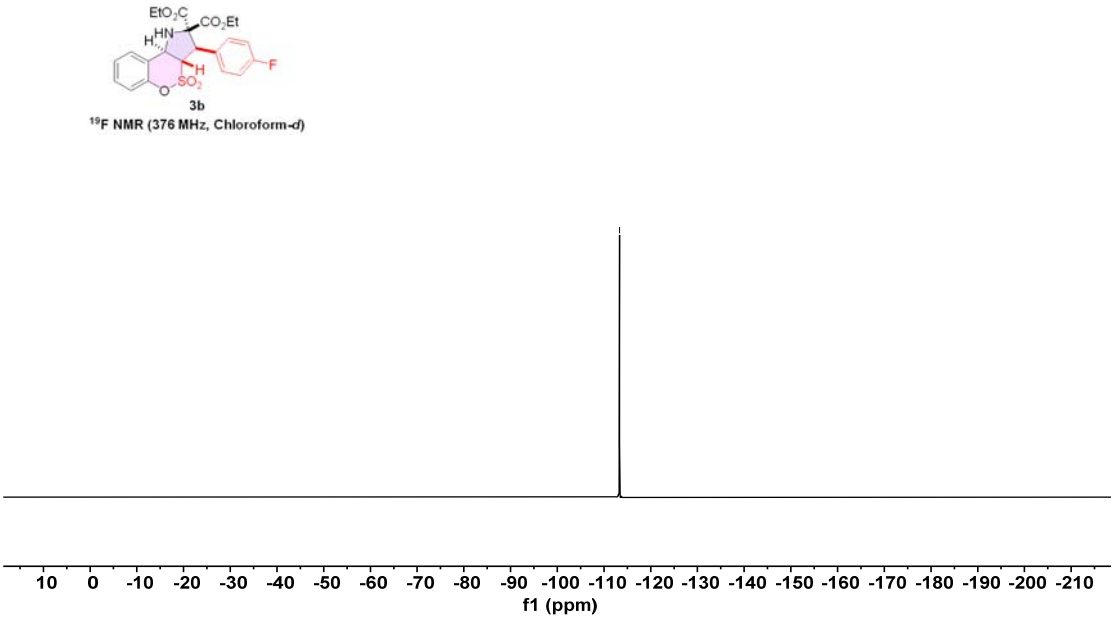




3b

^{13}C NMR (100 MHz, Chloroform-*d*)

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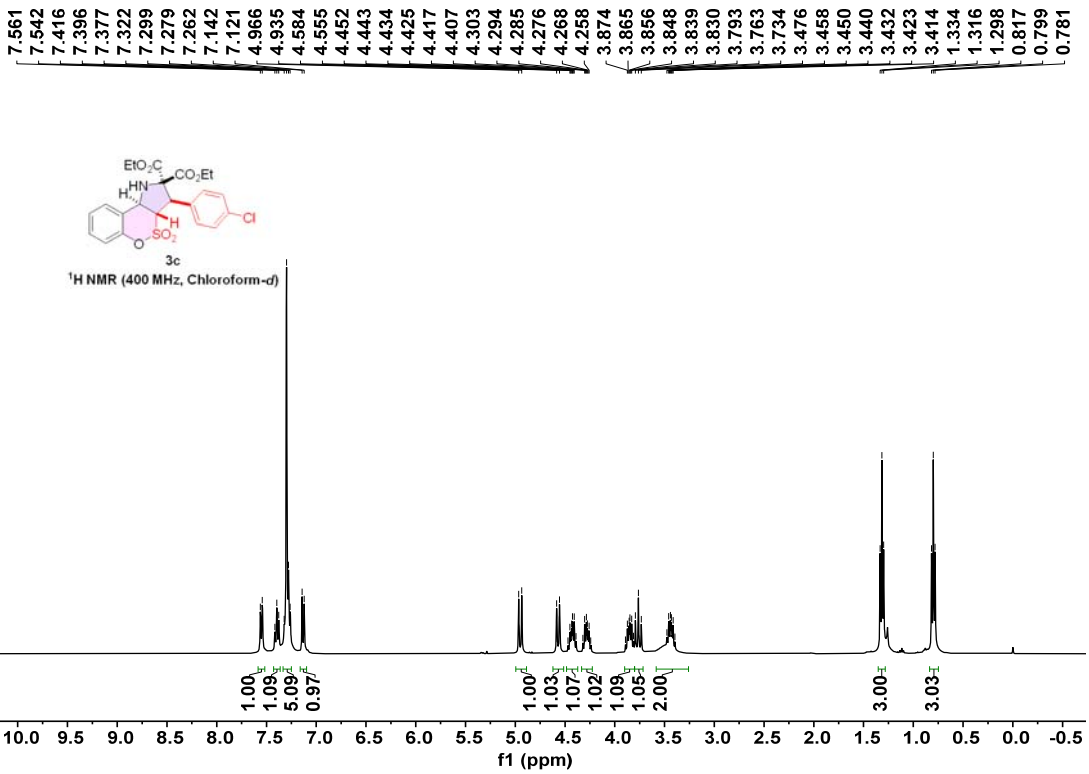
EtO2C
CO2Et
HN
H
H
SO2
O
F
3b
19F NMR (376 MHz, Chloroform-d)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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7.542
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7.322
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7.279
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7.142
7.121
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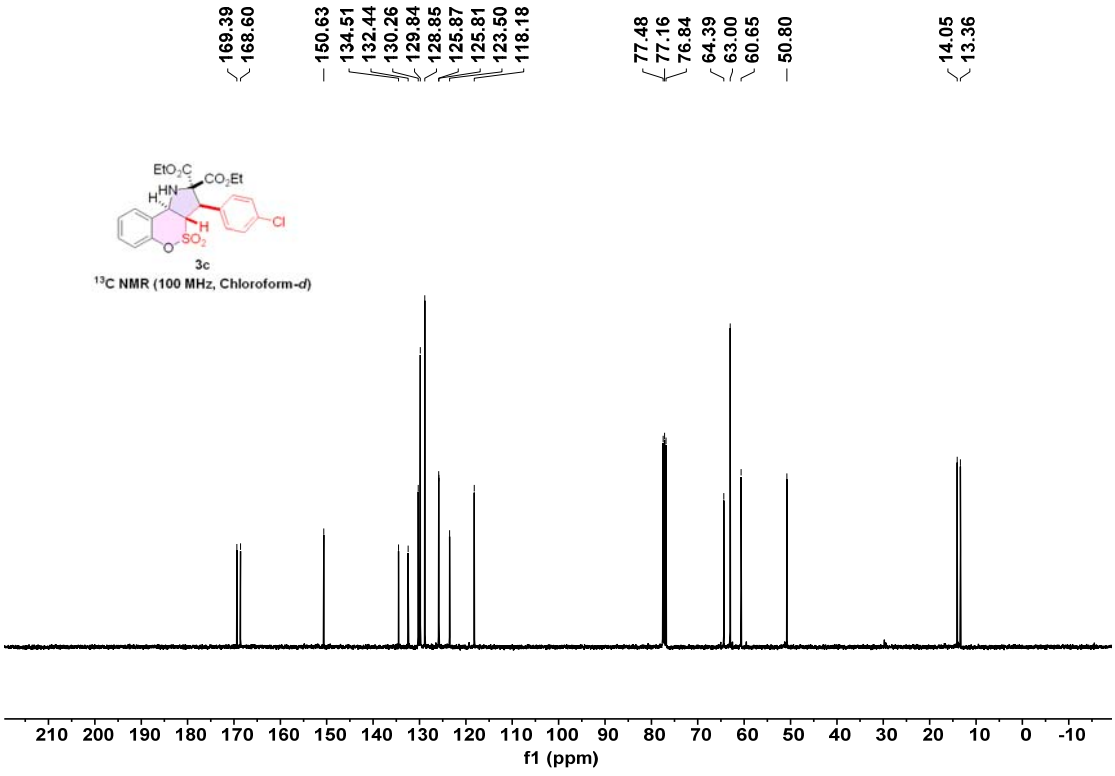
4.935
4.584
4.555
4.452
4.443
4.434
4.425
4.417
4.407
4.303
4.294
4.285
4.276
4.268
4.258
3.874
3.865
3.856
3.848
3.839
3.830
3.793
3.763
3.734
3.476
3.458
3.450
3.440
3.432
3.423
3.414
1.334
1.316
1.298
0.817
0.799
0.781
3c
1H NMR (400 MHz, Chloroform-d)
1.00
1.09
5.09
0.97
1.00
1.03
1.07
1.02
1.09
1.05
2.00
3.00
3.03
f1 (ppm)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128.85
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125.81
123.50
118.18
77.48
77.16
76.84
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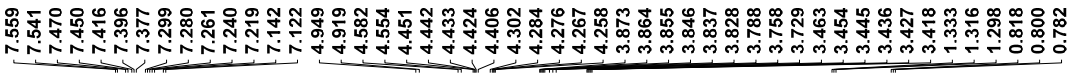
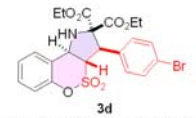
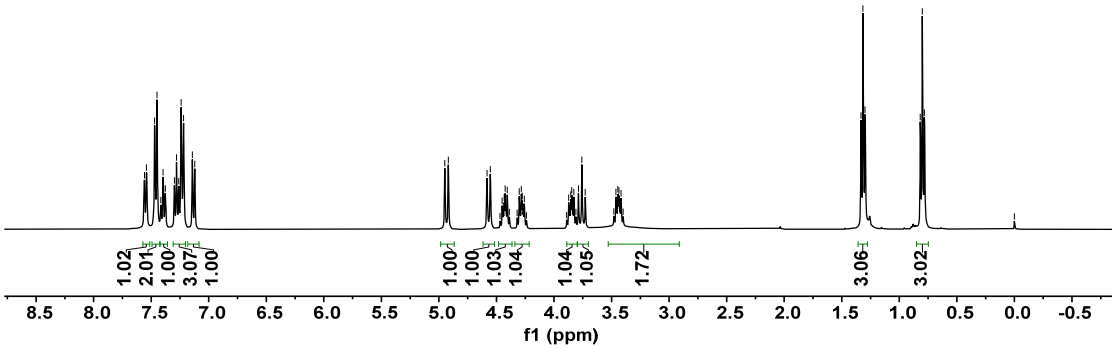
63.00
60.65
50.80
14.05
13.36
3c
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

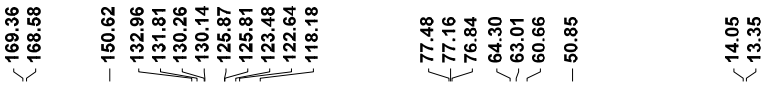


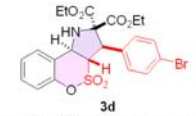


3d

^{1}H NMR (400 MHz, Chloroform-*d*)

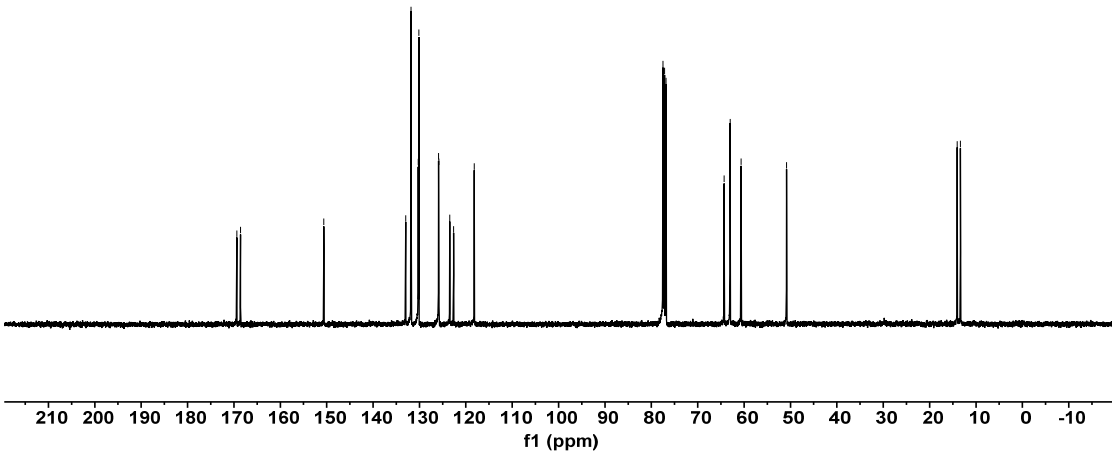


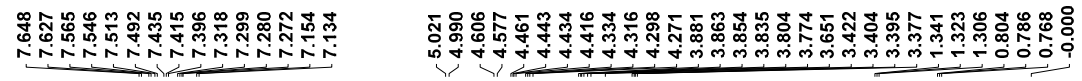


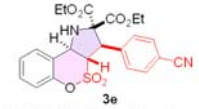


3d

^{13}C NMR (100 MHz, Chloroform-*d*)







3e

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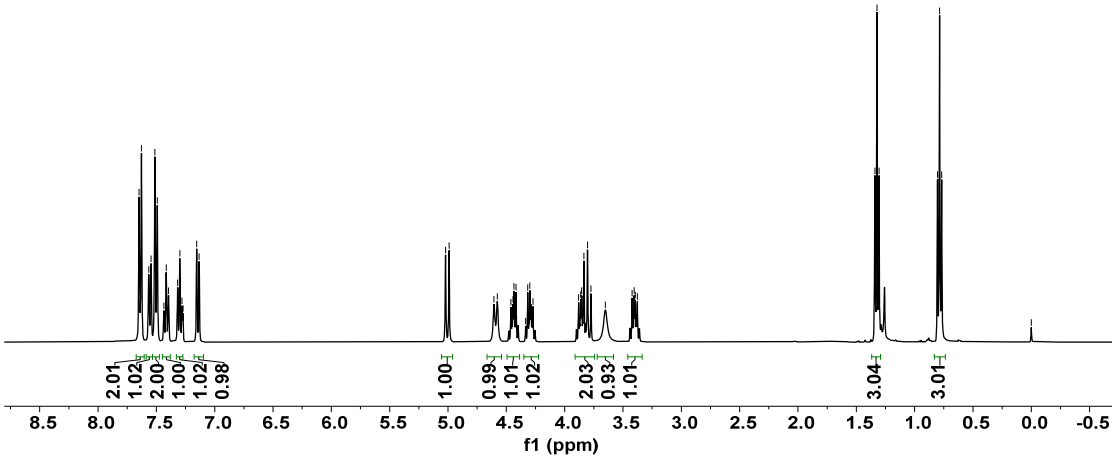
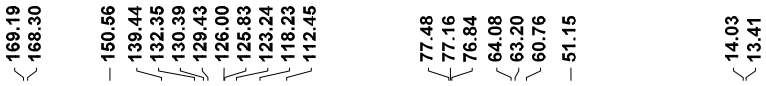
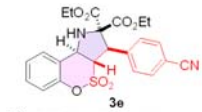
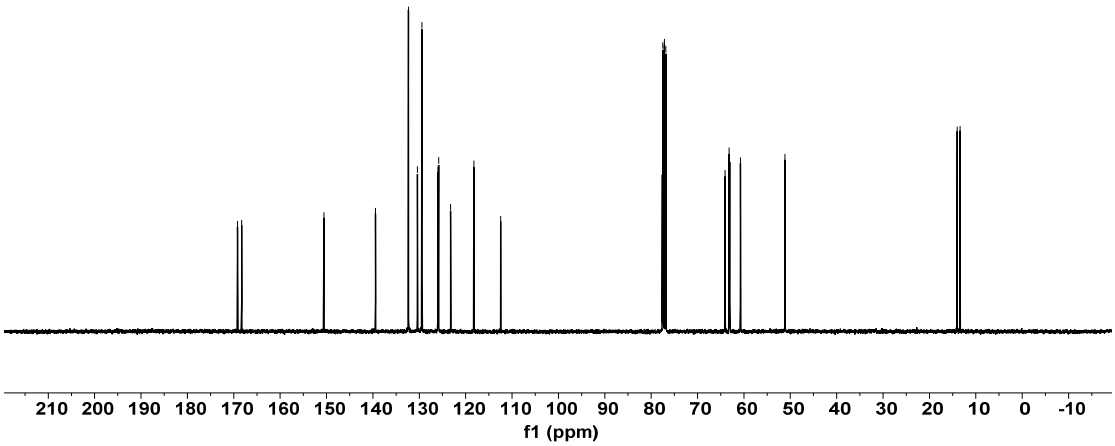


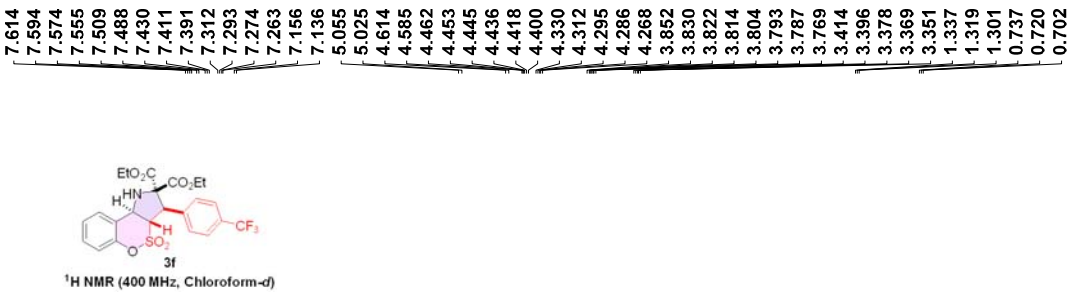




3e

^{13}C NMR (100 MHz, Chloroform-*d*)





3f

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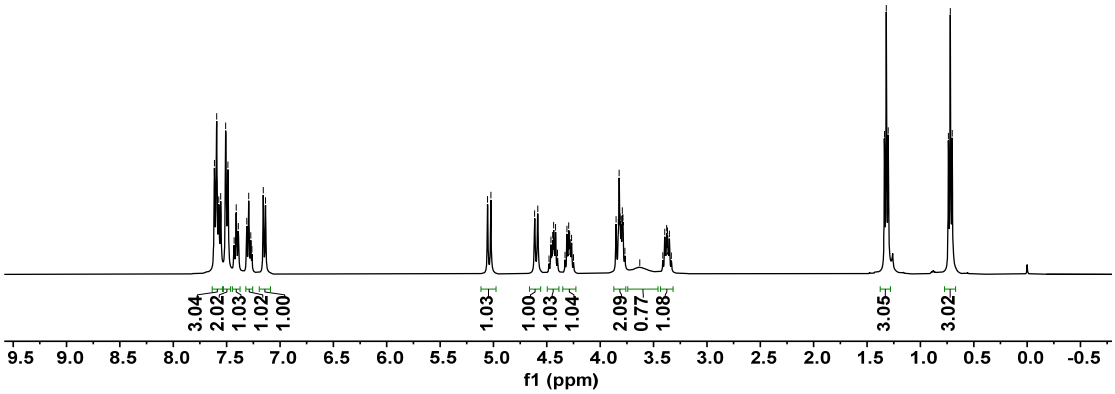

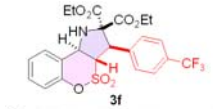

3f

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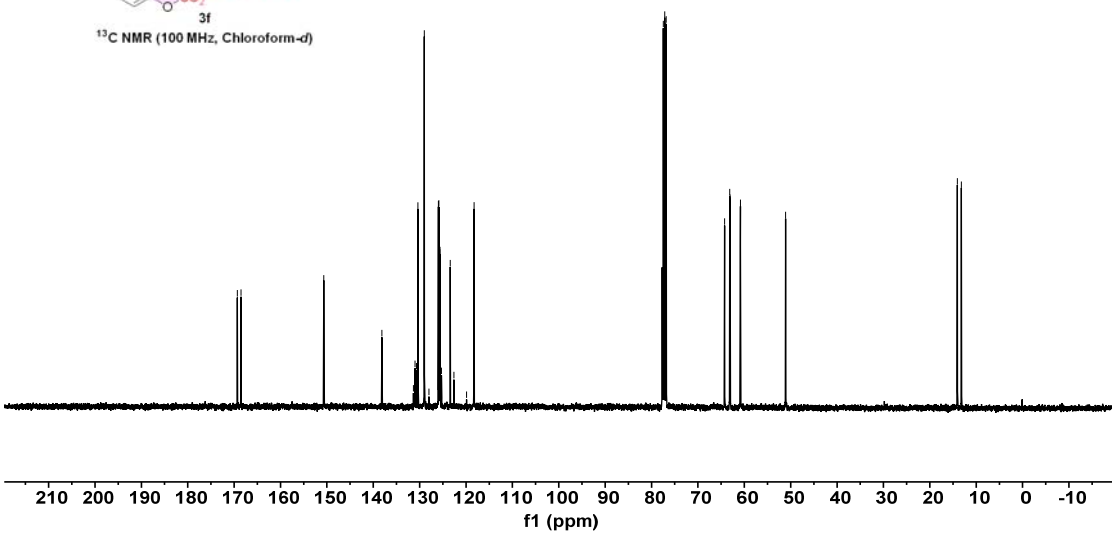

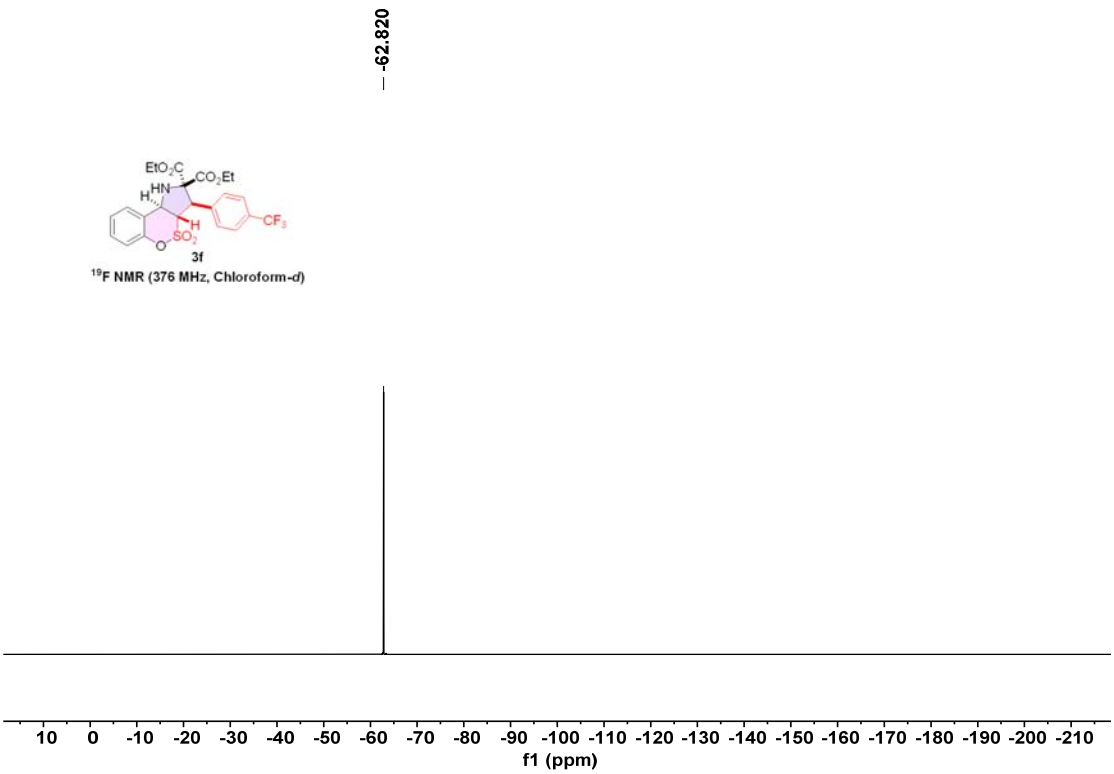
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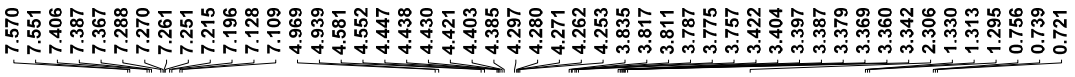
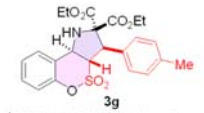
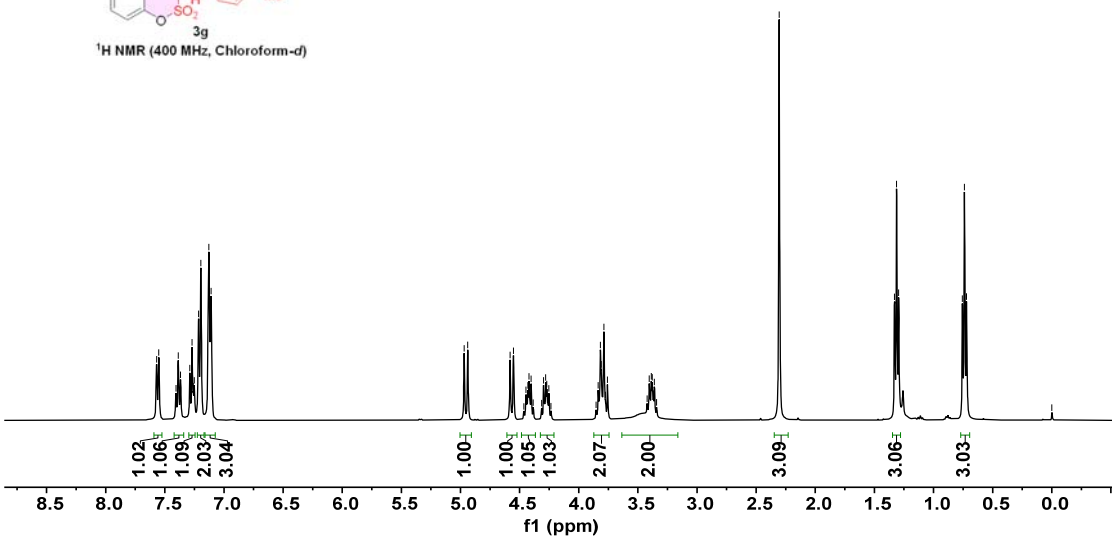
HN
H
H
SO2
O
CF3
3f
19F NMR (376 MHz, Chloroform-d)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

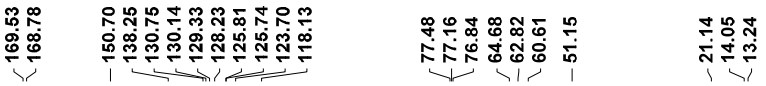


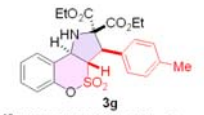


3g

^{1}H NMR (400 MHz, Chloroform-*d*)

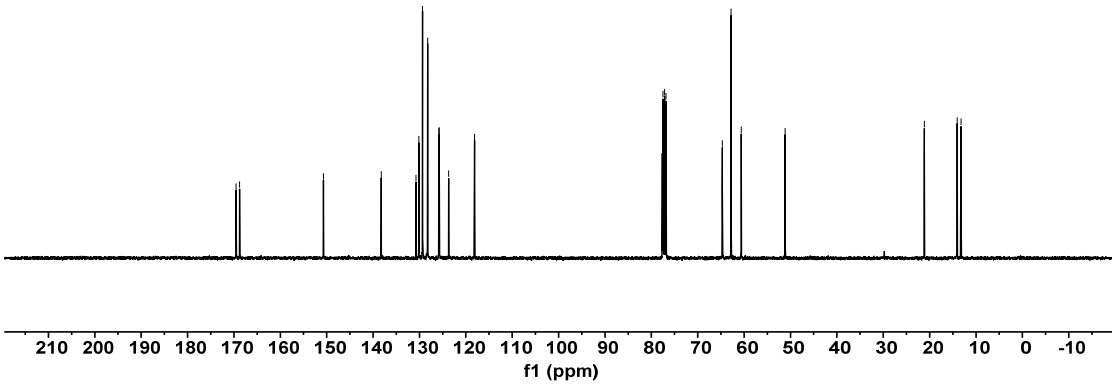


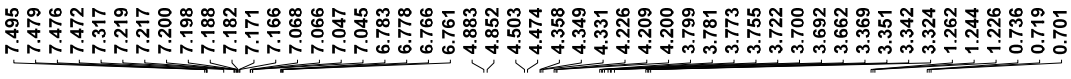


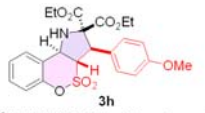


3g

^{13}C NMR (100 MHz, Chloroform-*d*)

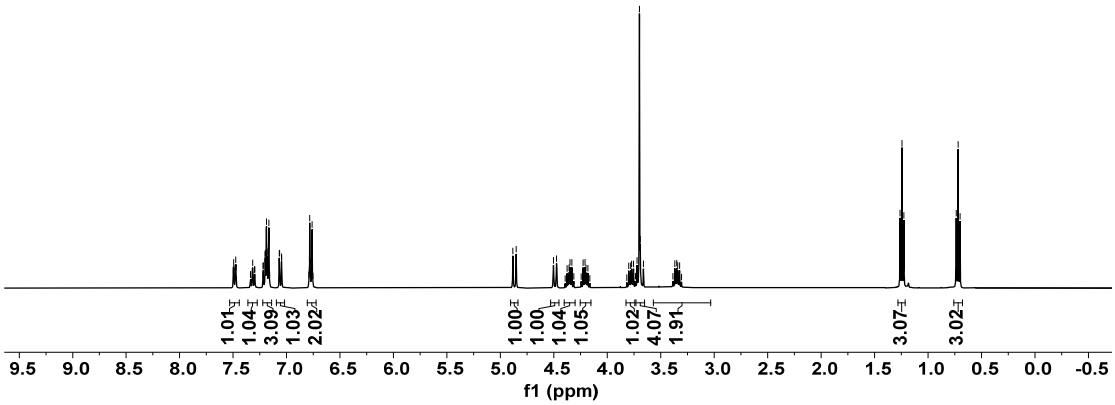


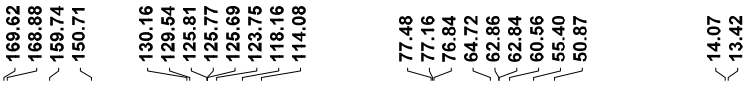


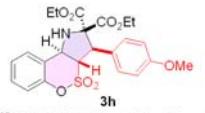


3h

^{1}H NMR (400 MHz, Chloroform-*d*)

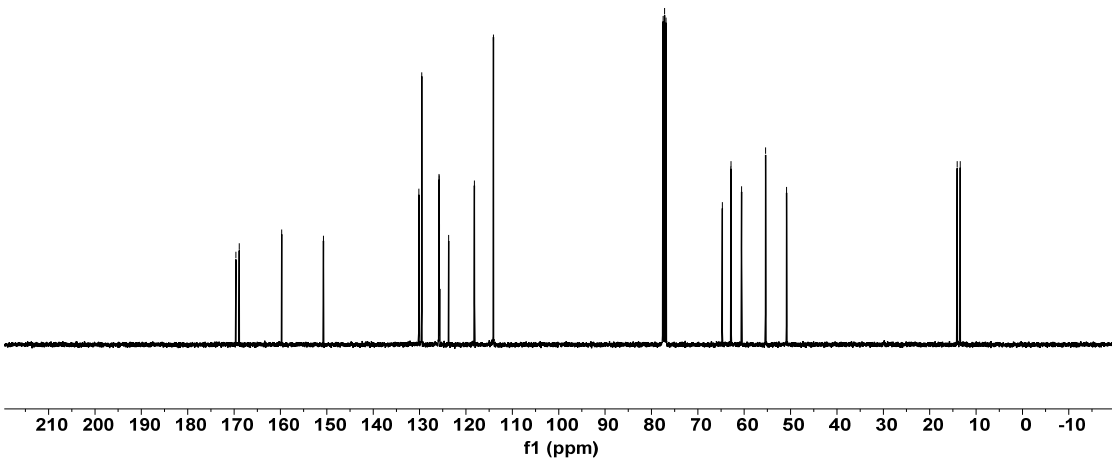


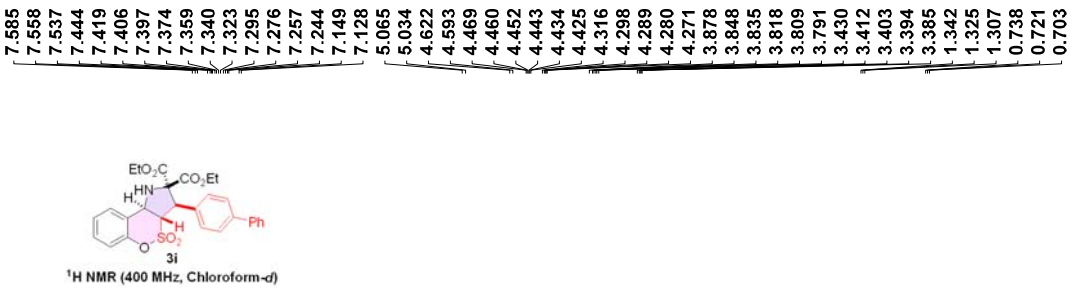




3h

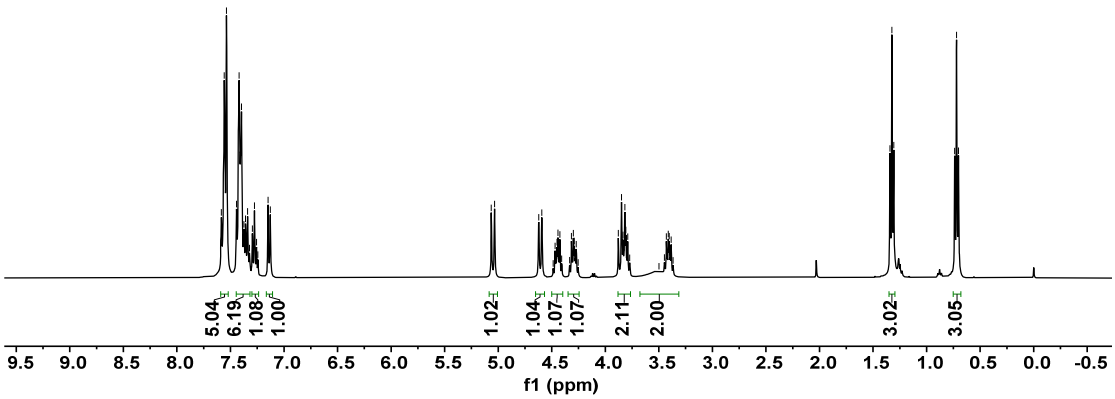
^{13}C NMR (100 MHz, Chloroform-*d*)

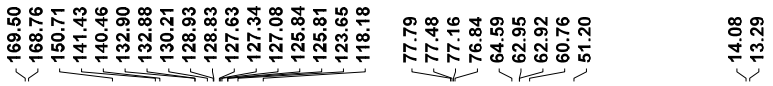


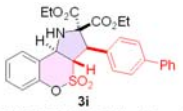


3i

^{1}H NMR (400 MHz, Chloroform-*d*)

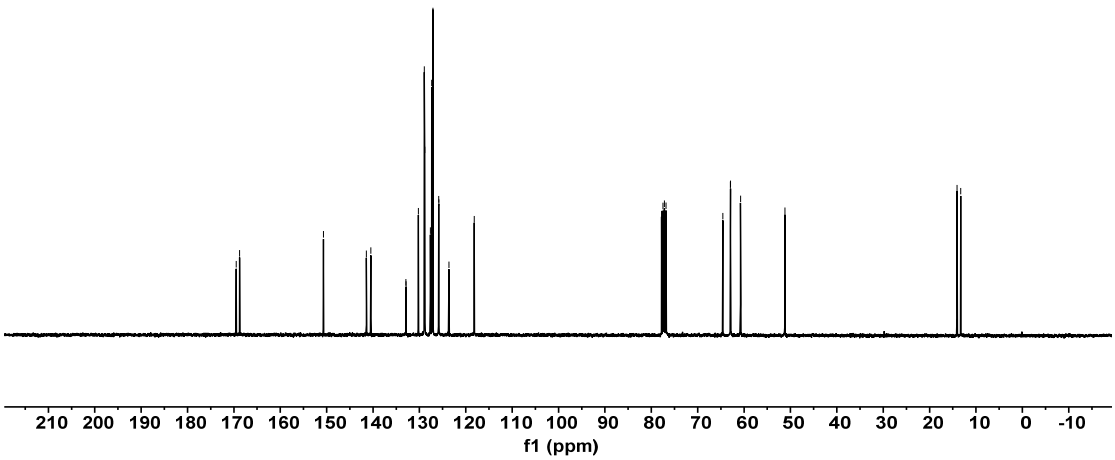


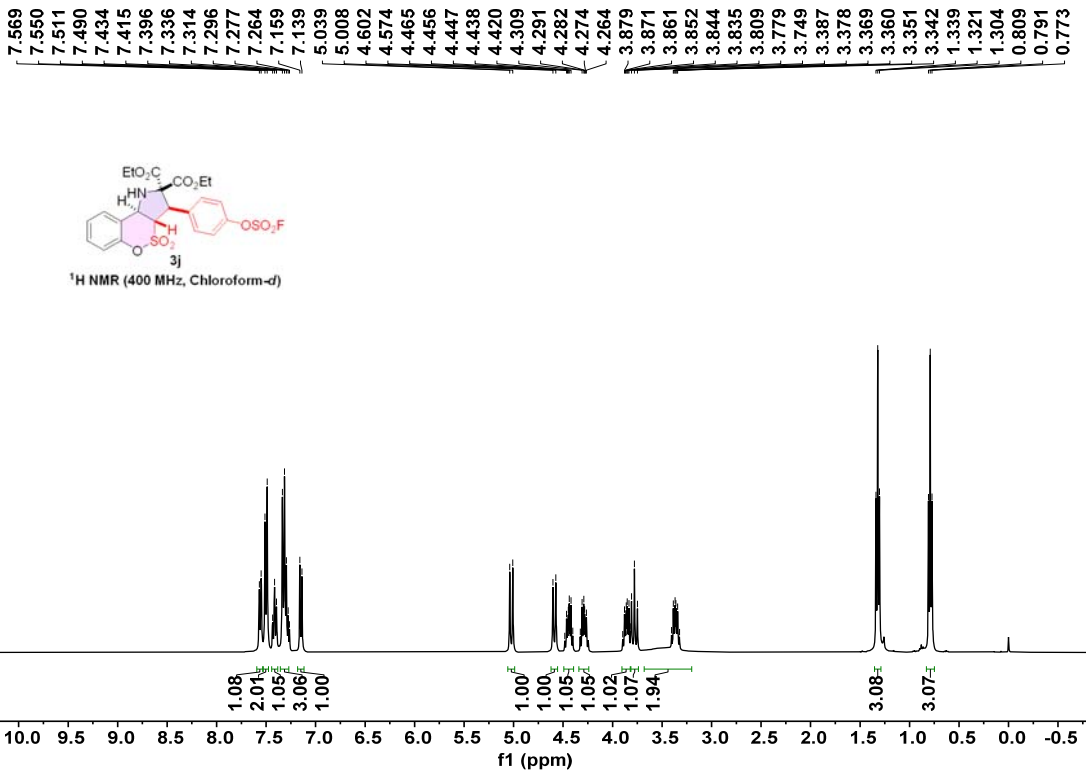


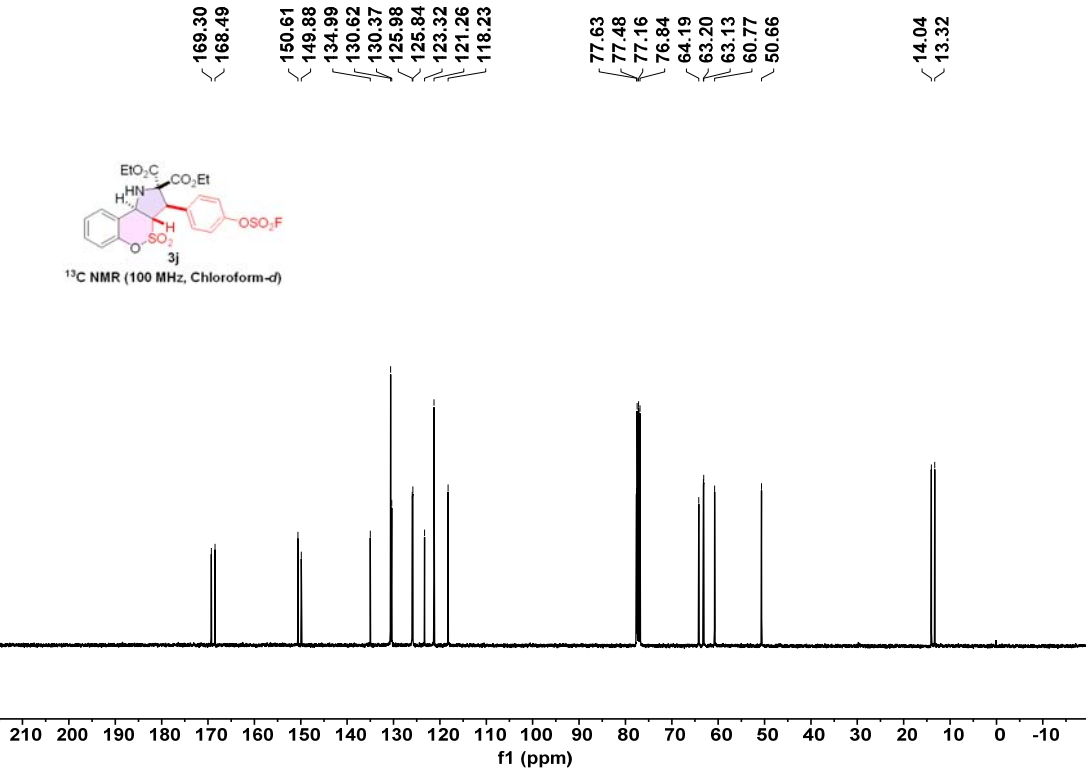


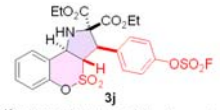
3i

^{13}C NMR (100 MHz, Chloroform-*d*)



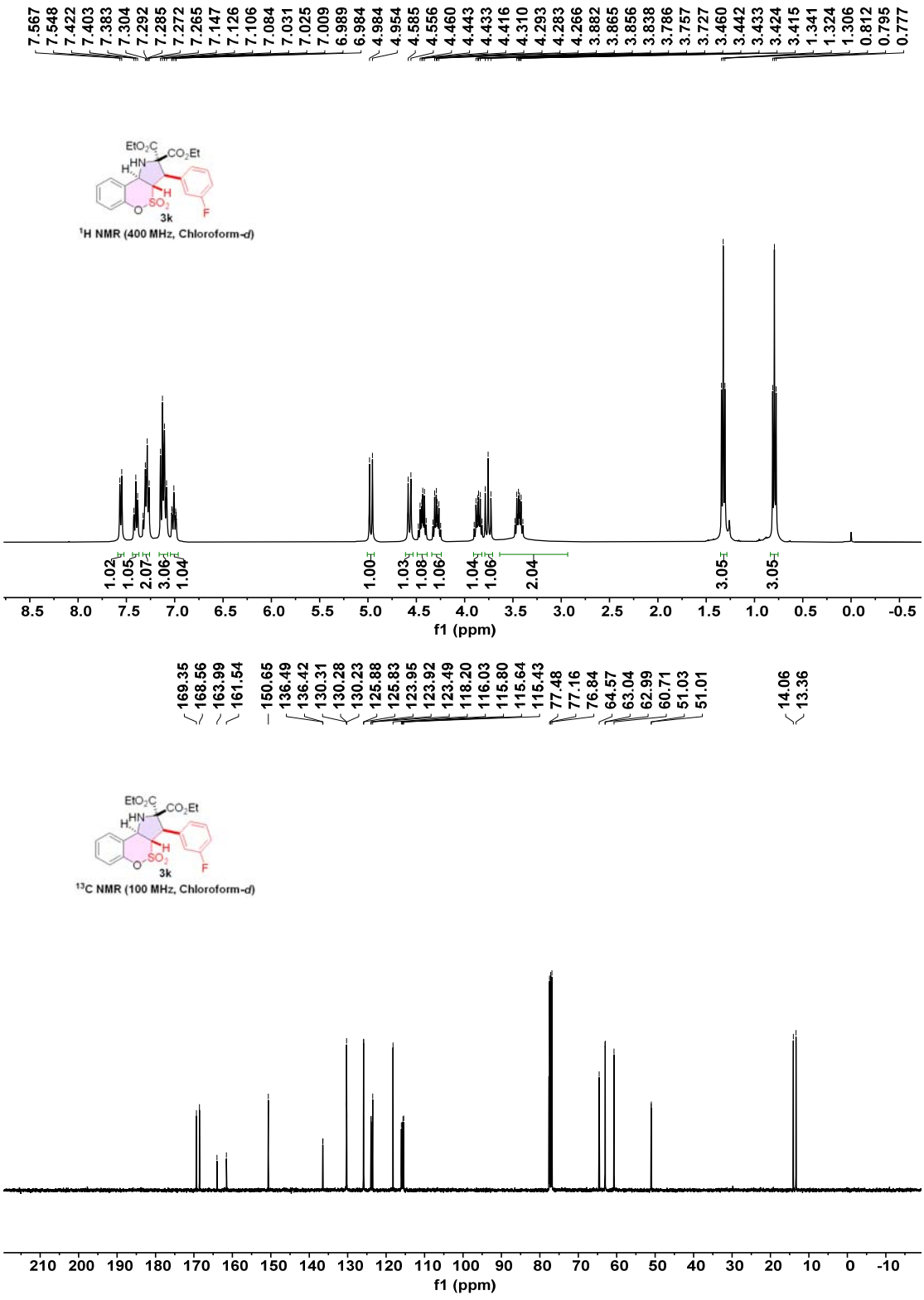

7.569
7.550
7.511
7.490
7.434
7.415
7.396
7.336
7.314
7.296
7.277
7.264
7.159
7.139
5.039
5.008
4.602
4.574
4.465
4.456
4.447
4.438
4.420
4.309
4.291
4.282
4.274
4.264
3.879
3.871
3.861
3.852
3.844
3.835
3.809
3.779
3.749
3.387
3.378
3.369
3.360
3.351
3.342
1.339
1.321
1.304
0.809
0.791
0.773
3j
1H NMR (400 MHz, Chloroform-d)
1.08
2.01
1.05
3.06
1.00
1.00
1.00
1.05
1.05
1.02
1.07
1.94
3.08
3.07
f1 (ppm)

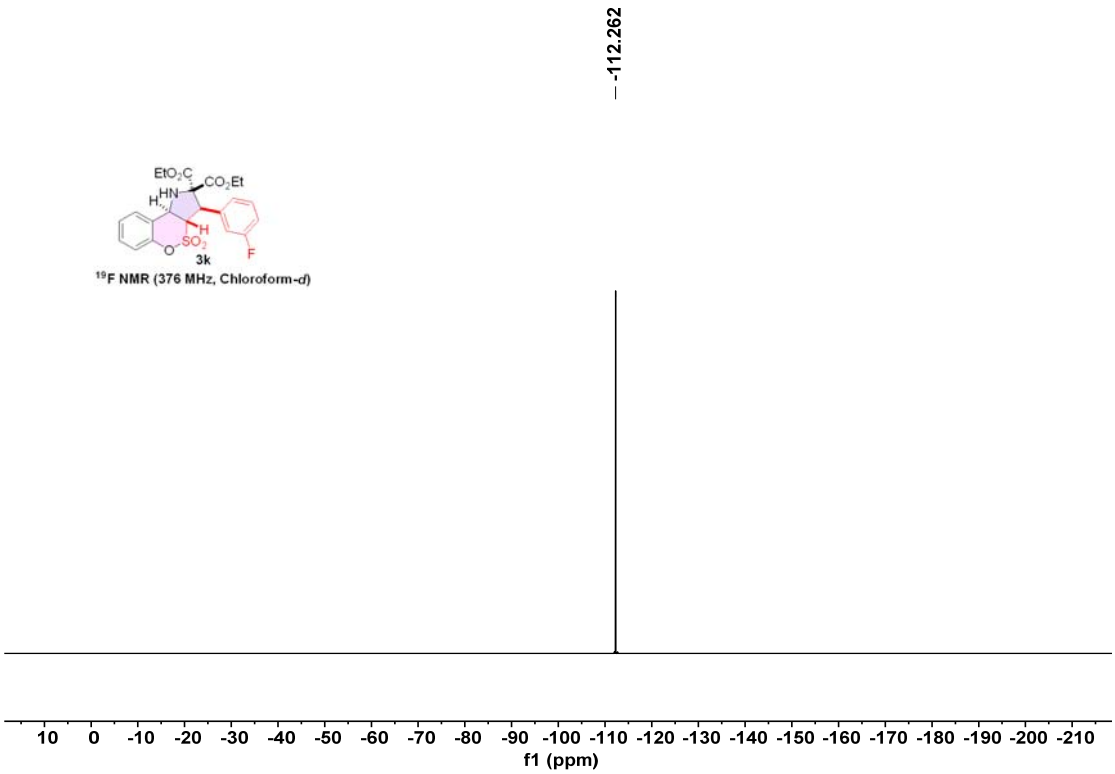

169.30
168.49
150.61
149.88
134.99
130.62
130.37
125.98
125.84
123.32
121.26
118.23
77.63
77.48
77.16
76.84
64.19
63.20
63.13
60.77
50.66
14.04
13.32
3j
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

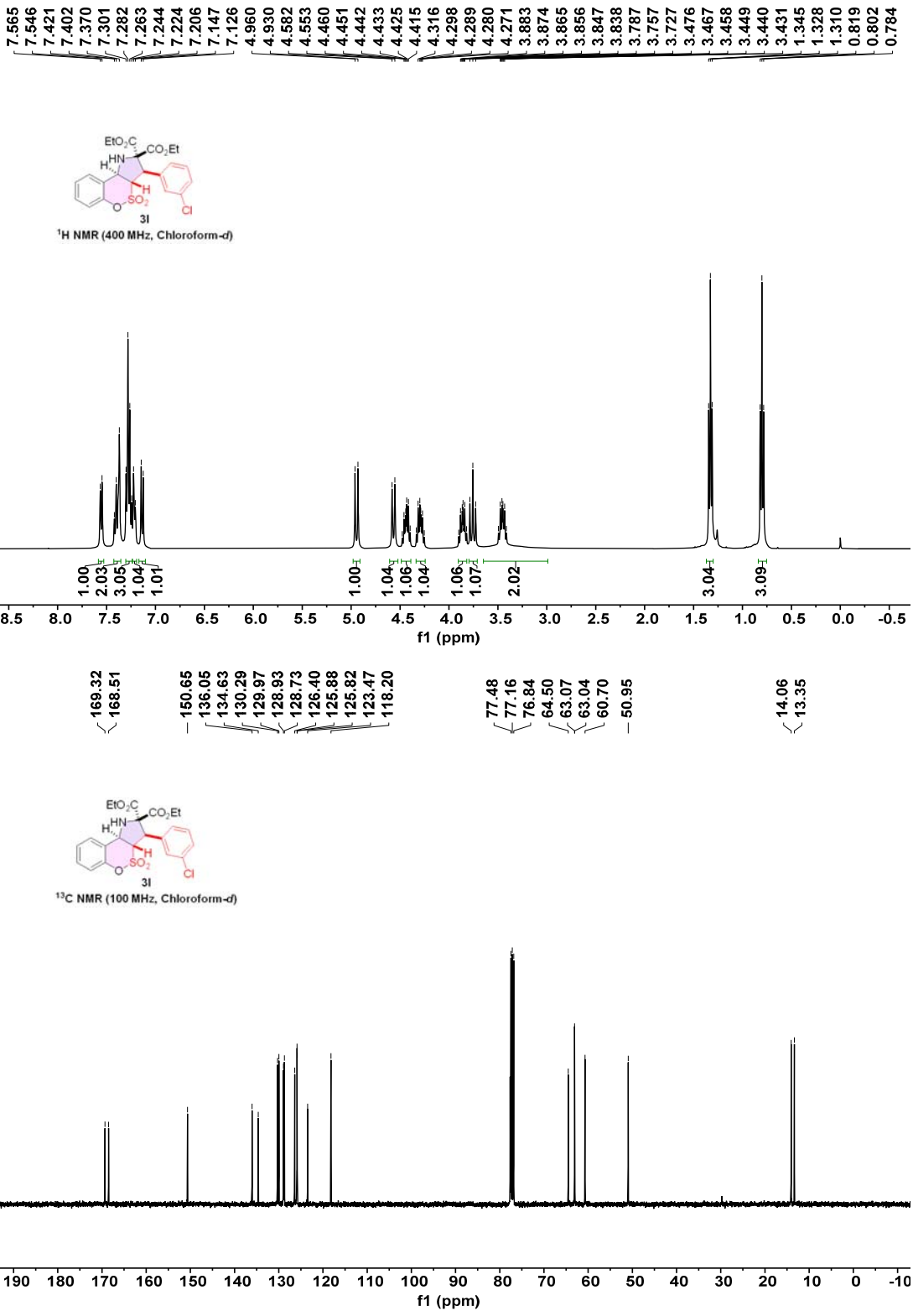


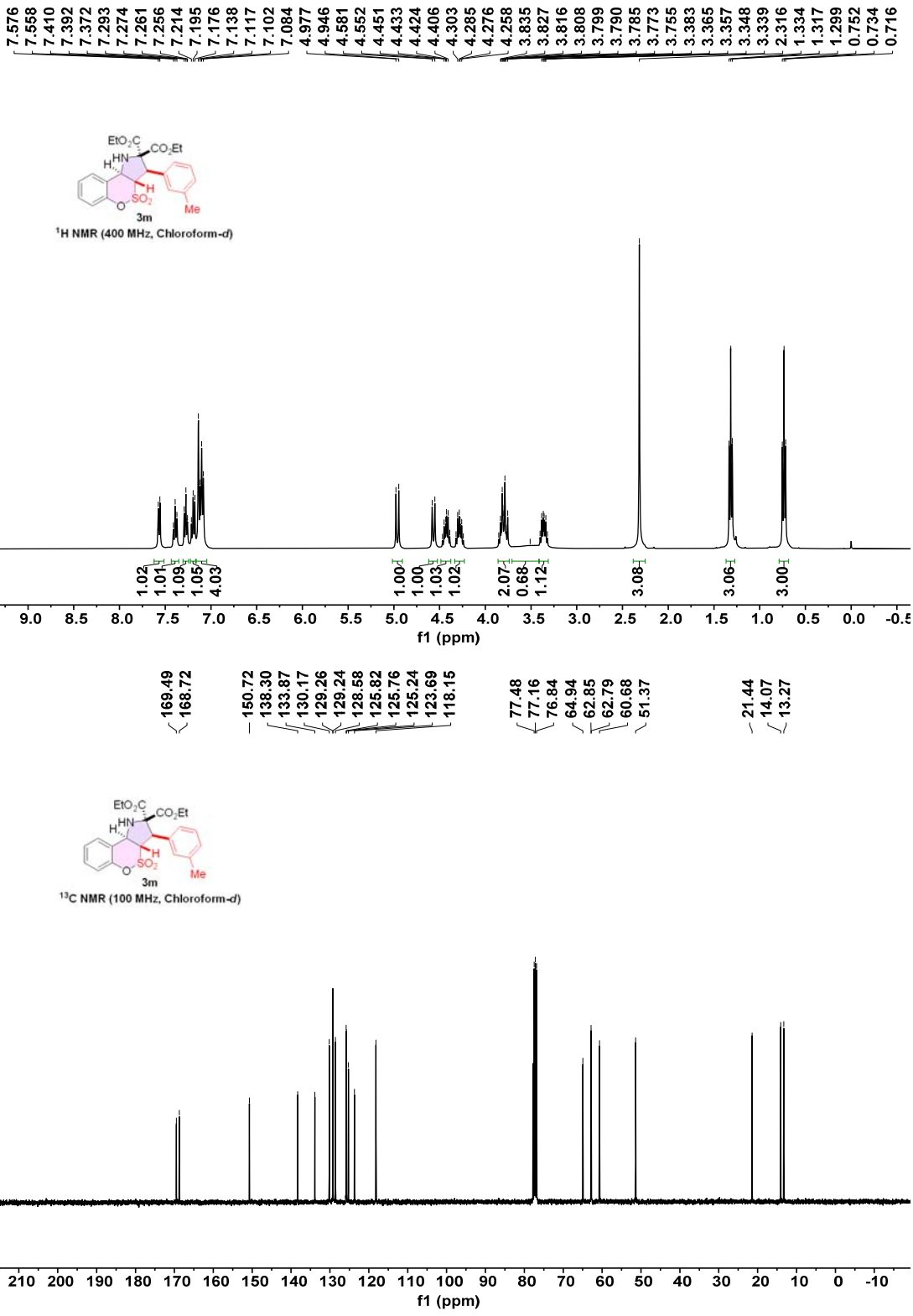
3j

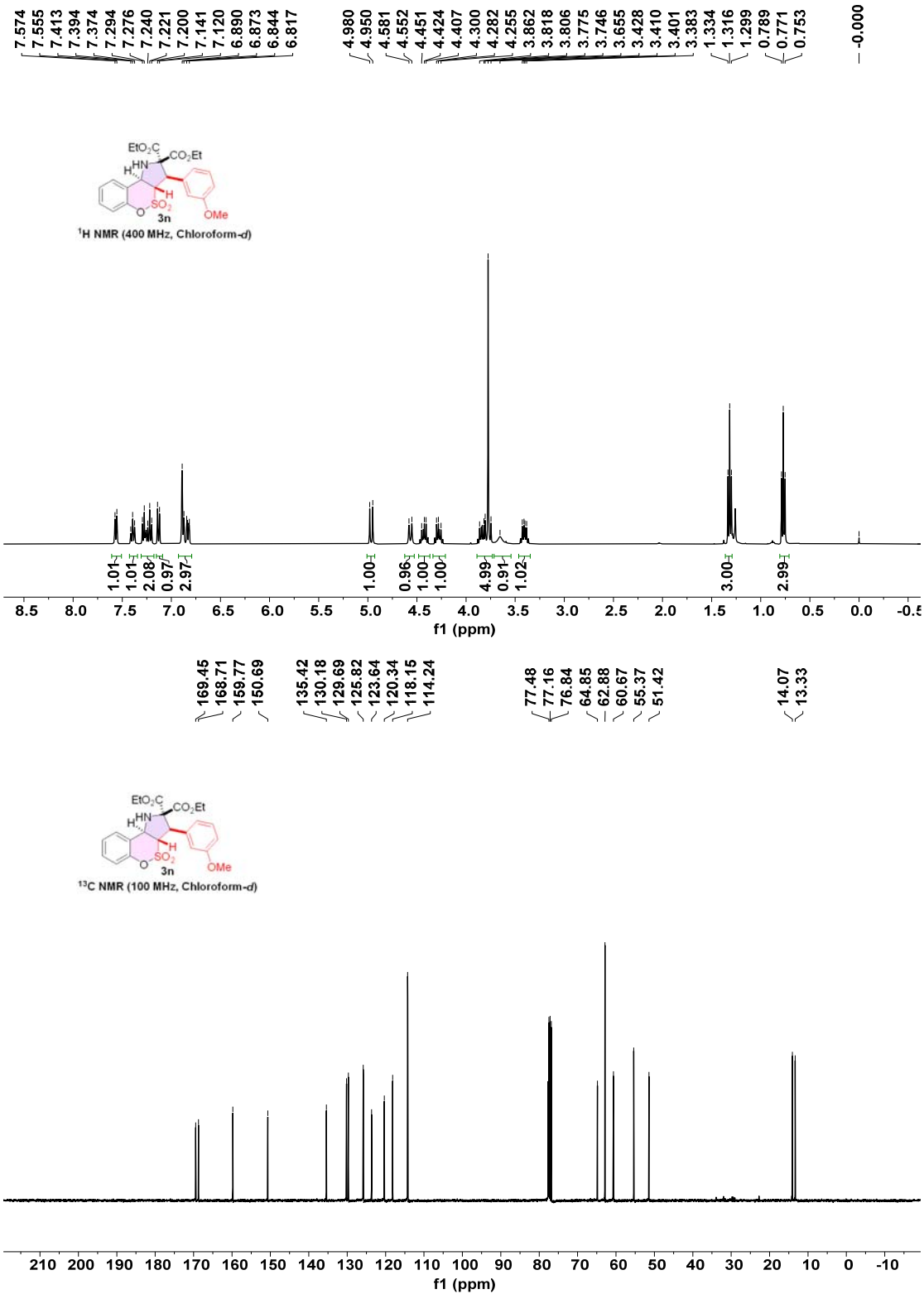
^{19}F NMR (376 MHz, Chloroform-*d*)

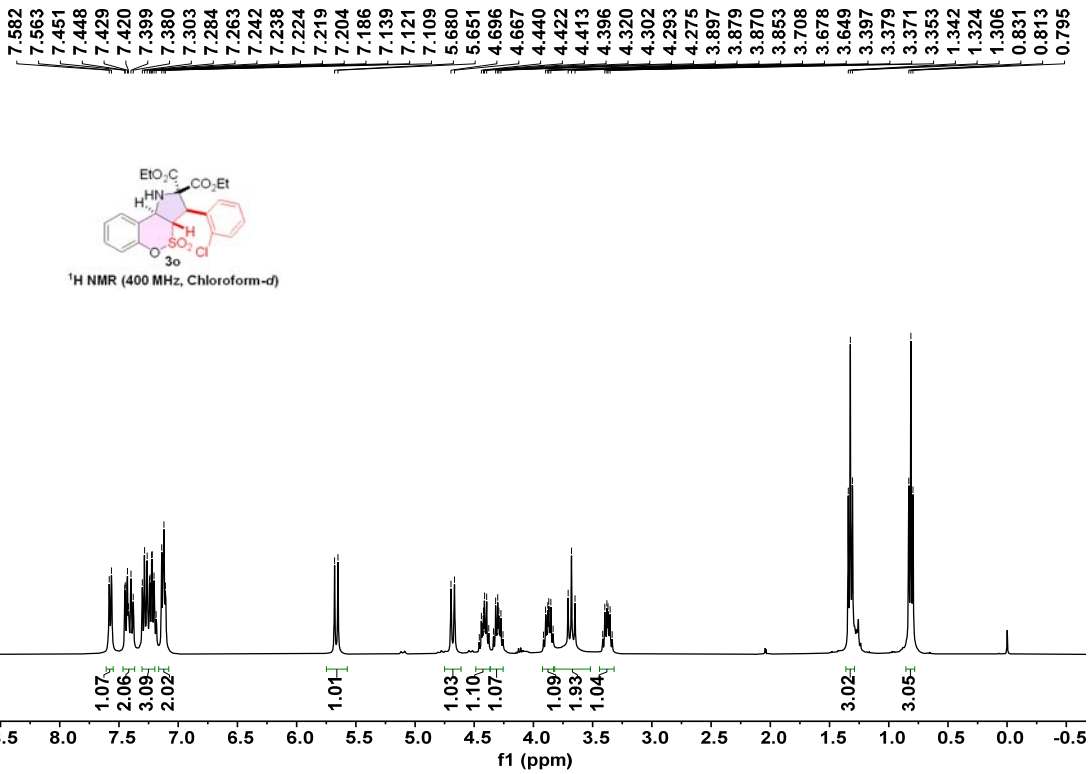

7.567
7.548
7.422
7.403
7.383
7.304
7.292
7.285
7.272
7.265
7.147
7.126
7.106
7.084
7.031
7.025
7.009
6.989
6.984
4.984
4.954
4.585
4.556
4.460
4.443
4.433
4.416
4.310
4.293
4.283
4.266
3.882
3.865
3.856
3.838
3.786
3.757
3.727
3.460
3.442
3.433
3.424
3.415
1.341
1.324
1.306
0.812
0.795
0.777
3k
1H NMR (400 MHz, Chloroform-d)
1.02
1.05
2.07
3.06
1.04
1.00
1.03
1.08
1.06
1.04
1.06
2.04
3.05
3.05
f1 (ppm)
169.35
168.56
163.99
161.54
150.65
136.49
136.42
130.31
130.28
130.23
125.88
125.83
123.95
123.92
123.49
118.20
116.03
115.80
115.64
115.43
77.48
77.16
76.84
64.57
63.04
62.99
60.71
51.03
51.01
14.06
13.36
3k
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

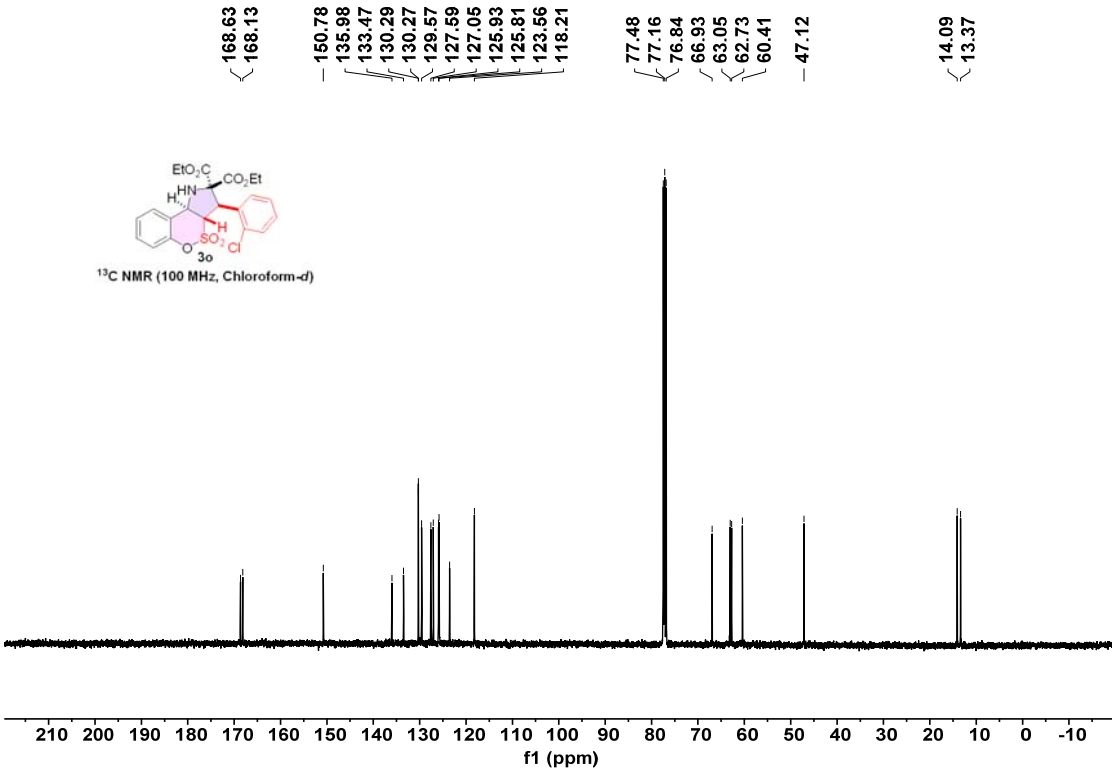

-112.262
EtO2C
CO2Et
HN
H
H
SO2
O
F
3k
19F NMR (376 MHz, Chloroform-d)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

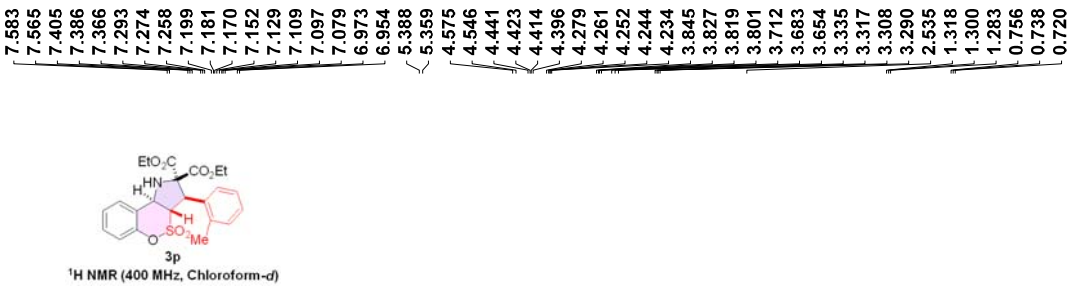

7.565
7.546
7.421
7.402
7.370
7.301
7.282
7.263
7.244
7.224
7.206
7.147
7.126
4.960
4.930
4.582
4.553
4.460
4.451
4.442
4.433
4.425
4.415
4.316
4.298
4.289
4.280
4.271
3.883
3.874
3.865
3.856
3.847
3.838
3.787
3.757
3.727
3.476
3.467
3.458
3.449
3.440
3.431
1.345
1.328
1.310
0.819
0.802
0.784
EtO2C
CO2Et
HN
H
H
SO2
O
Cl
3l
1H NMR (400 MHz, Chloroform-d)
1.00
2.03
3.05
1.04
1.01
1.00
1.04
1.06
1.04
1.06
1.07
2.02
3.04
3.09
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)
169.32
168.51
150.65
136.05
134.63
130.29
129.97
128.93
128.73
126.40
125.88
125.82
123.47
118.20
77.48
77.16
76.84
64.50
63.07
63.04
60.70
50.95
14.06
13.35
EtO2C
CO2Et
HN
H
H
SO2
O
Cl
3l
13C NMR (100 MHz, Chloroform-d)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.576
7.558
7.410
7.392
7.372
7.293
7.274
7.261
7.256
7.214
7.195
7.176
7.138
7.117
7.102
7.084
4.977
4.946
4.581
4.552
4.451
4.433
4.424
4.406
4.303
4.285
4.276
4.258
3.835
3.827
3.816
3.808
3.799
3.790
3.785
3.773
3.755
3.383
3.365
3.357
3.348
3.339
2.316
1.334
1.317
1.299
0.752
0.734
0.716
3m
1H NMR (400 MHz, Chloroform-d)
1.02
1.01
1.09
1.05
4.03
1.00
1.00
1.03
1.02
2.07
0.68
1.12
3.08
3.06
3.00
f1 (ppm)
169.49
168.72
150.72
138.30
133.87
130.17
129.26
129.24
128.58
125.82
125.76
125.24
123.69
118.15
77.48
77.16
76.84
64.94
62.85
62.79
60.68
51.37
21.44
14.07
13.27
3m
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)


7.574
7.555
7.413
7.394
7.374
7.294
7.276
7.240
7.221
7.200
7.141
7.120
6.890
6.873
6.844
6.817
4.980
4.950
4.581
4.552
4.451
4.424
4.407
4.300
4.282
4.255
3.862
3.818
3.806
3.775
3.746
3.655
3.428
3.410
3.401
3.383
1.334
1.316
1.299
0.789
0.771
0.753
-0.000
3n
OMe
1H NMR (400 MHz, Chloroform-d)
1.01
1.01
2.08
0.97
2.97
1.00
0.96
1.00
1.00
4.99
0.91
1.02
3.00
2.99
f1 (ppm)
169.45
168.71
159.77
150.69
135.42
130.18
129.69
125.82
123.64
120.34
118.15
114.24
77.48
77.16
76.84
64.85
62.88
60.67
55.37
51.42
14.07
13.33
3n
OMe
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

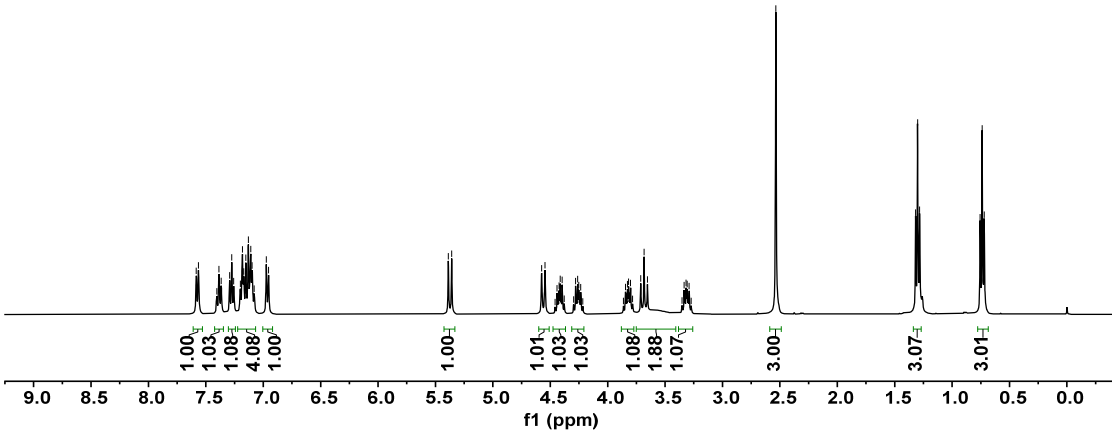

7.582
7.563
7.451
7.448
7.429
7.420
7.399
7.380
7.303
7.284
7.263
7.242
7.238
7.224
7.219
7.204
7.186
7.139
7.121
7.109
5.680
5.651
4.696
4.667
4.440
4.422
4.413
4.396
4.320
4.302
4.293
4.275
3.897
3.879
3.870
3.853
3.708
3.678
3.649
3.397
3.379
3.371
3.353
1.342
1.324
1.306
0.831
0.813
0.795
3o
1H NMR (400 MHz, Chloroform-d)
1.07
2.06
3.09
2.02
1.01
1.03
1.10
1.07
1.09
1.93
1.04
3.02
3.05
f1 (ppm)

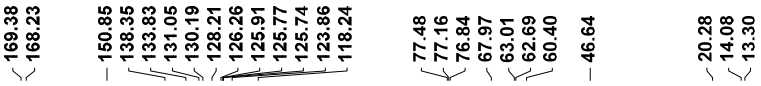

168.63
168.13
150.78
135.98
133.47
130.29
130.27
129.57
127.59
127.05
125.93
125.81
123.56
118.21
77.48
77.16
76.84
66.93
63.05
62.73
60.41
47.12
14.09
13.37
3o
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

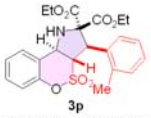


3p

^{1}H NMR (400 MHz, Chloroform-*d*)

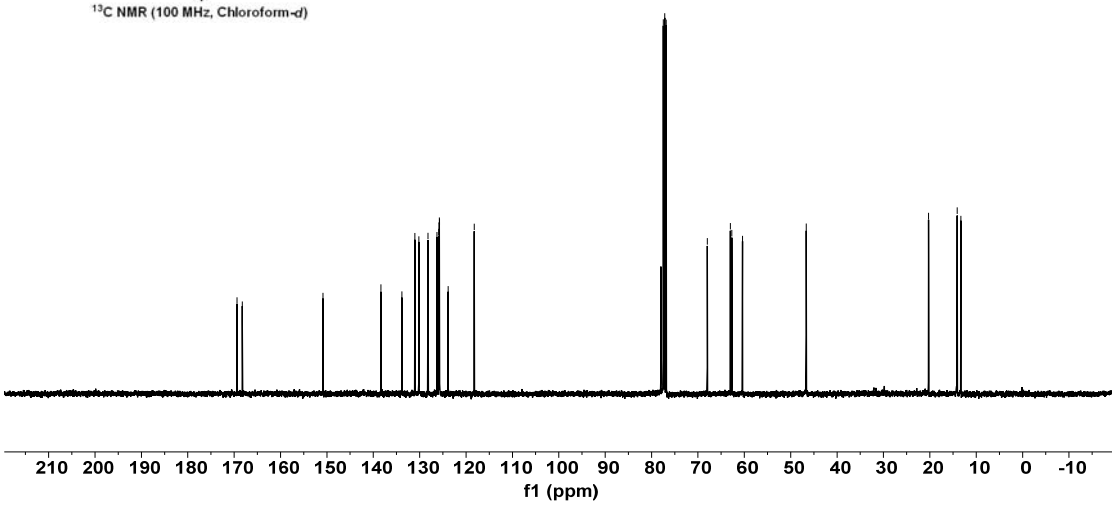


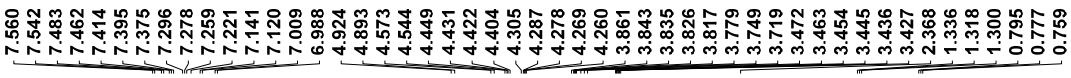


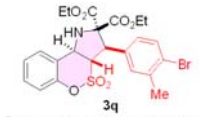


3p

^{13}C NMR (100 MHz, Chloroform-*d*)

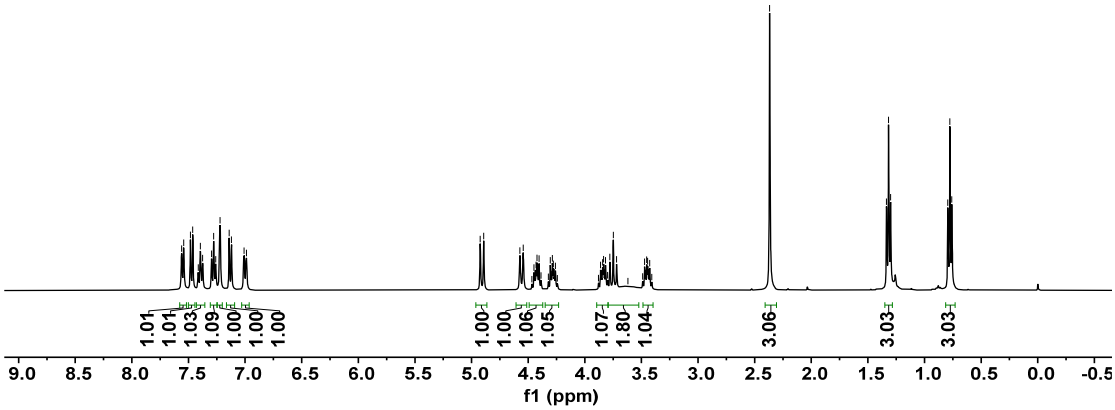


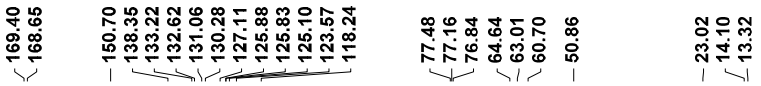


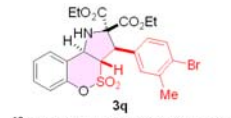


3q

^{1}H NMR (400 MHz, Chloroform-*d*)

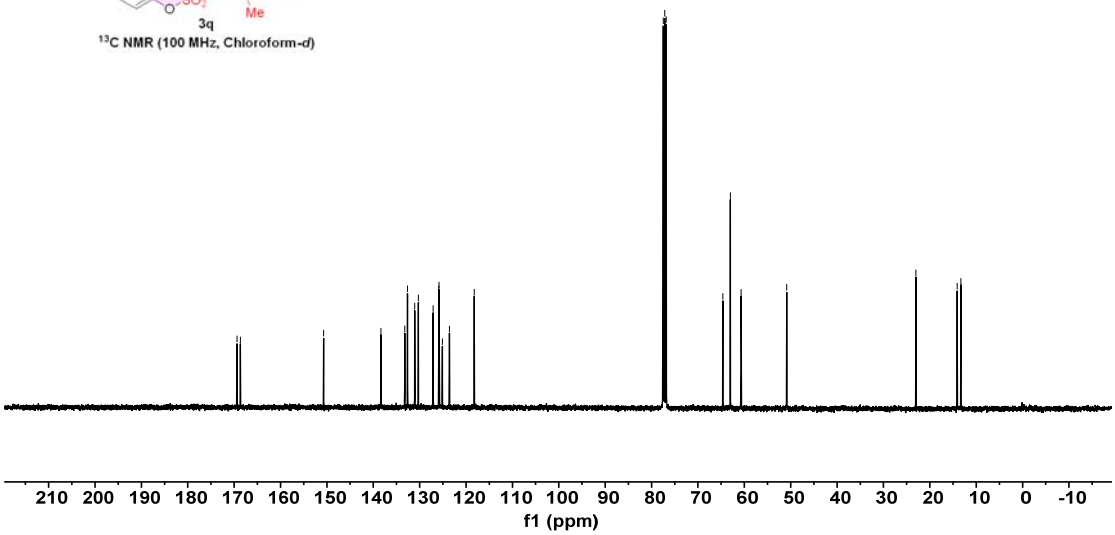


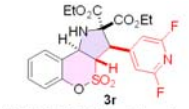




3q

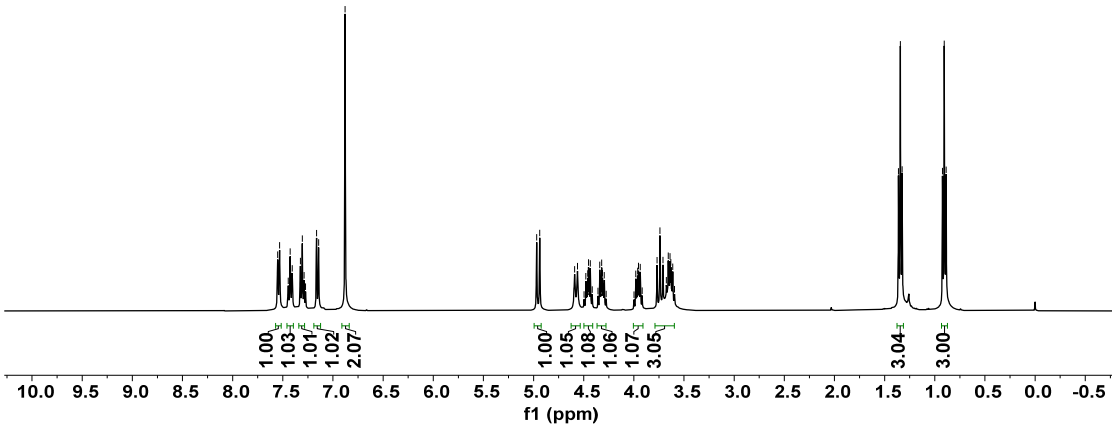
^{13}C NMR (100 MHz, Chloroform-*d*)

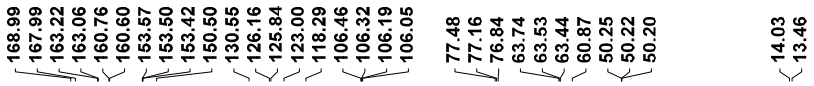


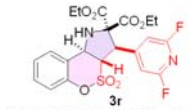


3r

^{1}H NMR (400 MHz, Chloroform-*d*)

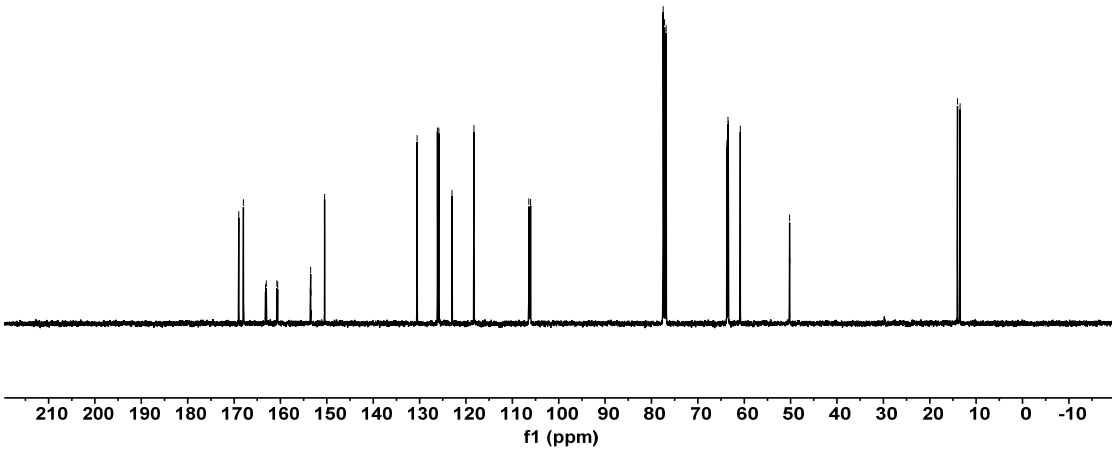


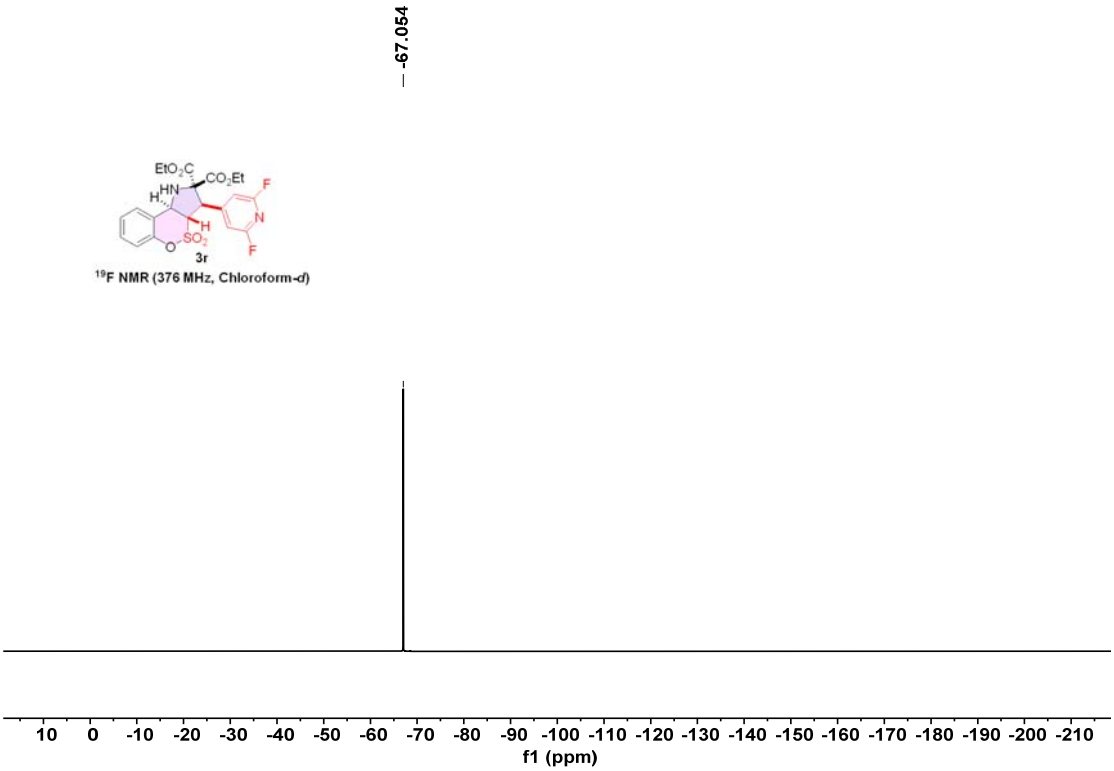




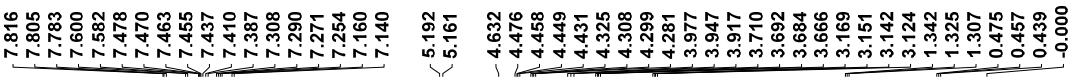
3r

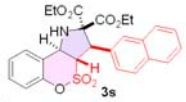
^{13}C NMR (100 MHz, Chloroform-*d*)



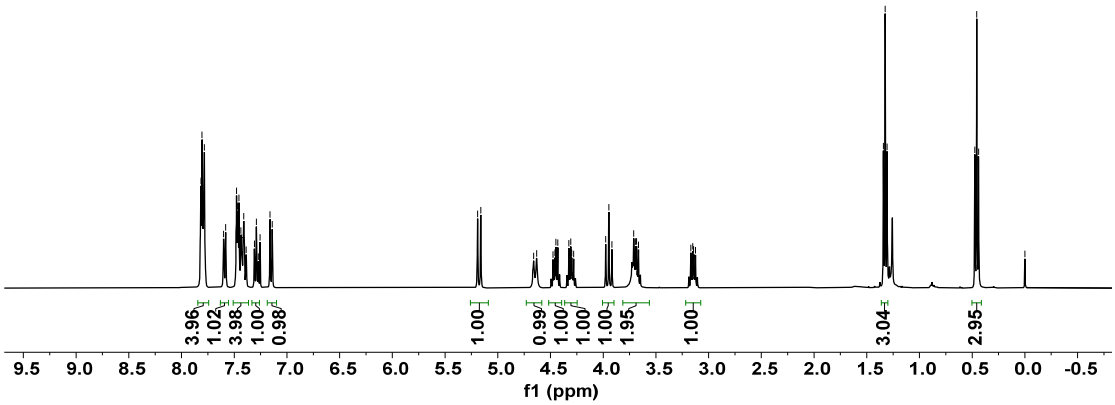


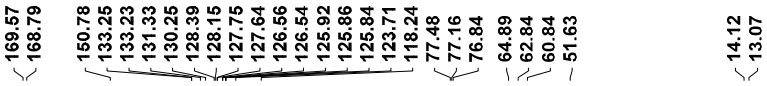
^{19}F NMR (376 MHz, Chloroform-*d*)

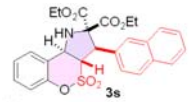




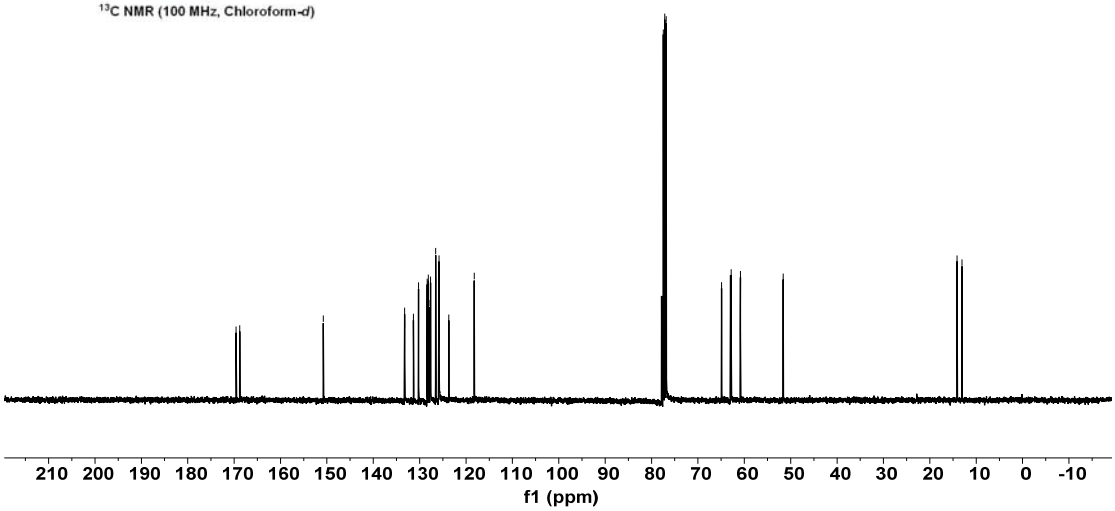
^{1}H NMR (400 MHz, Chloroform-*d*)

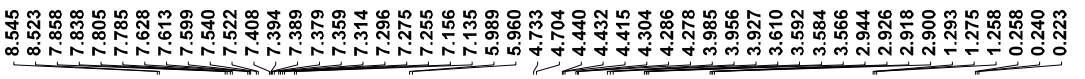


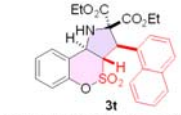




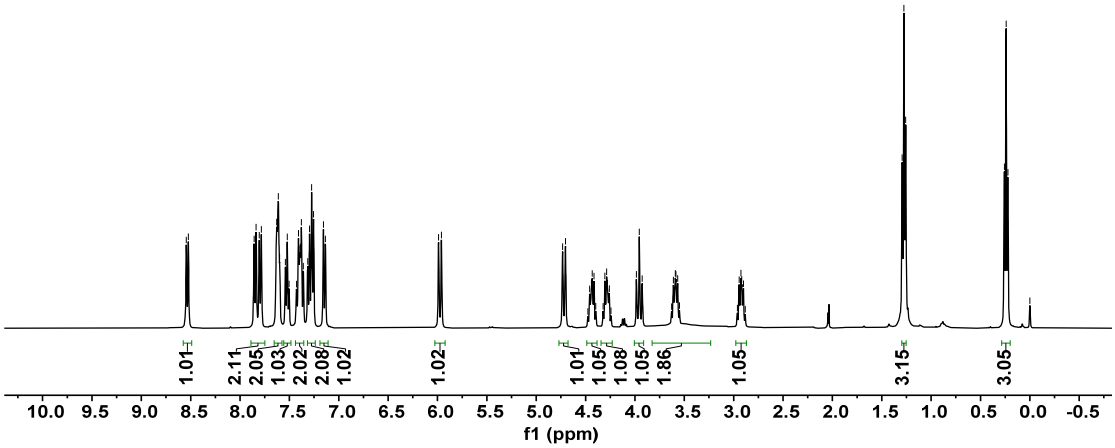
^{13}C NMR (100 MHz, Chloroform-*d*)

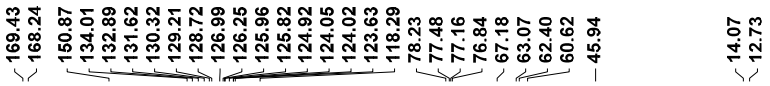


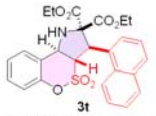




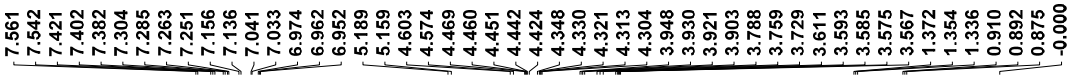
^{1}H NMR (400 MHz, Chloroform-*d*)

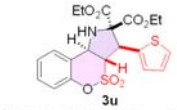






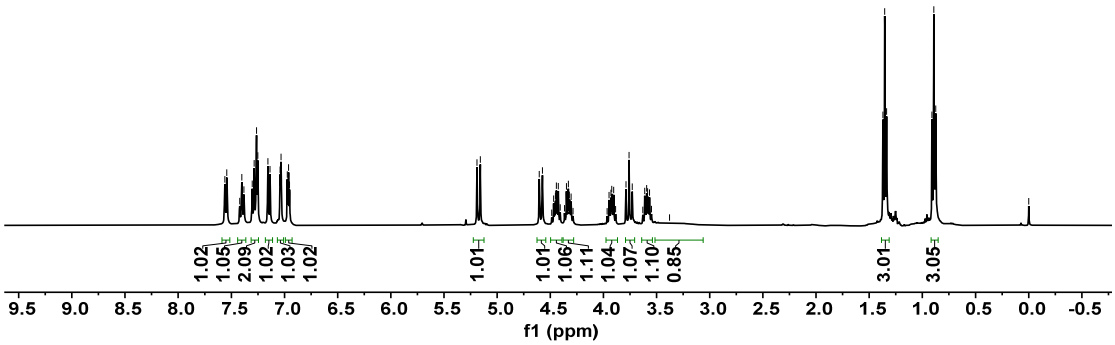
^{13}C NMR (100 MHz, Chloroform-*d*)

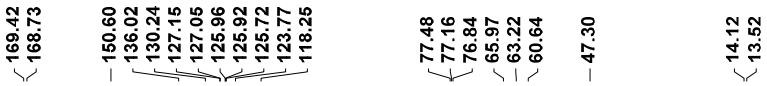


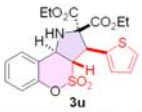


3u

^{1}H NMR (400 MHz, Chloroform-*d*)

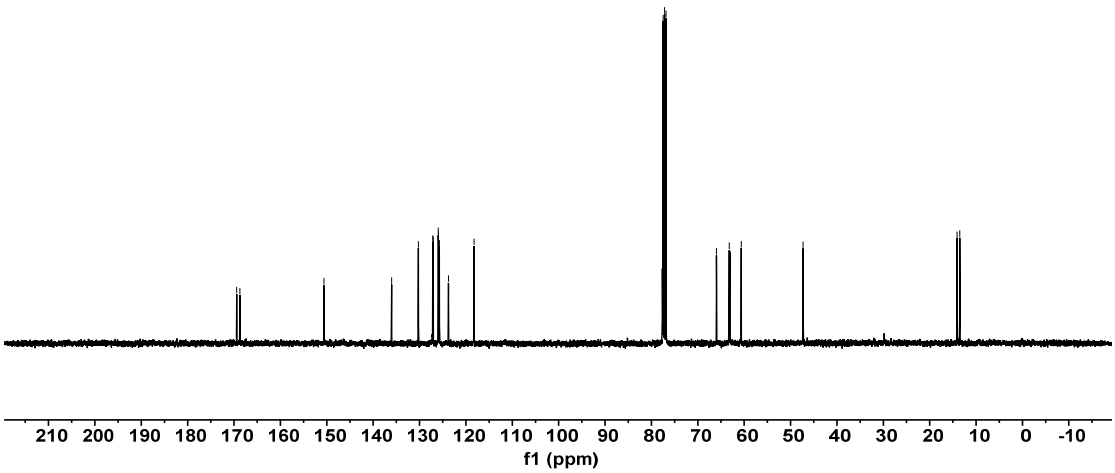


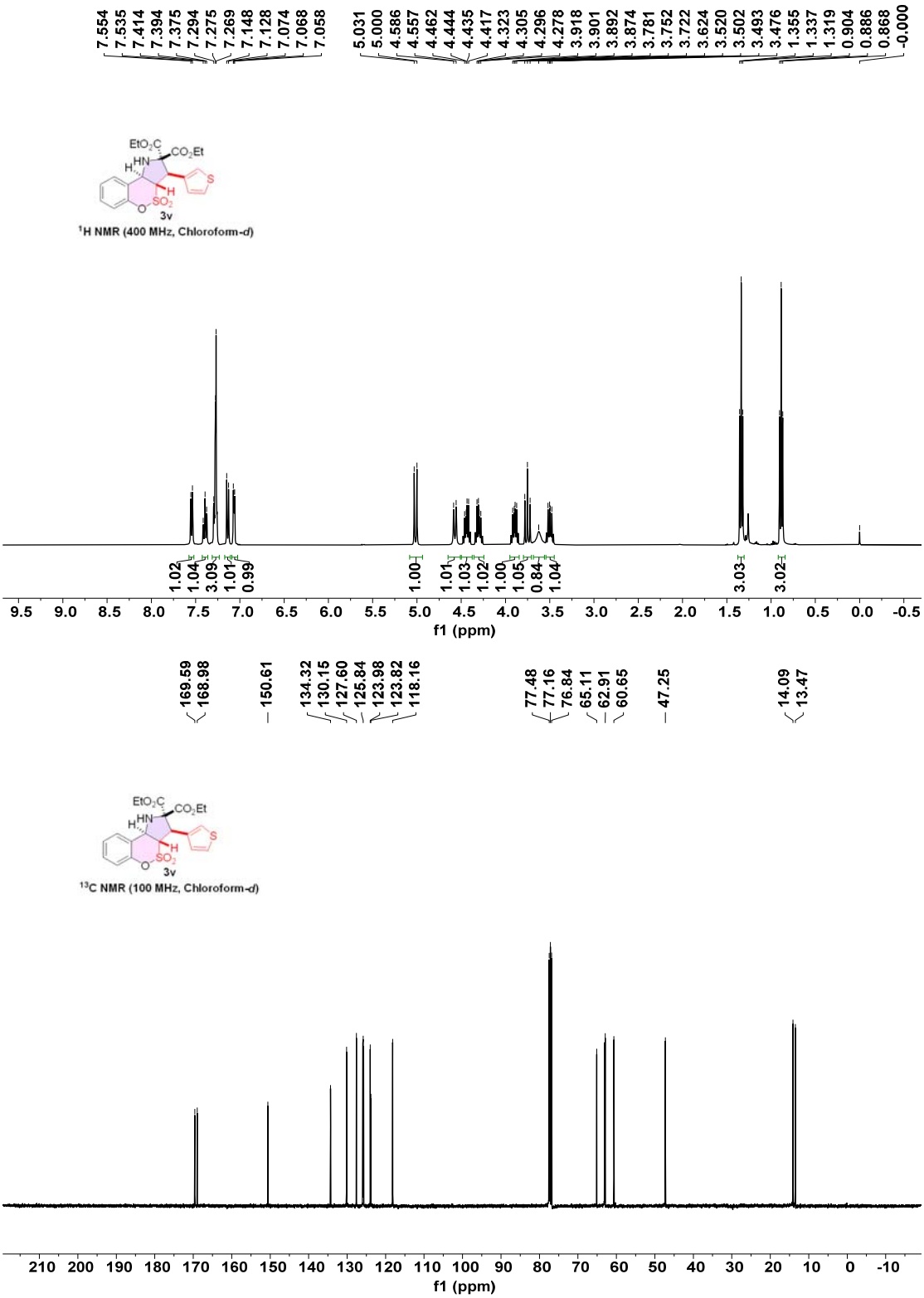


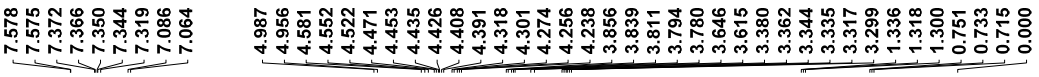


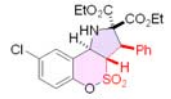
3u

^{13}C NMR (100 MHz, Chloroform-*d*)



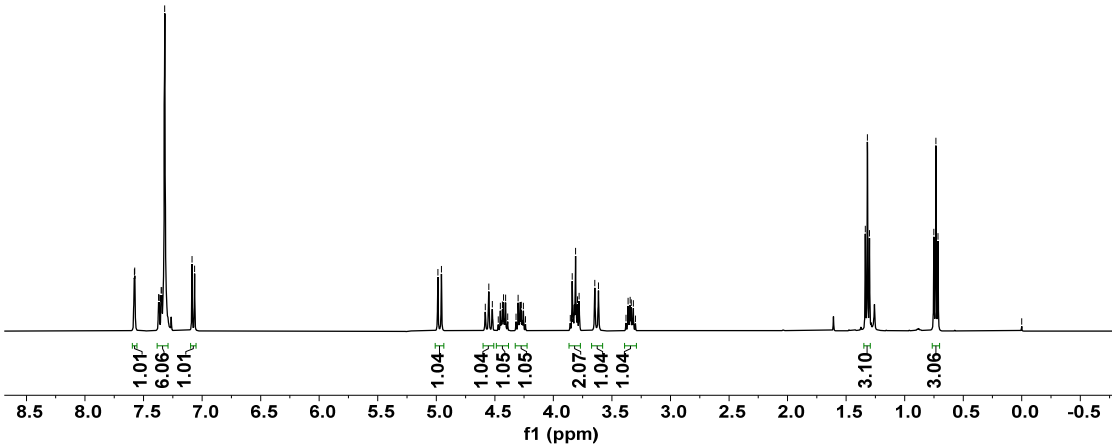

7.554
7.535
7.414
7.394
7.375
7.294
7.275
7.269
7.148
7.128
7.074
7.068
7.058
5.031
5.000
4.586
4.557
4.462
4.444
4.435
4.417
4.323
4.305
4.296
4.278
3.918
3.901
3.892
3.874
3.781
3.752
3.722
3.624
3.520
3.502
3.493
3.476
1.355
1.337
1.319
0.904
0.886
0.868
-0.000
3v
1H NMR (400 MHz, Chloroform-d)
1.02
1.04
3.09
1.01
0.99
1.00
1.01
1.03
1.02
1.00
1.05
0.84
1.04
3.03
3.02
f1 (ppm)
169.59
168.98
150.61
134.32
130.15
127.60
125.84
123.98
123.82
118.16
77.48
77.16
76.84
65.11
62.91
60.65
47.25
14.09
13.47
3v
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

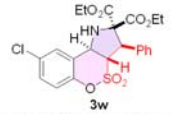




3w

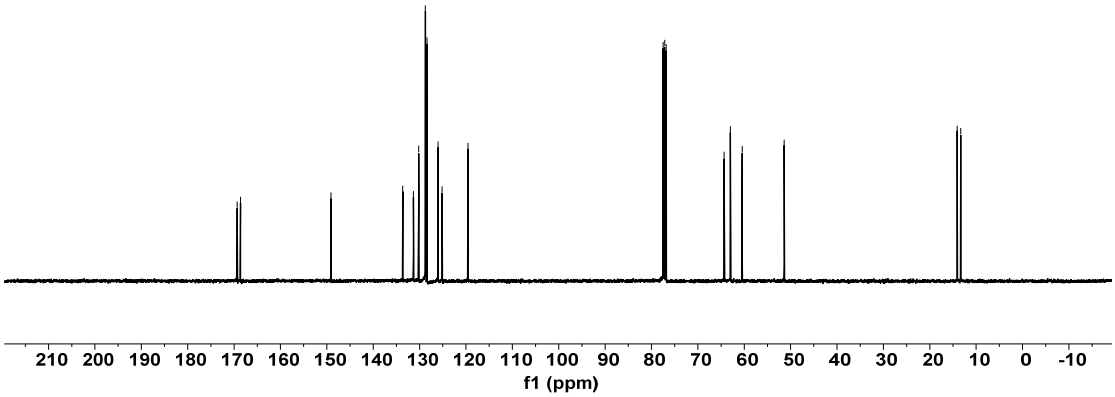
^{1}H NMR (400 MHz, Chloroform-*d*)

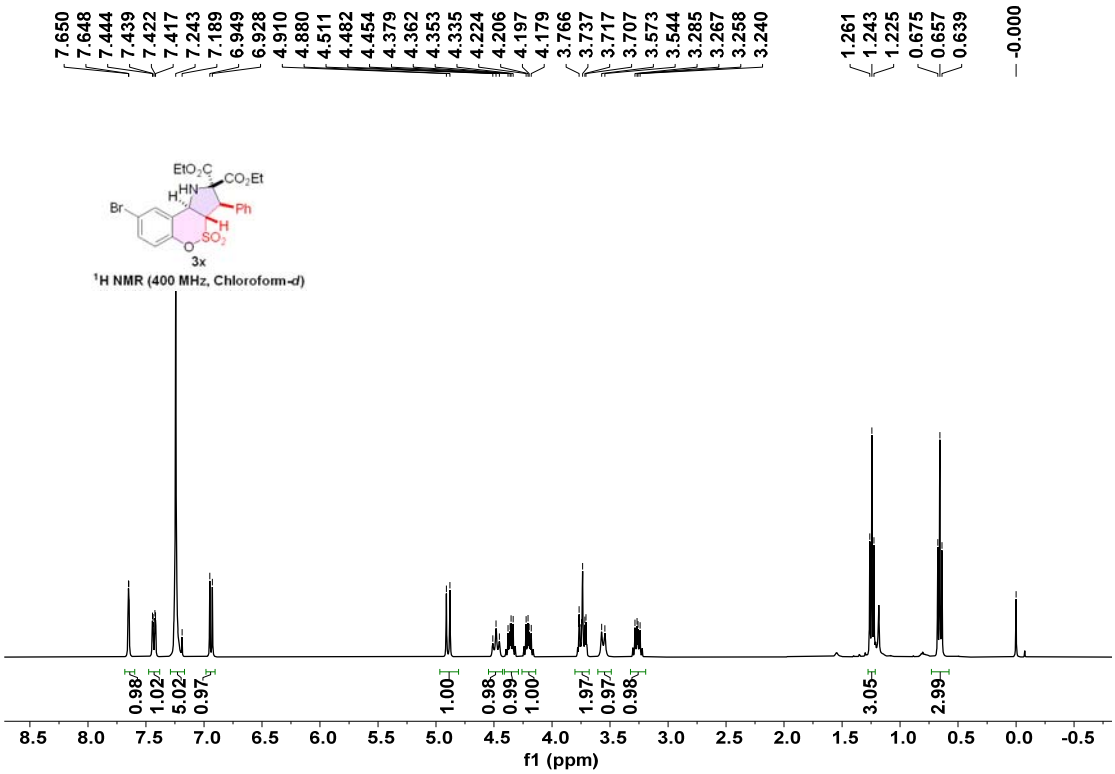


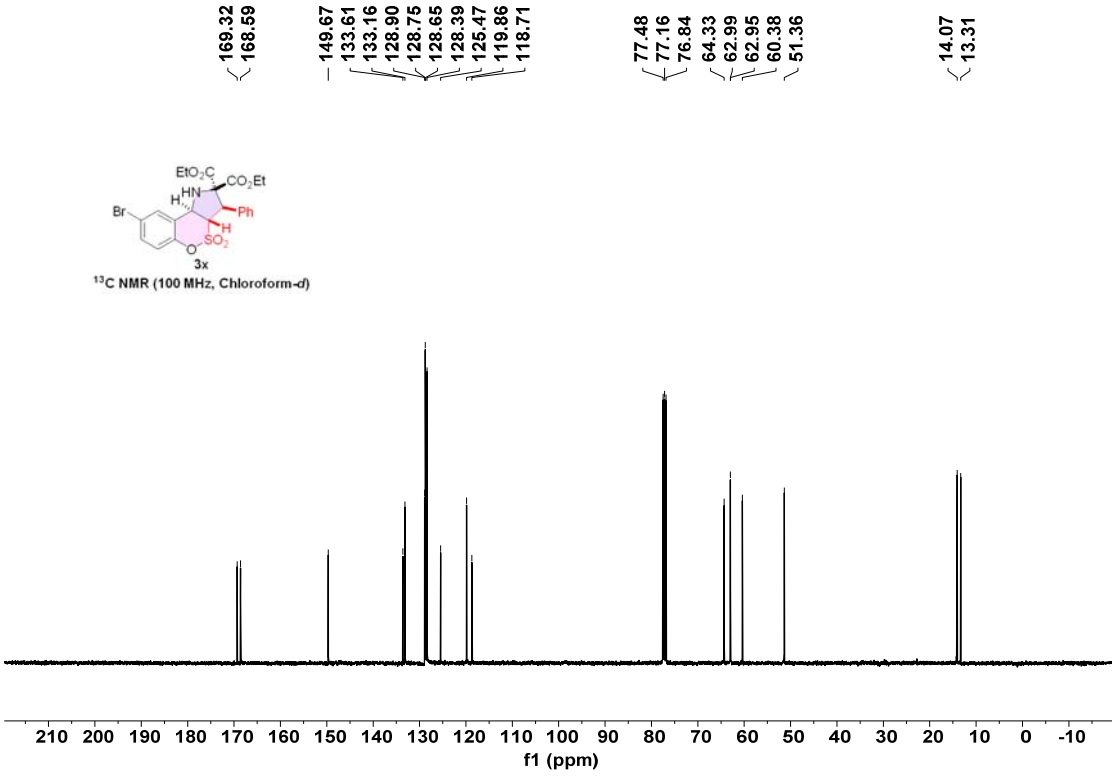


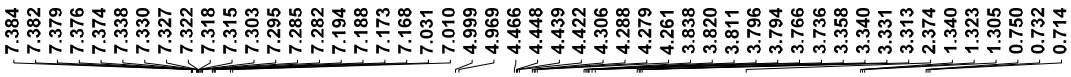
3w

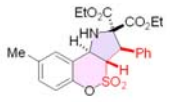
^{13}C NMR (100 MHz, Chloroform-*d*)




7.650
7.648
7.444
7.439
7.422
7.417
7.243
7.189
6.949
6.928
4.910
4.880
4.511
4.482
4.454
4.379
4.362
4.353
4.335
4.224
4.206
4.197
4.179
3.766
3.737
3.717
3.707
3.573
3.544
3.285
3.267
3.258
3.240
1.261
1.243
1.225
0.675
0.657
0.639
-0.000
3x
¹H NMR (400 MHz, Chloroform-d)
0.98
1.02
5.02
0.97
1.00
0.98
0.99
1.00
1.97
0.97
0.98
3.05
2.99
f1 (ppm)

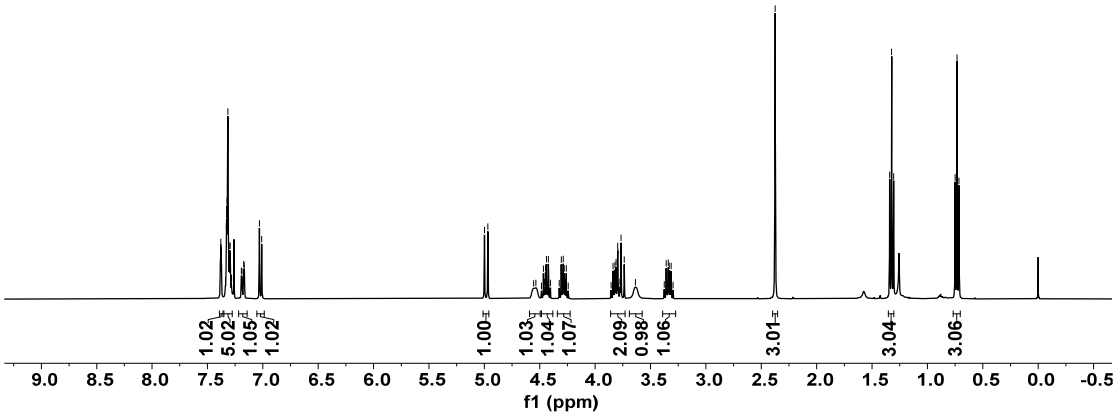

169.32
168.59
149.67
133.61
133.16
128.90
128.75
128.65
128.39
125.47
119.86
118.71
77.48
77.16
76.84
64.33
62.99
62.95
60.38
51.36
14.07
13.31
3x
¹³C NMR (100 MHz, Chloroform-d)
f1 (ppm)

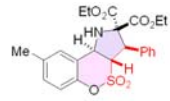




3y

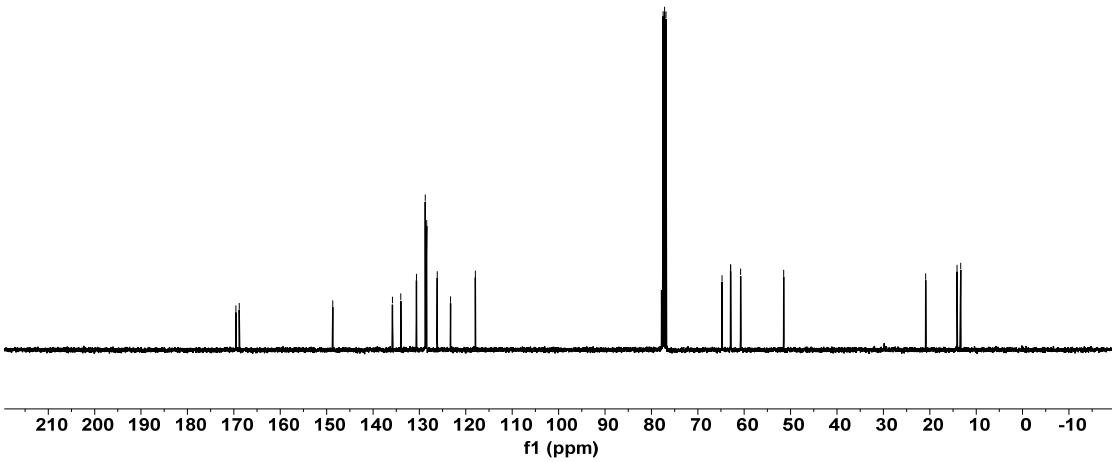
^{1}H NMR (400 MHz, Chloroform-*d*)

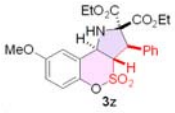




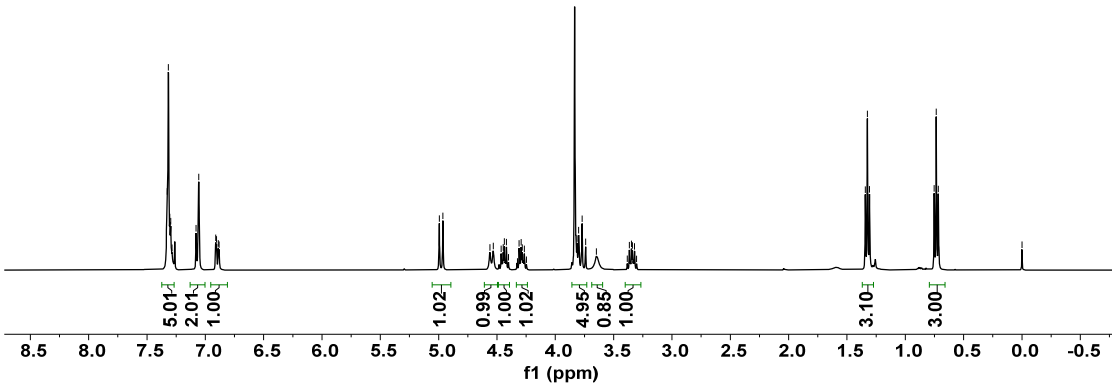
3y

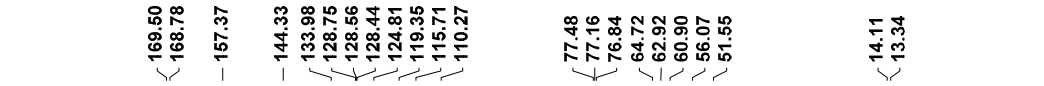
^{13}C NMR (100 MHz, Chloroform-*d*)

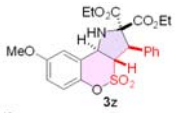




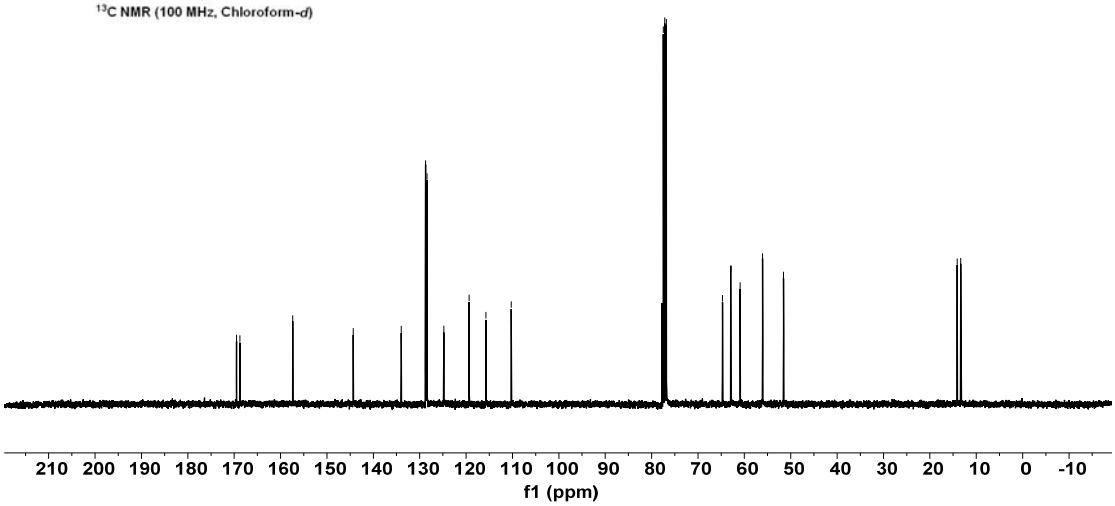
^{1}H NMR (400 MHz, Chloroform-*d*)

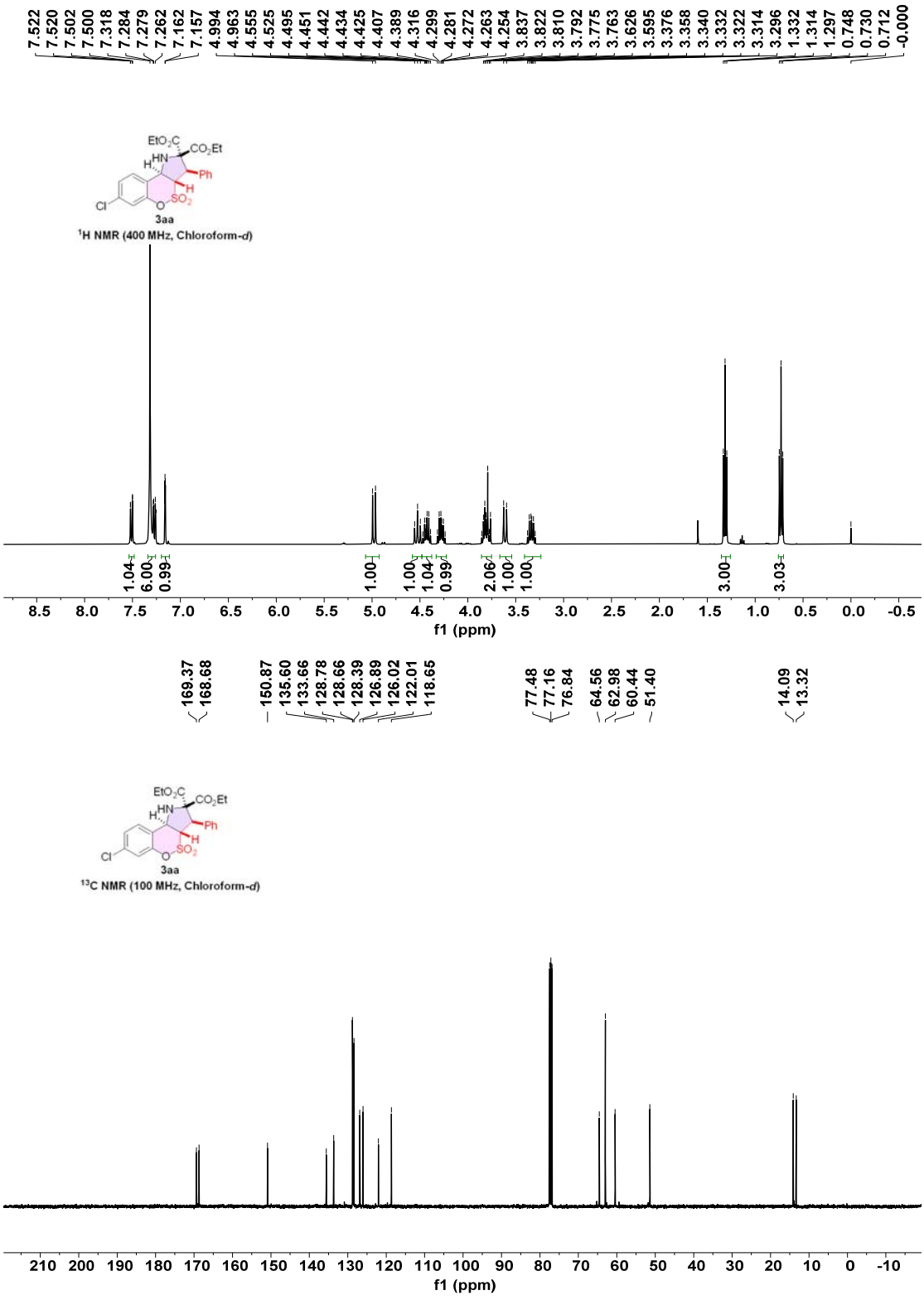


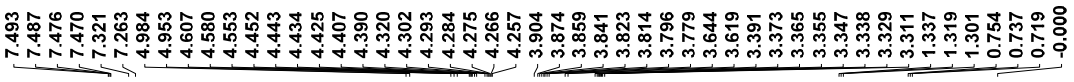


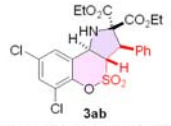


^{13}C NMR (100 MHz, Chloroform-*d*)



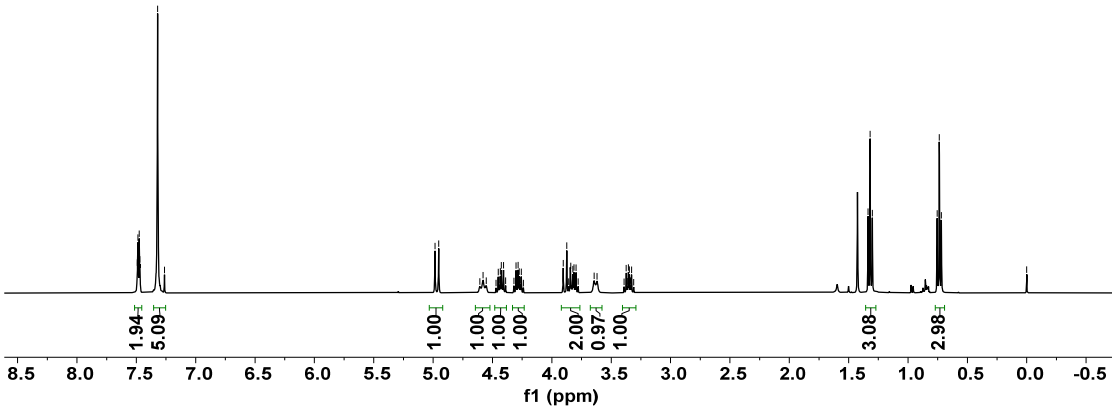

7.522
7.520
7.502
7.500
7.318
7.284
7.279
7.262
7.162
7.157
4.994
4.963
4.555
4.525
4.495
4.451
4.442
4.434
4.425
4.407
4.389
4.316
4.299
4.281
4.272
4.263
4.254
3.837
3.822
3.810
3.792
3.775
3.763
3.626
3.595
3.376
3.358
3.340
3.332
3.322
3.314
3.296
1.332
1.314
1.297
0.748
0.730
0.712
-0.000
3aa
1H NMR (400 MHz, Chloroform-d)
1.04
6.00
0.99
1.00
1.00
1.04
0.99
2.06
1.00
1.00
3.00
3.03
f1 (ppm)
169.37
168.68
150.87
135.60
133.66
128.78
128.66
128.39
126.89
126.02
122.01
118.65
77.48
77.16
76.84
64.56
62.98
60.44
51.40
14.09
13.32
3aa
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

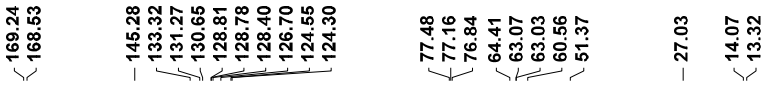


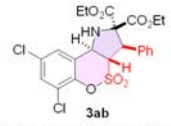


3ab

^{1}H NMR (400 MHz, Chloroform-*d*)

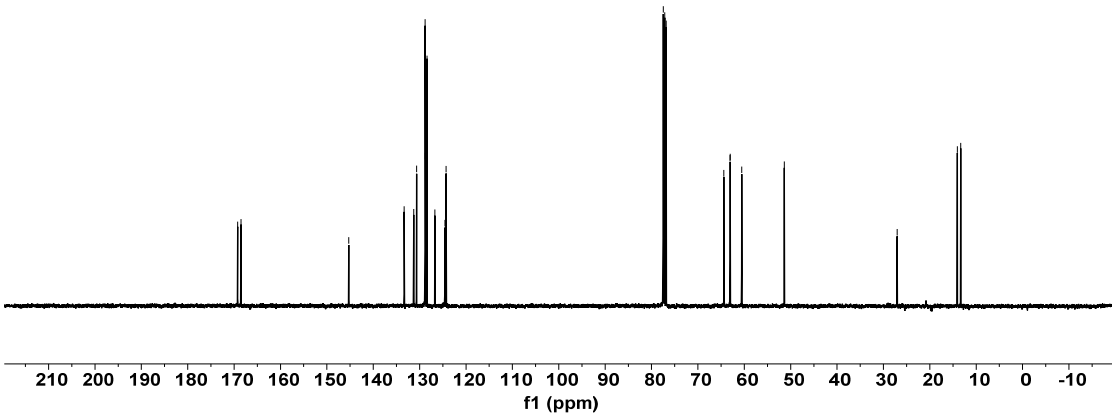


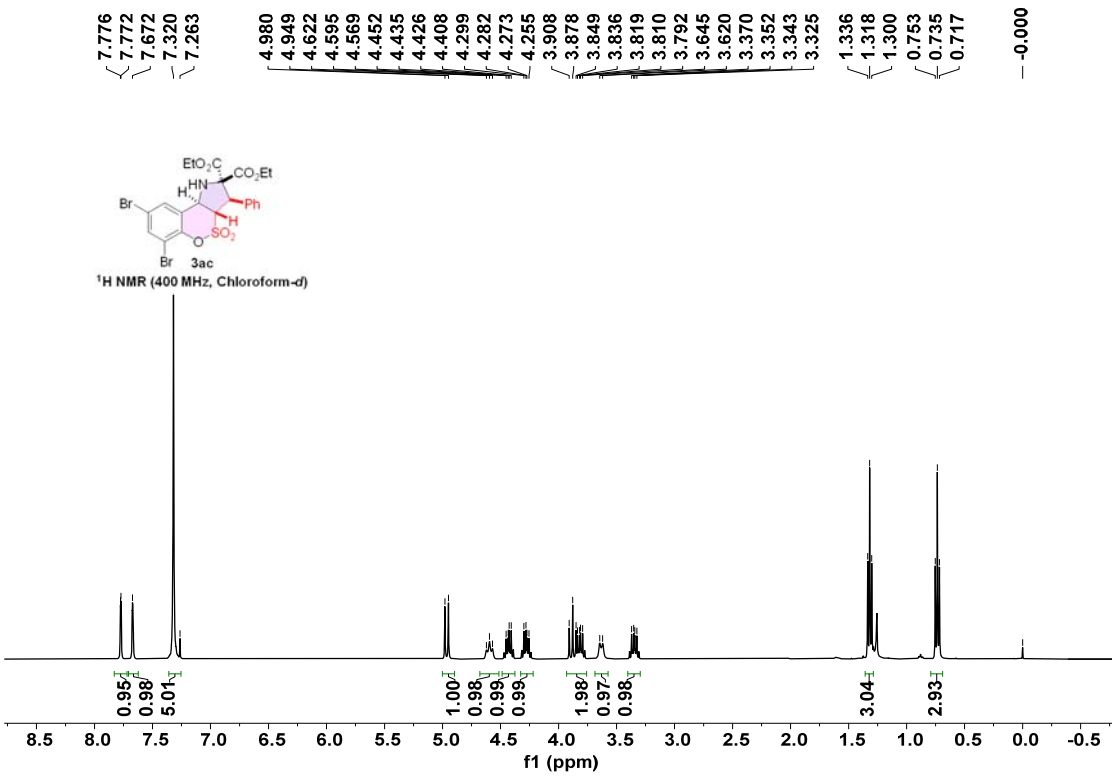




3ab

^{13}C NMR (100 MHz, Chloroform-*d*)

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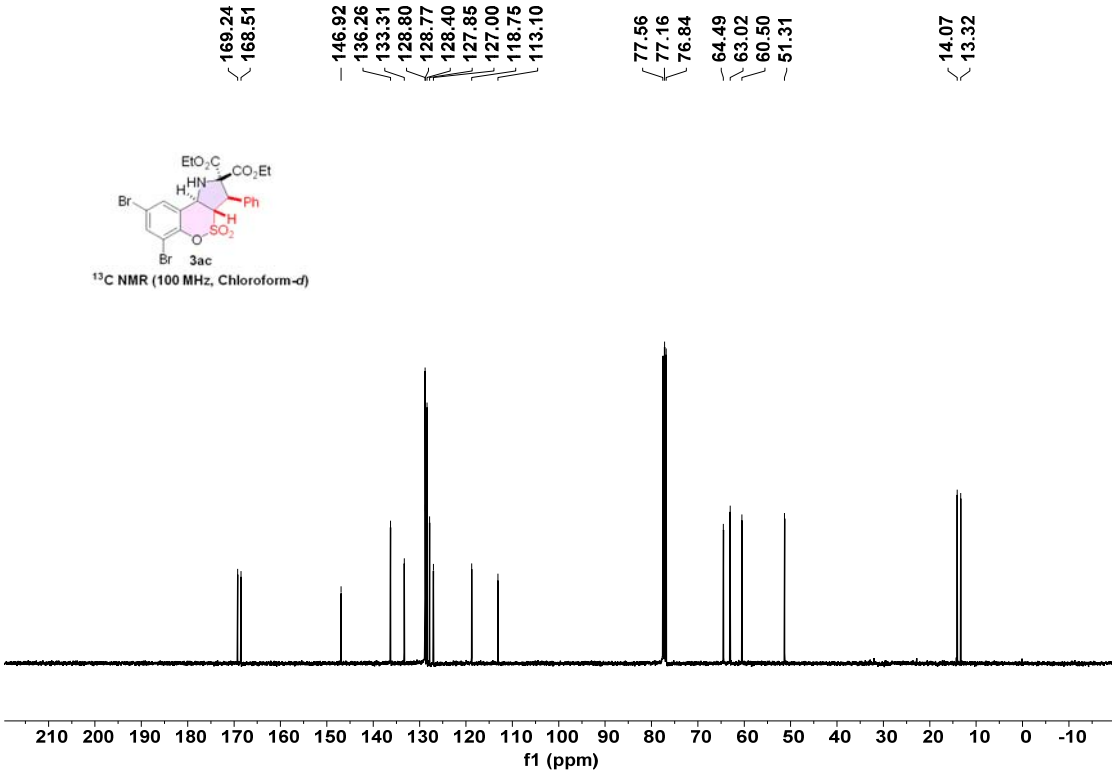
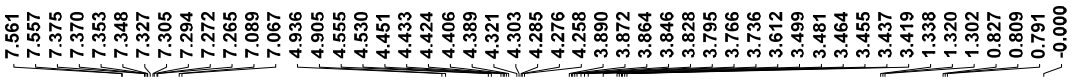
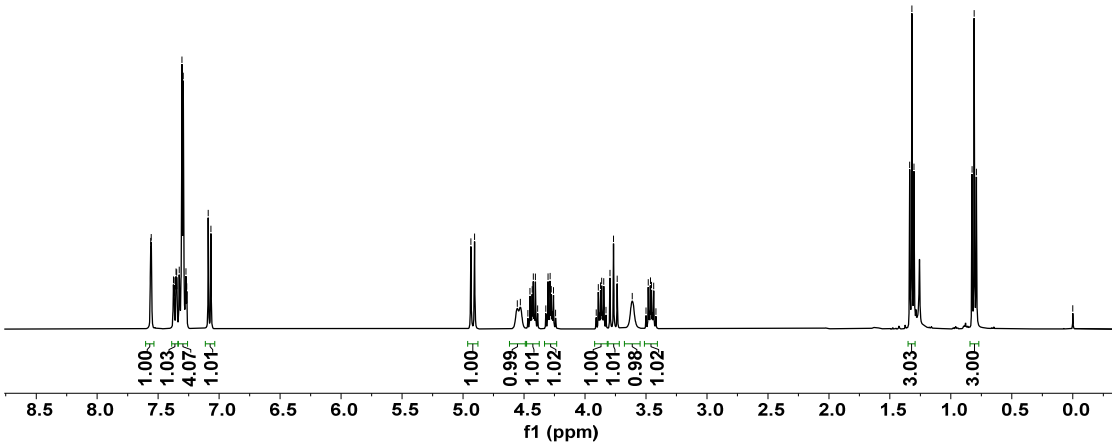
7.772
7.672
7.320
7.263
4.980
4.949
4.622
4.595
4.569
4.452
4.435
4.426
4.408
4.299
4.282
4.273
4.255
3.908
3.878
3.849
3.836
3.819
3.810
3.792
3.645
3.620
3.370
3.352
3.343
3.325
1.336
1.318
1.300
0.753
0.735
0.717
-0.000
3ac
¹H NMR (400 MHz, Chloroform-d)
0.95
0.98
5.01
1.00
0.98
0.99
0.99
1.98
0.97
0.98
3.04
2.93
f1 (ppm)

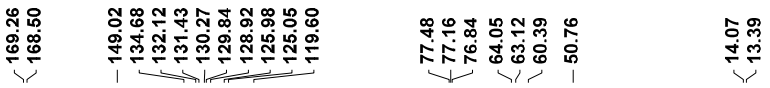

169.24
168.51
146.92
136.26
133.31
128.80
128.77
128.40
127.85
127.00
118.75
113.10
77.56
77.16
76.84
64.49
63.02
60.50
51.31
14.07
13.32
3ac
¹³C NMR (100 MHz, Chloroform-d)
f1 (ppm)

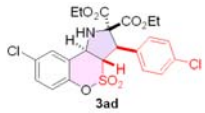


3ad

^{1}H NMR (400 MHz, Chloroform-*d*)

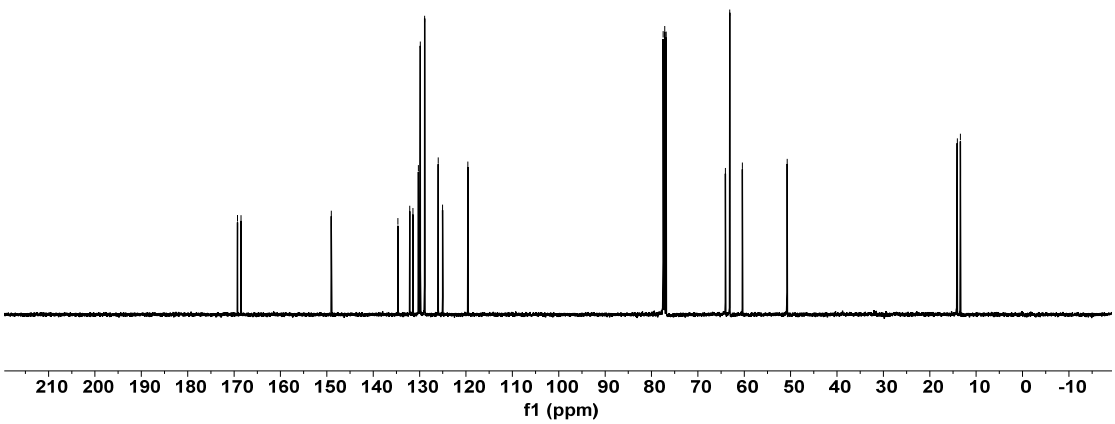


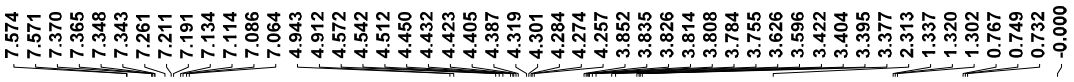


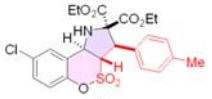


3ad

^{13}C NMR (100 MHz, Chloroform-*d*)

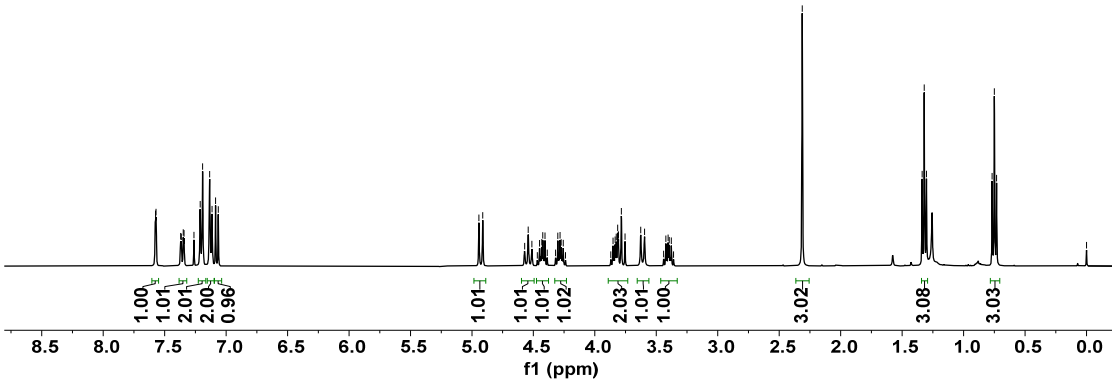


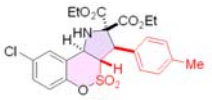




3ae

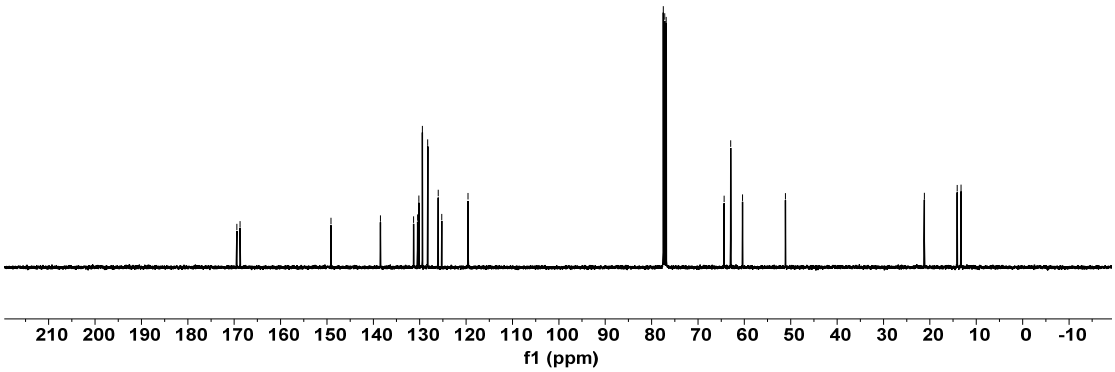
^{1}H NMR (400 MHz, Chloroform-*d*)

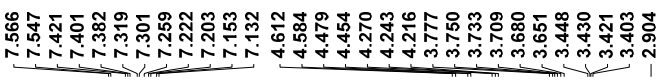


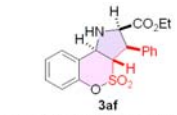


3ae

^{13}C NMR (100 MHz, Chloroform-*d*)

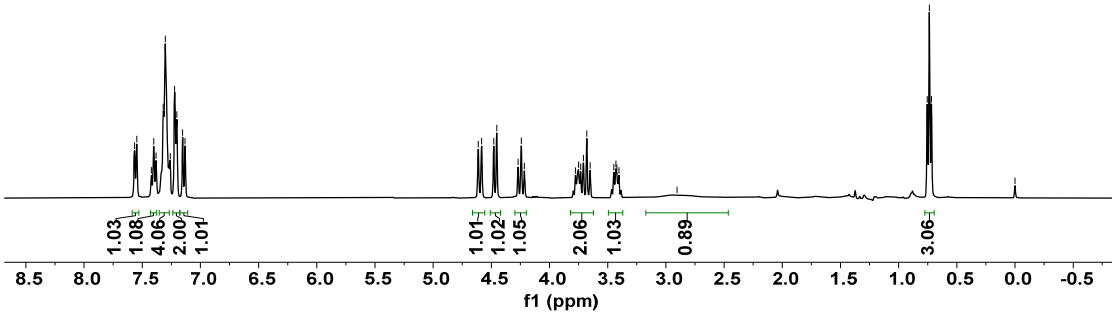


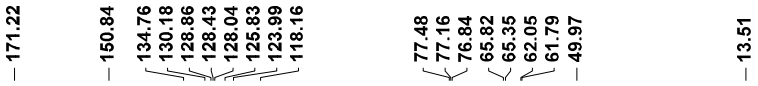


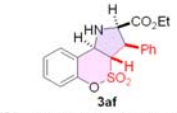


3af

^{1}H NMR (400 MHz, Chloroform-*d*)

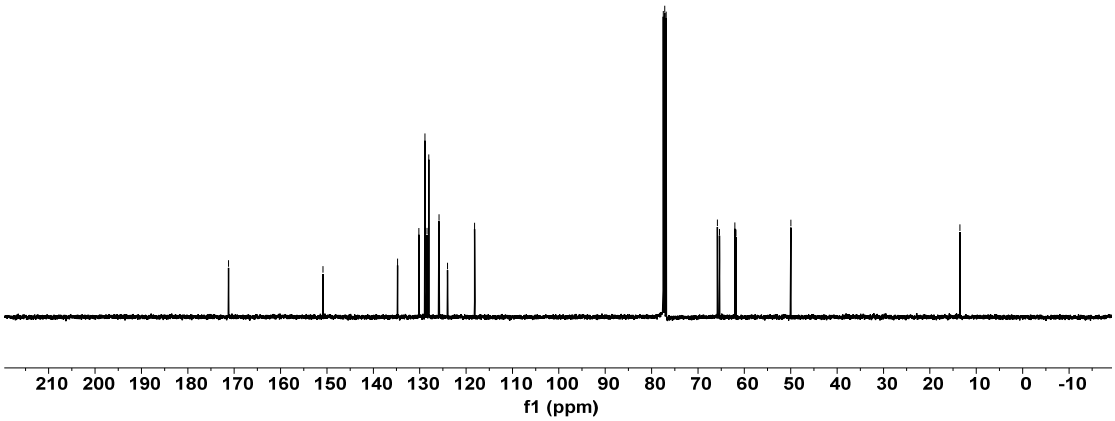


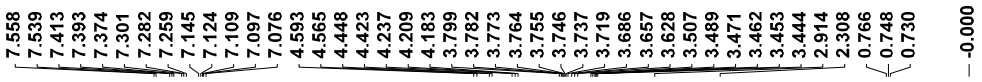


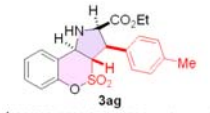


3af

^{13}C NMR (100 MHz, Chloroform-*d*)

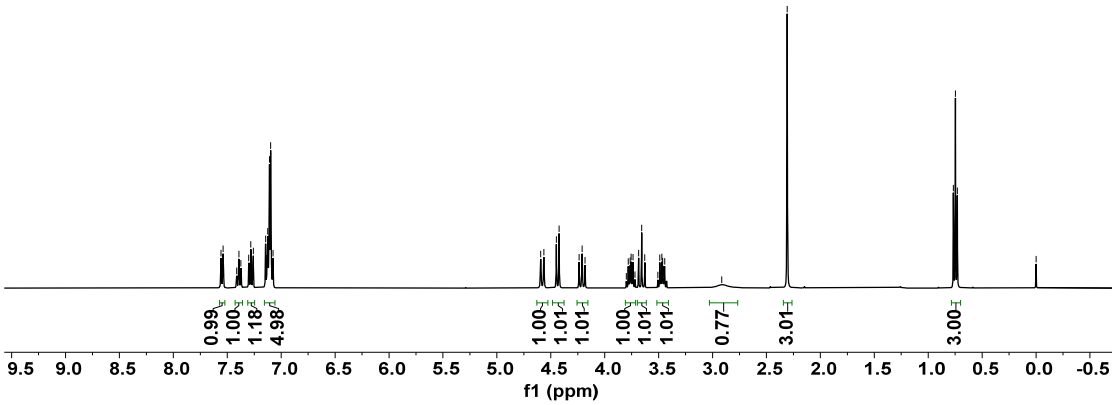


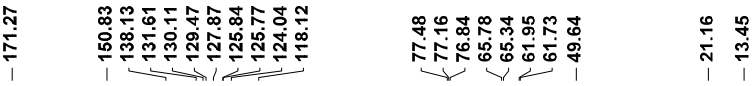


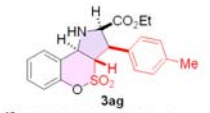


3ag

^{1}H NMR (400 MHz, Chloroform-*d*)

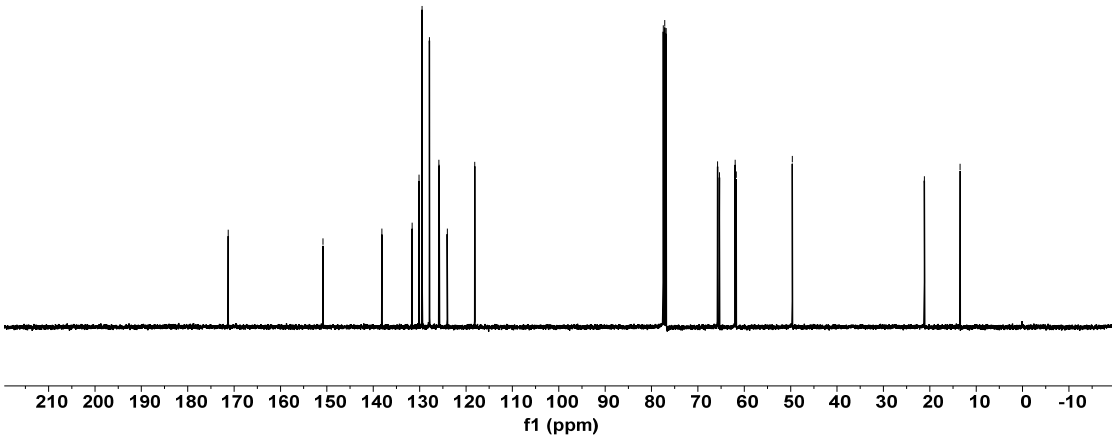


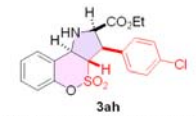




3ag

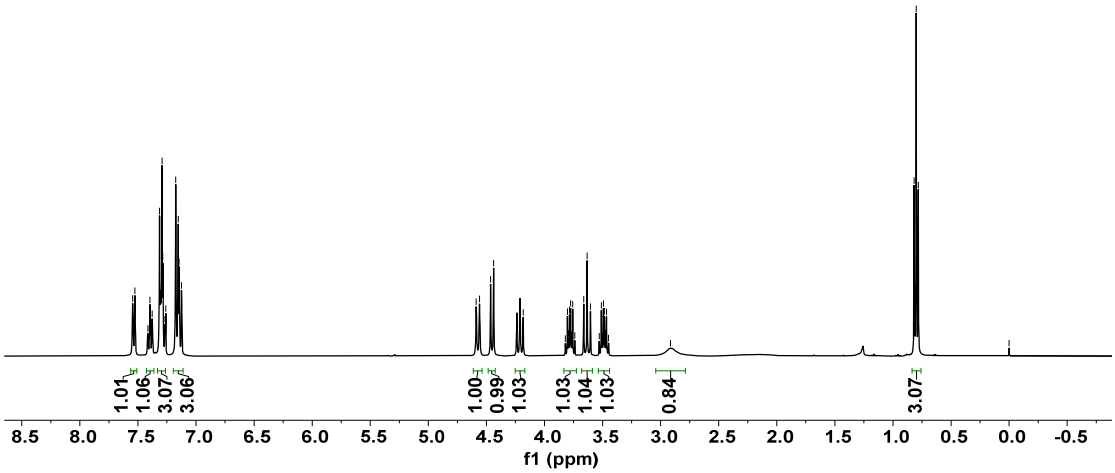
^{13}C NMR (100 MHz, Chloroform-*d*)

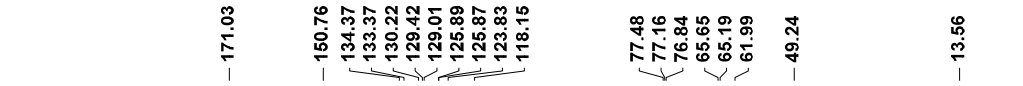


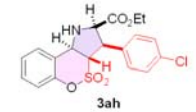


3ah

^{1}H NMR (400 MHz, Chloroform-*d*)

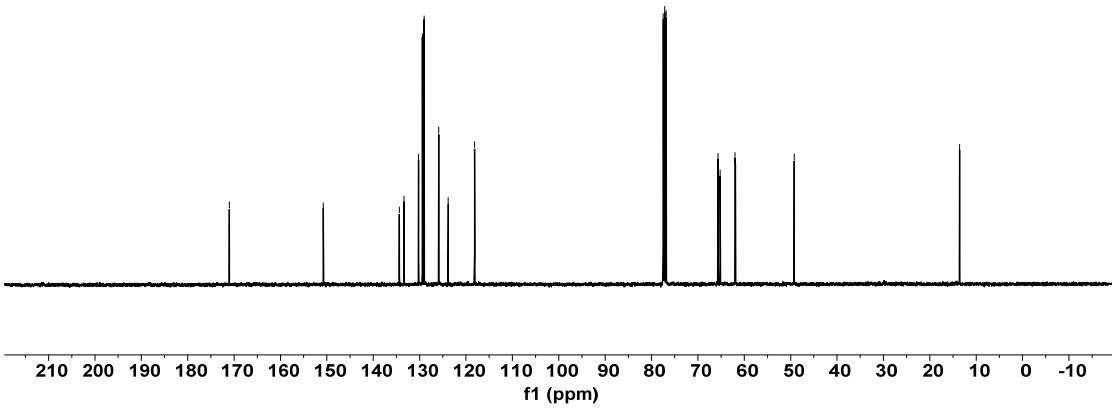


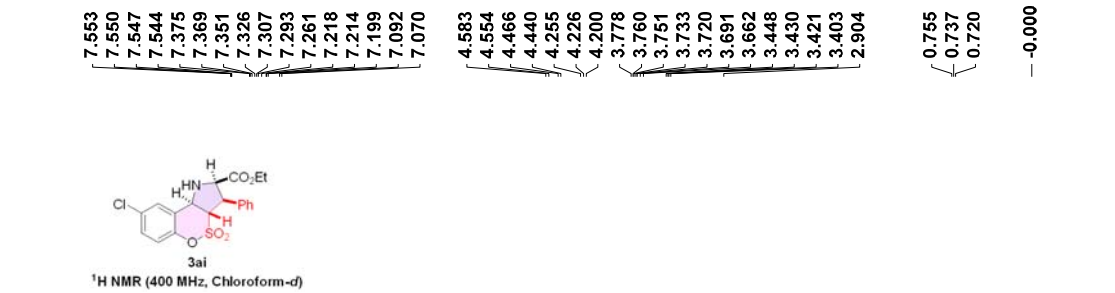




3ah

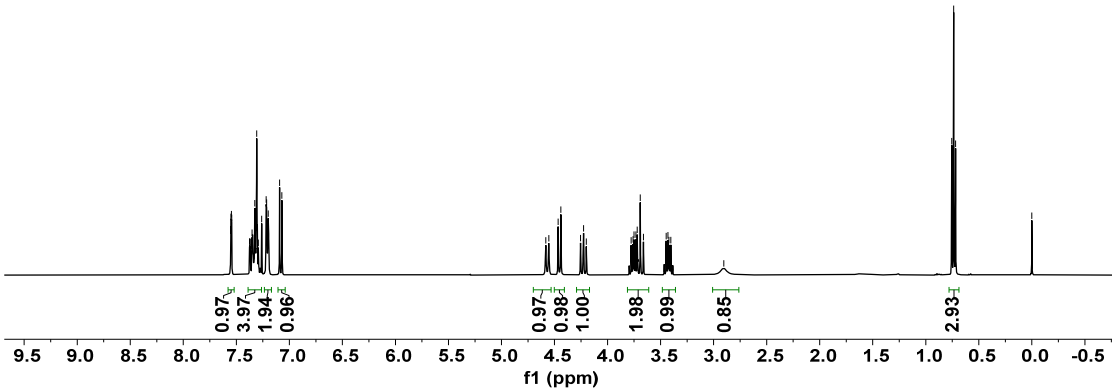
^{13}C NMR (100 MHz, Chloroform-*d*)

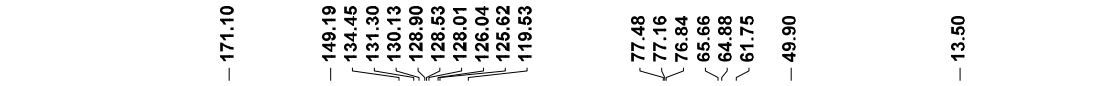


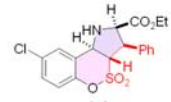


3ai

^{1}H NMR (400 MHz, Chloroform-*d*)

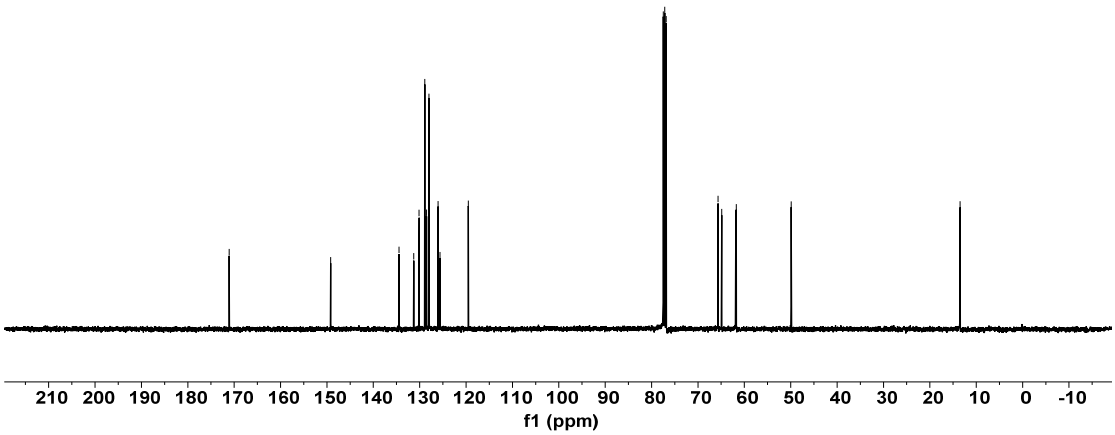


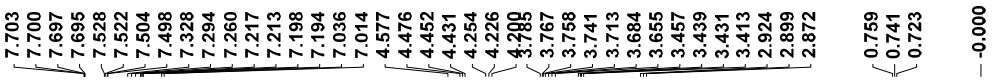


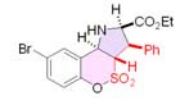


3ai

^{13}C NMR (100 MHz, Chloroform-*d*)

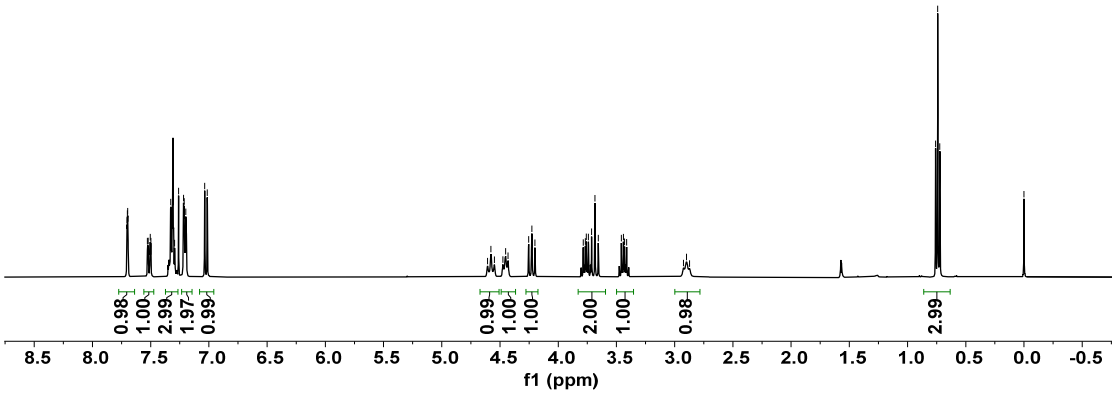


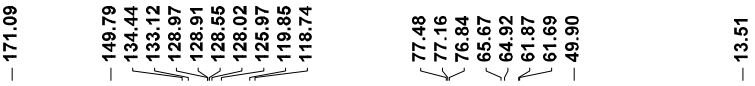


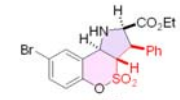


3aj

^{1}H NMR (400 MHz, Chloroform-*d*)

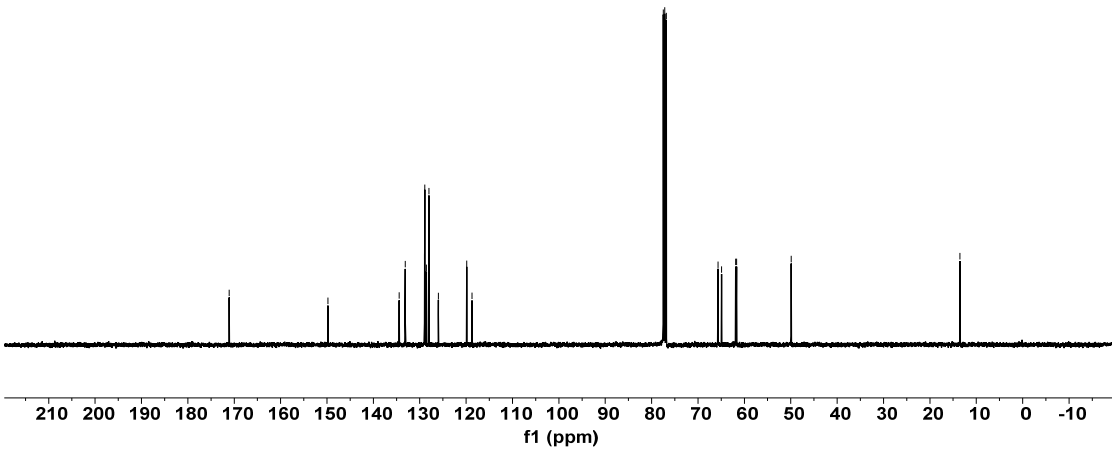


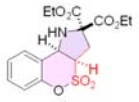




3aj

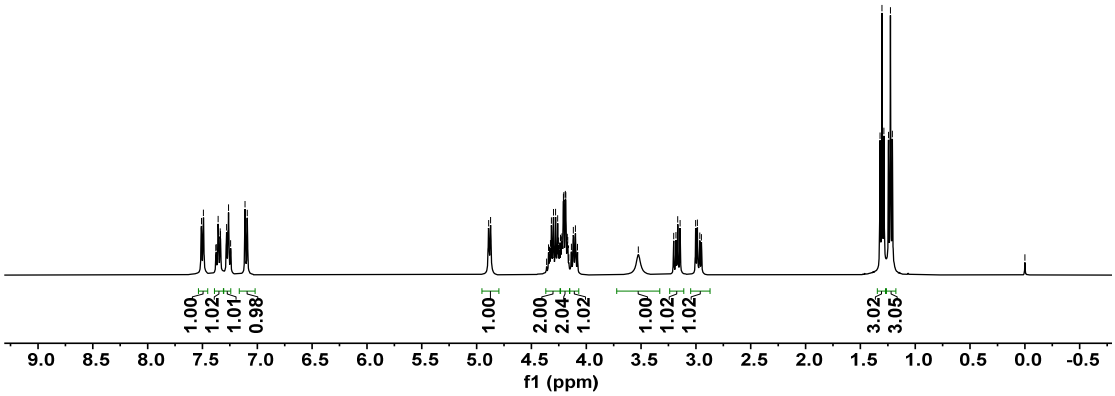
^{13}C NMR (100 MHz, Chloroform-*d*)

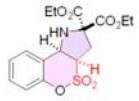




3am

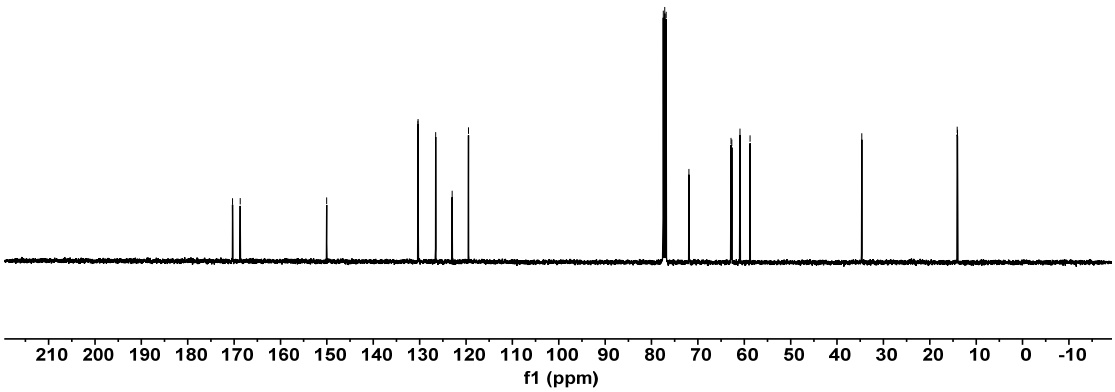
^{1}H NMR (400 MHz, Chloroform-*d*)

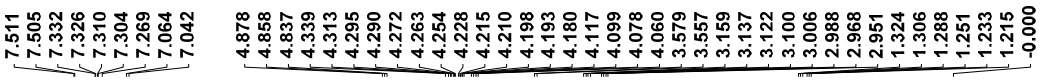


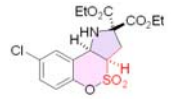


3am

^{13}C NMR (100 MHz, Chloroform-*d*)

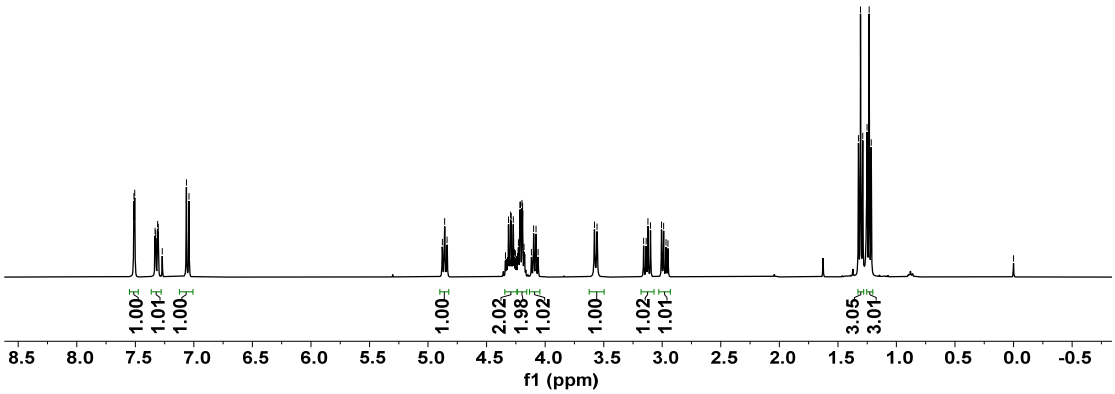


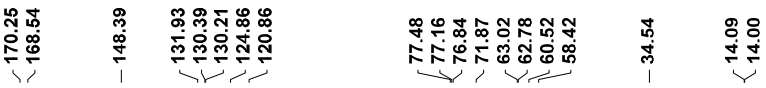


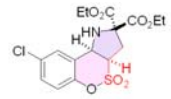


3an

^{1}H NMR (400 MHz, Chloroform-*d*)

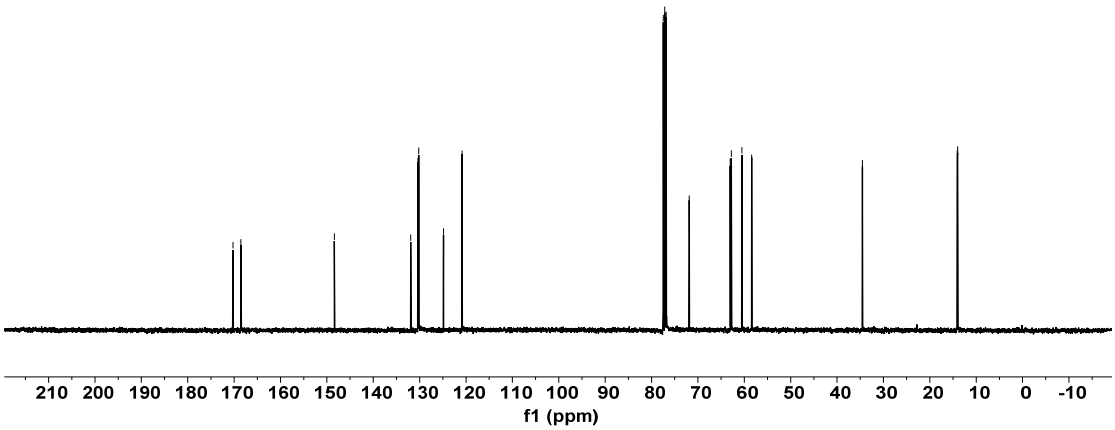


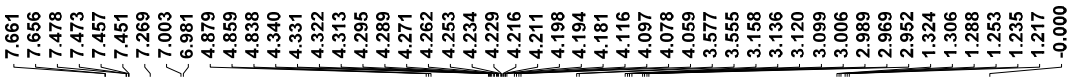


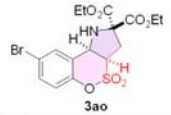


3an

^{13}C NMR (100 MHz, Chloroform-*d*)

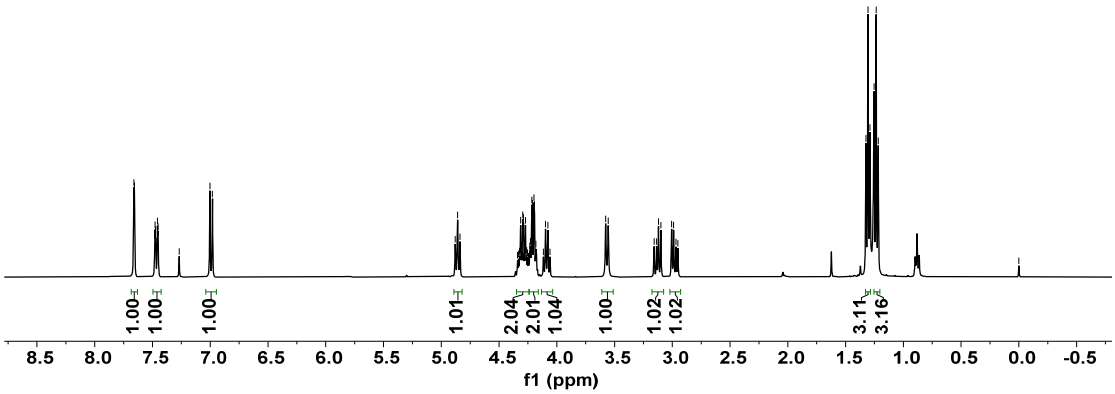


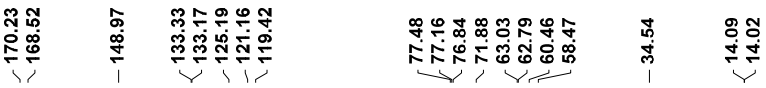


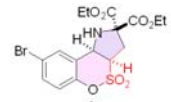


3ao

^{1}H NMR (400 MHz, Chloroform-*d*)

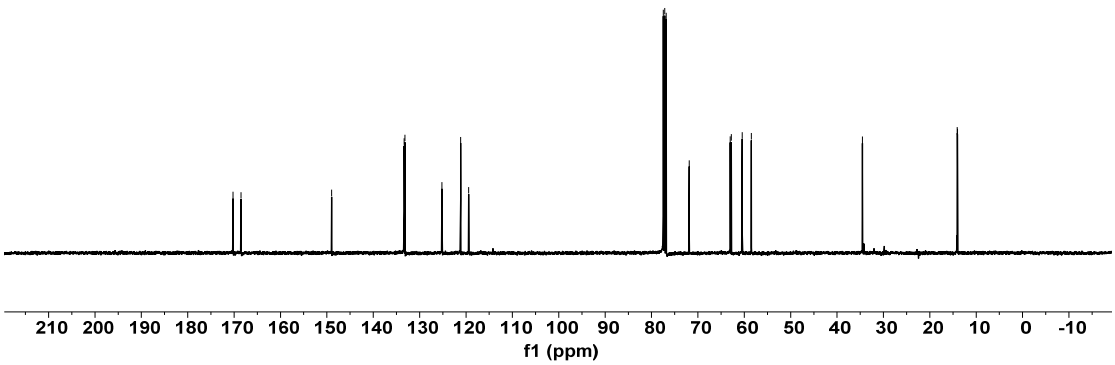






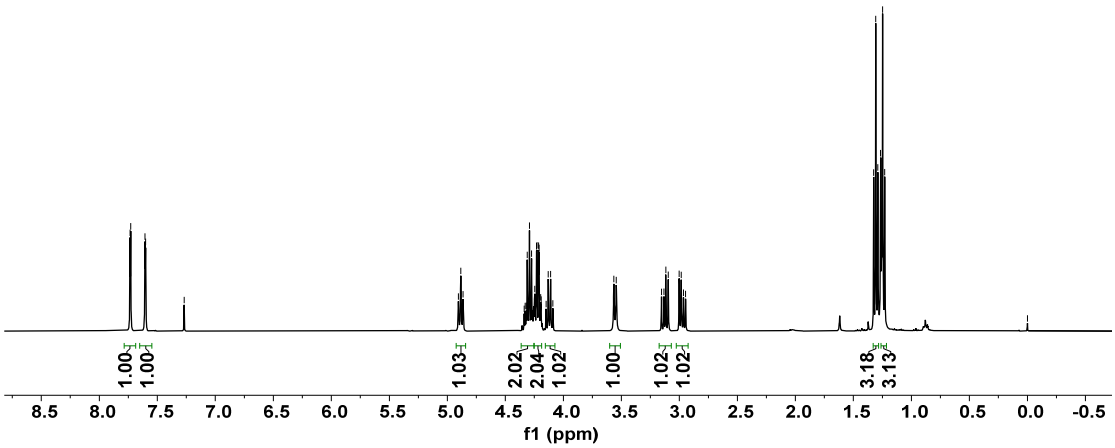
3ao

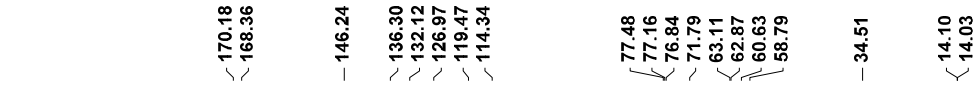
^{13}C NMR (100 MHz, Chloroform-*d*)



3ap

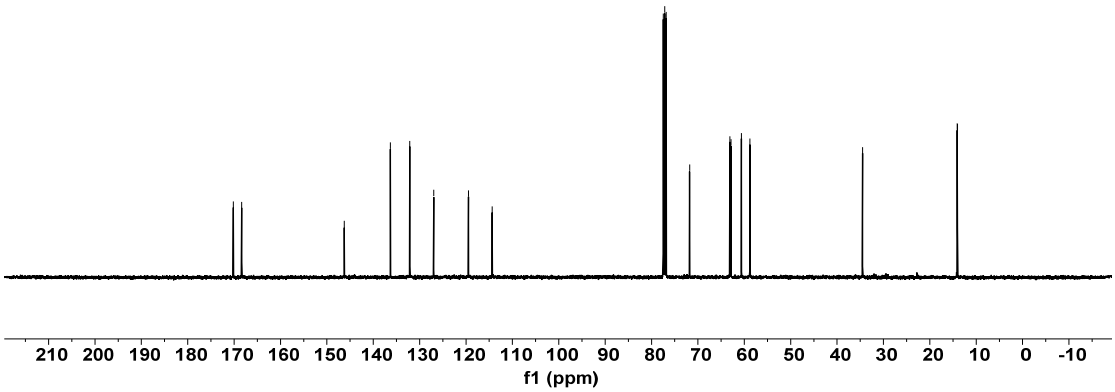
^{1}H NMR (400 MHz, Chloroform-*d*)

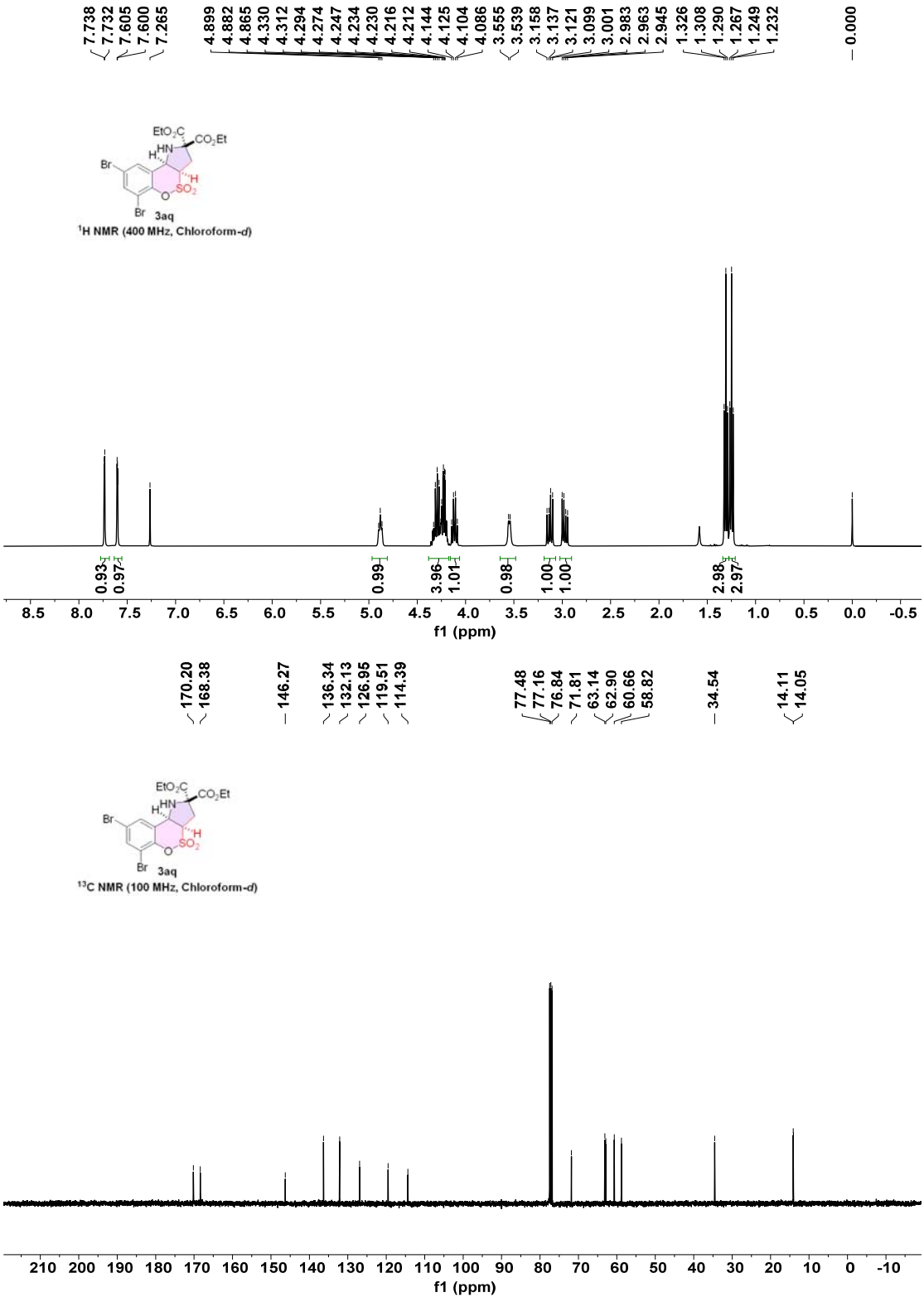


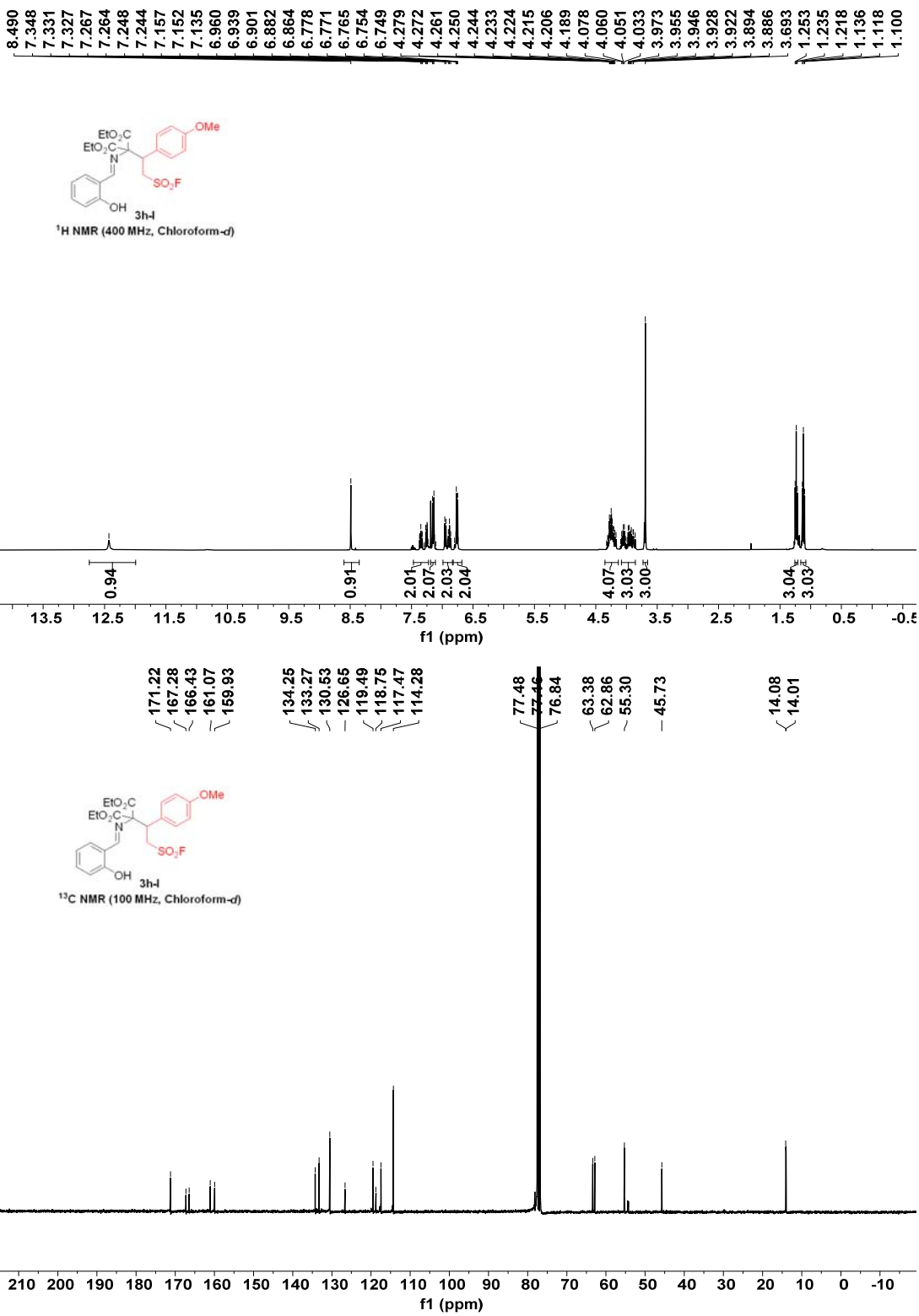


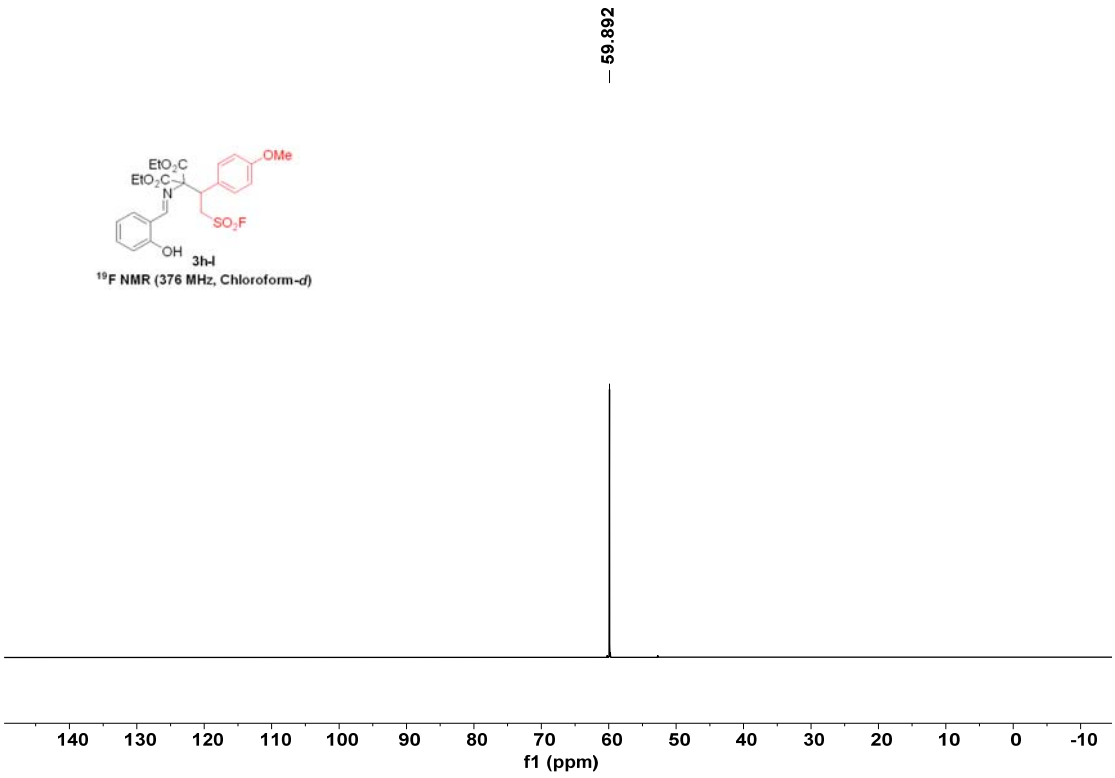
3ap

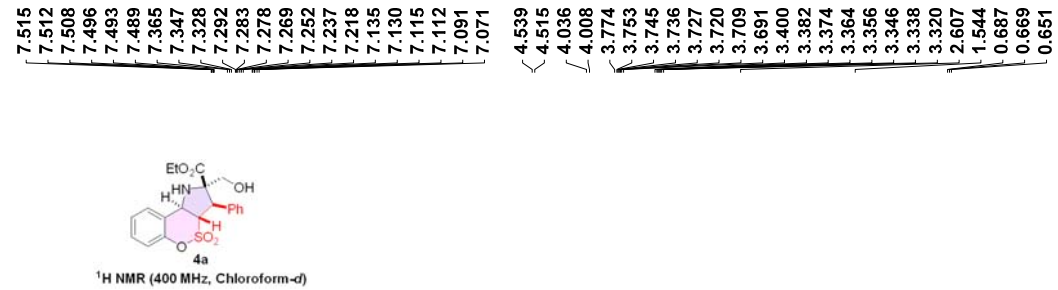
^{13}C NMR (100 MHz, Chloroform-*d*)




7.738
7.732
7.605
7.600
7.265
4.899
4.882
4.865
4.330
4.312
4.294
4.274
4.247
4.234
4.230
4.216
4.212
4.144
4.125
4.104
4.086
3.555
3.539
3.158
3.137
3.121
3.099
3.001
2.983
2.963
2.945
1.326
1.308
1.290
1.267
1.249
1.232
0.000
3aq
¹H NMR (400 MHz, Chloroform-d)
0.93
0.97
0.99
3.96
1.01
0.98
1.00
1.00
2.98
2.97
f1 (ppm)
170.20
168.38
146.27
136.34
132.13
126.95
119.51
114.39
77.48
77.16
76.84
71.81
63.14
62.90
60.66
58.82
34.54
14.11
14.05
3aq
¹³C NMR (100 MHz, Chloroform-d)
f1 (ppm)

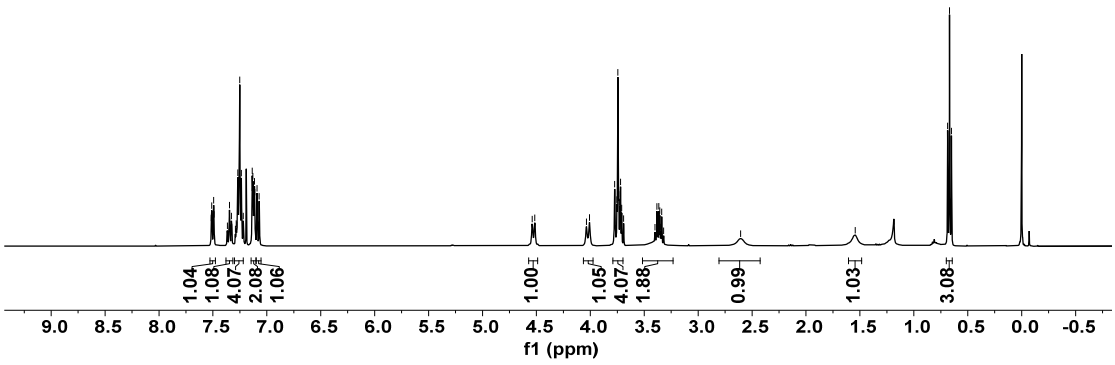

8.490
7.348
7.331
7.327
7.267
7.264
7.248
7.244
7.157
7.152
7.135
6.960
6.939
6.901
6.882
6.864
6.778
6.771
6.765
6.754
6.749
4.279
4.272
4.261
4.250
4.244
4.233
4.224
4.215
4.206
4.189
4.078
4.060
4.051
4.033
3.973
3.955
3.946
3.928
3.922
3.894
3.886
3.693
1.253
1.235
1.218
1.136
1.118
1.100
EtO2C
EtO2C
N
OMe
SO2F
OH
3h-I
1H NMR (400 MHz, Chloroform-d)
0.94
0.91
2.01
2.07
2.03
2.04
4.07
3.03
3.00
3.04
3.03
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)
171.22
167.28
166.43
161.07
159.93
134.25
133.27
130.53
126.65
119.49
118.75
117.47
114.28
77.48
76.84
63.38
62.86
55.30
45.73
14.08
14.01
EtO2C
EtO2C
N
OMe
SO2F
OH
3h-I
13C NMR (100 MHz, Chloroform-d)
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)

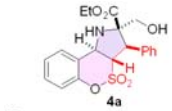

-59.892
EtO2C
EtO2C
N
OMe
SO2F
OH
3h-I
19F NMR (376 MHz, Chloroform-d)
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



4a

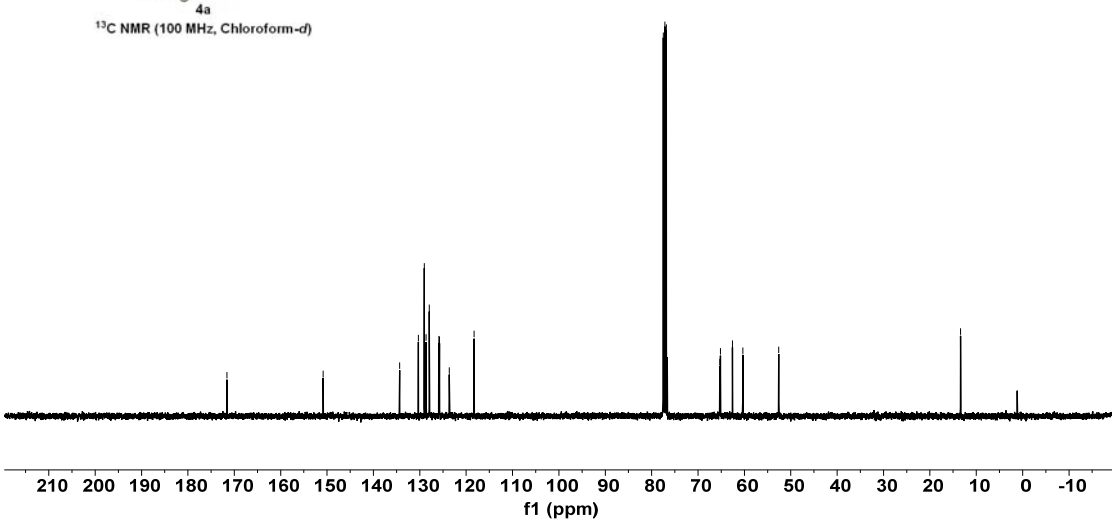
^{1}H NMR (400 MHz, Chloroform-*d*)

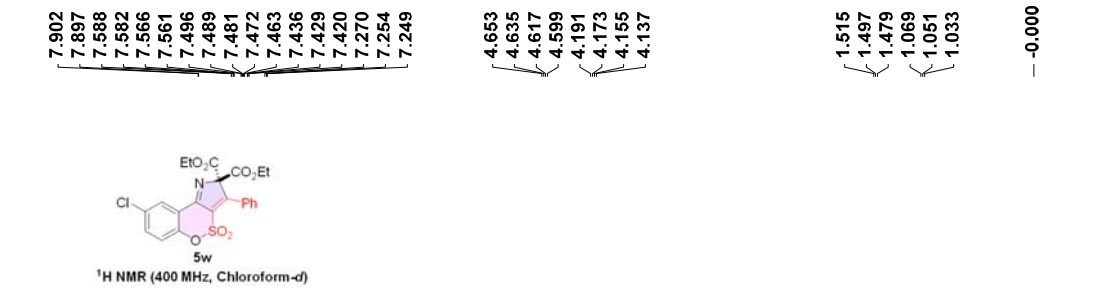




4a

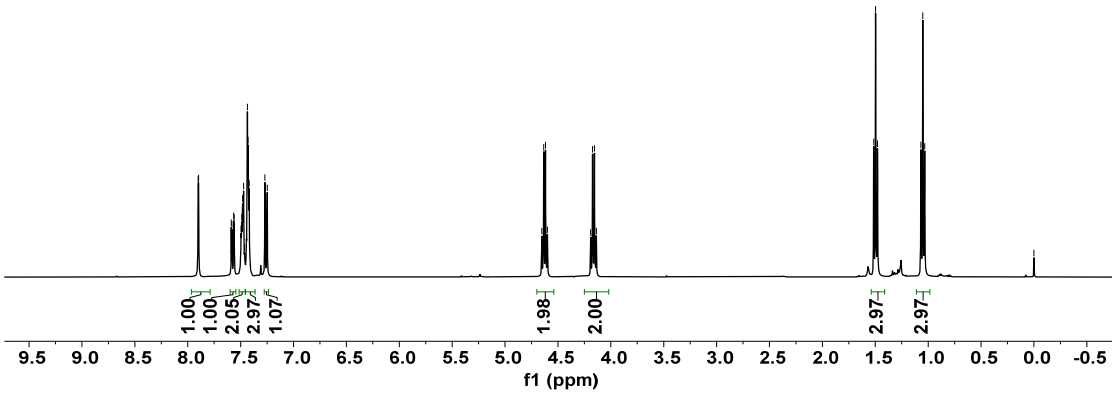
^{13}C NMR (100 MHz, Chloroform-*d*)

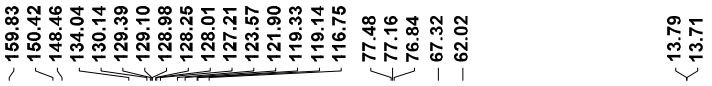


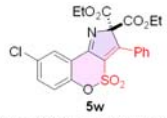


5w

^{1}H NMR (400 MHz, Chloroform-*d*)

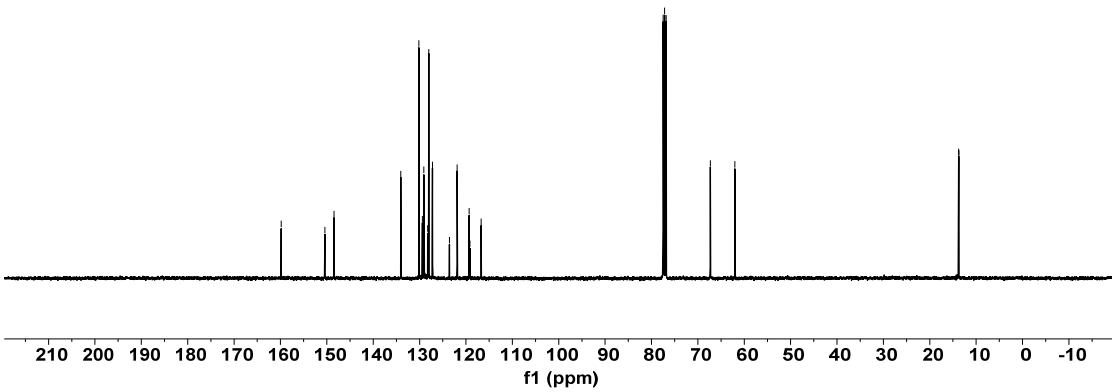


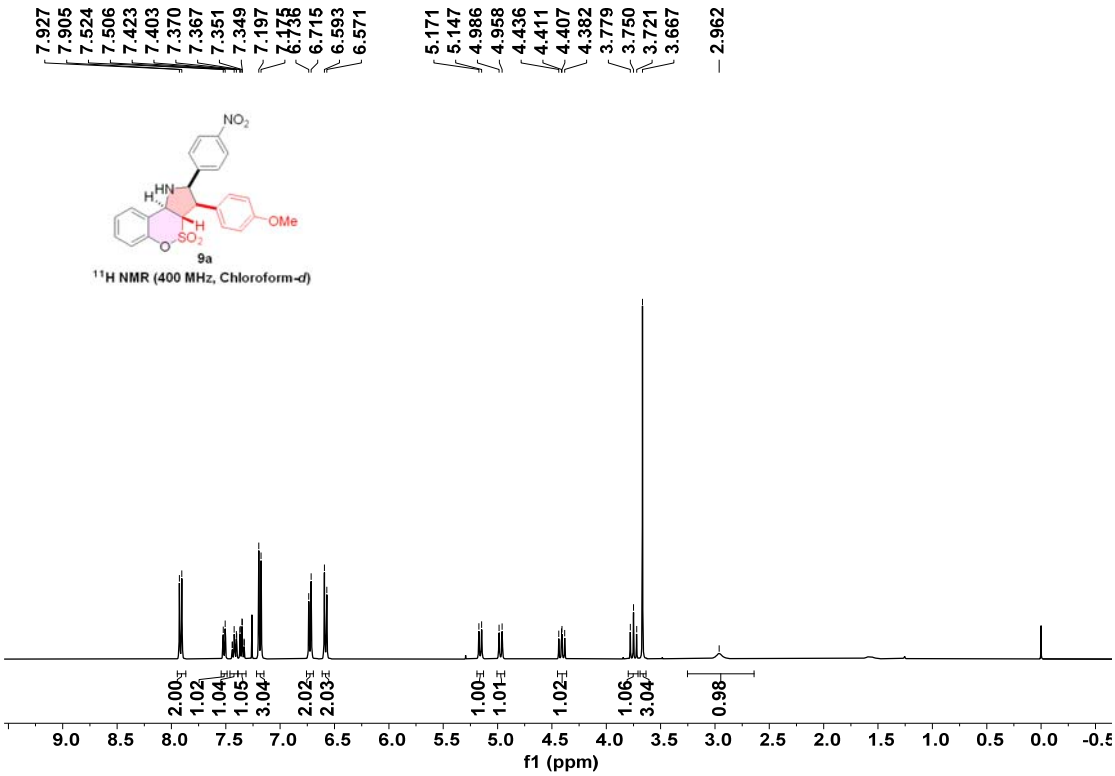


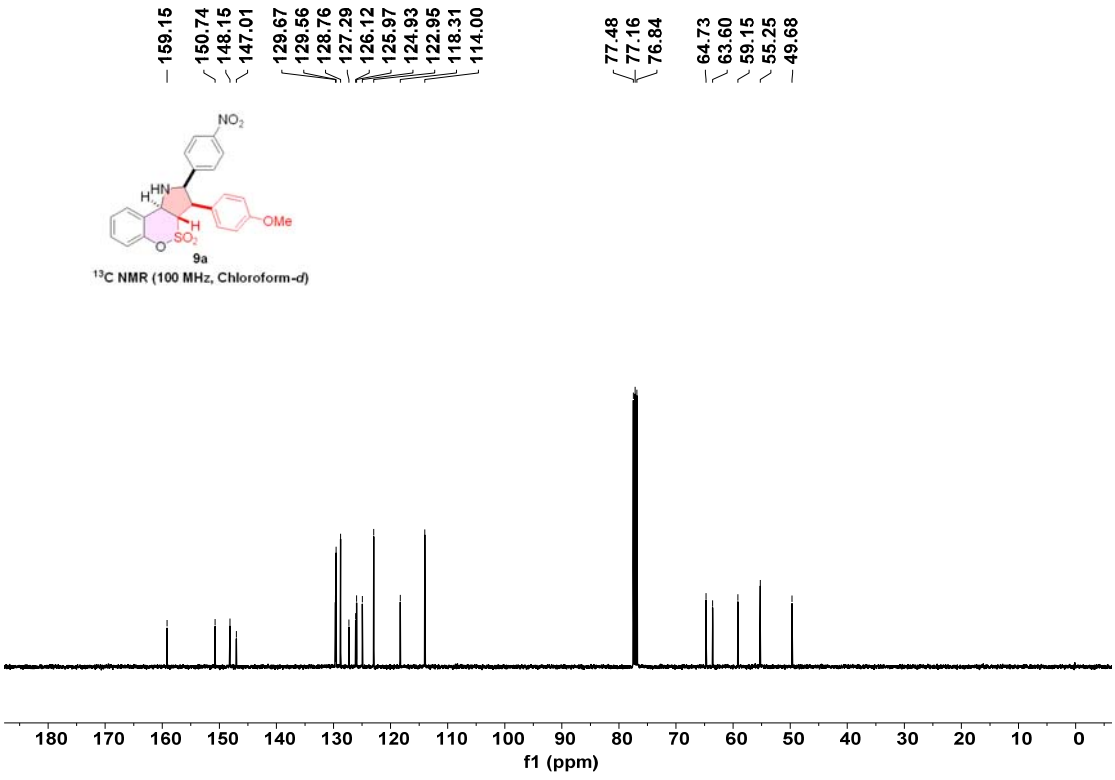


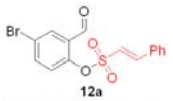
5w

^{13}C NMR (100 MHz, Chloroform-*d*)



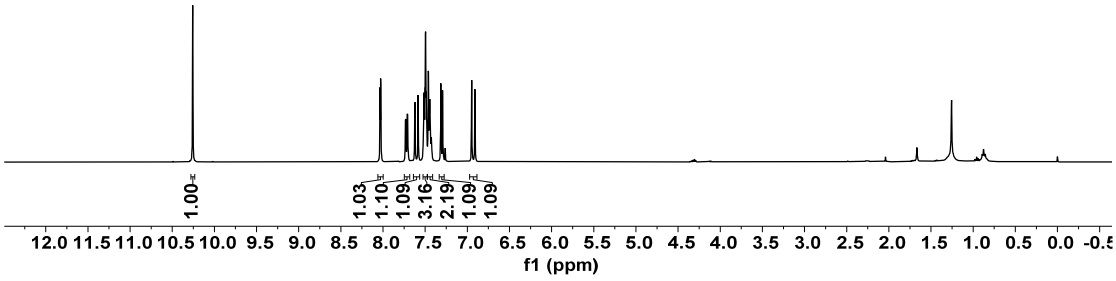

7.927
7.905
7.524
7.506
7.423
7.403
7.370
7.367
7.351
7.349
7.197
6.715
6.593
6.571
5.171
5.147
4.986
4.958
4.436
4.411
4.407
4.382
3.779
3.750
3.721
3.667
2.962
NO2
HN
H
H
SO2
O
OMe
9a
11H NMR (400 MHz, Chloroform-d)
2.00
1.02
1.04
1.05
3.04
2.02
2.03
1.00
1.01
1.02
1.06
3.04
0.98
f1 (ppm)

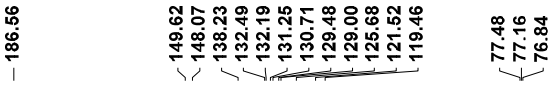

159.15
150.74
148.15
147.01
129.67
129.56
128.76
127.29
126.12
125.97
124.93
122.95
118.31
114.00
77.48
77.16
76.84
64.73
63.60
59.15
55.25
49.68
NO2
HN
H
H
SO2
O
OMe
9a
13C NMR (100 MHz, Chloroform-d)
f1 (ppm)

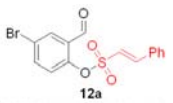


12a

^{1}H NMR (400 MHz, Chloroform-*d*)

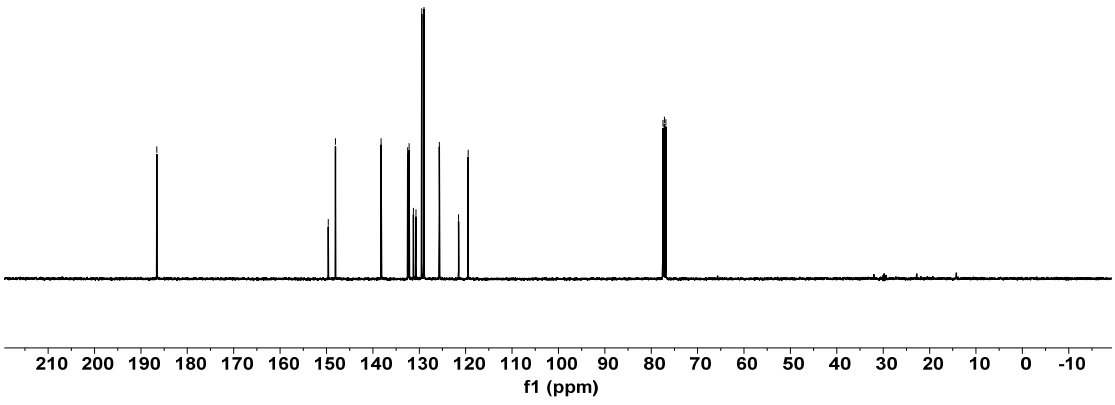


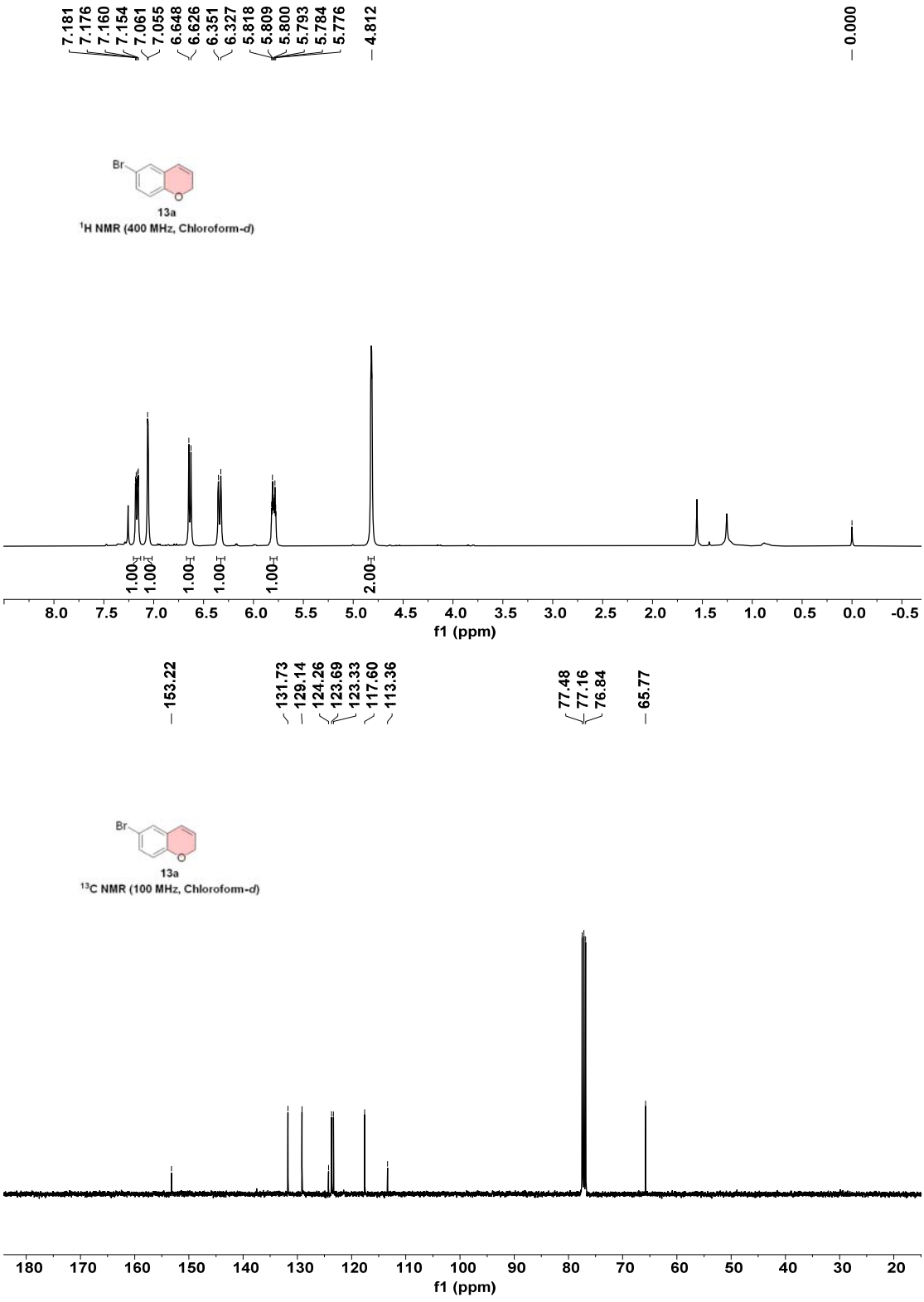




12a

^{13}C NMR (100 MHz, Chloroform-*d*)




7.181
7.176
7.160
7.154
7.061
7.055
6.648
6.626
6.351
6.327
5.818
5.809
5.800
5.793
5.784
5.776
4.812
0.000
Br
O
13a
1H NMR (400 MHz, Chloroform-d)
1.00
1.00
1.00
1.00
1.00
2.00
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)
153.22
131.73
129.14
124.26
123.69
123.33
117.60
113.36
77.48
77.16
76.84
65.77
Br
O
13a
13C NMR (100 MHz, Chloroform-d)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)