Supporting Information

Pd(II)-catalyzed asymmetric addition of arylboronic acids to cyclic *N*-sulfonyl ketimine esters and a DFT study of its mechanism

Mao Quan,[a,‡] Guoqiang Yang,[a,‡] Fang Xie,[a,*] Ilya D. Gridnev,[b] and Wanbin Zhang[a*]

[a] *School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, P. R. China. Fax: +86-21-5474-3265; Tel: +86-21-5474-3265; E-mail: xiefang@sju.edu.cn; wanbin@sjtu.edu.cn.*

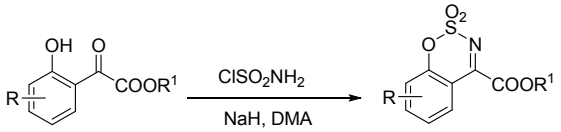
[b] *Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki 3-6, Aoba-ku, Sendai 9808578, Japan.*

CONTENTS

1. General

All air and moisture sensitive manipulations were carried out with standard Schlenk techniques nitrogen atmosphere. Column chromatography was performed using 100-200 mesh silica gels. DMA was distilled before use from CaH_2 under nitrogen. All solvents were refined by the standard of solvent manual. The other reagents were purchased from Adamas-Beta Ltd., Energy Chemical Inc. or J&K Scientific Inc. and used without further purification unless otherwise specified. The NMR spectra were recorded on a Varian MERCURY plus-400 (400 MHz, ^1H; 100 MHz, ^{13}C) spectrometer with chemical shifts reported in ppm relative to the residual deuterated solvents. Mass spectrometry analysis was carried out using an electrospray spectrometer Waters Micromass Q-TOF Premier Mass Spectrometer. Melting points were measured with SGW X-4 micro melting point apparatus. Optical rotations were measured on a Rudolph Research Analytical Autopol VI automatic polarimeter using a 50 mm path-length cell at 589 nm. Chiral analyses were performed on a Shimadzu LC-2010 HPLC system and using Daicel Chiralcel AD-H, and IE-H columns with *n*-hexane / *i*-propyl alcohol as an eluent.

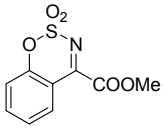
2. Synthesis of Substrates[1]



A **1a-1k**

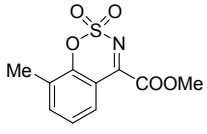
A were synthesized based on the literature.[2] To a solution of **A** (2.78 mmol) in 5.0 mL of DMA was quickly transferred solid H_2NSO_2Cl (1.12 g, 9.71 mmol, 3.5 equiv) and stirred for 1 h. NaH (60% in mineral oil, 388 mg, 9.71 mmol, 3.5 equiv) was added for 3 potions in 2 h and stirred for another 2 h at room temperature. After stirring at 50 °C for 12 h, the reaction was quenched by the addition of 5 mL of H_2O and transferred to a separatory funnel with 20 mL of Et_2O. The organic layer was separated, and the aqueous layer was extracted with 2 x 15 mL of Et_2O. The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. Purification by chromatography on silica gel (EtOAc/petroleum ether=1:4) afforded the product as a light yellow solid.

Methyl benzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1a)

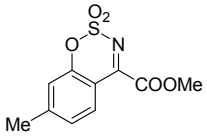


Light yellow solid, 342 mg, yield: 51%, Mp: 80-81 °C. ^1H NMR (400 MHz, $CDCl_3$): δ = 8.03 (d, *J* = 8.4 Hz, 1H), 7.79 (t, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 4.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 161.4, 155.0, 138.5, 130.5, 126.6, 119.4, 113.8, 54.4; IR (ν/cm^{-1}): 2961, 1743, 1589, 1549, 1387, 1231, 1024, 929, 864, 758; HRMS (ESI) calcd for $C_9H_8NO_5S$ $(M+H)^+$ 242.0123, found 242.0129

Methyl 8-methylbenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1b)



Light brown solid, 432 mg, yield: 61%, Mp: 71-72 °C. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 4.05 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.7, 161.6, 153.3, 140.0, 129.3, 128.0, 125.9, 113.6, 54.3, 15.1; IR (ν/cm^{-1}): 2595, 2922, 1746, 1563, 1557, 1393, 1236, 1204, 1098, 882, 732, 573; HRMS (ESI) calcd for $C_{10}H_{10}NO_5S$ $(M+H)^+$ 256.0280, found 256.0282.

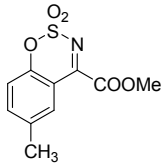


Methyl 7-methylbenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1c)

Light yellow solid, 404 mg, yield: 57%, Mp: 57-58 °C. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.89 (d, *J* = 8.2 Hz, 1H), 7.21 (d, *J* = 8.2 Hz, 1H), 7.14 (s, 1H), 4.04 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (100

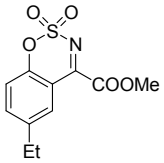
MHz, $CDCl_3$): δ = 164.8, 161.6, 155.2, 151.5, 130.2, 127.6, 119.5, 111.5, 54.3, 22.6; IR (ν/cm^{-1}): 2965, 2925, 1746, 1621, 1509, 1541, 1395, 1229, 1197, 1125, 567; HRMS (ESI) calcd for $C_{10}H_{10}NO_5S$ $(M+H)^+$ 256.0280, found 256.0278.

Methyl 6-methylbenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1d)



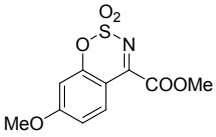
Yellow solid, 376 mg, yield: 53%, Mp: 65-66 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.76 (s, 1H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.24 (t, *J* = 7.8 1H), 4.06 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.2, 161.5, 153.0, 139.3, 136.8, 130.1, 119.1, 113.5, 54.3, 21.1; IR (ν/cm^{-1}): 2953, 2923, 1747, 1556, 1456, 1376, 1242, 1189, 596; HRMS (ESI) calcd for $C_{10}H_{10}NO_5S$ $(M+H)^+$ 256.0280, found 256.0280.

Methyl 6-ethylbenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1e)



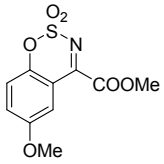
Colorless gummy oil, 386 mg, yield: 49%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 2.1 Hz, 1H), 7.61 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.28 – 7.24 (m 1H), 4.07 (s, 3H), 2.72 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.2, 161.6, 153.1, 143.1, 138.3, 129.1, 119.2, 113.6, 54.3, 28.5 15.5; IR (ν/cm^{-1}): 2953, 2920, 2854, 1757, 1556, 1458, 1377, 1242, 1191, 785, 608; HRMS (ESI) calcd for $C_{11}H_{12}NO_5S$ $(M+H)^+$ 270.0436, found 270.0438.

Mthyl 7-methoxybenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1f)



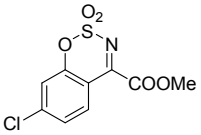
Yellow solid, 444 mg, yield: 59%, Mp: 107-108 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.98 (d, *J* = 9.1 Hz, 1H), 6.89 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.78 (d, *J* = 2.4, 1H), 4.03 (s, 3H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.9, 164.0, 161.8, 157.8, 132.3, 114.1, 107.5, 103.6, 56.8, 54.2; IR (ν/cm^{-1}): 3110, 2969, 1746, 1621, 1578, 1536, 1505, 1384, 1301, 1200, 1129, 1032, 863, 785, 685, 564; HRMS (ESI) calcd for $C_{10}H_{10}NO_6S$ $(M+H)^+$ 272.0229, found 272.0225.

Mthyl 6-methoxybenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1g)



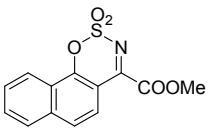
Yellow solid, 467 mg, yield: 62%, Mp: 80-81 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.50 (d, *J* = 2.8 Hz, 1H), 7.34 – 7.27 (m, 2H), 4.06 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.5, 161.5, 157.2, 148.9, 125.4, 120.4, 114.3, 113.0, 56.3, 54.4; IR (ν/cm^{-1}): 2920, 2849, 1740, 1562, 1503, 1382, 1282, 1259, 1206, 1174, 1035, 837, 823, 711, 695, 530; HRMS (ESI) calcd for $C_{10}H_{10}NO_6S$ $(M+H)^+$ 272.0229, found 272.0235.

Methyl 7-chlorobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1h)



Yellow solid, 428 mg, yield: 56%, Mp: 127-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.05 (d, *J* = 8.6 Hz, 1H), 7.43 – 7.34 (m, 2H), 4.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.8, 161.2, 155.4, 144.9, 131.5, 127.2, 119.9, 112.4, 54.5; IR (ν/cm^{-1}): 3100, 2963, 1743, 1582, 1434, 1393, 1263, 1203, 795, 627; HRMS (ESI) calcd for $C_9H_7NO_5SCl$ $(M+H)^+$ 275.9733, found 275.9733.

Methyl naphtho[2,1-*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1i)



Yellow solid, 380 mg, yield: 47%, Mp: 137-138 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.43 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.78 (ddd, *J* = 22.3, 15.2, 8.4 Hz 1H), 4.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.8, 161.8, 154.7, 138.0, 132.4, 128.7, 128.3, 125.9, 123.4, 123.0, 122.7, 109.3, 54.3; IR (ν/cm^{-1}): 2949, 2920, 1739, 1580, 1402, 1256, 1229, 1204, 1112, 1054, 896, 839, 775, 676, 568; HRMS (ESI) calcd for $C_{13}H_{10}NO_5S$ $(M+H)^+$ 292.0280, found 292.0288.

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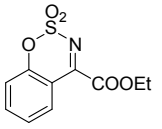
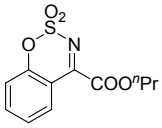
Ethyl benzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1j)



Colorless gummy oil, 362 mg, yield: 51%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.85 – 7.71 (m, 1H), 7.41 (td, *J* = 7.7, 1.0 Hz, 1H), 7.31 (dd, *J* = 8.4, 1.0 Hz, 1H), 4.50 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.7, 161.0, 154.9, 138.6, 130.5, 126.7, 119.3, 113.7, 64.3, 14.2; IR (ν/cm^{-1}): 2962, 2920, 1750, 1566, 1460, 1338, 1241, 1180, 1095, 893, 615; HRMS (ESI) calcd for $C_{10}H_{10}NO_5S$ $(M+H)^+$ 256.0280, found 256.0288.

Propyl benzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (1j)



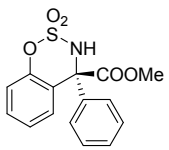
Colorless gummy oil, 426 mg, yield: 54%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.78 (ddd, *J* = 8.3, 7.6, 1.6 Hz, 1H), 7.41 (ddd, *J* = 8.0, 7.5, 1.0 Hz, 1H), 7.32 (dd, *J* = 8.4, 0.7 Hz, 1H), 4.41 (t, *J* = 6.7 Hz, 2H), 1.82 (tq, *J* = 14.17.1 Hz, 2H), 1.01 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.8, 161.1, 154.9, 138.6, 130.4, 126.6,119.4, 113.7, 69.6, 22.0, 10.5; IR (ν/cm^{-1}): 2972, 2882, 1741, 1597, 1556, 1401, 1206, 1189, 1123, 1016, 864, 749; HRMS (ESI) calcd for $C_{11}H_{12}NO_5S$ $(M+H)^+$ 270.0436, found 270.0436.

3. Asymmetric Catalysis

General procedure A: (in test tube opened to air): A test tube (20 mL) was charged with $Pd(TFA)_2$ (3.3 mg, 0.010 mmol, 0.050 equiv), **L1a** (3.9 mg, 0.015 mmol, 0.075 equiv) and unpurified TFE (1.0 mL). The solution was stirred at 30 °C for 2 h, then substrate (0.20 mmol, 1.0 equiv) and arylboronic acid (0.30 mmol, 1.5 equiv) were added into the tube. The wall of the tube was rinsed with an additional portion of TFE (1.0 mL). After stirring at 60 °C for 24 h in air, the reaction mixture was cooled to room temperature and the solvent was removed by rotary evaporation. The residue was purified by preparative TLC on silica gel (petroleum ether/EtOAc = 5/1) to give the product.

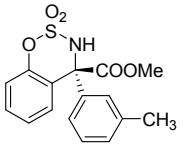
General procedure B: (in sealed tube charged with O_2): $Pd(TFA)_2$ (3.3 mg, 0.010 mmol, 0.050 equiv) and **L1a** (3.9 mg, 0.015 mmol, 0.075 equiv) were weighted in air and placed in a vial. The unpurified TFE (1.0 mL) was added and the solution was stirred at 30 °C for 2 h to afford the catalyst solution. A sealed tube (25 mL) was charged with substrate (0.20 mmol, 1.0 equiv) and arylboronic acid (0.30 mmol, 1.5 equiv), then degassed and recharged with O_2 (balloon) three times. The above catalyst solution was added to the tube via syringe. The wall of the tube was rinsed with TFE (1.0 mL). The tube was sealed and heated to 60 °C. After stirring for a certain time, the reaction mixture was cooled to room temperature, and the solvent was removed by rotary evaporation. The residue was purified by preparative TLC on silica gel (petroleum ether/EtOAc = 5/1) to give the product.

(*R*)-Methyl 4-phenyl-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3aa**).



General procedure A, colorless gummy oil, 63 mg, yield: 99%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.48 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.44 (td, *J* = 8.0, 1.4 Hz, 1H), 7.38 – 7.34 (m, 3H), 7.26 – 7.20 (m, 3H), 7.13 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.45 (br, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 170.8, 151.2, 139.4, 131.1, 130.7, 129.3, 128.9 127.8, 125.3, 119.9, 119.0, 71.5, 54.8; IR (ν/cm^{-1}): 3206, 2963, 1732, 1485, 1413, 1262, 1207, 1105, 1020, 803, 691, 579; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 30.6 min (major), t_{R2} = 46.2 min (minor)]; ee = 98%, $[\alpha]^{25}_D$ = +36.7 (c = 0.63, $CHCl_3$); HRMS (ESI) calcd for $C_{15}H_{14}NO_5S$ $(M+H)^+$ 320.0593, found 320.0590.

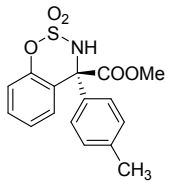
(*R*)-Methyl 4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ab**).



General procedure A, colorless gummy oil, 66 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.47 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.42 (td, *J* = 8.0, 1.4 Hz, 3H), 7.27 – 7.16 (m, 3H), 7.13 (dd, *J* = 8.4, 0.8

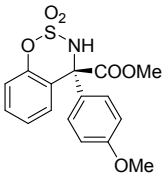
Hz, 1H), 7.02 (m, 2H), 6.39 (s, 1H), 3.89 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.9, 151.1, 139.3, 138.7, 131.0, 130.8, 130.1, 128.7, 128.3, 125.2, 124.8, 119.8, 119.2, 71.5, 54.7, 21.8; IR (ν/cm^{-1}): 3208, 2963, 1732, 1460, 1405, 1260, 1095, 1023, 863, 800; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 18.2 min (major), t_{R2} = 21.0 min (minor)]; ee = 99%, $[\alpha]^{25}_D$ = +31.5 (c = 0.66, $CHCl_3$); HRMS (ESI) calcd for $C_{16}H_{16}NO_5S$ $(M+H)^+$ 334.0749, found 334.0740.

(*R*)-Methyl 4-(*p*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ac**).



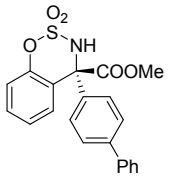
General procedure A, colorless gummy oil, 66 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.46 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.41 (td, *J* = 8.0, 1.4 Hz, 1H), 7.21 (td, *J* = 8.0, 1.2 Hz, 1H), 7.17 – 7.09 (m, 5H), 6.39 (s, 1H), 3.89 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.9, 151.2, 139.3, 136.5, 131.0, 130.7, 129.6, 127.6, 125.2, 119.8, 119.3, 71.3, 54.7, 21.4; IR (ν/cm^{-1}): 3254, 2963, 1732, 1614, 1580, 1507, 1416, 1261, 1100, 1020, 799, 705; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 23.3 min (major), t_{R2} = 35.2 min (minor)]; ee = 98%, $[\alpha]^{25}_D$ = +42.3 (c = 0.66, $CHCl_3$); HRMS (ESI) calcd for $C_{16}H_{16}NO_5S$ $(M+H)^+$ 334.0749, found 334.0744.

(*R*)-Methyl 4-(4-methoxyphenyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ad**).



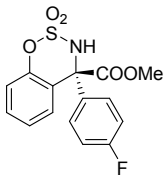
General procedure A, colorless gummy oil, 69 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.46 (d, *J* = 8.0 Hz, 1H), 7.42 (td, *J* = 8.0, 1.4 Hz, 1H), 7.22 (td, *J* = 8.0, 1.4 Hz, 1H), 7.13 (d, *J* = 9.2 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.86 (d, *J* = 9.6 Hz, 2H), 6.36 (s, 1H), 3.89 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 171.0, 160.1, 151.1, 131.4, 131.0, 130.8, 129.1, 125.2, 119.8, 119.6, 114.1, 71.2, 55.5, 54.6; IR (ν/cm^{-1}): 3271, 2960, 2052, 1646, 1608, 1507, 1488, 1472, 1259, 1173, 1104, 1019, 894, 799; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 35.5 min (major), t_{R2} = 42.8 min (minor)]; ee = 98%, $[\alpha]^{25}_D$ = +45.3 (c = 0.70, $CHCl_3$); HRMS (ESI) calcd for $C_{16}H_{16}NO_6S$ $(M+H)^+$ 350.0698, found 350.0691.

(*R*)-Methyl 4-([1,1'-biphenyl]-4-yl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ae**).



General procedure A, colorless gummy oil, 73 mg, yield: 92%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.59 – 7.56 (m, 4H), 7.54 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.48 – 7.42 (m, 3H), 7.36 (tt, *J* = 7.4, 1.6 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.26 (td, *J* = 7.6, 1.2 Hz, 1H), 7.16 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.50 (s, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.8, 151.2, 142.1, 140.2, 138.3, 131.2, 130.7, 129.1, 128.2, 128.0, 127.5, 127.4, 125.4, 120.0, 119.0, 71.3, 54.9; IR (ν/cm^{-1}): 3264, 2961, 2851, 1739, 1486, 1418, 1258, 1175, 1107, 863, 804, 699; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 36.7 min (minor), t_{R2} = 47.6 min (major)]; ee = 98%, $[\alpha]^{25}_D$ = +36.0 (c = 0.70, $CHCl_3$); HRMS (ESI) calcd for $C_{21}H_{18}NO_5S$ $(M+H)^+$ 396.0906, found 396.0915.

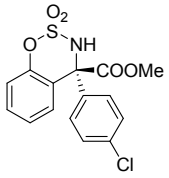
(*R*)-Methyl 4-(4-fluorophenyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3af**).



General procedure A, colorless gummy oil, 61 mg, yield: 90%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.50 – 7.43 (m, 2H), 7.26 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.23 – 7.19 (m, 2H), 7.15 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.06 (m, 2H), 6.47 (s, 1H). 3.89 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.6, 163.0 (d, *J* = 247.3 Hz), 151.3, 135.2 (d, *J* = 3.5 Hz), 131.4, 130.2, 129.8 (d, *J* = 8.4 Hz), 125.4, 120.1, 118.7, 115.8 (q, *J* = 22.4 Hz) 70.9, 54.9; IR (ν/cm^{-1}): 3254, 2961, 2852, 1733, 1605, 1508, 1417, 1260,

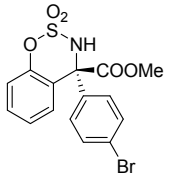
1104, 1016, 802, 711, 623; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 19.1 min (major), t_{R2} = 23.0 min (minor)]; ee = 98%, $[\alpha]^{25}_D$ = +63.7 (c = 0.60, $CHCl_3$); HRMS (ESI) calcd for $C_{15}H_{13}FNO_5S$ $(M+H)^+$ 338.0498, found 338.0494.

(*R*)-Methyl 4-(4-chlorophenyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ag**).



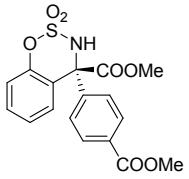
General procedure A, colorless gummy oil, 66 mg, yield: 94%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.50 – 7.43 (m, 2H), 7.25 (td, *J* = 7.6, 1.6 Hz, 1H), 7.18 – 7.13 (m, 3H), 6.50 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.4, 151.3, 137.8, 135.3, 131.4, 130.1, 129.3, 129.0, 125.4, 120.2, 118.3, 70.8, 55.0; IR (ν/cm^{-1}): 3257, 2960, 2862, 1732, 1580, 1489, 1417, 1260, 1174, 1095, 935, 831, 761; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 20.9 min (major), t_{R2} = 24.4 min (minor)]; ee = 98%, $[\alpha]^{25}_D$ = +63.9 (c = 0.66, $CHCl_3$); HRMS (ESI) calcd for $C_{15}H_{13}ClNO_5S$ $(M+H)^+$ 354.0203, found 354.0200.

(*R*)-Methyl 4-(4-bromophenyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ah**).



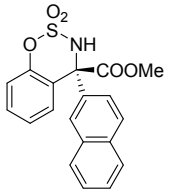
General procedure A, colorless gummy oil, 73 mg, yield: 92%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.55 – 7.40 (m, 4H), 7.35 – 7.20 (m, 1H), 7.18 – 7.06 (m, 3H), 6.52 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.4, 151.3, 138.4, 132.0, 131.5, 130.1, 129.6, 125.5, 123.5, 120.2, 118.1, 70.9, 55.1; IR (ν/cm^{-1}): 3293, 2958, 1735, 1578, 1485, 1413, 1395, 1175, 1007, 893, 743; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 32.5 min (major), t_{R2} = 37.2 min (minor)]; ee = 98%, $[\alpha]^{20}_D$ = +40.1 (c = 1.0, $CHCl_3$); HRMS (ESI) calcd for $C_{15}H_{12}BrNO_5SNa$ $(M+Na)^+$ 419.9517, found 419.9519.

(*R*)-Methyl 4-(4-(methoxycarbonyl)phenyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ai**).



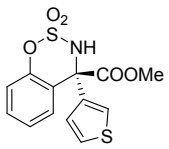
General procedure A, colorless gummy oil, 39 mg, yield: 52%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 8.01 (d, *J* = 8.4 Hz, 2H), 7.51 – 7.45 (m, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 6.55 (s, 1H), 3.90 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.3, 166.5, 151.4, 143.9, 131.5, 130.9, 130.1, 130.0, 127.9, 125.5, 120.3, 118.0, 71.0, 55.1, 52.5; IR (ν/cm^{-1}): 3260, 2962, 1716, 1614, 1580, 1507, 1485, 1417, 1261, 1104, 1019, 865, 803, 698; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 38.8 min (major), t_{R2} = 44.4 min (minor)]; ee = 97%, $[\alpha]^{25}_D$ = +35.1 (c = 0.22, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{16}NO_7S$ $(M+H)^+$ 378.0647, found 378.0658.

(*R*)-Methyl 4-(naphthalen-2-yl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3aj**).



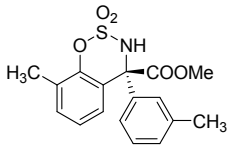
General procedure A, colorless gummy oil, 55 mg, yield: 74%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.84 (t, *J* = 8.0 Hz, 2H), 7.75 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.61 (d, *J* = 1.6 Hz, 1H), 7.54 (td, *J* = 8.0, 1.6 Hz, 2H), 7.51 – 7.45 (m, 2H), 7.36 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.26 (td, *J* = 8.0, 1.0 Hz, 1H), 7.18 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.54 (br, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.8, 151.3, 136.4, 133.4, 132.7, 131.3, 130.7, 129.1, 128.7, 127.8, 127.4, 127.3, 126.9, 125.3, 124.9, 120.0, 118.8, 71.6, 54.8; IR (ν/cm^{-1}): 3256, 2963, 1733, 1716, 1508, 1412, 1261, 1093, 1020, 864, 799, 704; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 35.8 min (major), t_{R2} = 50.4 min (minor)]; ee = 99%, $[\alpha]^{25}_D$ = +17.6 (c = 0.26, $CHCl_3$); HRMS (ESI) calcd for $C_{19}H_{16}NO_5S$ $(M+H)^+$ 370.0749, found 370.0746.

(*S*)-Methyl 4-(thiophen-3-yl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (**3ak**).



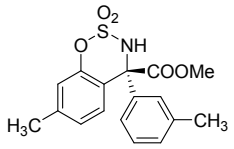
General procedure A, colorless gummy oil, 49 mg, yield: 67%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.55 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.34 (dd, *J* = 5.0, 2.6 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.14 (dd, *J* = 2.8, 1.2 Hz, 1H), 7.11 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.00 (dd, *J* = 5.2, 1.6 Hz, 1H), 6.32 (s, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.2, 150.7, 139.9, 131.1, 130.3, 127.1, 126.7, 125.4, 125.4, 119.8, 119.6, 68.2, 54.8; IR (ν/cm^{-1}): 3245, 2962, 1731, 1580, 1417, 1261, 1019, 799, 699; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 85/15, 210 nm, 0.5 mL/min. t_{R1} = 26.0 min (major), t_{R2} = 30.4 min (minor)]; ee = 96%, $[\alpha]^{25}_D$ = +30.2 (c = 0.28, $CHCl_3$); HRMS (ESI) calcd for $C_{13}H_{12}NO_5S_2$ $(M+H)^+$ 326.0157, found 326.0150.

(*R*)-Methyl 8-methyl-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3bb).



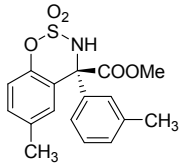
General procedure A, colorless gummy oil, 69 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.29 – 7.20 (m, 3H), 7.18 – 7.00 (m, 4H), 6.37 (s, 1H), 3.88 (s, 3H), 2.32 (s, 6H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 171.0, 149.5, 139.4, 138.6, 132.4, 130.0, 129.2, 128.6, 128.4, 128.2, 124.9, 124.5, 119.4, 71.6, 54.6, 21.8, 16.0; IR (ν/cm^{-1}): 3259, 2956, 2925, 1738, 1607, 1488, 1422, 1362, 1259, 1209, 1161, 1077, 879, 786, 568; HPLC [Daicel Chiralpak IE-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 28.6 min (minor), t_{R2} = 31.6 min (major)]; ee = 95%, $[\alpha]^{20}_D$ = +19.3 (c = 0.73, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{18}NO_5S$ $(M+H)^+$ 348.0906, found 348.0902.

(*R*)-Methyl 7-methyl-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3cb).



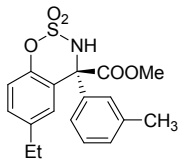
General procedure A, white solid, 69 mg, yield: 99%, Mp: 137-138 °C. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.25 (ddd, *J* = 32.4, 30.2, 7.9 Hz, 4H), 7.07 – 7.00 (m, 3H), 6.94 (s, 1H), 3.88 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 171.0, 150.9, 141.8, 139.5, 138.7, 130.5, 130.0, 128.7, 128.3, 126.2, 121.8, 120.0, 116.1, 71.3, 54.6, 21.8, 21.3; IR (ν/cm^{-1}): 3257, 2969, 2923, 1732, 1622, 1497, 1423, 1350, 1259, 1203, 1117, 904, 807, 703; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 31.5 min (major), t_{R2} = 50.5 min (minor)]; ee = 97%, $[\alpha]^{20}_D$ = +33.9 (c = 0.73, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{18}NO_5S$ $(M+H)^+$ 348.0906, found 348.0916.

(*R*)-Methyl 6-methyl-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3db).



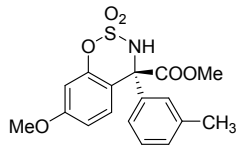
General procedure A, colorless gummy oil, 69 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.28 – 7.15 (m, 4H), 7.07 – 6.99 (m, 3H), 6.31 (s, 1H), 3.90 (s, 3H), 2.34 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.9, 149.0, 139.4, 138.7, 135.0, 131.7, 130.8, 130.1, 128.7, 128.3, 124.9, 119.5, 119.0, 71.5, 54.6, 21.8, 21.2; IR (ν/cm^{-1}): 3281, 2960, 1730, 1661, 1608, 1488, 1417, 1260, 1178, 1116, 1024, 801, 700; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 20.4 min (major), t_{R2} = 25.7 min (minor)]; ee = 96%, $[\alpha]^{20}_D$ = +22.9 (c = 0.95, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{18}NO_5S$ $(M+H)^+$ 348.0906, found 348.0909.

(*R*)-Methyl 6-ethyl-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3eb).



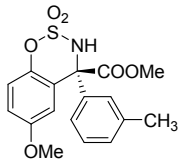
General procedure A, colorless gummy oil, 72 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.26 (ddd, *J* = 7.6, 5.6, 2.8 Hz, 3H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.04 (dd, *J* = 10.7, 4.6 Hz, 3H), 6.37 (s, 1H), 3.90 (s, 3H), 2.62 (q, *J* = 7.6 Hz, 2H), 2.34 (s, 3H) 1.19 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 171.0, 149.2, 141.3, 139.4, 138.7, 130.6, 130.0, 129.8, 128.7, 128.4, 124.9, 119.6, 118.8, 71.5, 54.6, 28.5, 21.8, 15.8; IR (ν/cm^{-1}): 3261, 2964, 2862, 1734, 1614, 1580, 1488, 1417, 1262, 1120, 1116, 1019, 803, 698; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 20.4 min (major), t_{R2} = 25.7 min (minor)]; ee = 96%, $[\alpha]^{20}_D$ = +22.9 (c = 0.95, $CHCl_3$); HRMS (ESI) calcd for $C_{18}H_{20}NO_5S$ $(M+H)^+$ 362.1062, found 362.1065.

(*R*)-Methyl 7-methoxy-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3fb).



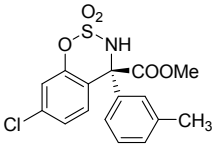
General procedure A, white solid, 72 mg, yield: 99%, Mp: 166-167 °C. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.37 (d, *J* = 8.9 Hz, 1H), 7.20 (dd, *J* = 25.9, 7.9 Hz, 2H), 7.06 – 6.98 (m, 2H), 6.78 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.62 (d, *J* = 2.6 Hz, 1H), 6.39 (s, 1H), 3.88 (s, 3H), 3.83 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 171.1, 161.3, 152.0, 139.6, 138.7, 131.5, 130.0, 128.7, 128.2, 124.8, 112.4, 110.7, 104.1, 71.0, 55.9, 54.6, 21.8; IR (ν/cm^{-1}): 3214, 2955, 1738, 1620, 1573, 1505, 1412, 1261, 1190, 1157, 1027, 939, 814, 707; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 48.4 min (major), t_{R2} = 65.1 min (minor)]; ee = 96%, $[\alpha]^{20}_D$ = +17.5 (c = 1.0, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{18}NO_6S$ $(M+H)^+$ 364.0855, found 364.0861.

(*R*)-Methyl 6-methoxy-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3gb).



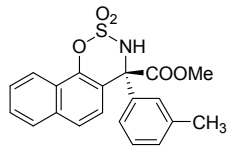
General procedure A, colorless gummy oil, 72 mg, yield: 99%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.25 (dd, *J* = 10.8, 4.3 Hz, 1H), 7.17 (d, *J* = 7.9 Hz, 1H), 7.10 – 7.01 (m, 3H), 6.96 (dq, *J* = 5.8, 3.0 Hz, 1H), 6.33 (s, 1H), 3.90 (s, 3H), 3.75 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.8, 156.4, 144.9, 139.2, 138.7, 130.1, 128.7, 128.3, 124.8, 120.5, 120.2, 116.4, 115.8, 71.6, 56.0, 51.7, 21.8; IR (ν/cm^{-1}): 3257, 2956, 1744, 1608, 1491, 1419, 1250, 1175, 1036, 855, 702; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 31.9 min (major), t_{R2} = 37.7 min (minor)]; ee = 98%, $[\alpha]^{20}_D$ = +45.9 (c = 1.0, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{18}NO_5S$ $(M+H)^+$ 364.0855, found 364.0865.

(*R*)-Methyl 7-chloro-4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3hb).



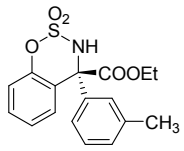
General procedure A, colorless gummy oil, 71 mg, yield: 97%. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.38 (d, *J* = 8.6, Hz, 1H), 7.25 – 7.12 (m, 4H), 7.00 (dd, *J* = 5.5, 4.8 Hz, 2H), 6.42 (s, 1H), 3.89 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.6, 151.3, 139.0, 136.4, 132.2, 130.4, 128.9, 128.1, 125.7, 124.7, 119.9, 118.1, 71.3, 54.8, 21.8; IR (ν/cm^{-1}): 3257, 2961, 2926, 2855, 1732, 1607, 1568, 1417, 1260, 1089, 1016, 799, 700; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 22.8 min (major), t_{R2} = 36.0 min (minor)]; ee = 96%, $[\alpha]^{20}_D$ = +7.4 (c = 0.5, $CHCl_3$); HRMS (ESI) calcd for $C_{16}H_{15}NO_5SCl$ $(M+H)^+$ 368.0359, found 368.0361.

(*R*)-Methyl 4-(*m*-tolyl)-3,4-dihydronaphtho[2,1-*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3ib).



General procedure A, white solid, 74 mg, yield: 96%, Mp: 185-186 °C. ^{1}H NMR (400 MHz $CDCl_3$) δ = 8.25 (dd, *J* = 6.1, 3.6, Hz, 1H), 7.86 (dd, *J* = 6.2, 3.2 Hz, 1H), 7.64 (ddd, *J* = 10.2, 6.7, 3.2 Hz, 3H), 7.46 (d, *J* = 8.8 Hz, 1H), 7.24 (dt, *J* = 23.6, 6.7 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H), 6.49 (s, 1H), 3.93 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.9, 147.0, 130.2, 128.8, 128.5, 128.4, 127.7, 127.6, 125.0, 124.4, 114.6, 71.9, 54.6, 21.7; IR (ν/cm^{-1}): 3260, 2962, 1736, 1603, 1404, 1260, 1176, 1095, 927, 811; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 66.4 min (major), t_{R2} = 120.0 min (minor)]; ee = 98%, $[\alpha]^{20}_D$ = -17.8 (c = 1.2, $CHCl_3$); HRMS (ESI) calcd for $C_{20}H_{18}NO_5S$ $(M+H)^+$ 384.0906, found 384.0894.

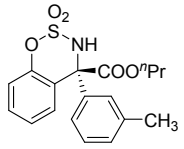
(*R*)-Ethyl 4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3jb).



General procedure B, white solid, 69 mg, yield: 99%, Mp: 122-123 °C. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.52 – 7.38 (m, 2H), 7.25 – 7.19 (m, 2H), 7.18 – 6.99 (m, 4H), 6.41 (s, 1H), 4.37 (q, *J* = 7.2 Hz, 2H), 2.33 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.3, 151.2, 139.5, 138.6, 131.0, 130.9, 130.0, 128.6, 128.3, 125.1, 124.8, 119.8, 119.3, 71.4, 61.3, 21.8, 14.1; IR

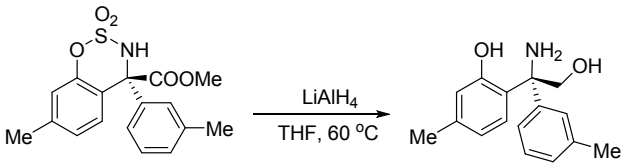
(ν/cm^{-1}): 3239, 2963, 2921, 1720, 1610, 1445, 1421, 1285, 1237, 1176, 1107, 870, 691; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90/10, 210 nm, 0.5 mL/min. t_{R1} = 23.2 min (major), t_{R2} = 25.2 min (minor)]; ee = 92%, $[\alpha]^{20}_D$ = +28.4 (c = 0.26, $CHCl_3$); HRMS (ESI) calcd for $C_{17}H_{18}NO_5S$ $(M+H)^+$ 348.0906, found 348.0909.

(*R*)-Propyl 4-(*m*-tolyl)-3,4-dihydrobenzo[*e*][1,2,3]oxathiazine-4-carboxylate 2,2-dioxide (3kb).



General procedure B, white solid, 71 mg, yield: 98%, Mp: 130-131 °C. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.54 – 7.38 (m, 2H), 7.26 – 7.19 (m, 2H), 7.18 – 7.09 (m, 2H), 7.08 – 6.98 (m, 2H), 6.43 (s, 1H), 4.26 (ddd, *J* = 17.3, 10.6, 4.0 Hz, 2H), 2.32 (s, 3H), 1.66 (dd, *J* = 14.2, 7.0 Hz, 2H) , 0.84 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 170.4, 151.2, 139.6, 138.6, 131.0, 131.0, 130.0, 128.6, 128.3, 125.1, 124.9, 119.8, 119.4, 71.5, 69.8, 21.9, 21.8, 10.4; IR (ν/cm^{-1}): 3229, 2967, 2877, 1716, 1609, 1483, 1420, 1287, 1263, 1177, 1070, 1051, 950, 868, 609; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 95/5, 210 nm, 0.5 mL/min. t_{R1} = 38.7 min (major), t_{R2} = 41.0 min (minor)]; ee = 98%, $[\alpha]^{20}_D$ = +22.1 (c = 0.65, $CHCl_3$); HRMS (ESI) calcd for $C_{18}H_{20}NO_5S$ $(M+H)^+$ 362.1062, found 362.1060.

4. **Reduction of arylation product 3cb**



3cb
ee: 97%

4
yield: 86%
ee: 99.9%

The reaction was carried out in a modified procedure of Hon Wai Lam.[3] To a solution of the arylation product **3cb** (208 mg, 0.6 mmol) in THF (2 mL) at room temperature was added $LiAlH_4$ (1.0 M in THF, 2.4 mL, 2.4 mmol) dropwise over 2 min. The mixture was heated at 55 °C overnight, cooled naturally to room temperature, and then to 0 °C with an ice bath. The reaction was quenched carefully with EtOAc (5 mL) followed by EtOH (5 mL). The solution was concentrated in vacuo. Purification of the residue by column chromatography (2:1 petroleum ether:EtOAc →1:1 petroleum ether:EtOAc) gave the product **4** (133 mg, 86%) as a yellow ointment. ^{1}H NMR (400 MHz $CDCl_3$) δ = 7.30 – 7.05 (m, 4H), 6.55 – 6.75 (m, 3H), 5.10 (brs, 4H), 4.15 (d, *J* = 12.0 Hz, 1H), 3.92 (d, *J* = 8.0 Hz, 1H), 2.34 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz $CDCl_3$) δ = 158.4, 143.3, 139.7, 138.6, 128.8, 128.5, 128.0, 127.0, 123.8, 123.5, 120.1, 118.7, 68.5, 63.7, 22.0, 21.3; IR (ν/cm^{-1}): 3363, 2922, 1621, 1578, 1490, 1452, 1384, 1298, 1270, 1163, 1040, 950, 781, 704; HPLC [Daicel Chiralpak AD-H, hexane/*i*-PrOH = 95/5, 210 nm, 0.5 mL/min. t_{R1} = 40.9 min (minor), t_{R2} = 46.9 min (major)]; ee = 99.9%, $[\alpha]^{20}_D$ = +3.6 (c = 1.0, $CHCl_3$); HRMS (ESI) calcd for $C_{16}H_{17}O_2$ $(M-NH_2)^+$ 241.1229, found 241.1233.

5. Computational Details

All computations were carried out using the Hybrid Becke functional (B3)[4] for electron exchange and the correlation functional of Lee, Yang and Parr (LYP),[5] as implemented in the Gaussian 09 software package.[6] For palladium the GEN basis set with the associated effective Core Potential was employed.[7] All other atoms were modeled at the 6-31G(d,p) level of theory.[8]

Geometry optimizations were performed with the account of the solvent effects (CPCM, Ethanol) without applying any geometry Constraints (C1 symmetry).

Starting geometries for the transition state search were located either by QST2 or QST3 procedures, or by the guess based on the structure of the previously found TS. The transition states were subsequently fully optimized as saddle points of first order, employing the Berny algorithm.[9] Frequency Calculations were carried out to confirm the nature of the stationary points, yielding zero imaginary frequencies for all Pd complexes and one imaginary frequency for all transition states, which represented the vector for the appropriate bond formation.

Energies and Free Energies of Computed Structures

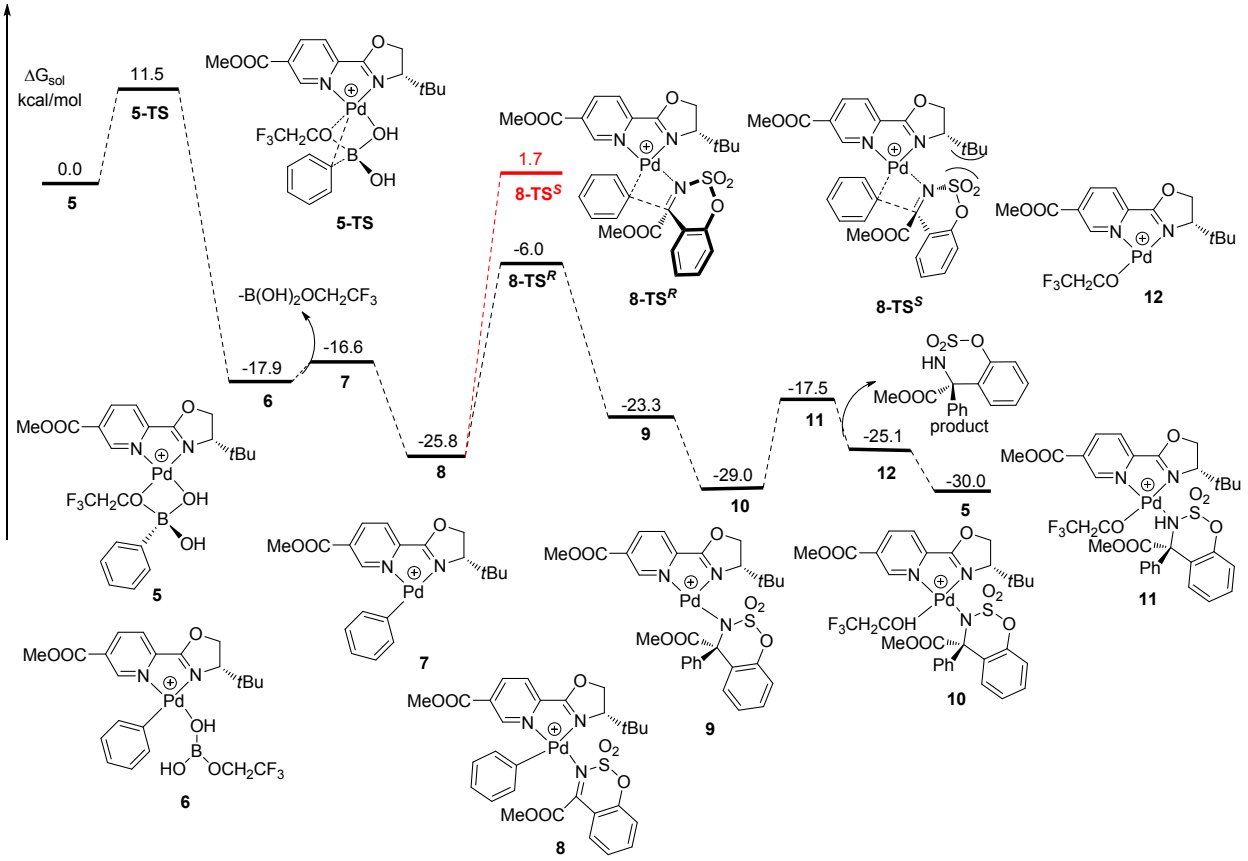


Figure 1. Catalytic circle of Pd(II)-catalyzed asymmetric addition of phenylboronic acid to substrate **1a**.

Compound, Mechanism	ZPVE Corrected Energy, a.u.	Free Energy (298 K), a.u.
5	**-1866.831838**	**-1866.898422**
5TS	**-1866.814831**	**-1866.880147**
6	**-1866.857112**	**-1866.926947**
7	**-1238.246302**	**-1238.304735**
8	**-2414.030638**	**-2414.104011**
8TS^R	**-2413.999566**	**-2414.072414**
8TS^S	**-2414.990022**	**-2414.061573**
9	**-2414.028763**	**-2414.100067**
10	**-2866.653407**	**-2866.733166**
11	**-2866.634719**	**-2866.714825**
12	**-1458.764723**	**-1458.823013**
1a	**-1175.743245**	**-1175.784588**

2a	**-408.035010**	**-408.067570**
3aa	**-1407.857238**	**-1407.903903**
$B(OH)_2OCH_2CF_3$	**-628.585403**	**-628.620145**
CF_3CH_2OH	**-452.592870**	**-452.624038**

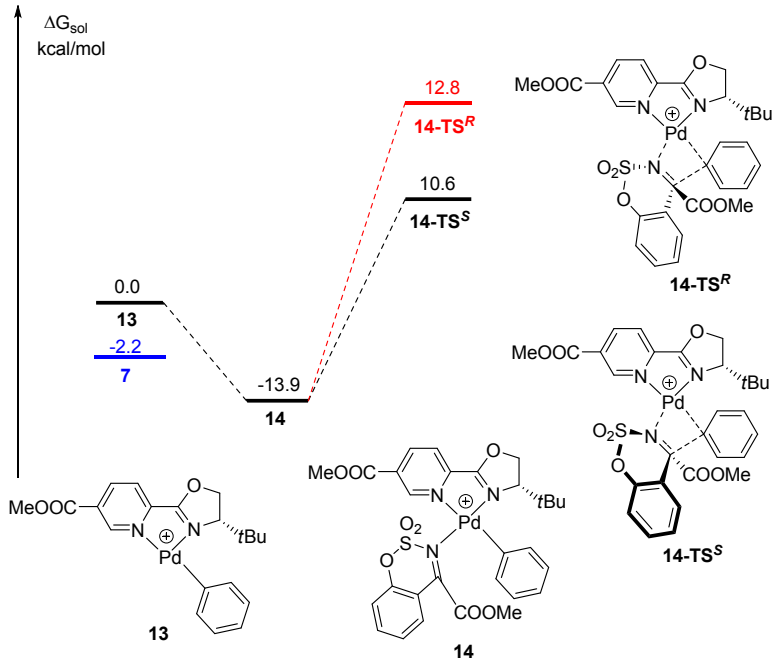


Figure 2 Alternative pathways of arylation.

Compound, Mechanism	ZPVE Corrected Energy, a.u.	Free Energy (298 K), a.u.
13	**-1238.245439**	**-1238.301173**
14	**-2414.032364**	**-2414.107870**
$14TS^R$	**-2413.994120**	**-2414.065395**
$14TS^S$	**-2413.997013**	**-2414.068774**

Reference

[1] B. H. Brodsky and J. D. Bois, *J. Am. Chem. Soc.*, 2005, **127**, 15391.

[2] F. Hu, X. Guan and M. Shi, *Tetrahedron*, 2012, **68**, 4782.

[3] Y. Luo, A. J. Carnell and H. W. Lam, *Angew. Chem. Int. Ed.*, 2012, **51**, 6762.

[4] (a) A. D. Becke, J. Chem. Phys., 1993, 98, 1372; (b) A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648.

[5] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785.

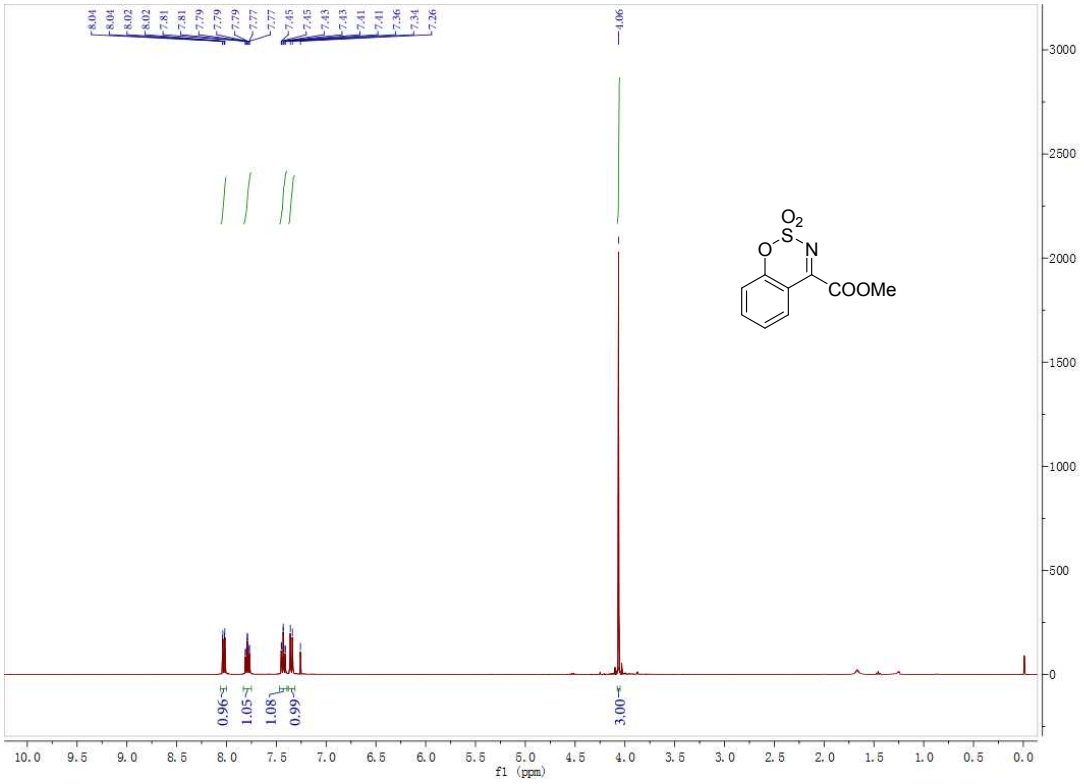
[6] Gaussian 09, Revision A.02, M. J. Frisch , G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. 10 Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

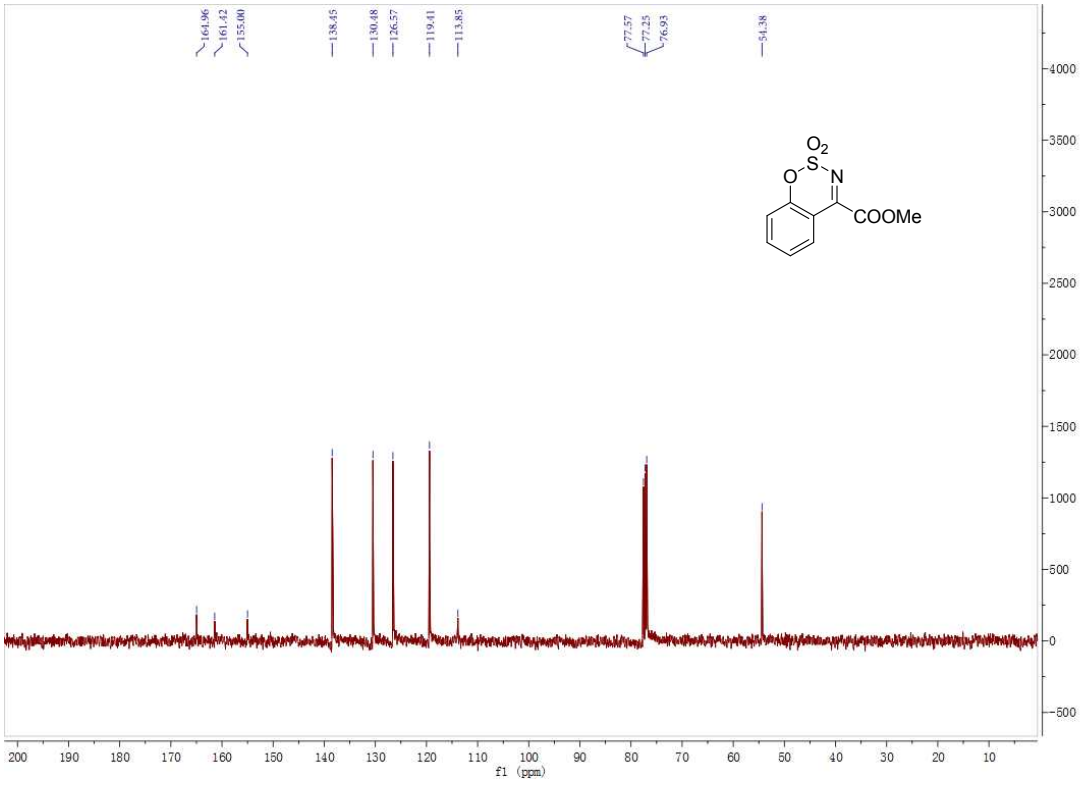
[7] D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta*, 1990, **77**, 123.

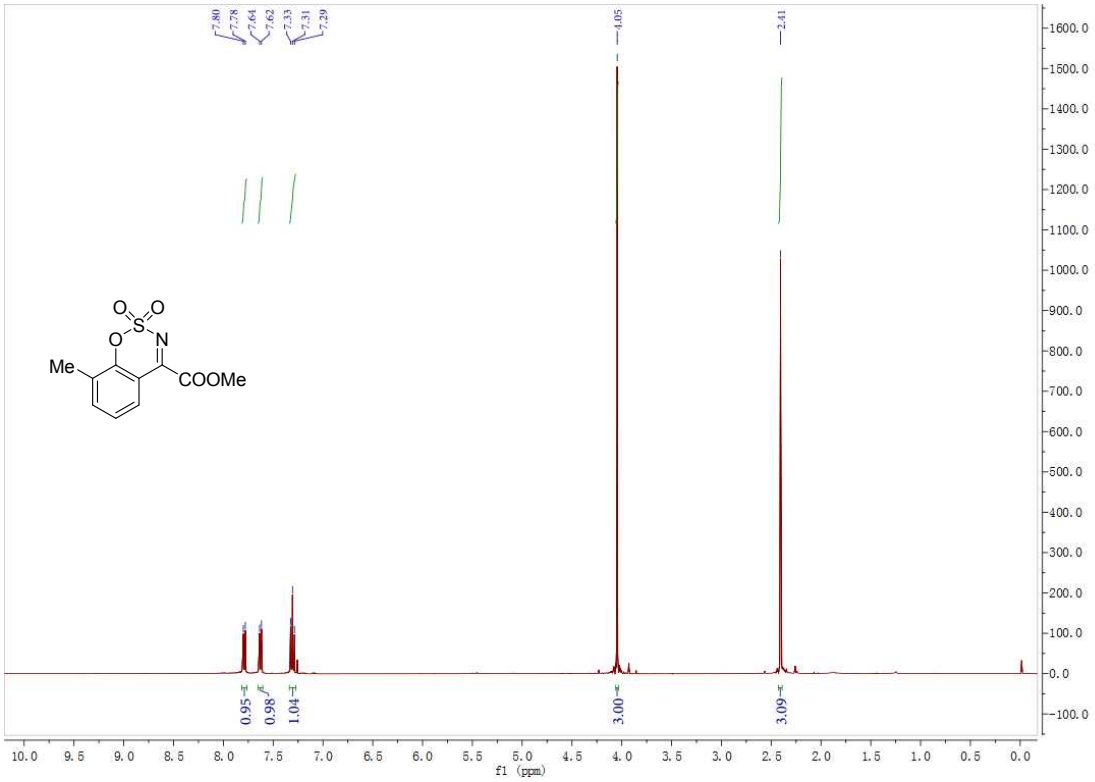
[8] (a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724; (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257; (c) P. C. Hariharan, J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213; (d) P. C. Hariharan, J. A. Pople, Mol. Phys. 1974, **27**, 209; (e) M. S. Gordon, *Chem. Phys. Lett.*, 1980 , 76, 163.

[9] C. Y. Peng, B. Schlegel, *Isr. J. Chem.*, 1994, **34**, 449.

6. NMR Spectrua



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Me
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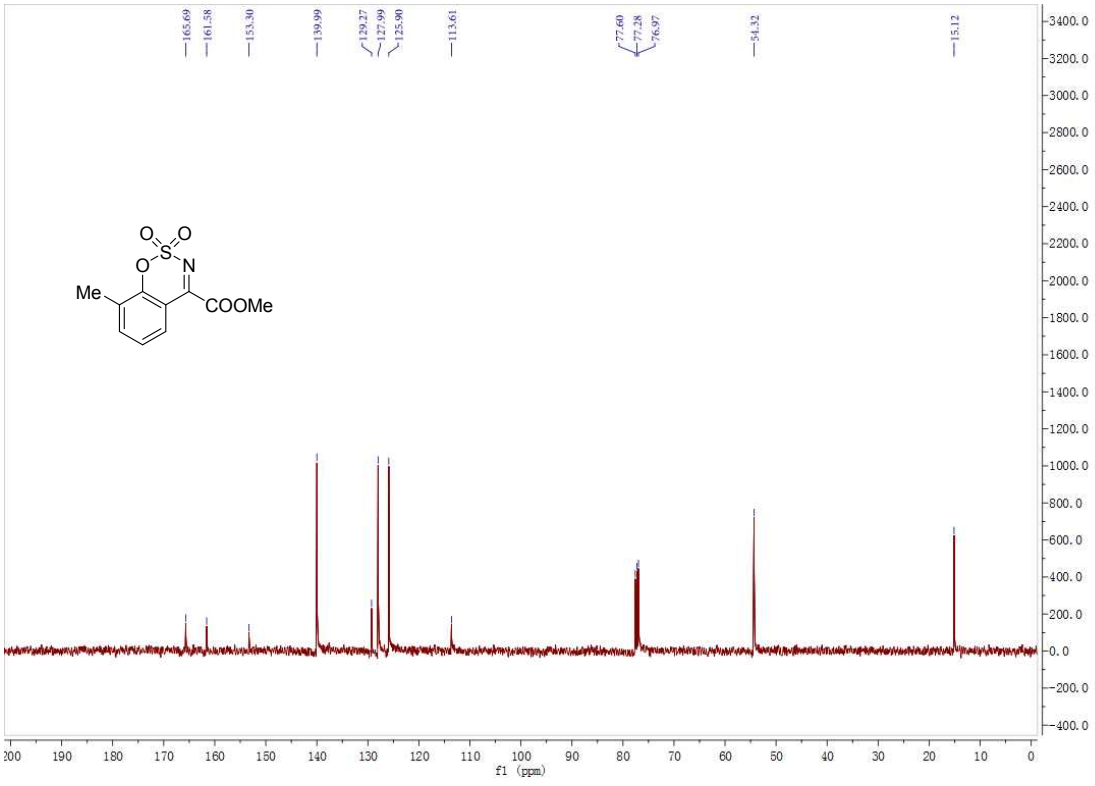
f1 (ppm)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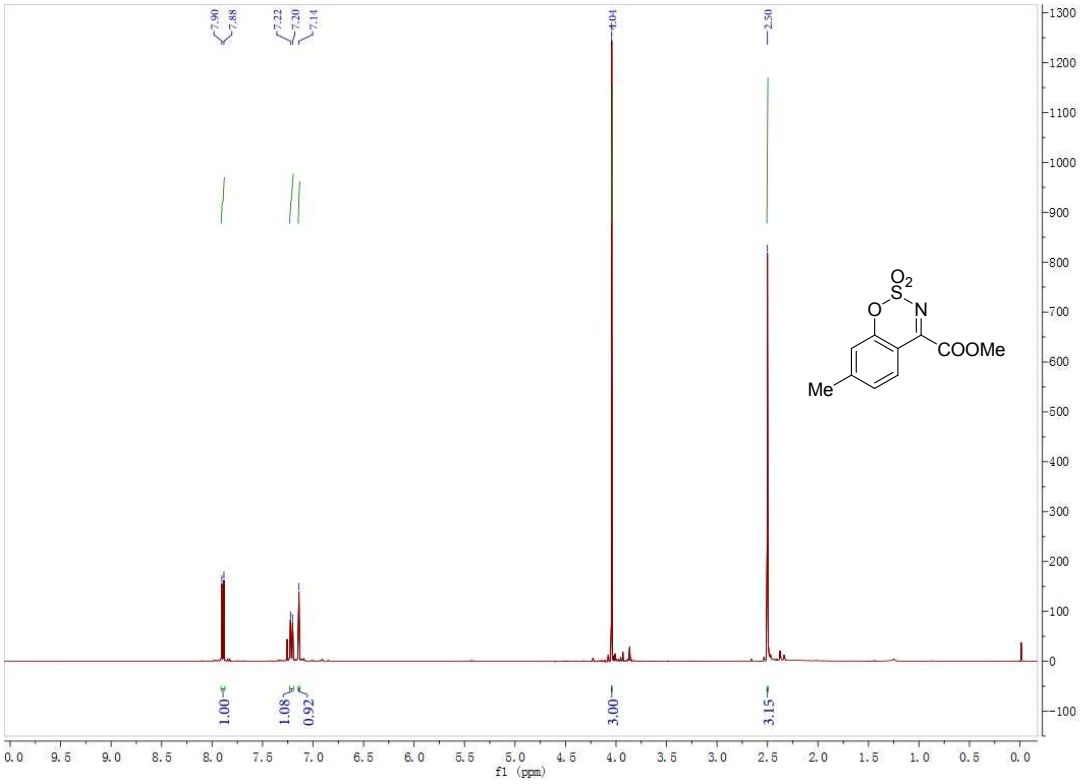
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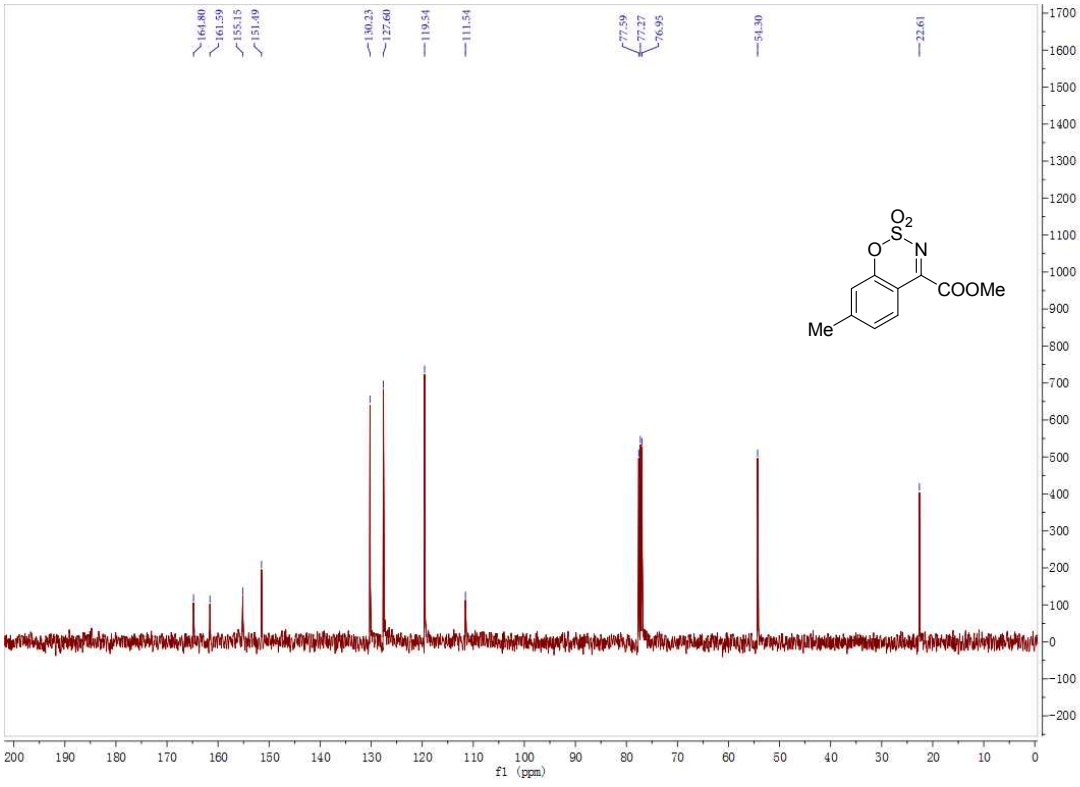
O
N
COOMe
Me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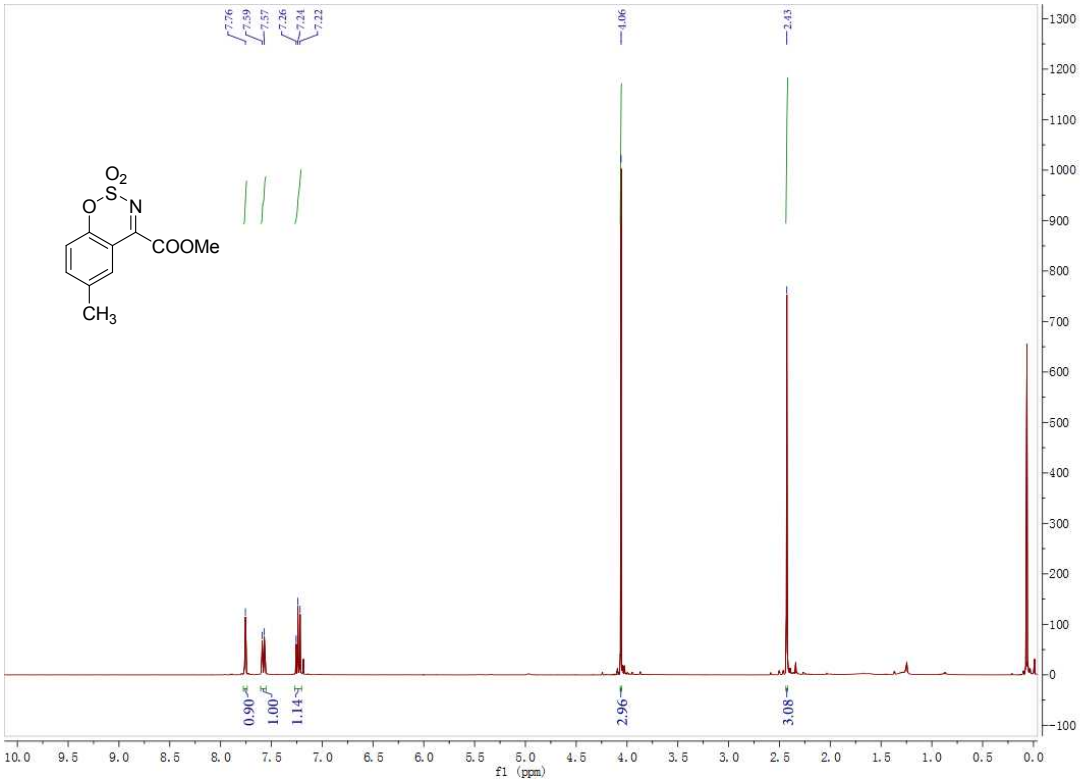
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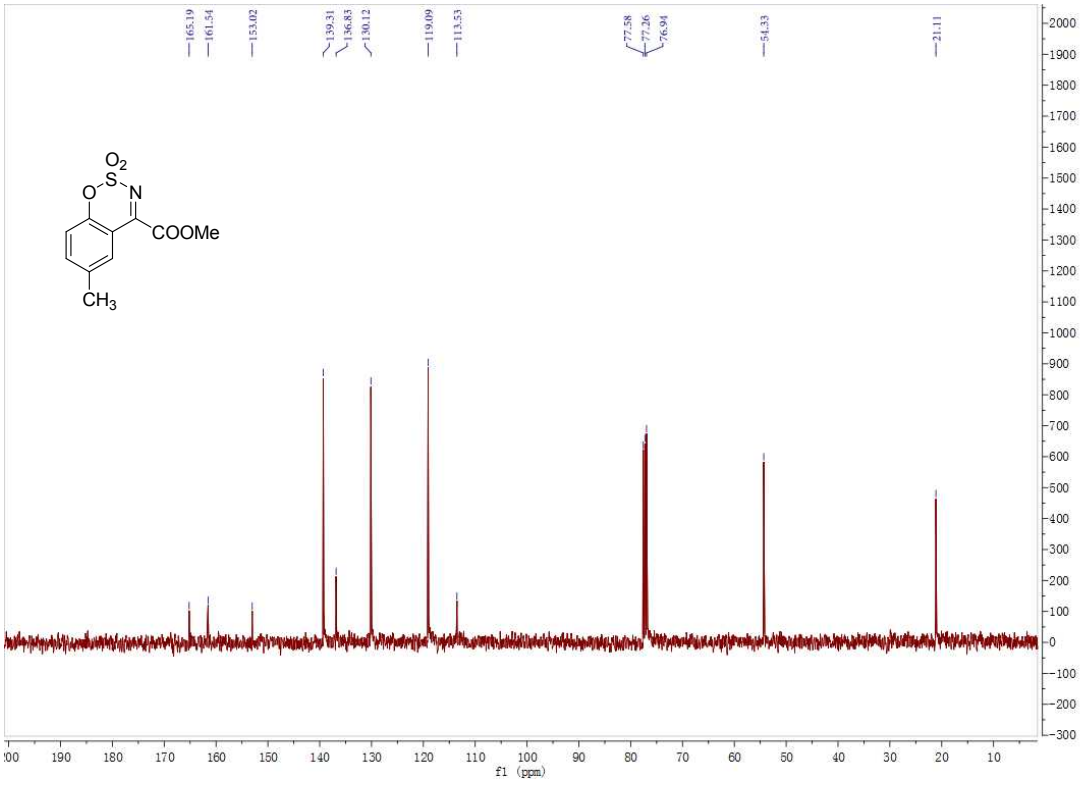
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COOMe
CH3
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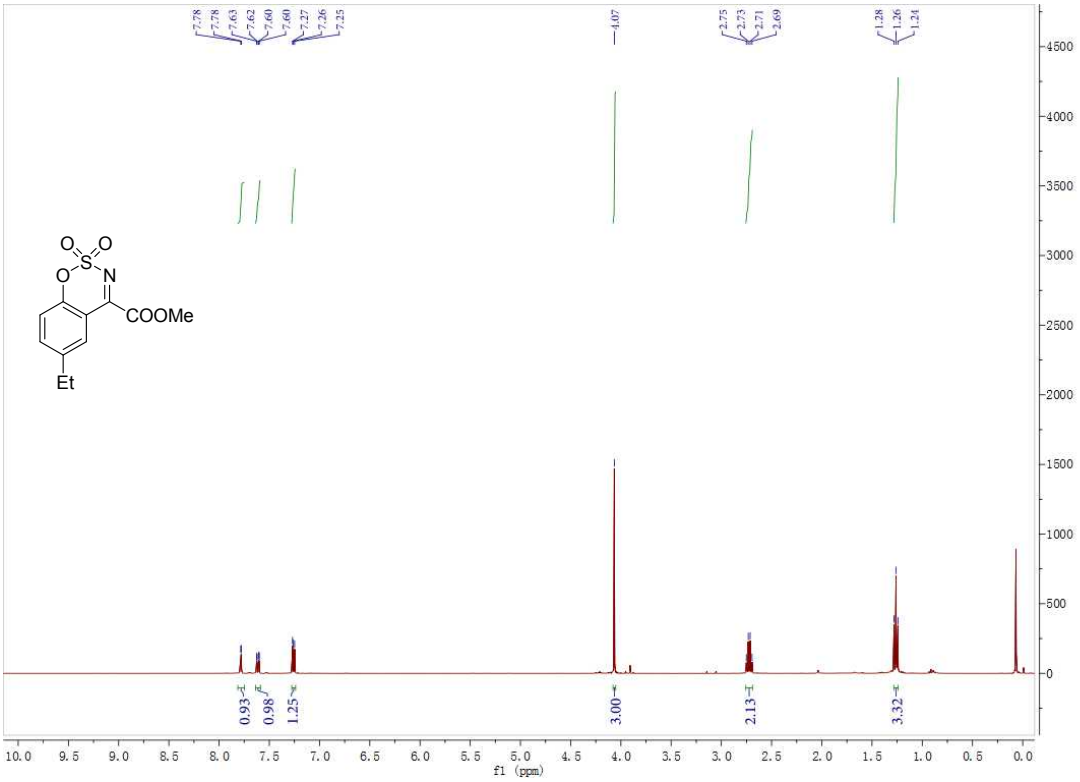
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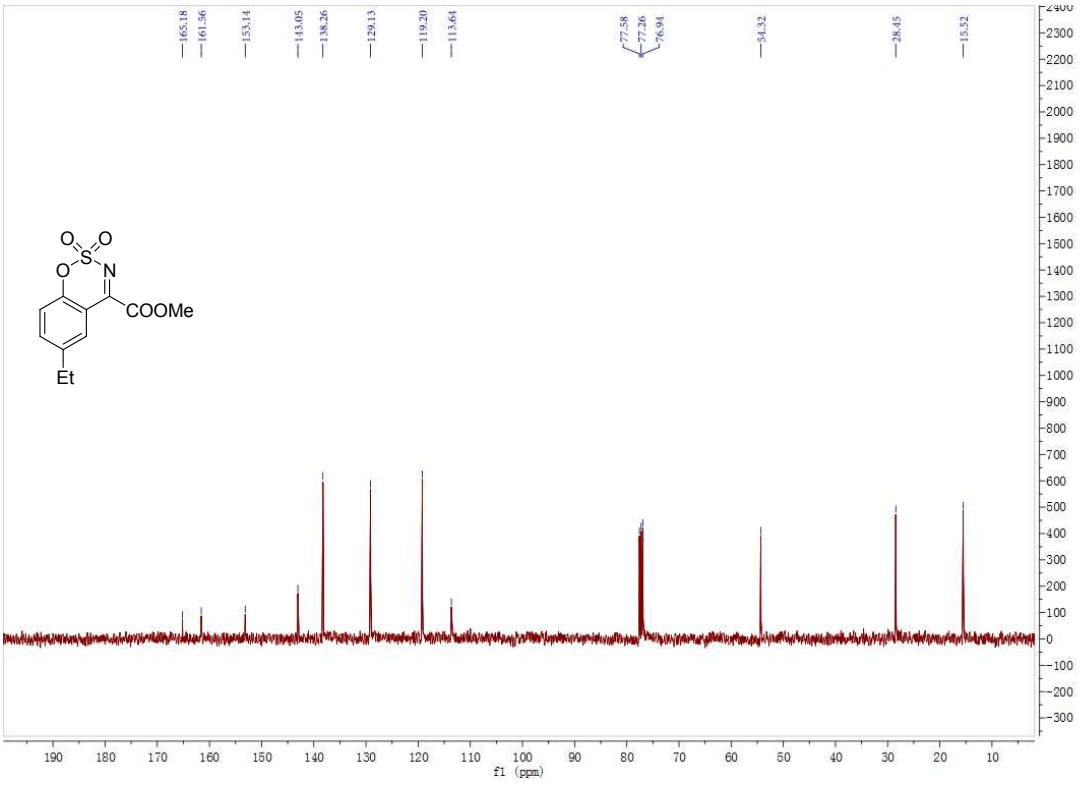
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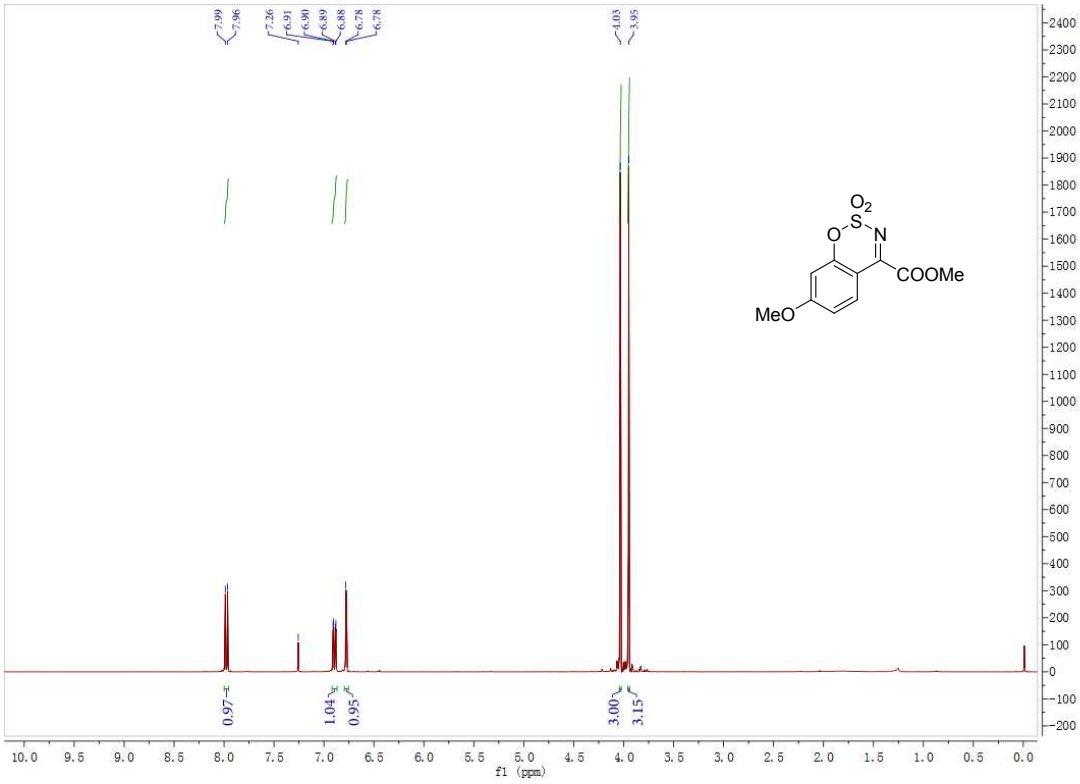
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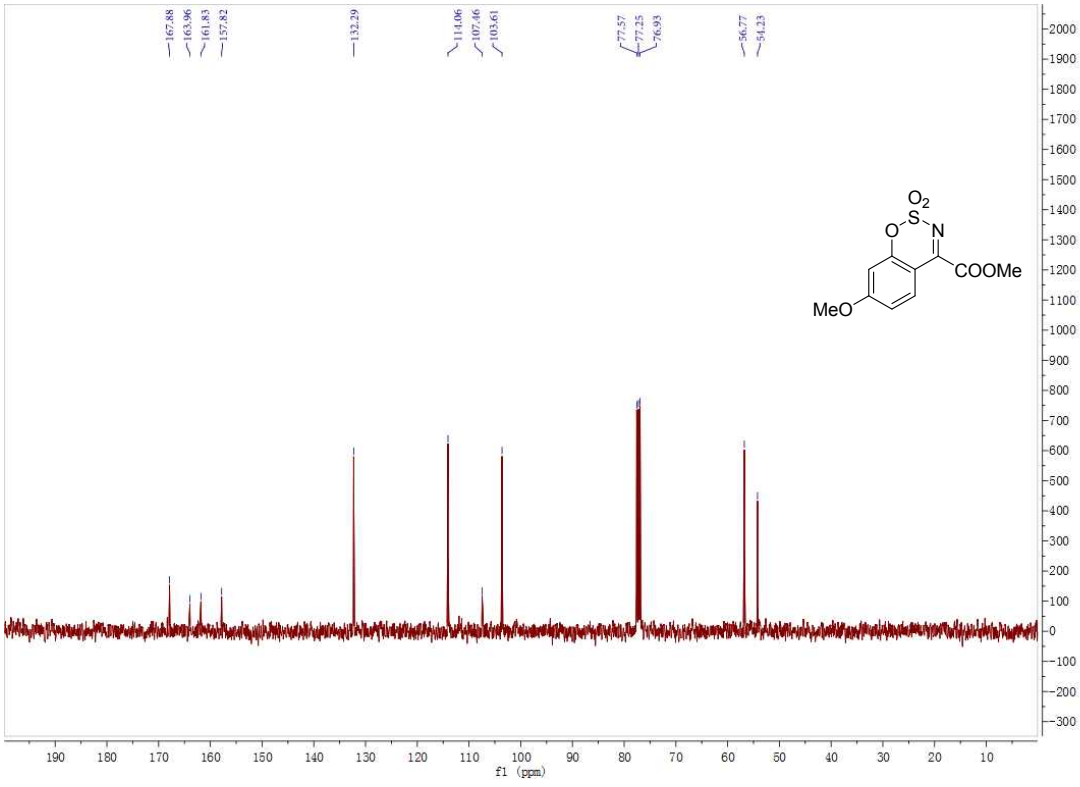
MeO
f1 (ppm)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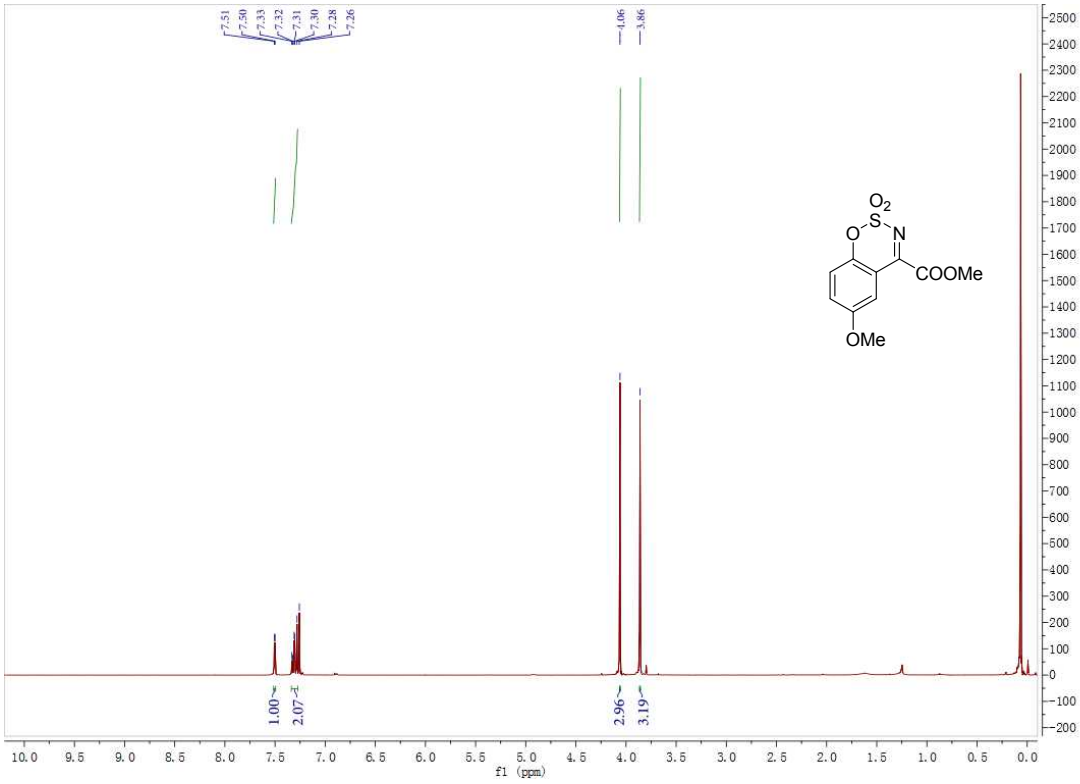
161.83
157.82
132.29
114.06
107.46
103.61
77.57
77.25
76.93
56.77
54.23
O2
S
O
N
COOMe
MeO
f1 (ppm)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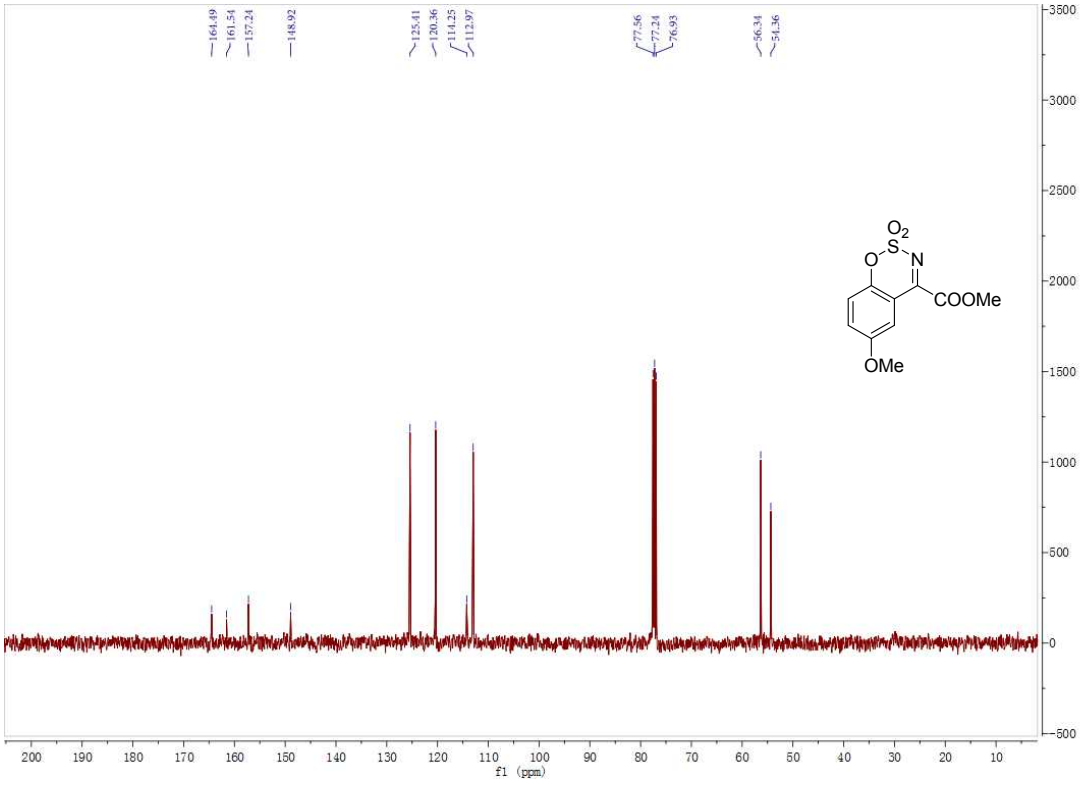
7.33
7.32
7.31
7.30
7.28
7.26
4.06
3.86
1.00
2.07
2.96
3.19
f1 (ppm)
O2
S
O
N
COOMe
OMe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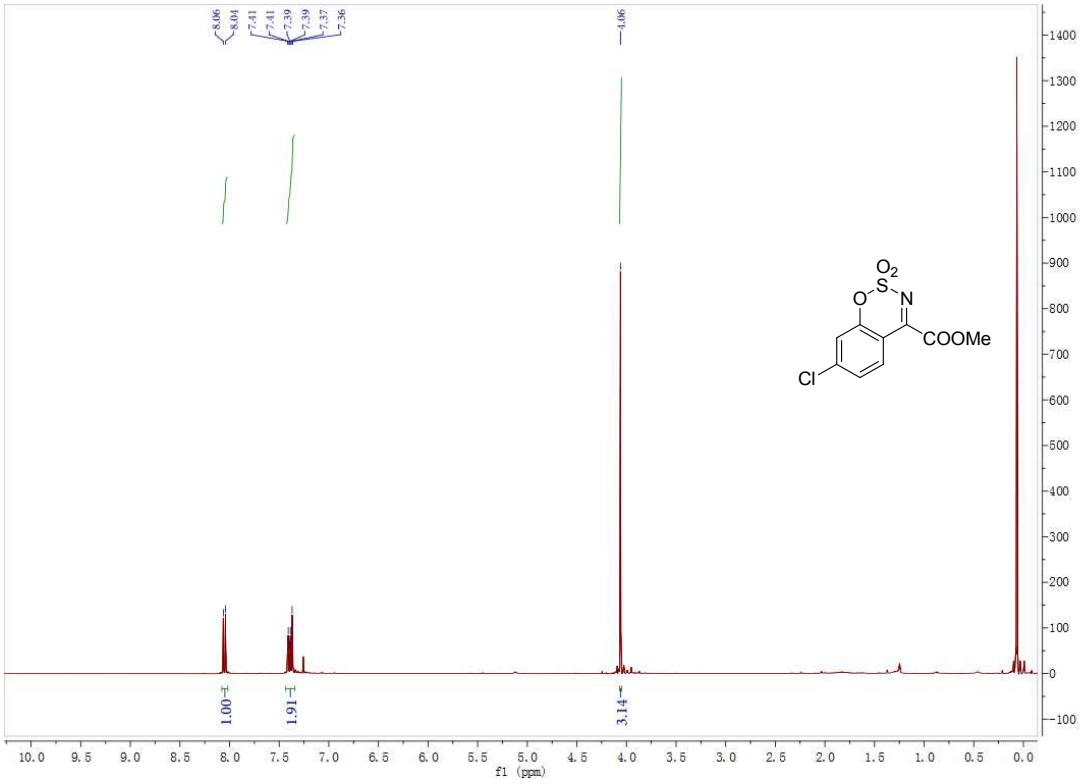
157.24
148.92
125.41
120.36
114.25
112.97
77.56
77.24
76.93
56.34
54.36
f1 (ppm)
O2
S
O
N
COOMe
OMe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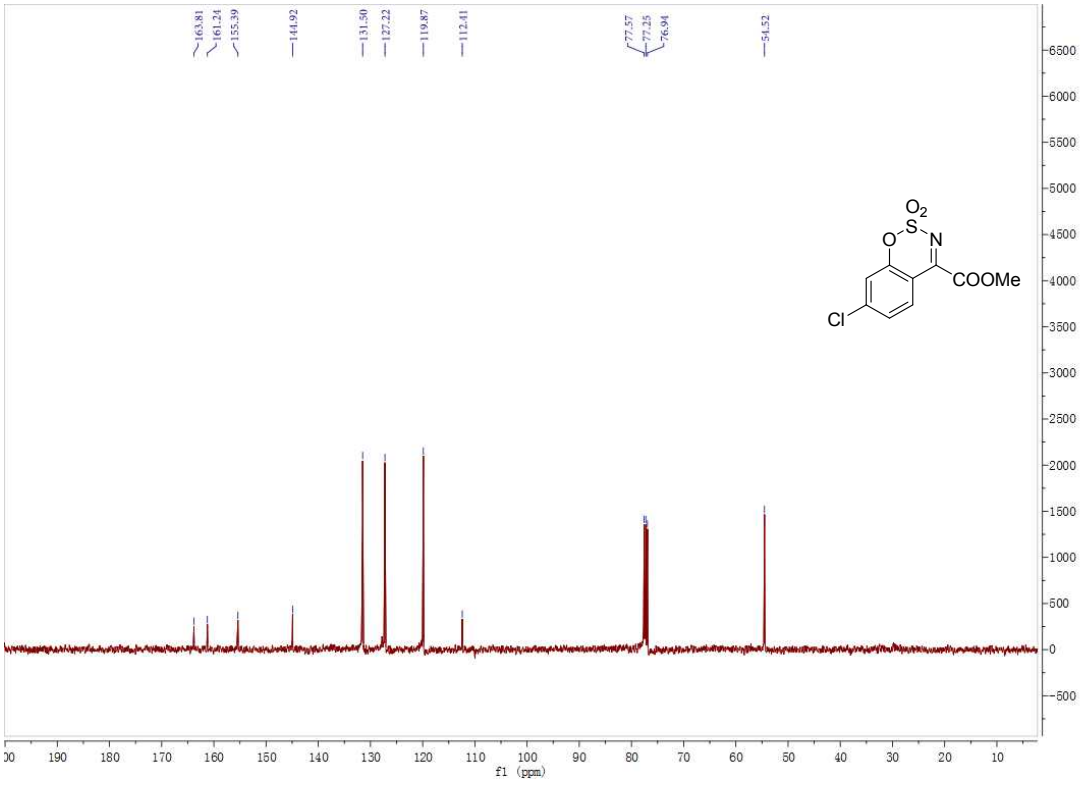
7.41
7.41
7.39
7.39
7.37
7.36
4.06
1.00
1.91
3.14
O2
S
O
N
COOMe
Cl
f1 (ppm)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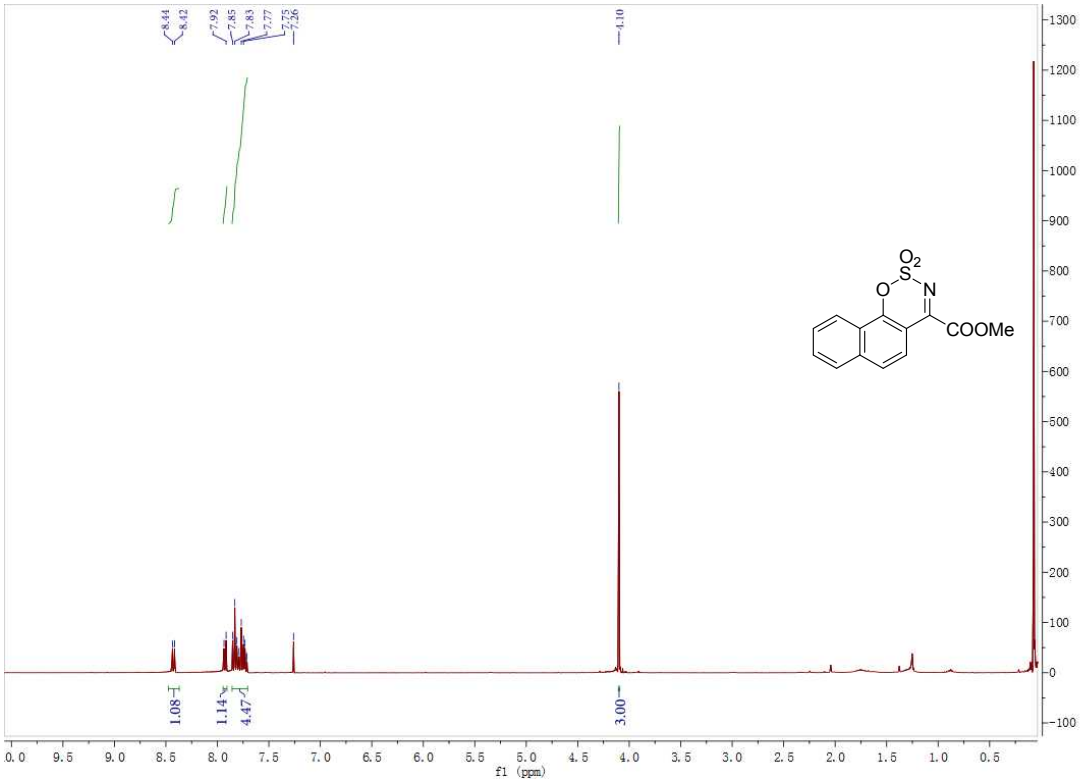
161.24
155.39
144.92
131.50
127.22
119.87
112.41
77.57
77.25
76.94
54.52
O2
S
O
N
COOMe
Cl
f1 (ppm)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7.83
7.77
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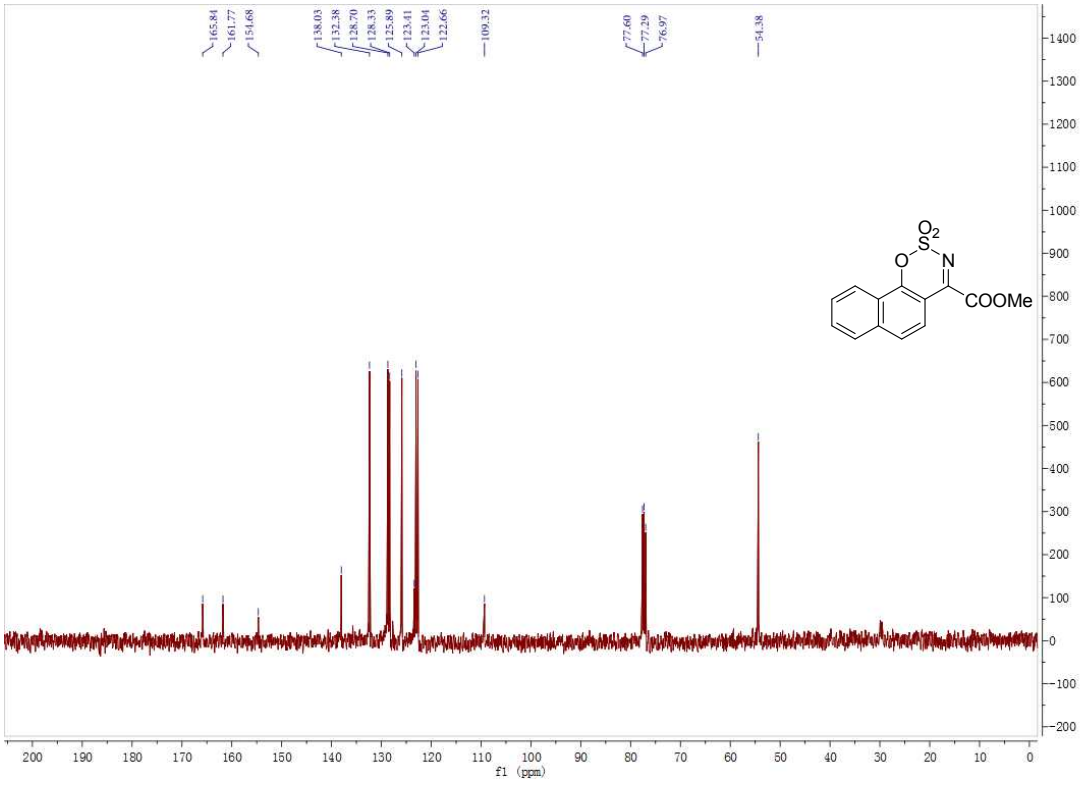
7.26
4.10
O2
S
O
N
COOMe
1.08
1.14
4.47
3.00
f1 (ppm)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161.77
154.68
138.03
132.38
128.70
128.33
125.89
123.41
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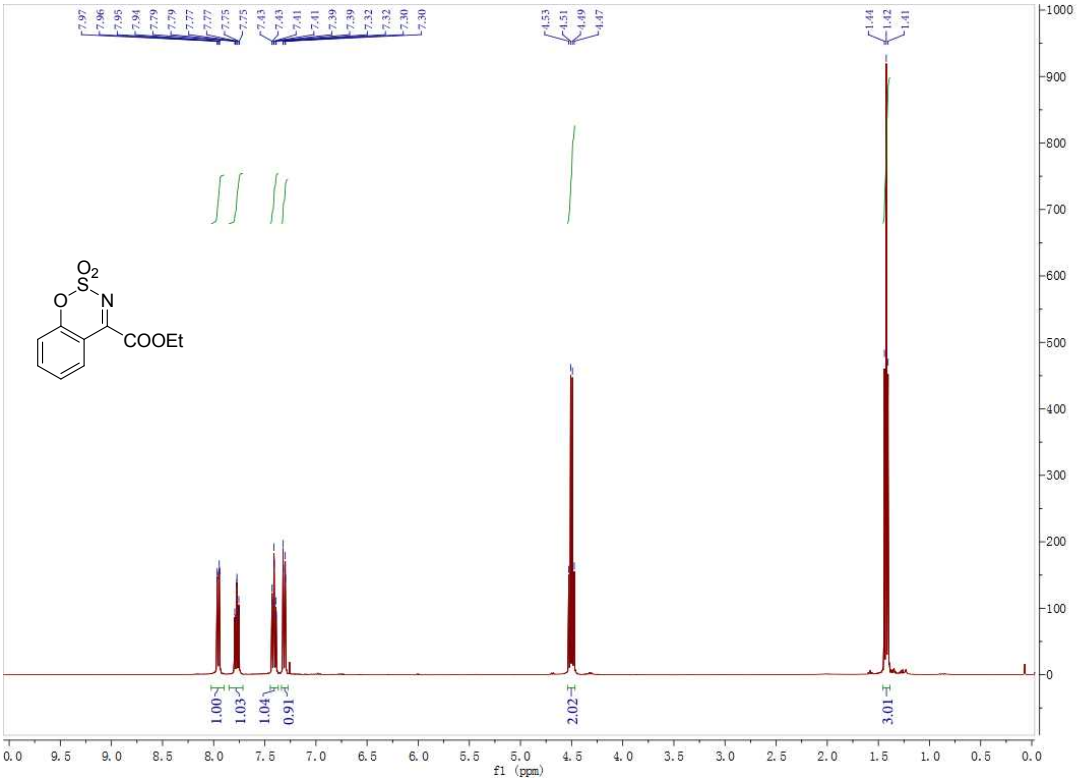
109.32
77.60
77.29
76.97
54.38
O2
S
O
N
COOMe
f1 (ppm)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7.79
7.77
7.77
7.75
7.75
7.43
7.43
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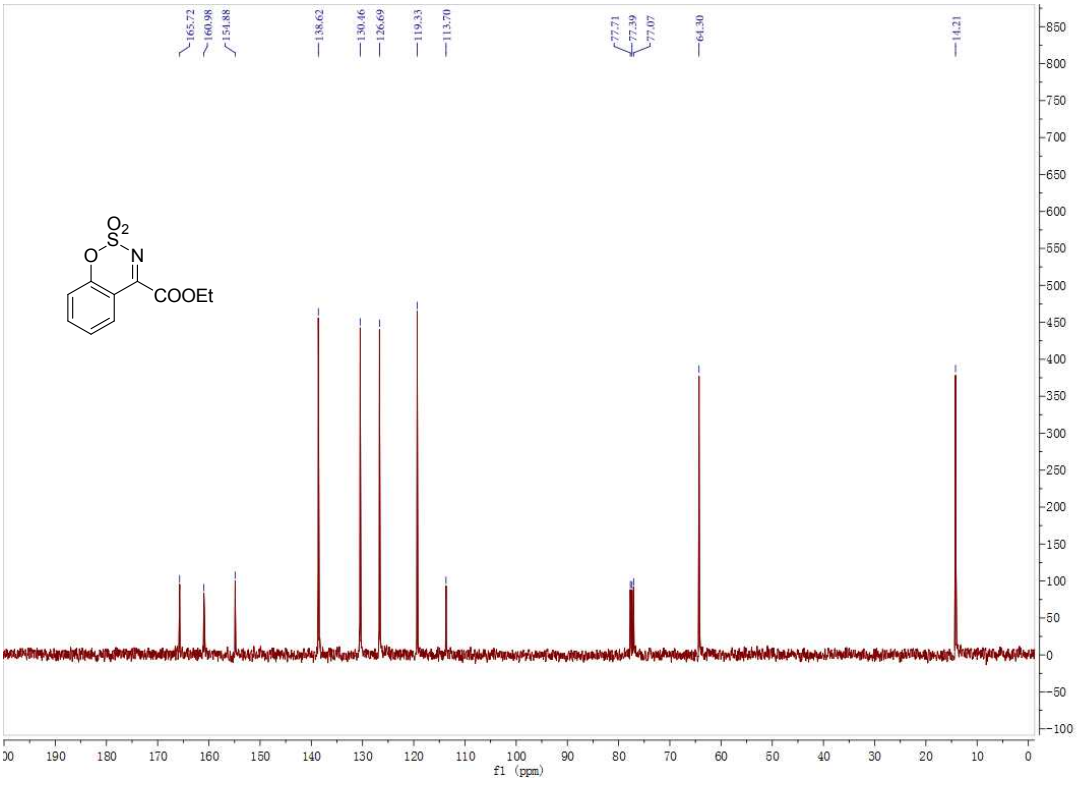
7.41
7.39
7.39
7.32
7.32
7.30
7.30
4.53
4.51
4.49
4.47
1.44
1.42
1.41
O2
S
O
N
COOEt
1.00
1.03
1.04
0.91
2.02
3.01
f1 (ppm)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126.69
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113.70
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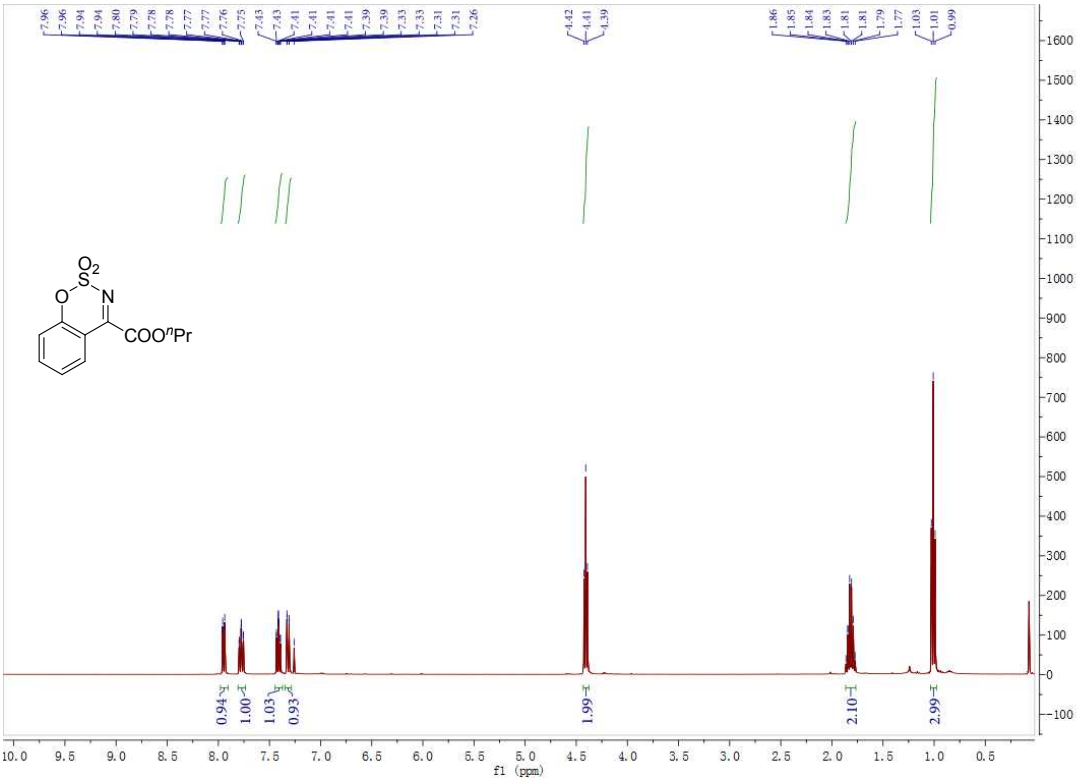
77.59
77.07
64.30
14.21
O2
S
O
N
COOEt
f1 (ppm)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7.96
7.94
7.94
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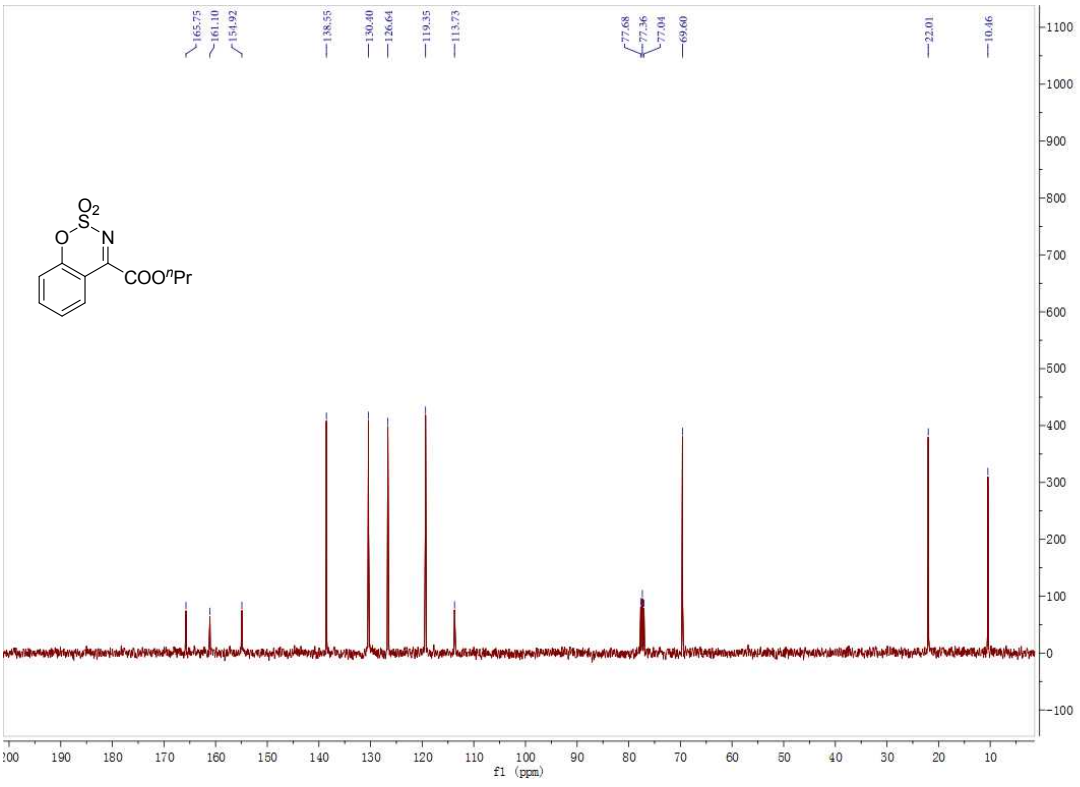
7.79
7.78
7.78
7.77
7.77
7.76
7.75
7.43
7.43
7.41
7.41
7.41
7.41
7.39
7.39
7.33
7.33
7.31
7.31
7.26
4.42
4.41
4.39
1.86
1.85
1.84
1.83
1.81
1.81
1.79
1.77
1.03
1.01
0.99
O2
S
O
N
COOnPr
0.94
1.00
1.03
0.93
1.99
2.10
2.99
f1 (ppm)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126.64
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77.04
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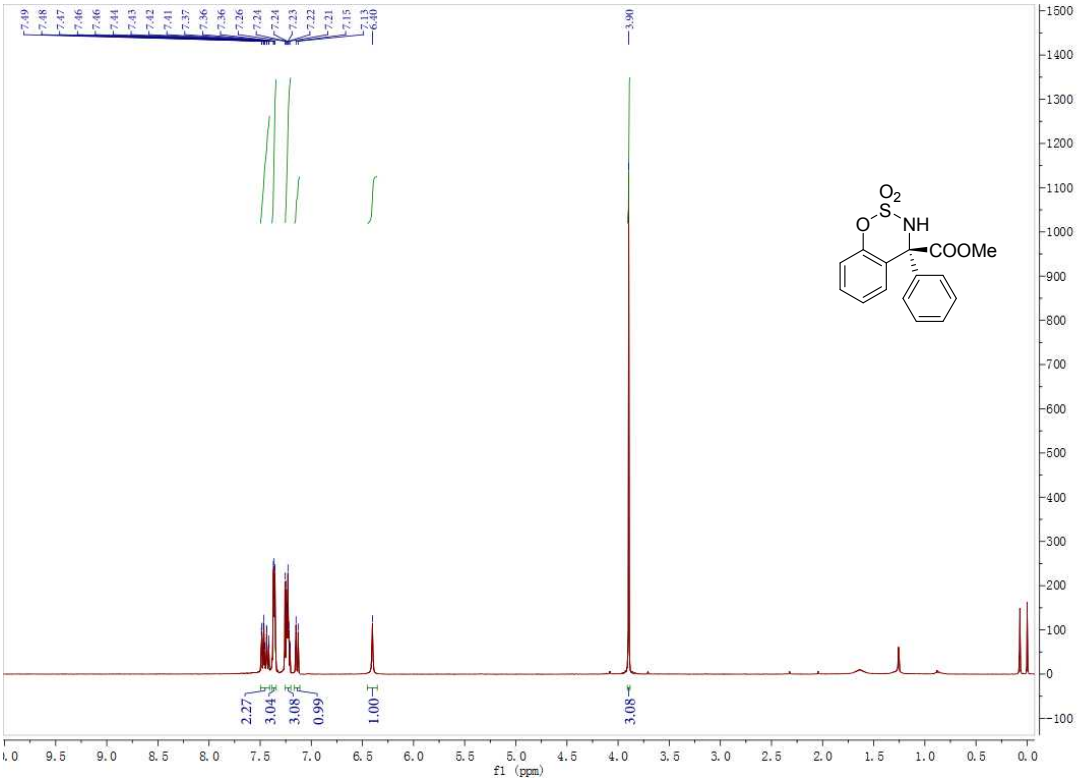
22.01
10.46
O2
S
O
N
COOnPr
f1 (ppm)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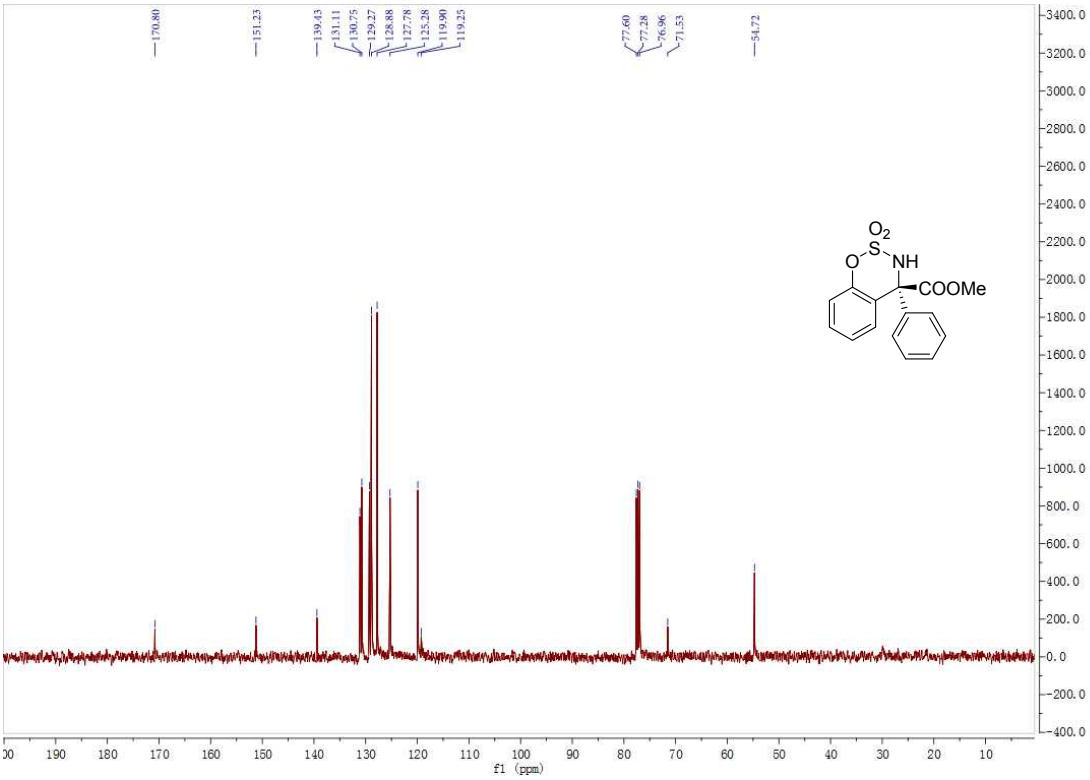
7.41
7.37
7.36
7.36
7.26
7.24
7.24
7.23
7.22
7.21
7.15
7.13
6.40
3.90
O2
S
O
NH
COOMe
2.27
3.04
3.08
0.99
1.00
3.08
f1 (ppm)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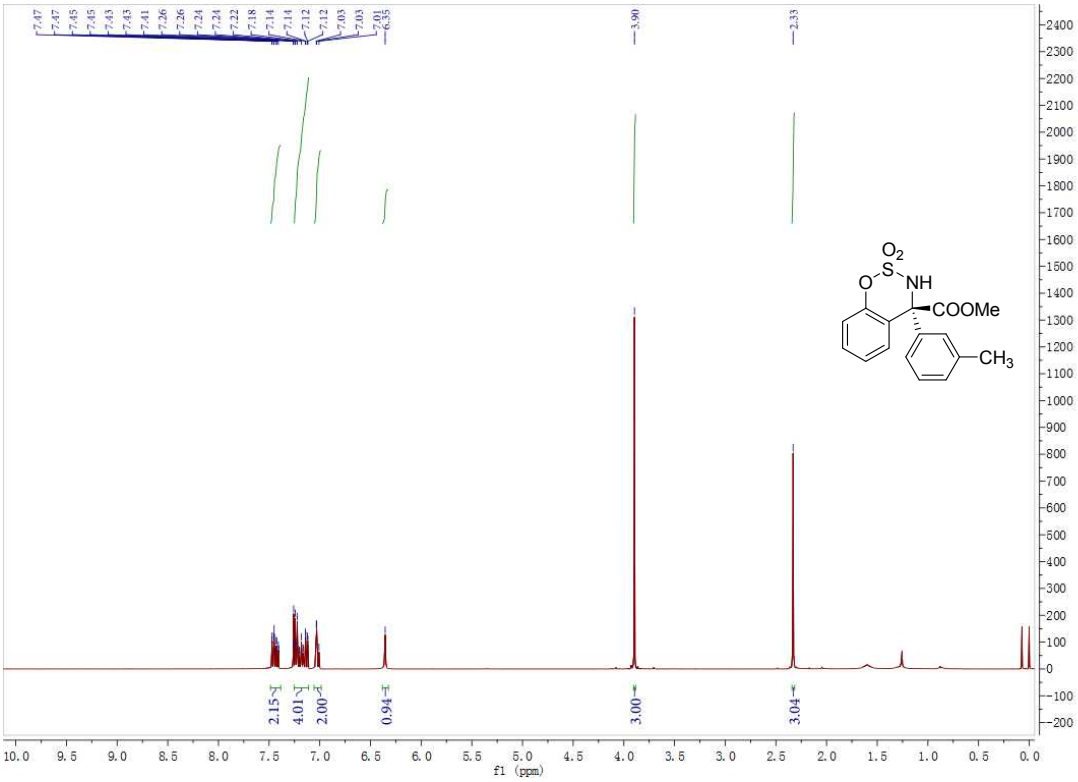
77.28
76.96
71.53
54.72
O2
S
O
NH
COOMe
f1 (ppm)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7.45
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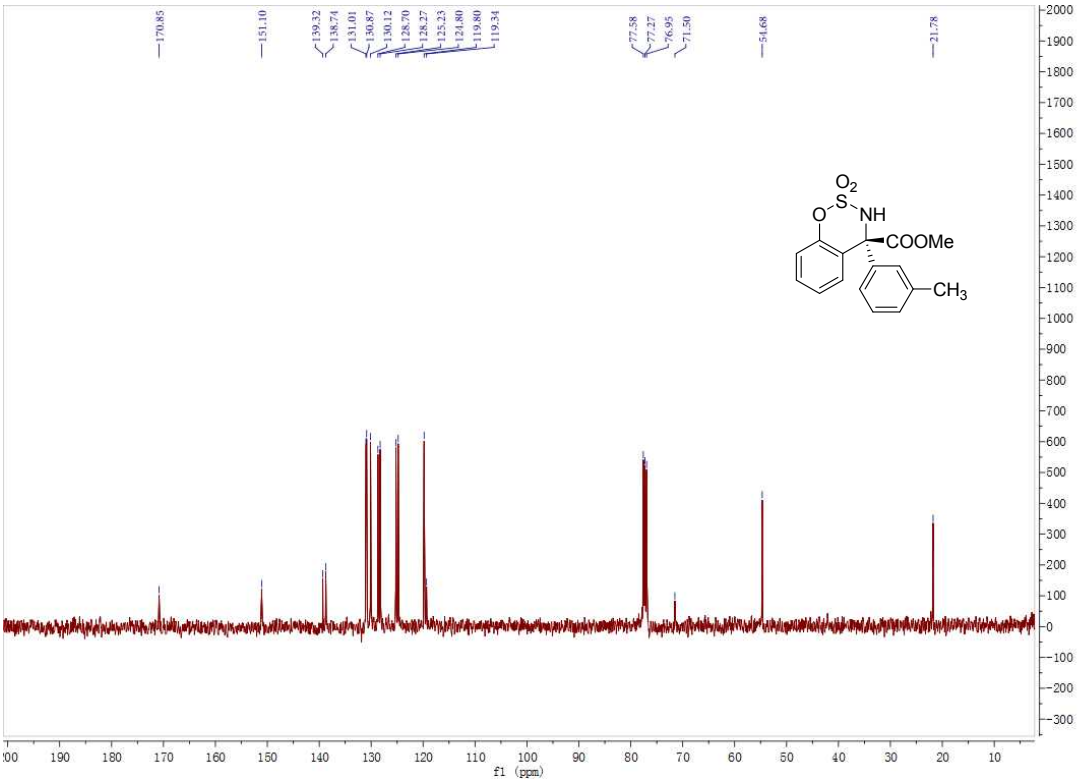
7.41
7.26
7.24
7.24
7.22
7.18
7.14
7.14
7.12
7.12
7.03
7.01
6.35
3.90
2.33
O2
S
O
NH
COOMe
CH3
2.15
4.01
2.00
0.94
3.00
3.04
f1 (ppm)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124.80
119.80
119.34
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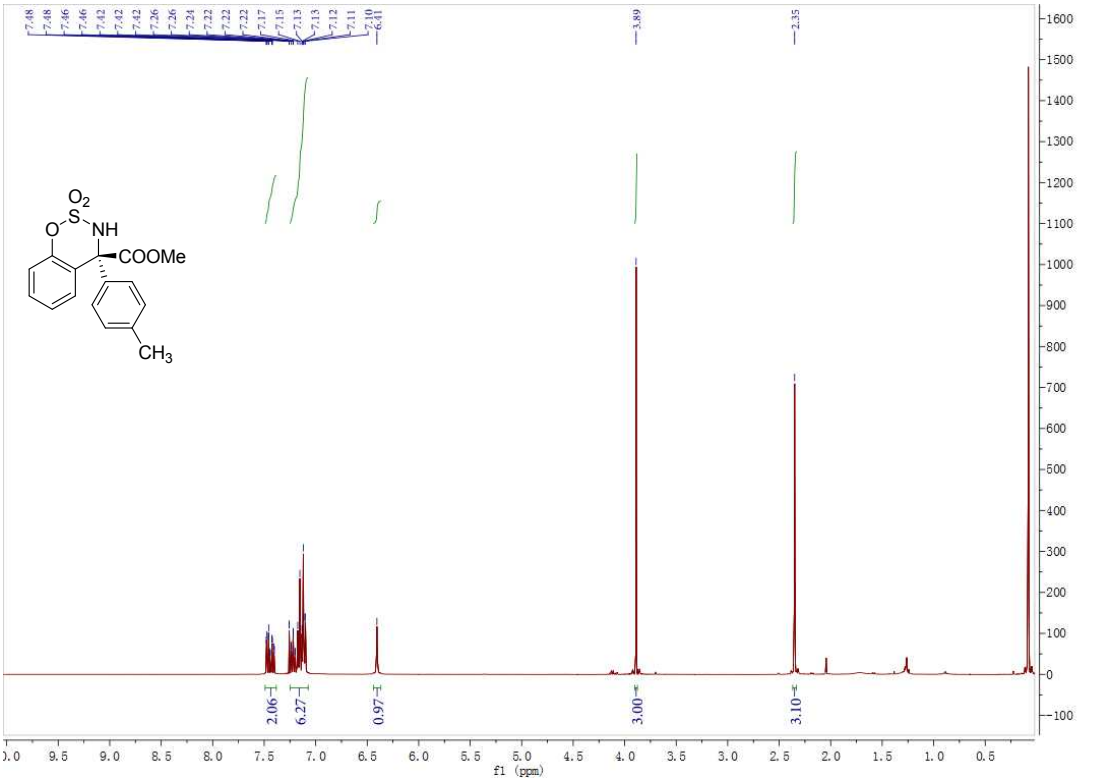
76.95
71.50
54.68
21.78
O2
S
O
NH
COOMe
CH3
f1 (ppm)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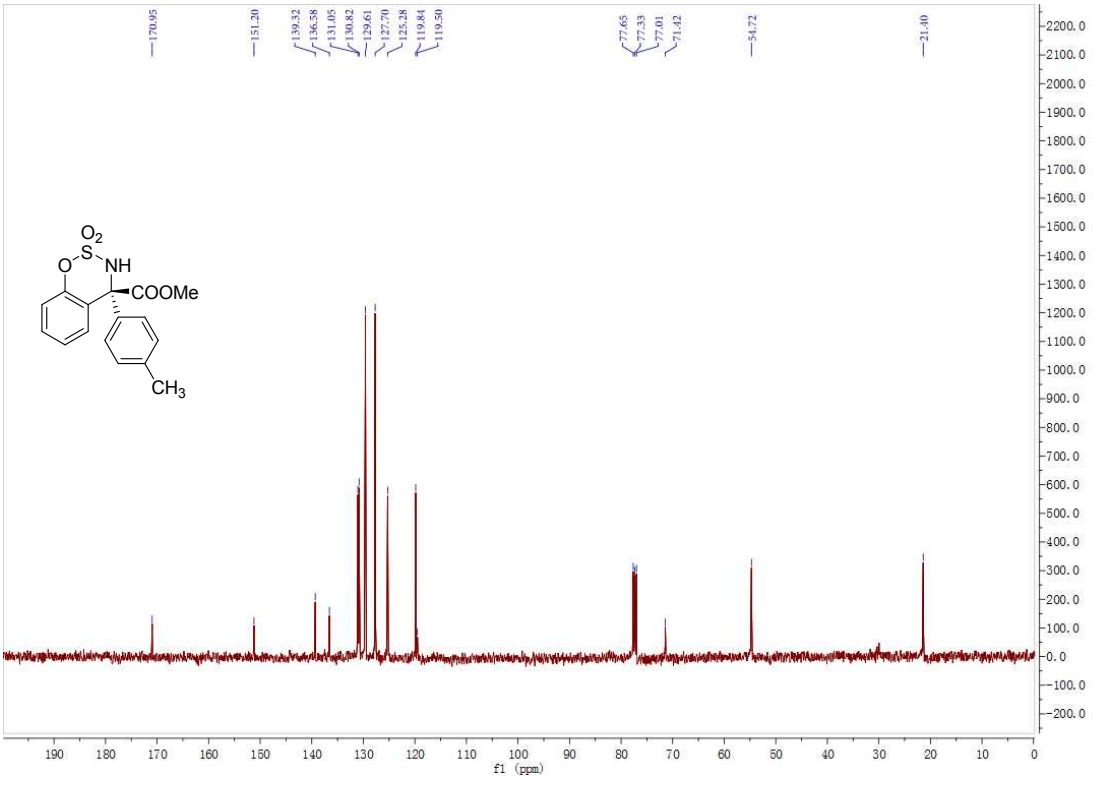
7.17
7.15
7.13
7.13
7.12
7.11
6.41
3.89
2.35
O2
S
O
NH
COOMe
CH3
2.06
6.27
0.97
3.00
3.10
f1 (ppm)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119.84
119.50
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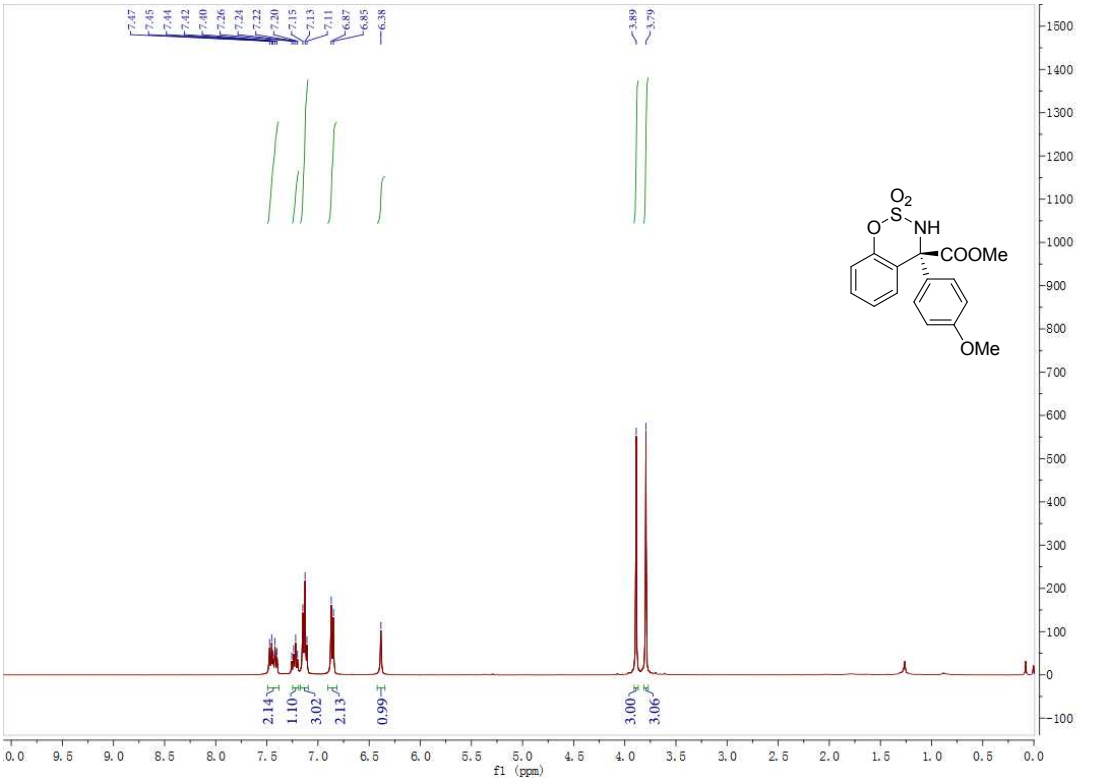
77.01
71.42
54.72
21.40
O2
S
O
NH
COOMe
CH3
f1 (ppm)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7.15
7.13
7.11
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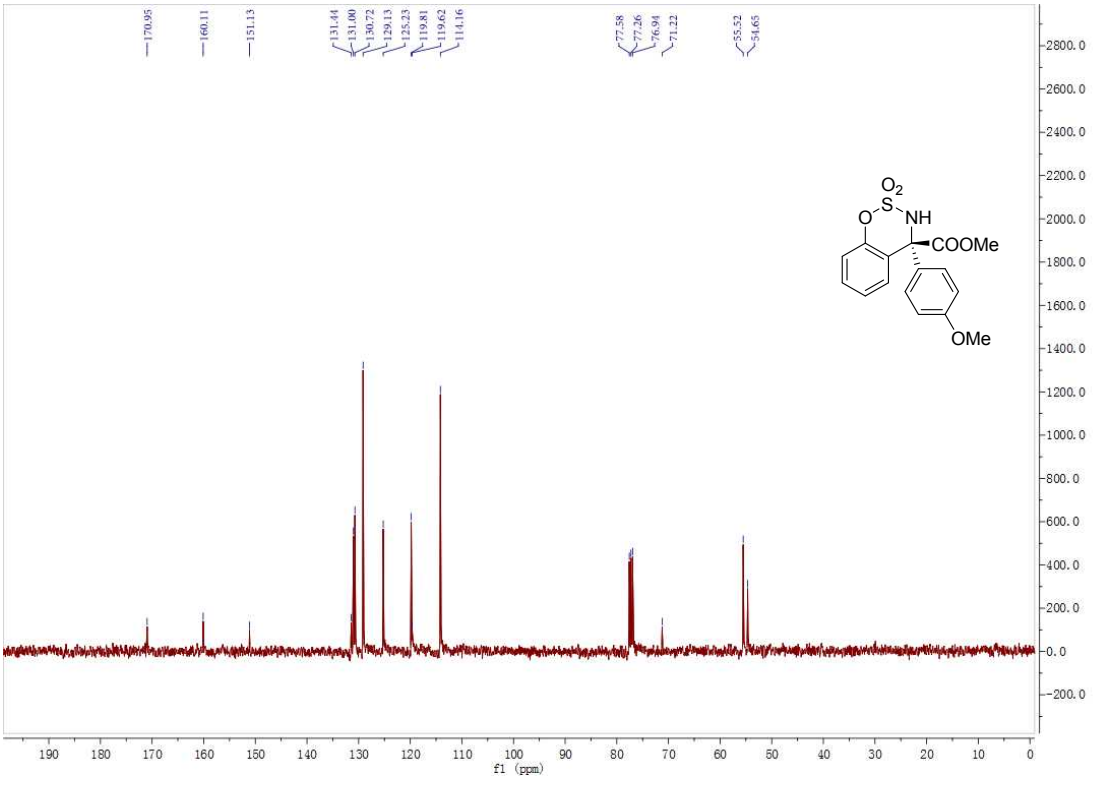
6.85
6.38
3.89
3.79
O2
S
O
NH
COOMe
OMe
2.14
1.10
3.02
2.13
0.99
3.00
3.06
f1 (ppm)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114.16
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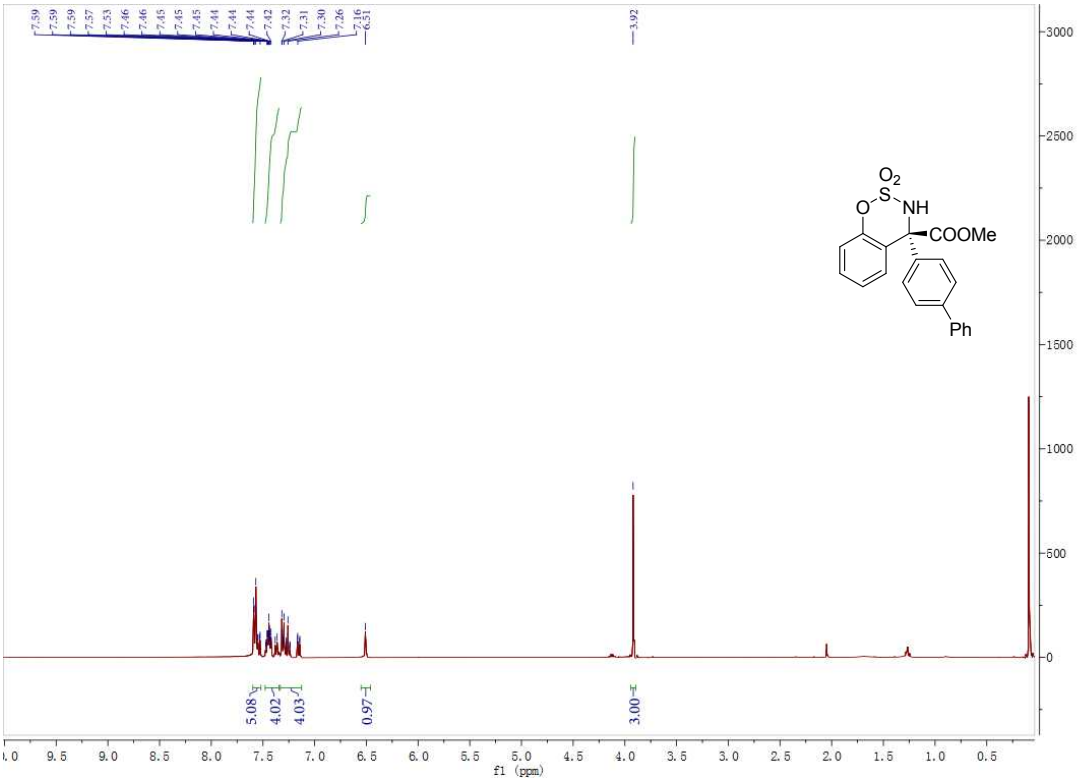
76.94
71.22
55.52
54.65
O2
S
O
NH
COOMe
OMe
f1 (ppm)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7.45
7.45
7.44
7.44
7.44
7.42
7.32
7.31
7.30
7.26
7.16
6.51
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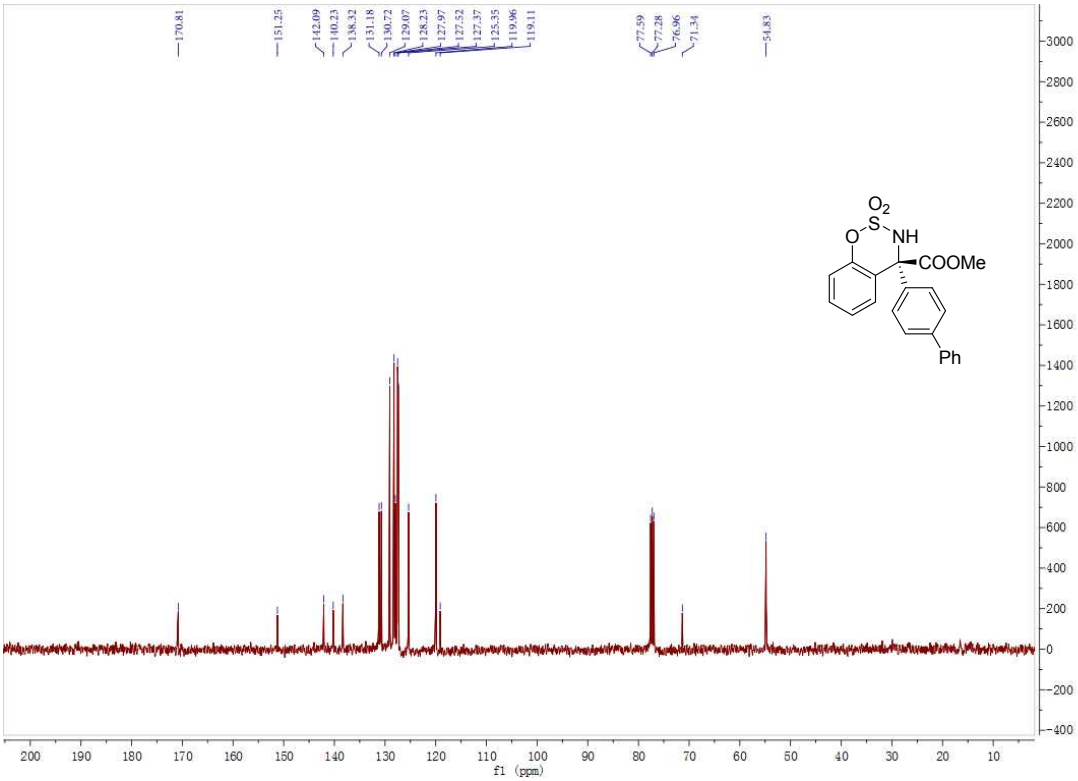
5.08
4.02
4.03
0.97
3.00
f1 (ppm)
O2
S
O
NH
COOMe
Ph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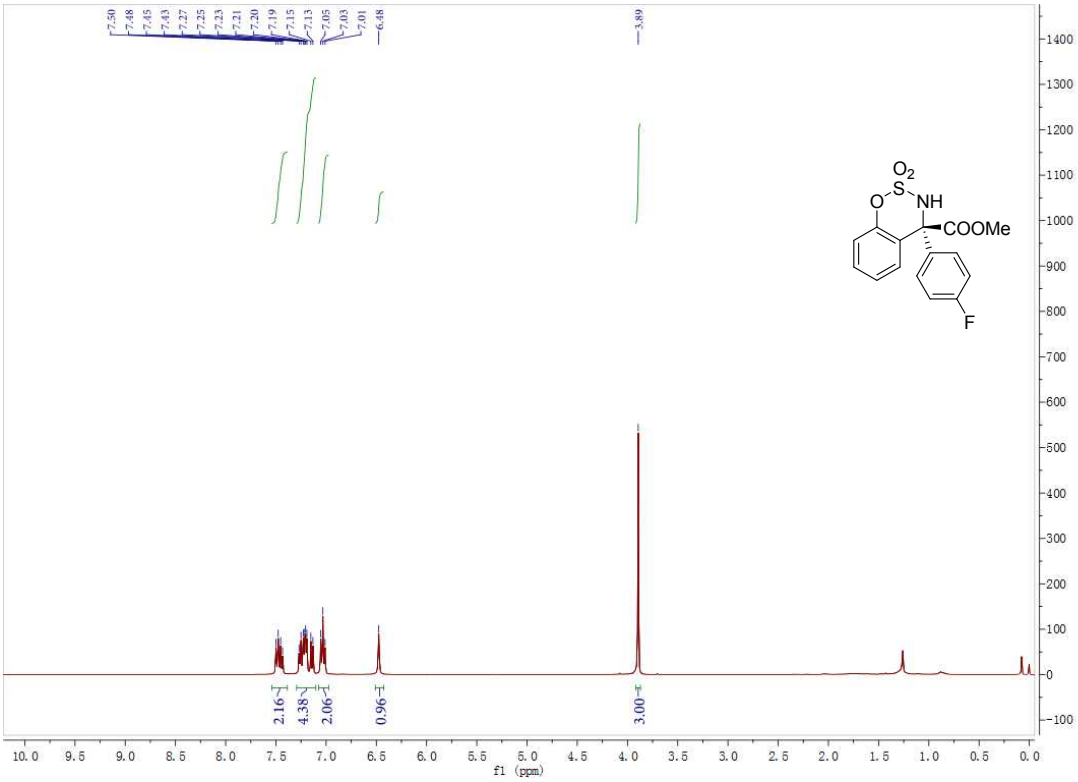
129.07
128.23
127.97
127.52
127.37
125.35
119.96
119.11
77.59
77.28
76.96
71.34
54.83
f1 (ppm)
O2
S
O
NH
COOMe
Ph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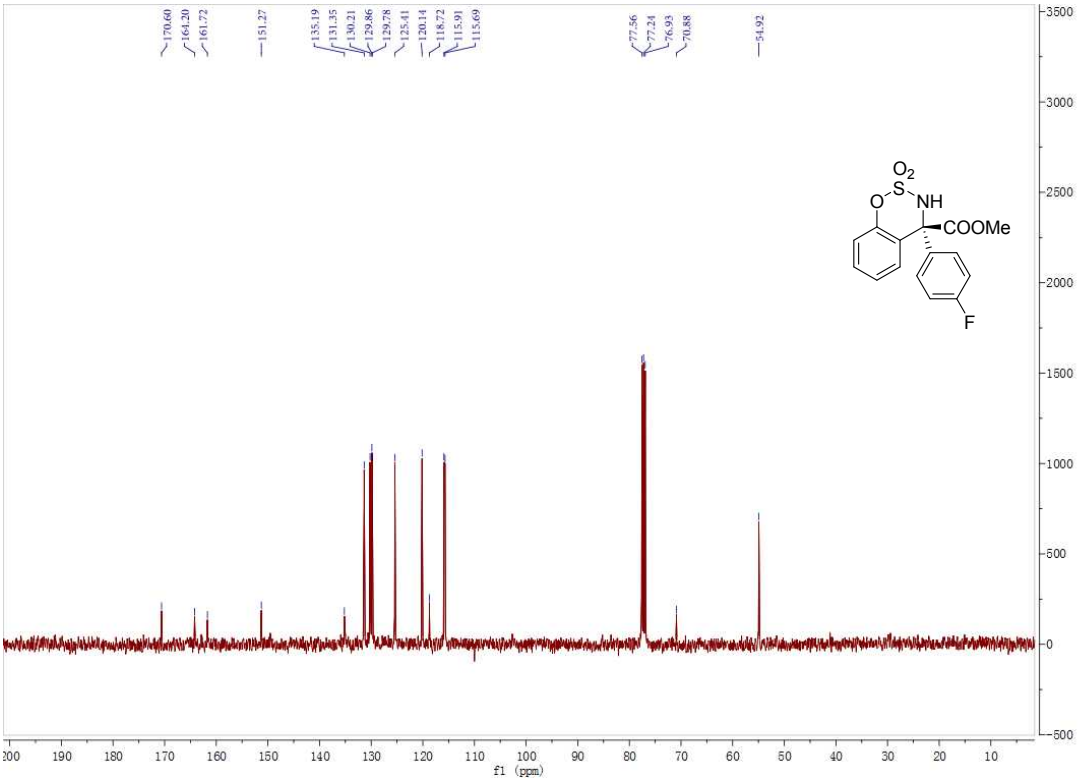
7.19
7.15
7.13
7.05
7.03
7.01
6.48
3.89
O2
S
O
NH
COOMe
F
2.16
4.38
2.06
0.96
3.00
f1 (ppm)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120.14
118.72
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115.69
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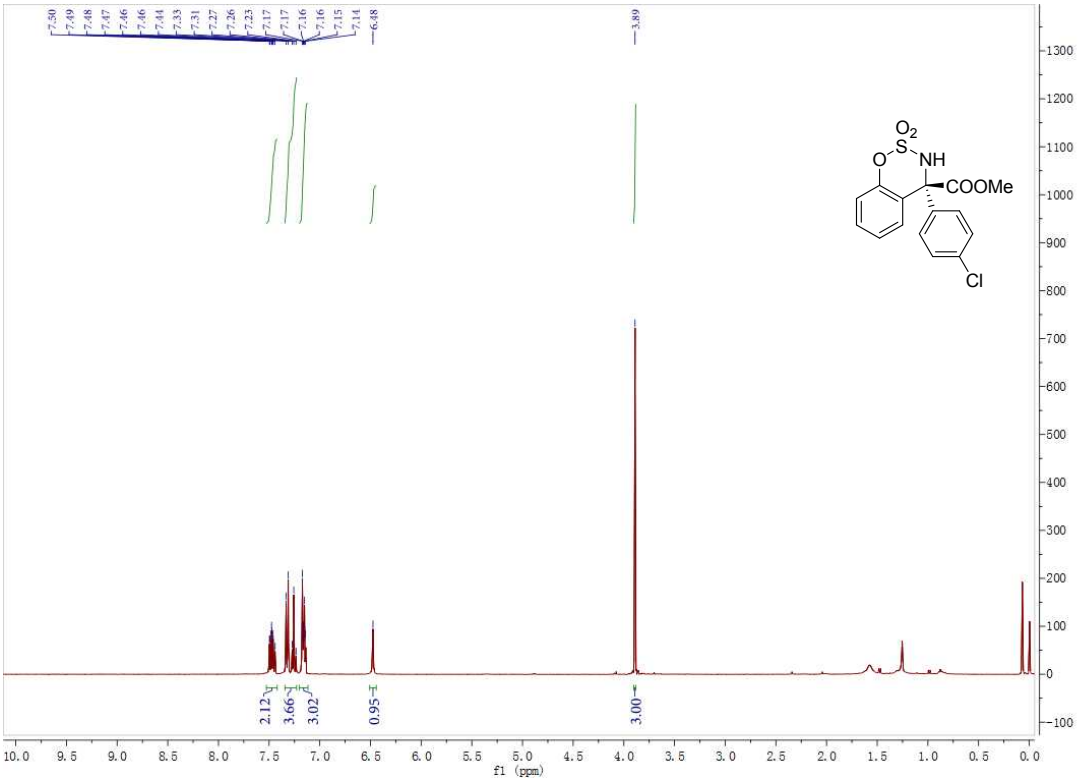
77.24
76.93
70.88
54.92
O2
S
O
NH
COOMe
F
f1 (ppm)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7.46
7.44
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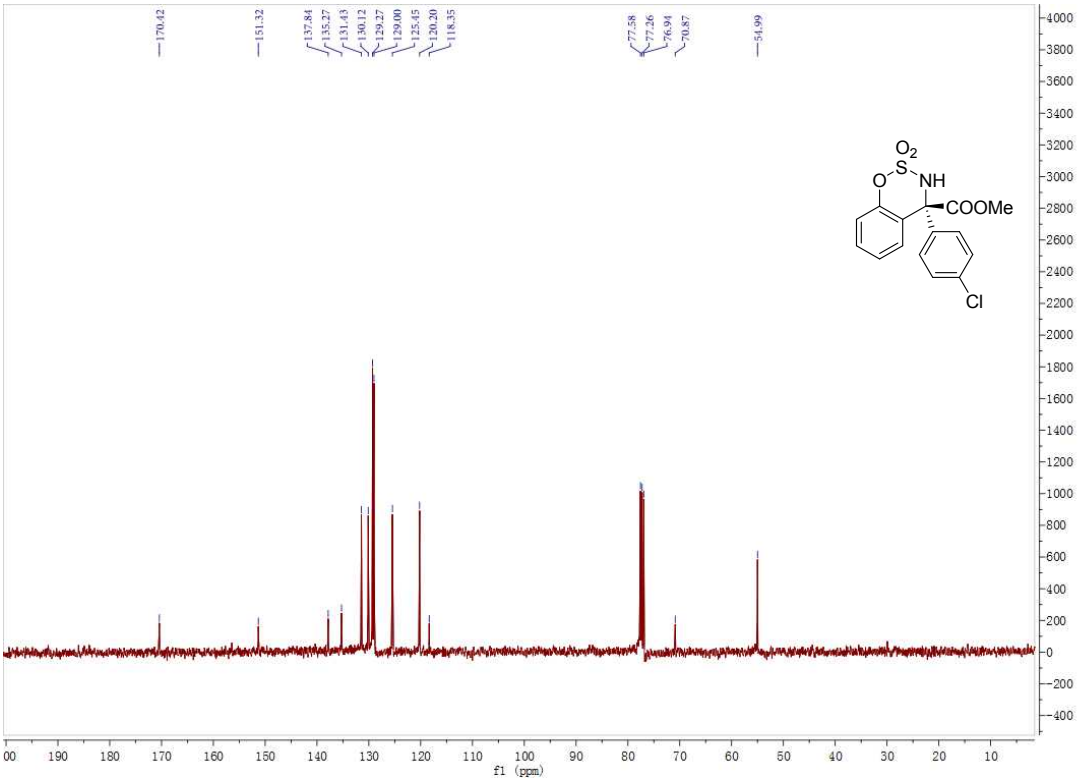
7.31
7.27
7.26
7.23
7.17
7.17
7.16
7.16
7.15
7.14
6.48
3.89
O2
S
O
NH
COOMe
Cl
2.12
3.66
3.02
0.95
3.00
f1 (ppm)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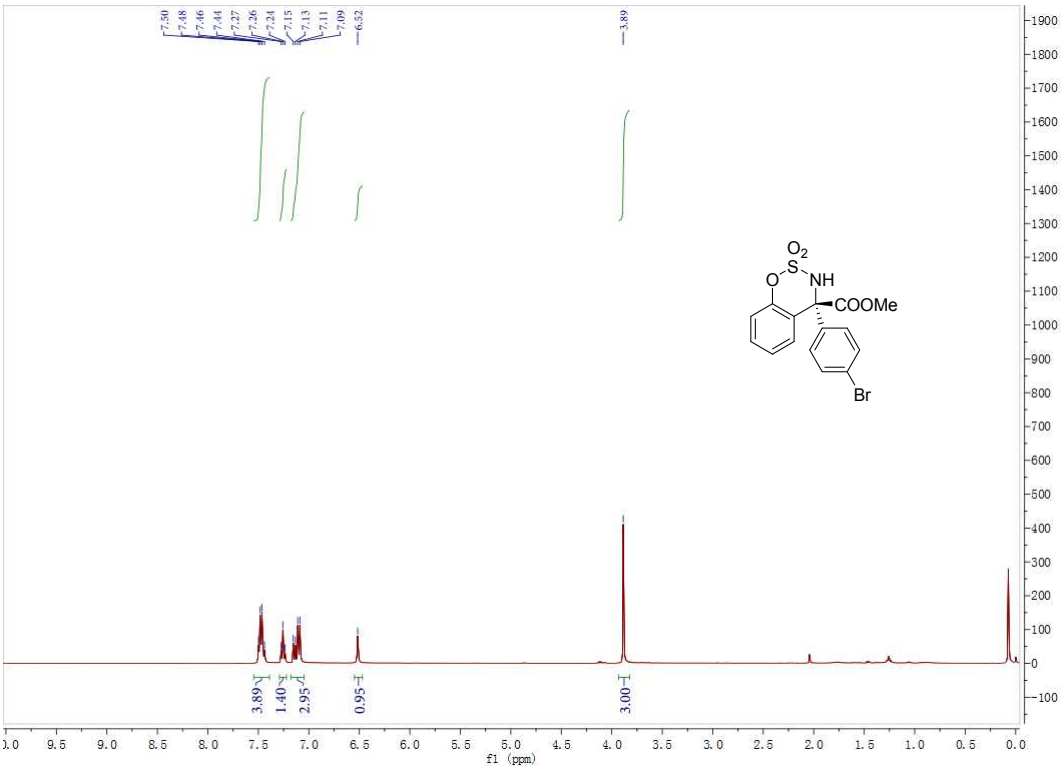
77.26
76.94
70.87
54.99
O2
S
O
NH
COOMe
Cl
f1 (ppm)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7.26
7.24
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7.13
7.11
7.09
6.52
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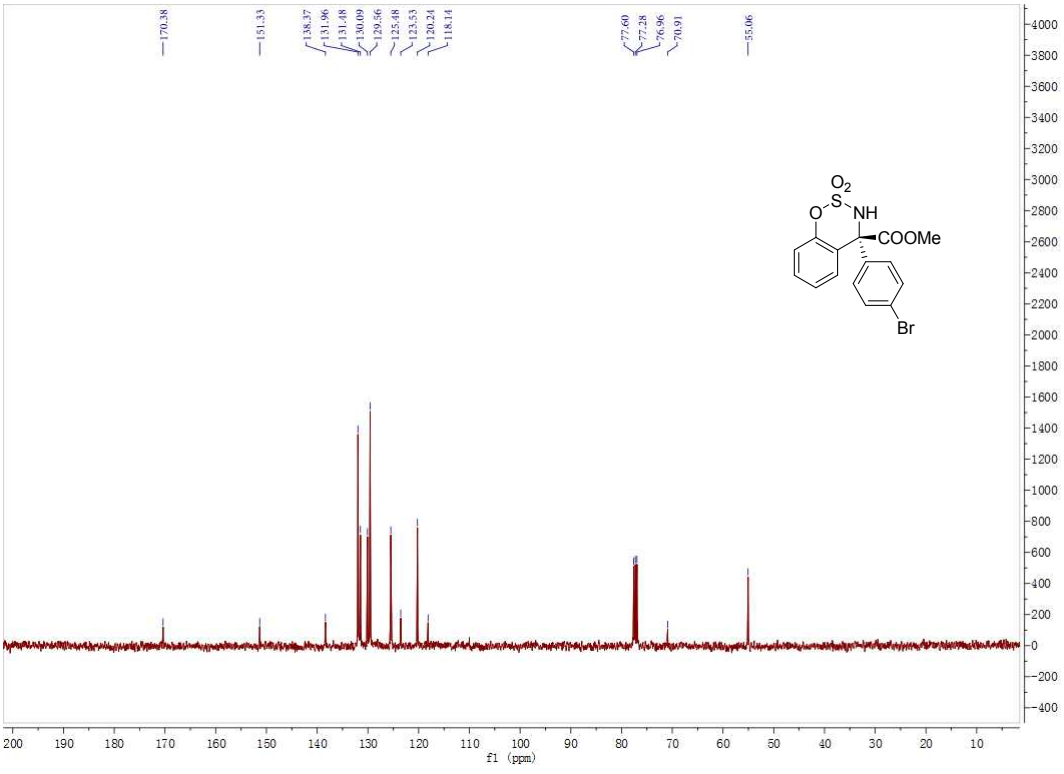
S
O
NH
COOMe
Br
3.89
1.40
2.95
0.95
3.00
f1 (ppm)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131.48
130.09
129.56
125.48
123.53
120.24
118.14
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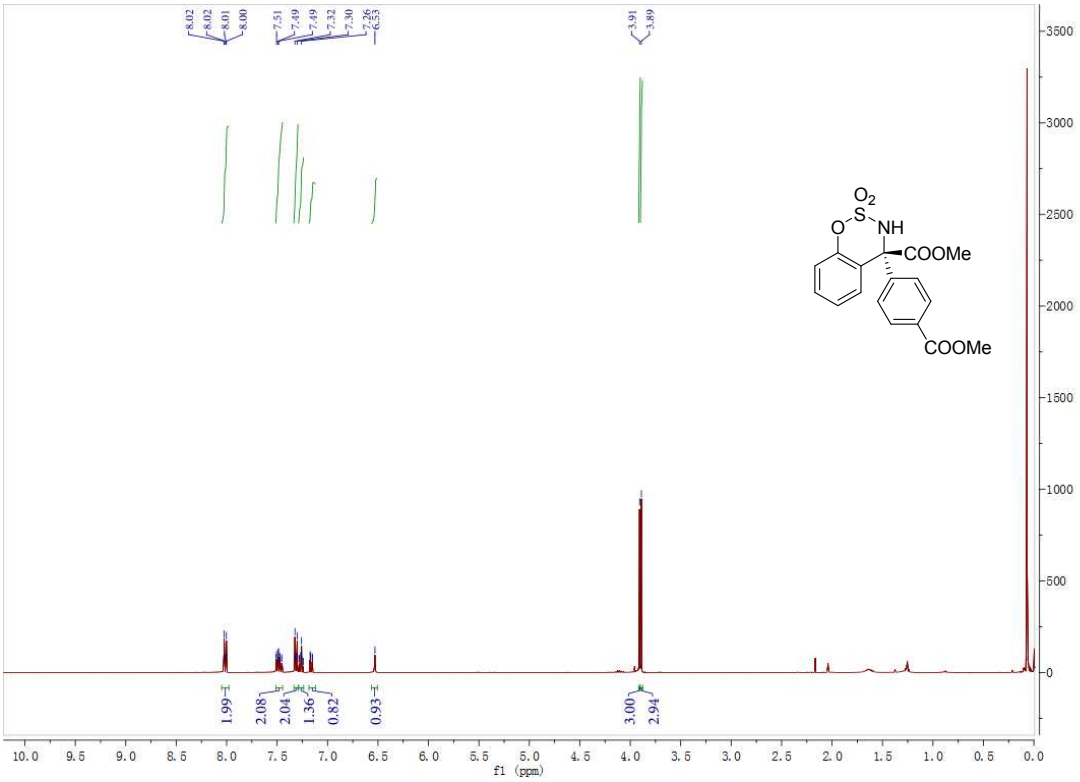
77.28
76.96
70.91
55.06
O2
S
O
NH
COOMe
Br
f1 (ppm)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8.02
8.01
8.00
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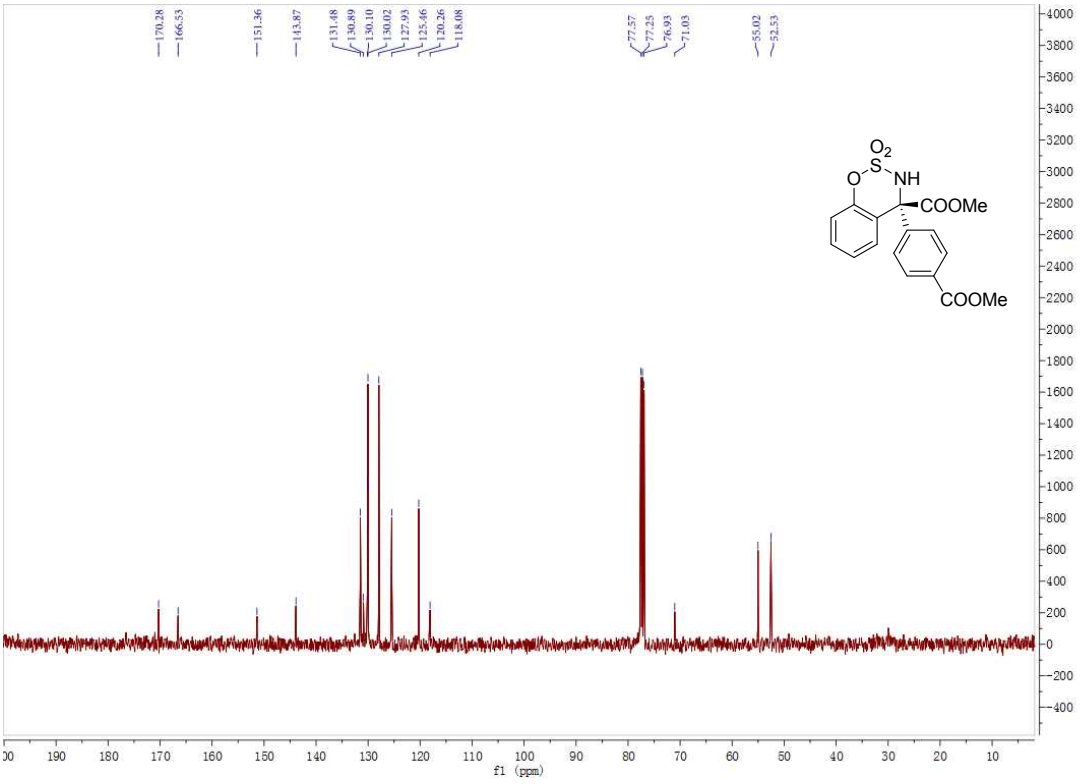
7.49
7.49
7.32
7.30
7.26
6.55
3.91
3.89
O2
S
O
NH
COOMe
COOMe
1.99
2.08
2.04
1.36
0.82
0.93
3.00
2.94
f1 (ppm)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143.87
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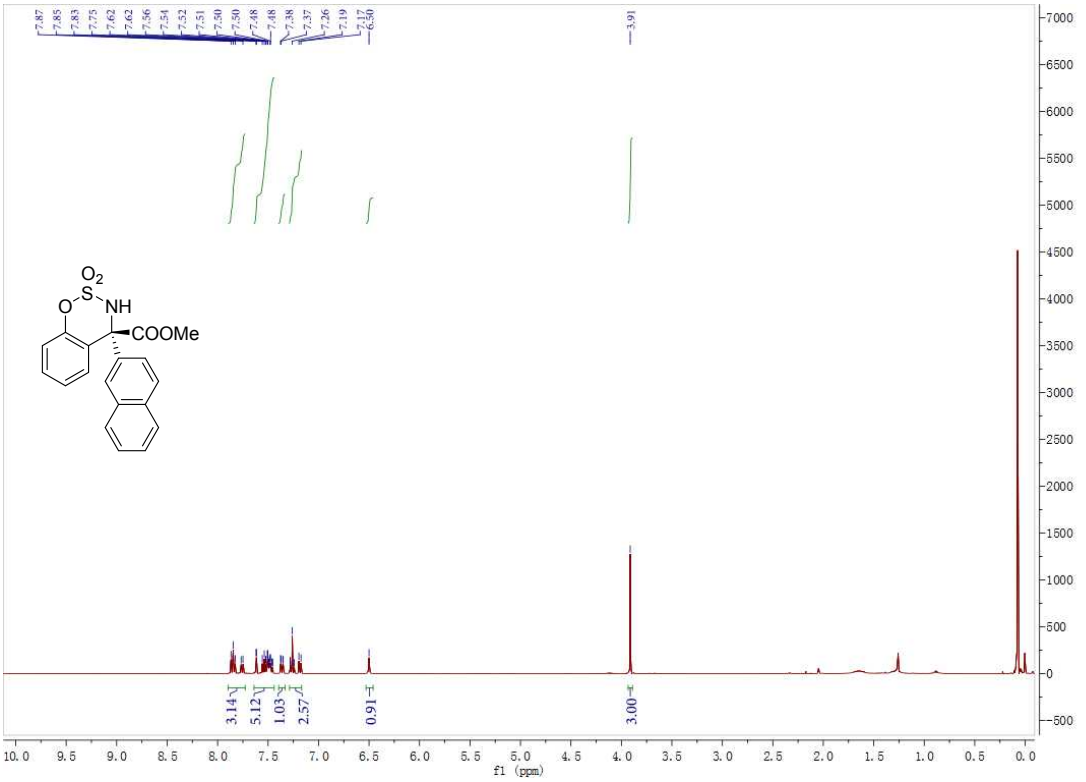
130.02
127.93
125.46
120.26
118.08
77.57
77.25
76.93
71.03
55.02
52.53
O2
S
O
NH
COOMe
COOMe
f1 (ppm)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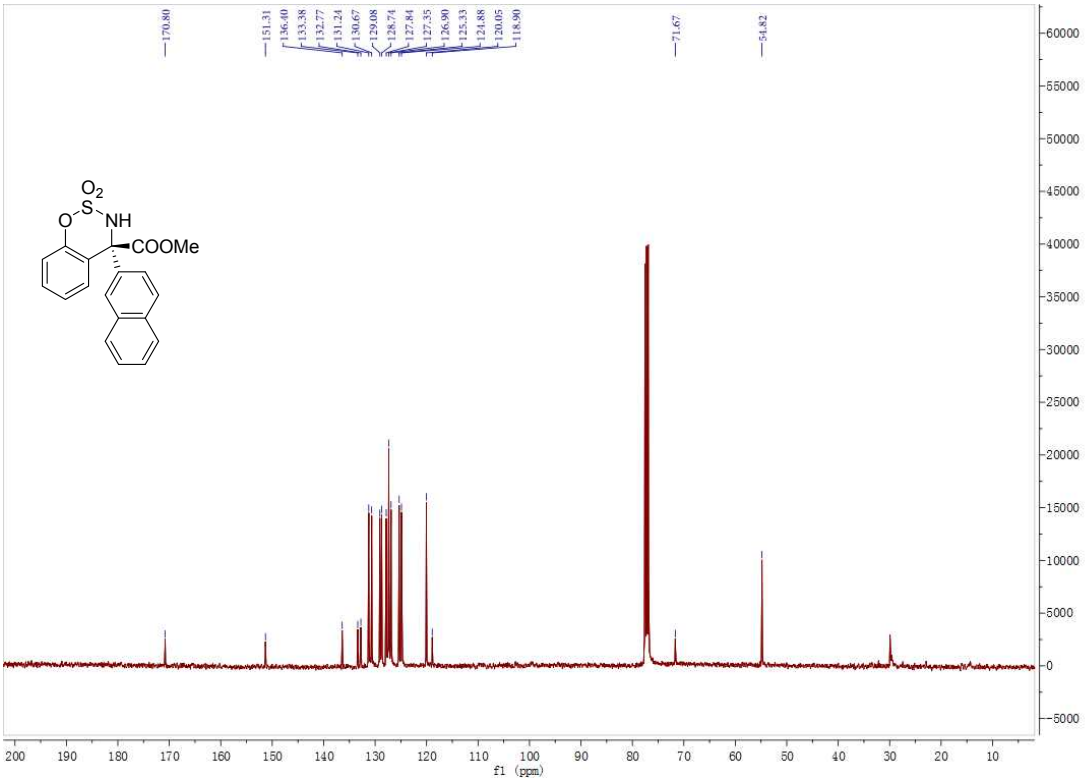
7.50
7.50
7.48
7.48
7.38
7.37
7.26
7.19
7.17
6.50
3.91
O2
S
O
NH
COOMe
3.14
5.12
1.03
2.57
0.91
3.00
f1 (ppm)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127.35
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125.33
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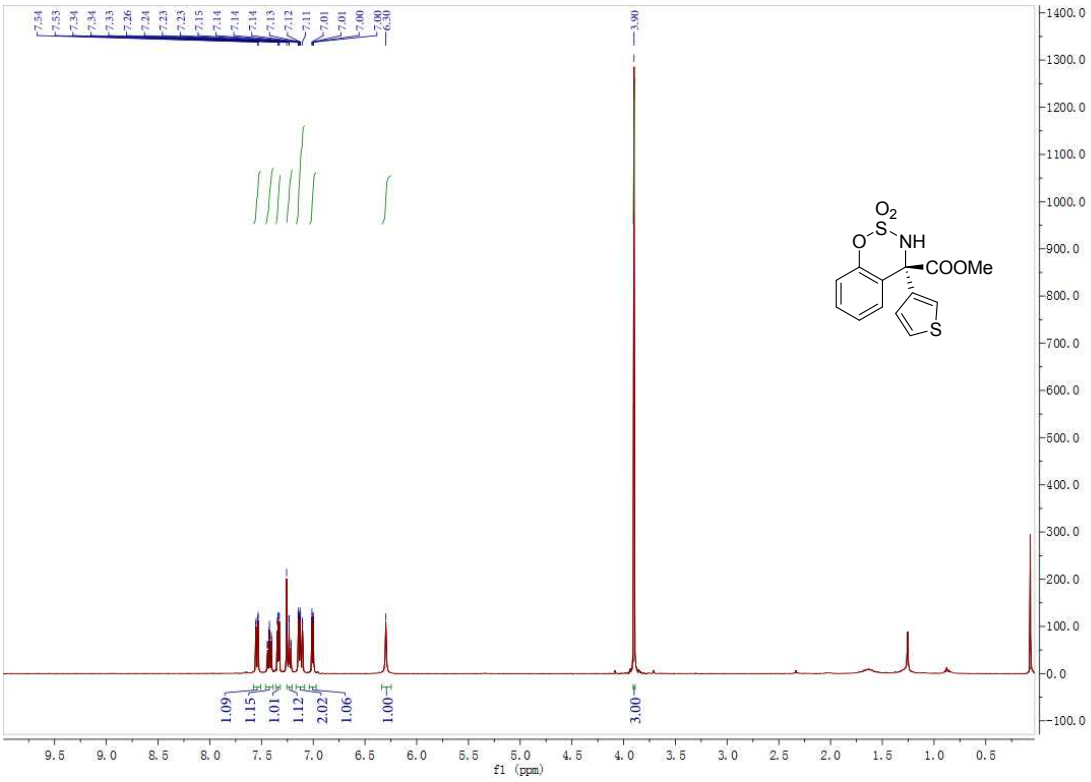
120.05
118.90
71.67
54.82
O2
S
O
NH
COOMe
f1 (ppm)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7.14
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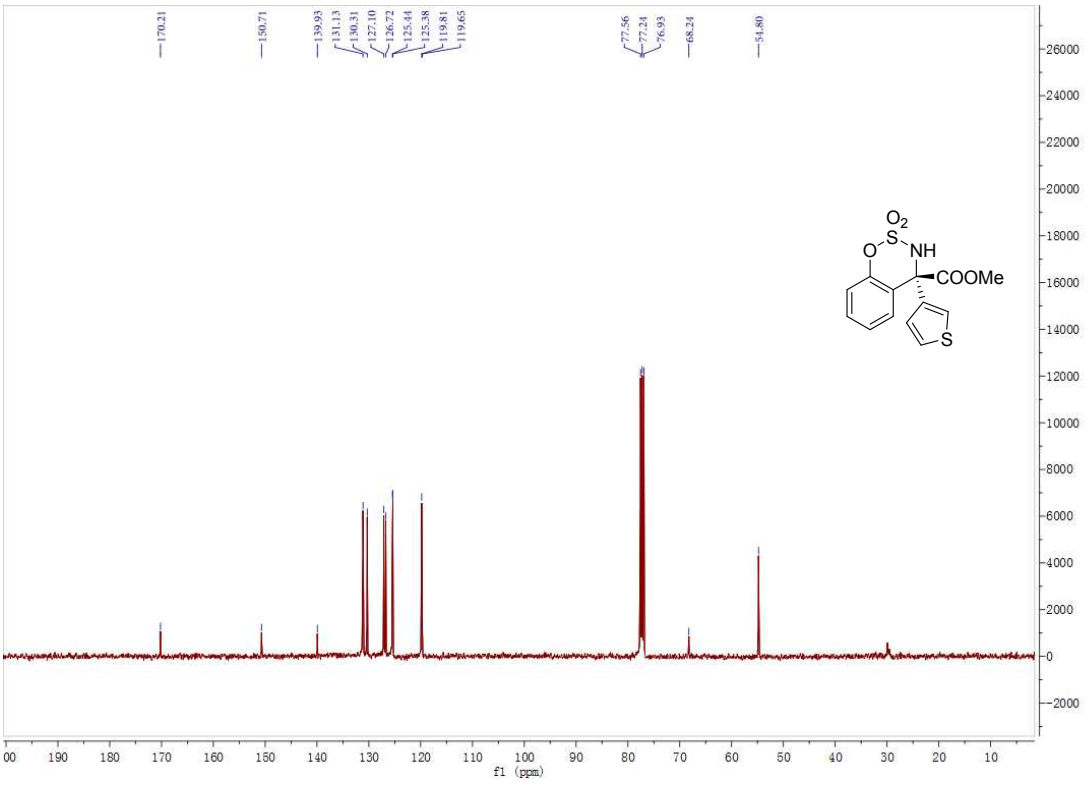
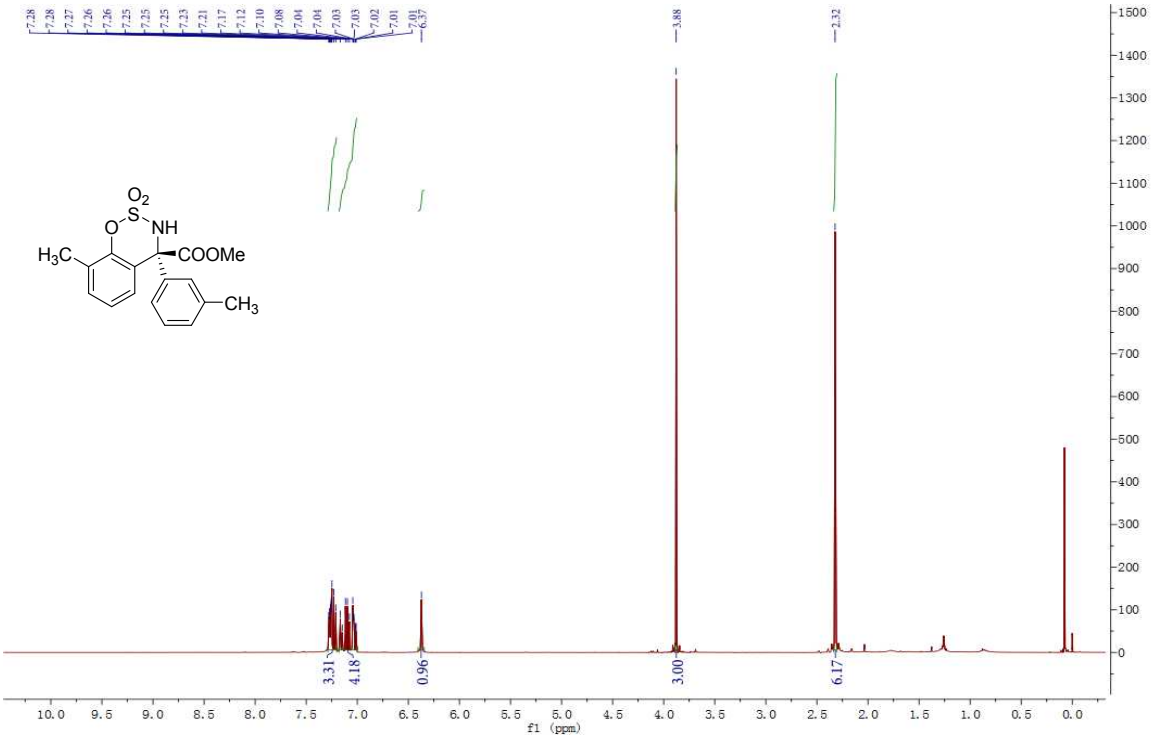
7.12
7.11
7.01
7.01
7.00
7.00
6.30
3.90
1.09
1.15
1.01
1.12
2.02
1.06
1.00
3.00
f1 (ppm)
O2
S
O
NH
COOMe
S


170.21
150.71
139.93
131.13
130.31
127.10
126.72
125.44
125.38
119.81
119.65
77.56
77.24
76.93
68.24
54.80
f1 (ppm)
O2
S
O
NH
COOMe
S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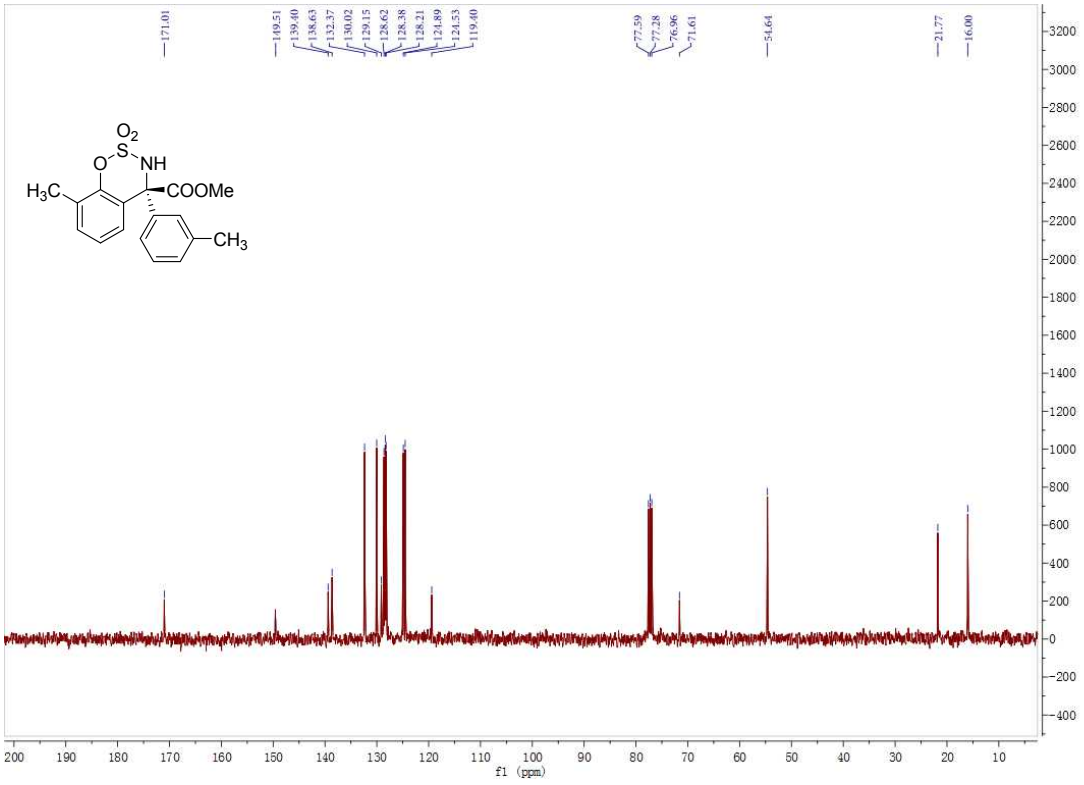
7.28
7.27
7.26
7.26
7.25
7.25
7.25
7.23
7.21
7.17
7.12
7.10
7.08
7.04
7.04
7.03
7.03
7.02
7.01
7.01
6.37
3.88
2.32
O2
S
O
NH
H3C
COOMe
CH3
3.31
4.18
0.96
3.00
6.17
f1 (ppm)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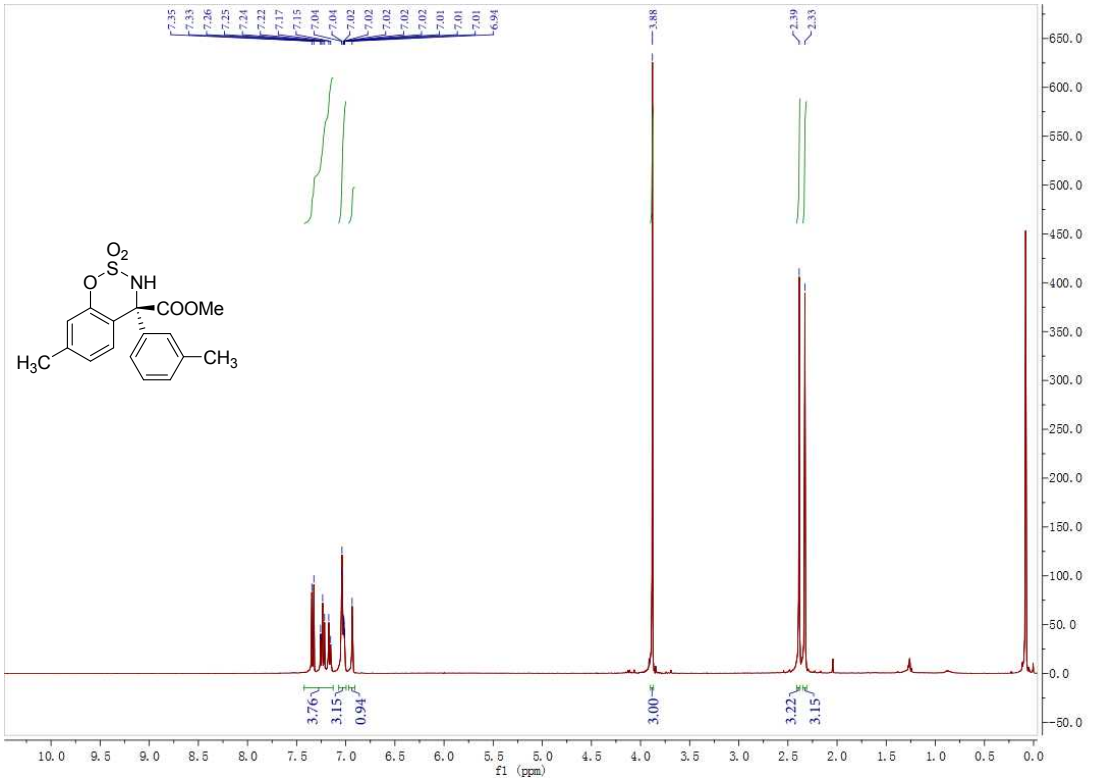
129.15
128.62
128.38
128.21
124.89
124.53
119.40
77.59
77.28
76.96
71.61
54.64
21.77
16.00
O2
S
O
NH
H3C
COOMe
CH3
f1 (ppm)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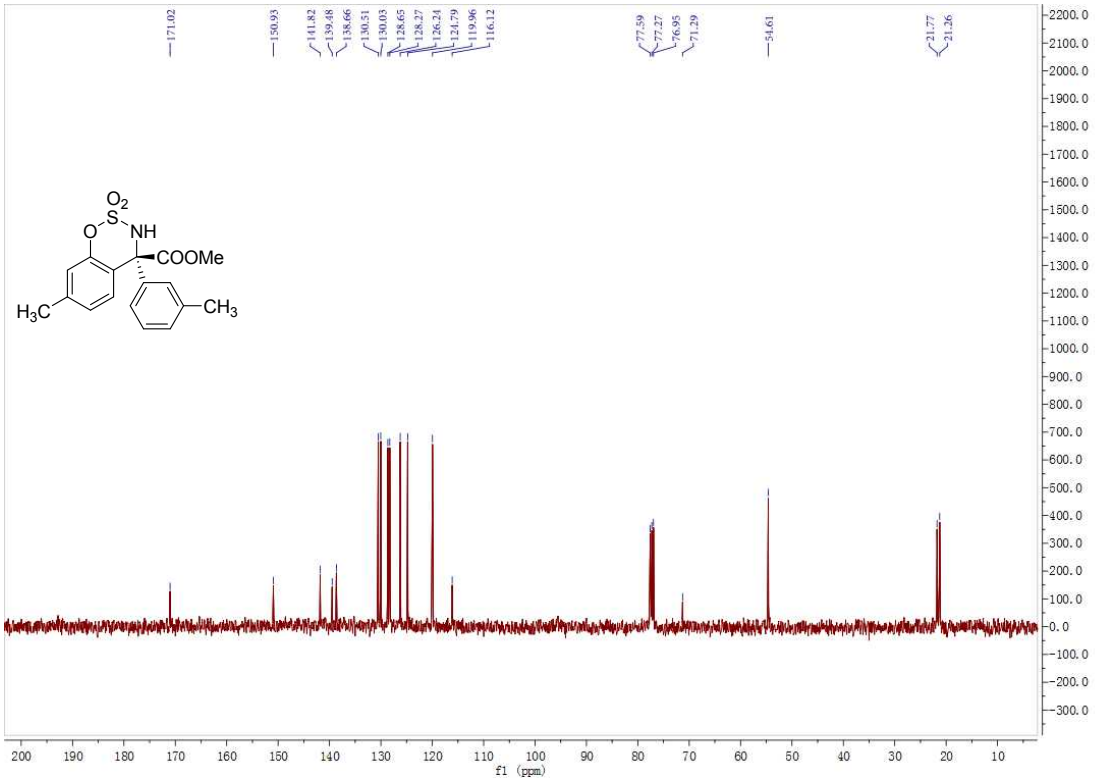
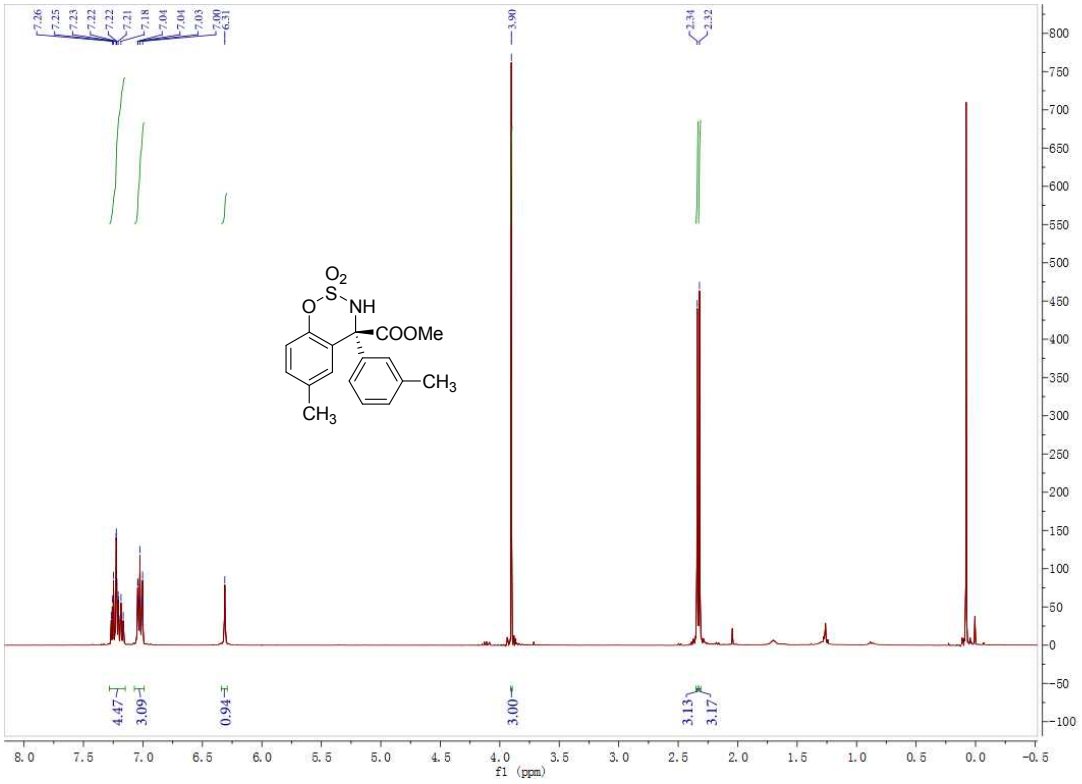
7.33
7.26
7.25
7.24
7.22
7.17
7.15
7.04
7.04
7.02
7.02
7.02
7.02
7.02
7.01
7.01
7.01
6.94
3.88
2.39
2.33
O2
S
O
NH
COOMe
H3C
CH3
3.76
3.15
0.94
3.00
3.22
3.15
f1 (ppm)


171.02
150.93
141.82
139.48
138.66
130.51
130.03
128.65
128.27
126.24
124.79
119.96
116.12
77.59
77.27
76.95
71.29
54.61
21.77
21.26
O2
S
O
NH
COOMe
H3C
CH3
f1 (ppm)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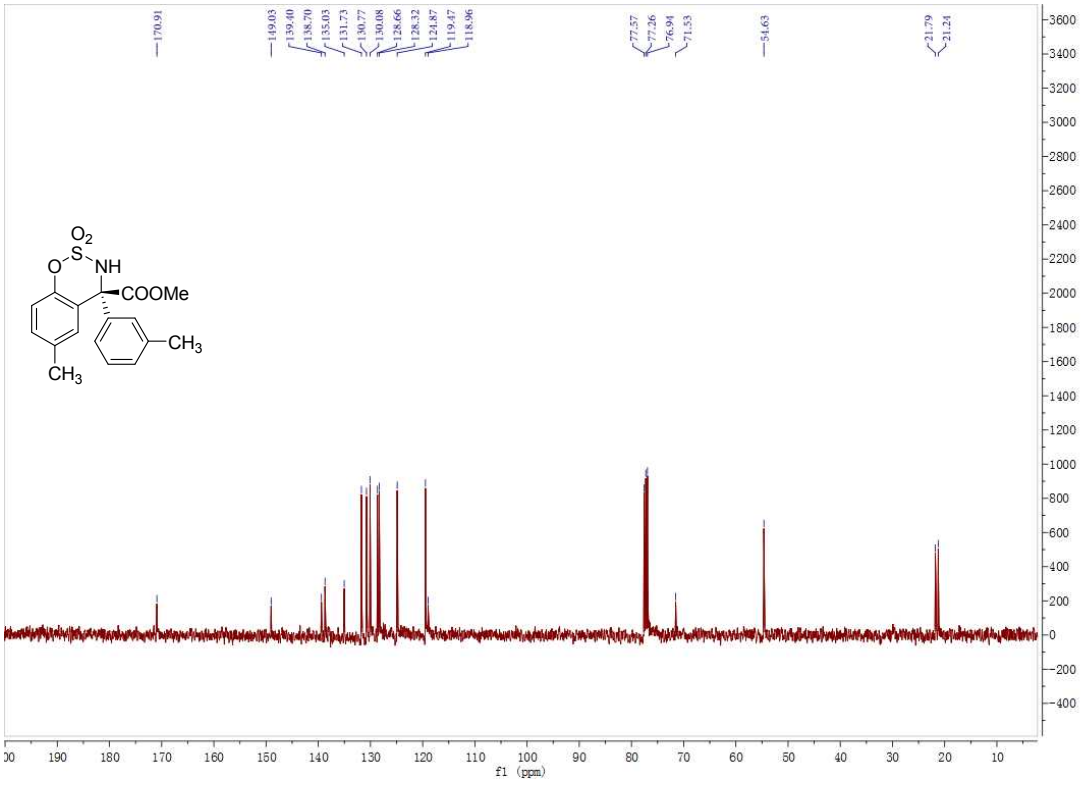
7.25
7.23
7.22
7.22
7.21
7.18
7.04
7.04
7.03
7.00
6.91
3.90
2.34
2.32
O2
S
O
NH
COOMe
CH3
CH3
4.47
3.09
0.94
3.00
3.13
3.17
f1 (ppm)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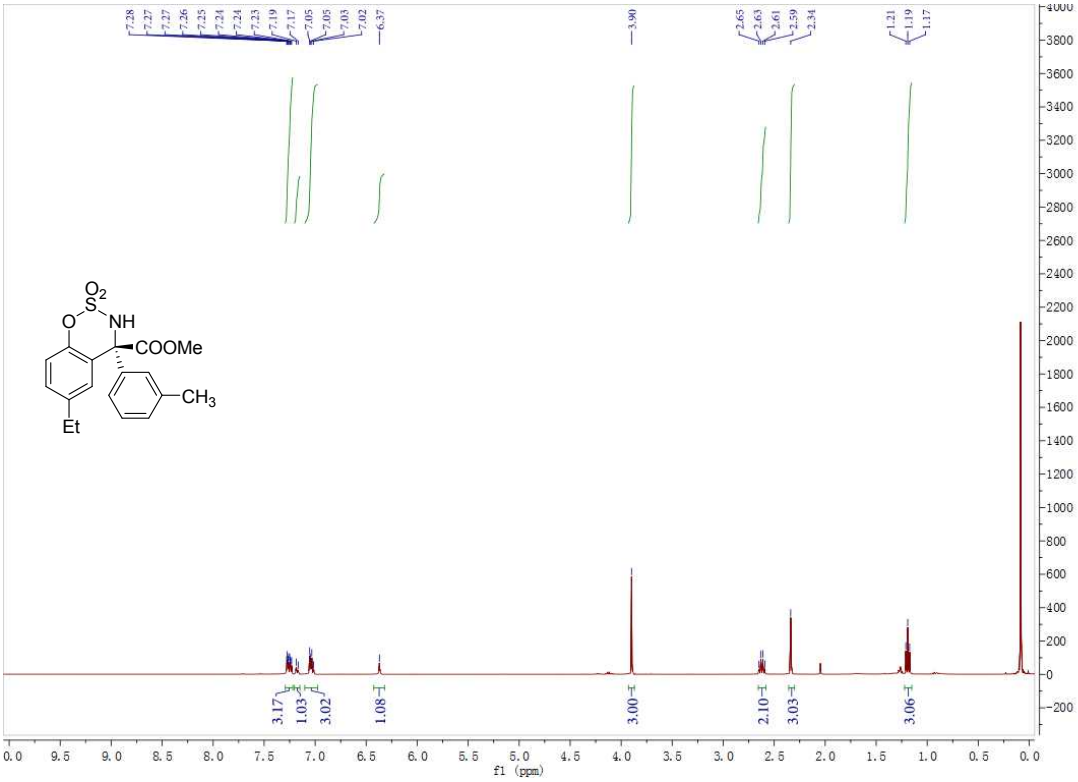
149.03
139.40
138.70
135.03
131.73
130.77
130.08
128.66
128.32
124.87
119.47
118.96
77.57
77.26
76.94
71.53
54.63
21.79
21.24
O2
S
O
NH
COOMe
CH3
CH3
f1 (ppm)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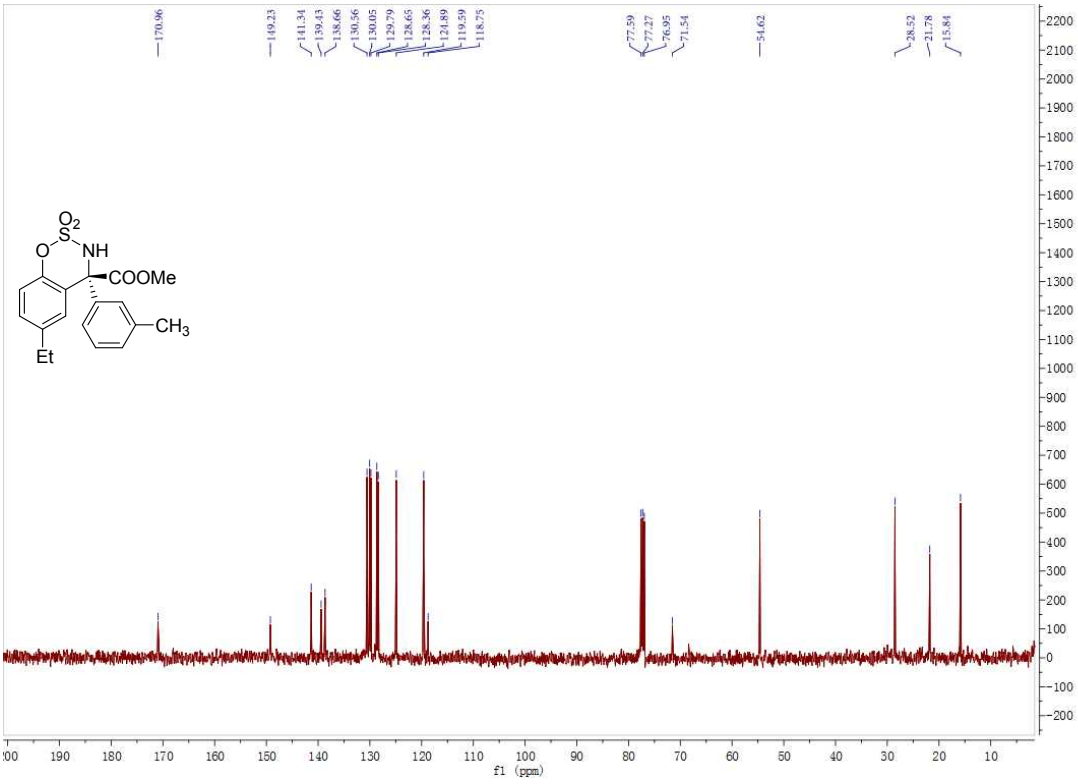
7.27
7.27
7.26
7.25
7.24
7.24
7.23
7.19
7.17
7.05
7.05
7.03
7.02
6.37
3.90
2.65
2.63
2.61
2.59
2.34
1.21
1.19
1.17
O2
S
O
NH
COOMe
CH3
Et
3.17
1.03
3.02
1.08
3.00
2.10
3.03
3.06
f1 (ppm)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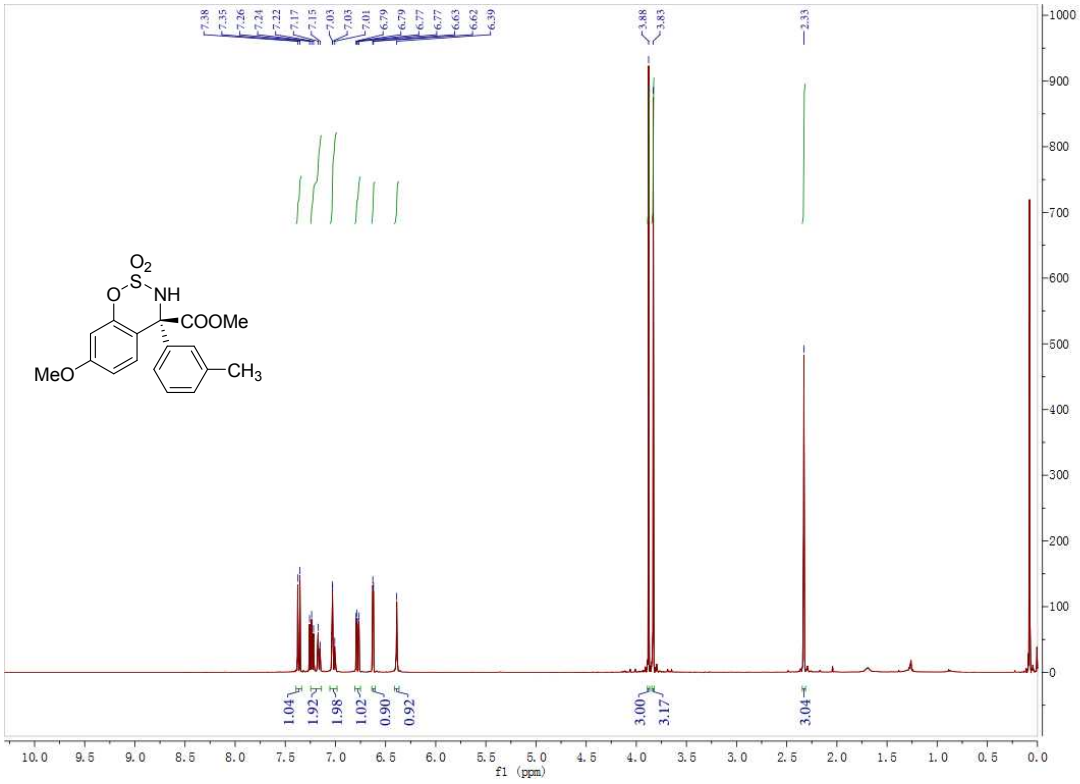
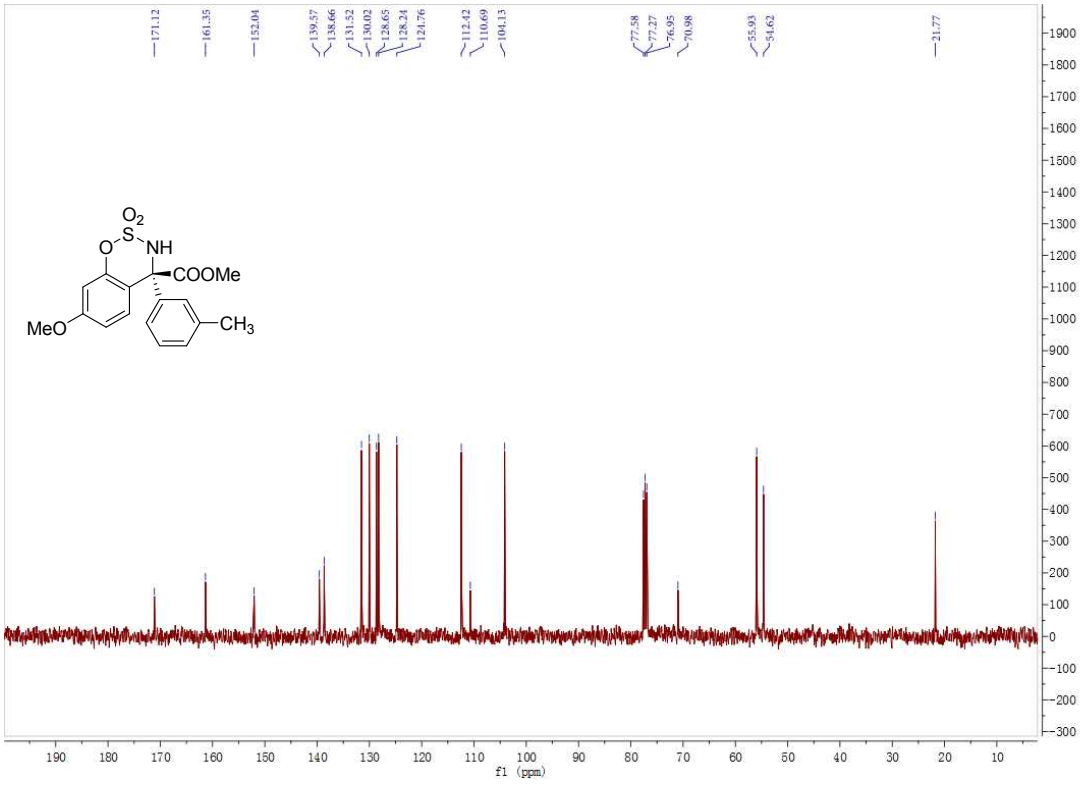
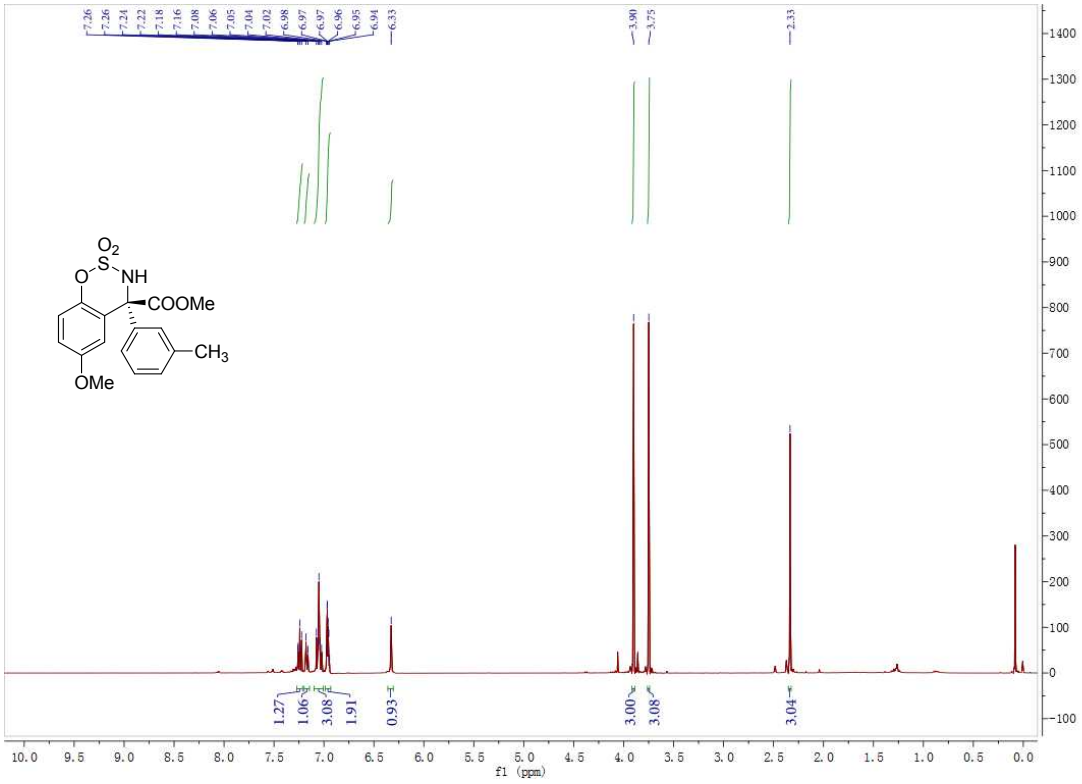
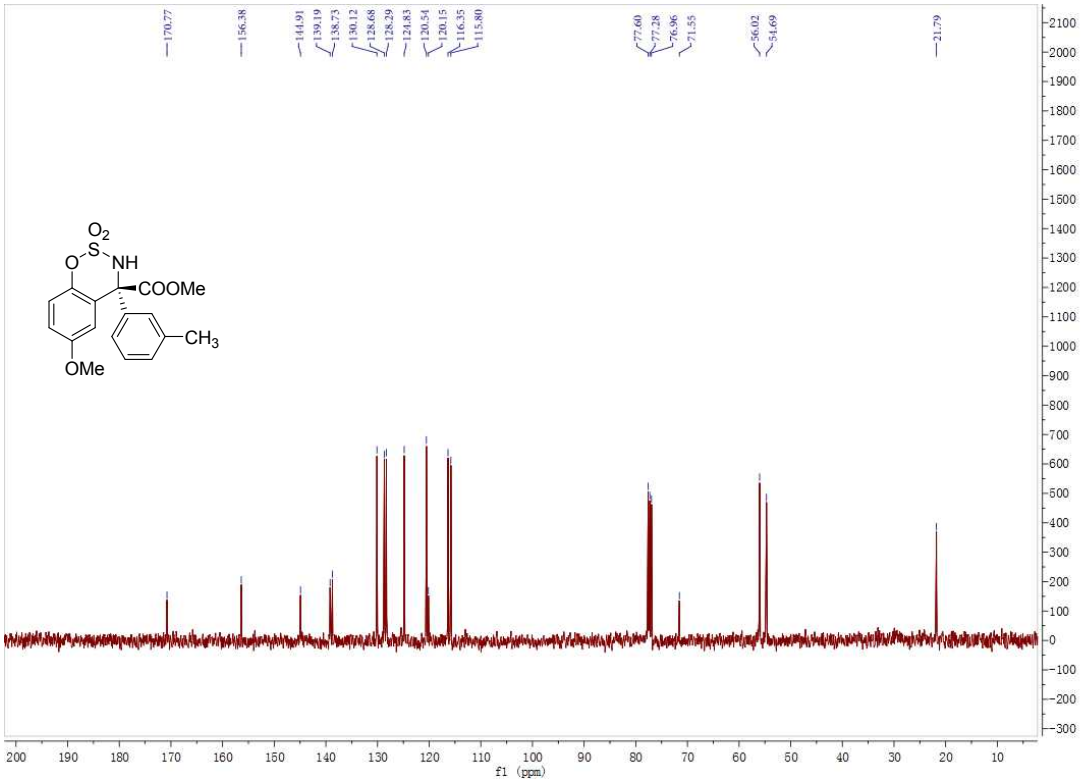
149.23
141.34
139.43
138.66
130.56
130.05
129.79
128.65
128.36
124.89
119.59
118.75
77.59
77.27
76.95
71.54
54.62
28.52
21.78
15.84
O2
S
O
NH
COOMe
CH3
Et
f1 (ppm)


7.38
7.35
7.26
7.24
7.22
7.17
7.15
7.03
7.03
7.01
6.79
6.79
6.77
6.77
6.63
6.62
6.39
3.88
3.83
2.33
O2
S
O
NH
COOMe
MeO
CH3
1.04
1.92
1.98
1.02
0.90
0.92
3.00
3.17
3.04
f1 (ppm)


171.12
161.35
152.04
139.57
138.66
131.52
130.02
128.65
128.24
124.76
112.42
110.69
104.13
77.58
77.27
76.95
70.98
55.93
54.62
21.77
O2
S
O
NH
COOMe
MeO
CH3
f1 (ppm)


7.26
7.26
7.24
7.22
7.18
7.16
7.08
7.06
7.05
7.04
7.02
6.98
6.97
6.97
6.96
6.95
6.94
6.33
3.90
3.75
2.33
O2
O
S
NH
COOMe
CH3
OMe
1.27
1.06
3.08
1.91
0.93
3.00
3.08
3.04
f1 (ppm)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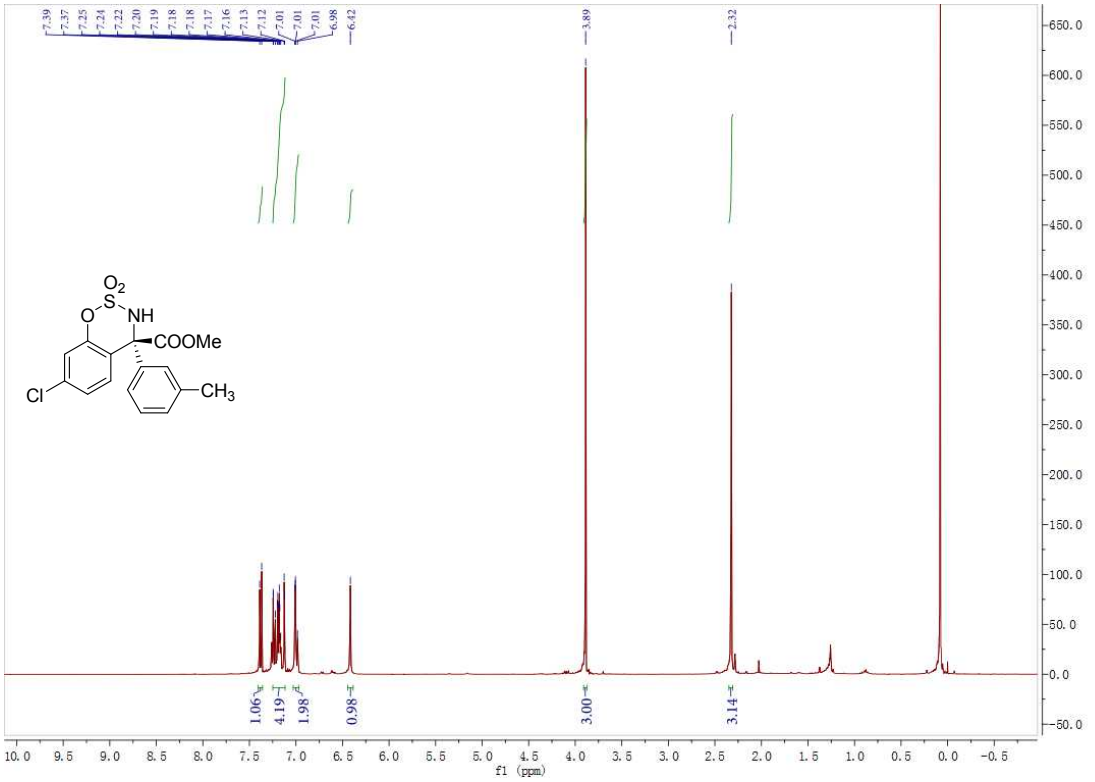
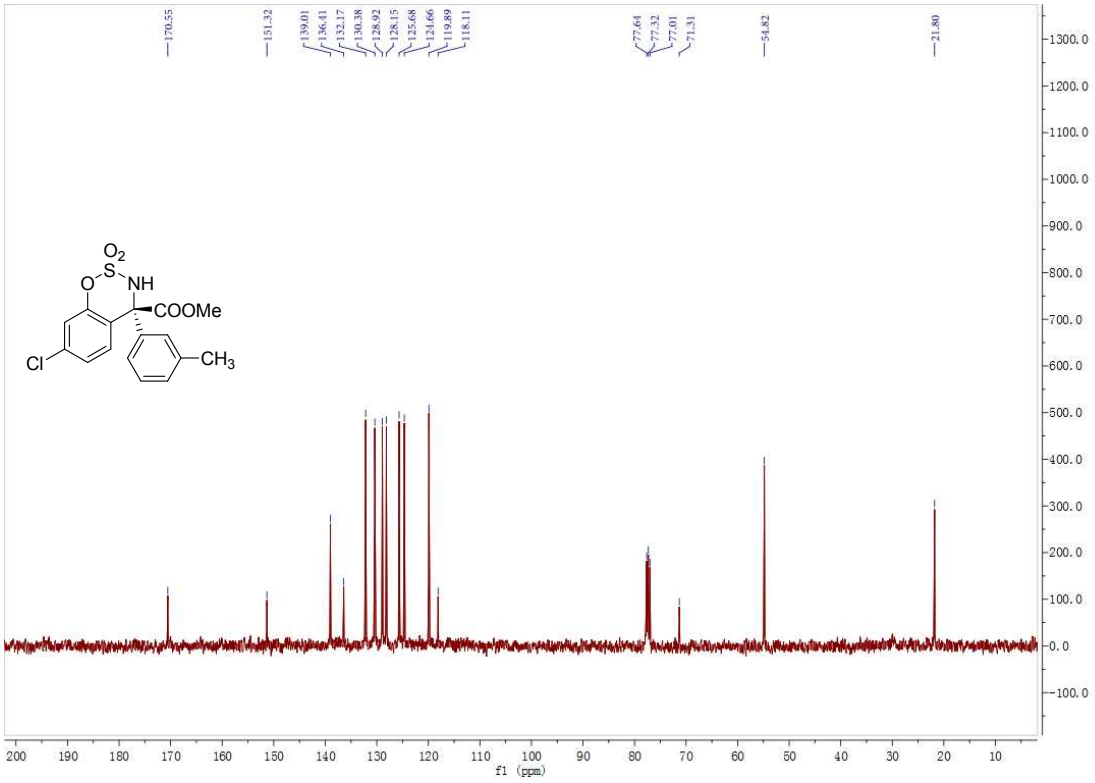
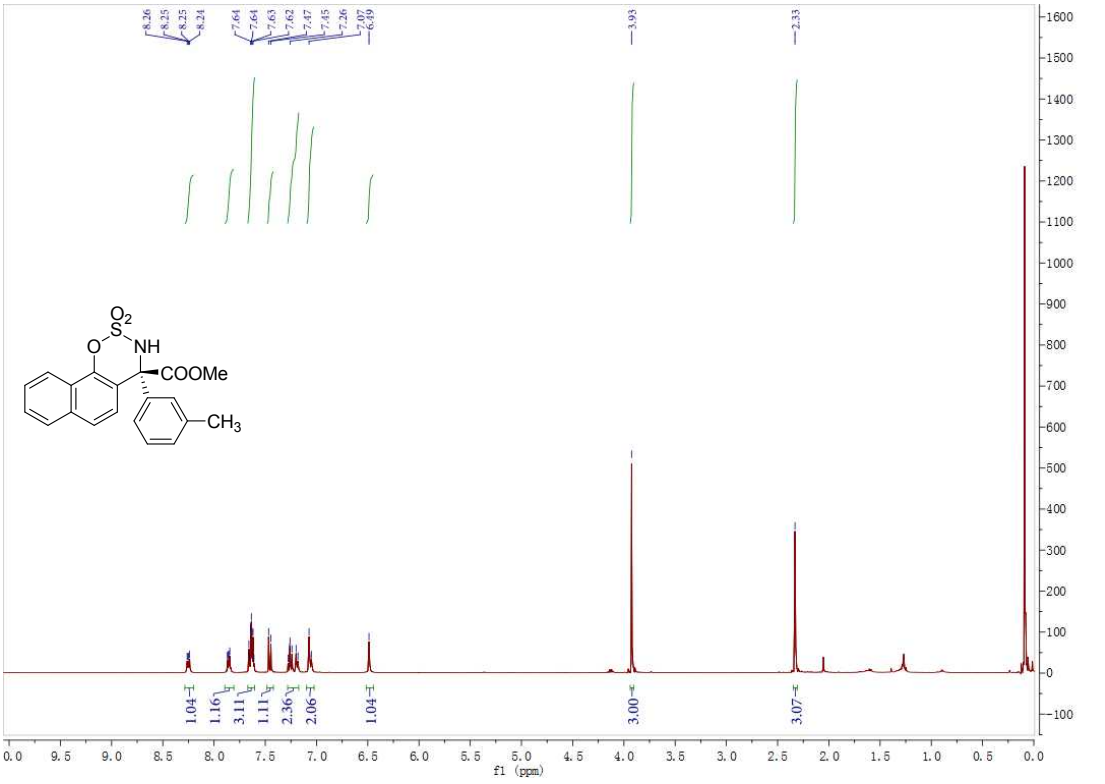
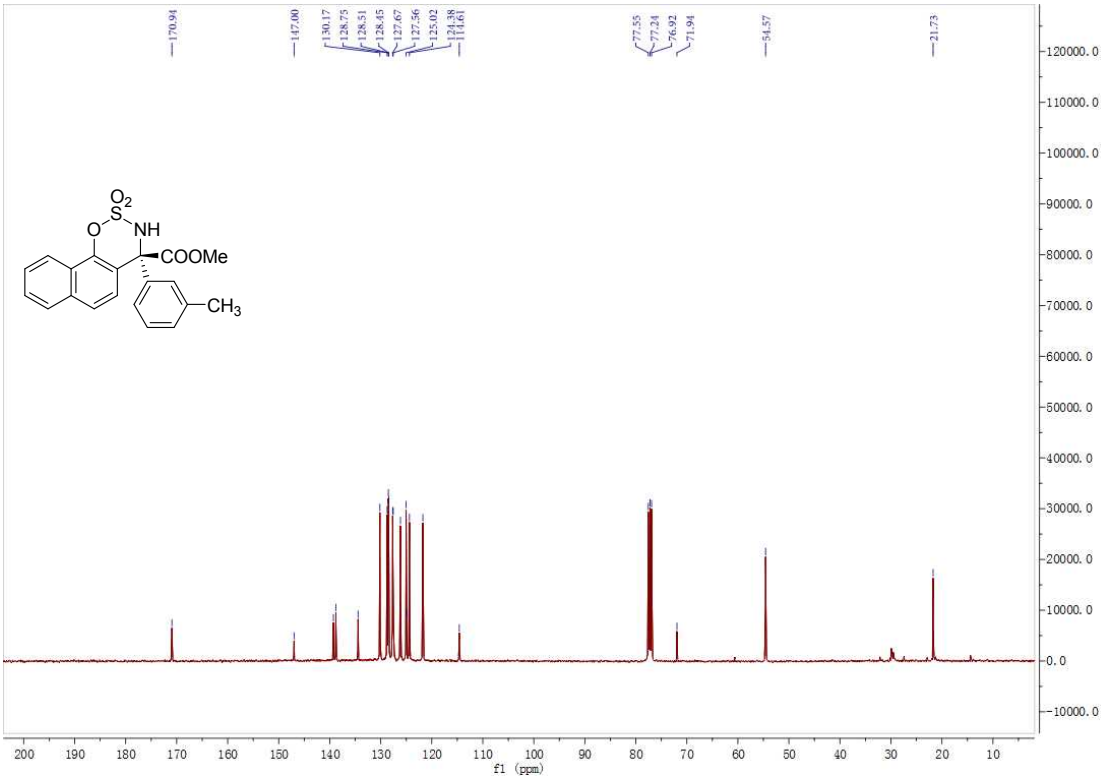
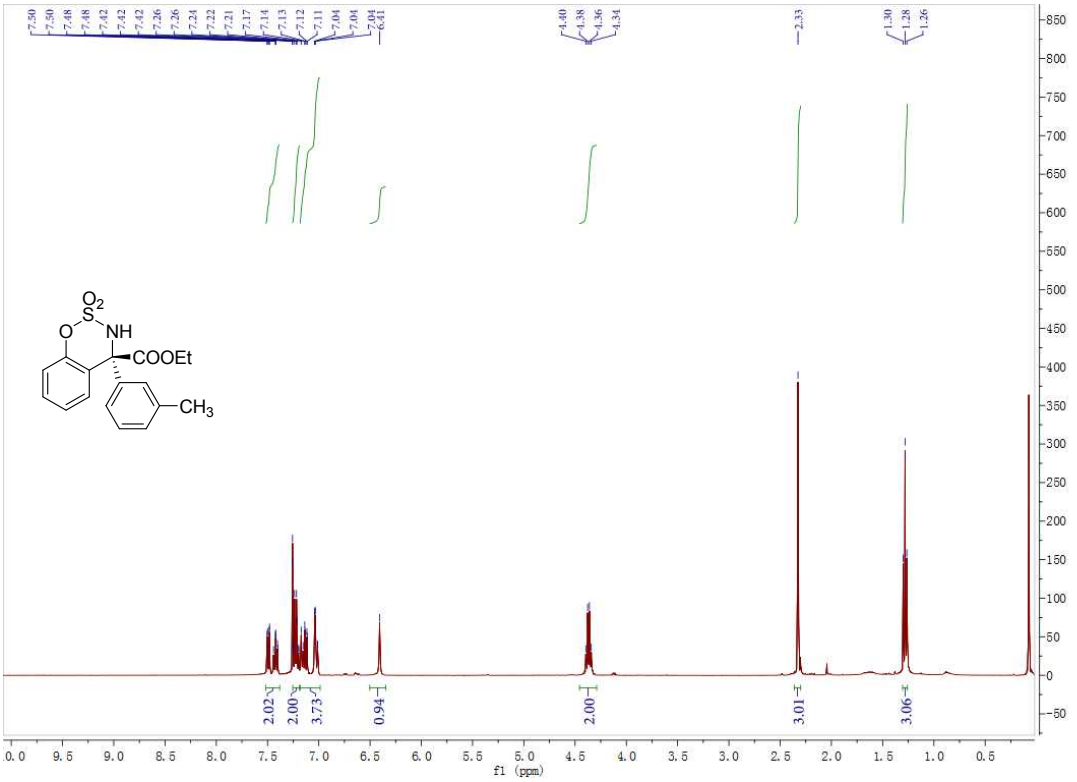
156.38
144.91
139.19
138.73
130.12
128.68
128.29
124.83
120.54
120.15
116.35
115.80
77.60
77.28
76.96
71.55
56.02
54.69
21.79
O2
O
S
NH
COOMe
CH3
OMe
f1 (ppm)

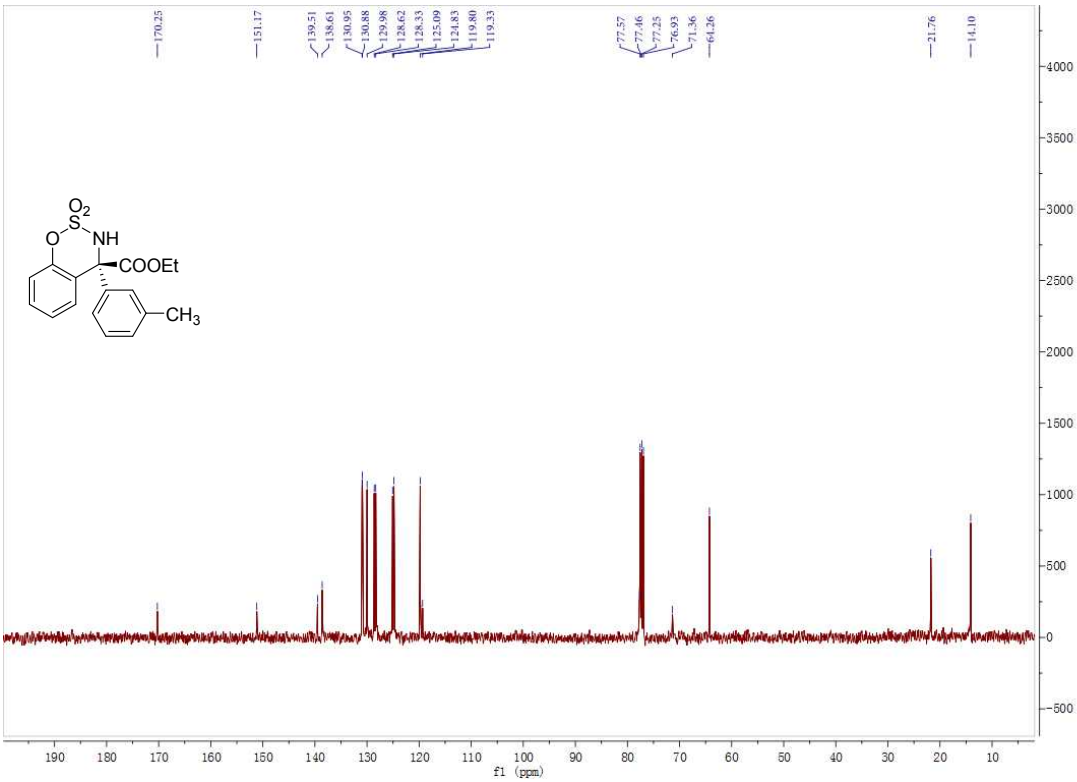

7.39
7.37
7.25
7.24
7.22
7.20
7.19
7.18
7.18
7.17
7.16
7.13
7.12
7.01
7.01
7.01
6.98
6.42
3.89
2.32
O2
S
O
NH
COOMe
Cl
CH3
1.06
4.19
1.98
0.98
3.00
3.14
f1 (ppm)

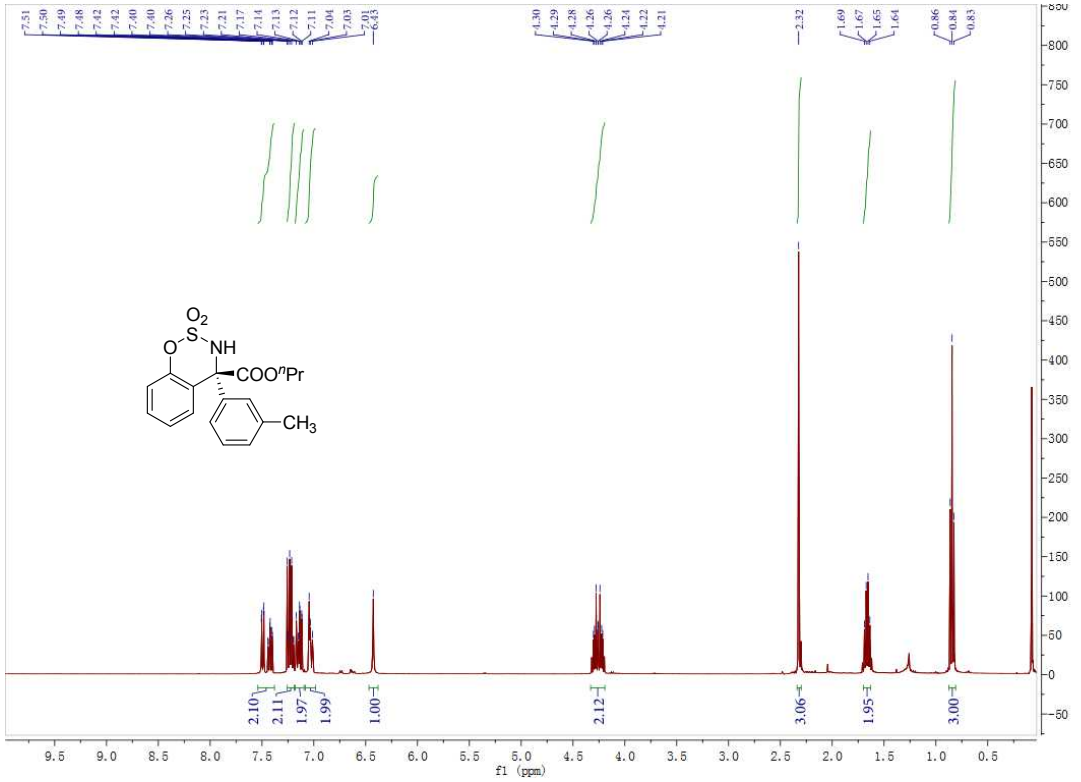

170.55
151.32
139.01
136.41
132.17
130.38
128.92
128.15
125.68
124.66
119.89
118.11
77.64
77.32
77.01
71.31
54.82
21.80
O2
S
O
NH
COOMe
Cl
CH3
f1 (ppm)


8.26
8.25
8.25
8.24
7.64
7.64
7.63
7.62
7.47
7.45
7.26
7.07
6.49
3.93
2.33
O2
S
O
NH
COOMe
CH3
1.04
1.16
3.11
1.11
2.36
2.06
1.04
3.00
3.07
f1 (ppm)


170.94
147.00
130.17
128.75
128.51
128.45
127.67
127.56
125.02
77.55
77.24
76.92
71.94
54.57
21.73
O2
S
O
NH
COOMe
CH3
f1 (ppm)


O2
S
O
NH
COOEt
CH3
f1 (ppm)


O2
S
O
NH
COOEt
CH3
f1 (ppm)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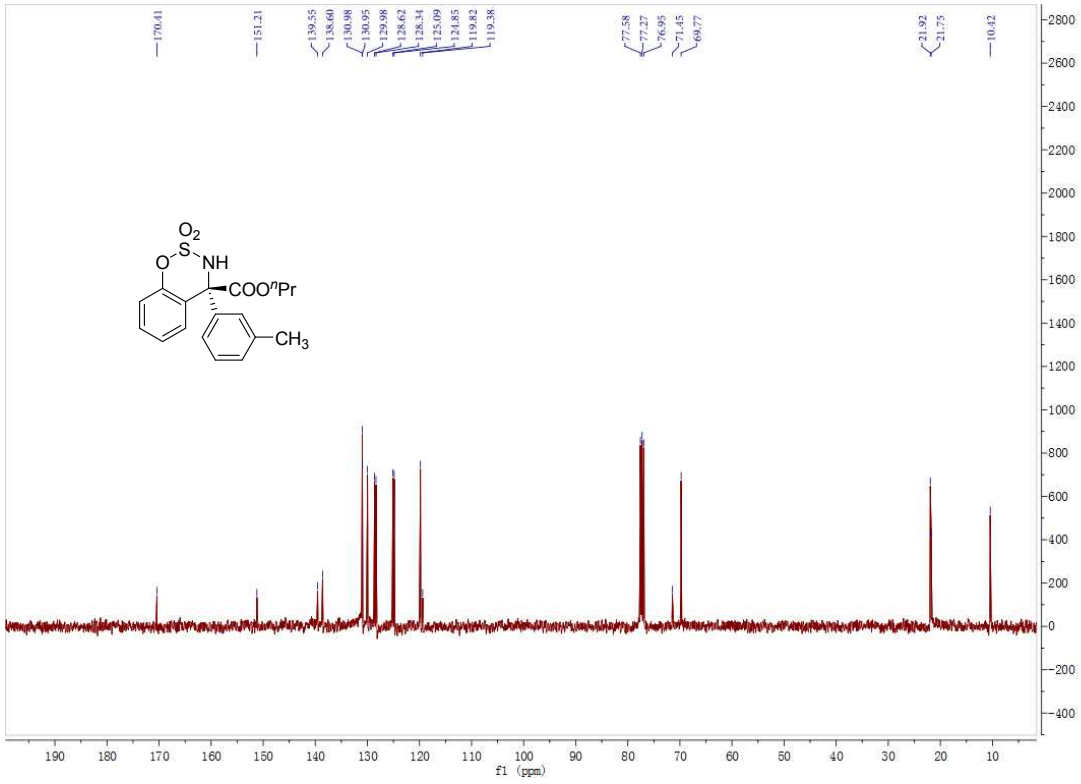
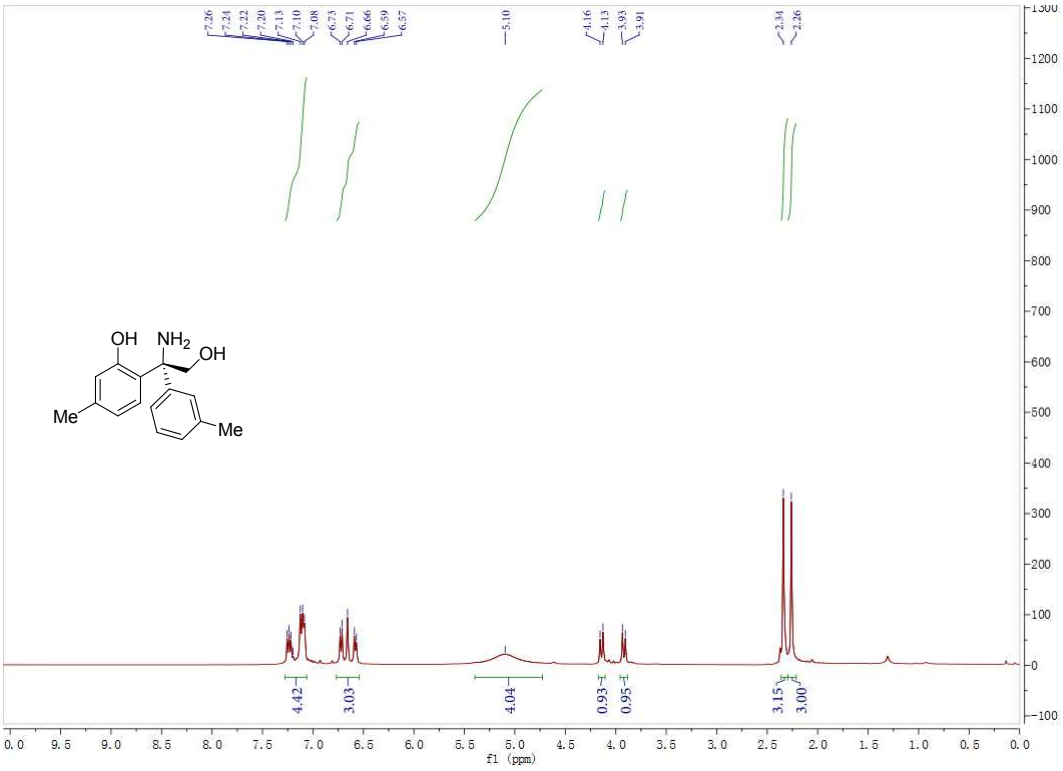
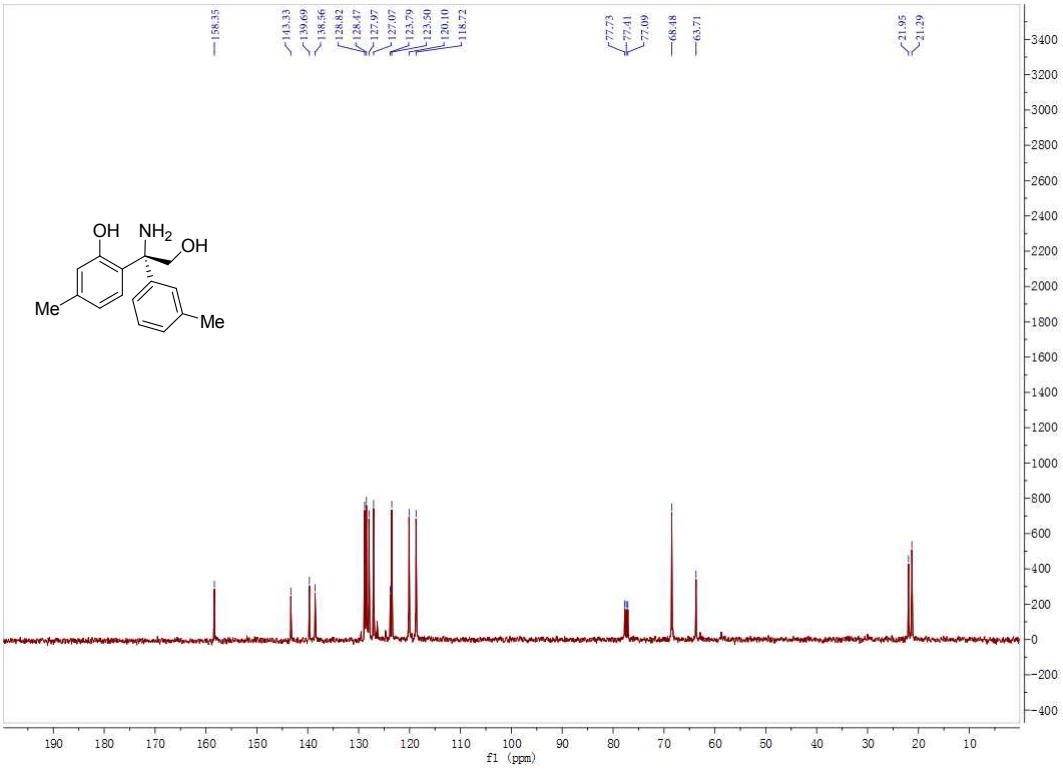
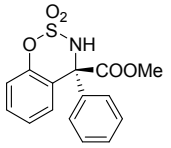
7.50
7.49
7.48
7.42
7.42
7.40
7.40
7.26
7.25
7.23
7.21
7.17
7.14
7.13
7.12
7.11
7.04
7.03
7.01
6.43
4.30
4.29
4.28
4.26
4.26
4.24
4.22
4.21
2.32
1.69
1.67
1.65
1.64
0.86
0.84
0.83
O2
S
O
NH
COOnPr
CH3
2.10
2.11
1.97
1.99
1.00
2.12
3.06
1.95
3.00
f1 (ppm)

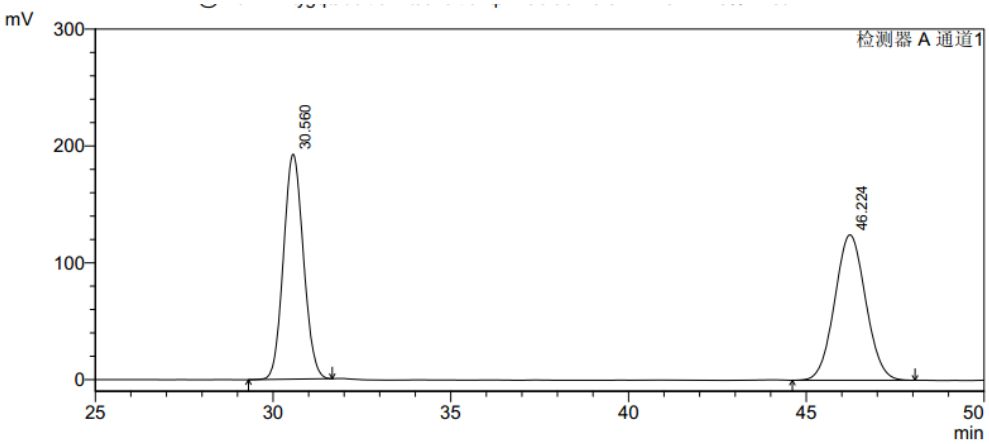

170.41
151.21
139.55
138.60
130.98
130.95
129.98
128.62
128.34
125.09
124.85
119.82
119.38
77.58
77.27
76.95
71.45
69.77
21.92
21.75
10.42
O2
S
O
NH
COOnPr
CH3
f1 (ppm)


7.26
7.24
7.22
7.20
7.13
7.10
7.08
6.73
6.71
6.66
6.59
6.57
5.10
4.16
4.13
3.93
3.91
2.34
2.26
OH
NH2
OH
Me
Me
4.42
3.03
4.04
0.93
0.95
3.15
3.00
f1 (ppm)


158.35
143.33
139.69
138.56
128.82
128.47
127.97
127.07
123.79
123.50
120.10
118.72
77.73
77.41
77.09
68.48
63.71
21.95
21.29
OH
NH2
OH
Me
Me
f1 (ppm)

7. HPLC Spectra of Products



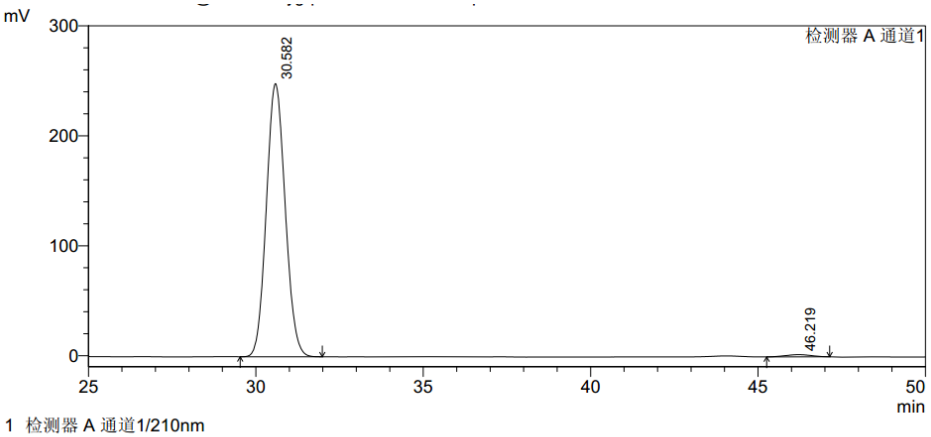


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition2\condition\ph-rac-adh-0.5ml-210nm-10%-2.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	30.560	7487859	192569	49.822	60.729
2	46.224	7541513	124527	50.178	39.271
总计		15029371	317096	100.000	100.000

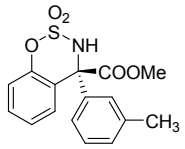


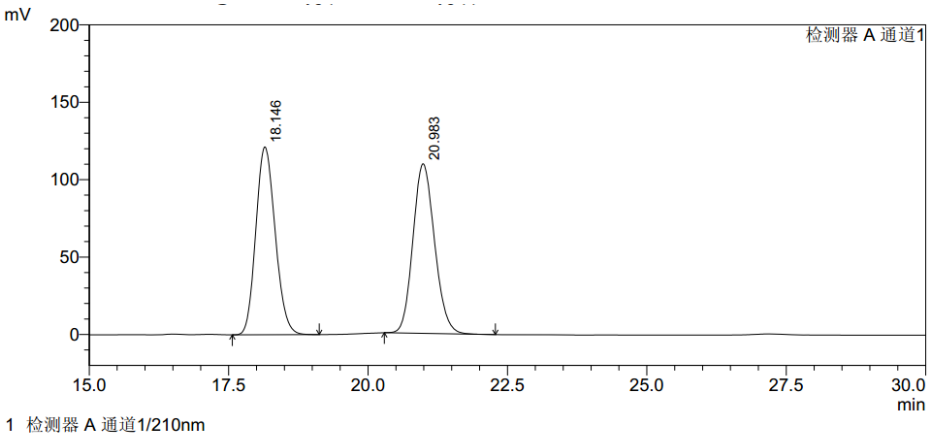
1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition2\condition\ph-cat-adh-0.5ml-210nm-10%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	30.582	9725318	248407	98.901	99.200
2	46.219	108029	2004	1.099	0.800
总计		9833347	250411	100.000	100.000



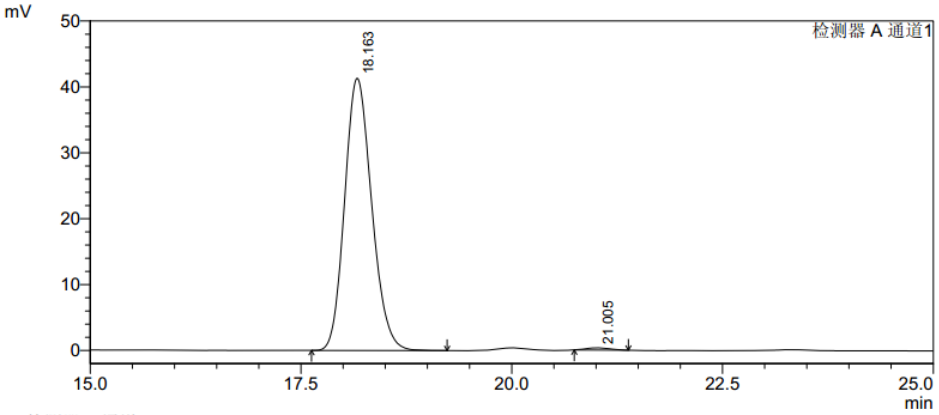


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-mMeB-rac-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	18.146	2930379	121381	49.775	52.557
2	20.983	2956866	109572	50.225	47.443
总计		5887245	230953	100.000	100.000

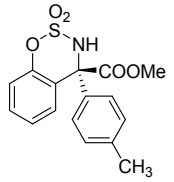


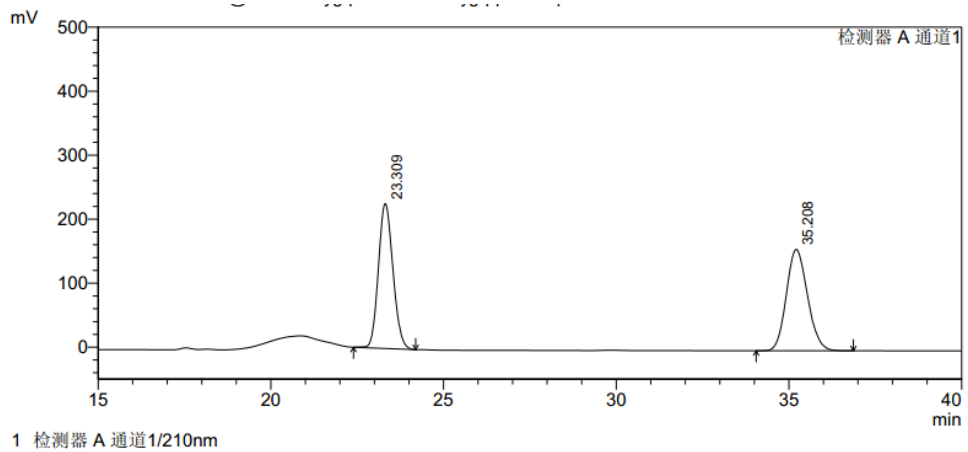
1 检测器 A 通道1/230nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-mMeB-cat-adh-15%.lcd

检测器 A Ch1 230nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	18.163	922241	41326	99.259	99.188
2	21.005	6887	338	0.741	0.812
总计		929128	41664	100.000	100.000

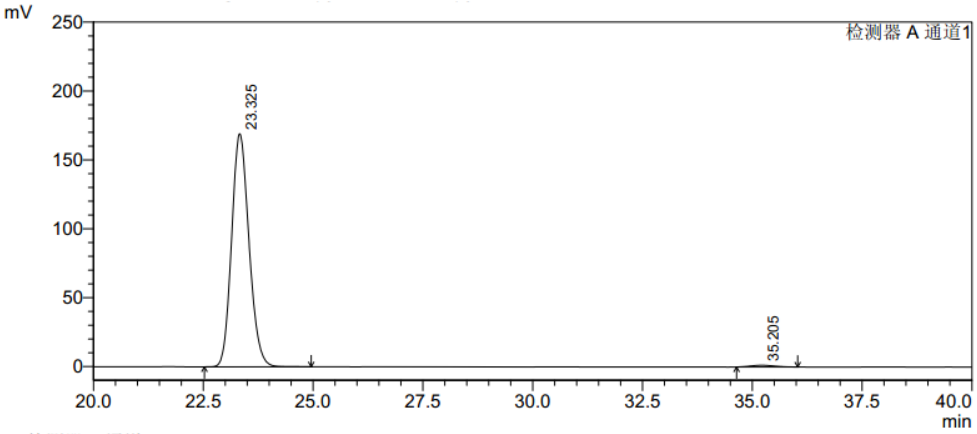




1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pMeB-rac-adh-15%.lcd
检测器 A Ch1 210nm

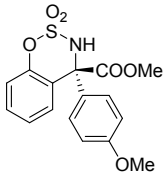
峰#	保留时间	面积	高度	面积 %	高度 %
1	23.309	6617489	226548	49.533	58.834
2	35.208	6742286	158514	50.467	41.166
总计		13359775	385062	100.000	100.000

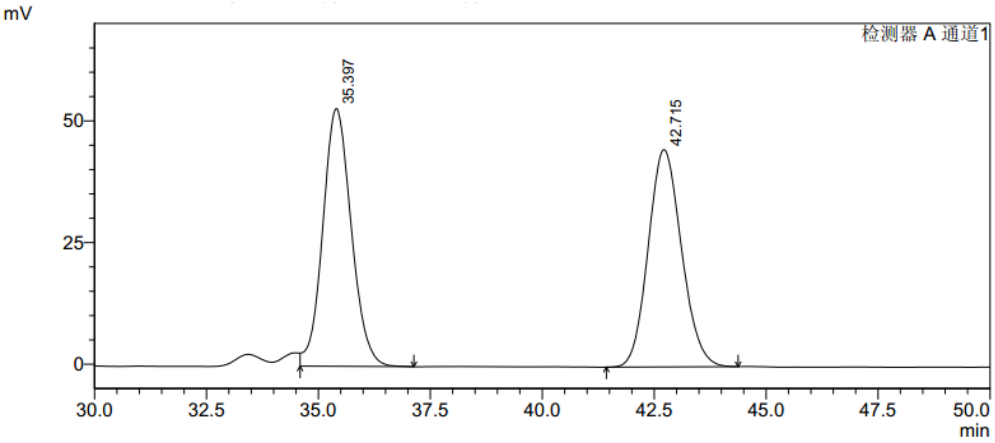


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pMeB-cat-adh-15%-2.lcd
检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	23.325	4654959	169153	98.989	99.270
2	35.205	47539	1245	1.011	0.730
总计		4702498	170398	100.000	100.000



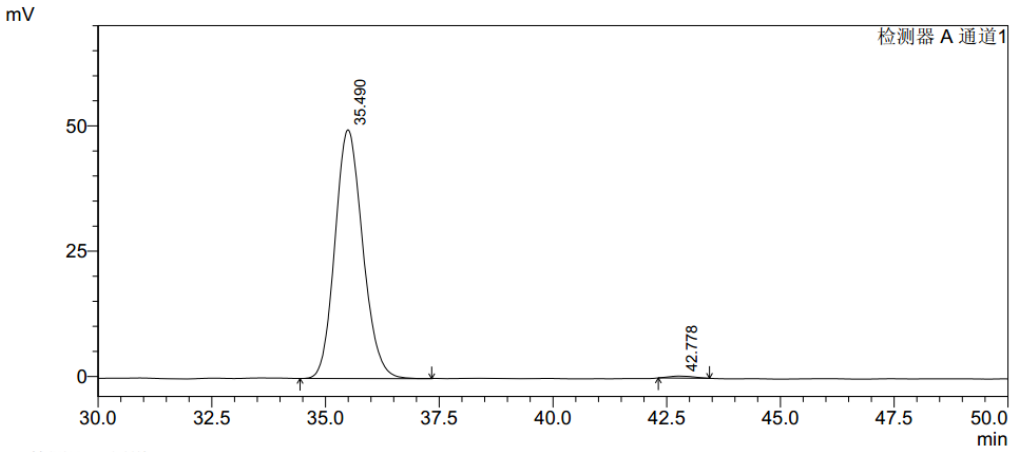


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pMeOB-rac-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	35.397	2345013	52936	50.382	54.252
2	42.715	2309452	44639	49.618	45.748
总计		4654466	97574	100.000	100.000

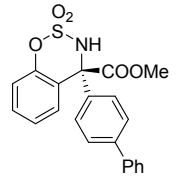


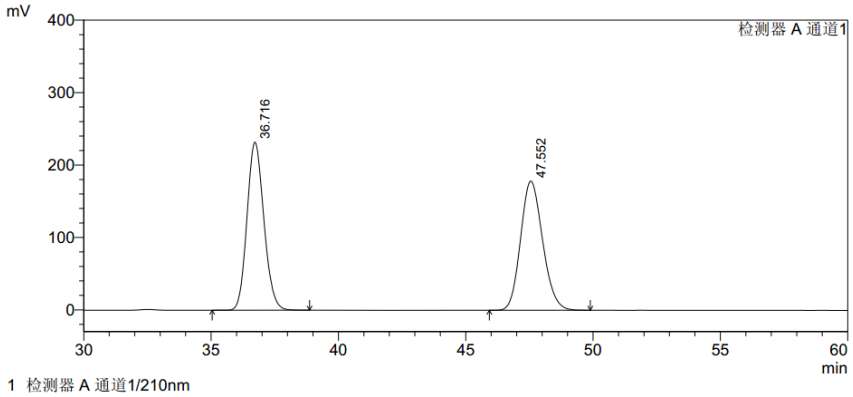
1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pMeOB-cat-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	35.490	2106845	49637	99.280	99.194
2	42.778	15283	403	0.720	0.806
总计		2122128	50040	100.000	100.000



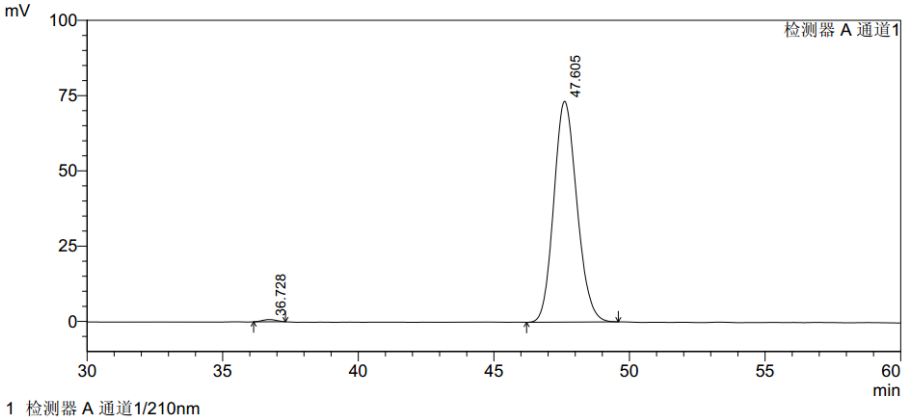


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pPhB-rac-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	36.716	10691310	231993	49.904	56.533
2	47.552	10732399	178375	50.096	43.467
总计		21423709	410368	100.000	100.000

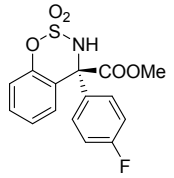


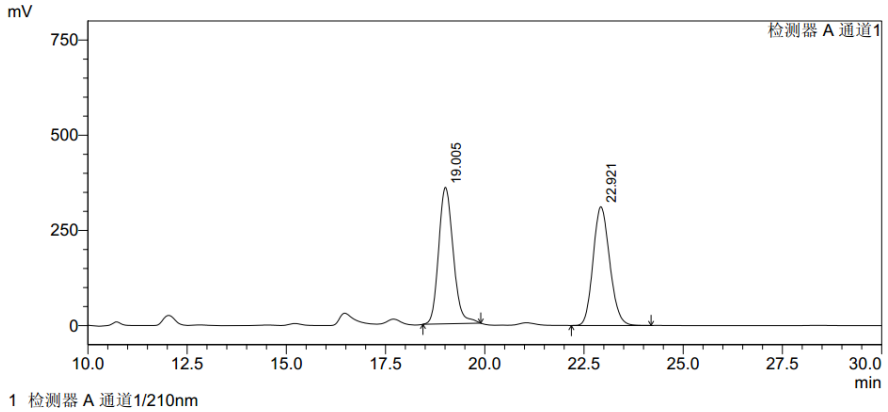
1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pPhB-cat-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	36.728	27158	741	0.622	1.000
2	47.605	4341598	73376	99.378	99.000
总计		4368757	74118	100.000	100.000



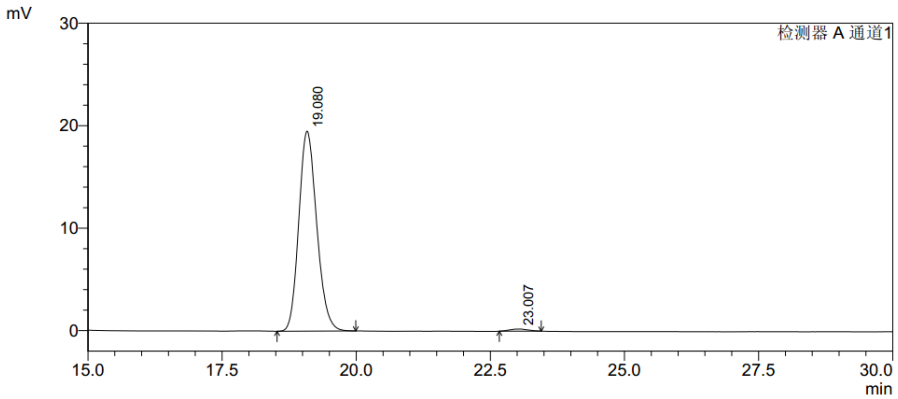


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pFB-rac-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	19.005	9138178	358527	50.120	53.475
2	22.921	9094447	311925	49.880	46.525
总计		18232625	670452	100.000	100.000

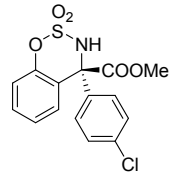


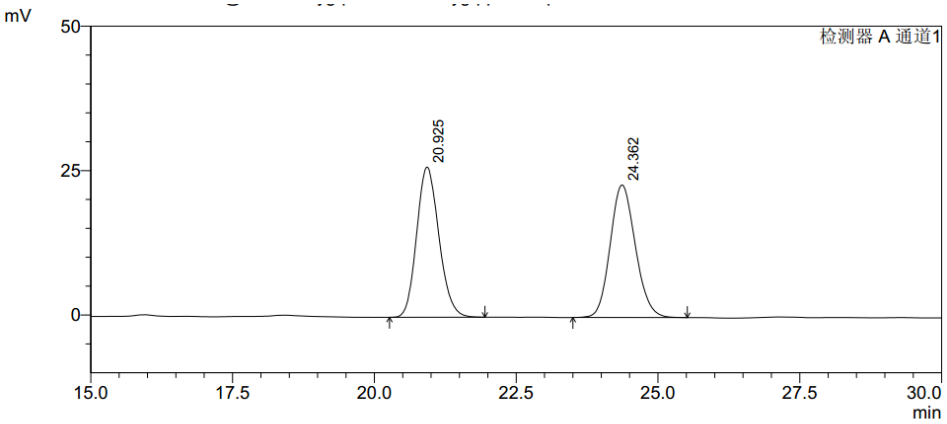
1 检测器 A 通道1/230nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pFB-cat-adh-15%.lcd

检测器 A Ch1 230nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	19.080	453741	19530	98.927	98.954
2	23.007	4921	206	1.073	1.046
总计		458662	19736	100.000	100.000

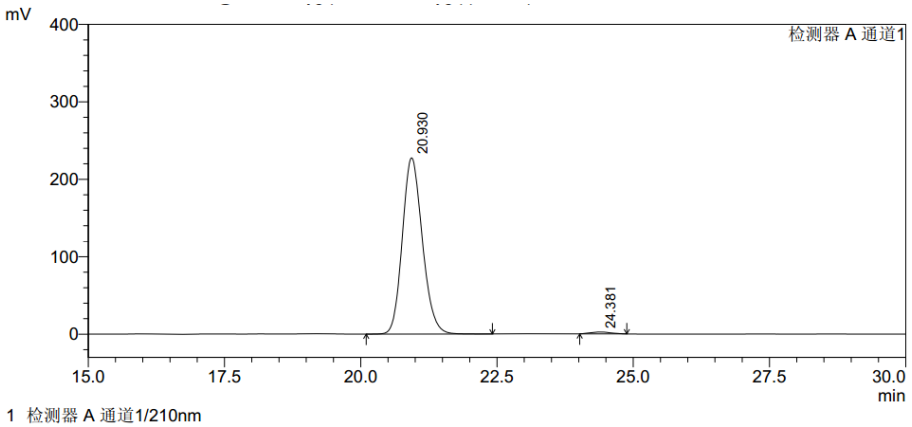




1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pClB-rac-adh-15%.lcd
检测器 A Ch1 210nm

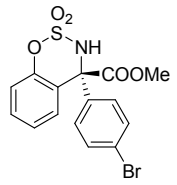
峰#	保留时间	面积	高度	面积 %	高度 %
1	20.925	710172	26000	50.054	53.098
2	24.362	708630	22965	49.946	46.902
总计		1418802	48965	100.000	100.000

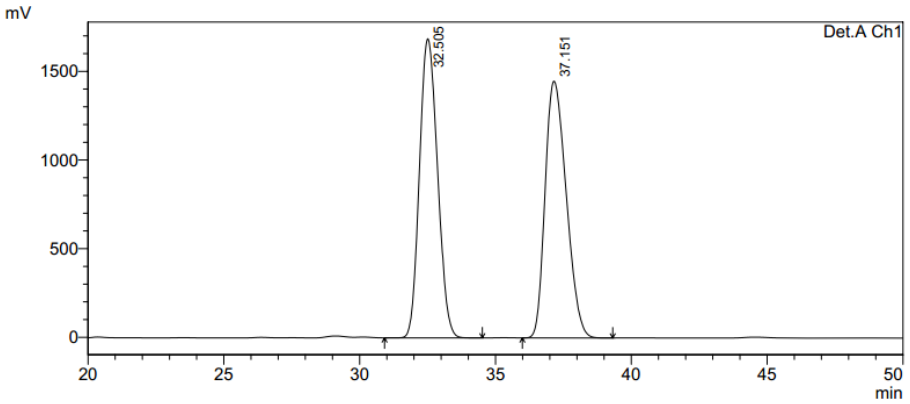


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pClB-cat-adh-15%.lcd
检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	20.930	5813886	227558	98.946	98.959
2	24.381	61906	2394	1.054	1.041
总计		5875792	229951	100.000	100.000



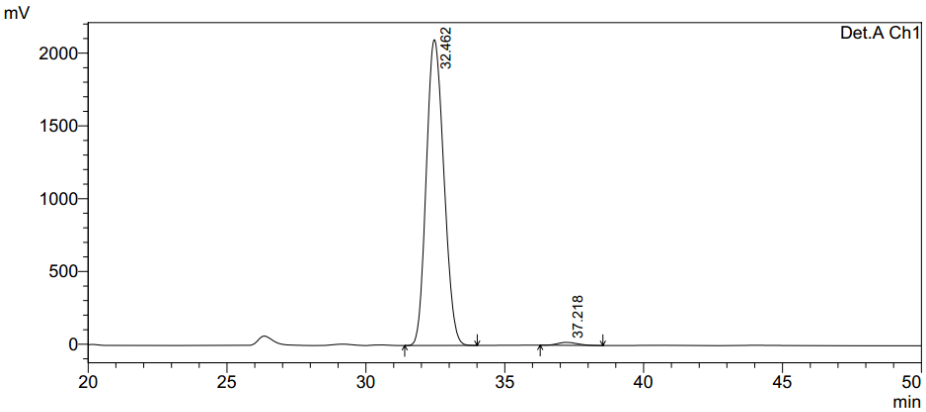


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.505	77939393	1687177	49.847	53.812
2	37.151	78418612	1448160	50.153	46.188
Total		156358005	3135337	100.000	100.000

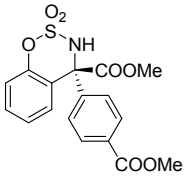


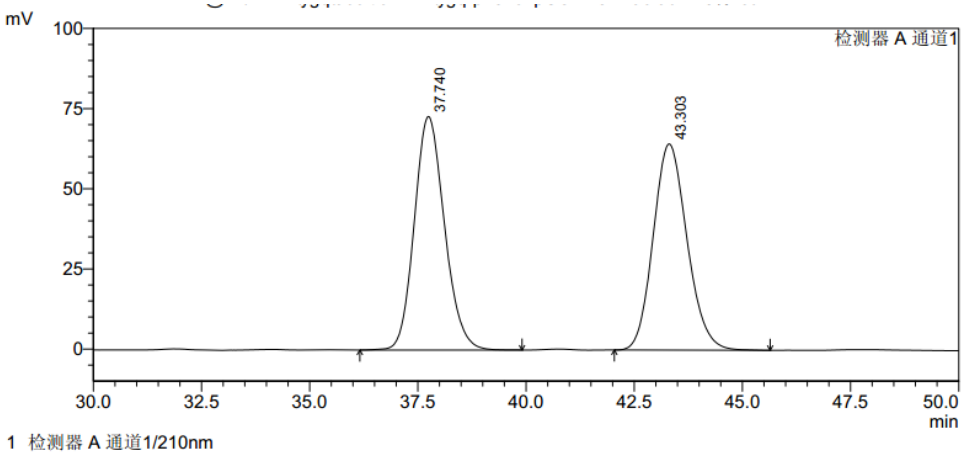
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.462	92522803	2100969	98.923	99.039
2	37.218	1007612	20381	1.077	0.961
Total		93530415	2121350	100.000	100.000



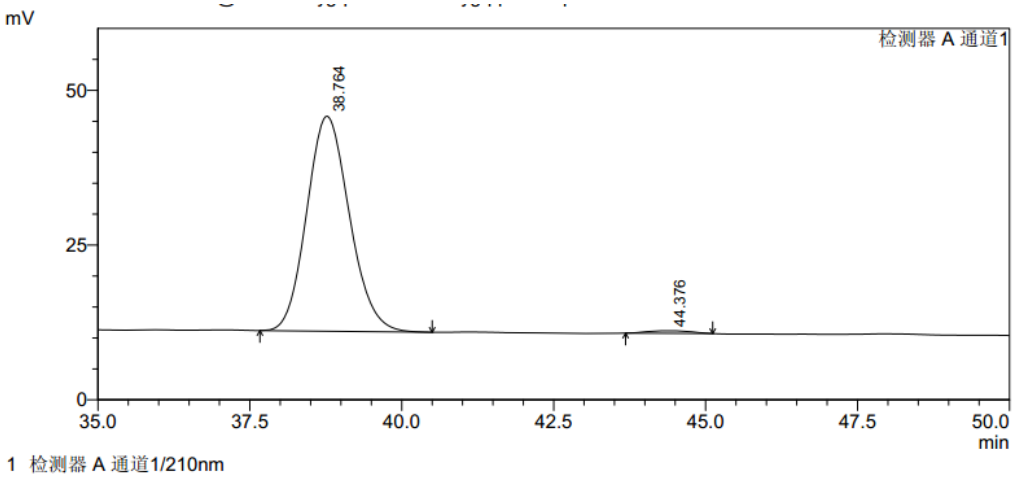


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pCO2MeB-rac-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	37.740	3534063	72849	50.281	53.112
2	43.303	3494609	64311	49.719	46.888
总计		7028672	137160	100.000	100.000

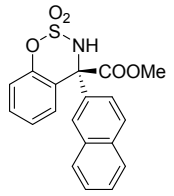


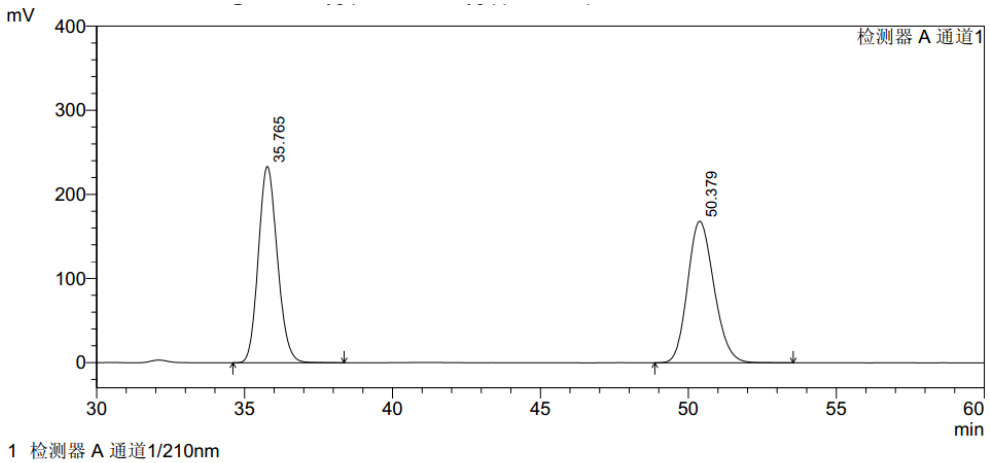
1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-pCO2MeB-cat-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	38.764	1700597	34748	98.746	98.702
2	44.376	21593	457	1.254	1.298
总计		1722189	35205	100.000	100.000

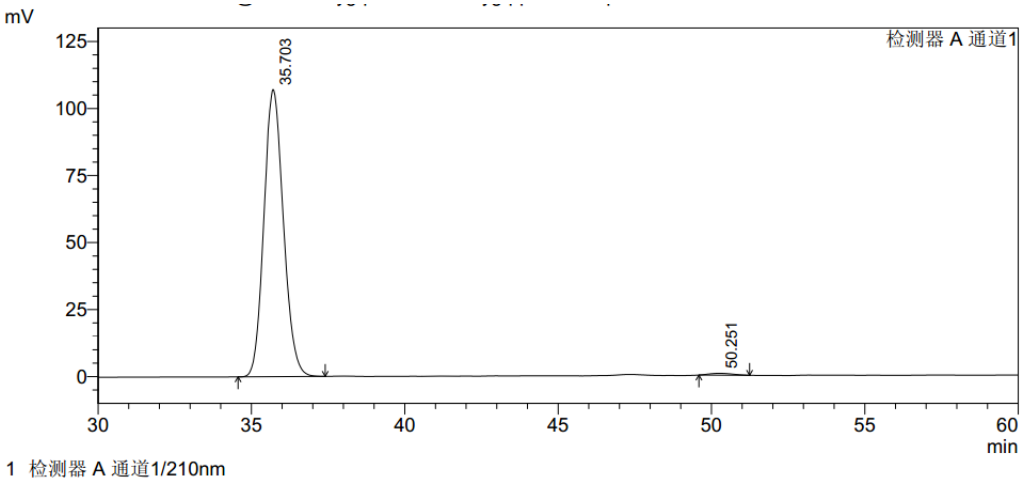




1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-naphB-rac-adh-15%.lcd
检测器 A Ch1 210nm

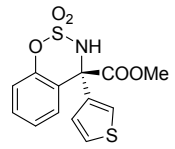
峰#	保留时间	面积	高度	面积 %	高度 %
1	35.765	10433154	233544	50.007	58.111
2	50.379	10430265	168350	49.993	41.889
总计		20863418	401894	100.000	100.000

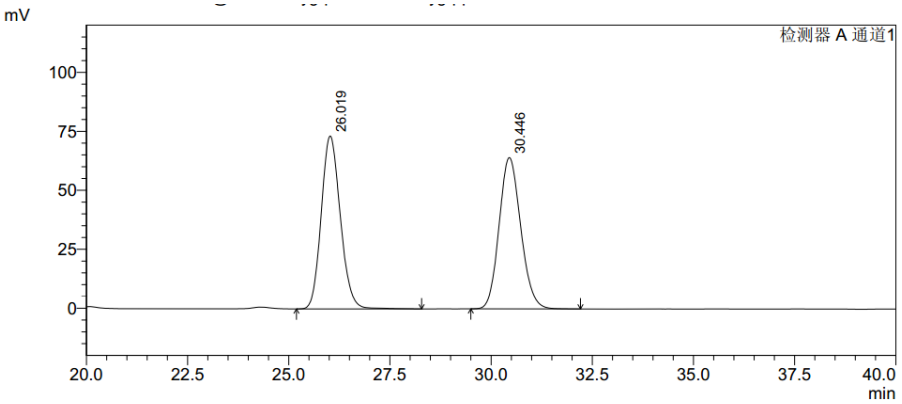


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-naphB-cat-adh-15%.lcd
检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	35.703	4738557	107127	99.257	99.377
2	50.251	35492	672	0.743	0.623
总计		4774049	107799	100.000	100.000



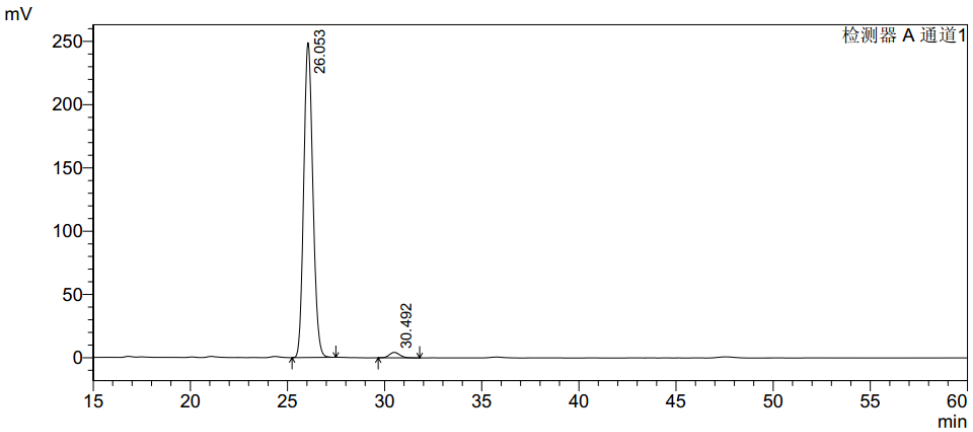


1 检测器 A 通道1/210nm

峰表 @D:\DATA\ygq\addition B-2\ygq-phenol-thioB-rac-adh-15%.lcd

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	26.019	2404308	73301	50.217	53.322
2	30.446	2383491	64168	49.783	46.678
总计		4787799	137469	100.000	100.000

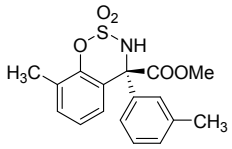


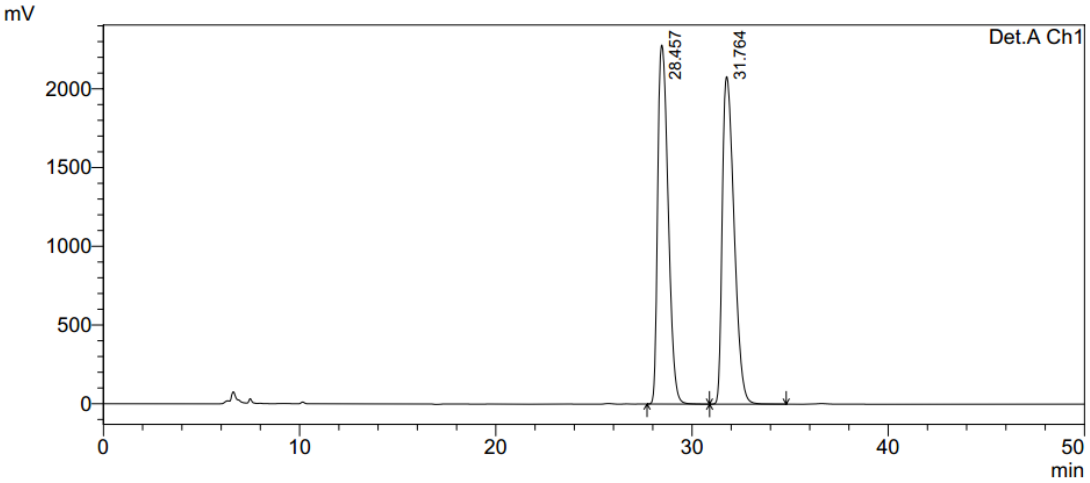
1 检测器 A 通道1/210nm

峰表

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	26.053	8131315	248936	98.060	98.302
2	30.492	160833	4300	1.940	1.698
总计		8292147	253237	100.000	100.000



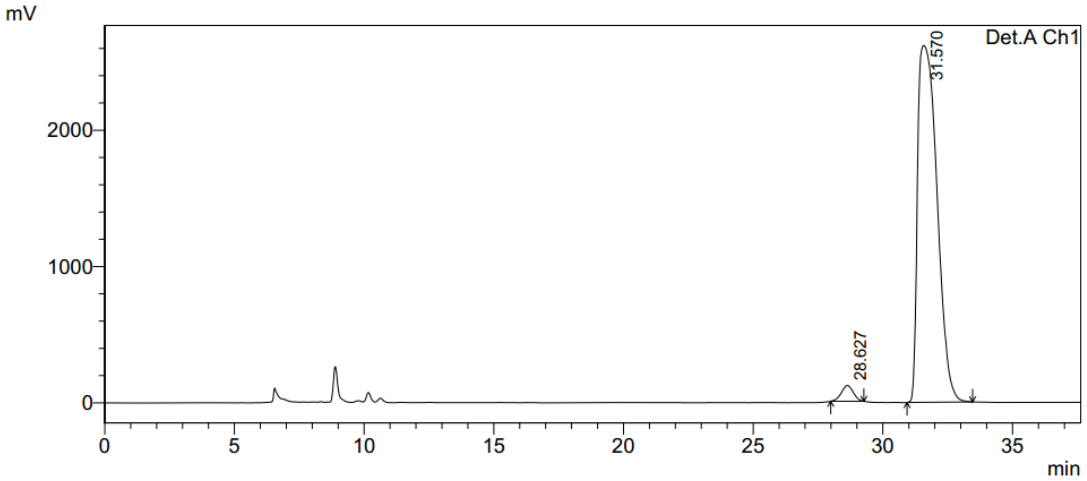


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.457	84244746	2280623	49.174	52.293
2	31.764	87073805	2080589	50.826	47.707
Total		171318551	4361212	100.000	100.000

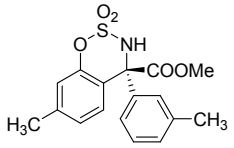


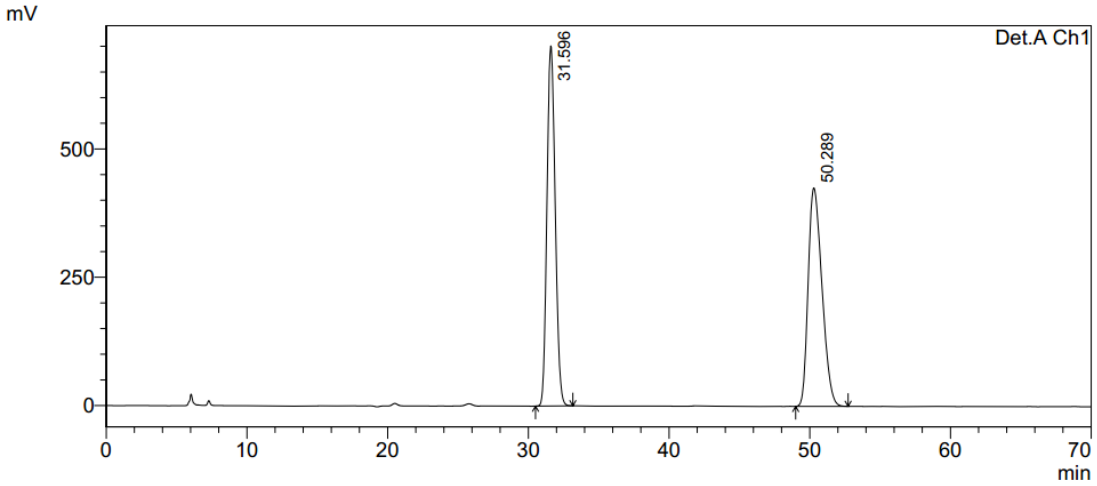
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.627	3724016	116085	2.666	4.245
2	31.570	135955777	2618303	97.334	95.755
Total		139679792	2734388	100.000	100.000



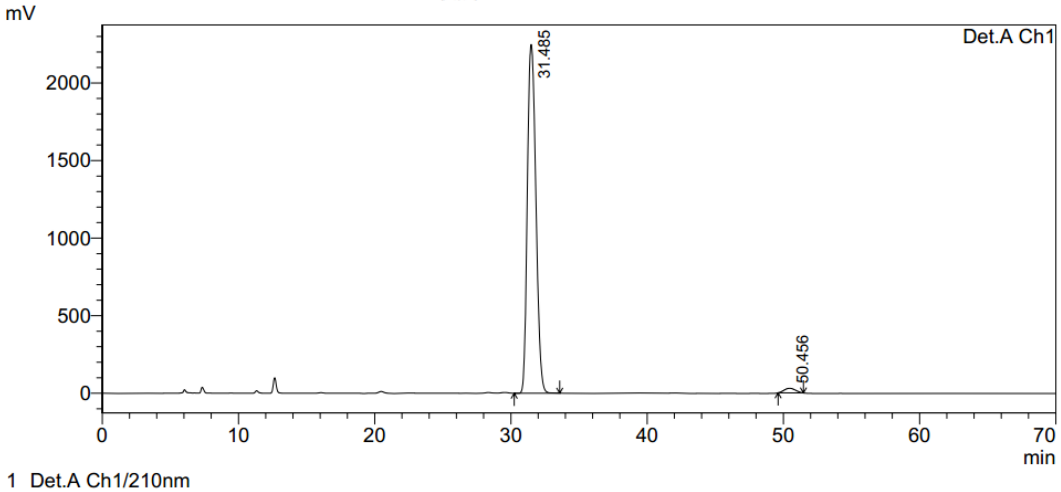


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.596	28683985	701816	49.747	62.249
2	50.289	28975499	425616	50.253	37.751
Total		57659484	1127432	100.000	100.000

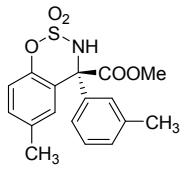


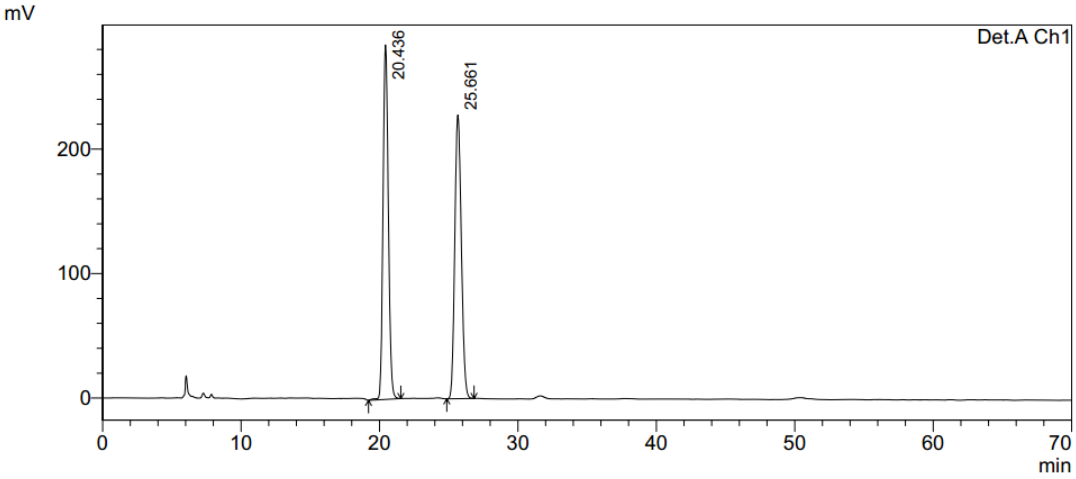
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.485	97857532	2248796	98.271	98.701
2	50.456	1721831	29589	1.729	1.299
Total		99579362	2278385	100.000	100.000



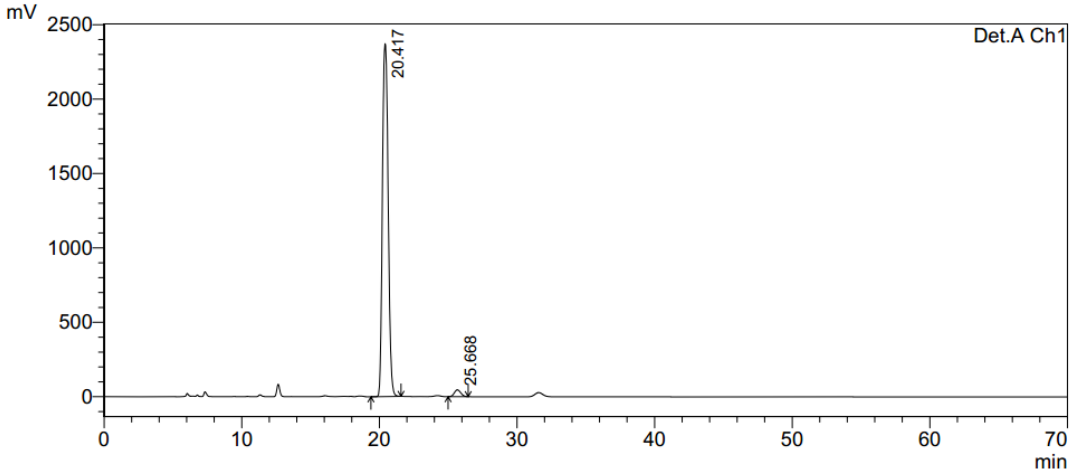


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.436	7567629	284816	50.310	55.546
2	25.661	7474448	227941	49.690	44.454
Total		15042077	512756	100.000	100.000

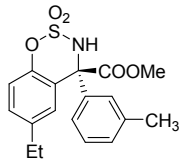


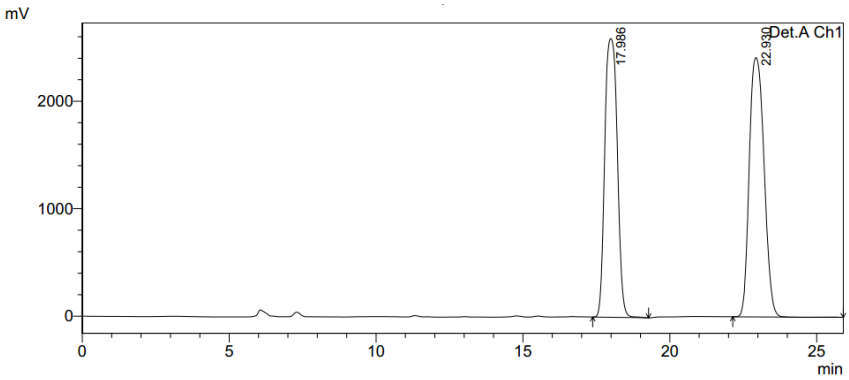
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.417	68737819	2371872	97.863	98.096
2	25.668	1501297	46045	2.137	1.904
Total		70239116	2417916	100.000	100.000



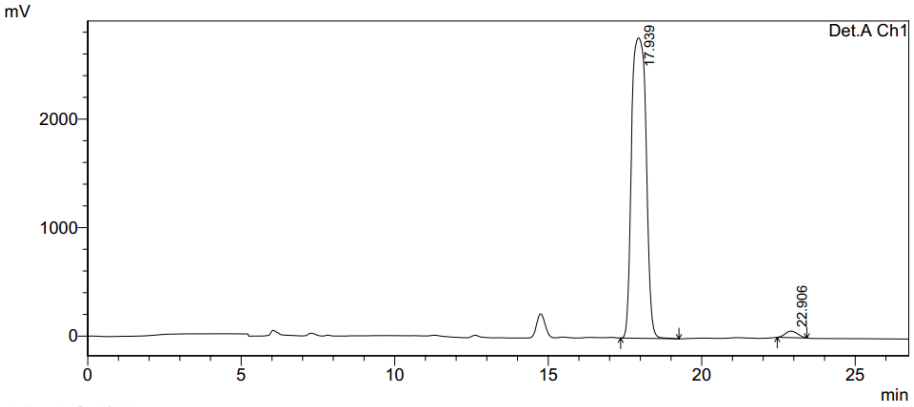


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.986	76848396	2593494	47.695	51.795
2	22.930	84276837	2413718	52.305	48.205
Total		161125232	5007212	100.000	100.000

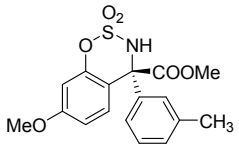


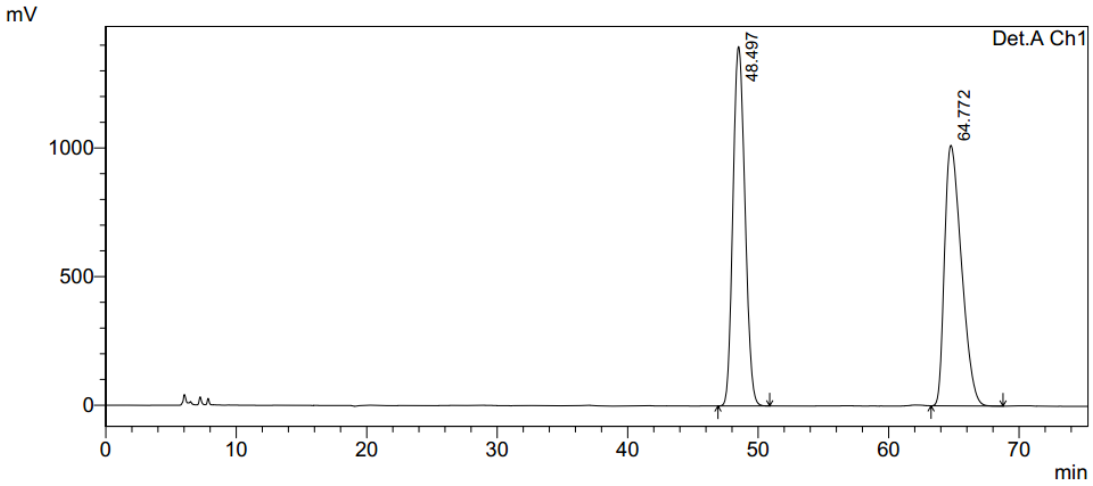
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.939	91168448	2769129	98.177	97.890
2	22.906	1692667	59698	1.823	2.110
Total		92861115	2828827	100.000	100.000



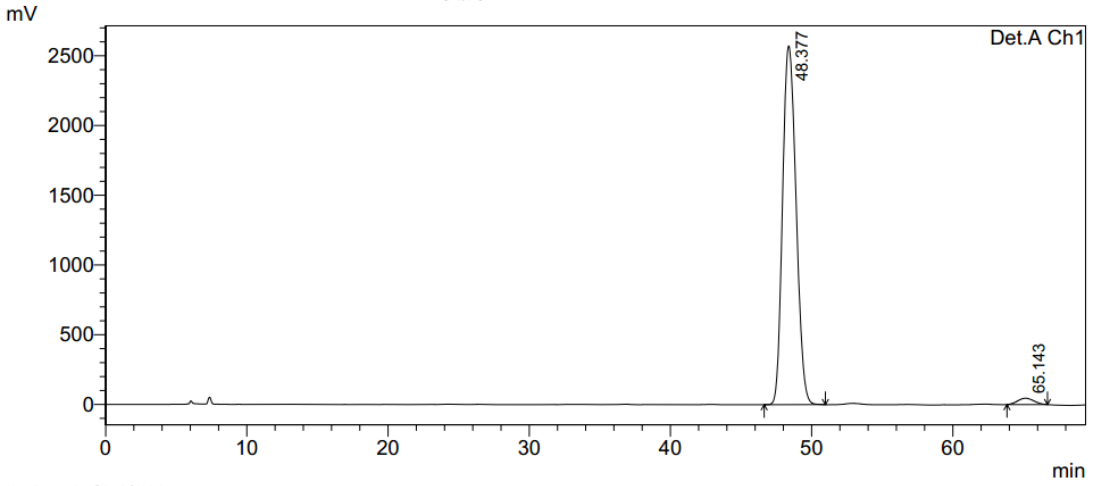


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	48.497	89551579	1397433	49.537	57.975
2	64.772	91225085	1012956	50.463	42.025
Total		180776664	2410389	100.000	100.000

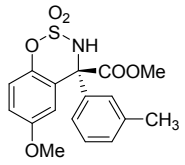


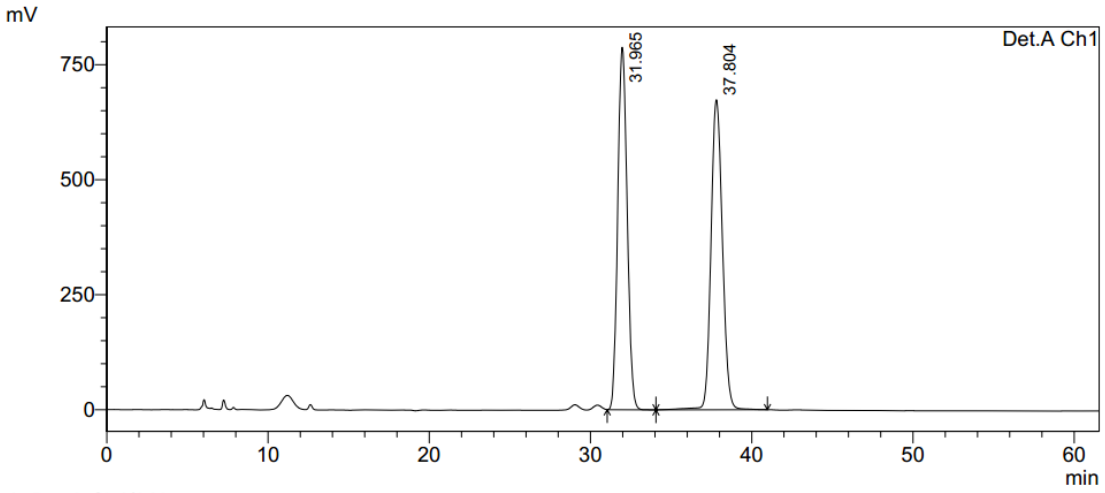
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	48.377	171002535	2572520	97.925	98.268
2	65.143	3624224	45350	2.075	1.732
Total		174626759	2617870	100.000	100.000



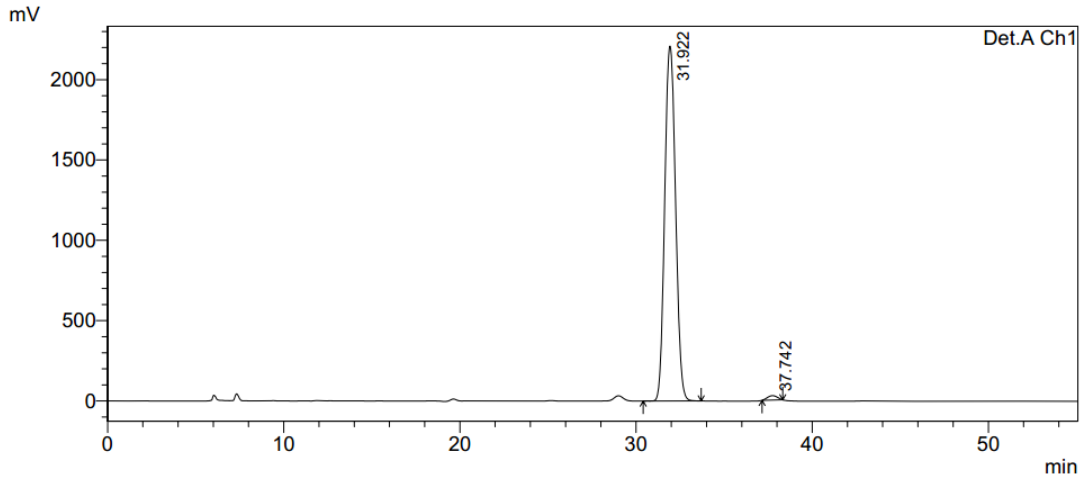


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.965	31964299	788250	49.055	53.906
2	37.804	33195389	674025	50.945	46.094
Total		65159687	1462275	100.000	100.000

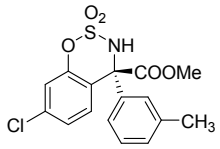


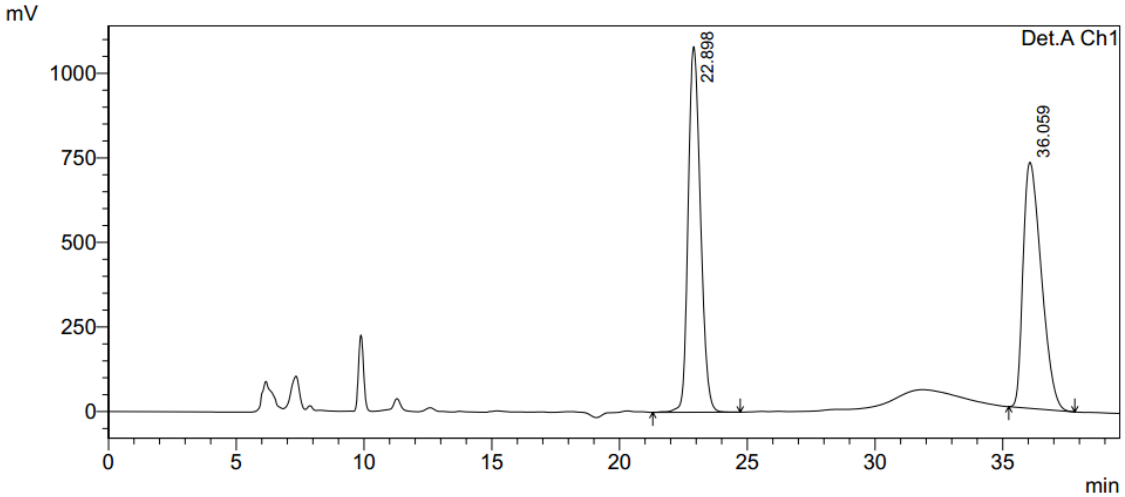
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.922	94520714	2209166	98.875	98.767
2	37.742	1075528	27568	1.125	1.233
Total		95596242	2236734	100.000	100.000



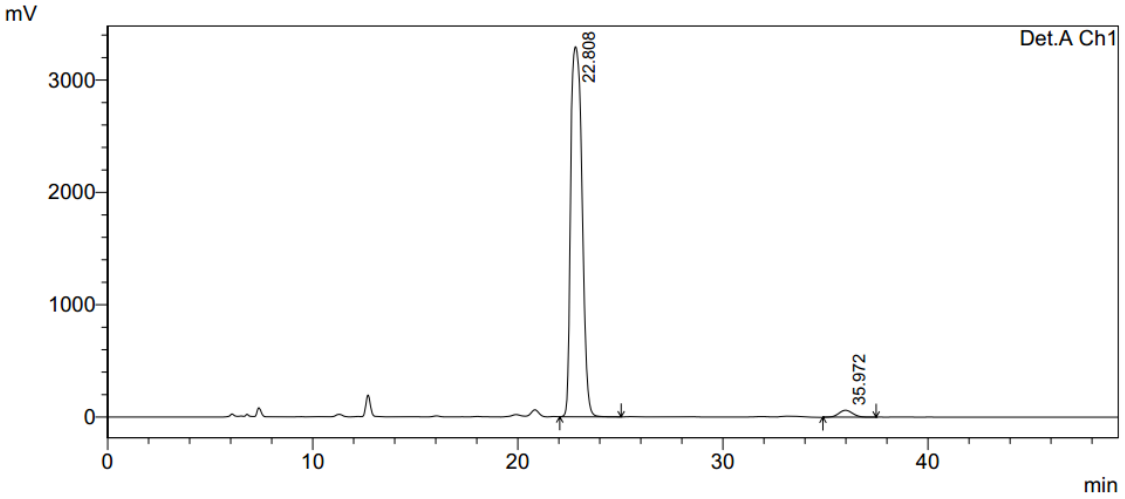


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.898	36239394	1081140	50.078	59.780
2	36.059	36126637	727380	49.922	40.220
Total		72366030	1808520	100.000	100.000

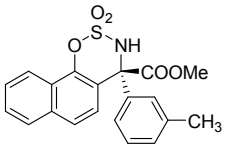


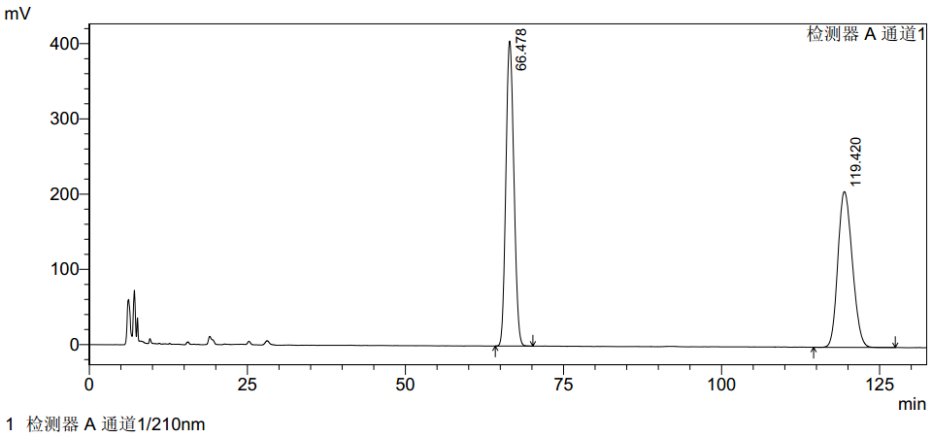
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.808	126726961	3294454	97.825	98.189
2	35.972	2817420	60758	2.175	1.811
Total		129544381	3355212	100.000	100.000



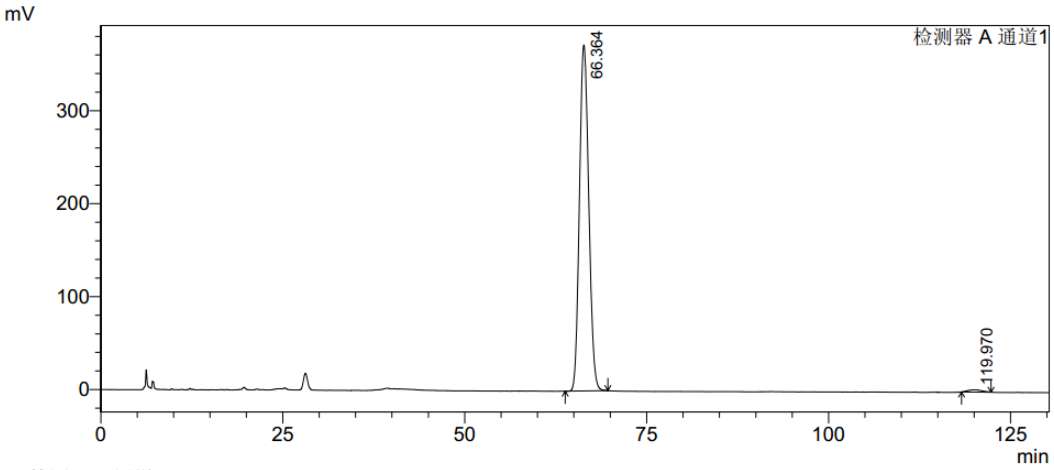


1 检测器 A 通道1/210nm

峰表

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	66.478	35659953	405467	52.042	66.197
2	119.420	32861905	207052	47.958	33.803
总计		68521858	612519	100.000	100.000

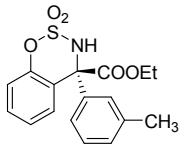


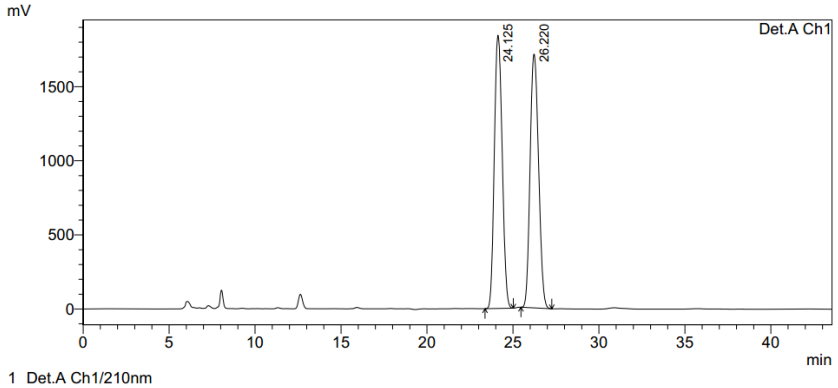
1 检测器 A 通道1/210nm

峰表

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	66.364	33099666	372266	99.043	99.374
2	119.970	319803	2343	0.957	0.626
总计		33419469	374610	100.000	100.000



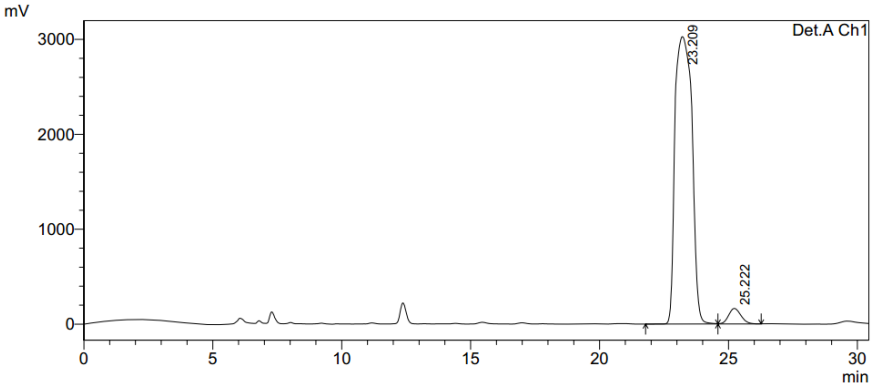


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.125	58484602	1843357	49.922	51.842
2	26.220	58667615	1712354	50.078	48.158
Total		117152217	3555711	100.000	100.000

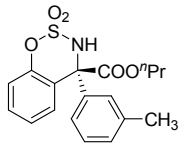


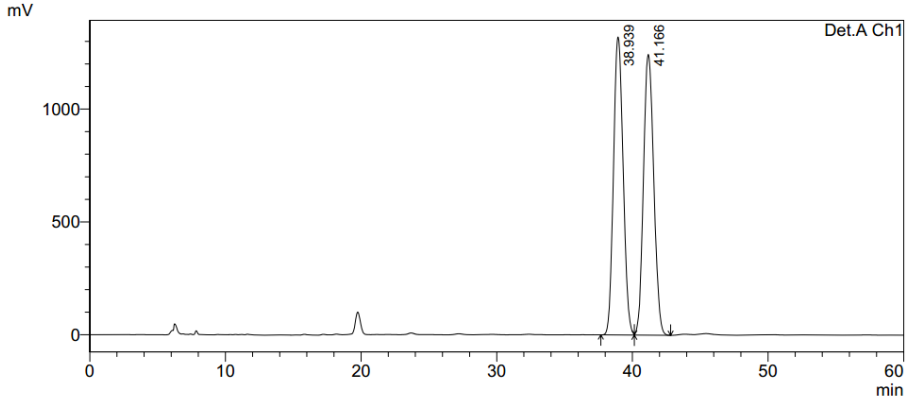
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.209	138359432	3027200	96.193	94.872
2	25.222	5476404	163638	3.807	5.128
Total		143835836	3190838	100.000	100.000



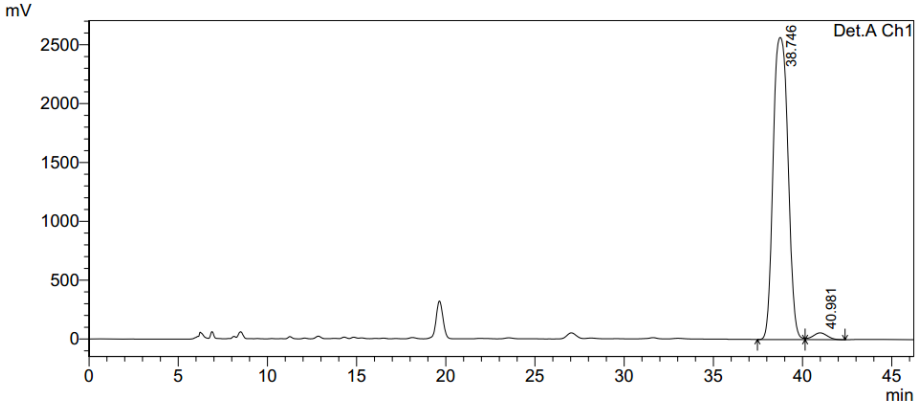


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.939	65354610	1321190	49.921	51.493
2	41.166	65562398	1244561	50.079	48.507
Total		130917008	2565751	100.000	100.000

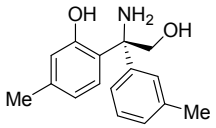


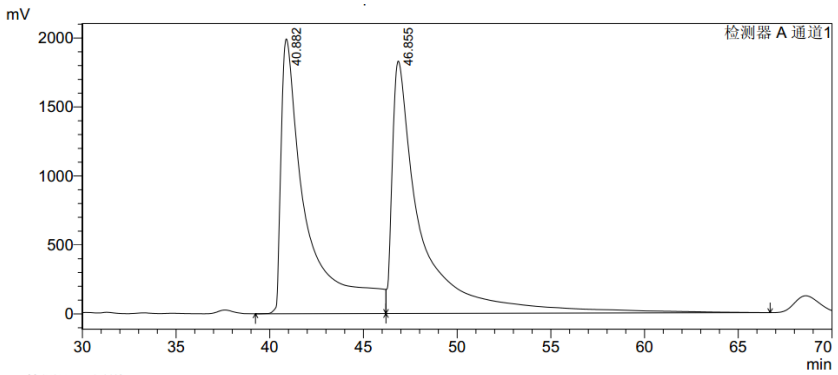
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.746	148633153	2566717	97.879	97.798
2	40.981	3221338	57781	2.121	2.202
Total		151854491	2624498	100.000	100.000



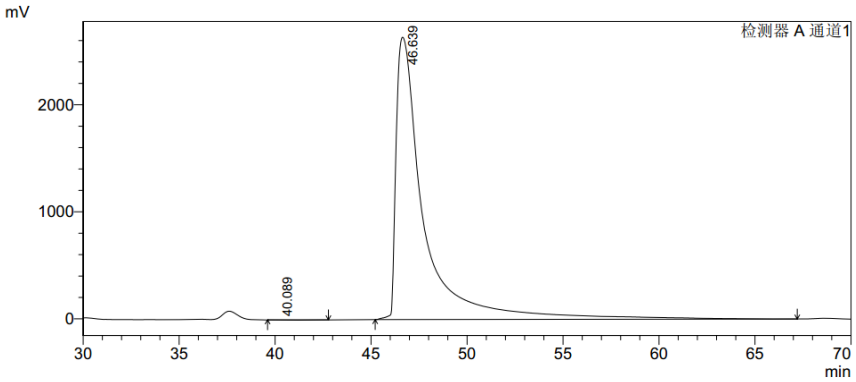


1 检测器 A 通道1/210nm

峰表

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	40.882	188080643	1991912	48.669	52.123
2	46.855	198365639	1829619	51.331	47.877
总计		386446283	3821531	100.000	100.000



1 检测器 A 通道1/210nm

峰表

检测器 A Ch1 210nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	40.089	9673	214	0.004	0.008
2	46.639	267555071	2637632	99.996	99.992
总计		267564744	2637846	100.000	100.000

8. Cartesian Coordinates

5:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.744252	-2.731416	0.166995
2	6	0	-1.711970	-3.639588	0.542157
3	6	0	-3.023906	-3.186273	0.667161
4	6	0	-3.299629	-1.846791	0.423378
5	6	0	-2.262625	-0.989482	0.055312
6	7	0	-1.016092	-1.430488	-0.081101
7	1	0	-3.812461	-3.870647	0.956283
8	1	0	-1.447988	-4.673009	0.730729
9	1	0	-2.446834	0.062357	-0.120987
10	6	0	0.675416	-3.037886	0.000598
11	8	0	1.129317	-4.256215	0.177321
12	6	0	2.583094	-4.131583	0.134920
13	6	0	2.824140	-2.784618	-0.566843
14	1	0	2.922328	-4.145492	1.173492
15	1	0	2.973634	-4.988308	-0.408777
16	1	0	2.903003	-2.944143	-1.648880
17	7	0	1.511873	-2.115401	-0.335378
18	6	0	4.082025	-2.018827	-0.098103
19	6	0	4.487130	-1.025661	-1.197537
20	1	0	3.640666	-0.438064	-1.556674
21	1	0	5.254455	-0.335620	-0.831200
22	1	0	4.899789	-1.560302	-2.059853
23	6	0	3.831046	-1.310346	1.237082
24	1	0	3.057613	-0.539590	1.156489
25	1	0	3.512720	-2.017185	2.011540
26	1	0	4.751453	-0.829679	1.582943
27	6	0	5.234829	-3.025514	0.065048
28	1	0	5.368084	-3.625342	-0.842027
29	1	0	6.168873	-2.483757	0.244343
30	1	0	5.084417	-3.704662	0.910035
31	46	0	0.606879	-0.289814	-0.573817
32	8	0	-0.190524	1.580612	-0.802746
33	6	0	-1.128523	1.886296	-1.811615
34	1	0	-1.675183	0.989670	-2.111491
35	1	0	-0.645411	2.327393	-2.685599
36	6	0	-2.119989	2.882034	-1.249994
37	8	0	2.068987	1.079425	-1.002395
38	1	0	2.797430	1.050442	-0.369407
39	5	0	1.203137	2.328012	-0.779140
40	6	0	1.417127	2.960244	0.682587
41	6	0	0.882479	2.364261	1.835609
42	6	0	2.185292	4.119122	0.856620
43	6	0	1.097603	2.901037	3.102846
44	1	0	0.279230	1.462723	1.741200
45	6	0	2.405852	4.667607	2.119621
46	1	0	2.620266	4.607846	-0.012771
47	6	0	1.860909	4.058891	3.247655
48	1	0	0.666130	2.421391	3.977321
49	1	0	2.999734	5.571540	2.223531
50	1	0	2.026626	4.485271	4.232969
51	8	0	1.371306	3.170560	-1.897993
52	1	0	1.097976	4.073027	-1.711176
53	9	0	-3.049621	3.189843	-2.165531
54	9	0	-1.524971	4.025155	-0.867988
55	9	0	-2.758912	2.397394	-0.166675
56	6	0	-4.668138	-1.254736	0.536791
57	8	0	-4.902494	-0.084750	0.314403
58	8	0	-5.572020	-2.150672	0.900244
59	6	0	-6.921040	-1.672021	1.033754
60	1	0	-7.280548	-1.284782	0.078142
61	1	0	-7.506519	-2.538113	1.337154
62	1	0	-6.968327	-0.892061	1.796148

5-TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.738652	-2.196785	-0.551410
2	6	0	-1.743862	-3.112376	-0.782444
3	6	0	-3.062892	-2.660921	-0.751490
4	6	0	-3.314507	-1.316742	-0.503104
5	6	0	-2.244910	-0.448009	-0.291163
6	7	0	-0.992591	-0.892578	-0.305193
7	1	0	-3.878827	-3.354431	-0.917415
8	1	0	-1.504161	-4.150888	-0.975378
9	1	0	-2.395626	0.607369	-0.103591
10	6	0	0.695974	-2.483316	-0.548951
11	8	0	1.148207	-3.691996	-0.793841
12	6	0	2.580956	-3.627172	-0.518897
13	6	0	2.903396	-2.121688	-0.538712

14	1	0	2.727157	-4.091563	0.459214
15	1	0	3.092280	-4.194731	-1.292811
16	1	0	3.212420	-1.825788	-1.548389
17	7	0	1.549663	-1.543480	-0.328319
18	6	0	3.995460	-1.668483	0.455744
19	6	0	4.538892	-0.308159	-0.002490
20	1	0	3.743662	0.419560	-0.170329
21	1	0	5.225981	0.100782	0.746028
22	1	0	5.091166	-0.416717	-0.942518
23	6	0	3.444108	-1.591242	1.883205
24	1	0	2.667193	-0.825822	1.979292
25	1	0	3.009670	-2.545706	2.201346
26	1	0	4.249903	-1.342702	2.581147
27	6	0	5.153711	-2.679309	0.401338
28	1	0	5.493168	-2.841071	-0.627958
29	1	0	6.002775	-2.291525	0.973056
30	1	0	4.885353	-3.648669	0.833037
31	46	0	0.594226	0.259216	0.119741
32	8	0	0.169331	2.657651	-0.372398
33	6	0	0.759056	3.304676	-1.466533
34	1	0	1.804820	3.577300	-1.292632
35	1	0	0.201222	4.213387	-1.718607
36	6	0	0.717821	2.407594	-2.686777
37	8	0	2.031913	1.621621	0.600395
38	1	0	2.571728	1.390142	1.368130
39	5	0	0.903961	2.635188	0.925113
40	6	0	-0.157578	1.899828	1.939531
41	6	0	-1.542048	2.141048	1.824621
42	6	0	0.252245	1.030961	2.973172
43	6	0	-2.464832	1.539694	2.673189
44	1	0	-1.897880	2.801573	1.038773
45	6	0	-0.665973	0.424926	3.829950
46	1	0	1.310566	0.828868	3.122033
47	6	0	-2.027375	0.671839	3.674738
48	1	0	-3.525726	1.734846	2.546316
49	1	0	-0.318205	-0.242093	4.613318
50	1	0	-2.746140	0.195348	4.335094
51	8	0	1.521326	3.848331	1.326700
52	1	0	0.919929	4.377046	1.858069
53	9	0	1.024301	3.103376	-3.792506
54	9	0	-0.498101	1.858927	-2.872834
55	9	0	1.593980	1.380859	-2.615069
56	6	0	-4.688456	-0.734219	-0.414893
57	8	0	-4.894005	0.438476	-0.176591
58	8	0	-5.630707	-1.642176	-0.610602
59	6	0	-6.987818	-1.176882	-0.519735
60	1	0	-7.179920	-0.424709	-1.287597
61	1	0	-7.607444	-2.055970	-0.685942
62	1	0	-7.175207	-0.756614	0.470277

6:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.327896	1.908512	-0.004012
2	6	0	3.520467	2.567302	0.234085
3	6	0	4.690087	1.820032	0.322543
4	6	0	4.612304	0.442040	0.165353
5	6	0	3.370610	-0.150006	-0.058680
6	7	0	2.247521	0.564918	-0.138044
7	1	0	5.640263	2.308397	0.503415
8	1	0	3.530658	3.644622	0.343197
9	1	0	3.285239	-1.222094	-0.176443
10	6	0	1.054031	2.627636	-0.156817
11	8	0	1.071172	3.947946	-0.023928
12	6	0	-0.323596	4.351695	-0.041397
13	6	0	-1.054411	3.129594	-0.624852
14	1	0	-0.600482	4.571817	0.993138
15	1	0	-0.406506	5.249833	-0.650180
16	1	0	-1.176497	3.259134	-1.707702
17	7	0	-0.053691	2.047033	-0.435836
18	6	0	-2.449724	2.853558	-0.022087
19	6	0	-3.203423	1.900379	-0.956239
20	1	0	-2.604421	1.020790	-1.192968
21	1	0	-4.138598	1.562893	-0.499467
22	1	0	-3.449663	2.399045	-1.900288
23	6	0	-2.330517	2.251097	1.380785
24	1	0	-1.837520	1.275193	1.356394
25	1	0	-1.756610	2.898406	2.053372
26	1	0	-3.325616	2.118107	1.818559
27	6	0	-3.231231	4.175432	0.040593
28	1	0	-3.239619	4.679148	-0.932572
29	1	0	-4.271249	3.974107	0.317833
30	1	0	-2.823355	4.869304	0.782973
31	46	0	0.325603	-0.175842	-0.411228
32	6	0	0.952638	-2.035148	-0.293669
33	6	0	1.161460	-2.631595	0.952426

34	6	0	1.195613	-2.763540	-1.460535
35	6	0	1.620307	-3.947852	1.027398
36	1	0	0.979404	-2.075499	1.868276
37	6	0	1.658238	-4.078485	-1.378794
38	1	0	1.035810	-2.310859	-2.436105
39	6	0	1.872005	-4.671876	-0.136441
40	1	0	1.782261	-4.405905	1.999384
41	1	0	1.852308	-4.636524	-2.290754
42	1	0	2.234483	-5.693732	-0.074887
43	8	0	-1.620669	-1.044504	-0.658959
44	1	0	-1.979631	-1.068346	-1.554159
45	5	0	-2.547065	-1.247679	0.356533
46	8	0	-2.043195	-1.304238	1.611280
47	1	0	-2.685752	-1.439239	2.315077
48	8	0	-3.849847	-1.357339	-0.026043
49	6	0	-4.882009	-1.469794	0.925932
50	1	0	-4.881669	-2.452344	1.406412
51	1	0	-4.820847	-0.689047	1.690991
52	6	0	-6.193858	-1.297272	0.195805
53	9	0	-6.366999	-2.228969	-0.753287
54	9	0	-7.215512	-1.393223	1.059907
55	9	0	-6.278283	-0.098398	-0.405542
56	6	0	5.803009	-0.458279	0.217160
57	8	0	5.739665	-1.657386	0.035859
58	8	0	6.921780	0.202816	0.478723
59	6	0	8.125796	-0.579933	0.518248
60	1	0	8.298086	-1.053216	-0.450643
61	1	0	8.922717	0.126433	0.743662
62	1	0	8.059318	-1.340991	1.298469

7:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.129381	-1.820604	-0.231204
2	6	0	-0.886888	-2.975192	-0.184886
3	6	0	-2.268393	-2.861838	-0.059840
4	6	0	-2.830441	-1.594228	0.014724
5	6	0	-1.999889	-0.474352	-0.035566
6	7	0	-0.678173	-0.582848	-0.154630
7	1	0	-2.889917	-3.748758	-0.023281
8	1	0	-0.403068	-3.941976	-0.249209
9	1	0	-2.416129	0.523304	0.021109
10	6	0	1.335569	-1.836271	-0.374882
11	8	0	1.981950	-2.989934	-0.379454
12	6	0	3.396086	-2.657392	-0.509107
13	6	0	3.434447	-1.108275	-0.572618
14	1	0	3.899840	-3.085259	0.357938
15	1	0	3.760383	-3.131960	-1.419767
16	1	0	3.809623	-0.779284	-1.547274
17	7	0	2.009855	-0.755911	-0.490838
18	6	0	4.278711	-0.405050	0.518483
19	6	0	4.248149	1.110518	0.274871
20	1	0	3.250195	1.535581	0.440763
21	1	0	4.931175	1.616694	0.964921
22	1	0	4.557504	1.355520	-0.747377
23	6	0	3.740950	-0.710404	1.920870
24	1	0	2.713810	-0.347841	2.040434
25	1	0	3.752518	-1.783217	2.142547
26	1	0	4.359828	-0.212756	2.674513
27	6	0	5.728699	-0.892993	0.386205
28	1	0	6.122242	-0.696803	-0.617529
29	1	0	6.366520	-0.369168	1.105435
30	1	0	5.825912	-1.965677	0.584084
31	46	0	0.716903	0.971434	-0.294428
32	6	0	-0.517015	2.463023	-0.088473
33	6	0	-1.326248	2.667862	1.030009
34	6	0	-0.417870	3.443440	-1.079452
35	6	0	-2.019921	3.871636	1.165975
36	1	0	-1.414217	1.902574	1.797642
37	6	0	-1.115944	4.644010	-0.935367
38	1	0	0.196899	3.279795	-1.963304
39	6	0	-1.915484	4.857318	0.186139
40	1	0	-2.640455	4.037691	2.041995
41	1	0	-1.040205	5.407126	-1.704777
42	1	0	-2.458617	5.791143	0.295668
43	6	0	-4.299060	-1.356089	0.146554
44	8	0	-4.786646	-0.248612	0.248504
45	8	0	-4.993543	-2.484564	0.136443
46	6	0	-6.419163	-2.350744	0.256212
47	1	0	-6.810775	-3.365579	0.217517
48	1	0	-6.675172	-1.878277	1.206695
49	1	0	-6.812763	-1.758908	-0.572585

8:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.869004	1.640848	-0.288010
2	6	0	4.197831	2.005261	-0.397558
3	6	0	5.166723	1.007254	-0.363605
4	6	0	4.756726	-0.312521	-0.227586
5	6	0	3.395240	-0.599616	-0.135948
6	7	0	2.466116	0.353953	-0.159275
7	1	0	6.217950	1.257945	-0.442254
8	1	0	4.464991	3.049423	-0.504214
9	1	0	3.056667	-1.623102	-0.039113
10	6	0	1.778346	2.626063	-0.284986
11	8	0	2.064392	3.910631	-0.426316
12	6	0	0.773975	4.578757	-0.541005
13	6	0	-0.237489	3.531778	-0.032877
14	1	0	0.827851	5.495091	0.044324
15	1	0	0.630324	4.818140	-1.596552
16	1	0	-1.090383	3.467115	-0.711822
17	7	0	0.552177	2.286177	-0.132075
18	6	0	-0.775019	3.771277	1.403411
19	6	0	-1.690625	2.609227	1.804302
20	1	0	-1.142991	1.665434	1.853927
21	1	0	-2.122216	2.796100	2.793690
22	1	0	-2.515985	2.491504	1.094559
23	6	0	0.370463	3.886193	2.417474
24	1	0	0.957187	2.961929	2.466852
25	1	0	1.049441	4.713285	2.183954
26	1	0	-0.037925	4.069095	3.416699
27	6	0	-1.596700	5.067663	1.389084
28	1	0	-2.397469	5.017904	0.642700
29	1	0	-2.058481	5.226754	2.369018
30	1	0	-0.982649	5.947348	1.169604
31	46	0	0.376811	0.108123	-0.138839
32	6	0	0.038788	-2.605519	-1.267613
33	6	0	0.476016	-1.870620	-0.161240
34	6	0	0.098963	-3.999818	-1.254820
35	6	0	0.971496	-2.550790	0.956381
36	6	0	0.590278	-4.672541	-0.138005
37	1	0	-0.241258	-4.559004	-2.122122
38	6	0	1.028094	-3.945505	0.966466
39	1	0	1.314194	-1.998305	1.828088
40	1	0	0.633332	-5.757619	-0.129296
41	1	0	1.412534	-4.460155	1.842624
42	1	0	-0.354835	-2.099721	-2.145664
43	6	0	-2.569502	-0.747211	0.381777
44	6	0	-3.968742	-0.926494	0.063664
45	6	0	-4.395012	-0.737767	-1.258435
46	1	0	-4.626429	-1.466406	2.054295
47	6	0	-4.918336	-1.329994	1.018658
48	6	0	-5.695937	-0.961302	-1.659211
49	6	0	-6.615227	-1.360912	-0.693894
50	6	0	-6.233325	-1.533560	0.639059
51	1	0	-5.974545	-0.817001	-2.696436
52	1	0	-7.646347	-1.531080	-0.984726
53	1	0	-6.966245	-1.834819	1.378297
54	8	0	-3.461747	-0.384398	-2.226060
55	16	0	-2.319695	0.656345	-1.757711
56	8	0	-1.311305	0.599773	-2.779950
57	8	0	-2.931899	1.903961	-1.374989
58	7	0	-1.717021	-0.109450	-0.366303
59	6	0	-2.021977	-1.357339	1.664692
60	8	0	-2.275292	-2.645713	1.695265
61	8	0	-1.469038	-0.703021	2.515825
62	6	0	-1.874365	-3.352648	2.888205
63	1	0	-2.044541	-4.404109	2.668283
64	1	0	-0.820965	-3.167734	3.099027
65	1	0	-2.494995	-3.026643	3.724992
66	6	0	5.706570	-1.462886	-0.161964
67	8	0	5.349205	-2.614193	-0.014039
68	8	0	6.969527	-1.077047	-0.273657
69	6	0	7.960046	-2.111539	-0.167217
70	1	0	7.831149	-2.845406	-0.965576
71	1	0	8.919489	-1.607503	-0.268634
72	1	0	7.887517	-2.602790	0.805153

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.844188	1.453391	-0.394794
2	6	0	4.214377	1.565290	-0.530385
3	6	0	4.992256	0.422961	-0.356472
4	6	0	4.359524	-0.778537	-0.064769
5	6	0	2.970618	-0.806013	0.057952
6	7	0	2.228124	0.286405	-0.094214
7	1	0	6.069824	0.474308	-0.458974
8	1	0	4.662181	2.521346	-0.772388

9	1	0	2.458390	-1.733037	0.281215
10	6	0	1.917642	2.579393	-0.578683
11	8	0	2.376604	3.767450	-0.923654
12	6	0	1.190630	4.571805	-1.202719
13	6	0	0.029093	3.771181	-0.574447
14	1	0	1.361669	5.555778	-0.770629
15	1	0	1.106248	4.649711	-2.288205
16	1	0	-0.803848	3.688443	-1.276235
17	7	0	0.651537	2.439484	-0.422105
18	6	0	-0.509075	4.336938	0.767614
19	6	0	-1.608614	3.419001	1.314089
20	1	0	-1.219549	2.437287	1.592590
21	1	0	-2.056546	3.868711	2.206860
22	1	0	-2.407196	3.271702	0.578584
23	6	0	0.612293	4.462420	1.806588
24	1	0	1.065082	3.489226	2.026758
25	1	0	1.404333	5.144209	1.478496
26	1	0	0.207982	4.858424	2.743854
27	6	0	-1.123932	5.715881	0.485943
28	1	0	-1.906816	5.650313	-0.278141
29	1	0	-1.578527	6.112275	1.399585
30	1	0	-0.381967	6.447126	0.149314
31	46	0	0.124811	0.416411	-0.066776
32	6	0	-0.158478	-2.257430	-1.094033
33	6	0	-0.168839	-1.619237	0.158437
34	6	0	0.293744	-3.565227	-1.208193
35	6	0	0.241197	-2.326365	1.299248
36	6	0	0.694234	-4.263227	-0.067350
37	1	0	0.321021	-4.046455	-2.180529
38	6	0	0.663967	-3.647175	1.182754
39	1	0	0.238849	-1.848821	2.272259
40	1	0	1.024868	-5.293635	-0.154078
41	1	0	0.976051	-4.192392	2.067884
42	1	0	-0.502906	-1.733972	-1.982065
43	6	0	-2.121684	-0.741852	0.524062
44	6	0	-2.966952	-1.792084	-0.064732
45	6	0	-3.336496	-1.705345	-1.412572
46	1	0	-2.982786	-3.092595	1.655276
47	6	0	-3.297129	-2.968250	0.626604
48	6	0	-4.045350	-2.703569	-2.055814
49	6	0	-4.379484	-3.847186	-1.340884
50	6	0	-4.000317	-3.980950	-0.004334
51	1	0	-4.308271	-2.580700	-3.100359
52	1	0	-4.929413	-4.642104	-1.833454
53	1	0	-4.247284	-4.883654	0.543348
54	8	0	-2.910820	-0.640174	-2.203293
55	16	0	-2.757602	0.801513	-1.465941
56	8	0	-1.945483	1.588964	-2.360377
57	8	0	-4.075418	1.254659	-1.082289
58	7	0	-1.916856	0.457699	-0.091777
59	6	0	-2.052814	-0.523330	2.044613
60	8	0	-3.164961	-0.919629	2.623213
61	8	0	-1.140234	0.046136	2.598013
62	6	0	-3.271831	-0.664554	4.039261
63	1	0	-4.227593	-1.092378	4.333992
64	1	0	-2.450577	-1.152980	4.566400
65	1	0	-3.256641	0.411102	4.222399
66	6	0	5.084041	-2.072394	0.113451
67	8	0	4.519618	-3.123367	0.342532
68	8	0	6.395403	-1.935195	-0.014575
69	6	0	7.173392	-3.136116	0.112951
70	1	0	6.867962	-3.863850	-0.641391
71	1	0	8.206625	-2.833362	-0.047096
72	1	0	7.050654	-3.561528	1.111241

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.770176	1.328777	0.350420
2	6	0	-4.136841	1.413533	0.533398
3	6	0	-4.908215	0.281639	0.277649
4	6	0	-4.277151	-0.879191	-0.154189
5	6	0	-2.891696	-0.885392	-0.305326
6	7	0	-2.155717	0.191174	-0.044952
7	1	0	-5.983119	0.312541	0.412548
8	1	0	-4.587263	2.342076	0.862255
9	1	0	-2.376229	-1.775997	-0.641882
10	6	0	-1.838678	2.450667	0.542794
11	8	0	-2.227463	3.534577	1.188353
12	6	0	-1.007490	4.303149	1.418450
13	6	0	0.026457	3.671339	0.462223
14	1	0	-1.238335	5.348477	1.221531
15	1	0	-0.745682	4.169443	2.469879
16	1	0	0.957678	3.450282	0.991082
17	7	0	-0.626984	2.391267	0.120387
18	6	0	0.366900	4.515583	-0.791237

19	6	0	1.316100	3.710894	-1.681280
20	1	0	0.830706	2.813660	-2.070022
21	1	0	1.638367	4.314236	-2.536628
22	1	0	2.213617	3.408894	-1.129247
23	6	0	-0.897233	4.872383	-1.583916
24	1	0	-1.427532	3.973852	-1.918661
25	1	0	-1.592676	5.485103	-1.000378
26	1	0	-0.626826	5.445923	-2.476543
27	6	0	1.079090	5.792642	-0.326517
28	1	0	1.986665	5.554110	0.239627
29	1	0	1.373021	6.391024	-1.195114
30	1	0	0.440864	6.421359	0.303434
31	46	0	-0.079191	0.328336	-0.167311
32	6	0	-0.384236	-2.378314	1.097511
33	6	0	0.275557	-1.702161	0.056708
34	6	0	-0.885036	-3.656304	0.889555
35	6	0	0.427578	-2.331628	-1.193029
36	6	0	-0.742684	-4.266658	-0.357410
37	1	0	-1.394869	-4.173095	1.696223
38	6	0	-0.097478	-3.602172	-1.399827
39	1	0	0.932328	-1.833067	-2.013245
40	1	0	-1.139216	-5.264529	-0.517033
41	1	0	0.003657	-4.075382	-2.371072
42	1	0	-0.518179	-1.903820	2.061725
43	6	0	2.049496	-0.717036	0.703217
44	6	0	3.072501	-1.774727	0.526400
45	6	0	3.674666	-1.937470	-0.725890
46	1	0	3.021625	-2.556134	2.533189
47	6	0	3.471182	-2.641493	1.553362
48	6	0	4.633917	-2.899977	-0.977085
49	6	0	5.009593	-3.748926	0.058238
50	6	0	4.430107	-3.616587	1.318589
51	1	0	5.066472	-2.975957	-1.968293
52	1	0	5.760135	-4.511290	-0.121338
53	1	0	4.725507	-4.278340	2.125283
54	8	0	3.258404	-1.167418	-1.806572
55	16	0	2.885957	0.389647	-1.516266
56	8	0	4.109672	1.097631	-1.213319
57	8	0	2.082191	0.767518	-2.653703
58	7	0	1.966222	0.358075	-0.143573
59	6	0	1.700916	-0.326976	2.151839
60	8	0	1.791913	0.979314	2.326616
61	8	0	1.413661	-1.117963	3.021326
62	6	0	1.410808	1.472386	3.622742
63	1	0	1.610222	2.541784	3.593561
64	1	0	0.348179	1.283628	3.790633
65	1	0	2.007109	0.994782	4.401862
66	6	0	-4.997009	-2.151543	-0.459114
67	8	0	-4.424287	-3.174251	-0.778007
68	8	0	-6.310646	-2.030781	-0.340634
69	6	0	-7.079684	-3.208825	-0.634198
70	1	0	-8.119428	-2.924444	-0.482885
71	1	0	-6.914402	-3.516709	-1.668614
72	1	0	-6.804677	-4.018534	0.044720

9:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.028256	1.016249	0.726233
2	6	0	-4.322271	0.959112	1.198272
3	6	0	-5.116983	-0.116301	0.804689
4	6	0	-4.572508	-1.081979	-0.031898
5	6	0	-3.247970	-0.957095	-0.453744
6	7	0	-2.498168	0.079212	-0.095540
7	1	0	-6.141563	-0.193744	1.148545
8	1	0	-4.697795	1.735004	1.854500
9	1	0	-2.800908	-1.707364	-1.091756
10	6	0	-2.083784	2.099571	0.982896
11	8	0	-2.429030	3.204142	1.594209
12	6	0	-1.200372	4.004971	1.652895
13	6	0	-0.314132	3.397506	0.555263
14	1	0	-1.483946	5.043462	1.498588
15	1	0	-0.780401	3.865398	2.650732
16	1	0	0.723887	3.364212	0.879390
17	7	0	-0.884122	2.028935	0.508834
18	6	0	-0.398876	4.109902	-0.826471
19	6	0	0.335014	3.298740	-1.903236
20	1	0	-0.171674	2.350678	-2.114005
21	1	0	0.357927	3.871939	-2.836245
22	1	0	1.364837	3.079528	-1.611468
23	6	0	-1.852022	4.317136	-1.276089
24	1	0	-2.377490	3.363556	-1.405688
25	1	0	-2.425853	4.938401	-0.581134
26	1	0	-1.861509	4.822443	-2.246969
27	6	0	0.302534	5.467273	-0.670752
28	1	0	1.351833	5.333952	-0.386083

29	1	0	0.276351	6.009063	-1.621410
30	1	0	-0.177823	6.100924	0.082137
31	46	0	-0.437648	0.267847	-0.358100
32	6	0	1.021622	-1.908932	1.874700
33	6	0	2.066830	-2.072952	0.963965
34	6	0	0.924889	-2.738056	2.989301
35	6	0	2.997921	-3.093101	1.169701
36	6	0	1.864599	-3.743333	3.199771
37	1	0	0.113313	-2.591963	3.695541
38	6	0	2.899185	-3.919840	2.284597
39	1	0	3.805793	-3.245995	0.461858
40	1	0	1.790327	-4.386098	4.071458
41	1	0	3.635695	-4.702794	2.436158
42	1	0	0.279010	-1.129343	1.729583
43	6	0	2.154571	-1.201835	-0.317623
44	6	0	3.604076	-1.061488	-0.791234
45	6	0	4.381830	-0.230945	0.012913
46	1	0	3.646292	-2.286839	-2.562160
47	6	0	4.209062	-1.636349	-1.905290
48	6	0	5.716753	0.030818	-0.227863
49	6	0	6.310545	-0.571578	-1.334910
50	6	0	5.556963	-1.391221	-2.169266
51	1	0	6.268279	0.686576	0.436652
52	1	0	7.359096	-0.389833	-1.546160
53	1	0	6.018267	-1.851304	-3.036870
54	8	0	3.769679	0.323448	1.137141
55	16	0	2.385900	1.142846	0.851465
56	8	0	1.774284	1.246595	2.167587
57	8	0	2.733642	2.399693	0.203546
58	7	0	1.610259	0.174130	-0.196181
59	6	0	1.315308	-1.980674	-1.327632
60	8	0	1.628966	-3.023960	-1.831901
61	8	0	0.109405	-1.409695	-1.569945
62	6	0	-0.705444	-2.021531	-2.610650
63	1	0	-0.075574	-2.209400	-3.478500
64	1	0	-1.137682	-2.946943	-2.230628
65	1	0	-1.467220	-1.282498	-2.847374
66	6	0	-5.334387	-2.269878	-0.526184
67	8	0	-4.843337	-3.113500	-1.248358
68	8	0	-6.584790	-2.281552	-0.094027
69	6	0	-7.397905	-3.381267	-0.537929
70	1	0	-8.368658	-3.232586	-0.068680
71	1	0	-7.493328	-3.361601	-1.625510
72	1	0	-6.959156	-4.328168	-0.217704

10:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.791352	-2.067852	-0.588608
2	6	0	-4.034762	-2.551390	-0.934130
3	6	0	-5.146046	-1.752274	-0.663355
4	6	0	-4.960957	-0.515090	-0.058743
5	6	0	-3.668288	-0.091475	0.254548
6	7	0	-2.615451	-0.856608	-0.005416
7	1	0	-6.140496	-2.096870	-0.921614
8	1	0	-4.133662	-3.523127	-1.402585
9	1	0	-3.482699	0.873480	0.711796
10	6	0	-1.518587	-2.781475	-0.726700
11	8	0	-1.424998	-4.020098	-1.148481
12	6	0	0.019416	-4.301879	-1.163886
13	6	0	0.601501	-3.254541	-0.202311
14	1	0	0.148424	-5.337767	-0.858758
15	1	0	0.356352	-4.157966	-2.192275
16	1	0	1.560611	-2.874280	-0.560224
17	7	0	-0.431856	-2.210060	-0.329612
18	6	0	0.735643	-3.730893	1.276089
19	6	0	1.020100	-2.534328	2.191934
20	1	0	0.173547	-1.840628	2.228707
21	1	0	1.206598	-2.885952	3.211932
22	1	0	1.904816	-1.988868	1.861789
23	6	0	-0.538466	-4.425675	1.778644
24	1	0	-1.405419	-3.755118	1.758058
25	1	0	-0.781980	-5.329140	1.211025
26	1	0	-0.393181	-4.725846	2.821202
27	6	0	1.916573	-4.708924	1.334496
28	1	0	2.842491	-4.227611	1.003699
29	1	0	2.063195	-5.056803	2.362048
30	1	0	1.748480	-5.591934	0.708814
31	46	0	-0.650736	-0.260423	0.040682
32	6	0	2.481428	3.152830	0.058714
33	6	0	3.211148	1.961710	0.036328
34	6	0	3.115598	4.373057	-0.137089
35	6	0	4.589850	2.011897	-0.164191
36	6	0	4.491953	4.418671	-0.352461
37	1	0	2.533007	5.289141	-0.122051
38	6	0	5.224813	3.236473	-0.363415

39	1	0	5.178631	1.101075	-0.167803
40	1	0	4.988978	5.371297	-0.507853
41	1	0	6.297776	3.260506	-0.527288
42	1	0	1.411552	3.131775	0.225412
43	6	0	2.480275	0.618909	0.314664
44	6	0	3.382670	-0.582606	-0.001629
45	6	0	3.495910	-0.884175	-1.363857
46	1	0	4.062165	-1.195018	1.945277
47	6	0	4.087377	-1.398021	0.883637
48	6	0	4.219108	-1.962316	-1.845036
49	6	0	4.897461	-2.770063	-0.937685
50	6	0	4.837400	-2.478441	0.420466
51	1	0	4.258178	-2.141900	-2.913996
52	1	0	5.475123	-3.616124	-1.295003
53	1	0	5.374620	-3.094321	1.134186
54	8	0	2.946751	-0.024048	-2.307561
55	16	0	1.415998	0.518705	-2.068358
56	8	0	1.463015	1.855038	-2.645249
57	8	0	0.494183	-0.413644	-2.708498
58	7	0	1.242957	0.455328	-0.477469
59	6	0	2.047673	0.787152	1.780253
60	8	0	3.040950	0.613489	2.622536
61	8	0	0.934606	1.145247	2.126406
62	8	0	-1.147221	1.705491	0.545590
63	6	0	-1.375697	2.639160	-0.503881
64	1	0	-2.147981	2.222774	-1.151231
65	1	0	-0.468007	2.828466	-1.081841
66	6	0	-1.875907	3.935307	0.093364
67	6	0	2.751815	0.810138	4.018995
68	1	0	3.698439	0.648887	4.530763
69	1	0	2.392350	1.826607	4.187210
70	1	0	2.007227	0.083240	4.349113
71	1	0	-0.371979	1.938811	1.100420
72	9	0	-3.003897	3.756602	0.796740
73	9	0	-2.124585	4.825522	-0.873923
74	9	0	-0.966749	4.472275	0.928244
75	6	0	-6.081735	0.416219	0.274538
76	8	0	-5.910691	1.478012	0.837863
77	8	0	-7.256799	-0.050107	-0.117292
78	6	0	-8.394570	0.780520	0.168366
79	1	0	-9.254799	0.240367	-0.222469
80	1	0	-8.493306	0.928931	1.245521
81	1	0	-8.290075	1.745083	-0.332555

11:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.797773	1.977995	-0.592929
2	6	0	4.043313	2.486029	-0.896626
3	6	0	5.160798	1.709220	-0.592149
4	6	0	4.979689	0.465484	0.000331
5	6	0	3.685679	0.013036	0.260743
6	7	0	2.625981	0.755163	-0.035914
7	1	0	6.156403	2.077144	-0.810597
8	1	0	4.138125	3.464857	-1.351057
9	1	0	3.504970	-0.955503	0.711327
10	6	0	1.526993	2.695373	-0.735893
11	8	0	1.438754	3.882893	-1.294250
12	6	0	-0.001467	4.166099	-1.339095
13	6	0	-0.583738	3.234123	-0.265418
14	1	0	-0.131192	5.229615	-1.150988
15	1	0	-0.340930	3.912553	-2.345542
16	1	0	-1.536510	2.803372	-0.584383
17	7	0	0.451937	2.183202	-0.244108
18	6	0	-0.745423	3.892927	1.136395
19	6	0	-1.038873	2.814542	2.183427
20	1	0	-0.193775	2.130972	2.304800
21	1	0	-1.236270	3.281007	3.154257
22	1	0	-1.918061	2.229798	1.908055
23	6	0	0.520676	4.650354	1.563277
24	1	0	1.387004	3.983453	1.639944
25	1	0	0.772696	5.470387	0.883935
26	1	0	0.362855	5.086895	2.554626
27	6	0	-1.929863	4.864968	1.057676
28	1	0	-2.850970	4.340398	0.783746
29	1	0	-2.087424	5.341347	2.030645
30	1	0	-1.763015	5.660796	0.323643
31	46	0	0.665345	0.172181	0.084866
32	6	0	-2.632516	-3.227118	0.435964
33	6	0	-3.335740	-2.032171	0.250019
34	6	0	-3.288525	-4.448021	0.330641
35	6	0	-4.703552	-2.074174	-0.013376
36	6	0	-4.652798	-4.487568	0.050784
37	1	0	-2.732221	-5.369115	0.471765
38	6	0	-5.357243	-3.299490	-0.115606
39	1	0	-5.266858	-1.155880	-0.139294

40	1	0	-5.163471	-5.441571	-0.034266
41	1	0	-6.421701	-3.320183	-0.326991
42	1	0	-1.569431	-3.227240	0.669930
43	6	0	-2.587142	-0.691890	0.399607
44	6	0	-3.412413	0.509535	-0.044768
45	6	0	-3.584604	0.670930	-1.417197
46	1	0	-3.976262	1.337780	1.862278
47	6	0	-4.037898	1.436894	0.785846
48	6	0	-4.283310	1.712669	-1.993016
49	6	0	-4.880262	2.638954	-1.141664
50	6	0	-4.766438	2.490693	0.236995
51	1	0	-4.368412	1.779187	-3.071570
52	1	0	-5.441184	3.467733	-1.559635
53	1	0	-5.247215	3.201448	0.900367
54	8	0	-3.080735	-0.344103	-2.251391
55	16	0	-1.510247	-0.617599	-2.125512
56	8	0	-1.272808	-1.920583	-2.694556
57	8	0	-0.785356	0.537598	-2.597226
58	7	0	-1.313603	-0.717193	-0.411599
59	6	0	-2.138081	-0.590591	1.872866
60	8	0	-3.177231	-0.671444	2.677397
61	8	0	-0.987610	-0.484776	2.234602
62	8	0	1.028000	-1.767194	0.330072
63	6	0	1.641634	-2.472872	-0.705293
64	1	0	2.484456	-1.943328	-1.171391
65	1	0	0.946631	-2.759898	-1.507960
66	6	0	2.201581	-3.755434	-0.128182
67	6	0	-2.904700	-0.546000	4.086527
68	1	0	-3.874382	-0.623179	4.573674
69	1	0	-2.246851	-1.353433	4.411818
70	1	0	-2.446063	0.423574	4.291050
71	1	0	-0.845645	-1.626087	-0.248049
72	9	0	2.774023	-4.506177	-1.085064
73	9	0	3.139370	-3.520210	0.810600
74	9	0	1.246565	-4.503904	0.453539
75	6	0	6.106420	-0.441012	0.377693
76	8	0	5.934450	-1.548310	0.844675
77	8	0	7.290167	0.106106	0.148059
78	6	0	8.434487	-0.691229	0.495147
79	1	0	9.300586	-0.089557	0.225039
80	1	0	8.434839	-0.899955	1.567066
81	1	0	8.429753	-1.626755	-0.067652

12:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.783214	-1.865030	-0.396565
2	6	0	-1.812899	-2.775023	-0.508421
3	6	0	-3.114256	-2.326879	-0.284875
4	6	0	-3.327677	-0.991412	0.034939
5	6	0	-2.235197	-0.128024	0.134001
6	7	0	-1.000462	-0.566374	-0.076788
7	1	0	-3.946459	-3.016680	-0.361687
8	1	0	-1.604306	-3.807321	-0.762082
9	1	0	-2.348824	0.921432	0.383224
10	6	0	0.638879	-2.161683	-0.602324
11	8	0	1.066800	-3.366755	-0.900817
12	6	0	2.514375	-3.245769	-1.083404
13	6	0	2.852521	-1.789874	-0.669179
14	1	0	2.975237	-4.015196	-0.465509
15	1	0	2.717068	-3.440935	-2.136251
16	1	0	3.335524	-1.265325	-1.498678
17	7	0	1.508089	-1.222770	-0.482722
18	6	0	3.739579	-1.624962	0.590171
19	6	0	3.977676	-0.129384	0.846545
20	1	0	3.074888	0.379728	1.206749
21	1	0	4.736919	0.001366	1.624500
22	1	0	4.330054	0.381392	-0.056317
23	6	0	3.081029	-2.258697	1.820669
24	1	0	2.117523	-1.786334	2.042412
25	1	0	2.912397	-3.333114	1.690960
26	1	0	3.724767	-2.129368	2.696387
27	6	0	5.092799	-2.291319	0.302797
28	1	0	5.566493	-1.856300	-0.584394
29	1	0	5.769079	-2.144393	1.150740
30	1	0	4.997082	-3.370133	0.143124
31	46	0	0.684600	0.569597	0.058039
32	8	0	-0.315167	2.153902	0.612700
33	6	0	0.580471	3.178396	0.883380
34	1	0	0.223915	3.799812	1.715223
35	1	0	1.580806	2.800679	1.170491
36	6	0	0.780161	4.083177	-0.319471
37	9	0	-0.374323	4.623229	-0.741501
38	9	0	1.623474	5.089895	-0.034706
39	9	0	1.302642	3.414891	-1.373356
40	6	0	-4.684866	-0.412752	0.276884

41	8	0	-4.866588	0.752532	0.563701
42	8	0	-5.644751	-1.314301	0.138064
43	6	0	-6.988633	-0.845830	0.337739
44	1	0	-7.624759	-1.715191	0.182582
45	1	0	-7.108424	-0.460950	1.352496
46	1	0	-7.226931	-0.065416	-0.387628

1a:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745050	-0.029495	-0.095124
2	6	0	0.348268	0.928491	-0.007738
3	6	0	1.655907	0.470602	-0.229219
4	1	0	-0.833719	2.668533	0.470998
5	6	0	0.163723	2.289175	0.290932
6	6	0	2.749910	1.318211	-0.188691
7	6	0	2.537642	2.659318	0.103346
8	6	0	1.250823	3.143381	0.350518
9	1	0	3.739648	0.920342	-0.376290
10	1	0	3.385661	3.333765	0.145352
11	1	0	1.100130	4.190452	0.584146
12	8	0	1.885664	-0.845947	-0.574395
13	16	0	0.886278	-1.972046	0.071244
14	8	0	1.017062	-3.106258	-0.803286
15	8	0	1.170925	-2.086911	1.482301
16	7	0	-0.623776	-1.314678	-0.118583
17	6	0	-2.171964	0.479113	-0.251085
18	8	0	-2.440849	1.461762	-0.901059
19	8	0	-3.032863	-0.291656	0.383898
20	6	0	-4.415030	0.088706	0.265503
21	1	0	-4.562008	1.090643	0.671409
22	1	0	-4.720913	0.064769	-0.781212
23	1	0	-4.967695	-0.645951	0.845453

2a:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.765519	-0.000004	-0.000008
2	8	0	-2.510310	1.074232	-0.403186
3	1	0	-1.979397	1.792792	-0.759475
4	8	0	-2.510292	-1.074239	0.403197
5	1	0	-1.979368	-1.792785	0.759493
6	6	0	-0.187449	0.000002	-0.000011
7	6	0	0.538240	1.180918	0.217856
8	6	0	0.538243	-1.180916	-0.217862
9	6	0	1.930478	1.184234	0.224255
10	1	0	0.010815	2.115222	0.397060
11	6	0	1.930481	-1.184230	-0.224254
12	1	0	0.010820	-2.115221	-0.397065
13	6	0	2.629172	0.000003	0.000003
14	1	0	2.469587	2.109983	0.402684
15	1	0	2.469592	-2.109979	-0.402674
16	1	0	3.715376	0.000003	0.000012

3aa:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.343149	-1.012463	-0.229162
2	6	0	1.328406	-0.279526	0.391839
3	6	0	3.387702	-1.535164	0.523211
4	6	0	1.372638	-0.070663	1.767978
5	6	0	3.428338	-1.329570	1.901430
6	1	0	4.171417	-2.103773	0.032564
7	6	0	2.420392	-0.597739	2.520136
8	1	0	0.594754	0.502528	2.261293
9	1	0	4.243760	-1.739855	2.488993
10	1	0	2.444827	-0.432788	3.592725
11	1	0	2.309893	-1.176840	-1.301939
12	6	0	0.221472	0.326744	-0.472527
13	6	0	-0.980015	0.832752	0.325415
14	6	0	-1.900336	-0.126749	0.745708
15	1	0	-0.555877	2.943987	0.326050
16	6	0	-1.249407	2.165652	0.625020
17	6	0	-3.057887	0.189788	1.431969
18	6	0	-3.305584	1.528164	1.724927
19	6	0	-2.404428	2.509535	1.324079
20	1	0	-3.738614	-0.598813	1.732145
21	1	0	-4.206292	1.799436	2.265218
22	1	0	-2.598674	3.552214	1.551214
23	8	0	-1.606480	-1.479259	0.543422
24	16	0	-1.109858	-1.955901	-0.931688
25	8	0	-0.253868	-3.081683	-0.641281

26	8	0	-2.242515	-2.133328	-1.817020
27	7	0	-0.262755	-0.655471	-1.466775
28	6	0	0.780813	1.475648	-1.336308
29	8	0	1.608747	2.239535	-0.651293
30	8	0	0.458674	1.650897	-2.490435
31	6	0	2.138236	3.386184	-1.342784
32	1	0	1.328041	4.059015	-1.629694
33	1	0	2.802539	3.869900	-0.629714
34	1	0	2.692718	3.065638	-2.226389
35	1	0	-0.748877	-0.202790	-2.240758

$B(OH)_2OCH_2CF_3$:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.858820	0.020981	0.067905
2	8	0	-1.902448	1.383573	0.051166
3	1	0	-1.091864	1.835743	0.297460
4	8	0	-2.979220	-0.617672	-0.379531
5	1	0	-2.898415	-1.575248	-0.325504
6	8	0	-0.806070	-0.760222	0.504431
7	6	0	0.384614	-0.247506	1.041366
8	1	0	0.246912	0.692975	1.585068
9	1	0	0.797833	-0.983879	1.734386
10	6	0	1.407092	-0.021730	-0.053787
11	9	0	0.997698	0.904424	-0.942961
12	9	0	2.566881	0.405550	0.469618
13	9	0	1.656677	-1.143810	-0.744983

TFE:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.415188	0.016676	0.000001
2	6	0	-0.907438	0.745080	-0.000013
3	1	0	-0.931228	1.384973	0.890405
4	1	0	-0.931206	1.384960	-0.890443
5	8	0	-1.925092	-0.225045	-0.000025
6	1	0	-2.769035	0.239170	0.000140
7	9	0	1.432537	0.896143	-0.000125
8	9	0	0.560756	-0.769038	1.080654
9	9	0	0.560675	-0.769247	-1.080509

13:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.503811	1.075003	-0.439251
2	6	0	2.639994	1.813132	-0.714460
3	6	0	3.877308	1.215081	-0.490727
4	6	0	3.918416	-0.086151	-0.003372
5	6	0	2.718466	-0.758729	0.241818
6	7	0	1.536670	-0.190630	0.028655
7	1	0	4.792740	1.758295	-0.693950
8	1	0	2.561612	2.824245	-1.095488
9	1	0	2.716559	-1.776614	0.615572
10	6	0	0.142020	1.601121	-0.619067
11	8	0	-0.043631	2.830909	-1.054564
12	6	0	-1.482096	2.947122	-1.284846
13	6	0	-2.086345	1.788345	-0.469822
14	1	0	-1.779509	3.944944	-0.970107
15	1	0	-1.640868	2.828674	-2.358574
16	1	0	-2.858811	1.273779	-1.044165
17	7	0	-0.907170	0.903624	-0.347904
18	6	0	-2.681401	2.195962	0.906784
19	6	0	-3.132745	0.950685	1.679470
20	1	0	-2.286914	0.313210	1.953346
21	1	0	-3.635416	1.254983	2.603651
22	1	0	-3.835466	0.350674	1.092434
23	6	0	-1.664570	2.973837	1.751797
24	1	0	-0.776628	2.370294	1.971994
25	1	0	-1.340424	3.899806	1.265658
26	1	0	-2.117450	3.249133	2.709689
27	6	0	-3.916108	3.067859	0.633189
28	1	0	-4.648811	2.530207	0.020906
29	1	0	-4.399161	3.333151	1.579059
30	1	0	-3.665828	4.002728	0.121493
31	46	0	-0.506664	-1.064760	0.042012
32	6	0	-2.330312	-1.701274	-0.189586
33	6	0	-2.825095	-2.558519	0.795402
34	6	0	-3.079878	-1.440995	-1.337642
35	6	0	-4.068337	-3.169144	0.620027
36	1	0	-2.256696	-2.747394	1.704410
37	6	0	-4.322770	-2.053594	-1.504588
38	1	0	-2.704760	-0.766166	-2.102848

39	6	0	-4.818097	-2.914630	-0.527023
40	1	0	-4.451906	-3.837071	1.386214
41	1	0	-4.902917	-1.854739	-2.401379
42	1	0	-5.787920	-3.385421	-0.657189
43	6	0	5.194155	-0.810563	0.273631
44	8	0	5.236565	-1.924706	0.755523
45	8	0	6.259449	-0.098746	-0.066580
46	6	0	7.536368	-0.715275	0.161006
47	1	0	8.272187	0.000000	-0.202442
48	1	0	7.681450	-0.901639	1.227175
49	1	0	7.609240	-1.652371	-0.394745

14:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.942245	2.771029	-0.539481
2	6	0	-0.659476	4.117567	-0.676845
3	6	0	0.674541	4.514026	-0.618769
4	6	0	1.657422	3.547097	-0.442061
5	6	0	1.280136	2.207963	-0.325641
6	7	0	0.007629	1.830931	-0.359830
7	1	0	0.937426	5.560822	-0.715754
8	1	0	-1.455591	4.837622	-0.822226
9	1	0	2.025153	1.431703	-0.200577
10	6	0	-2.306026	2.220402	-0.560348
11	8	0	-3.337772	3.009961	-0.781513
12	6	0	-4.483810	2.113519	-0.916195
13	6	0	-4.009593	0.805821	-0.257598
14	1	0	-5.330979	2.600745	-0.438636
15	1	0	-4.671395	1.997913	-1.985849
16	1	0	-4.309687	-0.060492	-0.850286
17	7	0	-2.542139	0.970710	-0.352811
18	6	0	-4.497498	0.602727	1.204888
19	6	0	-3.876121	-0.665132	1.800906
20	1	0	-2.789051	-0.582646	1.886621
21	1	0	-4.282018	-0.834691	2.804140
22	1	0	-4.103379	-1.545038	1.191013
23	6	0	-4.136644	1.803811	2.088925
24	1	0	-3.051978	1.943145	2.160061
25	1	0	-4.580707	2.736775	1.726270
26	1	0	-4.510716	1.638817	3.104471
27	6	0	-6.022642	0.419762	1.164174
28	1	0	-6.301884	-0.420280	0.518260
29	1	0	-6.397007	0.208328	2.170898
30	1	0	-6.544394	1.312371	0.805226
31	46	0	-0.842419	-0.198147	-0.340642
32	6	0	-1.653111	-2.945384	0.434680
33	6	0	-1.813057	-1.919982	-0.501693
34	6	0	-2.372051	-4.133344	0.307292
35	6	0	-2.682612	-2.110222	-1.579247
36	6	0	-3.248344	-4.314613	-0.761518
37	1	0	-2.246743	-4.918572	1.048101
38	6	0	-3.397480	-3.303058	-1.707181
39	1	0	-2.816849	-1.328321	-2.322990
40	1	0	-3.806100	-5.241276	-0.859890
41	1	0	-4.074603	-3.436181	-2.546654
42	1	0	-0.978125	-2.819545	1.276683
43	6	0	1.706799	-1.407068	0.780576
44	6	0	2.985225	-2.071141	0.802106
45	6	0	3.640151	-2.317293	-0.413977
46	1	0	3.141644	-2.255863	2.951680
47	6	0	3.633817	-2.421460	1.999020
48	6	0	4.901466	-2.873527	-0.472761
49	6	0	5.519758	-3.216308	0.726158
50	6	0	4.890251	-2.998714	1.954809
51	1	0	5.378513	-3.034383	-1.432411
52	1	0	6.506454	-3.666076	0.699339
53	1	0	5.388031	-3.278521	2.875990
54	8	0	3.048154	-1.912456	-1.603453
55	16	0	1.437281	-2.044882	-1.698856
56	8	0	1.055320	-1.230252	-2.820002
57	8	0	1.063293	-3.432592	-1.607101
58	7	0	0.963844	-1.254681	-0.277973
59	6	0	1.142545	-0.788437	2.048437
60	8	0	1.575071	0.442704	2.181826
61	8	0	0.398858	-1.392023	2.784568
62	6	0	1.005502	1.218241	3.257827
63	1	0	1.476736	2.195559	3.181681
64	1	0	-0.073932	1.297738	3.114784
65	1	0	1.233568	0.750727	4.216629
66	6	0	3.114761	3.862354	-0.369052
67	8	0	3.970199	3.015178	-0.205916
68	8	0	3.358038	5.158522	-0.500396
69	6	0	4.737545	5.554976	-0.439464
70	1	0	4.735740	6.634353	-0.581050
71	1	0	5.161751	5.297533	0.533164

72	1	0	5.305036	5.067886	-1.235063

14-TS^{R}

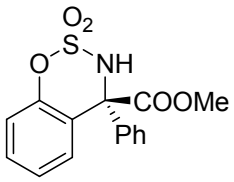
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.786024	1.119164	-0.750936
2	6	0	4.122991	1.110831	-1.096230
3	6	0	4.889672	0.009331	-0.720006
4	6	0	4.285046	-1.022525	-0.012998
5	6	0	2.925308	-0.935016	0.293510
6	7	0	2.193115	0.109874	-0.074639
7	1	0	5.942122	-0.036657	-0.974190
8	1	0	4.555257	1.942075	-1.639885
9	1	0	2.425313	-1.725160	0.840315
10	6	0	1.875436	2.241724	-1.017321
11	8	0	2.277581	3.295271	-1.698257
12	6	0	1.077513	4.116370	-1.867662
13	6	0	0.133133	3.611415	-0.763482
14	1	0	1.383338	5.156676	-1.782234
15	1	0	0.695419	3.915860	-2.870874
16	1	0	-0.896135	3.539032	-1.122798
17	7	0	0.674645	2.252732	-0.550690
18	6	0	0.170194	4.458192	0.543160
19	6	0	-0.684897	3.795084	1.627831
20	1	0	-0.370686	2.764734	1.823833
21	1	0	-0.596426	4.356518	2.563934
22	1	0	-1.740033	3.788675	1.342323
23	6	0	1.603664	4.618526	1.069441
24	1	0	2.046533	3.653874	1.341748
25	1	0	2.262946	5.109022	0.346293
26	1	0	1.594083	5.236261	1.973125
27	6	0	-0.428247	5.837995	0.231462
28	1	0	-1.426255	5.743821	-0.211357
29	1	0	-0.524680	6.414928	1.156967
30	1	0	0.195320	6.422621	-0.452248
31	46	0	0.058638	0.353970	0.009727
32	6	0	-2.759539	1.524476	0.465709
33	6	0	-1.964474	0.664880	-0.305546
34	6	0	-3.842515	2.183009	-0.108379
35	6	0	-2.293836	0.451483	-1.657037
36	6	0	-4.143121	1.984309	-1.454325
37	1	0	-4.453940	2.842962	0.498808
38	6	0	-3.364867	1.123172	-2.230299
39	1	0	-1.717166	-0.246466	-2.255257
40	1	0	-4.994644	2.490374	-1.898642
41	1	0	-3.603626	0.963956	-3.277080
42	1	0	-2.545286	1.684427	1.516165
43	6	0	-1.863029	-1.245774	0.737155
44	6	0	-2.973969	-2.022283	0.151792
45	6	0	-2.705393	-3.272399	-0.408985
46	1	0	-4.530872	-0.589002	0.540253
47	6	0	-4.300372	-1.569980	0.141365
48	6	0	-3.694601	-4.079224	-0.944221
49	6	0	-5.003141	-3.613189	-0.932256
50	6	0	-5.303329	-2.358937	-0.396412
51	1	0	-3.430659	-5.044455	-1.360888
52	1	0	-5.791305	-4.228142	-1.353529
53	1	0	-6.324665	-1.994770	-0.404426
54	8	0	-1.406595	-3.782015	-0.381640
55	16	0	-0.237243	-2.706661	-0.680992
56	8	0	0.991944	-3.368936	-0.323339
57	8	0	-0.400986	-2.185110	-2.023389
58	7	0	-0.563997	-1.560681	0.486277
59	6	0	-2.096861	-0.701535	2.155617
60	8	0	-1.041661	-0.073477	2.635648
61	8	0	-3.132920	-0.882572	2.749295
62	6	0	-1.169740	0.481239	3.958111
63	1	0	-0.200356	0.923594	4.177245
64	1	0	-1.950812	1.244318	3.964016
65	1	0	-1.404432	-0.307379	4.674519
66	6	0	5.011153	-2.249333	0.431852
67	8	0	4.466435	-3.165668	1.013344
68	8	0	6.297909	-2.217625	0.116653
69	6	0	7.069981	-3.368645	0.495144
70	1	0	8.088463	-3.154376	0.176333
71	1	0	7.031708	-3.510844	1.577014
72	1	0	6.690938	-4.259110	-0.010533

14-TS^{S}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.928304	-1.223494	0.380979
2	6	0	4.287871	-1.256581	0.624526
3	6	0	5.010395	-0.075924	0.468186

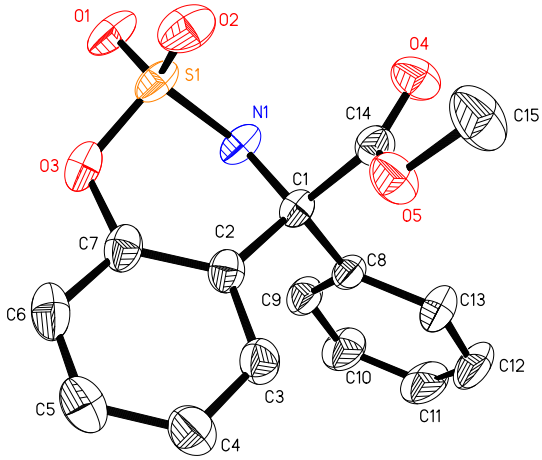
4	6	0	4.337698	1.078167	0.085695
5	6	0	2.960285	1.022499	-0.135632
6	7	0	2.272799	-0.105216	0.001914
7	1	0	6.078668	-0.060028	0.649585
8	1	0	4.768654	-2.177767	0.930616
9	1	0	2.413293	1.909617	-0.428687
10	6	0	2.049077	-2.393644	0.500668
11	8	0	2.522169	-3.543414	0.938416
12	6	0	1.346014	-4.390257	1.127614
13	6	0	0.268147	-3.714722	0.263900
14	1	0	1.618146	-5.400118	0.827700
15	1	0	1.108233	-4.366063	2.193346
16	1	0	-0.693457	-3.696447	0.780638
17	7	0	0.801633	-2.337230	0.185374
18	6	0	0.074838	-4.349786	-1.140608
19	6	0	-0.873479	-3.481257	-1.970708
20	1	0	-0.450433	-2.491049	-2.163492
21	1	0	-1.067583	-3.958530	-2.937106
22	1	0	-1.831423	-3.351321	-1.460182
23	6	0	1.410003	-4.492861	-1.883630
24	1	0	1.888207	-3.520313	-2.046750
25	1	0	2.115943	-5.139689	-1.352647
26	1	0	1.236437	-4.938770	-2.868220
27	6	0	-0.568009	-5.729785	-0.940680
28	1	0	-1.535995	-5.641262	-0.434487
29	1	0	-0.737326	-6.206567	-1.911540
30	1	0	0.063609	-6.402654	-0.351266
31	46	0	0.133254	-0.380339	-0.053268
32	6	0	-2.551641	-0.591466	-1.232201
33	6	0	-1.913309	-0.685115	0.019009
34	6	0	-3.685474	-1.343013	-1.503855
35	6	0	-2.425698	-1.572273	0.984528
36	6	0	-4.194216	-2.200319	-0.528350
37	1	0	-4.175374	-1.256427	-2.467970
38	6	0	-3.553739	-2.331364	0.705990
39	1	0	-1.939948	-1.671786	1.949514
40	1	0	-5.094148	-2.773118	-0.730643
41	1	0	-3.941304	-3.018008	1.451752
42	1	0	-2.172092	0.084507	-1.991677
43	6	0	-1.696567	1.313608	0.694291
44	6	0	-2.929882	2.002122	0.231604
45	6	0	-2.964336	2.553540	-1.060184
46	1	0	-4.135789	1.689598	1.990771
47	6	0	-4.104755	2.101419	0.992809
48	6	0	-4.083957	3.165062	-1.588818
49	6	0	-5.235288	3.237142	-0.812924
50	6	0	-5.239653	2.710378	0.475916
51	1	0	-4.039939	3.572690	-2.592379
52	1	0	-6.123816	3.711017	-1.216205
53	1	0	-6.134564	2.769955	1.085492
54	8	0	-1.863921	2.446382	-1.910954
55	16	0	-0.420524	2.606472	-1.181095
56	8	0	0.544435	2.140247	-2.148561
57	8	0	-0.333239	3.950307	-0.654053
58	7	0	-0.497713	1.545475	0.067214
59	6	0	-1.466894	1.077344	2.201982
60	8	0	-2.517065	0.595254	2.830034
61	8	0	-0.410753	1.342334	2.728668
62	6	0	-2.365461	0.362392	4.243066
63	1	0	-3.312953	-0.064221	4.565414
64	1	0	-1.548214	-0.338873	4.420475
65	1	0	-2.174440	1.306317	4.756315
66	6	0	5.012129	2.399394	-0.089629
67	8	0	4.417806	3.413641	-0.393593
68	8	0	6.317022	2.330593	0.131373
69	6	0	7.044675	3.563734	0.015303
70	1	0	6.673695	4.289307	0.742400
71	1	0	8.082385	3.311783	0.226868
72	1	0	6.949104	3.966674	-0.995050

9. X-Ray Crystal Structure Data



The crystal data of compound **3aa** have been deposited in CCDC with number 1047798. Empirical Formula: $C_{15}H_{13}NO_5S$; Formula Weight: 319.32; Crystal Color, Habit: colorless; Crystal Dimensions: 0.38 x 0.30 x 0.25 mm; Crystal System: Trigonal; Lattice Parameters: a = 10.3879(15) Å, b = 10.3879(15) Å, c = 24.218(5) Å, α = 90 °C, β = 90 °C, γ = 120 °C, V = 2263.2(6) Å^3; Space group: P 32; Z = 6; D_{calc} = 1.406 g/cm3; F_{000} = 996; Final R indices [I>2sigma(I)]: R1 = 0.0326; wR2 = 0.0873.

The crystal was obtained from a petroleum ether/dichloromethane solution at room temperature under air.



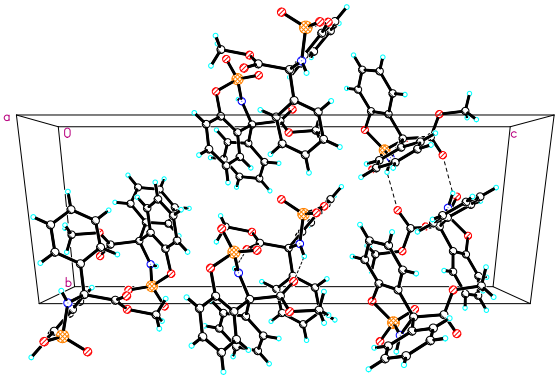


Table 1. Crystal data and structure refinement for **3aa**.

Identification code	271
Empirical formula	C15 H13 N O5 S
Formula weight	319.32
Temperature	296(2) K
Wavelength	1.54178 A
Crystal system, space group	Trigonal, P 32
Unit cell dimensions	a = 10.3879(15) A alpha = 90 deg.
	b = 10.3879(15) A beta = 90 deg.
	c = 24.218(5) A gamma = 120 deg.
Volume	2263.2(6) A^3
Z, Calculated density	6, 1.406 Mg/m^3
Absorption coefficient	2.126 mm^-1
F(000)	996
Crystal size	0.38 x 0.30 x 0.25 mm
Theta range for data collection	4.92 to 67.23 deg.
Limiting indices	-12<=h<=12, -12<=k<=11, -28<=l<=27
Reflections collected / unique	13604 / 5193 [R(int) = 0.0283]
Completeness to theta = 67.23	98.6 %

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7529 and 0.5198
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5193 / 1 / 398
Goodness-of-fit on F^2	1.094
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0873
R indices (all data)	R1 = 0.0328, wR2 = 0.0875
Absolute structure parameter	0.069(13)
Extinction coefficient	0.0056(3)
Largest diff. peak and hole	0.218 and -0.241 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3aa**.

	x	y	z	U(eq)
S(1)	4840(1)	9495(1)	2075(1)	55(1)
S(2)	2829(1)	1507(1)	634(1)	55(1)
O(1)	4941(2)	10759(2)	2333(1)	74(1)
O(2)	5690(2)	9650(2)	1601(1)	75(1)
O(3)	5275(2)	8687(2)	2532(1)	66(1)
O(4)	2767(2)	7784(2)	854(1)	67(1)
O(5)	3708(3)	6294(2)	944(1)	66(1)
O(6)	2981(2)	2361(2)	1107(1)	76(1)
O(7)	4092(2)	1607(2)	375(1)	75(1)
O(8)	2018(2)	1941(2)	177(1)	65(1)
O(9)	1118(2)	-566(2)	1855(1)	67(1)
O(10)	-372(2)	378(3)	1765(1)	66(1)
N(1)	3112(2)	8271(2)	1997(1)	52(1)
N(2)	1606(2)	-222(2)	713(1)	51(1)
C(1)	2792(2)	6842(2)	1761(1)	44(1)
C(2)	3716(2)	6297(3)	2068(1)	46(1)
C(3)	3414(3)	4839(3)	2013(1)	56(1)
C(4)	4199(4)	4303(3)	2292(1)	67(1)
C(5)	5330(4)	5235(4)	2643(1)	72(1)
C(6)	5671(3)	6677(4)	2712(1)	70(1)
C(7)	4876(3)	7202(3)	2422(1)	54(1)
C(8)	1131(2)	5757(2)	1856(1)	46(1)
C(9)	472(3)	5858(3)	2339(1)	59(1)
C(10)	-999(4)	4854(4)	2450(1)	79(1)
C(11)	-1821(4)	3738(4)	2088(2)	88(1)
C(12)	-1197(4)	3611(3)	1616(2)	87(1)
C(13)	278(3)	4616(3)	1491(1)	67(1)
C(14)	3098(3)	7045(2)	1130(1)	49(1)
C(15)	4022(5)	6401(5)	356(1)	91(1)
C(16)	173(2)	-540(2)	947(1)	44(1)
C(17)	-370(3)	384(2)	639(1)	46(1)
C(18)	-1827(3)	80(3)	697(1)	56(1)
C(19)	-2364(3)	866(4)	417(1)	67(1)
C(20)	-1436(4)	1994(4)	67(1)	71(1)
C(21)	10(4)	2339(3)	-3(1)	70(1)
C(22)	539(3)	1543(3)	287(1)	55(1)
C(23)	-911(2)	-2203(2)	852(1)	46(1)
C(24)	-811(3)	-2861(3)	369(1)	60(1)
C(25)	-1812(4)	-4334(4)	261(1)	79(1)

C(26)	-2925(4)	-5153(4)	623(2)	89(1)
C(27)	-3056(3)	-4532(4)	1095(2)	87(1)
C(28)	-2049(3)	-3059(3)	1217(1)	67(1)
C(29)	376(2)	-236(3)	1578(1)	49(1)
C(30)	-264(5)	692(5)	2353(1)	90(1)
H(1B)	2415	8447	2088	62
H(2B)	1783	-920	623	61
H(3A)	2653	4203	1777	67
H(4A)	3971	3323	2245	80
H(5A)	5864	4879	2834	86
H(6B)	6429	7300	2951	84
H(9A)	1028	6610	2591	71
H(10A)	-1431	4940	2773	95
H(11A)	-2812	3063	2165	106
H(12A)	-1762	2841	1371	104
H(13A)	693	4524	1164	80
H(15A)	4467	5810	266	136
H(15B)	4693	7419	260	136
H(15C)	3112	6044	153	136
H(18A)	-2461	-681	932	67
H(19A)	-3344	637	464	81
H(20A)	-1794	2528	-124	86
H(21A)	632	3099	-241	84
H(24A)	-62	-2305	116	71
H(25A)	-1725	-4769	-62	95
H(26A)	-3599	-6144	546	106
H(27A)	-3828	-5096	1338	104
H(28A)	-2138	-2645	1546	80
H(30A)	-856	1136	2443	135
H(30B)	754	1364	2449	135
H(30C)	-619	-217	2556	135

Table 3. Bond lengths [A] and angles [deg] for **3aa**.

S(1)-O(2)	1.4082(19)	C(10)-C(11)	1.360(5)
S(1)-O(1)	1.4098(19)	C(10)-H(10A)	0.9300
S(1)-O(3)	1.585(2)	C(11)-C(12)	1.354(6)
S(1)-N(1)	1.6101(18)	C(11)-H(11A)	0.9300
S(2)-O(6)	1.4094(19)	C(12)-C(13)	1.389(5)
S(2)-O(7)	1.4106(19)	C(12)-H(12A)	0.9300
S(2)-O(8)	1.587(2)	C(13)-H(13A)	0.9300
S(2)-N(2)	1.6109(18)	C(15)-H(15A)	0.9600
O(3)-C(7)	1.407(3)	C(15)-H(15B)	0.9600
O(4)-C(14)	1.190(3)	C(15)-H(15C)	0.9600
O(5)-C(14)	1.308(3)	C(16)-C(17)	1.528(3)
O(5)-C(15)	1.453(3)	C(16)-C(23)	1.536(3)
O(8)-C(22)	1.403(3)	C(16)-C(29)	1.555(3)
O(9)-C(29)	1.193(3)	C(17)-C(18)	1.389(3)
O(10)-C(29)	1.308(3)	C(17)-C(22)	1.390(3)
O(10)-C(30)	1.454(3)	C(18)-C(19)	1.376(4)
N(1)-C(1)	1.465(3)	C(18)-H(18A)	0.9300
N(1)-H(1B)	0.8600	C(19)-C(20)	1.375(4)
N(2)-C(16)	1.468(3)	C(19)-H(19A)	0.9300
N(2)-H(2B)	0.8600	C(20)-C(21)	1.369(5)
C(1)-C(2)	1.528(3)	C(20)-H(20A)	0.9300
C(1)-C(8)	1.535(3)	C(21)-C(22)	1.390(4)
C(1)-C(14)	1.553(3)	C(21)-H(21A)	0.9300
C(2)-C(3)	1.391(3)	C(23)-C(28)	1.385(3)
C(2)-C(7)	1.394(3)	C(23)-C(24)	1.385(4)
C(3)-C(4)	1.374(4)	C(24)-C(25)	1.379(4)
C(3)-H(3A)	0.9300	C(24)-H(24A)	0.9300
C(4)-C(5)	1.379(4)	C(25)-C(26)	1.359(5)
C(4)-H(4A)	0.9300	C(25)-H(25A)	0.9300
C(5)-C(6)	1.366(5)	C(26)-C(27)	1.352(6)
C(5)-H(5A)	0.9300	C(26)-H(26A)	0.9300
C(6)-C(7)	1.386(4)	C(27)-C(28)	1.387(5)
C(6)-H(6B)	0.9300	C(27)-H(27A)	0.9300
C(8)-C(9)	1.385(4)	C(28)-H(28A)	0.9300
C(8)-C(13)	1.386(3)	C(30)-H(30A)	0.9600
C(9)-C(10)	1.379(4)	C(30)-H(30B)	0.9600
C(9)-H(9A)	0.9300	C(30)-H(30C)	0.9600

O(2)-S(1)-O(1)	120.32(12)	O(1)-S(1)-N(1)	108.78(11)
O(2)-S(1)-O(3)	107.55(13)	O(3)-S(1)-N(1)	99.45(10)
O(1)-S(1)-O(3)	105.99(13)	O(6)-S(2)-O(7)	120.57(12)
O(2)-S(1)-N(1)	112.46(12)	O(6)-S(2)-O(8)	107.28(13)

O(7)-S(2)-O(8)	105.97(13)	C(11)-C(10)-C(9)	120.4(3)
O(6)-S(2)-N(2)	112.51(12)	C(11)-C(10)-H(10A)	119.8
O(7)-S(2)-N(2)	108.69(11)	C(9)-C(10)-H(10A)	119.8
O(8)-S(2)-N(2)	99.48(10)	C(12)-C(11)-C(10)	120.0(3)
C(7)-O(3)-S(1)	116.34(15)	C(12)-C(11)-H(11A)	120.0
C(14)-O(5)-C(15)	116.7(2)	C(10)-C(11)-H(11A)	120.0
C(22)-O(8)-S(2)	116.32(15)	C(11)-C(12)-C(13)	120.8(3)
C(29)-O(10)-C(30)	116.7(2)	C(11)-C(12)-H(12A)	119.6
C(1)-N(1)-S(1)	116.40(14)	C(13)-C(12)-H(12A)	119.6
C(1)-N(1)-H(1B)	121.8	C(8)-C(13)-C(12)	119.8(3)
S(1)-N(1)-H(1B)	121.8	C(8)-C(13)-H(13A)	120.1
C(16)-N(2)-S(2)	116.24(14)	C(12)-C(13)-H(13A)	120.1
C(16)-N(2)-H(2B)	121.9	O(4)-C(14)-O(5)	125.0(2)
S(2)-N(2)-H(2B)	121.9	O(4)-C(14)-C(1)	122.3(2)
N(1)-C(1)-C(2)	108.63(17)	O(5)-C(14)-C(1)	112.68(19)
N(1)-C(1)-C(8)	106.73(17)	O(5)-C(15)-H(15A)	109.5
C(2)-C(1)-C(8)	109.79(18)	O(5)-C(15)-H(15B)	109.5
N(1)-C(1)-C(14)	108.56(18)	H(15A)-C(15)-H(15B)	109.5
C(2)-C(1)-C(14)	113.87(17)	O(5)-C(15)-H(15C)	109.5
C(8)-C(1)-C(14)	109.01(17)	H(15A)-C(15)-H(15C)	109.5
C(3)-C(2)-C(7)	116.2(2)	H(15B)-C(15)-H(15C)	109.5
C(3)-C(2)-C(1)	121.03(19)	N(2)-C(16)-C(17)	108.81(17)
C(7)-C(2)-C(1)	122.8(2)	N(2)-C(16)-C(23)	106.66(17)
C(4)-C(3)-C(2)	122.5(2)	C(17)-C(16)-C(23)	109.94(18)
C(4)-C(3)-H(3A)	118.7	N(2)-C(16)-C(29)	108.31(18)
C(2)-C(3)-H(3A)	118.7	C(17)-C(16)-C(29)	114.01(17)
C(3)-C(4)-C(5)	119.3(3)	C(23)-C(16)-C(29)	108.84(17)
C(3)-C(4)-H(4A)	120.3	C(18)-C(17)-C(22)	116.7(2)
C(5)-C(4)-H(4A)	120.3	C(18)-C(17)-C(16)	120.72(19)
C(6)-C(5)-C(4)	120.5(3)	C(22)-C(17)-C(16)	122.6(2)
C(6)-C(5)-H(5A)	119.8	C(19)-C(18)-C(17)	122.3(2)
C(4)-C(5)-H(5A)	119.8	C(19)-C(18)-H(18A)	118.8
C(5)-C(6)-C(7)	119.4(3)	C(17)-C(18)-H(18A)	118.8
C(5)-C(6)-H(6B)	120.3	C(20)-C(19)-C(18)	119.4(3)
C(7)-C(6)-H(6B)	120.3	C(20)-C(19)-H(19A)	120.3
C(6)-C(7)-C(2)	122.0(2)	C(18)-C(19)-H(19A)	120.3
C(6)-C(7)-O(3)	115.4(2)	C(21)-C(20)-C(19)	120.5(3)
C(2)-C(7)-O(3)	122.4(2)	C(21)-C(20)-H(20A)	119.7
C(9)-C(8)-C(13)	118.3(2)	C(19)-C(20)-H(20A)	119.7
C(9)-C(8)-C(1)	119.20(19)	C(20)-C(21)-C(22)	119.4(3)
C(13)-C(8)-C(1)	122.4(2)	C(20)-C(21)-H(21A)	120.3
C(10)-C(9)-C(8)	120.6(2)	C(22)-C(21)-H(21A)	120.3
C(10)-C(9)-H(9A)	119.7	C(21)-C(22)-C(17)	121.7(2)
C(8)-C(9)-H(9A)	119.7	C(21)-C(22)-O(8)	115.5(2)

C(17)-C(22)-O(8)	122.8(2)	C(26)-C(27)-H(27A)	119.8
C(28)-C(23)-C(24)	118.2(2)	C(28)-C(27)-H(27A)	119.8
C(28)-C(23)-C(16)	122.5(2)	C(23)-C(28)-C(27)	120.2(3)
C(24)-C(23)-C(16)	119.13(19)	C(23)-C(28)-H(28A)	119.9
C(25)-C(24)-C(23)	120.5(3)	C(27)-C(28)-H(28A)	119.9
C(25)-C(24)-H(24A)	119.7	O(9)-C(29)-O(10)	125.0(2)
C(23)-C(24)-H(24A)	119.7	O(9)-C(29)-C(16)	122.4(2)
C(26)-C(25)-C(24)	120.3(3)	O(10)-C(29)-C(16)	112.62(19)
C(26)-C(25)-H(25A)	119.8	O(10)-C(30)-H(30A)	109.5
C(24)-C(25)-H(25A)	119.8	O(10)-C(30)-H(30B)	109.5
C(27)-C(26)-C(25)	120.3(3)	H(30A)-C(30)-H(30B)	109.5
C(27)-C(26)-H(26A)	119.9	O(10)-C(30)-H(30C)	109.5
C(25)-C(26)-H(26A)	119.8	H(30A)-C(30)-H(30C)	109.5
C(26)-C(27)-C(28)	120.5(3)	H(30B)-C(30)-H(30C)	109.5

Table 4. Torsion angles [deg] for **3aa**.

O(2)-S(1)-O(3)-C(7)	-66.71(19)
O(1)-S(1)-O(3)-C(7)	163.38(17)
N(1)-S(1)-O(3)-C(7)	50.60(18)
O(6)-S(2)-O(8)-C(22)	-66.66(19)
O(7)-S(2)-O(8)-C(22)	163.32(17)
N(2)-S(2)-O(8)-C(22)	50.63(18)
O(2)-S(1)-N(1)-C(1)	47.4(2)
O(1)-S(1)-N(1)-C(1)	-176.72(18)
O(3)-S(1)-N(1)-C(1)	-66.14(19)
O(6)-S(2)-N(2)-C(16)	47.5(2)
O(7)-S(2)-N(2)-C(16)	-176.32(18)
O(8)-S(2)-N(2)-C(16)	-65.77(18)
S(1)-N(1)-C(1)-C(2)	48.2(2)
S(1)-N(1)-C(1)-C(8)	166.57(15)
S(1)-N(1)-C(1)-C(14)	-76.1(2)
N(1)-C(1)-C(2)-C(3)	166.4(2)
C(8)-C(1)-C(2)-C(3)	50.1(3)
C(14)-C(1)-C(2)-C(3)	-72.5(3)
N(1)-C(1)-C(2)-C(7)	-12.4(3)
C(8)-C(1)-C(2)-C(7)	-128.8(2)
C(14)-C(1)-C(2)-C(7)	108.7(2)
C(7)-C(2)-C(3)-C(4)	0.5(4)
C(1)-C(2)-C(3)-C(4)	-178.4(2)
C(2)-C(3)-C(4)-C(5)	0.1(4)
C(3)-C(4)-C(5)-C(6)	-0.1(5)
C(4)-C(5)-C(6)-C(7)	-0.4(4)
C(5)-C(6)-C(7)-C(2)	1.1(4)
C(5)-C(6)-C(7)-O(3)	178.2(3)
C(3)-C(2)-C(7)-C(6)	-1.1(3)
C(1)-C(2)-C(7)-C(6)	177.8(2)
C(3)-C(2)-C(7)-O(3)	-178.0(2)
C(1)-C(2)-C(7)-O(3)	0.9(3)
S(1)-O(3)-C(7)-C(6)	158.81(19)
S(1)-O(3)-C(7)-C(2)	-24.1(3)
N(1)-C(1)-C(8)-C(9)	-36.1(3)
C(2)-C(1)-C(8)-C(9)	81.5(2)
C(14)-C(1)-C(8)-C(9)	-153.2(2)
N(1)-C(1)-C(8)-C(13)	147.9(2)
C(2)-C(1)-C(8)-C(13)	-94.6(3)
C(14)-C(1)-C(8)-C(13)	30.8(3)
C(13)-C(8)-C(9)-C(10)	-0.6(4)
C(1)-C(8)-C(9)-C(10)	-176.7(3)

C(8)-C(9)-C(10)-C(11)	0.7(5)
C(9)-C(10)-C(11)-C(12)	-0.1(6)
C(10)-C(11)-C(12)-C(13)	-0.5(6)
C(9)-C(8)-C(13)-C(12)	-0.1(4)
C(1)-C(8)-C(13)-C(12)	175.9(3)
C(11)-C(12)-C(13)-C(8)	0.7(5)
C(15)-O(5)-C(14)-O(4)	1.0(4)
C(15)-O(5)-C(14)-C(1)	179.3(3)
N(1)-C(1)-C(14)-O(4)	-40.2(3)
C(2)-C(1)-C(14)-O(4)	-161.3(2)
C(8)-C(1)-C(14)-O(4)	75.7(3)
N(1)-C(1)-C(14)-O(5)	141.5(2)
C(2)-C(1)-C(14)-O(5)	20.3(3)
C(8)-C(1)-C(14)-O(5)	-102.6(2)
S(2)-N(2)-C(16)-C(17)	48.0(2)
S(2)-N(2)-C(16)-C(23)	166.56(15)
S(2)-N(2)-C(16)-C(29)	-76.4(2)
N(2)-C(16)-C(17)-C(18)	166.6(2)
C(23)-C(16)-C(17)-C(18)	50.2(3)
C(29)-C(16)-C(17)-C(18)	-72.4(3)
N(2)-C(16)-C(17)-C(22)	-12.4(3)
C(23)-C(16)-C(17)-C(22)	-128.9(2)
C(29)-C(16)-C(17)-C(22)	108.6(2)
C(22)-C(17)-C(18)-C(19)	0.7(4)
C(16)-C(17)-C(18)-C(19)	-178.5(2)
C(17)-C(18)-C(19)-C(20)	0.0(4)
C(18)-C(19)-C(20)-C(21)	-0.2(5)
C(19)-C(20)-C(21)-C(22)	-0.4(4)
C(20)-C(21)-C(22)-C(17)	1.1(4)
C(20)-C(21)-C(22)-O(8)	178.1(3)
C(18)-C(17)-C(22)-C(21)	-1.2(3)
C(16)-C(17)-C(22)-C(21)	177.9(2)
C(18)-C(17)-C(22)-O(8)	-178.0(2)
C(16)-C(17)-C(22)-O(8)	1.1(3)
S(2)-O(8)-C(22)-C(21)	158.75(19)
S(2)-O(8)-C(22)-C(17)	-24.3(3)
N(2)-C(16)-C(23)-C(28)	147.4(2)
C(17)-C(16)-C(23)-C(28)	-94.8(3)
C(29)-C(16)-C(23)-C(28)	30.7(3)
N(2)-C(16)-C(23)-C(24)	-36.5(3)
C(17)-C(16)-C(23)-C(24)	81.3(2)
C(29)-C(16)-C(23)-C(24)	-153.2(2)
C(28)-C(23)-C(24)-C(25)	-0.7(4)
C(16)-C(23)-C(24)-C(25)	-176.9(3)

C(23)-C(24)-C(25)-C(26)	1.0(5)
C(24)-C(25)-C(26)-C(27)	-0.3(6)
C(25)-C(26)-C(27)-C(28)	-0.7(6)
C(24)-C(23)-C(28)-C(27)	-0.4(4)
C(16)-C(23)-C(28)-C(27)	175.8(3)
C(26)-C(27)-C(28)-C(23)	1.1(5)
C(30)-O(10)-C(29)-O(9)	0.8(4)
C(30)-O(10)-C(29)-C(16)	179.4(3)
N(2)-C(16)-C(29)-O(9)	-39.8(3)
C(17)-C(16)-C(29)-O(9)	-161.1(2)
C(23)-C(16)-C(29)-O(9)	75.8(3)
N(2)-C(16)-C(29)-O(10)	141.5(2)
C(17)-C(16)-C(29)-O(10)	20.2(3)
C(23)-C(16)-C(29)-O(10)	-102.9(2)

Table 5. Hydrogen bonds for **3aa** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1B)...O(9)#1	0.86	2.14	2.893(3)	146.4
N(2)-H(2B)...O(4)#2	0.86	2.13	2.892(3)	146.9

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z #2 x,y-1,z