Supporting Information

Chiral synthetic unprecedented spiro[indoline-2,3'-thiophen]-3-ones via organocatalytic asymmetric sulfa-Michael/aldol cascade reaction

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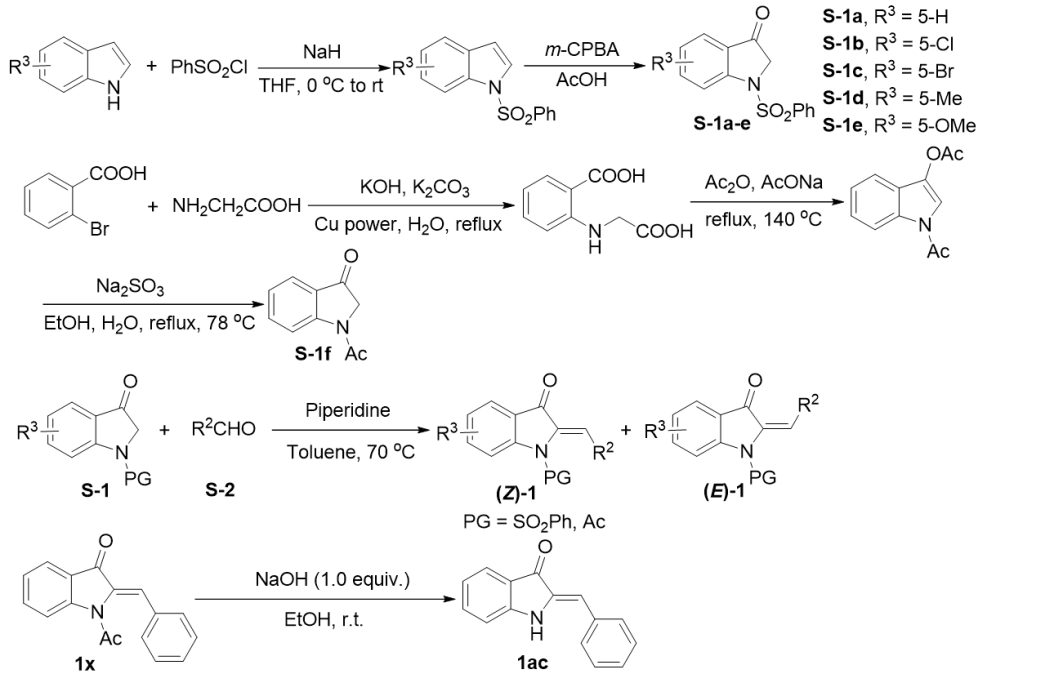
Table of Contents

1. General information

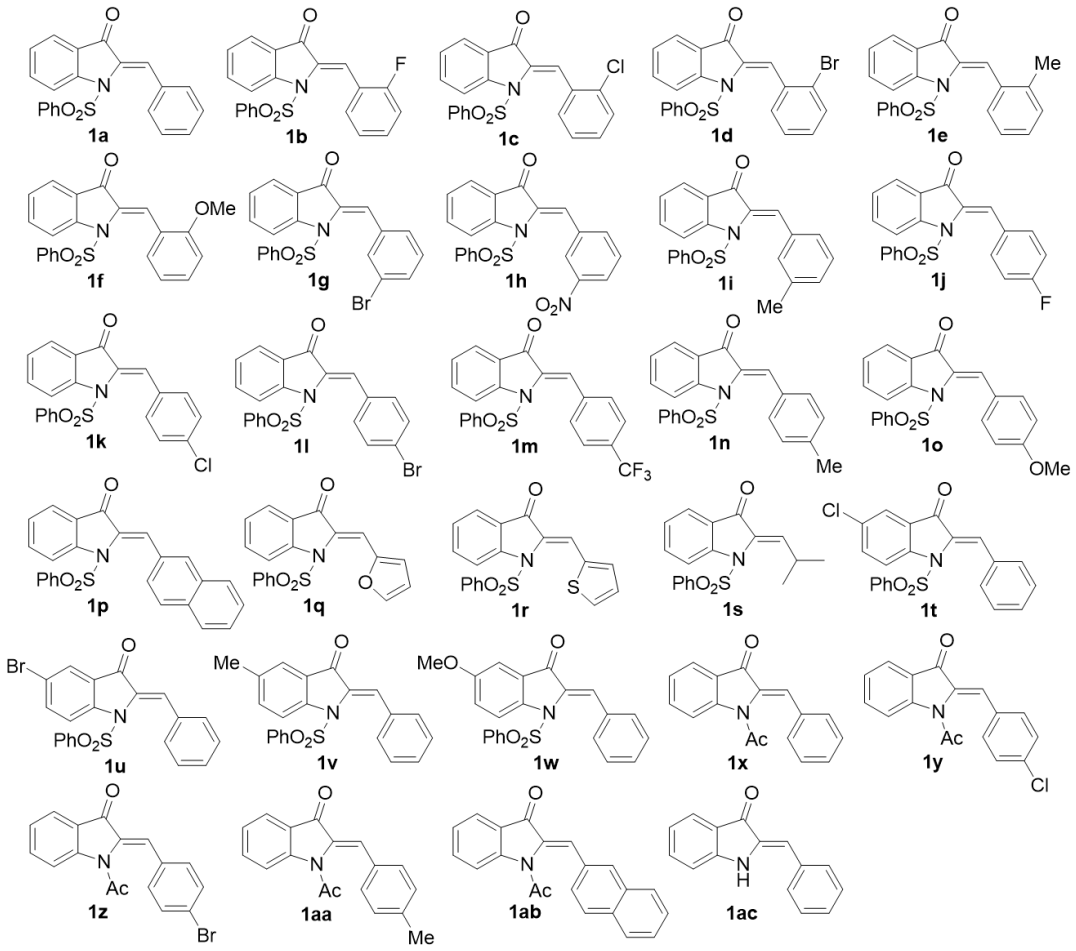
Chemicals and solvents were either purchased from commercial suppliers (such as Energy-chemical, Alfa, Aladdin) or purified by standard procedures as specified in Purification of Laboratory Chemicals, 4th Ed (Armarego, W. L. F.; Perrin, D. D. Butterworth Heinemann: 1997). Petroleum ether (PE) and ethyl acetate (EtOAc) were distilled. All experiments were monitored by analytical thin-layer chromatography (TLC). TLC was performed on silica gel plates with F-254 indicator and visualized by irradiation with UV light. Flash chromatography was performed using silica gel (200-300 mesh). Melting points were recorded on an electrothermal digital melting point apparatus. ^{1}H NMR, ^{13}C NMR spectra were recorded on a JNM-ECS400 (400 M) or 600 MHz Bruker Avance III HD spectrometer (400 or 600 MHz ^{1}H, 100 or 150 MHz ^{13}C). The spectra were recorded in DMSO-d_6 or $CDCl_3$ as the solvents at room temperature, ^{1}H and ^{13}C NMR chemical shifts are reported in ppm relative to the residual solvent peak as an internal standard: DMSO (^{1}H NMR: δ 2.50, ^{13}C NMR: δ 39.52); $CDCl_3$ (^{1}H NMR: δ 7.26, ^{13}C NMR: δ 77.00). Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet or combinations thereof), integration, coupling constant (Hz) and assignment. Data for ^{13}C NMR are reported as chemical shift. High resolution mass spectrometry (HRMS) were performed on a Thermofisher (Vanquish (UPLC)-Q-Exactive Plus) mass instrument (ESI) and methanol was used to dissolve the sample. Enantiomeric excess values were determined by HPLC using a Daicel Chirapak (IA-H, IB-H and IC-H) column on Essentia LC-16 series and eluting with *i*-PrOH and *n*-hexane. Optical rotation was measured on the IP-digi 300 polarimeter with $[\alpha]_D^{20}$ values reported in degrees at 20 °C; concentration (*c*) is in g/100 mL. 1,4-dithiane-2,5-diol or thiols were purchased from Energy Chemical (China). Chiral thiourea and squaramide catalysts were synthesized utilizing literature procedure.[1]

2. Preparation of substrates

2-ylideneoxindoles **1** were prepared by following the publish procedures.[2]

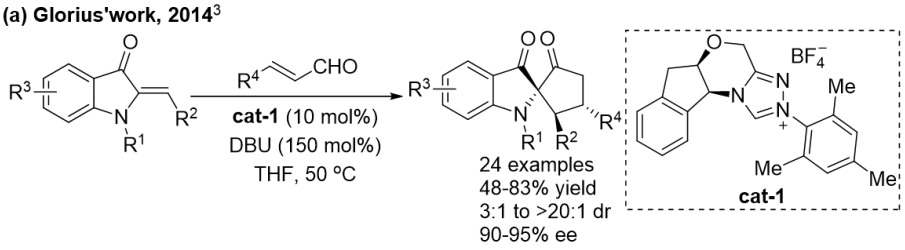


***List of (Z)-2-ylideneoxindoles* 1**

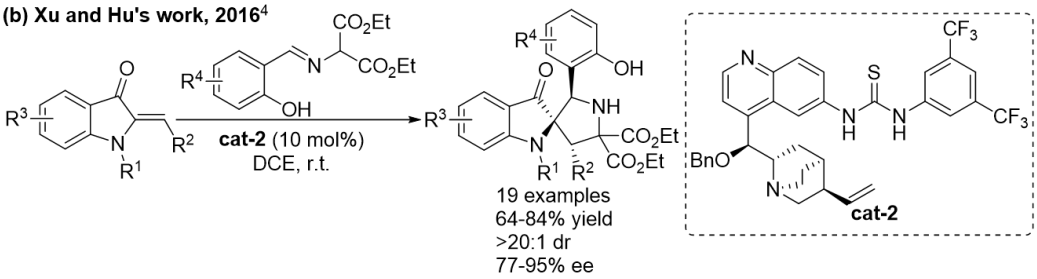


3. Reported examples of asymmetric synthesis of C2-spirooxindoles

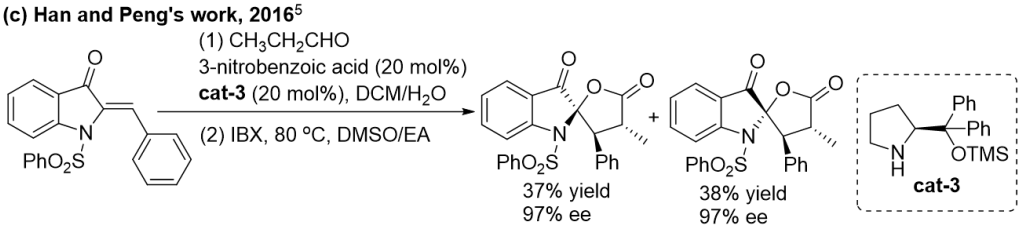
(a) Glorius'work, 2014[3]



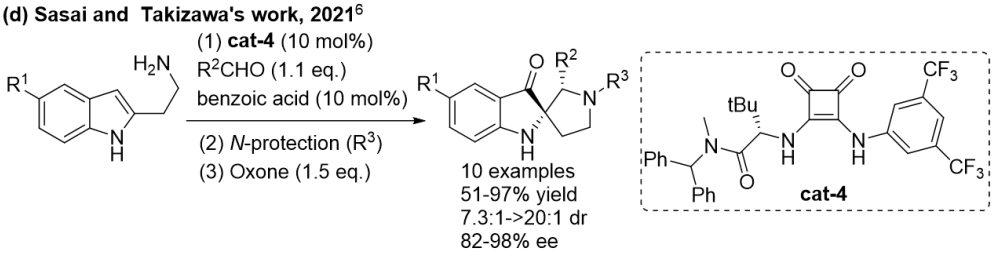
(b) Xu and Hu's work, 2016[4]



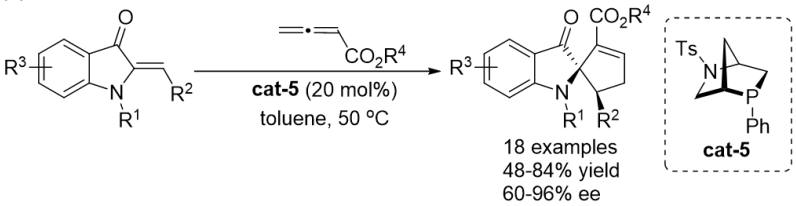
(c) Han and Peng's work, 2016[5]



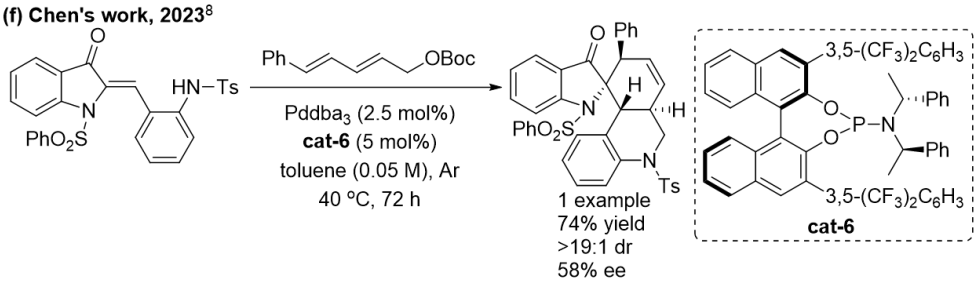
(d) Sasai and Takizawa's work, 2021[6]



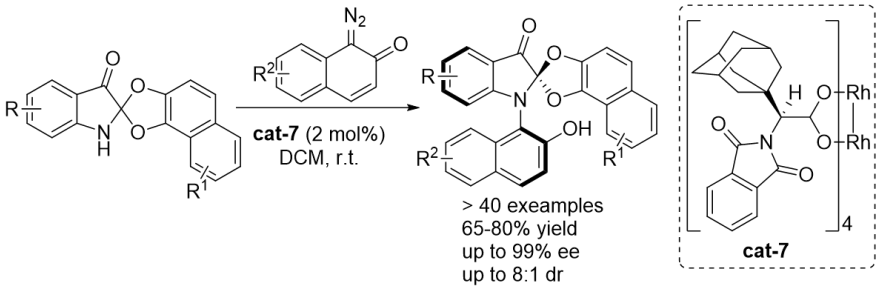
(e) Pirovano's work, 2022[7]



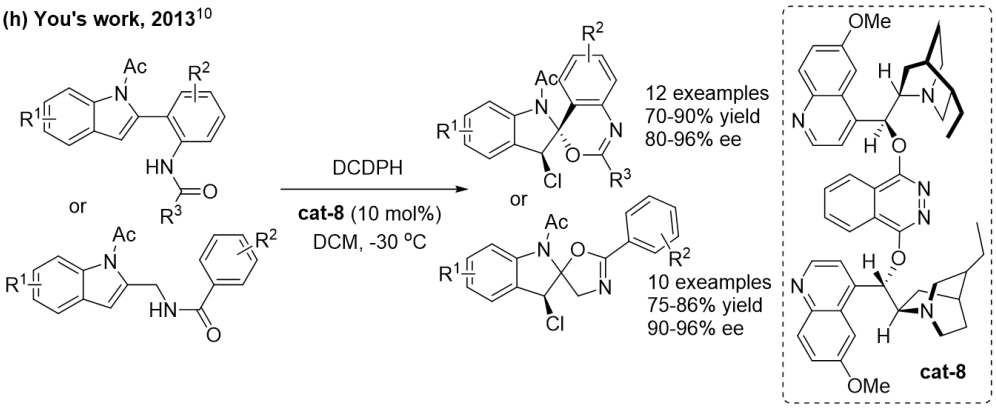
(f) Chen's work, 2023[8]



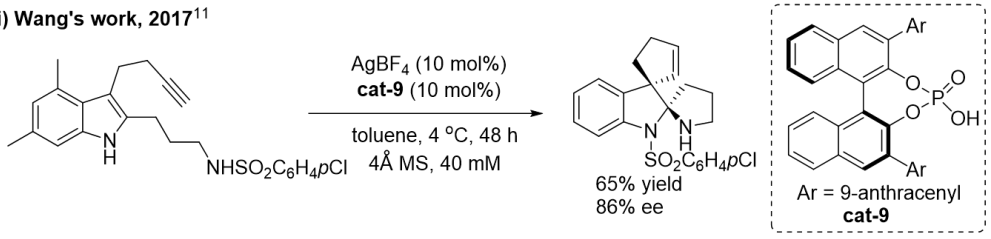
(g) Wang and Ren's work, 2023[9]



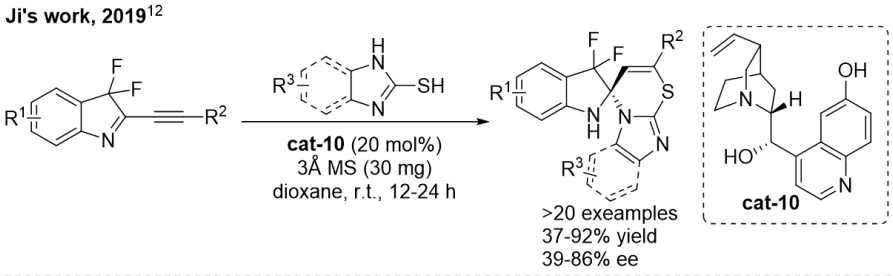
(h) You's work, 2013[10]



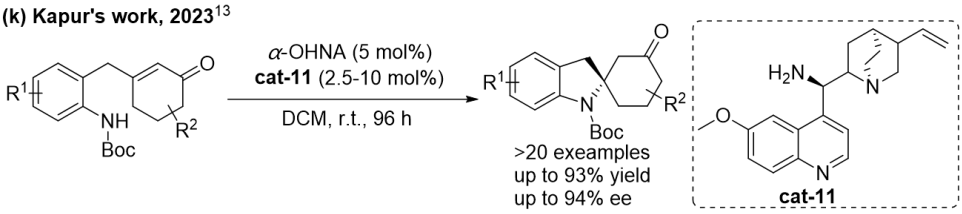
(i) Wang's work, 2017[11]



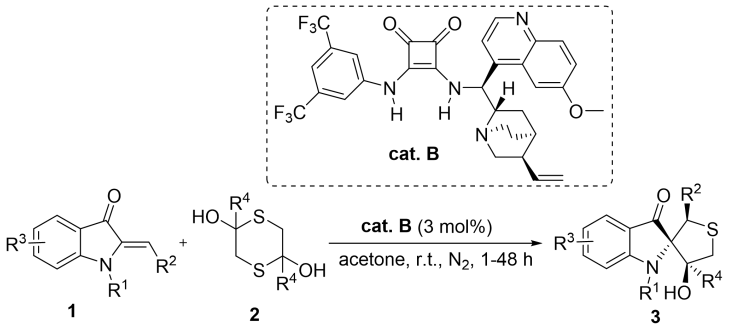
(j) Ji's work, 2019[12]



(k) Kapur's work, 2023[13]

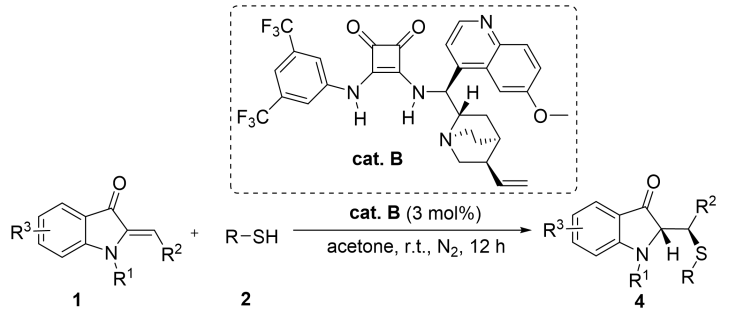


4. General procedure for the organocatalytic asymmetric *sulfa*-Michael/aldol cascade reaction of 2-ylideneoxindoles with 1,4-dithiane-2,5-diol



(*Z*)-2-ylideneoxindoles **1** (0.10 mmol, 1.0 equiv.), 1,4-dithiane-2,5-diol **2** (0.06 mmol, 0.60 equiv.) and catalyst **B** (1.89 mg, 0.003 mmol, 3 mol%) were added to a 5.0 mL Schlenk tube equipped with a stir bar. Then sealed with a rubber septum and vacuum purged five times with high pure nitrogen to remove air. Fresh distilled degassed acetone (1.0 mL) was added consecutively under a positive flow of high pure nitrogen. The reaction mixture was stirred at room temperature. After the required period of time (as judged by TLC analysis). The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1 to 5/1, v/v) to afford the desired spiro[indoline-2,3'-thiophen]-3-ones **3**.

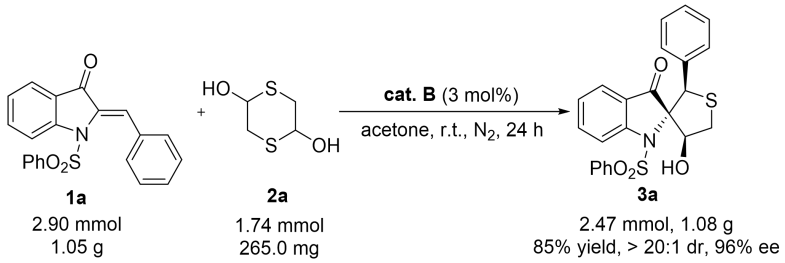
5. General procedure for *sulfa*-Michael addition of 2-ylideneoxindoles with thiol



(*Z*)-2-ylideneoxindoles **1** (0.10 mmol, 1.0 equiv.), thiol **2** (0.12 mmol, 1.2 equiv.) and catalyst **B** (1.89 mg, 0.003 mmol, 3 mol%) were added to a 5.0 mL Schlenk tube equipped with a stir bar. Then sealed with a rubber septum and vacuum purged five times with high pure nitrogen to remove air. Fresh distilled degassed acetone (1.0 mL) was added consecutively under a positive flow of high pure nitrogen. The reaction mixture was stirred at room temperature for 12 h. The resulting solution was

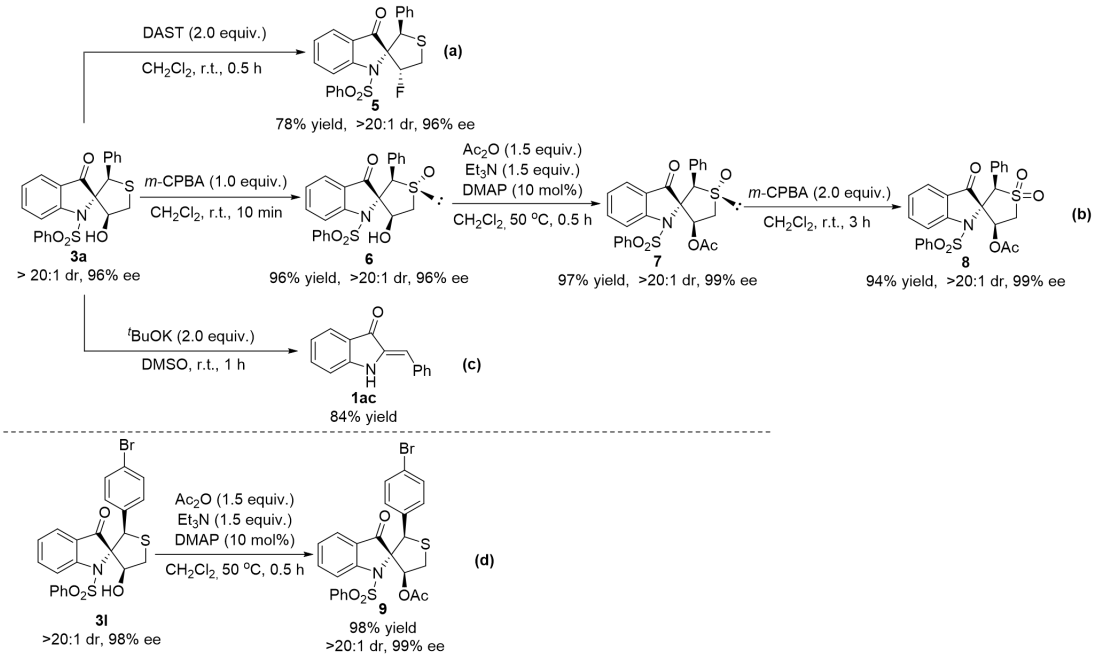
concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired products **4**.

6. The large-scale synthesis of the product 3a



(*Z*)-2-benzylidene-1-(phenylsulfonyl)indolin-3-one **1a** (2.90 mmol, 1.05 g), 1,4-dithiane-2,5-diol **2a** (1.74 mmol, 265.0 mg) and catalyst **B** (55.0 mg, 0.087 mmol) were added to a dry 50 mL round bottom flask with a stir bar. Then sealed with a rubber septum and vacuum purged five times with high pure nitrogen to remove air. Fresh distilled degassed acetone (20.0 mL) was added consecutively under a positive flow of high pure nitrogen. The reaction mixture was stirred at room temperature for 24 hours (as judged by TLC analysis). The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the white solid **3a** (85% yield, >20:1 dr and 96% ee).

7. Procedure for the synthesis of compounds 5 to 9 and 1ac



Synthesis of **5**: According to the literature,[16] in a test tube, **3a** (0.10 mmol, 43.7 mg, >20:1 dr and 96% ee) was dissolved in anhydrous CH_2Cl_2 (1.0 mL), DAST (2.0 equiv., 0.2 mmol, 32.2 mg) was added under N_2 atmosphere. The resulting solution was stirred at room temperature for 0.5 h. After the reaction was completed, which was determined by TLC, the mixture was directly purified by flash chromatography on silica gel was purified by silica gel flash chromatography (petroleum ether/ethyl acetate = 5/1, v/v) to yield the product **5** as a white solid (78% yield, 34.2 mg, >20:1 dr and 96% ee).

Synthesis of **6**: To a stirred solution of **3a** (0.10 mmol, 43.7 mg) in dry CH_2Cl_2 (1.0 mL) at room temperature, then slowly add *m*-CPBA (17.2 mg, 0.1 mmol). The reaction mixture was intense stirred for 10 min (as judged by TLC analysis). The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 1/1, v/v) to afford the white solid **6** (96% yield, >20:1 dr and 96% ee).

Synthesis of **7**: To a solution of **6** (0.10 mmol, 45.3 mg, >20:1 dr and 96% ee), DMAP (0.01 mmol, 1.2 mg), and Et_3N (0.15 mmol, 21.0 μL) in CH_2Cl_2 (1.0 mL) under stirring at 50 ℃ temperature, then slowly add Ac_2O (0.15 mmol, 14.0 μL) and keep the same temperature for 0.5 h (as judged by TLC analysis). The reaction mixture was then poured into saturated aqueous $NaHCO_3$ (5.0 mL), extracted with CH_2Cl_2 (3 × 5 mL), dried over Na_2SO_4 and evaporated under reduced pressure. The residue obtained was directly purified by flash chromatography (eluted with petroleum ether/ethyl acetate = 2/1, v/v) to afford the white solid **7** (97% yield, >20:1 dr and 99% ee).

Synthesis of **8**: In a test tube, **7** (0.05 mmol, 25.0 mg, >20:1 dr and 99% ee) was dissolved in CH_2Cl_2 (1.0 mL), then slowly add *m*-CPBA (17.2 mg, 0.10 mmol). The reaction mixture was intense stirred for 3 h (as judged by TLC analysis). The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 2/1, v/v) to afford the white solid **8** (94% yield, >20:1 dr and 99% ee).

Synthesis of **9**: To a solution of **3l** (0.06 mmol, 30.0 mg), DMAP (0.006 mmol, 0.73 mg), and Et_3N (0.09 mmol, 12.5 μL) in DCM (1.0 mL) under stirring at 50 ℃ temperature, then slowly add Ac_2O (0.09 mmol, 8.5 μL) and keep the same temperature for 0.5 h (as judged by TLC analysis). The reaction mixture was then poured into saturated aqueous $NaHCO_3$ (5.0 mL), extracted with CH_2Cl_2 (3 × 5 mL), dried over Na_2SO_4 and evaporated under reduced pressure. The residue obtained was directly purified by flash chromatography (eluted with petroleum ether/ethyl acetate = 15/1, v/v) to afford the white solid **9** (98% yield, >20:1 dr and 99% ee).

Synthesis of **1ac**: (2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-piro[indoline-2,3'-thiophen]-3-one **3a** (0.10 mmol, 43.7 mg, >20:1 dr, 96% ee), and ^{t}BuOK (0.20 mmol, 22.4 mg) were added to a 10 mL Shlenk tube equipped with a stir bar. Then, fresh dried and degassed DMSO (1.0 mL) was added, the reaction mixture was stirred at room temperature for 0.5 hours (as judged by TLC analysis). After completion the reaction was quenched by addition of H_2O (5.0 mL) and the aqueous layer was extracted with DCM (3 × 5 mL). The combined organic phases and washed with water (3 × 5 mL). Then organic extracts were dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude mixture was purified by flash chromatography (eluted with petroleum ether/ ethyl acetate = 10/1, v/v) to afford a brown solid **1ac** (84% yield, 18.6 mg).

8. Cocrystallization phenomenon of *rac*-3k and its application in further improving the optical purity of spiro[indoline-2,3'-thiophene]-3-ones

Some products **3** with poor enantioselectivity were selected as representatives for cocrystallization. The corresponding products **3** obtained under standard conditions was dissolved in 3 mL acetone, n-hexane (6-9 mL) is added to make the system into a transparent system, and the solvent system is crystallized at room temperature. After crystal precipitation, the solid and liquid phases are separated. After the solid is washed with *n*-hexane for several times, the washing liquid and liquid phase are enriched. Finally, the solid and liquid phases were analyzed by HPLC (**Table S1**).

Table S1 Further improving the optical purity via cocrystallization.

Compound	Data obtained under standard conditions		Data from cocrystallization			
			solid phase		liquid phase	
	M (mg)	ee (%)	M (mg)	ee (%)	M (mg)	ee (%)
3i	42.6	82	4.1	10	32.0	90
3k	41.0	91	12.6	84	21.0	98
3l	49.0	90	12.3	72	30.2	98
3o	41.7	86	14.0	70	24.5	99
3w	40.5	82	15.4	68	24.4	96

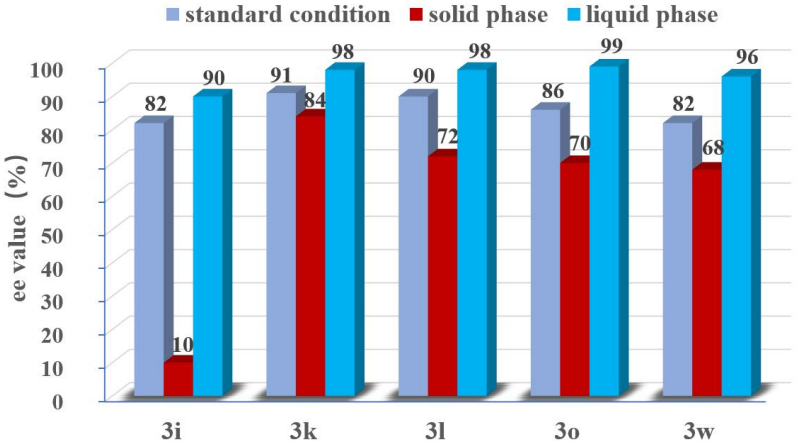


Figure S1. The ee values of each phase after evaporation crystallization.

The racemized **3k** cocrystal as shown in **Figure S2**, exhibited two hydrogen bonds between the hydroxyl group on the thiophene ring and the carbonyl group on the indole ring between the **3k** enantiomers. Additionglly weak π...π interactions might also occur between the *N*-benzenesulfonyl substitutes of indole ring. These interactions led to the formation of a racemized **3k** cocrystal during the crystallization process, where a small portion of the other enantiomer preferentially combined to precipitate.

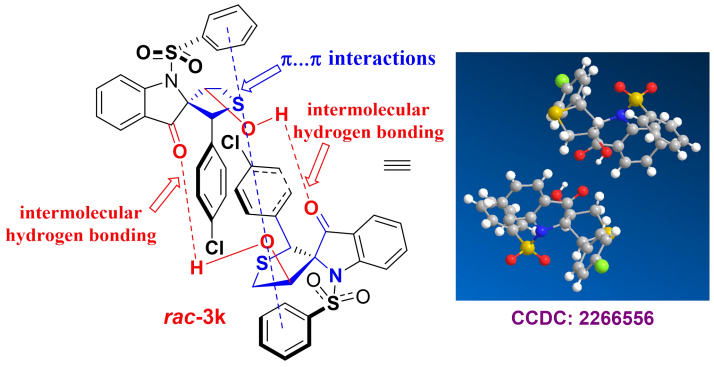


Figure S2. X-ray of ***rac*-3k** cocrystal.

9. The effects of Z/E configurations of 2-ylideneoxindole 1 for the asymmetric sulfa-Michael/aldol cascade reaction

To investigate the effects of ***Z/E*** configurations of 2-ylideneoxindole **1** on this asymmetric sulfa-Michael/aldol cascade reaction, (*E*)-2-ylideneoxindole **1** (**1a'** and **1x'**) was compared with (*Z*)-2-ylideneoxindole (**1a** and **1x**) under standard conditions, and the results are shown below.

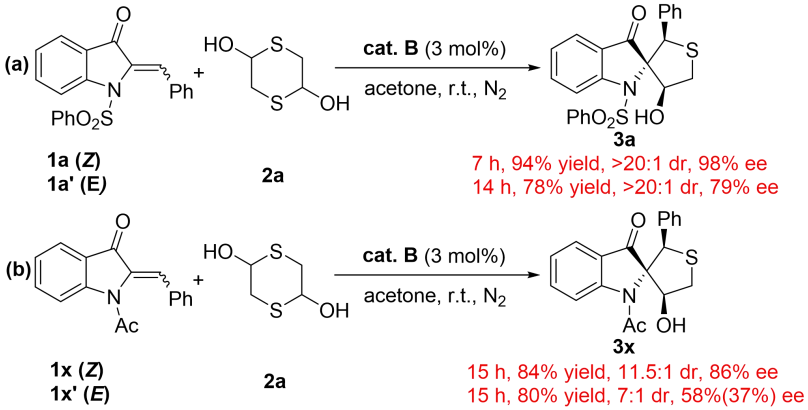
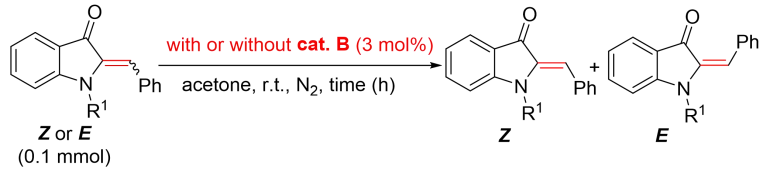


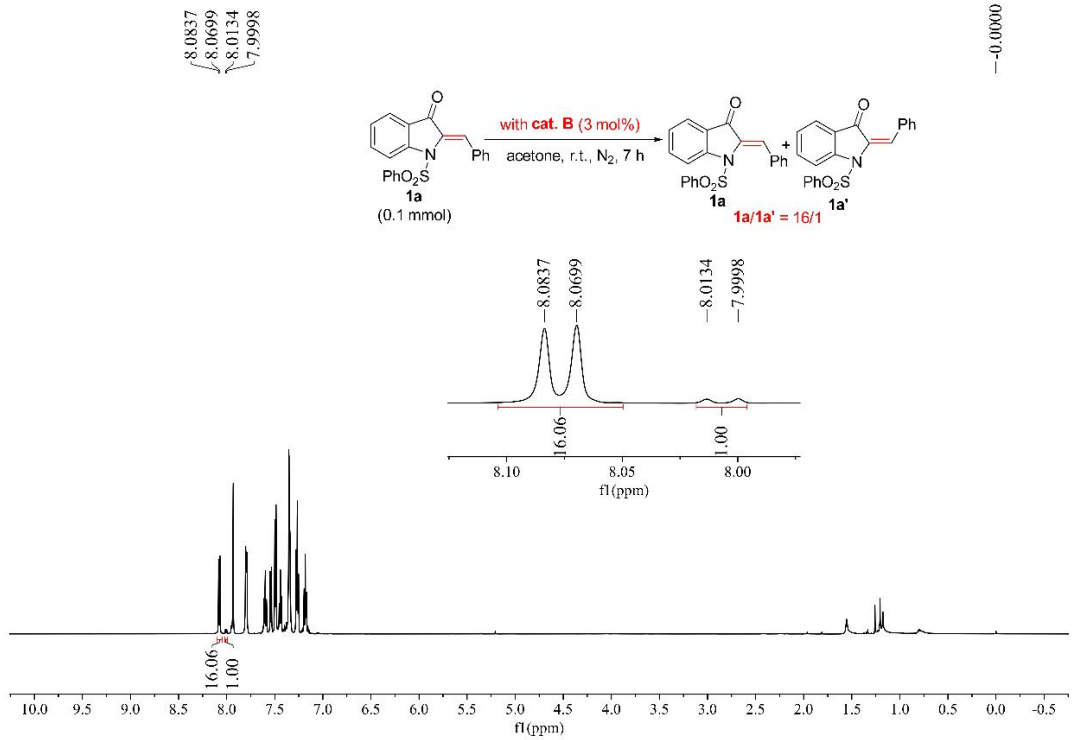
Table S2. Investigation the effects of catalyst **B** on the conformational transitions of various N1-substituted 2-ylideneoxindole substrates.

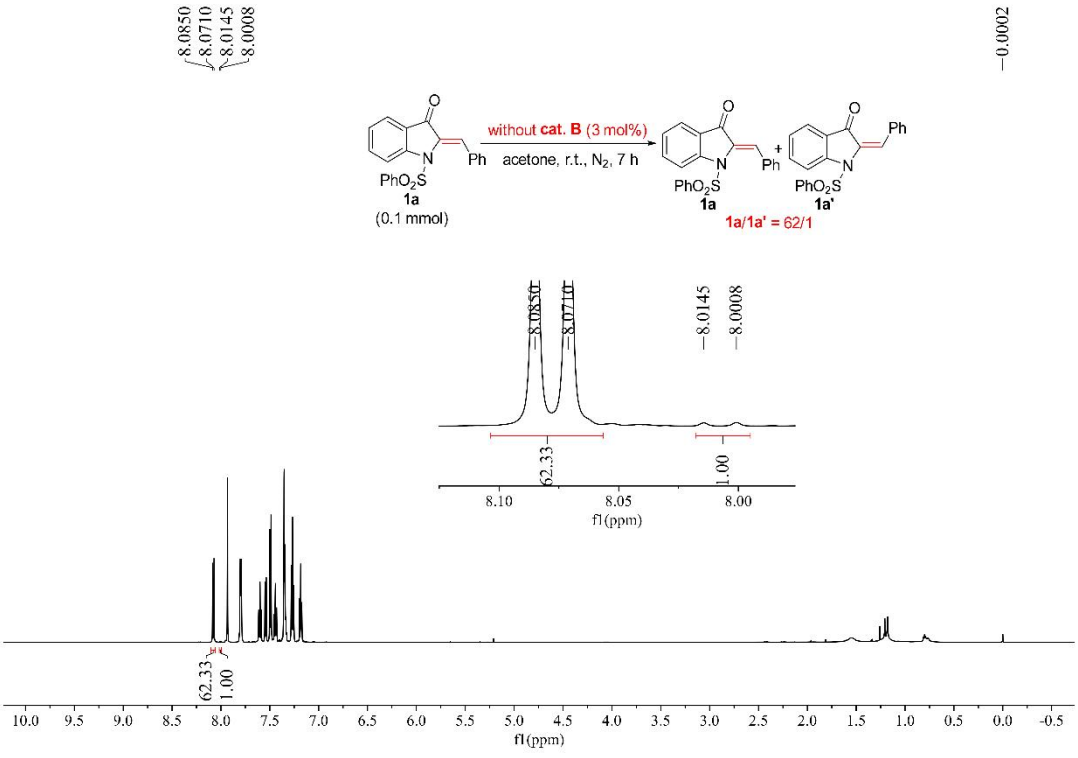


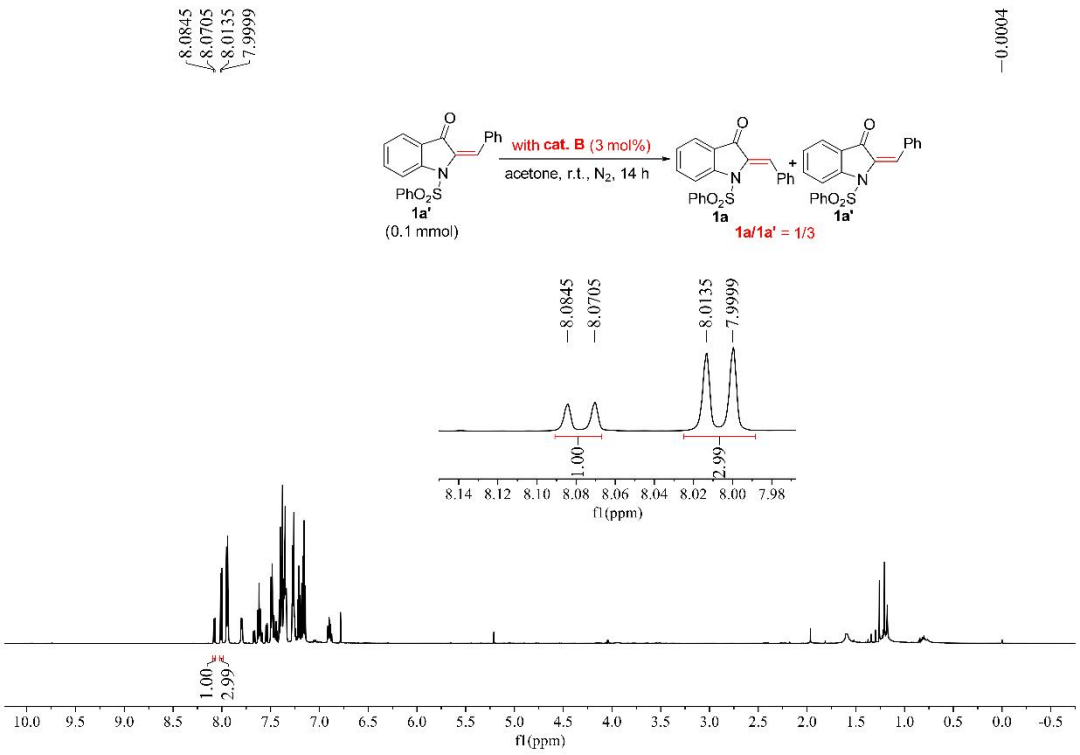
1	R^1	Time (h)	With **cat. B** Z/E	Without **cat. B** Z/E
1a (*Z*)	SO_2Ph	7	16/1	62/1
1a' (*E*)	SO_2Ph	14	1/3	1/15
1x (*Z*)	Ac	15	7/1	6.5/1
1x' (*E*)	Ac	15	1/2	1/16
1ac (*Z*)	H	20	100/-	100/-

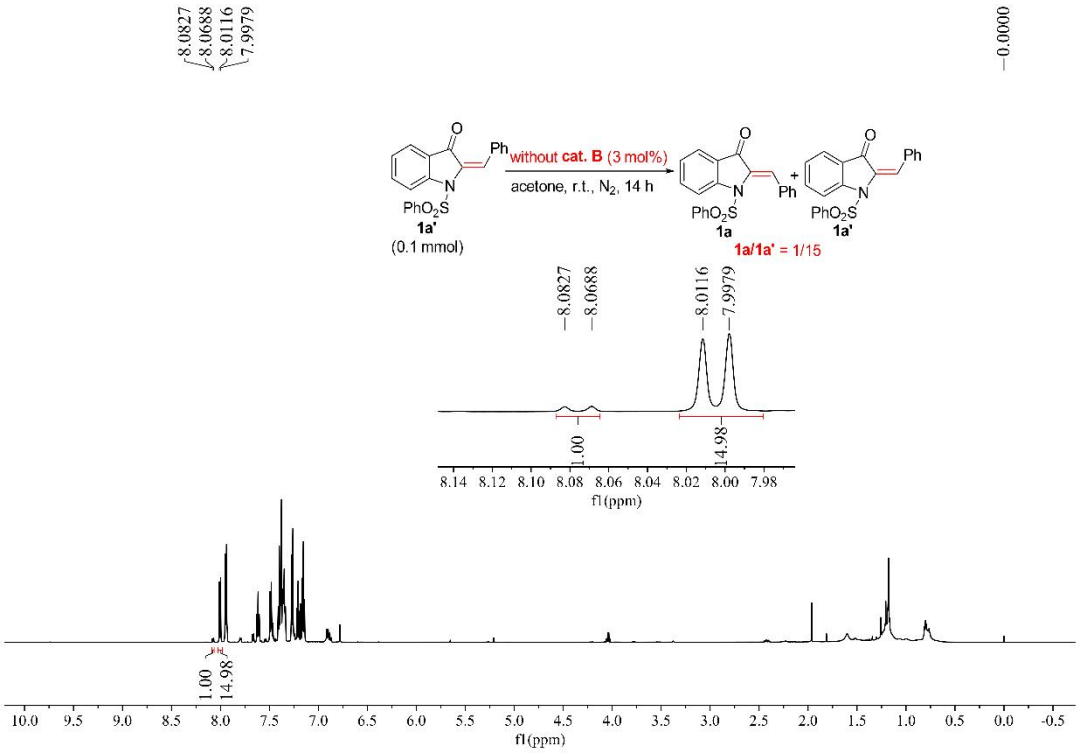
Under standard reaction conditions in the absence of thiol **2a**, we further investigated the effect of catalyst **B** on the conformational transitions of various N1-substituted 2-ylideneoxindole substrates. After the reaction time, the reaction mixture was filtered over a short pad of silica. The filtered solution was concentrated under reduced pressure. The residual crude reaction mixture was dissolved in $CDCl_3$ for ^{1}H-NMR spectra to detect the conformational transitions of 2-ylideneoxindole **1** in the reaction system, and the results are shown in **Table S2**.

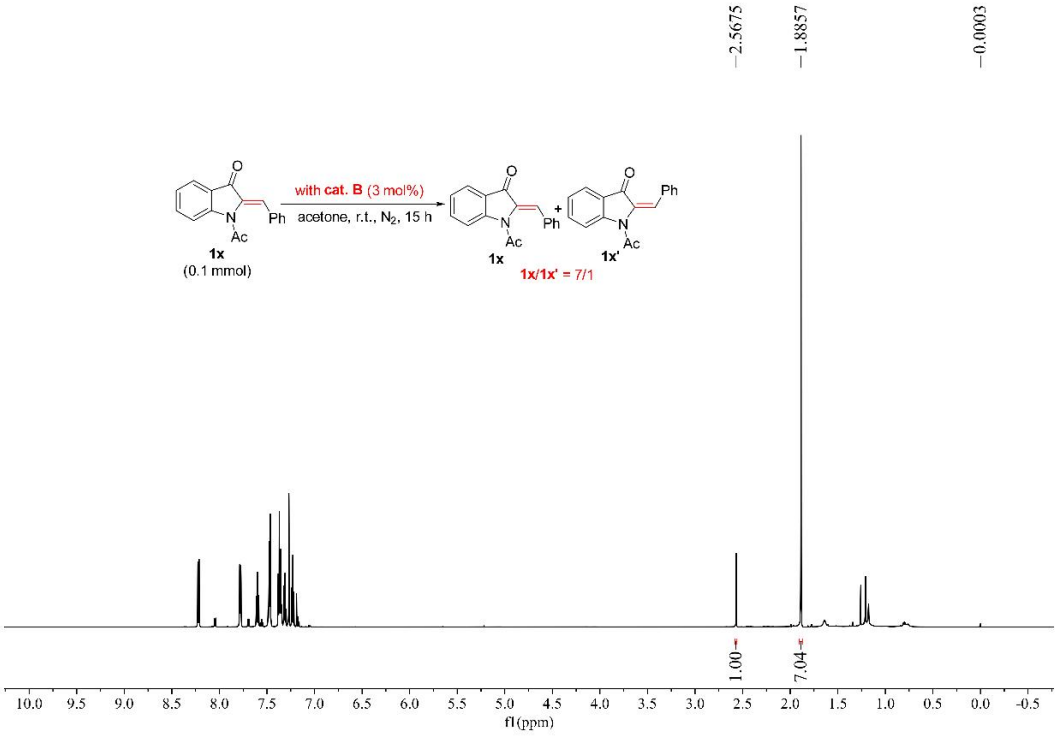
NMR spectra of the above reaction system

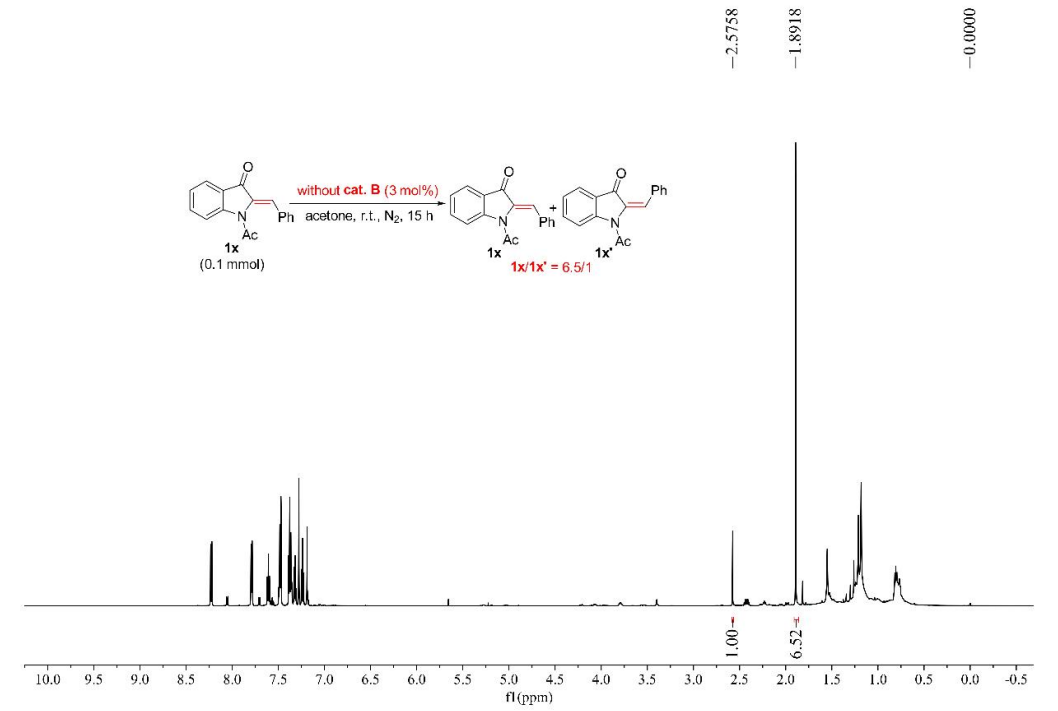


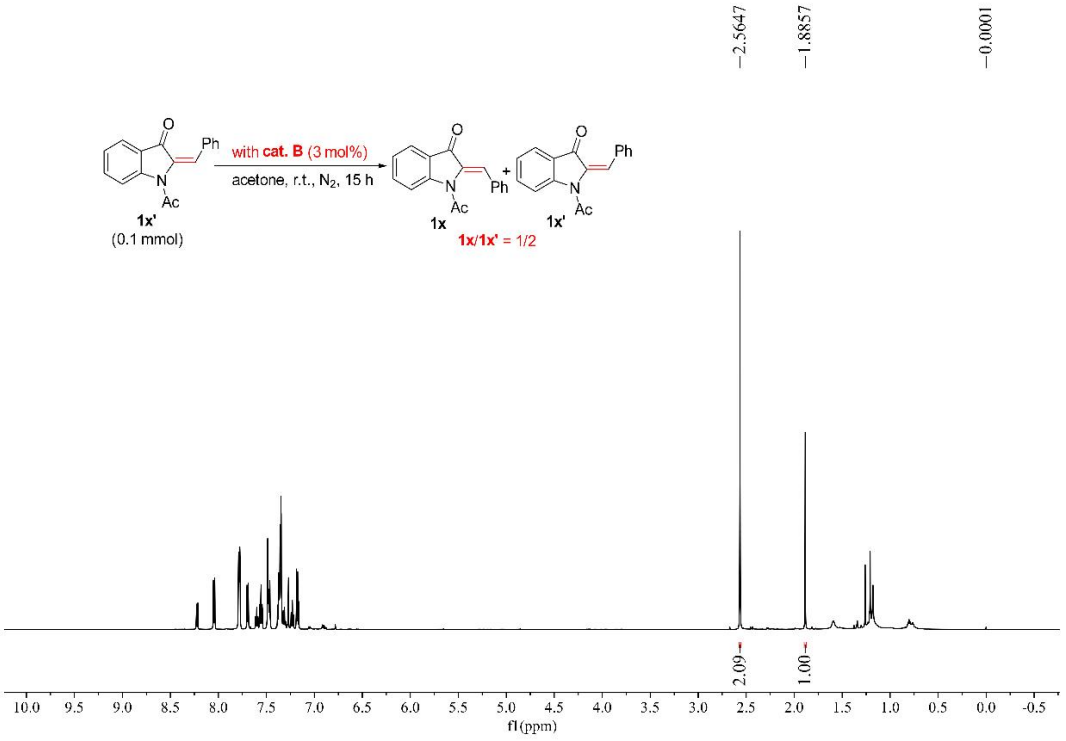


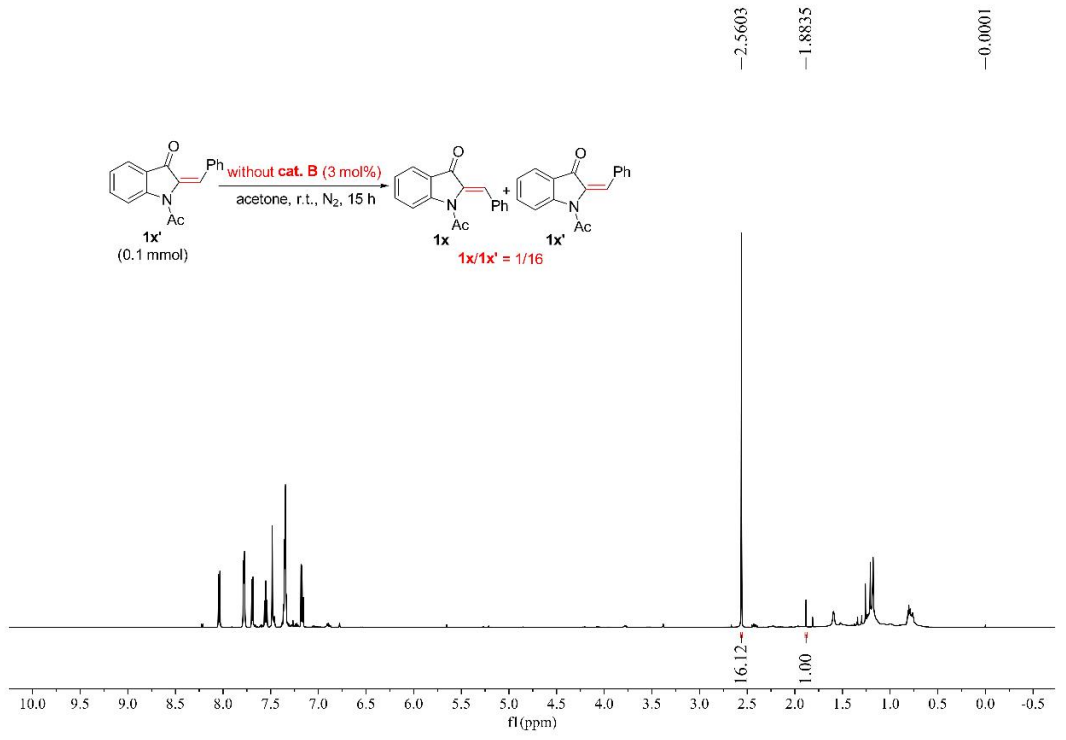

8.0845
8.0705
8.0135
7.9999
0.0004
with cat. B (3 mol%)
acetone, r.t., N2, 14 h
PhO2S
1a'
(0.1 mmol)
1a
1a/1a' = 1/3
1.00
2.99
f1 (ppm)

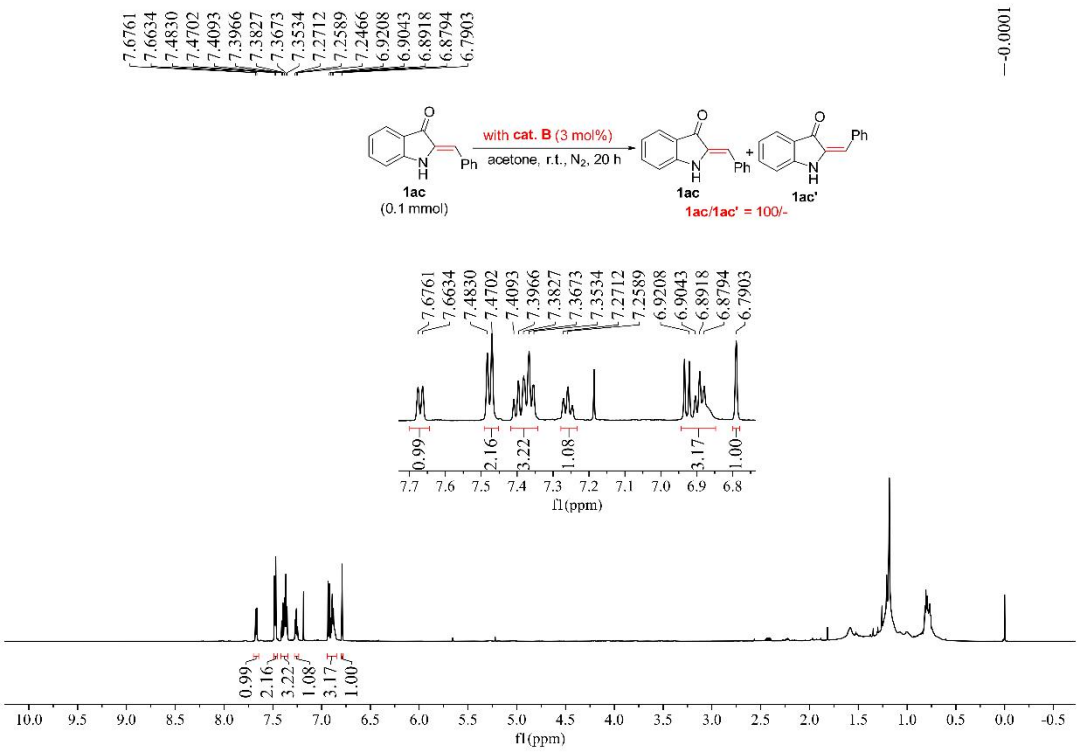

8.0827
8.0688
8.0116
7.9979
0.0000
without cat. B (3 mol%)
acetone, r.t., N2, 14 h
PhO2S
1a'
(0.1 mmol)
1a
1a/1a' = 1/15
1.00
14.98
f1 (ppm)

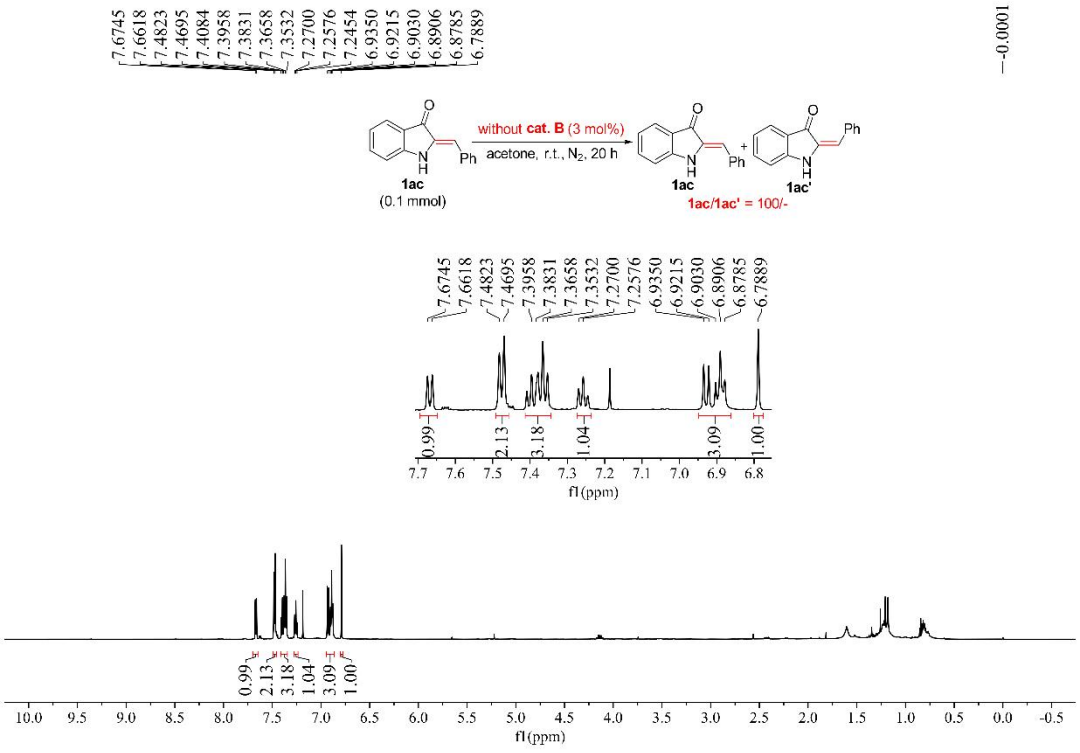

2.5675
1.8857
0.0003
with cat. B (3 mol%)
acetone, r.t., N2, 15 h
1x
(0.1 mmol)
1x
1x'
1x/1x' = 7/1
1.00
7.04
f1(ppm)


2.5758
1.8918
0.0000
without cat. B (3 mol%)
acetone, r.t., N2, 15 h
1x
(0.1 mmol)
1x
1x'
1x/1x' = 6.5/1
1.00
6.52
f1(ppm)

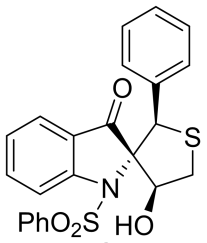

2.5647
1.8857
0.0001
with cat. B (3 mol%)
acetone, r.t., N2, 15 h
1x'
(0.1 mmol)
1x
1x'
1x/1x' = 1/2
2.09
1.00
f1 (ppm)


2.5603
1.8835
0.0001
without cat. B (3 mol%)
acetone, r.t., N2, 15 h
1x'
(0.1 mmol)
1x
1x'
1x/1x' = 1/16
16.12
1.00
f1 (ppm)


7.6761
7.6634
7.4830
7.4702
7.4093
7.3966
7.3827
7.3673
7.3534
7.2712
7.2589
7.2466
6.9208
6.9043
6.8918
6.8794
6.7903
-0.0001
with cat. B (3 mol%)
acetone, r.t., N2, 20 h
1ac
(0.1 mmol)
1ac
1ac'
1ac/1ac' = 100/-
0.99
2.16
3.22
1.08
3.17
1.00
f1 (ppm)


7.6745
7.6618
7.4823
7.4695
7.4084
7.3958
7.3831
7.3658
7.3532
7.2700
7.2576
7.2454
6.9350
6.9215
6.9030
6.8906
6.8785
6.7889
-0.0001
without cat. B (3 mol%)
acetone, r.t., N2, 20 h
1ac
(0.1 mmol)
1ac
1ac'
1ac/1ac' = 100/-
0.99
2.13
3.18
1.04
3.09
1.00
f1 (ppm)

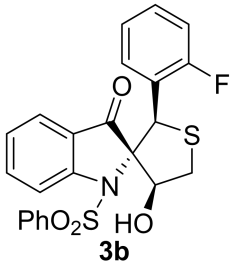
10. Characterization of products



3a

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3a)

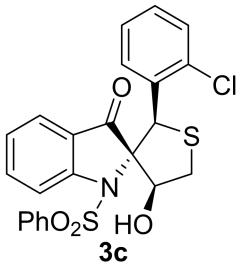
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1a** (36.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 7 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3a** as a white solid in 94% yield (41.2 mg, >20:1 dr, 98% ee). **m. p.**: 117 – 118 ℃. $[\alpha]_D^{20}$ = 49.182 (c 0.54, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 12.380 min (major), t_R = 13.966 min (minor), 98% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.25 – 8.15 (m, 2H), 7.77 – 7.71 (m, 1H), 7.67 – 7.60 (m, 2H), 7.53 – 7.35 (m, 4H), 7.34 – 7.28 (m, 1H), 7.19 – 7.05 (m, 3H), 6.99 – 6.89 (m, 1H), 5.99 (d, *J* = 4.6 Hz, 1H), 5.63 (s, 1H), 5.51 (ddd, *J* = 9.6, 7.6, 4.7 Hz, 1H), 3.72 (t, *J* = 9.6 Hz, 1H), 3.18 (dd, *J* = 9.5, 7.7 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.1, 151.4, 138.6, 137.0, 134.4, 134.3, 129.7, 128.8, 128.1, 128.0, 127.7, 123.4, 123.3, 122.8, 113.9, 85.1, 73.8, 48.8, 30.3. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{19}NNaO_4S_2^+$ $[M+Na]^+$: 460.0648, found: 460.0646.



3b

(2*R*,2'*R*,4'*S*)-2'-(2-fluorophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3b)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1b** (38.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 7.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3b** as a white solid in 92% yield (42.0 mg, >20:1 dr, 99% ee). **m. p.**: 103 – 104 ℃. $[\alpha]_D^{20}$ = 43.197 (*c* 0.71, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.195 min (major), t_R = 20.947 min (minor), 99% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.16 – 8.09 (m, 2H), 7.74 – 7.66 (m, 2H), 7.65 – 7.51 (m, 4H), 7.40 – 7.33 (m, 1H), 7.19 – 7.10 (m, 1H), 7.08 – 6.91 (m, 3H), 6.02 (s, 1H), 5.79 (d, *J* = 4.4 Hz, 1H), 5.50 (ddd, *J* = 9.7, 7.5, 4.4 Hz, 1H), 3.76 (t, *J* = 9.6 Hz, 1H), 3.18 (dd, *J* = 9.5, 7.5 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.4, 160.6 (d, *J* = 245.7 Hz), 151.7, 138.9, 137.3, 134.0, 131.5 (d, *J* = 3.1 Hz), 130.0 (d, *J* = 8.2 Hz), 129.5, 127.5, 123.9 (d, *J* = 3.2 Hz), 123.4 (d, *J* = 8.1 Hz), 122.7, 122.0 (d, *J* = 12.9 Hz), 115.0, 114.7, 114.3, 84.3, 74.1, 40.9, 30.6. **^{19}F NMR** (376 MHz, DMSO-d_6): δ -115.1 – -115.3 (m). **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}FNNaO_4S_2^+$ $[M+Na]^+$: 478.0553, found: 478.0548.

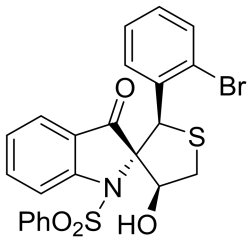


3c

(2*R*,2'*R*,4'*S*)-2'-(2-chlorophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3c)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1c** (39.6 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 11 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3c** as a white solid in 90% yield (42.5

mg, >20:1 dr, 85% ee). **m. p.**: 110 – 111 °C. $[\alpha]_D^{20}$ = 80.128 (*c* 0.58, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 15.608 min (major), t_R = 21.006 min (minor), 85% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.11 – 8.04 (m, 2H), 7.82 – 7.74 (m, 2H), 7.72 – 7.63 (m, 1H), 7.63 – 7.52 (m, 3H), 7.42 – 7.35 (m, 1H), 7.24 – 7.15 (m, 2H), 7.15 – 7.08 (m, 1H), 7.08 – 6.99 (m, 1H), 6.14 (s, 1H), 5.69 (d, *J* = 4.3 Hz, 1H), 5.53 (ddd, *J* = 9.7, 7.3, 4.1 Hz, 1H), 3.83 (t, *J* = 9.7 Hz, 1H), 3.17 (dd, *J* = 9.5, 7.3 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.5, 151.9, 139.1, 137.6, 134.0, 133.8, 133.4, 132.5, 129.7, 129.5, 129.1, 127.4, 126.7, 123.7, 123.6, 123.0, 114.7, 84.4, 74.4, 45.1, 31.0. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}ClNNaO_4S_2^+$ $[M+Na]^+$: 494.0258, found: 494.0255.

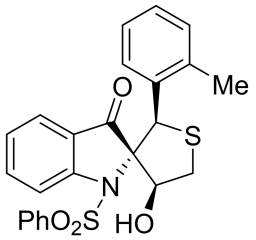


3d

(2*R*,2'*R*,4'*S*)-2'-(2-bromophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3d)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1d** (44.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 1.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3d** as a white solid in 90% yield (46.5 mg, >20:1 dr, 94% ee). **m. p.**: 167 – 168 °C. $[\alpha]_D^{20}$ = 22.602 (*c* 0.59, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 16.639 min (major), t_R = 21.025 min (minor), 94% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.08 – 8.01 (m, 2H), 7.83 – 7.70 (m, 2H), 7.71 – 7.50 (m, 4H), 7.45 – 7.35 (m, 2H), 7.26 – 7.17 (m, 1H), 7.09 – 6.99 (m, 2H), 6.08 (s, 1H), 5.68 (d, *J* = 4.4 Hz, 1H), 5.53 (ddd, *J* = 9.7, 7.3, 4.3

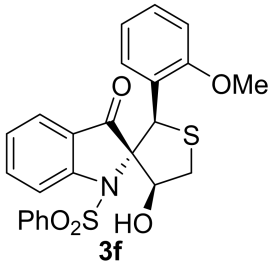
Hz, 1H), 3.83 (t, *J* = 9.7 Hz, 1H), 3.16 (dd, *J* = 9.6, 7.4 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.6, 151.9, 139.2, 137.5, 135.2, 133.9, 132.6, 132.5, 130.0, 129.4, 127.2, 127.2, 124.5, 123.7, 123.6, 123.1, 114.8, 84.3, 74.4, 47.8, 31.1. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}BrNNaO_4S_2^+$ [M+Na]$^+$: 537.9753, found: 537.9745.



3e

(2*R*,2'*R*,4'*S*)-4'-hydroxy-1-(phenylsulfonyl)-2'-(o-tolyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3e)

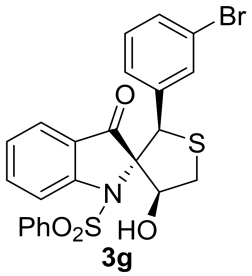
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1e** (37.5 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 2 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3e** as a white solid in 91% yield (41.0 mg, >20:1 dr, 97% ee). **m. p.**: 183 – 184 °C. **[α]** $^{20}_{D}$ = 22.602 (*c* 0.59, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 95/5, flow rate 1.0 mL/min, λ = 254 nm), t_R = 43.111 min (minor), t_R = 52.326 min (major), 97% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.12 – 8.05 (m, 2H), 7.73 – 7.62 (m, 3H), 7.60 – 7.52 (m, 3H), 7.46 – 7.40 (m, 1H), 7.07 – 6.94 (m, 4H), 5.90 (s, 1H), 5.66 (d, *J* = 4.4 Hz, 1H), 5.52 (ddd, *J* = 9.6, 7.5, 4.4 Hz, 1H), 3.81 (t, *J* = 9.6 Hz, 1H), 3.17 (dd, *J* = 9.5, 7.5 Hz, 1H), 2.45 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.7, 151.4, 138.6, 137.3, 137.2, 134.1, 133.4, 130.3, 130.1, 129.4, 127.7, 127.5, 125.5, 123.7, 123.6, 123.4, 114.5, 84.8, 73.9, 44.9, 30.8, 19.8. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_4S_2^+$ [M+Na]$^+$: 474.0804, found: 474.0801.



3f

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-(2-methoxyphenyl)-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3f)

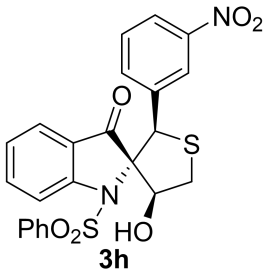
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1f** (39.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 1.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3f** as a white solid in 82% yield (38.4 mg, >20:1 dr, 83% ee). **m. p.**: 101 – 102 ℃. **[α]** $_{D}^{20}$ = -1.354 (*c* 0.64, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 95/5, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.158 min (minor), t_R = 22.560 min (major), 83% ee. **^{1}H NMR** (600 MHz, DMSO-d_6): δ 8.15 – 8.10 (m, 2H), 7.71 – 7.65 (m, 1H), 7.66 – 7.61 (m, 1H), 7.61 – 7.55 (m, 3H), 7.55 – 7.49 (m, 1H), 7.34 – 7.28 (m, 1H), 7.07 – 7.01 (m, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 6.79 – 6.73 (m, 1H), 6.70 – 6.66 (m, 1H), 6.16 (s, 1H), 5.74 (d, *J* = 4.5 Hz, 1H), 5.50 (ddd, *J* = 9.8, 7.3, 4.5 Hz, 1H), 3.76 (t, *J* = 9.7 Hz, 1H), 3.61 (s, 3H), 3.11 (dd, *J* = 9.6, 7.4 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 194.8, 157.5, 151.9, 139.4, 136.9, 133.8, 130.8, 129.4, 129.0, 127.4, 123.3, 123.2, 123.0, 122.8, 119.5, 114.0, 109.8, 84.5, 74.7, 55.0, 41.9, 30.8. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_5S_2^+$ $[M+Na]^+$: 490.0753, found: 490.0755.



3g

(2*R*,2'*R*,4'*S*)-2'-(3-bromophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3g)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1g** (44.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 2.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3g** as a white solid in 88% yield (45.4 mg, >20:1 dr, 93% ee). **m. p.**: 111 – 112 ℃. $[\alpha]_D^{20}$ = 42.684 (*c* 0.83, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.569 min (major), t_R = 11.732 min (minor), 93% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.27 – 8.19 (m, 2H), 7.79 – 7.70 (m, 1H), 7.69 – 7.57 (m, 3H), 7.56 – 7.47 (m, 1H), 7.45 – 7.26 (m, 4H), 7.10 (t, *J* = 7.9 Hz, 1H), 7.03 – 6.94 (m, 1H), 6.06 (d, *J* = 4.7 Hz, 1H), 5.61 (s, 1H), 5.51 (ddd, *J* = 9.8, 7.6, 4.6 Hz, 1H), 3.71 (t, *J* = 9.6 Hz, 1H), 3.19 (dd, *J* = 9.4, 7.6 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.0, 151.4, 138.4, 137.4, 137.3, 134.5, 131.4, 131.0, 130.1, 129.8, 127.7, 123.5, 123.5, 122.7, 121.2, 113.9, 99.5, 84.9, 73.9, 48.1, 30.3. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}BrNNaO_4S_2^+$ $[M+Na]^+$: 537.9753, found: 537.9755.

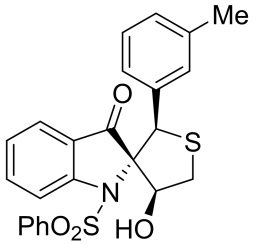


3h

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-(3-nitrophenyl)-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3h)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1h** (40.6 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 1 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl

acetate = 5/1, v/v) to afford the desired product **3h** as a white solid in 90% yield (43.5 mg, >20:1 dr, 98% ee). **m. p.**: 191 – 192 ℃. **[α]** $_D^{20}$ = 12.857 (*c* 0.84, $CHCl_3$); The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 23.225 min (minor), t_R = 30.140 min (major), 98% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.35 – 8.21 (m, 3H), 8.01 – 7.94 (m, 1H), 7.84 – 7.71 (m, 2H), 7.69 – 7.60 (m, 2H), 7.54 – 7.38 (m, 3H), 7.34 – 7.28 (m, 1H), 7.00 – 6.91 (m, 1H), 6.11 (d, *J* = 4.6 Hz, 1H), 5.76 (s, 1H), 5.55 (ddd, *J* = 9.7, 7.5, 4.6 Hz, 1H), 3.76 (t, *J* = 9.7 Hz, 1H), 3.23 (dd, *J* = 9.5, 7.5 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.0, 151.4, 147.3, 138.3, 137.4, 137.3, 135.2, 134.5, 129.8, 129.7, 127.7, 123.6, 123.5, 123.4, 123.1, 122.5, 113.9, 84.8, 74.0, 48.0, 30.4. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}N_2NaO_6S_2^+$ $[M+Na]^+$: 505.0498, found: 505.0498.

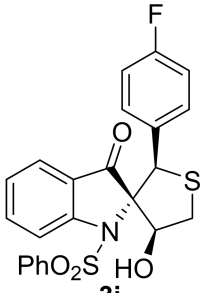


3i

(2*R*,2'*R*,4'*S*)-4'-hydroxy-1-(phenylsulfonyl)-2'-(*m*-tolyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3i)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1i** (37.5 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 2 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3i** as a white solid in 94% yield (42.6 mg, >20:1 dr, 82% ee). **m. p.**: 126-127 ℃. **[α]** $_D^{20}$ = 12.649 (*c* 0.37, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 34.691 min (major), t_R = 40.095 min (minor), 82% ee (recrystallization up to 90% ee). **^{1}H NMR** (400 MHz, DMSO-d_6): ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.25 – 8.18 (m, 2H), 7.77 – 7.71 (m,

1H), 7.67 – 7.59 (m, 2H), 7.51 – 7.45 (m, 1H), 7.42 – 7.30 (m, 2H), 7.26 – 7.19 (m, 2H), 7.02 – 6.87 (m, 3H), 5.97 (d, *J* = 4.6 Hz, 1H), 5.60 (s, 1H), 5.50 (ddd, *J* = 9.7, 7.6, 4.6 Hz, 1H), 3.70 (t, *J* = 9.6 Hz, 1H), 3.17 (dd, *J* = 9.5, 7.6 Hz, 1H), 2.10 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.0, 151.4, 138.6, 136.9, 136.9, 134.4, 134.3, 129.7, 129.4, 128.6, 127.8, 127.6, 125.8, 123.3, 123.2, 122.9, 113.9, 85.1, 73.9, 48.6, 30.2, 20.9. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_4S_2^+$ $[M+Na]^+$: 474.0804, found: 474.0803.

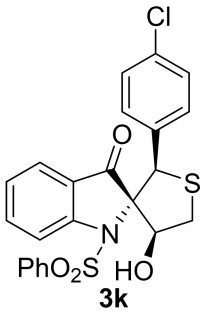


3j

(2*R*,2'*R*,4'*S*)-2'-(4-fluorophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3j)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1j** (38.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 7.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3j** as a white solid in 86% yield (39.0 mg, >20:1 dr, 98% ee). **m. p.**: 87 – 88 °C. **$[\alpha]_D^{20}$** = 48.998 (*c* 0.33, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.477 min (major), t_R = 38.764 min (minor), 98% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 8.16 – 8.10 (m, 2H), 7.74 – 7.66 (m, 2H), 7.65 – 7.48 (m, 4H), 7.40 – 7.33 (m, 1H), 7.19 – 7.11 (m, 1H), 7.08 – 6.92 (m, 3H), 6.02 (s, 1H), 5.79 (d, *J* = 4.4 Hz, 1H), 5.50 (ddd, *J* = 9.7, 7.5, 4.4 Hz, 1H), 3.76 (t, *J* = 9.6 Hz, 1H), 3.18 (dd, *J* = 9.5, 7.5 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.6, 160.8 (d, *J* = 246.8 Hz), 151.9, 139.1, 137.6, 134.2, 131.7 (d, *J* = 2.6 Hz), 130.2 (d, *J* = 8.1 Hz), 129.7, 127.7, 124.1 (d, *J* = 2.9 Hz), 123.7 (d, *J* = 8.1 Hz), 122.9, 122.2 (d, *J* = 13.1 Hz), 115.0 (d, *J* = 22.4 Hz), 114.5, 84.5, 74.3,

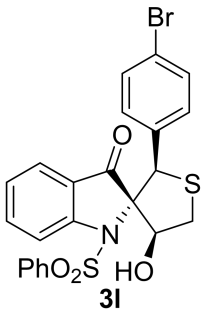
41.1, 30.8. **^{19}F NMR** (376 MHz, DMSO-d_6): δ -115.1 – -115.2 (m). **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}FNNaO_4S_2^+$ [M+Na]$^+$: 478.0553, found: 478.0550.



3k

(2*R*,2'*R*,4'*S*)-2'-(4-chlorophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3k)

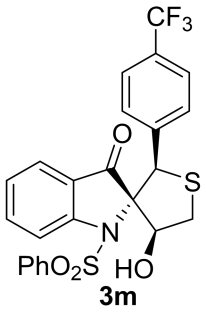
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1k** (39.6 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 11 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3k** as a white solid in 87% yield (41.0 mg, >20:1 dr, 91% ee). **m. p.**: 197 – 198 °C. **$[\alpha]_D^{20}$** = 65.079 (*c* 0.83, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 28.962 min (major), t_R = 40.891 min (minor), 91% ee (recrystallization up to 98% ee). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.25 – 8.18 (m, 2H), 7.79 – 7.70 (m, 1H), 7.69 – 7.60 (m, 2H), 7.56 – 7.47 (m, 1H), 7.47 – 7.31 (m, 4H), 7.26 – 7.18 (m, 2H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.02 (d, *J* = 4.6, 1H), 5.62 (s, 1H), 5.50 (ddd, *J* = 9.7, 7.5, 4.6 Hz, 1H), 3.71 (t, *J* = 9.6 Hz, 1H), 3.19 (dd, *J* = 9.5, 7.7 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.0, 151.4, 138.4, 137.3, 134.4, 133.6, 132.7, 130.6, 129.7, 128.0, 127.7, 123.5, 123.5, 122.7, 113.9, 85.0, 73.9, 48.1, 30.3. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}ClNNaO_4S_2^+$ [M+Na]$^+$: 494.0258, found: 494.0257.



3l

(2*R*,2'*R*,4'*S*)-2'-(4-bromophenyl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3l)

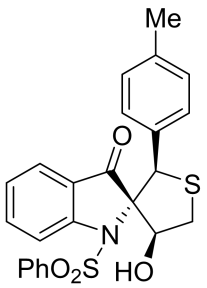
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1l** (44.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3l** as a white solid in 95% yield (49.0 mg, >20:1 dr, 90% ee). **m. p.**: 189 – 190 °C. **[α]** $_D^{20}$ = 2.679 (*c* 0.73, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 31.059 min (major), t_R = 45.987 min (minor), 90% ee (recrystallization up to 98% ee). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.25 – 8.18 (m, 2H), 7.79 – 7.70 (m, 1H), 7.68 – 7.60 (m, 2H), 7.55 – 7.47 (m, 1H), 7.44 – 7.32 (m, 6H), 7.03 – 6.95 (m, 1H), 6.02 (d, *J* = 4.6 Hz, 1H), 5.61 (s, 1H), 5.50 (ddd, *J* = 9.7, 7.6, 4.6 Hz, 1H), 3.71 (t, *J* = 9.6 Hz, 1H), 3.18 (dd, *J* = 9.5, 7.6 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.0, 151.4, 138.4, 137.3, 134.4, 134.1, 131.0, 130.9, 129.7, 127.7, 123.5, 123.5, 122.7, 121.3, 113.9, 84.9, 73.9, 48.1, 30.3. **HRMS** (ESI) m/z: calculated for $C_{23}H_{18}BrNNaO_4S_2^+$ $[M+Na]^+$: 537.9753, found: 537.9749.



3m

(2*R*,2'*R*,4'*S*)-4'-hydroxy-1-(phenylsulfonyl)-2'-(4-(trifluoromethyl)phenyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3m)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1m** (43.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 1 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3m** as a white solid in 88% yield (44.5 mg, >20:1 dr, 94% ee). **m. p.**: 152 – 153 ℃. $[\alpha]_D^{20}$ = 65.079 (*c* 0.83, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 11.875 min (major), t_R = 13.372 min (minor), 94% ee. **^{1}H NMR** (600 MHz, DMSO-d_6): δ 8.24 – 8.20 (m, 2H), 7.77 – 7.72 (m, 1H), 7.64 (t, *J* = 8.2 Hz, 4H), 7.55 – 7.49 (m, 3H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.34 – 7.31 (m, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 6.06 (d, *J* = 4.6 Hz, 1H), 5.71 (s, 1H), 5.53 (ddd, *J* = 9.7, 7.5, 4.6 Hz, 1H), 3.73 (t, *J* = 9.6 Hz, 1H), 3.21 (dd, *J* = 9.6, 7.6, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 194.0, 151.4, 139.7, 138.4, 137.4, 134.5, 129.8, 129.7, 128.7, 128.5, 127.7, 124.9, 123.5, 123.0, 122.6, 114.0, 84.9, 74.1, 48.3, 30.3. **^{19}F NMR** (565 MHz, DMSO-d_6): δ -61.1. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{18}F_3NNaO_4S_2^+$ $[M+Na]^+$: 528.0522, found: 528.0522.

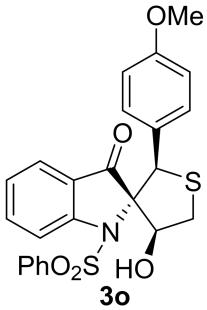


3n

(2*R*,2'*R*,4'*S*)-4'-hydroxy-1-(phenylsulfonyl)-2'-(*p*-tolyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3n)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1n** (37.5 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 2 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl

acetate = 5/1, v/v) to afford the desired product **3n** as a white solid in 90% yield (40.5 mg, >20:1 dr, 83% ee). **m. p.:** 181 – 182 ℃. $[\alpha]_D^{20}$ = 37.181 (*c* 0.28, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 14.300 min (major), t_R = 19.859 min (minor), 83% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): ^{1}H NMR (400 MHz, DMSO-d_6) δ = 8.24 – 8.17 (m, 2H), 7.77 – 7.71 (m, 1H), 7.66 – 7.59 (m, 2H), 7.52 – 7.45 (m, 1H), 7.39 – 7.28 (m, 4H), 7.00 – 6.90 (m, 3H), 5.95 (d, *J* = 4.6 Hz, 1H), 5.60 (s, 1H), 5.48 (ddd, *J* = 9.7, 7.6, 4.7 Hz, 1H), 3.69 (t, *J* = 9.6 Hz, 1H), 3.16 (dd, *J* = 9.4, 7.7 Hz, 1H), 2.11 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.1, 151.4, 138.6, 137.3, 137.0, 134.3, 131.4, 129.7, 128.7, 128.6, 127.6, 123.4, 123.2, 122.8, 113.9, 85.1, 73.8, 48.4, 30.2, 20.5. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_4S_2^+$ $[M+Na]^+$: 474.0804, found: 474.0804.

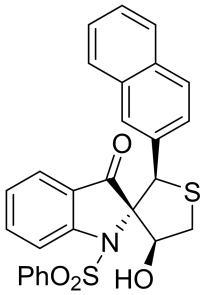


3o

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-(4-methoxyphenyl)-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3o)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1o** (39.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 1.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3o** as a white solid in 89% yield (41.7 mg, >20:1 dr, 86% ee). **m. p.**: 169 – 170 ℃. $[\alpha]_D^{20}$ = 120.659 (*c* 0.38, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 24.618 min (major), t_R = 29.009 min (minor), 86% ee (recrystallization up to 99% ee). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.24 – 8.17 (m, 2H), 7.78 – 7.69 (m, 1H), 7.67 – 7.59 (m, 2H), 7.52 –

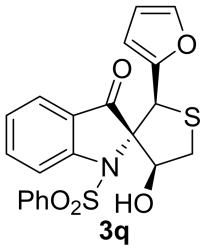
7.43 (m, 1H), 7.40 – 7.32 (m, 4H), 7.01 – 6.93 (m, 1H), 6.73 – 6.65 (m, 2H), 5.95 (d, *J* = 4.6 Hz, 1H), 5.59 (s, 1H), 5.48 (ddd, *J* = 9.6, 7.6, 4.6 Hz, 1H), 3.70 (t, *J* = 9.6 Hz, 1H), 3.60 (s, 3H), 3.16 (dd, *J* = 9.5, 7.6 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 194.2, 158.9, 151.4, 138.6, 137.0, 134.3, 130.0, 129.7, 127.7, 126.0, 123.4, 123.3, 122.8, 113.9, 113.4, 85.3, 73.7, 55.0, 48.2, 30.2. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_5S_2^+$ $[M+Na]^+$: 490.0753, found: 490.0753.



3p

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-(naphthalen-2-yl)-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3p)

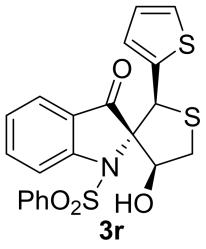
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1p** (41.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 48 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3p** as a white solid in 82% yield (40.0 mg, >20:1 dr, 88% ee). **m. p.**: 186-187 °C. **$[\alpha]_D^{20}$** = 83.954 (*c* 0.56, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 0.8 mL/min, λ = 254 nm), t_R = 17.648 min (major), t_R = 19.043 min (minor), 88% ee. **^{1}H NMR** (600 MHz, DMSO-d_6): δ 8.27 – 8.22 (m, 2H), 7.94 – 7.91 (m, 1H), 7.78 – 7.72 (m, 3H), 7.68 – 7.62 (m, 3H), 7.58 – 7.53 (m, 1H), 7.46 – 7.38 (m, 4H), 7.25 (d, *J* = 7.6 Hz, 1H), 6.89 – 6.83 (m, 1H), 6.07 (d, *J* = 4.7 Hz, 1H), 5.82 (s, 1H), 5.60 – 5.53 (m, 1H), 3.80 – 3.73 (m, 1H), 3.26 – 3.20 (m, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 194.3, 151.5, 138.7, 137.2, 134.5, 132.6, 132.3, 129.8, 128.3, 127.9, 127.8, 127.6, 127.5, 126.5, 126.4, 126.4, 123.5, 123.4, 122.8, 114.0, 85.2, 74.2, 48.9, 30.4. **HRMS** (ESI) *m/z*: calculated for $C_{27}H_{21}NNaO_4S_2^+$ $[M+Na]^+$: 510.0804, found: 510.0804.



3q

(2*R*,2'*S*,4'*S*)-2'-(furan-2-yl)-4'-hydroxy-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3q)

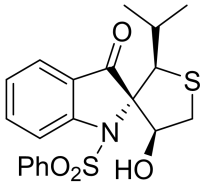
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1q** (35.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3q** as a white solid in 87% yield (37.0 mg, >20:1 dr, 90% ee). **m. p.**: 129-130 °C. $[\alpha]_D^{20}$ = 109.344 (*c* 0.82, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 85/15, flow rate 1.0 mL/min, λ = 254 nm), t_R = 25.472 min (major), t_R = 33.676 min (minor), 90% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.17 – 8.10 (m, 2H), 7.76 – 7.68 (m, 1H), 7.65 – 7.56 (m, 3H), 7.57 – 7.49 (m, 2H), 7.28 – 7.23 (m, 1H), 7.14 – 7.06 (m, 1H), 6.17 (dd, *J* = 3.3, 1.7 Hz, 1H), 6.12 (d, *J* = 3.3 Hz, 1H), 6.04 (d, *J* = 4.8 Hz, 1H), 5.63 (s, 1H), 5.40 (ddd, *J* = 9.7, 7.5, 4.8 Hz, 1H), 3.59 (t, *J* = 9.6 Hz, 1H), 3.10 (dd, *J* = 9.5, 7.5 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 193.8, 151.6, 149.3, 143.0, 138.9, 137.1, 134.2, 129.7, 127.3, 123.6, 123.4, 122.7, 114.2, 110.5, 109.2, 83.0, 74.5, 40.9, 29.9. **HRMS** (ESI) *m/z*: calculated for $C_{21}H_{17}NNaO_5S_2^+$ $[M+Na]^+$: 450.0440, found: 450.0438.



3r

(2*R*,2'*S*,4'*S*)-4'-hydroxy-1-(phenylsulfonyl)-2'-(thiophen-2-yl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3r)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1r** (36.7 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 4 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3r** as a white solid in 90% yield (40.0 mg, >20:1 dr, 93% ee). **m. p.**: 76 – 77 °C. $[\alpha]_D^{20}$ = 82.514 (*c* 0.52, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 85/15, flow rate 1.0 mL/min, λ = 254 nm), t_R = 17.153 min (minor), t_R = 18.729 min (major), 93% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.25 – 8.18 (m, 2H), 7.79 – 7.70 (m, 1H), 7.68 – 7.60 (m, 2H), 7.59 – 7.50 (m, 1H), 7.51 – 7.44 (m, 1H), 7.44 – 7.38 (m, 1H), 7.29 – 7.22 (m, 1H), 7.07 – 6.98 (m, 1H), 6.94 – 6.88 (m, 1H), 6.75 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.05 (d, *J* = 4.7 Hz, 1H), 5.85 (s, 1H), 5.45 (ddd, *J* = 9.6, 7.6, 4.6 Hz, 1H), 3.67 (t, *J* = 9.6 Hz, 1H), 3.15 (dd, *J* = 9.5, 7.7 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 193.9, 151.7, 138.6, 138.4, 137.1, 134.4, 129.8, 127.6, 126.9, 126.6, 126.6, 123.5, 123.4, 123.0, 114.0, 84.6, 73.7, 43.9, 30.4. **HRMS** (ESI) *m/z*: calculated for $C_{21}H_{17}NNaO_4S_3^+$ $[M+Na]^+$: 466.0212, found: 466.0213.

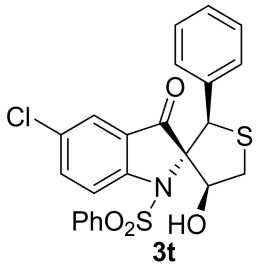


3s

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-isopropyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3s)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1s** (32.7 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 2 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the desired product **3s** as a colorless oil in 75% yield (30.3 mg, >20:1 dr, 93% ee). $[\alpha]_D^{20}$ = 161.519 (*c* 0.93, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0

mL/min, λ = 254 nm), t_R = 15.636 min (major), t_R = 19.194 min (minor), 93% ee. **^{1}H NMR** (600 MHz, DMSO-d_6): δ 8.19 – 8.15 (m, 2H), 7.78 – 7.70 (m, 1H), 7.70 – 7.62 (m, 4H), 7.59 (d, *J* = 8.7 Hz, 1H), 7.22 – 7.16 (m, 1H), 5.92 (d, *J* = 4.5 Hz, 1H), 5.29 (ddd, *J* = 10.1, 7.0, 4.6 Hz, 1H), 4.08 (d, *J* = 10.5 Hz, 1H), 3.30 (t, *J* = 9.9 Hz, 1H), 2.87 (dd, *J* = 9.7, 7.0 Hz, 1H), 1.74 – 1.64 (m, 1H), 0.81 (d, *J* = 6.5 Hz, 3H), 0.34 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 195.4, 151.7, 139.0, 137.3, 134.3, 129.7, 127.5, 123.5, 114.6, 83.1, 79.2, 76.2, 51.3, 31.4, 28.4, 22.5, 19.9. **HRMS** (ESI) *m/z*: calculated for $C_{20}H_{21}NNaO_4S_2^+$ $[M+Na]^+$: 426.0804, found: 426.0802.

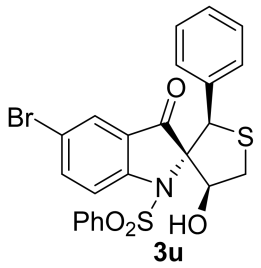


3t

(2*R*,2'*R*,4'*S*)-5-chloro-4'-hydroxy-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3t)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1t** (39.6 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 4 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3t** as a white solid in 90% yield (42.5 mg, >20:1 dr, 87% ee). **m. p.**: 76-77 °C. **[α]** $^{20}_{D}$ = 46.453 (*c* 0.56, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 9.548 min (minor), t_R = 12.115 min (major), 87% ee. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.24 – 8.17 (m, 2H), 7.79 – 7.71 (m, 1H), 7.68 – 7.60 (m, 2H), 7.53 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.50 – 7.39 (m, 3H), 7.37 (d, *J* = 2.3 Hz, 1H), 7.20 – 7.08 (m, 3H), 6.02 (d, *J* = 4.5 Hz, 1H), 5.63 (s, 1H), 5.50 (ddd, *J* = 9.6, 7.6, 4.5 Hz, 1H), 3.69 (t, *J* = 9.6 Hz, 1H), 3.20 (dd, *J* = 9.6, 7.6 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 193.0, 150.1, 138.3, 136.6, 134.5, 134.1, 129.8, 128.7, 128.3, 128.1, 127.7, 127.6, 124.1, 122.6, 115.7, 85.9, 73.8, 48.8,

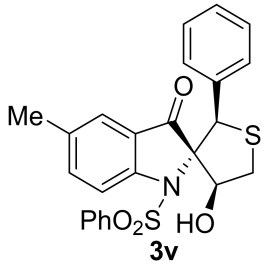
30.2. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}ClNNaO_4S_2^+$ [M+Na]$^+$: 494.0258, found: 494.0254.



3u

(2*R*,2'*R*,4'*S*)-5-bromo-4'-hydroxy-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3u)

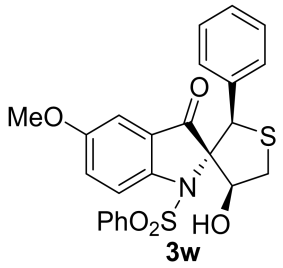
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1u** (44.0 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 4.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3u** as a white solid in 88% yield (45.3 mg, >20:1 dr, 70% ee). **m. p.**: 77-78 °C. **[α]** $_D^{20}$ = 27.636 (*c* 0.66, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.166 min (minor), t_R = 12.802 min (major), 70% ee. **^{1}H NMR** (600 MHz, DMSO-*d*$_6$): δ 8.22 – 8.17 (m, 2H), 7.78 – 7.73 (m, 1H), 7.68 – 7.61 (m, 3H), 7.48 (d, *J* = 2.2 Hz, 1H), 7.44 – 7.38 (m, 3H), 7.19 – 7.10 (m, 3H), 6.03 (d, *J* = 4.5 Hz, 1H), 5.62 (s, 1H), 5.48 (ddd, *J* = 9.6, 7.5, 4.5 Hz, 1H), 3.67 (t, *J* = 9.6 Hz, 1H), 3.19 (dd, *J* = 9.5, 7.7 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO-*d*$_6$): δ 192.9, 150.5, 139.4, 138.2, 134.6, 134.2, 129.8, 128.7, 128.3, 128.1, 127.6, 125.6, 124.5, 116.1, 115.4, 85.8, 73.9, 48.8, 30.2. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{18}BrNNaO_4S_2^+$ [M+Na]$^+$: 537.9753, found: 537.9752.



3v

(2*R*,2'*R*,4'*S*)-4'-hydroxy-5-methyl-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3v)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1v** (37.5 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 1.5 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3v** as a white solid in 71% yield (32.0 mg, >20:1 dr, 85% ee). **m. p.**: 77-78 °C. **[α]** $_{D}^{20}$ = 48.328 (*c* 0.55, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 17.718 min (minor), t_R = 21.523 min (major), 85% ee. **^{1}H NMR** (400 MHz, DMSO-*d*$_6$): δ 8.22 – 8.15 (m, 2H), 7.77 – 7.69 (m, 1H), 7.66 – 7.58 (m, 2H), 7.47 – 7.40 (m, 2H), 7.31 – 7.27 (m, 2H), 7.18 – 7.08 (m, 4H), 5.91 (d, *J* = 4.6 Hz, 1H), 5.62 (s, 1H), 5.47 (ddd, *J* = 9.7, 7.6, 4.5 Hz, 1H), 3.70 (t, *J* = 9.5 Hz, 1H), 3.16 (dd, *J* = 9.3, 7.7 Hz, 2H), 2.12 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-*d*$_6$): δ 194.0, 149.6, 138.7, 137.9, 134.5, 134.2, 132.8, 129.6, 128.8, 128.1, 128.0, 127.6, 122.9, 122.9, 113.7, 85.2, 73.9, 48.7, 30.2, 19.7. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_4S_2^+$ [M+Na]$^+$: 474.0804, found: 474.0804.

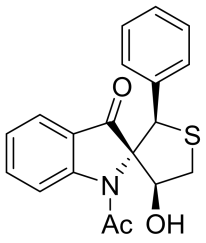


3w

(2*R*,2'*R*,4'*S*)-4'-hydroxy-5-methoxy-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3w)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1w** (39.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 4 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3w** as a white solid in 87% yield (40.5

mg, >20:1 dr, 82% ee). **m. p.**: 76 – 77 ℃. **[α]** $_{D}^{20}$ = 50.837 (*c* 0.28, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 22.434 min (minor), t_R = 30.381 min (major), 82% ee (recrystallization up to 96% ee). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.20 – 8.13 (m, 2H), 7.77 – 7.68 (m, 1H), 7.66 – 7.58 (m, 2H), 7.47 – 7.40 (m, 2H), 7.36 (d, J=9.1, 1H), 7.19 – 7.06 (m, 4H), 6.77 (d, *J* = 2.8 Hz, 1H), 5.90 (d, *J* = 4.5 Hz, 1H), 5.63 (s, 1H), 5.46 (ddd, *J* = 9.6, 7.6, 4.6 Hz, 1H), 3.69 (t, *J* = 9.6 Hz, 1H), 3.62 (s, 3H), 3.16 (dd, *J* = 9.4, 7.7 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 193.9, 155.3, 145.9, 138.8, 134.5, 134.2, 129.6, 128.8, 128.1, 128.0, 127.5, 125.1, 123.7, 115.1, 104.9, 85.5, 73.9, 55.7, 48.8, 30.2. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_5S_2^+$ $[M+Na]^+$: 490.0753, found: 490.0749.

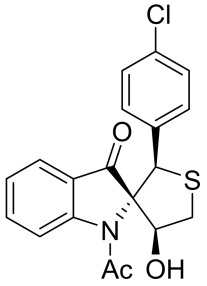


3x

(2*R*,2'*R*,4'*S*)-1-acetyl-4'-hydroxy-2'-phenyl-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3x)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1x** (26.3 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 15 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the desired product **3x** as a white solid in 84% yield (28.5 mg, 11.5:1 dr, 86% ee). **m. p.**: 114-115 ℃. **[α]** $_{D}^{20}$ = 35.158 (*c* 0.59, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.631 min (major), t_R = 23.023 min (minor), 86% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.45 (d, *J* = 7.7 Hz, 1H), 7, 7.34 – 7.30 (m, 2H), 7.29 – 7.27 (m, 1H), 7.16 – 7.09 (m, 3H), 6.73 – 6.65 (m, 2H), 5.63 (dd, *J* = 8.9, 7.3 Hz, 1H), 5.00 (s, 1H), 4.90 (s, 1H), 3.64 (dd, *J* = 10.7, 7.3 Hz,

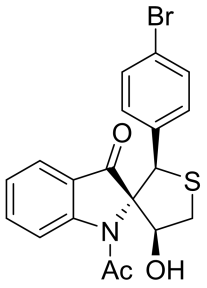
1H), 3.02 (dd, *J* = 10.7, 9.0 Hz, 1H), 1.89 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 198.5, 169.7, 160.8, 137.4, 133.4, 128.5, 128.3, 128.0, 124.3, 121.8, 119.4, 112.3, 78.4, 77.3, 53.9, 31.8, 20.6. **HRMS** (ESI) *m/z*: calculated for $C_{19}H_{17}NNaO_3S^+$ $[M+Na]^+$: 362.0821, found: 362.0821.



3y

(2*R*,2'*R*,4'*S*)-1-acetyl-2'-(4-chlorophenyl)-4'-hydroxy-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3y)

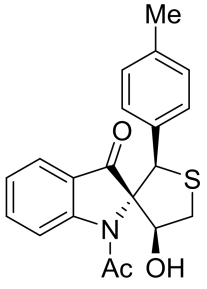
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1y** (29.8 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 9 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the desired product **3y** as a white solid in 82% yield (30.6 mg, 10:1 dr, 88% ee). **m. p.**: 121-122 ℃. **[α]** $_D^{20}$ = 31.701 (*c* 0.41, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.308 min (major), t_R = 23.942 min (minor), 88% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.7 Hz, 1H),, 7.36 – 7.30 (m, 1H), 7.30 – 7.26 (m, 2H), 7.14 – 7.09 (m, 2H), 6.76 – 6.70 (m, 2H), 5.61 (dd, *J* = 8.9, 7.4 Hz, 1H), 4.96 (s, 1H), 4.90 (s, 1H), 3.64 (dd, *J* = 10.8, 7.3 Hz, 1H), 3.02 (dd, *J* = 10.8, 8.9 Hz, 1H), 1.87 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 198.2, 169.6, 160.7, 137.7, 134.1, 132.2, 130.0, 128.2, 124.4, 121.6, 119.6, 112.3, 78.3, 77.3, 53.3, 31.9, 20.6. **HRMS** (ESI) *m/z*: calculated for $C_{19}H_{16}ClNNaO_3S^+$ $[M+Na]^+$: 396.0432, found:396.0431.



3z

(2*R*,2'*R*,4'*S*)-1-acetyl-2'-(4-bromophenyl)-4'-hydroxy-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3z)

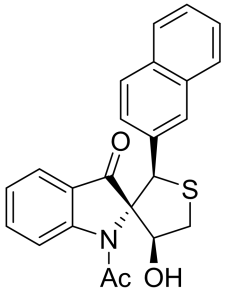
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1z** (34.2 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 8 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the desired product **3z** as a white solid in 78% yield (32.5 mg, 12:1 dr, 98% ee). **m. p.**: 118-119 °C. **[α]** $_{D}^{20}$ = 2.154 (*c* 0.38, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 11.380 min (major), t_R = 31.827 min (minor), 98% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.8 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.29 – 7.25 (m, 2H), 7.23 – 7.19 (m, 2H), 6.77 – 6.69 (m, 2H), 5.60 (dd, *J* = 8.9, 7.3 Hz, 1H), 4.93 (s, 1H), 4.86 (s, 1H), 3.63 (dd, *J* = 10.8, 7.3 Hz, 1H), 3.02 (dd, *J* = 10.9, 8.8 Hz, 1H), 1.87 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 198.2, 169.5, 160.7, 137.8, 132.8, 131.2, 130.4, 124.4, 122.3, 121.6, 119.6, 112.3, 78.3, 77.1, 53.4, 31.9, 20.6. **HRMS** (ESI) *m/z*: calculated for $C_{19}H_{16}BrNNaO_3S^+$ $[M+Na]^+$: 439.9926, found: 439.9924.



3aa

(2*R*,2'*R*,4'*S*)-1-acetyl-4'-hydroxy-2'-(*p*-tolyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3aa)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1aa** (27.7 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 34 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the desired product **3aa** as a white solid in 74% yield (26.0 mg, 15:1 dr, 72% ee). **m. p.**: 78-88 ℃. $[\alpha]_D^{20}$ = 39.147 (*c* 0.67, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.206 min (major), t_R = 16.548 min (minor), 72% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.45 (d, *J* = 7.7 Hz, 1H), 7.33 – 7.26 (m, 1H), 7.21 – 7.17 (m, 2H), 6.97 – 6.91 (m, 2H), 6.74 – 6.67 (m, 2H), 5.61 (dd, *J* = 8.9, 7.2 Hz, 1H), 4.97 (s, 1H), 4.88 (s, 1H), 3.62 (dd, *J* = 10.7, 7.3 Hz, 1H), 3.01 (dd, *J* = 10.7, 8.9 Hz, 1H), 2.19 (s, 3H), 1.88 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 198.6, 169.7, 160.9, 138.1, 137.4, 130.3, 128.8, 128.4, 124.3, 121.9, 119.4, 112.4, 78.5, 77.3, 53.6, 31.8, 21.0, 20.6. **HRMS** (ESI) *m/z*: calculated for $C_{20}H_{19}NNaO_3S^+$ $[M+Na]^+$: 376.0978, found: 376.0978.

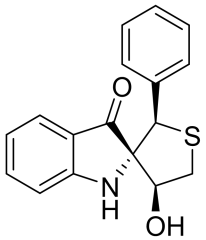


3ab

(2*R*,2'*R*,4'*S*)-1-acetyl-4'-hydroxy-2'-(naphthalen-2-yl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3ab)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1ab** (31.3 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 34 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl

acetate = 8/1, v/v) to afford the desired product **3ab** as a white solid in 72% yield (28.0 mg, 16:1 dr, 64% ee). **m. p.**: 115-116 ℃. **[α]**$_D^{20}$ = 23.144 (*c* 0.27, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.952 min (major), t_R = 19.273 min (minor), 64% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.87 – 7.84 (m, 1H), 7.75 – 7.73 (m, 1H), 7.72 – 7.66 (m, 1H), 7.62 – 7.57 (m, 1H), 7.47 – 7.37 (m, 4H), 7.23 – 7.17 (m, 1H), 6.68 – 6.64 (m, 1H), 6.62 (d, *J* = 8.3 Hz, 1H), 5.67 (dd, *J* = 8.8, 7.1 Hz, 1H), 5.17 (s, 1H), 4.91 (s, 1H), 3.68 (dd, J = 10.8, 7.2 Hz, 1H), 3.08 (dd, *J* = 10.8, 8.8 Hz, 1H), 1.89 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 198.6, 169.6, 160.8, 137.5, 133.1, 132.8, 131.3, 128.0, 127.9, 127.7, 127.5, 126.3, 126.2, 126.2, 124.4, 121.7, 119.5, 112.4, 78.6, 77.4, 53.9, 32.0, 20.6. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{19}NNaO_3S^+$ $[M+Na]^+$: 412.0978, found: 412.0977.

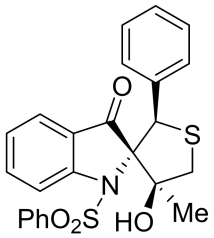


3ac

(2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-phenyl-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3ac)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1ac** (22.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2a** (9.1 mg, 0.06 mmol) at room temperature for 20 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 8/1, v/v) to afford the desired product **3ac** as a faint yellow solid in 75% yield (22.3 mg, 2:1 dr, 80% ee (major diastereomer), 81% ee (minor diastereomer)). **m. p.**: 180-181 ℃. **[α]**$_D^{20}$ = 98.807 (*c* 0.28, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.425 min (major), t_R = 29.692 min (minor), 80% ee (major diastereomer). The **enantiomeric excess** was determined by HPLC with an IA-

H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.488 min (major), t_R = 54.733 min (minor), 81% ee (minor diastereomer). **^{1}H NMR** (600 MHz, DMSO-d_6): δ 7.68 (s, 1H), 7.35 – 7.28 (m, 2H), 7.28 – 7.19 (m, 2H), 7.16 – 7.07 (m, 3H), 6.75 (d, *J* = 8.2 Hz, 1H), 6.49 (t, *J* = 7.4 Hz, 1H), 5.50 (d, *J* = 6.3 Hz, 1H), 4.78 (s, 1H), 4.55 – 4.48 (m, 1H), 3.17 (d, *J* = 8.8 Hz, 2H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 199.8, 162.1, 137.0, 135.6, 129.0, 127.6, 127.5, 123.2, 120.1, 116.5, 111.8, 78.8, 78.7, 53.6, 34.2. **HRMS** (ESI) *m/z*: calculated for $C_{17}H_{15}NNaO_2S^+$ $[M+Na]^+$: 320.0716, found: 320.0715.

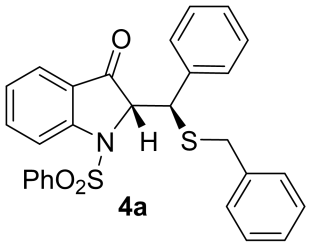


3ad

(2*R*,2'*R*,4'*S*)-4'-hydroxy-4'-methyl-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (3ad)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1a** (36.1 mg, 0.10 mmol) and 1,4-dithiane-2,5-diol **2b** (10.8 mg, 0.06 mmol) at room temperature for 16 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 5/1, v/v) to afford the desired product **3ad** as a faint yellow solid in 63% yield (28.5 mg, >20:1 dr, 64% ee). **m. p.**: 139-140 °C. **$[\alpha]_D^{20}$** = 27.713 (*c* 0.58, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 9.658 min (major), t_R = 10.189 min (minor), 64% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.2 Hz, 1H), 7.50 – 7.46 (m, 2H), 7.46 – 7.41 (m, 2H), 7.42 – 7.38 (m, 1H), 7.37 – 7.31 (m, 3H), 7.30 – 7.21 (m, 4H), 7.12 – 7.08 (m, 1H), 4.58 – 4.53 (m, 2H), 4.14 (s, 1H), 3.96 (s, 1H), 2.27 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 206.7, 141.2, 137.7, 136.4, 133.6, 133.5, 130.8, 128.9, 128.6, 128.5, 128.1, 127.5, 125.6, 123.7, 117.3, 90.6, 82.8,

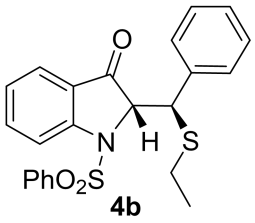
60.5, 56.5, 30.3. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_4S_2^+$ $[M+Na]^+$: 474.0804, found: 474.0805.



4a

(*R*)-2-((*R*)-(benzylthio)(phenyl)methyl)-1-(phenylsulfonyl)indolin-3-one (4a)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1a** (36.1 mg, 0.10 mmol) and thiol **2c** (15.0 mg, 0.12 mmol) at room temperature for 12 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired product **4a** as a yellow solid in 95% yield (46.0 mg, 7:1 dr, 63% ee). **m. p.**: 87 – 88 ℃. $[\alpha]_D^{20}$ = 67.143 (*c* 0.44, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.668 min (minor), t_R = 21.237 min (major), 63% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 1H), 7.50 – 7.41 (m, 3H), 7.41 – 7.35 (m, 1H), 7.35 – 7.26 (m, 8H), 7.24 – 7.17 (m, 2H), 7.06 – 6.97 (m, 3H), 6.93 (t, *J* = 7.4 Hz, 1H), 4.68 (d, *J* = 4.6 Hz, 1H), 4.19 (d, *J* = 4.6 Hz, 1H), 3.66 (d, *J* = 13.4 Hz, 1H), 3.58 (d, *J* = 13.3 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 196.0, 152.5, 137.6, 136.9, 136.0, 135.7, 133.9, 129.4, 129.3, 129.1, 128.5, 127.8, 127.7, 127.1, 127.1, 125.6, 124.7, 123.9, 116.7, 69.4, 51.3, 36.9. **HRMS** (ESI) *m/z*: calculated for $C_{28}H_{23}NNaO_3S_2^+$ $[M+Na]^+$: 508.1012, found: 508.1013.

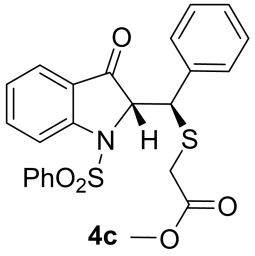


4b

(*R*)-2-((*R*)-(ethylthio)(phenyl)methyl)-1-(phenylsulfonyl)indolin-3-one (4b)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1a** (36.1 mg, 0.10 mmol) and thiol **2d** (7.5 mg, 0.12 mmol) at room

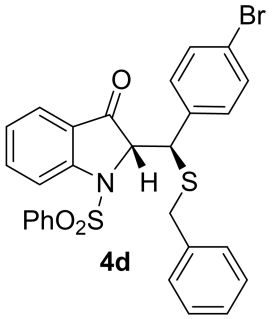
temperature for 12 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired product **4b** as a yellow solid in 97% yield (41.0 mg, 4:1 dr, 58% ee). **m. p.**: 82 – 83 ℃. $[\alpha]_D^{20}$ = 89.130 (*c* 0.32, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.850 min (minor), t_R = 14.017 min (major), 58% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.4 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.59 – 7.48 (m, 2H), 7.49 – 7.43 (m, 1H), 7.42 – 7.38 (m, 4H), 7.12 – 6.98 (m, 4H), 4.84 (d, *J* = 4.4 Hz, 1H), 4.37 (d, *J* = 4.5 Hz, 1H), 2.59 – 2.50 (m, 2H), 1.27 (t, *J* = 7.4 Hz, 3H).**^{13}C NMR** (150 MHz, $CDCl_3$): δ 196.0, 152.4, 136.9, 136.0, 136.0, 134.0, 129.4, 129.2, 127.8, 127.7, 127.1, 125.8, 124.7, 123.9, 116.7, 69.5, 51.7, 26.8, 14.3.**HRMS** (ESI) *m/z*: calculated for $C_{23}H_{21}NNaO_3S_2^+$ $[M+Na]^+$: 446.0855, found: 446.0854.



Methyl 2-(((*R*)-((*R*)-3-oxo-1-(phenylsulfonyl)indolin-2-yl)(phenyl)methyl)thio)acetate (4c)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1a** (36.1 mg, 0.10 mmol) and thiol **2e** (12.7 mg, 0.12 mmol) at room temperature for 12 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired product **4c** as a yellow solid in 97% yield (45.5 mg, 6:1 dr, 14% ee). **m. p.**: 89 – 90 ℃. $[\alpha]_D^{20}$ = 25.336 (*c* 0.27, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IB-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 0.7 mL/min, λ = 254 nm), t_R = 19.248 min (minor), t_R = 22.366 min (major), 14% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.4 Hz, 1H), 7.76 – 7.71 (m, 2H), 7.57 – 7.53 (m, 1H), 7.49 – 7.36 (m, 6H), 7.13 – 7.06 (m, 3H), 7.04 – 6.99 (m, 1H), 5.04 (d, *J* =

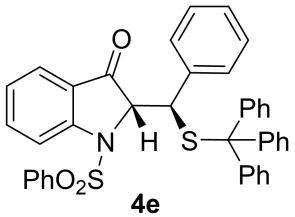
4.7 Hz, 1H), 4.47 (d, *J* = 4.6 Hz, 1H), 3.70 (s, 3H), 3.28 (d, *J* = 14.9 Hz, 1H), 3.18 (d, *J* = 14.9 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 195.9, 170.4, 152.5, 137.0, 136.0, 134.9, 134.1, 129.4, 129.4, 128.0, 127.9, 127.2, 125.5, 124.7, 123.9, 116.7, 68.9, 52.4, 52.2, 34.0. **HRMS** (ESI) *m/z*: calculated for $C_{24}H_{21}NNaO_5S_2^+$ $[M+Na]^+$: 490.0753, found: 490.0750.



4d

(*R*)-2-((*R*)-(benzylthio)(4-bromophenyl)methyl)-1-(phenylsulfonyl)indolin-3-one (4d)

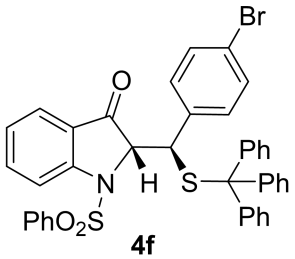
Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1l** (44.0 mg, 0.10 mmol) and thiol **2c** (15.0 mg, 0.12 mmol) at room temperature for 12 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired product **4d** as a yellow solid in 98% yield (55.3 mg, 8:1 dr, 84% ee). **m. p.**: 49 – 50 °C. $[\alpha]_D^{20}$ = 68.546 (*c* 0.54, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 0.7 mL/min, λ = 254 nm), t_R = 20.161 min (minor), t_R = 30.441 min (major), 84% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.4 Hz, 1H), 7.56 – 7.45 (m, 4H), 7.41 – 7.21 (m, 12H), 7.02 (t, *J* = 7.5 Hz, 1H), 4.71 (d, *J* = 4.6 Hz, 1H), 4.23 (d, *J* = 4.6 Hz, 1H), 3.71 (d, *J* = 13.4 Hz, 1H), 3.61 (d, *J* = 13.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 195.6, 152.4, 137.2, 137.2, 135.6, 135.0, 134.0, 131.0, 130.9, 129.3, 129.0, 128.4, 127.1, 127.0, 125.2, 124.8, 123.9, 121.7, 116.6, 69.2, 50.3, 36.9. **HRMS** (ESI) *m/z*: calculated for $C_{28}H_{22}BrNNaO_3S_2^+$ $[M+Na]^+$: 586.0117, found: 586.0117.



4e

(*R*)-2-((*R*)-phenyl(tritylthio)methyl)-1-(phenylsulfonyl)indolin-3-one (4e)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1a** (36.1 mg, 0.10 mmol) and thiol **2f** (33.2 mg, 0.12 mmol) at room temperature for 12 h. The resulting solution was concentrated and directly purified by flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired product **4e** as a yellow solid in 63% yield (40.2 mg, 12.5:1 dr, 63% ee). **m. p.**: 99 – 100 °C. $[\alpha]_D^{20}$ = 31.560 (*c* 1.09, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.936 min (major), t_R = 10.447 min (minor), 63% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.7 Hz, 1H), 7.62 – 7.54 (m, 3H), 7.46 – 7.40 (m, 8H), 7.39 – 7.35 (m, 2H), 7.22 – 7.12 (m, 9H), 6.98 – 6.92 (m, 1H), 6.88 – 6.77 (m, 5H), 4.46 – 4.43 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 196.7, 152.4, 144.3, 136.8, 136.5, 136.5, 133.9, 130.0, 129.4, 129.3, 127.7, 127.1, 127.0, 126.7, 126.6, 125.8, 124.4, 123.8, 116.4, 69.7, 69.3, 50.9. **HRMS** (ESI) *m/z*: calculated for $C_{40}H_{31}NNaO_3S_2^+$ $[M+Na]^+$: 660.1638, found: 660.1633.

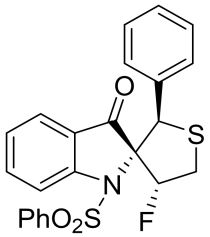


4f

(*R*)-2-((*R*)-(4-bromophenyl)(tritylthio)methyl)-1-(phenylsulfonyl)indolin-3-one (4f)

Following the general procedure, the reaction was performed with (*Z*)-2-ylideneoxindole **1l** (44.0 mg, 0.10 mmol) and thiol **2f** (33.2 mg, 0.12 mmol) at room temperature for 12 h. The resulting solution was concentrated and directly purified by

flash column chromatography (eluted with petroleum ether/ethyl acetate = 10/1, v/v) to afford the desired product **4f** as a yellow solid in 65% yield (46.6 mg, 15:1 dr, 86% ee). **m. p.**: 112 – 113 ℃. $[\alpha]_D^{20}$ = 8.136 (*c* 4.82, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.729 min (major), t_R = 10.331 min (minor), 86% ee (recrystallization up to 96% ee). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.73 (d, *J* = 8.5 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.62 – 7.56 (m, 1H), 7.50 – 7.36 (m, 10H), 7.24 – 7.13 (m, 9H), 7.02 – 6.90 (m, 3H), 6.75 – 6.71 (m, 2H), 4.58 – 4.54 (m, 1H), 4.48 – 4.44 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 196.4, 152.4, 144.0, 137.2, 136.2, 135.8, 134.0, 131.1, 130.0, 129.9, 129.4, 127.7, 127.1, 126.8, 125.4, 124.7, 123.9, 120.6, 116.4, 69.6, 69.2, 50.0. **HRMS** (ESI) *m/z*: calculated for $C_{40}H_{30}BrNNaO_3S_2^+$ $[M+Na]^+$: 738.0743, found: 738.0740.

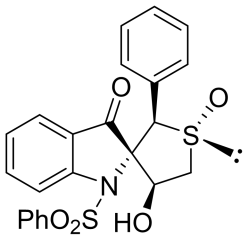


5

(2*S*,2'*R*,4'*R*)-4'-fluoro-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one (5)

White solid; reaction time: 0.5 h; 78% yield (34.2 mg), >20:1 dr. **m. p.**: 176 – 177 ℃. $[\alpha]_D^{20}$ = 76.654 (*c* 0.65, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.040 min (major), t_R = 11.746 min (minor), 96% ee. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.06 – 7.98 (m, 2H), 7.66 – 7.45 (m, 6H), 7.41 – 7.30 (m, 2H), 7.17 – 7.02 (m, 3H), 6.93 – 6.84 (m, 1H), 6.39 (ddd, *J* = 53.1, 9.2, 8.1 Hz, 1H), 5.70 (d, *J* = 1.5 Hz, 1H), 4.14 (dt, *J* = 15.8, 9.5 Hz, 1H), 3.31 (dd, *J* = 9.7, 8.1 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 192.1, 151.7, 139.4, 136.9, 133.9, 133.0, 129.5, 129.1, 128.4, 128.0, (127.1, 127.0), 124.1, 123.4, 122.9, 114.1, (92.2, 90.3), (83.0, 82.7), (48.9, 48.8), (27.7, 27.5). **^{19}F NMR** (376 MHz, $CDCl_3$): δ -186.5. **HRMS** (ESI) *m/z*:

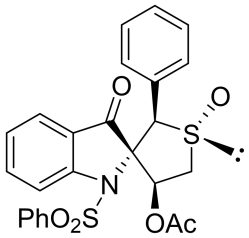
calculated for $C_{23}H_{19}FNO_3S_2^+$ $[M+H]^+$: 440.0785, found: 440.0785.



6

(1'*R*,2*R*,2'*R*,4'*S*)-4'-hydroxy-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-3-one 1'-oxide (6)

White solid; reaction time: 10 min; 96% yield (43.5 mg), >20:1 dr. **m. p.**: 97 – 98 °C. $[\alpha]_D^{20}$ = 54.644 (*c* 0.72, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 28.757 min (major), t_R = 61.545 min (minor), 96% ee. **^{1}H NMR** (600 MHz, DMSO-d_6): δ 8.17 – 8.13 (m, 2H), 7.76 – 7.70 (m, 1H), 7.64 – 7.53 (m, 4H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.34 – 7.22 (m, 5H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.12 (d, *J* = 4.6 Hz, 1H), 5.89 (td, *J* = 9.2, 4.6 Hz, 1H), 5.01 (s, 1H), 3.80 (dd, *J* = 13.7, 9.3 Hz, 1H), 3.24 (dd, *J* = 13.7, 9.2 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6): δ 197.2, 152.6, 138.4, 138.2, 134.5, 130.5, 129.8, 129.1, 128.9, 128.8, 127.5, 124.0, 123.9, 122.3, 114.3, 84.1, 74.5, 71.1, 53.0. **HRMS** (ESI) *m/z*: calculated for $C_{23}H_{19}NNaO_5S_2^+$ $[M+Na]^+$: 476.0597, found: 476.0591.

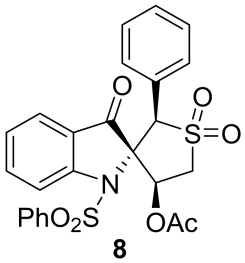


7

(1'*R*,2*R*,2'*R*,4'*S*)-1'-oxido-3-oxo-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-4'-yl acetate (7)

White solid; reaction time: 0.5 h; 97% yield (48.0 mg), >20:1 dr. **m. p.**: 257 – 258 °C. $[\alpha]_D^{20}$ = 85.816 (*c* 1.41, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 32.003 min (major), t_R = 47.945 min (minor), 99% ee. **^{1}H NMR** (600 MHz,

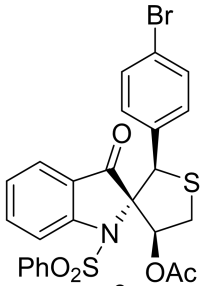
$CDCl_3$): δ 7.96 – 7.90 (m, 3H), 7.64 – 7.52 (m, 3H), 7.51 – 7.41 (m, 4H), 7.24 – 7.15 (m, 3H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.40 (t, *J* = 9.1 Hz, 1H), 5.23 (s, 1H), 3.78 (dd, *J* = 13.9, 8.7 Hz, 1H), 3.59 (dd, *J* = 13.9, 9.5 Hz, 1H), 1.35 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 196.1, 168.8, 153.5, 139.9, 138.4, 134.0, 129.6, 129.6, 129.0, 128.8, 128.7, 126.4, 124.5, 124.0, 122.5, 114.9, 80.8, 74.1, 72.1, 51.8, 19.8. **HRMS** (ESI) *m/z*: calculated for $C_{25}H_{22}NO_6S_2^+$ $[M+H]^+$: 496.0883, found: 496.0880.



8

(2*R*,2'*R*,4'*S*)-1',1'-dioxido-3-oxo-2'-phenyl-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-4'-yl acetate (8)

White solid; reaction time: 3 h; 94% yield (24.0 mg), >20:1 dr. **m. p.**: 222 – 223 °C. **$[\alpha]_D^{20}$** = 35.303 (*c* 1.32, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 45.516 min (major), t_R = 85.345 min (minor), 99% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95 – 7.89 (m, 3H), 7.67 – 7.54 (m, 3H), 7.53 – 7.43 (m, 4H), 7.25 – 7.16 (m, 3H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.15 (dd, *J* = 10.3, 8.4 Hz, 1H), 5.73 (s, 1H), 4.25 (dd, *J* = 12.4, 8.2 Hz, 1H), 4.18 (dd, *J* = 12.6, 10.3 Hz, 1H), 1.41 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 193.5, 168.9, 152.9, 140.0, 138.1, 134.1, 131.2, 129.7, 129.7, 128.6, 126.3, 124.9, 124.7, 124.3, 122.6, 114.8, 78.6, 70.8, 68.1, 54.4, 19.8. **HRMS** (ESI) *m/z*: calculated for $C_{25}H_{22}NO_7S_2^+$ $[M+H]^+$: 512.0832, found: 512.0831.

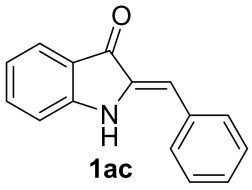


9

(2*R*,2'*R*,4'*S*)-2'-(4-bromophenyl)-3-oxo-1-(phenylsulfonyl)-4',5'-dihydro-2'*H*-spiro[indoline-2,3'-thiophen]-4'-yl acetate (9)

White solid; reaction time: 0.5 h; 98% yield (33.0 mg), >20:1 dr. **m. p.**: 234 – 235 ℃. $[\alpha]_D^{20}$ = 67.673 (c 0.65, $CHCl_3$). The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 15.735 min (major), t_R = 22.279 min (minor), 99% ee. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.99 – 7.91 (m, 3H), 7.64 – 7.58 (m, 1H), 7.58 – 7.52 (m, 1H), 7.52 – 7.46 (m, 2H), 7.43 – 7.37 (m, 3H), 7.24 – 7.20 (m, 2H), 7.04 – 6.99 (m, 1H), 6.06 (dd, *J* = 9.1, 7.8 Hz, 1H), 5.74 (s, 1H), 3.66 – 3.60 (m, 1H), 3.55 (dd, *J* = 9.8, 7.9 Hz, 1H), 1.34 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 192.8, 169.4, 152.1, 140.2, 137.3, 133.8, 132.4, 131.2, 130.8, 129.5, 126.4, 124.3, 123.8, 123.1, 122.4, 114.6, 82.0, 74.8, 48.4, 27.7, 20.1. **HRMS** (ESI) *m/z*: calculated for $C_{25}H_{20}BrNNaO_5S_2^+$ $[M+Na]^+$: 579.9858, found: 579.9849.

(*Z*)-2-benzylideneindolin-3-one (1ac)



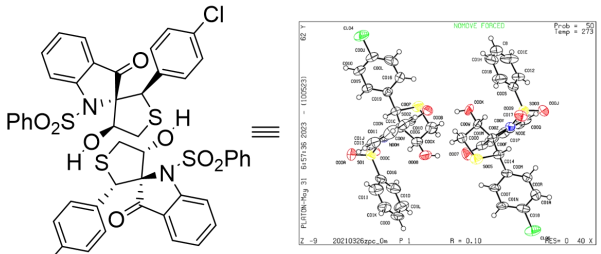
1ac

Brown solid; Reaction time: 1 h; Yield: 84% (18.6 mg); m. p.: 174–175 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6): δ 9.80 (s, 1H), 7.77 – 7.70 (m, 2H), 7.61 – 7.45 (m, 4H), 7.41 – 7.33 (m, 1H), 7.14 (d, *J* = 8.1 Hz, 1H), 6.96 – 6.88 (m, 1H), 6.64 (s, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): δ 186.4, 154.2, 136.4, 134.4, 134.2, 129.9, 129.0, 128.4, 124.1, 120.0, 119.8, 112.6, 109.8. **HRMS** (ESI) *m/z*: calculated for $C_{15}H_{12}NO^+$ $[M+H]^+$: 222.0913, found: 222.0917.

11. X-ray crystallographic data of products *rac*-3k, 4f, 7 and 9

The single crystals of compound ***rac*-3k** for X-ray analysis was grown from the mixed solution of hexane and acetone (*v*/*v* = 3/1). A suitable crystal was selected and X-ray on a Super Nova, Dual, Cu at zero, Atlas S2 diffractometer. The crystal was kept at 273.00(10) K during data collection, and the thermal ellipsoid was drawn at the 50% probability level.

Compound ***rac*-3k**:



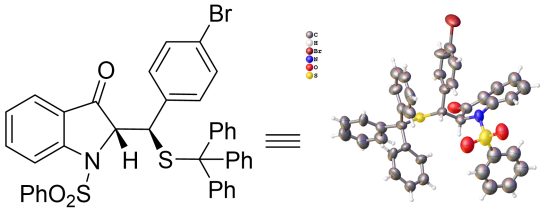
***rac*-3k** **CCDC 2266556 for *rac*-3k**

Table S3 Crystal data and structure refinement for *rac*-3k.

Bond precision:	C-C = 0.0226 A		Wavelength=1.54178
Cell:	a=8.968(4)	b=10.282(5)	c=12.508(6)
	alpha=66.07(2)	beta=86.01(2)	gamma=84.86(2)
Temperature: 273 K			
	Calculated		Reported
Volume	1049.3(9)		1049.2(8)
Space group	P 1		P 1
Hall group	P 1		P 1
Moiety formula	C23 H18 C1 N O4 S2		0.25(C23 H18 C1 N O4 S2)
Sum formula	C23 H18 C1 N O4 S2		C2 H2 C12 N2 O2 S2
Mr	471.95		221.08
Dx, g cm-3	1.494		2.799
Z	2		8
Mu (mm-1)	3.745		17.960
F000	488.0		880.0
F000'	491.31		
h, k, lmax	11, 13, 16		11, 12, 16
Nref	9420[4710]		7572
Tmin, Tmax			
Tmin'			
Correction method= Not given			
Data completeness= 1.61/0.80		Theta(max)= 83.755	
R(reflections)= 0.1021(5651)			wR2(reflections)= 0.2650(7572)
S = 1.679	Npar= 561		

Compound **4f**:

The single crystals of compound **4f** for X-ray analysis was grown from the mixed solution of dichloromethane and methanol (*v*/*v* = 3/1). Single crystals of compound **4f** were X-ray. A suitable crystal was selected and X-ray on a XtaLAB AFC12 (RINC): Kappa single diffractometer. The crystal was kept at 150.00(10) K during data collection. Using Olex2, the structure was solved with the SHELXS structure solution program using Direct Methods and refined with the SHELXL refinement package using Least Squares minimization. The thermal ellipsoid was drawn at the 50% probability level.



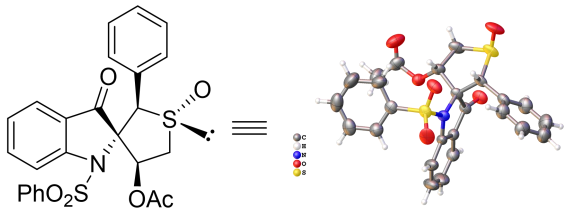
4f **CCDC: 2376029 for 4f**

Table S4 Crystal data and structure refinement 4f.

Identification code	**4f**
Empirical formula	$C_{40}H_{30}BrNO_3S_2$
Formula weight	716.68
Temperature/K	150
Crystal system	triclinic
Space group	P1
a/Å	10.0638(3)
b/Å	10.0887(3)
c/Å	21.2206(10)
α/°	77.031(3)
β/°	86.622(3)
γ/°	66.577(3)
Volume/Å^3	1925.46(13)
Z	2
ρ_{calc}g/cm^3	1.236
μ/mm^{-1}	2.746
F(000)	736.0
Crystal size/mm^3	0.58 × 0.47 × 0.33
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.276 to 133.198
Index ranges	-11 ≤ h ≤ 7, -12 ≤ k ≤ 11, -25 ≤ l ≤ 25
Reflections collected	18043
Independent reflections	8785 [R_{int} = 0.0478, R_{sigma} = 0.0603]
Data/restraints/parameters	8785/662/907
Goodness-of-fit on F^2	1.487
Final R indexes [I>=2σ (I)]	R_1 = 0.1140, wR_2 = 0.3387
Final R indexes [all data]	R_1 = 0.1220, wR_2 = 0.3527
Largest diff. peak/hole / e Å^{-3}	1.30/-0.58
Flack parameter	0.13(5)

Compound **7**:

The single crystals of compound **7** for X-ray analysis was grown from the mixed solution of hexane and chloroform (*v*/*v* = 3/1). Single crystals of compound **7** were X-ray. A suitable crystal was selected and X-ray on a XtaLAB AFC12 (RINC): Kappa single diffractometer. The crystal was kept at 150.00(10) K during data collection. Using Olex2, the structure was solved with the SHELXS structure solution program using Direct Methods and refined with the SHELXL refinement package using Least Squares minimization. The thermal ellipsoid was drawn at the 50% probability level.



7

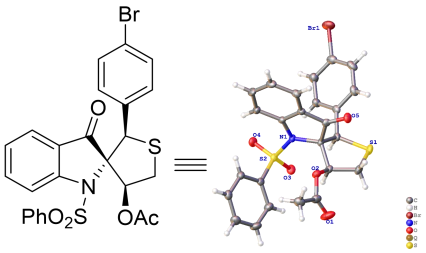
CCDC: 2370577 for 7

Table S5 Crystal data and structure refinement for 7.

Identification code	**7**
Empirical formula	$C_{25}H_{21}NO_6S_2$
Formula weight	495.55
Temperature/K	150
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.53006(13)
b/Å	14.5860(2)
c/Å	16.7204(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2324.24(6)
Z	4
ρ_{calc}g/cm^3	1.416
μ/mm^{-1}	2.444
F(000)	1032.0
Crystal size/mm^3	0.44 × 0.36 × 0.25
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.044 to 136.084
Index ranges	-11 ≤ h ≤ 11, -17 ≤ k ≤ 17, -19 ≤ l ≤ 20
Reflections collected	9405
Independent reflections	4067 [R_{int} = 0.0790, R_{sigma} = 0.0755]
Data/restraints/parameters	4067/0/309
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0729, wR_2 = 0.1972
Final R indexes [all data]	R_1 = 0.0774, wR_2 = 0.2051
Largest diff. peak/hole / e Å^{-3}	0.62/-0.52
Flack parameter	0.01(3)

Compound **9**:

The single crystals of compound **9** for X-ray analysis was grown from the mixed solution of hexane and chloroform (V/V = 10/1). Single crystals of compound **9** were X-ray. A suitable crystal was selected and X-ray on a XtaLAB AFC12 (RINC): Kappa single diffractometer. The crystal was kept at 150.00(10) K during data collection. Using Olex2, the structure was solved with the SHELXS structure solution program using Direct Methods and refined with the SHELXL refinement package using Least Squares minimization. The thermal ellipsoid was drawn at the 50% probability level.

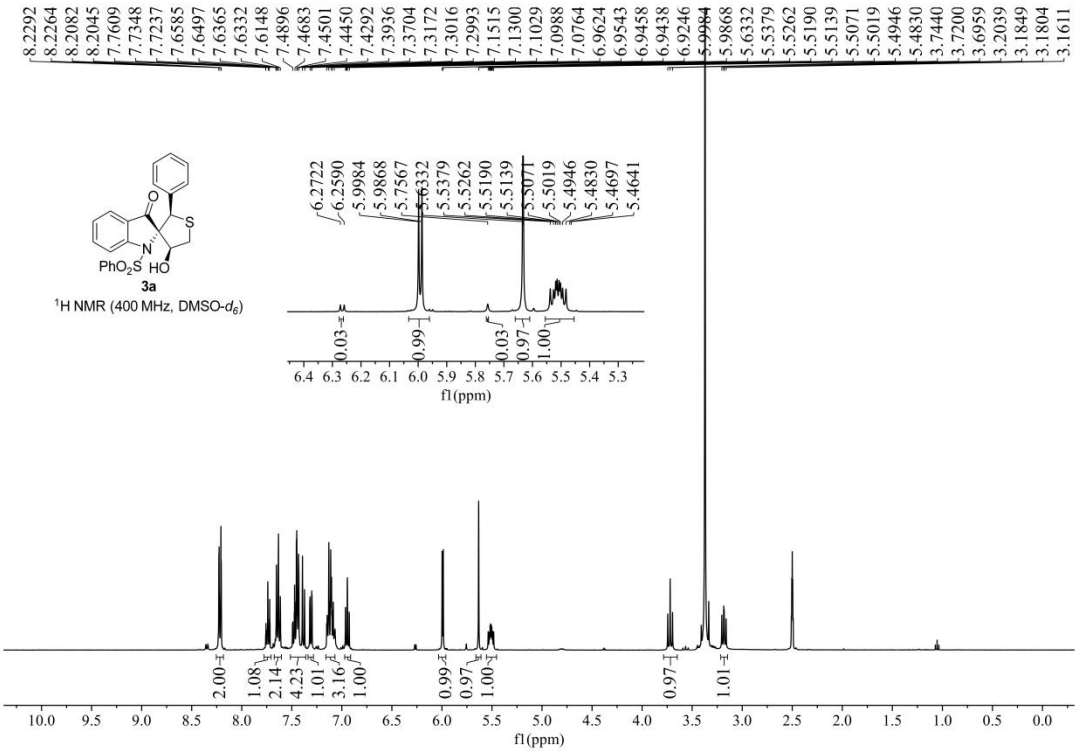


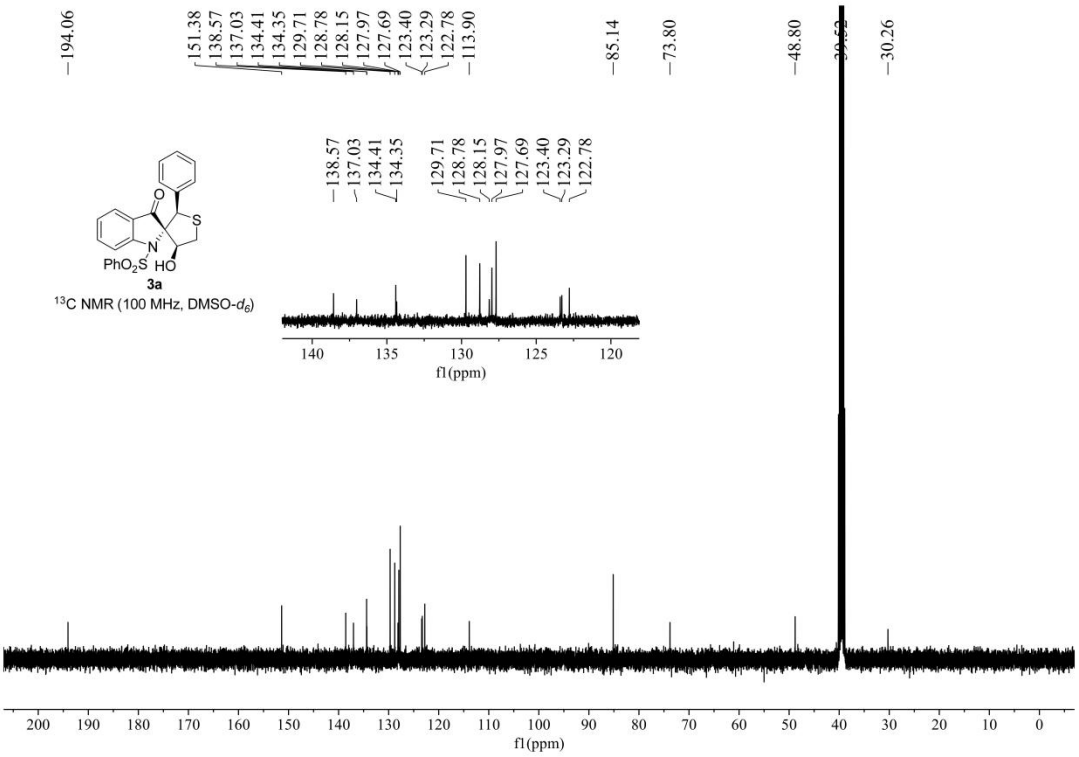
9 **CCDC 2266557 for 9**

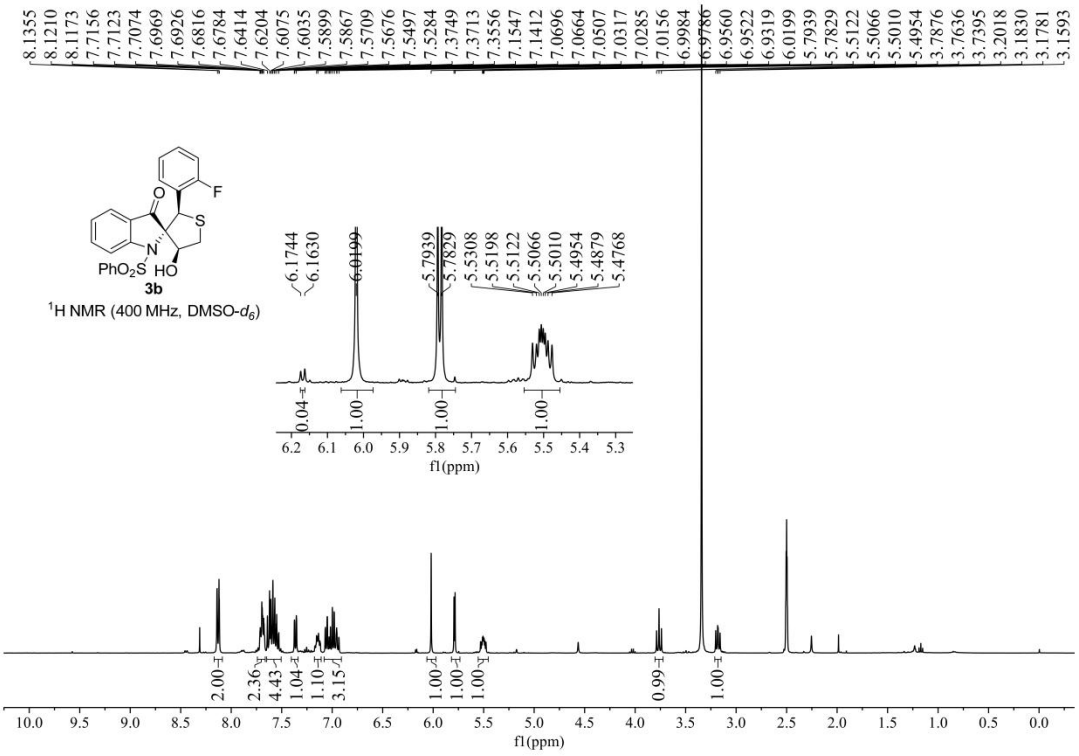
Table S6 Crystal data and structure refinement for 9.

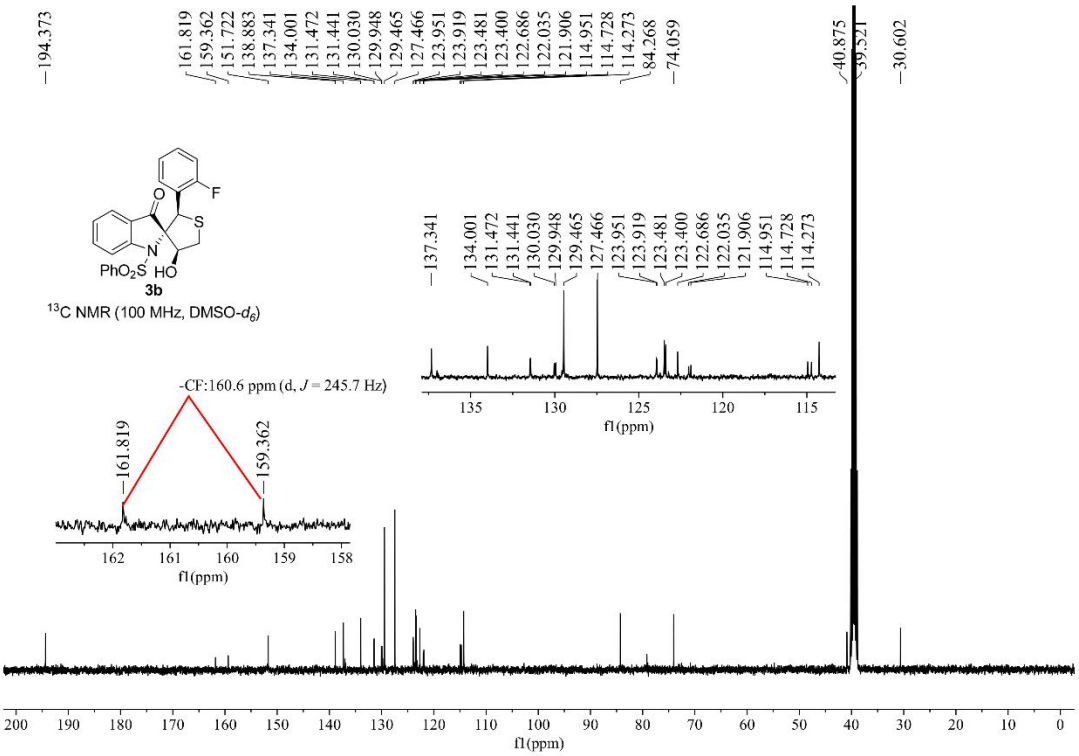
Identification code	9
Empirical formula	$C_{25}H_{20}BrNO_5S_2$
Formula weight	558.45
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.25447(8)
b/Å	13.91114(12)
c/Å	17.92573(13)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2307.76(3)
Z	4
ρ_{calc}g/cm^3	1.607
μ/mm^{-1}	4.453
F(000)	1136.0
Crystal size/mm^3	0.16 × 0.13 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.044 to 144.008
Index ranges	-10 ≤ h ≤ 11, -14 ≤ k ≤ 16, -21 ≤ l ≤ 21
Reflections collected	10959
Independent reflections	4423 [R_{int} = 0.0198, R_{sigma} = 0.0204]
Data/restraints/parameters	4423/0/309
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0249, wR_2 = 0.0658
Final R indexes [all data]	R_1 = 0.0250, wR_2 = 0.0659
Largest diff. peak/hole / e Å^{-3}	0.82/-0.41
Flack/Hooft parameter	0.001(5)/0.001(5)

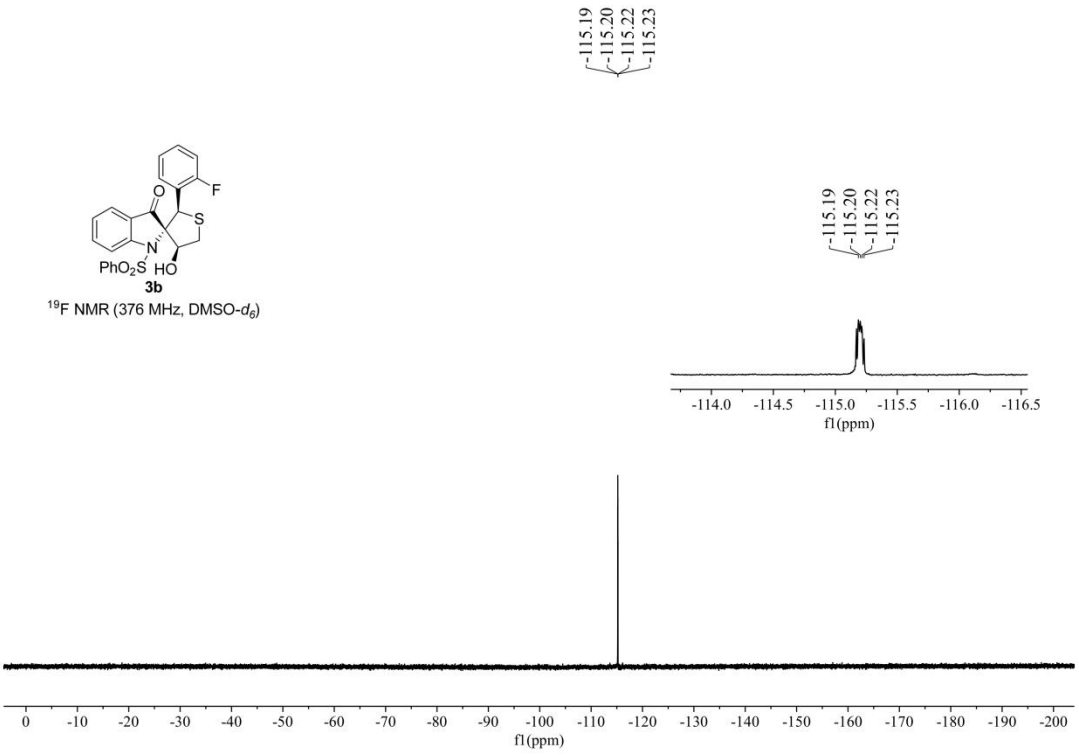
12. NMR spectra





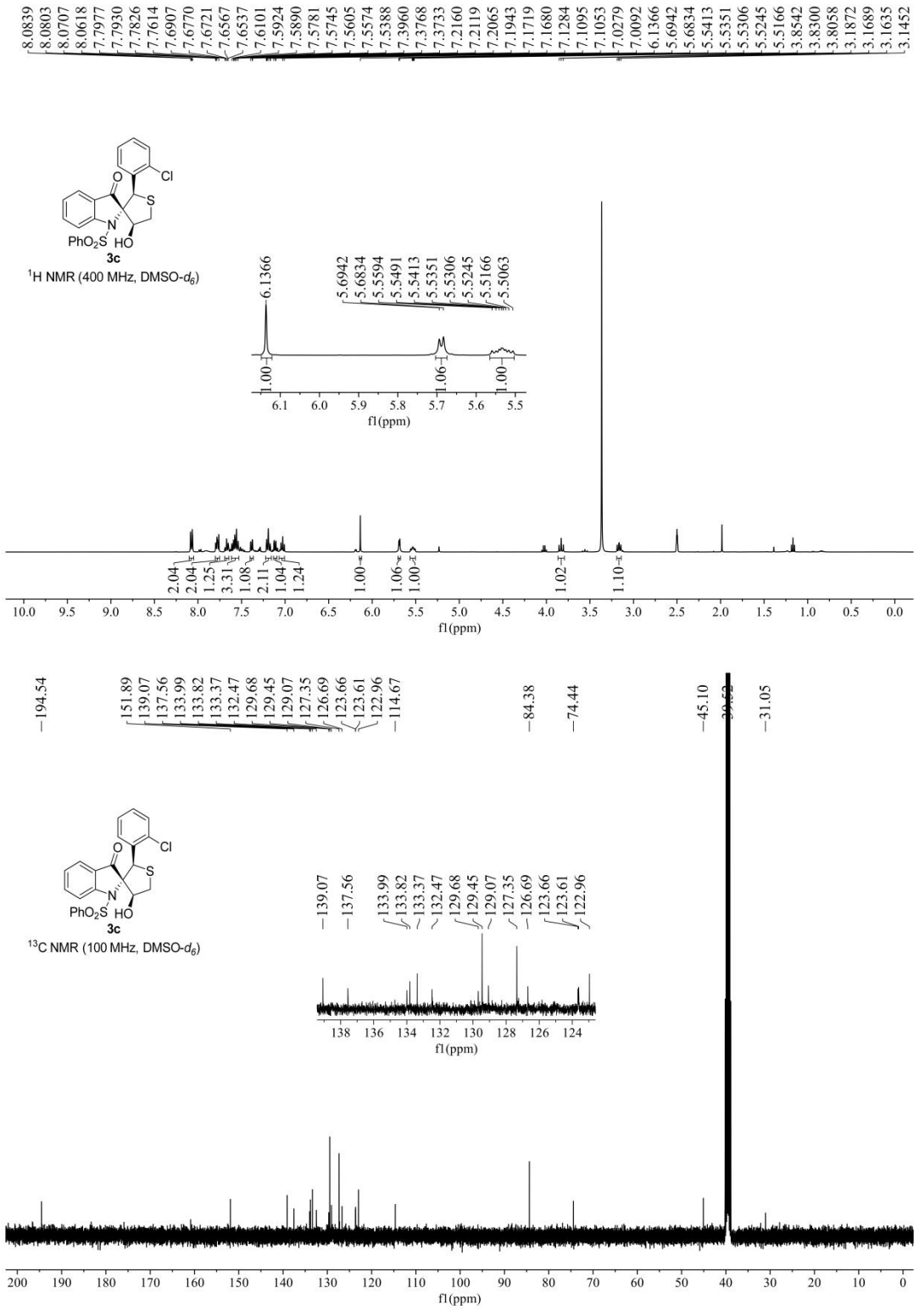

3b
^{1}H NMR (400 MHz, DMSO-d_6)
f1(ppm)

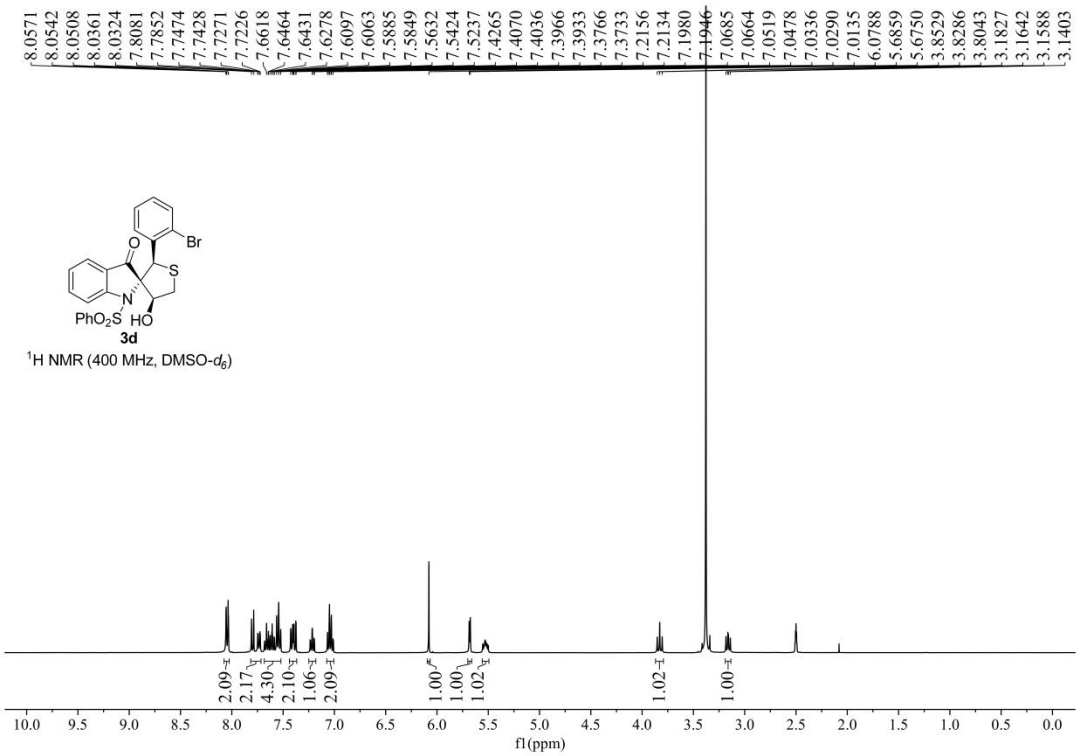

3b
^{13}C NMR (100 MHz, DMSO-d_6)
-CF:160.6 ppm (d, J = 245.7 Hz)
f1(ppm)



3b

^{19}F NMR (376 MHz, DMSO-d_6)


3c
1H NMR (400 MHz, DMSO-d6)
fl(ppm)
3c
13C NMR (100 MHz, DMSO-d6)
fl(ppm)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8.0361
8.0324
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7.7428
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7.6618
7.6464
7.6431
7.6278
7.6097
7.6063
7.5885
7.5849
7.5632
7.5424
7.5237
7.4265
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7.3933
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7.3733
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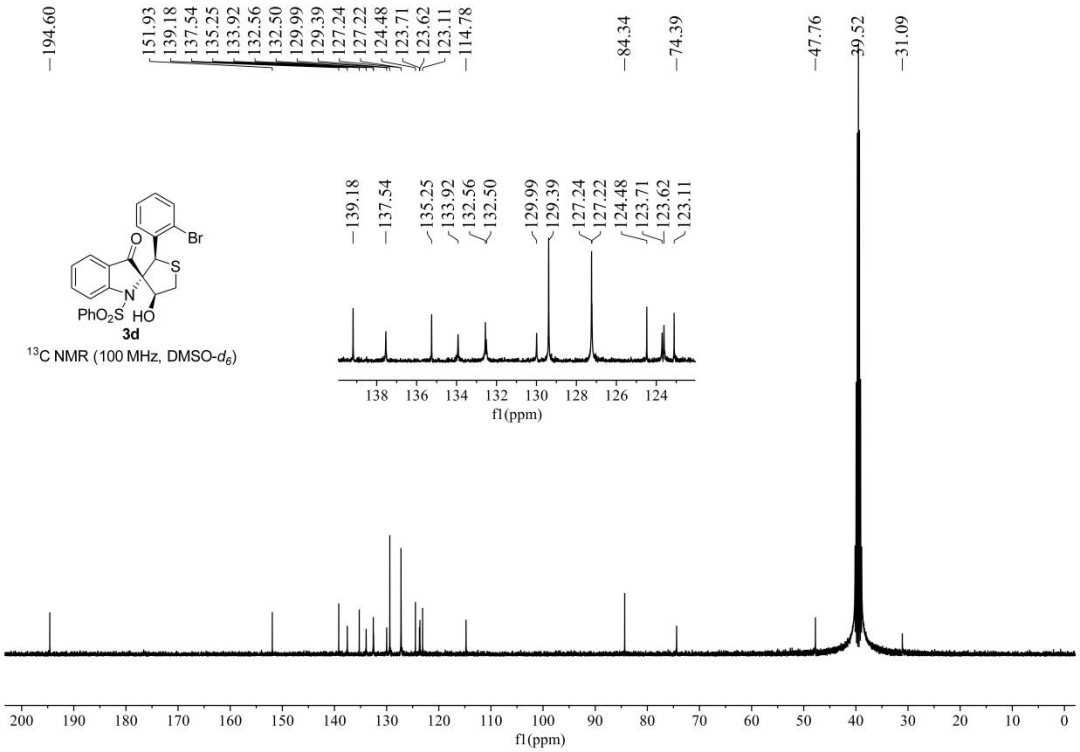
7.1980
7.1946
7.0685
7.0664
7.0519
7.0478
7.0336
7.0290
7.0135
6.0788
5.6859
5.6750
3.8529
3.8286
3.8043
3.1827
3.1642
3.1588
3.1403
Br
O
S
N
PhO2S
HO
3d
1H NMR (400 MHz, DMSO-d6)
2.09
2.17
4.30
2.10
1.06
2.09
1.00
1.00
1.02
1.02
1.00
f1 (ppm)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139.18
137.54
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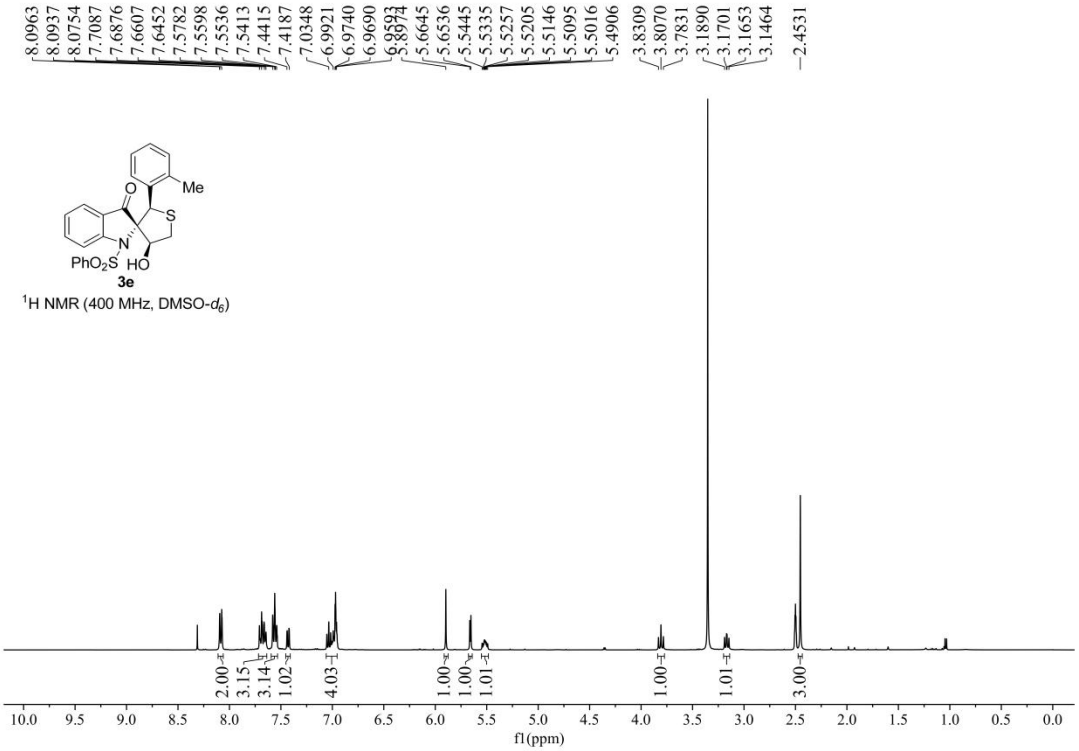
132.56
132.50
129.99
129.39
127.24
127.22
124.48
123.71
123.62
123.11
114.78
84.34
74.39
47.76
39.52
31.09
Br
O
S
N
PhO2S
HO
3d
13C NMR (100 MHz, DMSO-d6)
f1 (ppm)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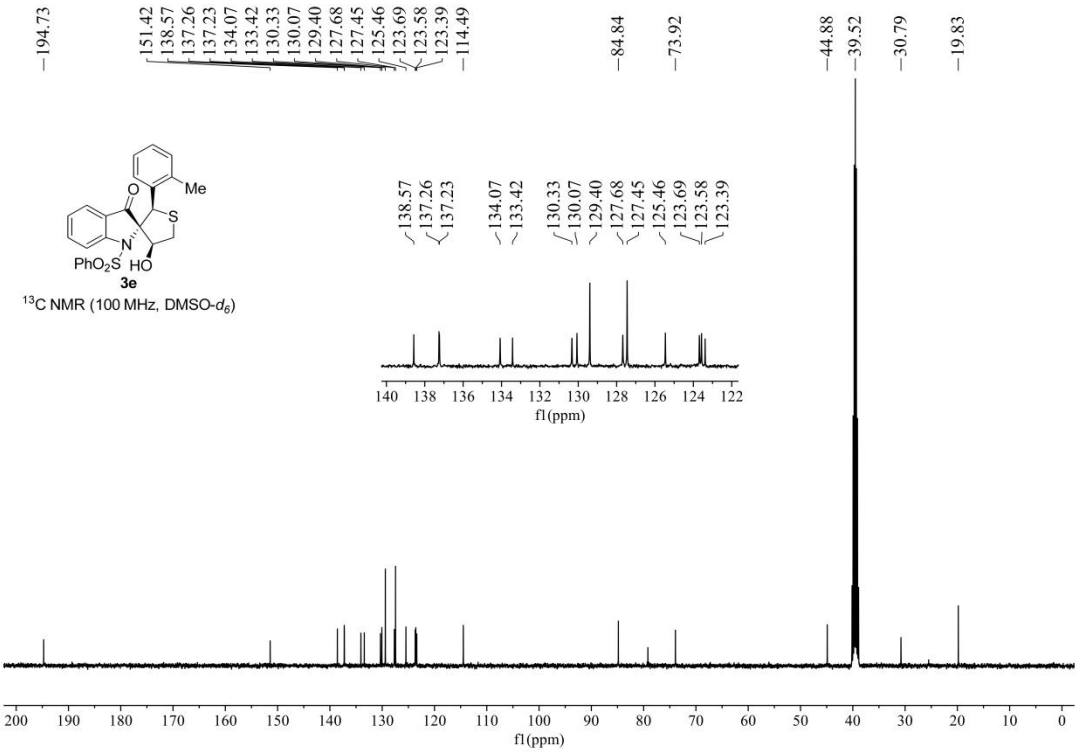
5.5205
5.5146
5.5095
5.5016
5.4906
3.8309
3.8070
3.7831
3.1890
3.1701
3.1653
3.1464
2.4531
Me
O
S
N
PhO2S HO
3e
1H NMR (400 MHz, DMSO-d6)
2.00
3.15
3.14
1.02
4.03
1.00
1.00
1.01
1.00
1.01
3.00
f1(ppm)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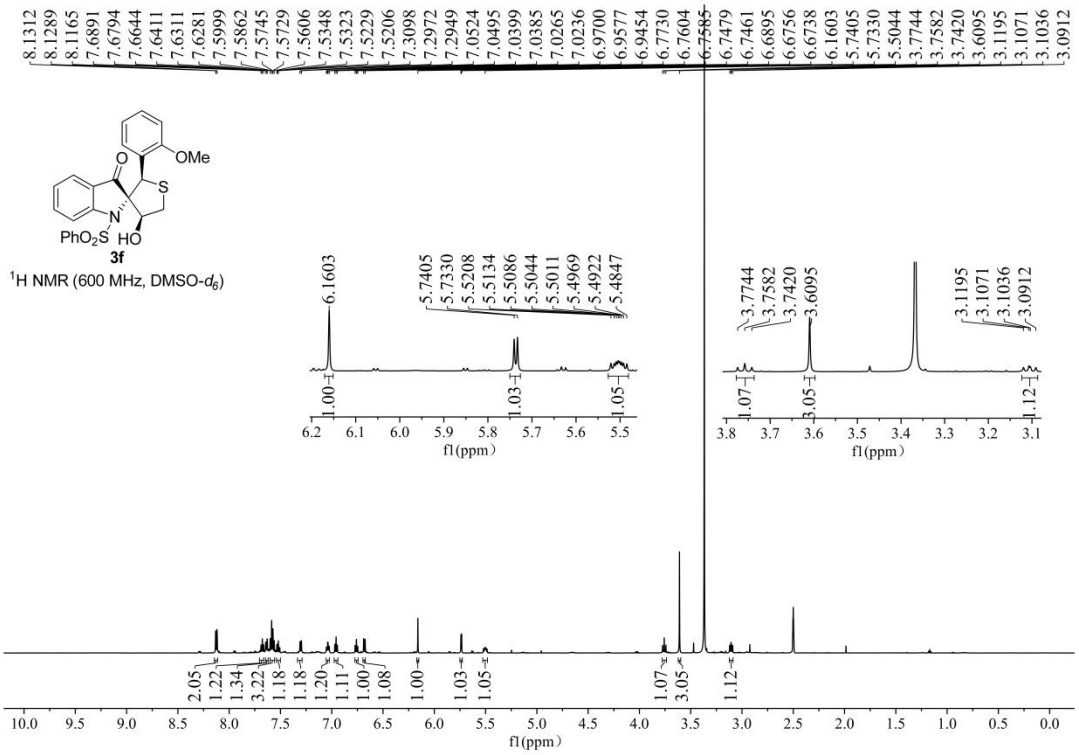
151.42
138.57
137.26
137.23
134.07
133.42
130.33
130.07
129.40
127.68
127.45
125.46
123.69
123.58
123.39
114.49
84.84
73.92
44.88
39.52
30.79
19.83
Me
O
S
N
PhO2S HO
3e
13C NMR (100 MHz, DMSO-d6)
f1(ppm)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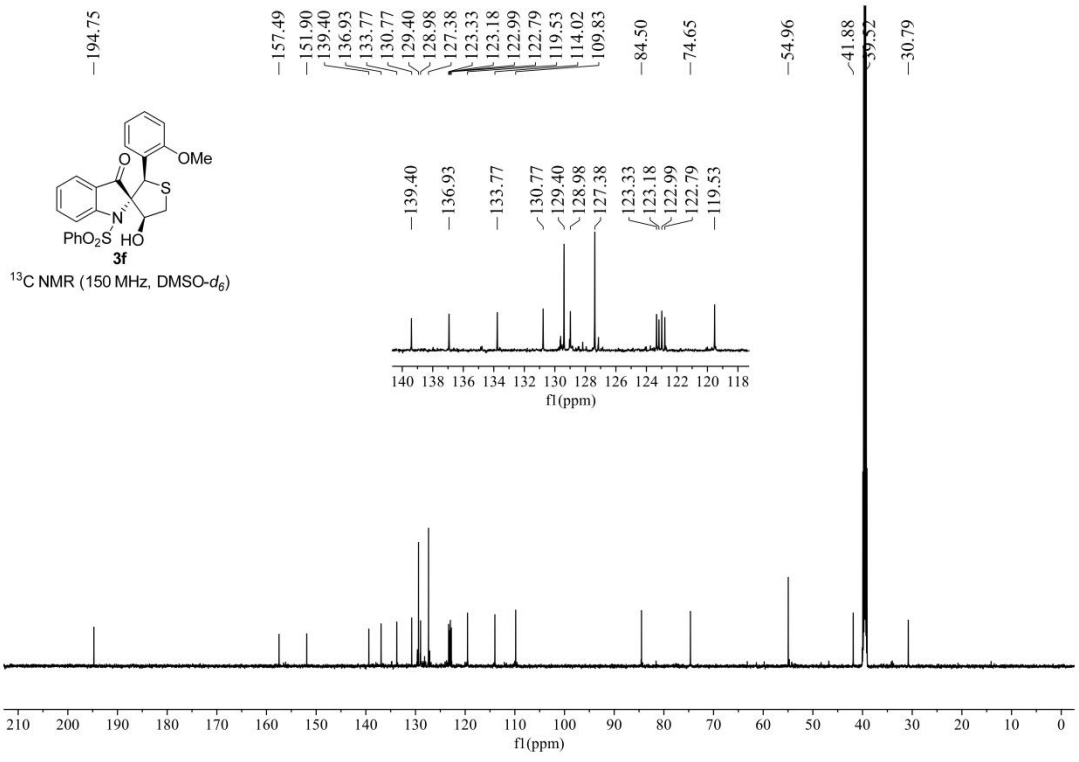
8.1165
7.6891
7.6794
7.6644
7.6411
7.6311
7.6281
7.5999
7.5862
7.5745
7.5729
7.5606
7.5348
7.5323
7.5229
7.5206
7.3098
7.2972
7.2949
7.0524
7.0495
7.0399
7.0385
7.0265
7.0236
6.9700
6.9577
6.9454
6.7730
6.7604
6.7585
6.7479
6.7461
6.6895
6.6756
6.6738
6.1603
5.7405
5.7330
5.5208
5.5134
5.5086
5.5044
5.5011
5.4969
5.4922
5.4847
3.7744
3.7582
3.7420
3.6095
3.1195
3.1071
3.1036
3.0912
OMe
O
S
N
PhO2S
HO
3f
1H NMR (600 MHz, DMSO-d6)
fl(ppm)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157.49
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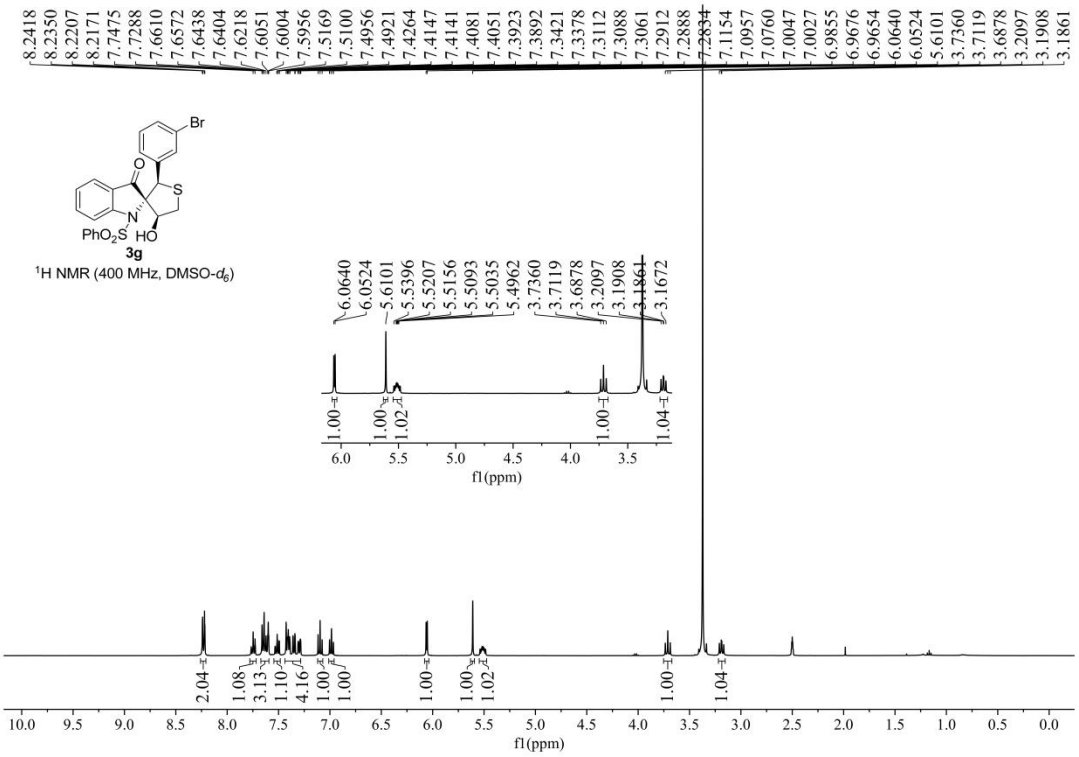
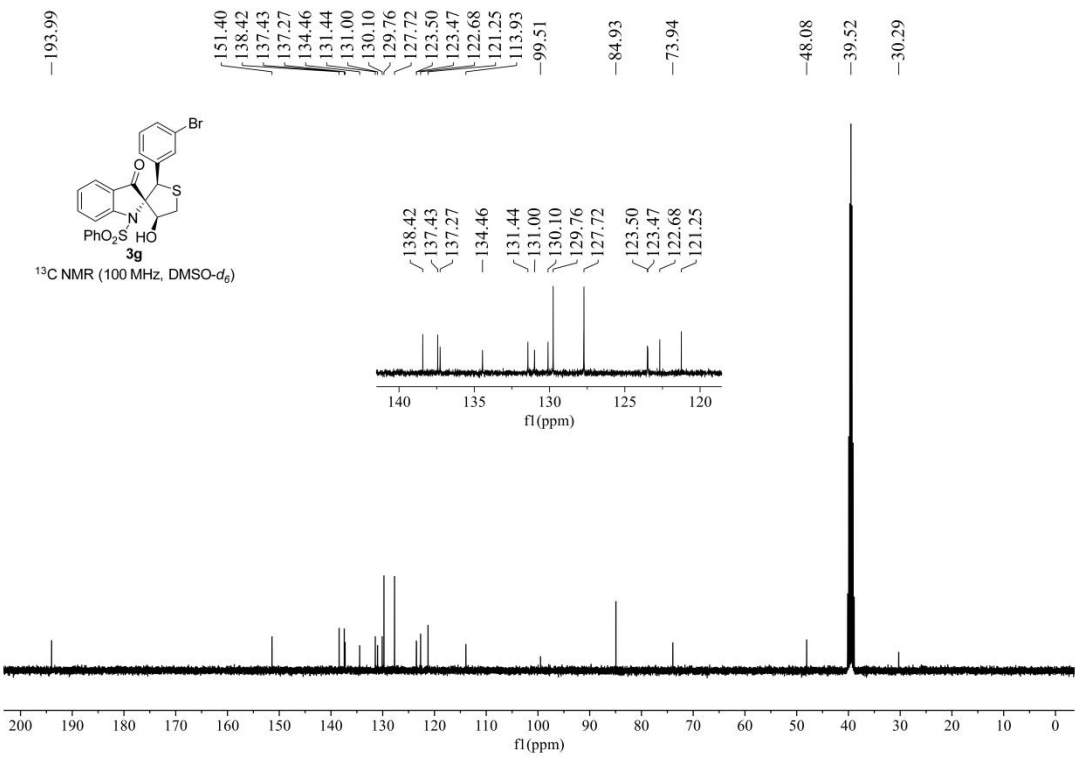
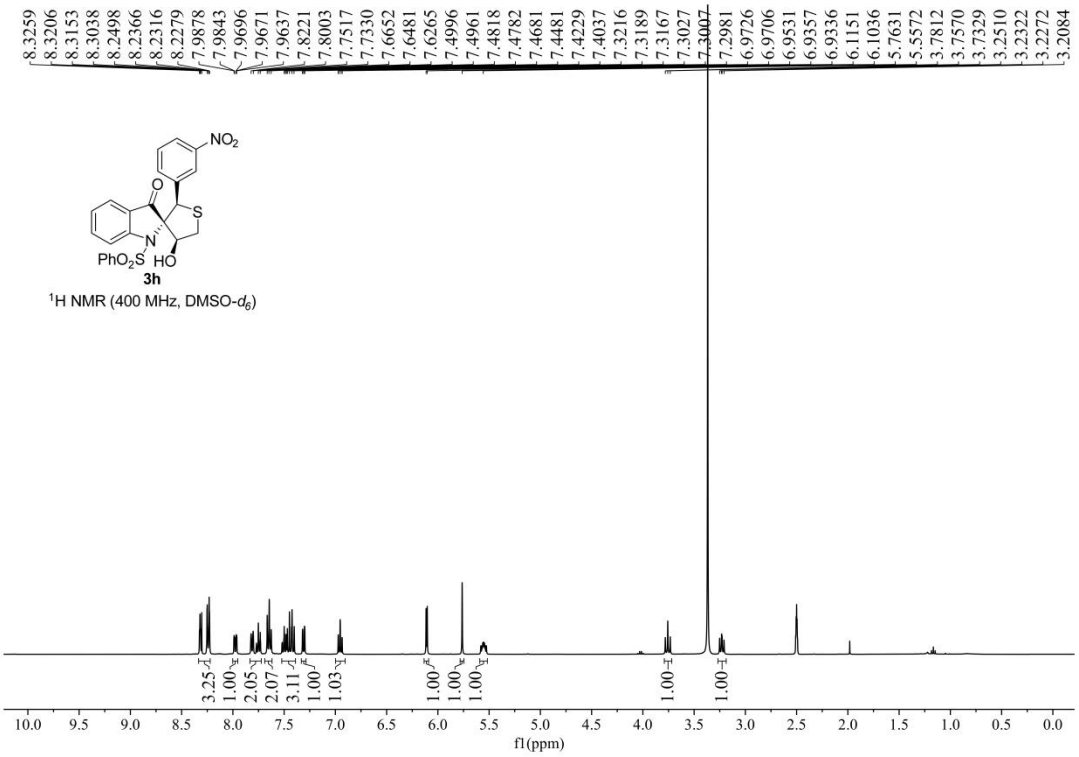
136.93
133.77
130.77
129.40
128.98
127.38
123.33
123.18
122.99
122.79
119.53
114.02
109.83
84.50
74.65
54.96
41.88
39.52
30.79
OMe
O
S
N
PhO2S
HO
3f
13C NMR (150 MHz, DMSO-d6)
fl(ppm)


3g
^{1}H NMR (400 MHz, DMSO-d_6)
f1 (ppm)


3g
^{13}C NMR (100 MHz, DMSO-d_6)
f1 (ppm)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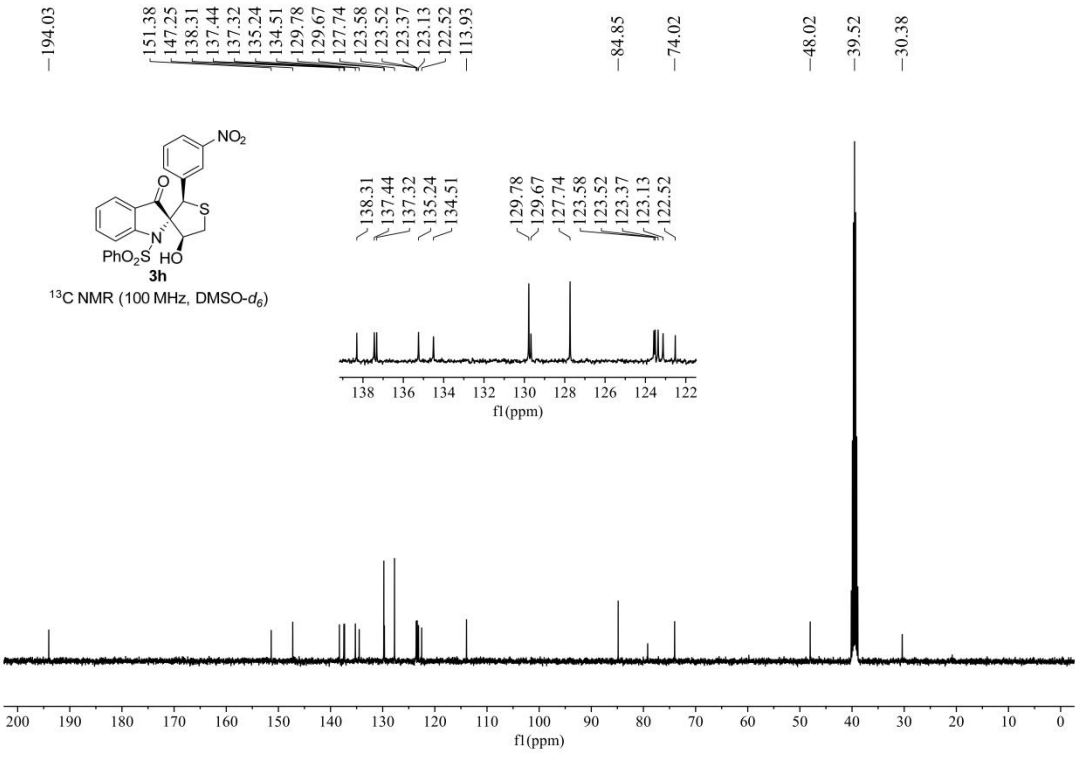
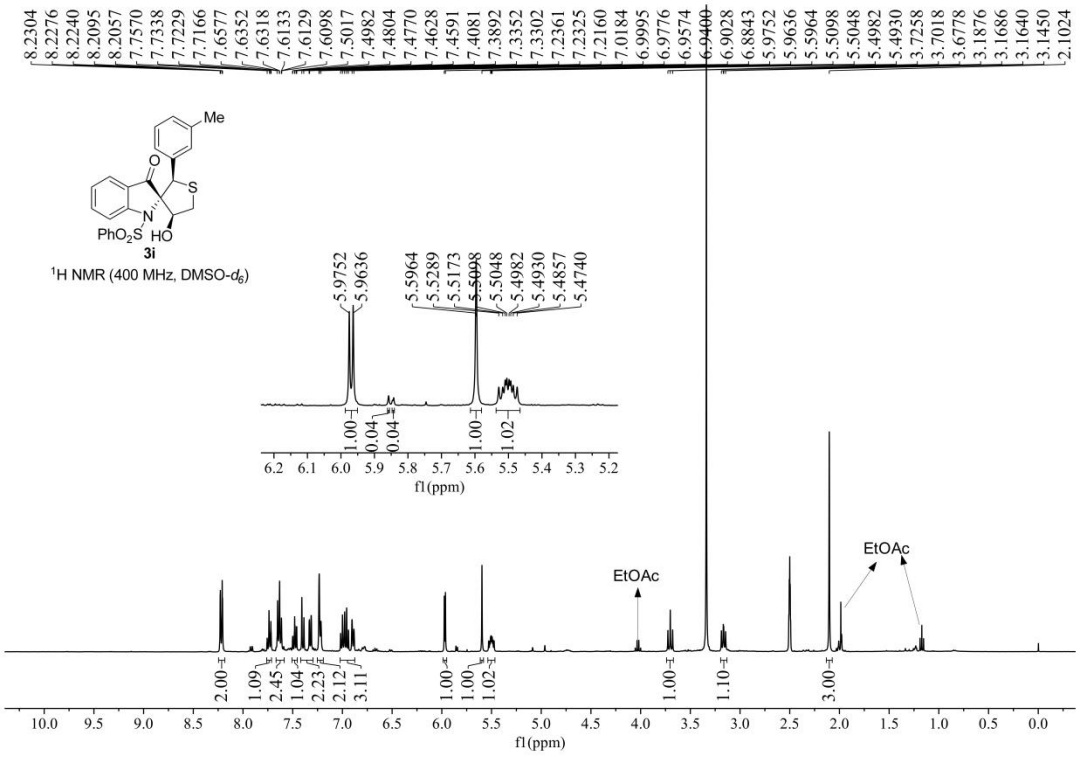
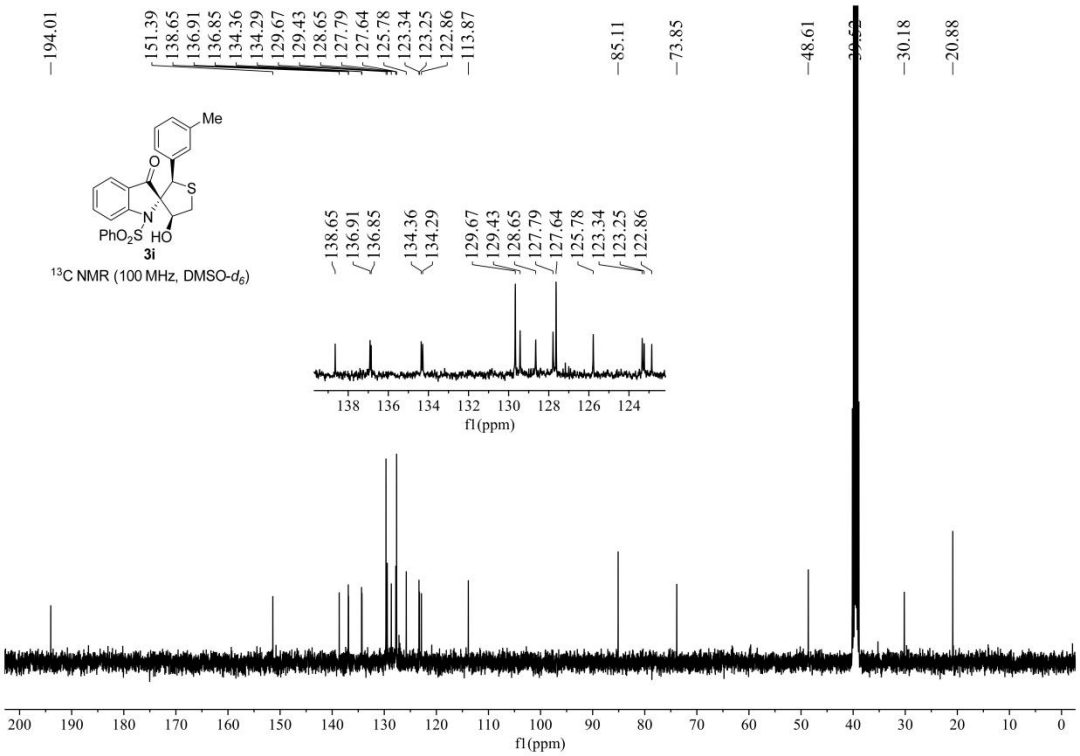
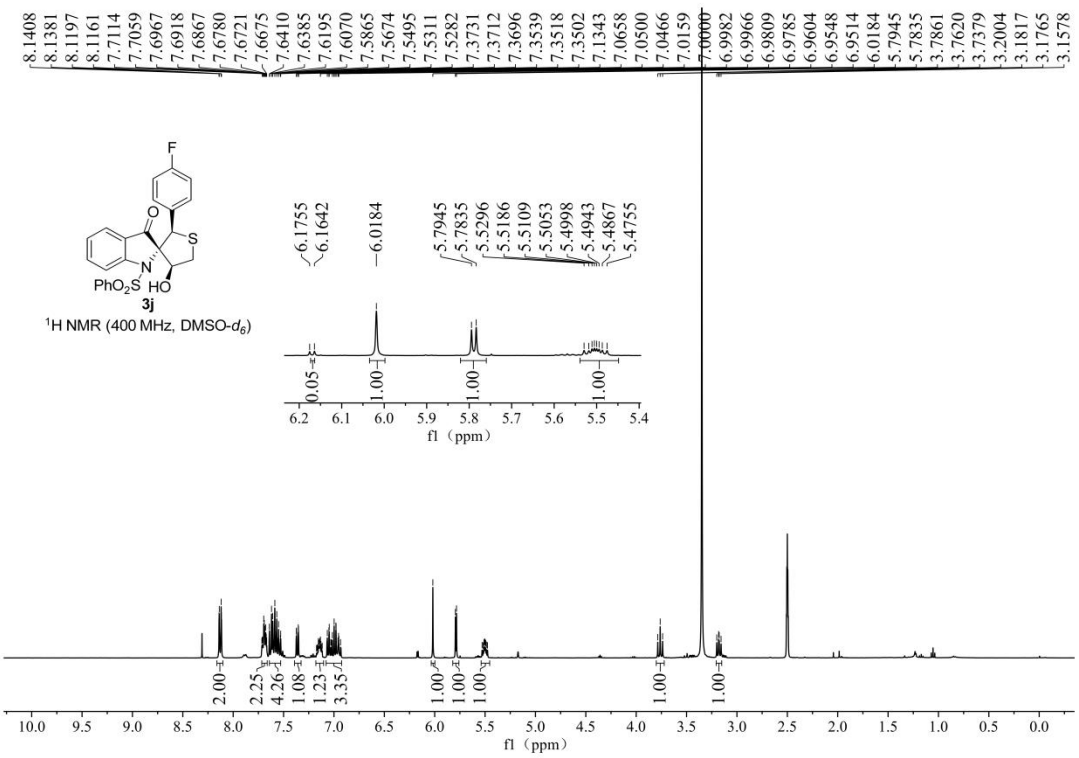
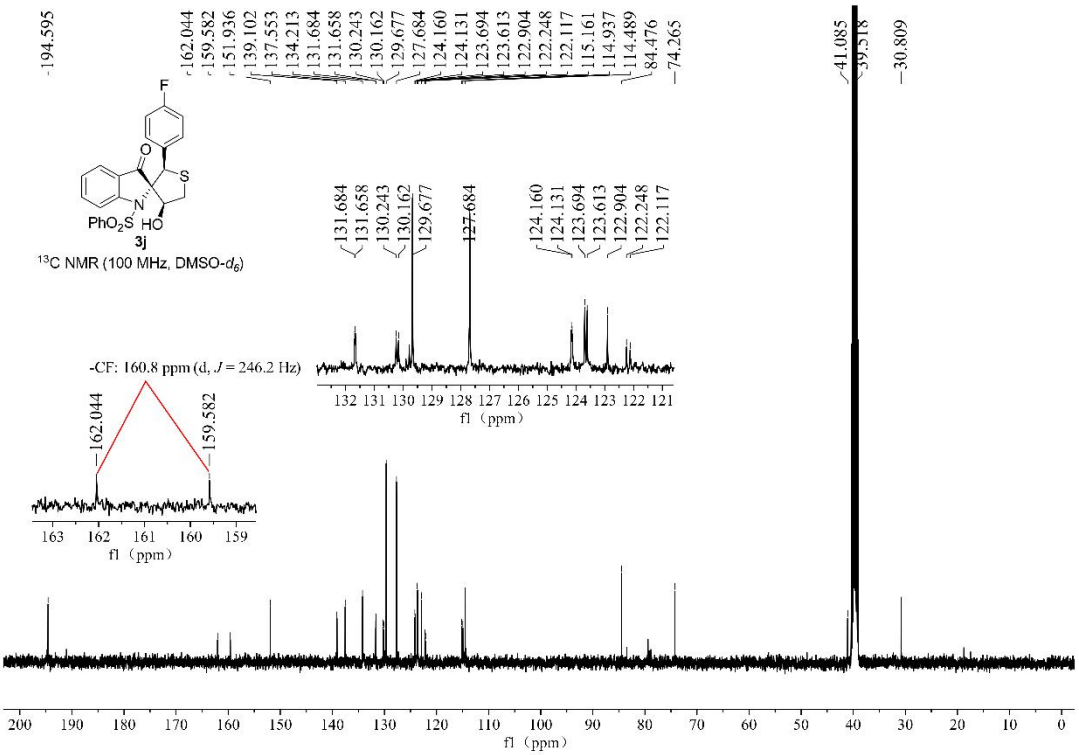
8.3206
8.3153
8.3038
8.2498
8.2366
8.2316
8.2279
7.9878
7.9843
7.9696
7.9671
7.9637
7.8221
7.8003
7.7517
7.7330
7.6652
7.6481
7.6265
7.4996
7.4961
7.4818
7.4782
7.4681
7.4481
7.4229
7.4037
7.3216
7.3189
7.3167
7.3027
7.3007
7.2981
6.9726
6.9706
6.9531
6.9357
6.9336
6.1151
6.1036
5.7631
5.5572
3.7812
3.7570
3.7329
3.2510
3.2322
3.2272
3.2084
NO2
O
S
N
PhO2S
HO
3h
1H NMR (400 MHz, DMSO-d6)
3.25
1.00
2.05
2.07
3.11
1.00
1.03
1.00
1.00
1.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

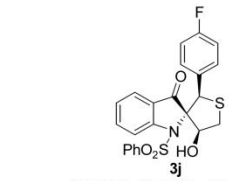

194.03
151.38
147.25
138.31
137.44
137.32
135.24
134.51
129.78
129.67
127.74
123.58
123.52
123.37
123.13
122.52
113.93
84.85
74.02
48.02
39.52
30.38
NO2
O
S
N
PhO2S
HO
3h
13C NMR (100 MHz, DMSO-d6)
138.31
137.44
137.32
135.24
134.51
129.78
129.67
127.74
123.58
123.52
123.37
123.13
122.52
138 136 134 132 130 128 126 124 122
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Me
O
S
N
PhO2S
HO
3i
1H NMR (400 MHz, DMSO-d6)
EtOAc
EtOAc
f1 (ppm)


Me
O
S
N
PhO2S
HO
3i
13C NMR (100 MHz, DMSO-d6)
f1 (ppm)

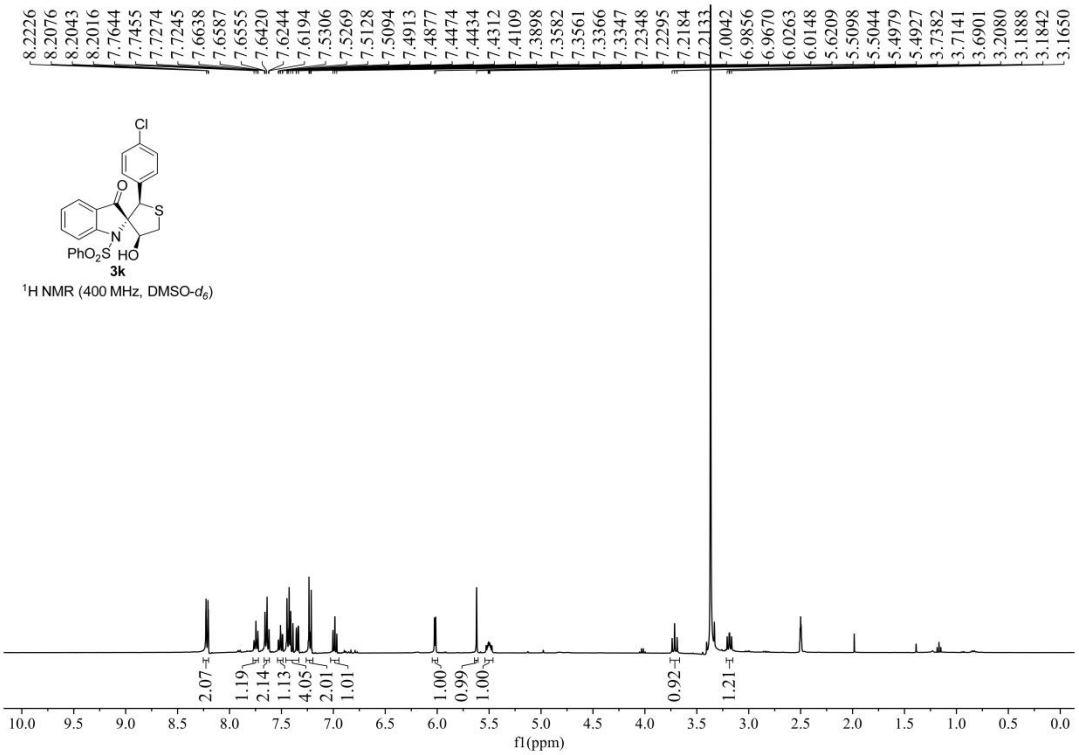

3j
^{1}H NMR (400 MHz, DMSO-d_6)
f1 (ppm)


3j
^{13}C NMR (100 MHz, DMSO-d_6)
-CF: 160.8 ppm (d, J = 246.2 Hz)
f1 (ppm)



3j

^{19}F NMR (376 MHz, DMSO-d_6)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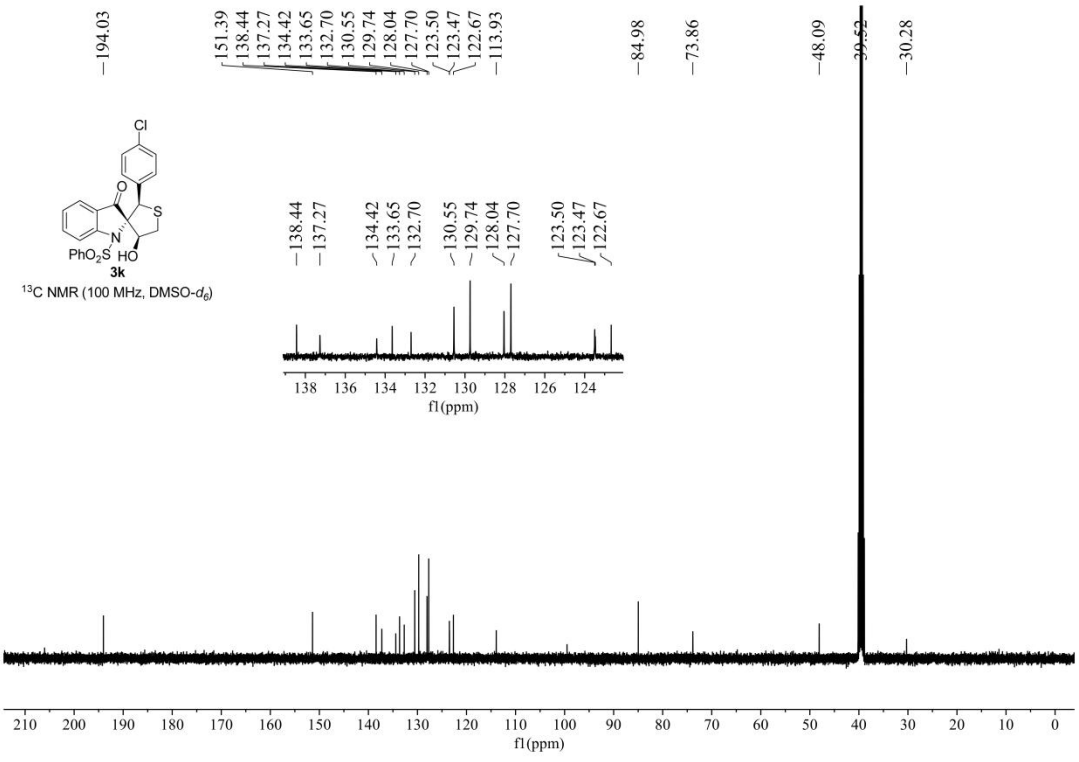
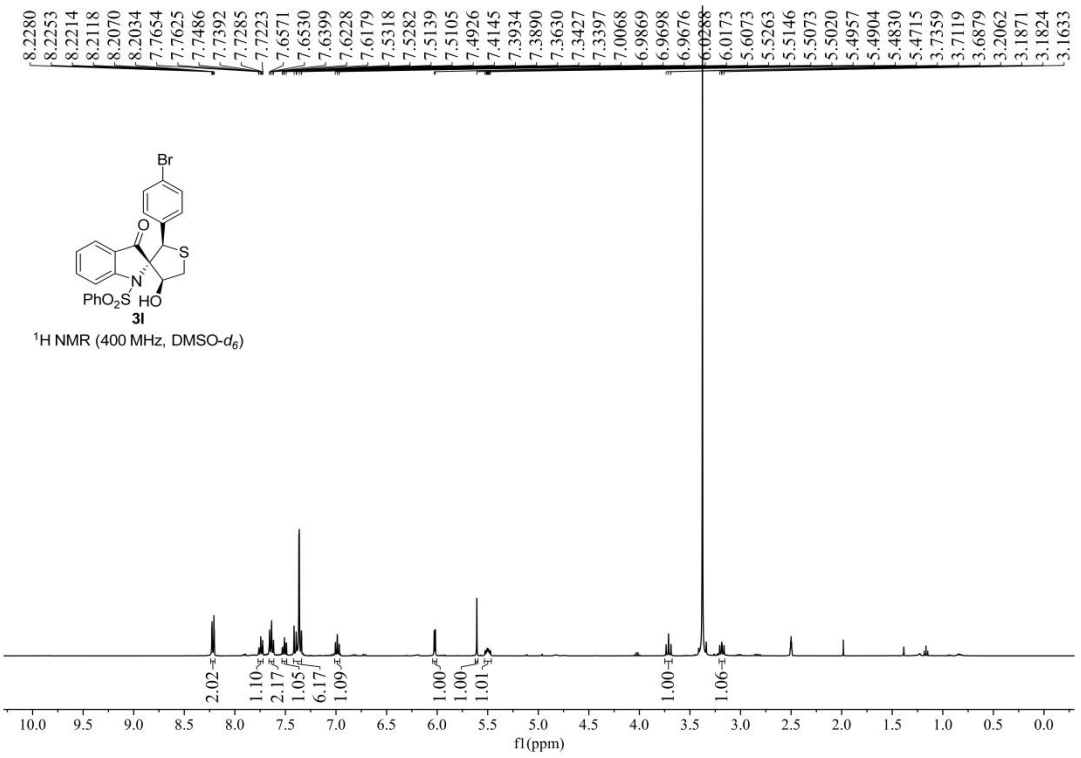
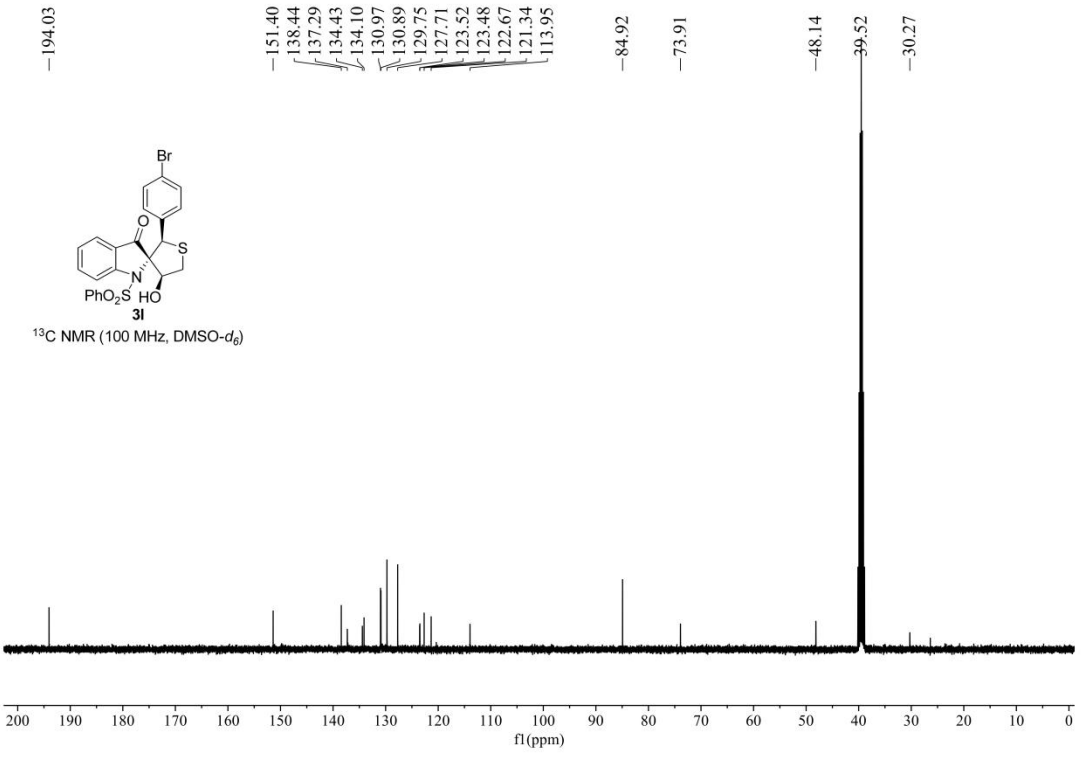
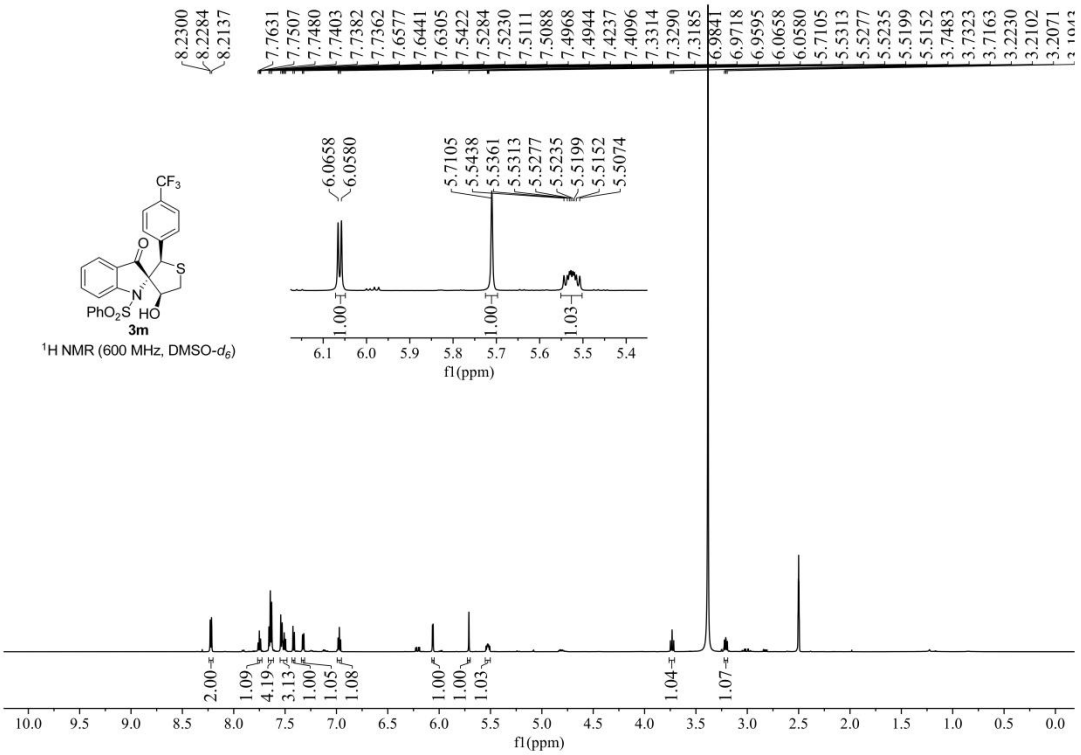
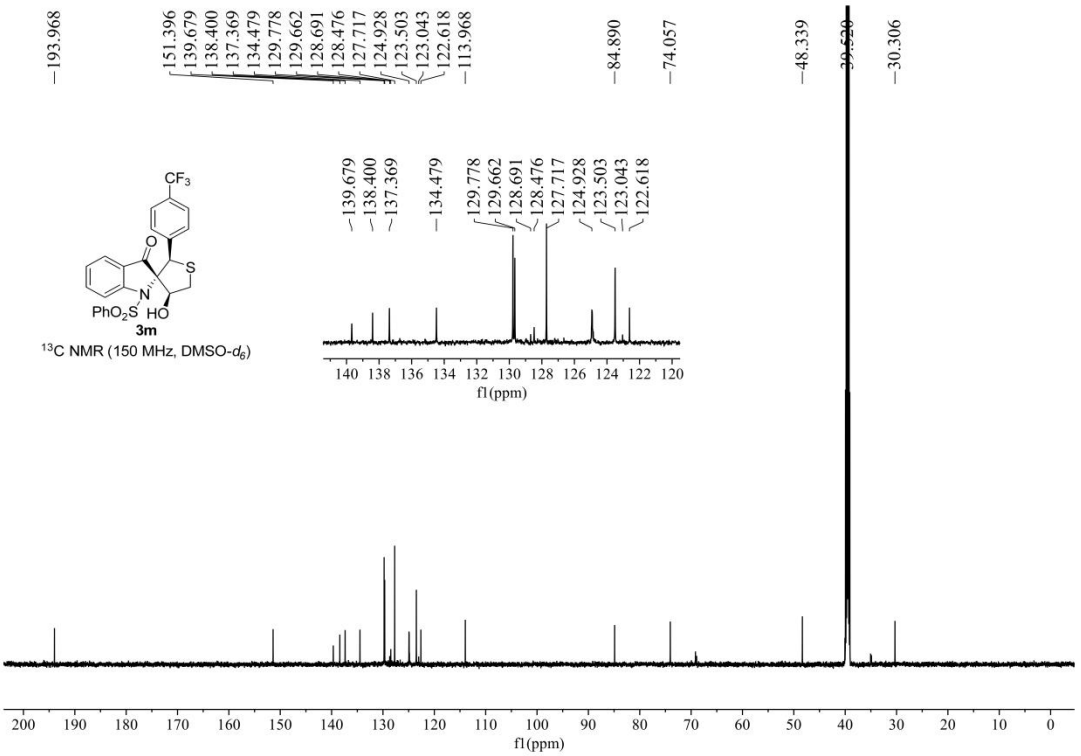
8.2076
8.2043
8.2016
7.7644
7.7455
7.7274
7.7245
7.6638
7.6587
7.6555
7.6420
7.6244
7.6194
7.5306
7.5269
7.5128
7.5094
7.4913
7.4877
7.4474
7.4434
7.4312
7.4109
7.3898
7.3582
7.3561
7.3366
7.3347
7.2348
7.2295
7.2184
7.2133
7.0042
6.9856
6.9670
6.0263
6.0148
5.6209
5.5098
5.5044
5.4979
5.4927
3.7382
3.7141
3.6901
3.2080
3.1888
3.1842
3.1650
Cl
O
S
N
PhO2S HO
3k
1H NMR (400 MHz, DMSO-d6)
2.07
1.19
2.14
1.13
4.05
2.01
1.01
1.00
0.99
1.00
0.92
1.21
f1 (ppm)

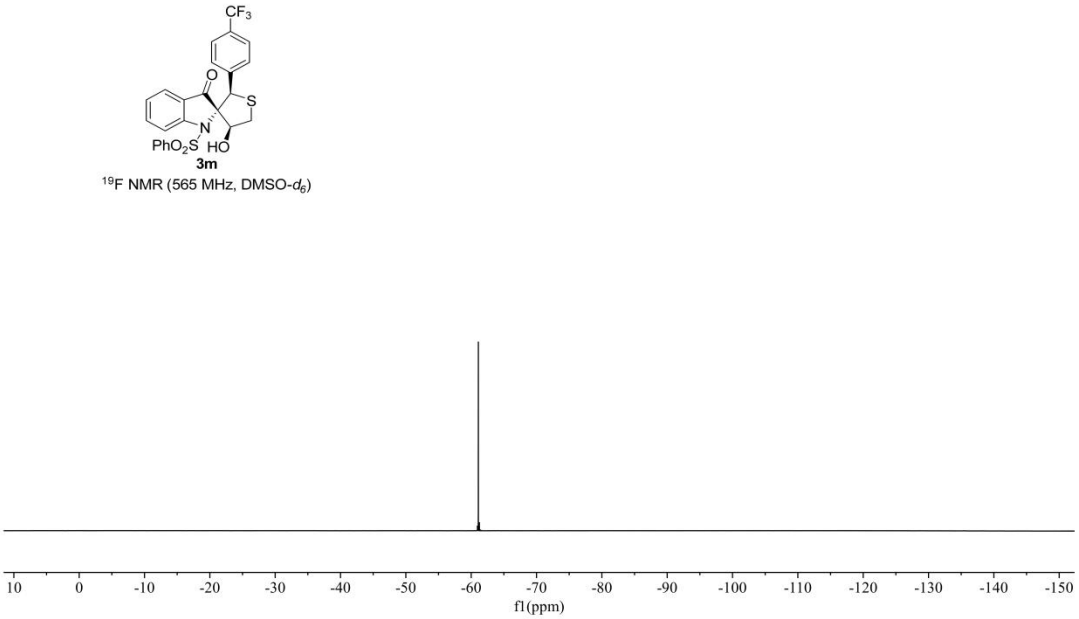

194.03
151.39
138.44
137.27
134.42
133.65
132.70
130.55
129.74
128.04
127.70
123.50
123.47
122.67
113.93
84.98
73.86
48.09
39.52
30.28
Cl
O
S
N
PhO2S HO
3k
13C NMR (100 MHz, DMSO-d6)
f1 (ppm)

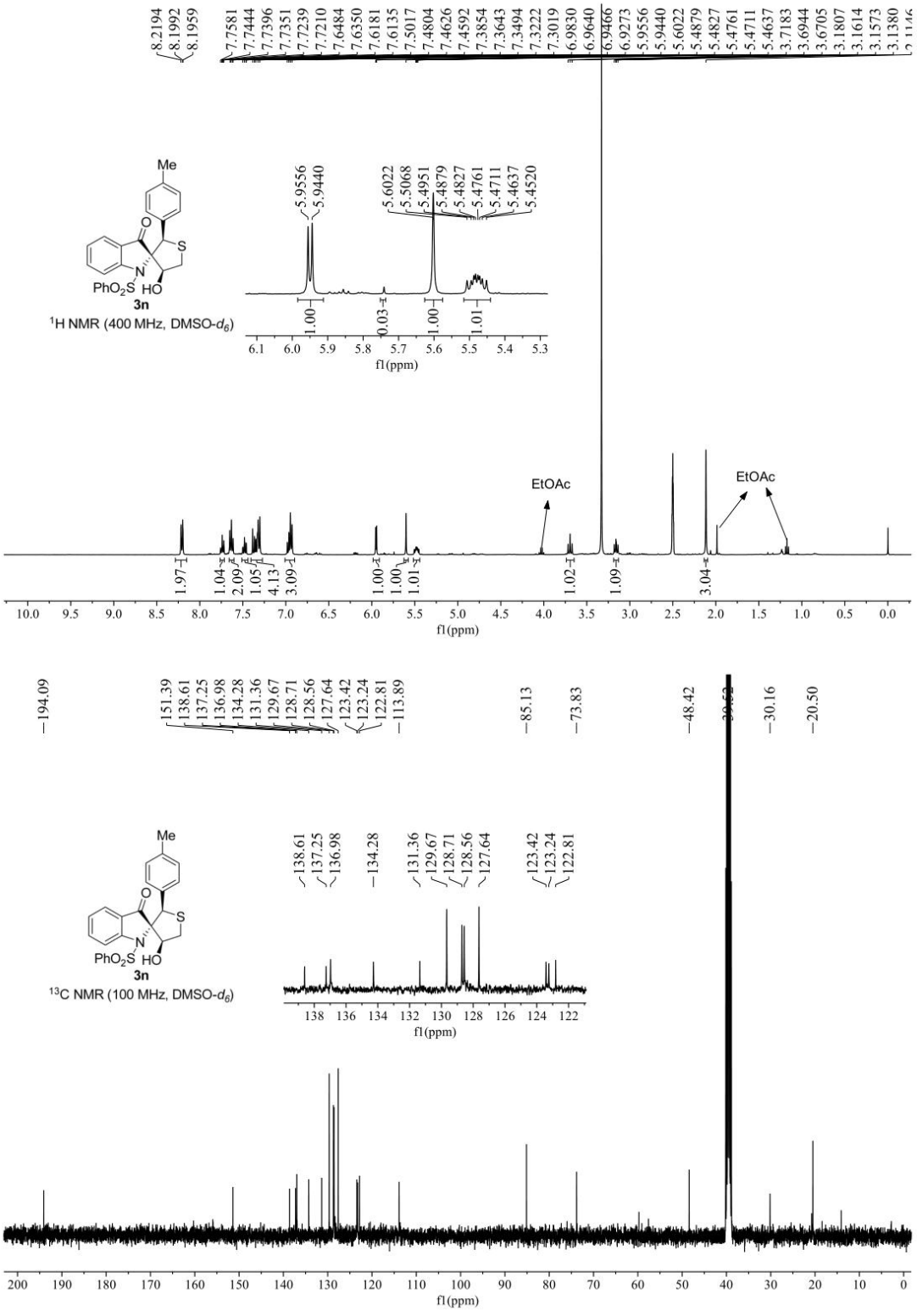

8.2280
8.2253
8.2214
8.2118
8.2070
8.2034
7.7654
7.7625
7.7486
7.7392
7.7285
7.7223
7.6571
7.6530
7.6399
7.6228
7.6179
7.5318
7.5282
7.5139
7.5105
7.4926
7.4145
7.3934
7.3890
7.3630
7.3427
7.3397
7.0068
6.9869
6.9698
6.9676
6.0288
6.0173
5.6073
5.5263
5.5146
5.5073
5.5020
5.4957
5.4904
5.4830
5.4715
3.7359
3.7119
3.6879
3.2062
3.1871
3.1824
3.1633
Br
O
S
N
PhO2S
HO
3l
1H NMR (400 MHz, DMSO-d6)
2.02
1.10
2.17
1.05
6.17
1.09
1.00
1.00
1.01
1.00
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

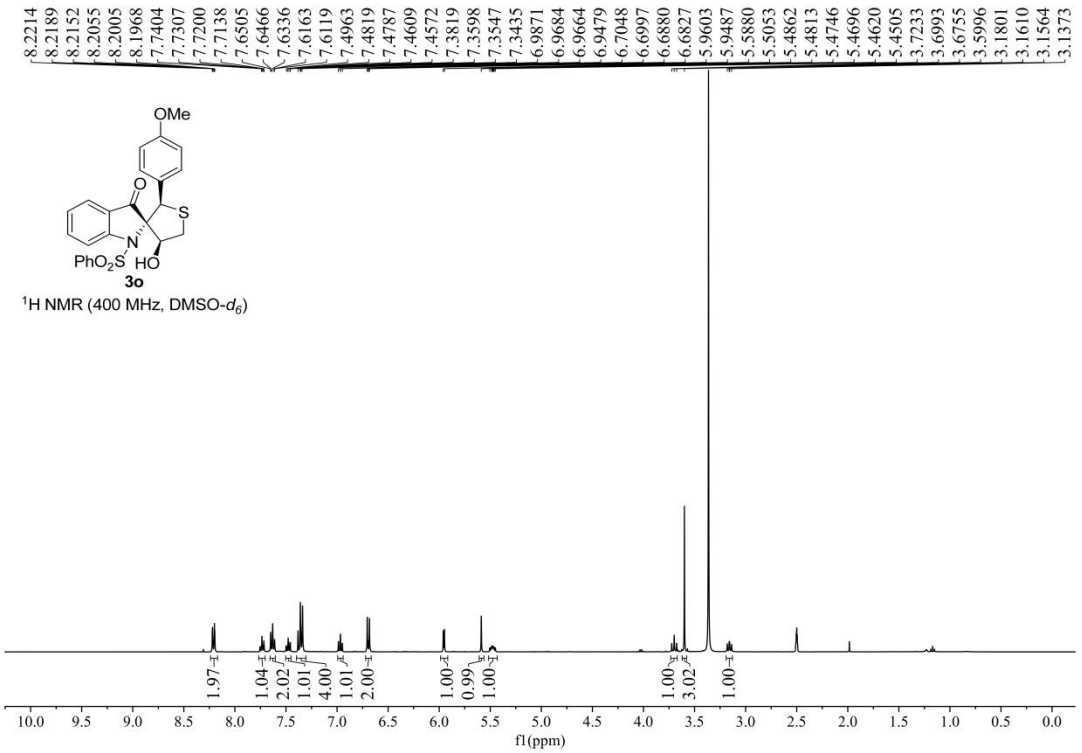

194.03
151.40
138.44
137.29
134.43
134.10
130.97
130.89
129.75
127.71
123.52
123.48
122.67
121.34
113.95
84.92
73.91
48.14
39.52
30.27
Br
O
S
N
PhO2S
HO
3l
13C NMR (100 MHz, DMSO-d6)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

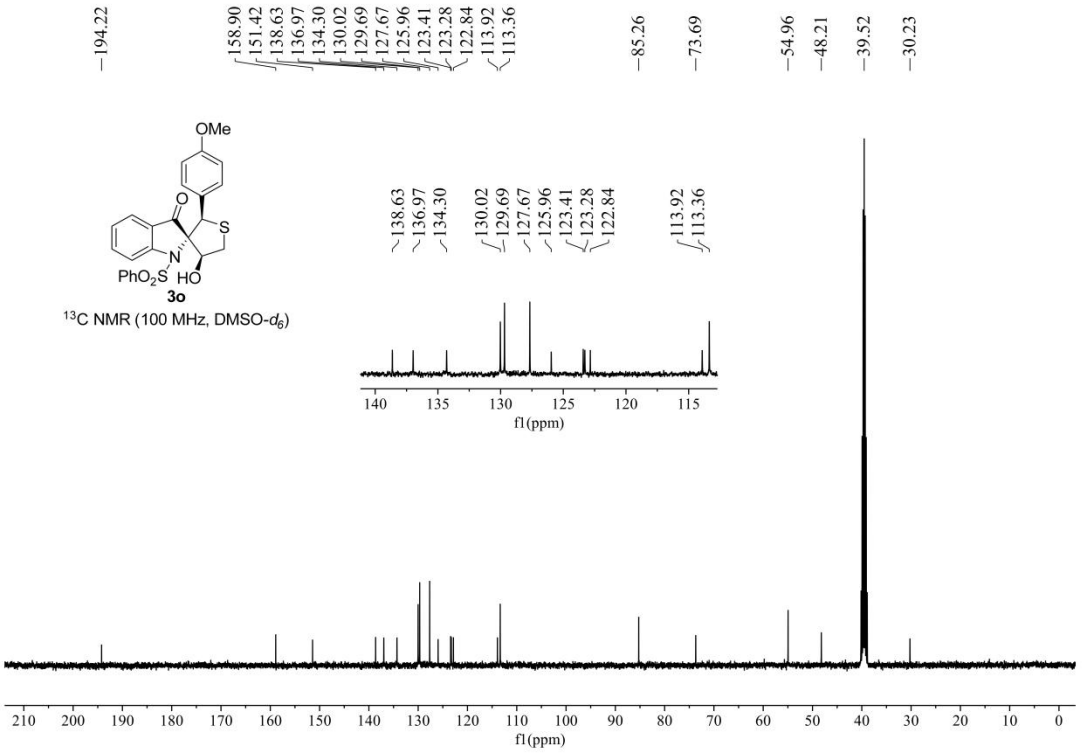

3m
^{1}H NMR (600 MHz, DMSO-d_6)
f1 (ppm)

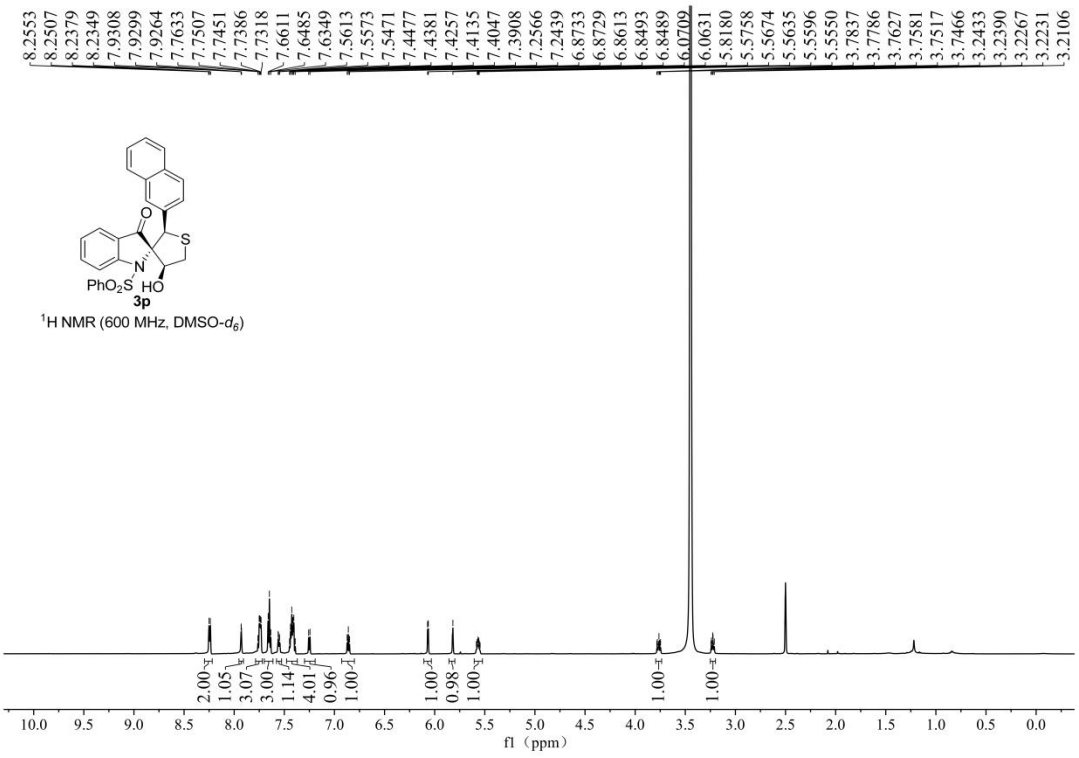

3m
^{13}C NMR (150 MHz, DMSO-d_6)
f1 (ppm)


-61.09
CF3
O
S
N
PhO2S
HO
3m
19F NMR (565 MHz, DMSO-d6)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)


Me
O
S
N
PhO2S HO
3n
1H NMR (400 MHz, DMSO-d6)
EtOAc
EtOAc
f1(ppm)
13C NMR (100 MHz, DMSO-d6)
f1(ppm)


OMe
O
S
N
PhO2S
HO
3o
1H NMR (400 MHz, DMSO-d6)
f1(ppm)


OMe
O
S
N
PhO2S
HO
3o
13C NMR (100 MHz, DMSO-d6)
f1(ppm)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8.2507
8.2379
8.2349
7.9308
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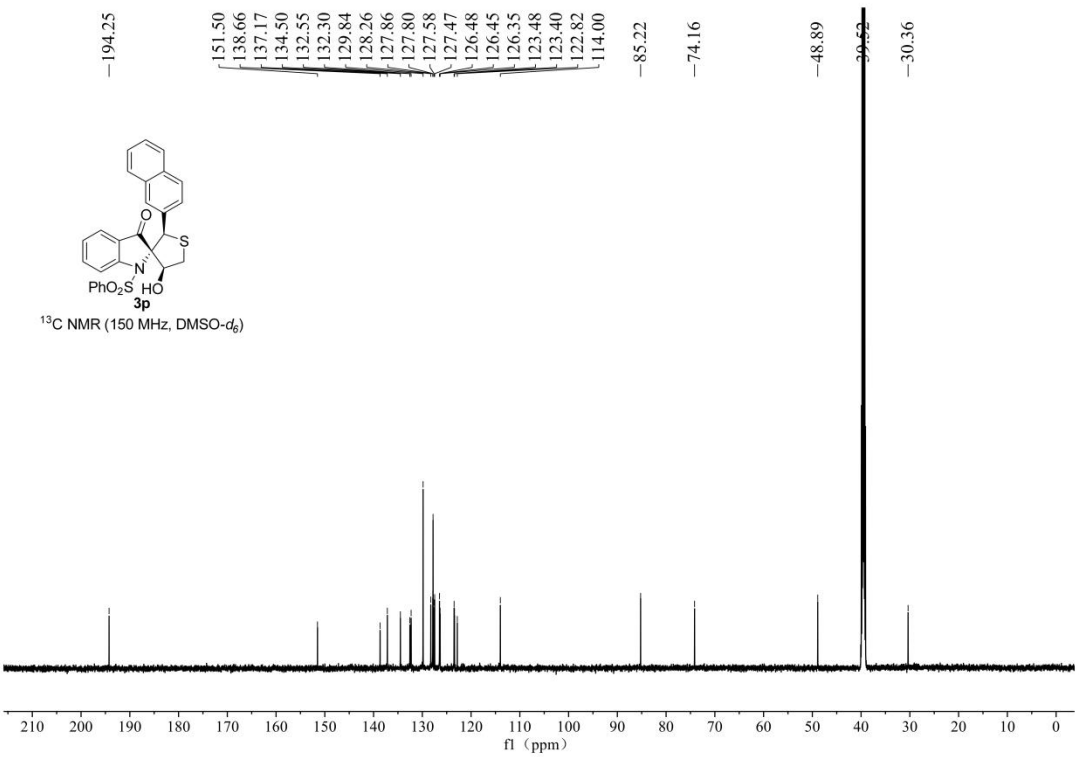
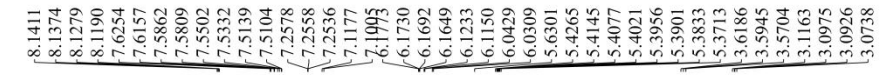
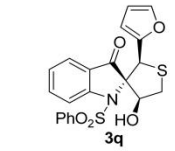
7.9264
7.7633
7.7507
7.7451
7.7386
7.7318
7.6611
7.6485
7.6349
7.5613
7.5573
7.5471
7.4477
7.4381
7.4257
7.4135
7.4047
7.3908
7.2566
7.2439
6.8733
6.8729
6.8613
6.8493
6.8489
6.0702
6.0631
5.8180
5.7758
5.5674
5.5635
5.5596
5.5550
3.7837
3.7786
3.7627
3.7581
3.7517
3.7466
3.2433
3.2390
3.2267
3.2231
3.2106
PhO2S HO
3p
1H NMR (600 MHz, DMSO-d6)
2.00
1.05
3.07
3.00
1.14
4.01
0.96
1.00
1.00
0.98
1.00
1.00
1.00
fl (ppm)

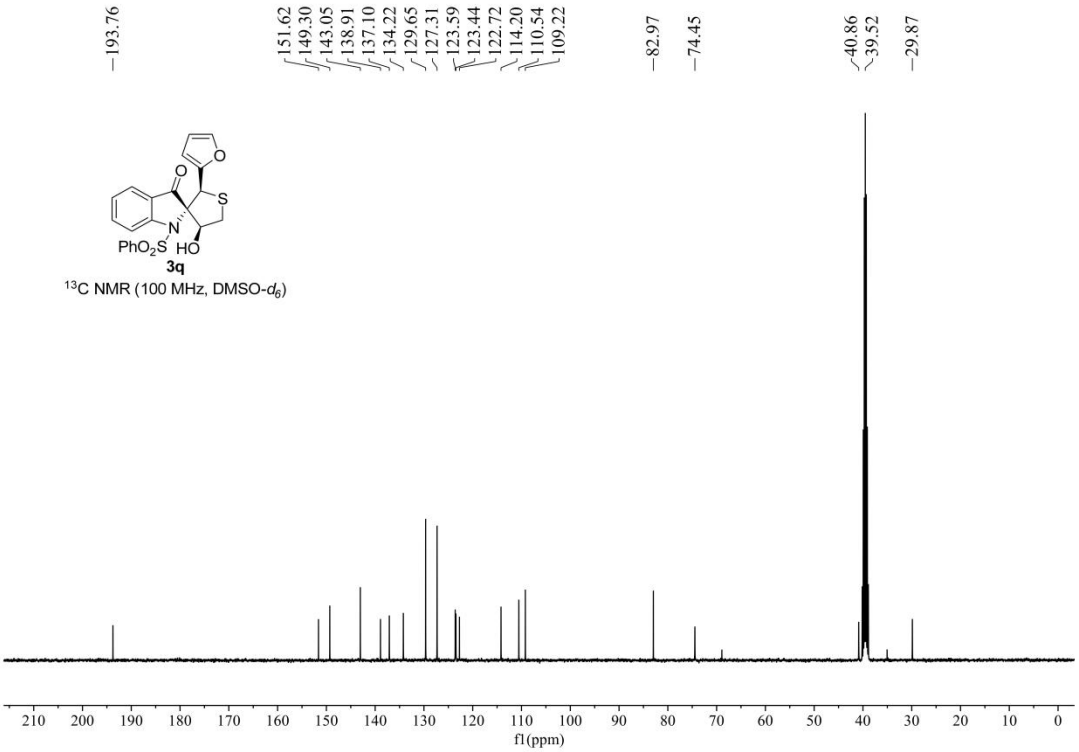

194.25
151.50
138.66
137.17
134.50
132.55
132.30
129.84
128.26
127.86
127.80
127.58
127.47
126.48
126.45
126.35
123.48
123.40
122.82
114.00
85.22
74.16
48.89
39.52
30.36
PhO2S HO
3p
13C NMR (150 MHz, DMSO-d6)
fl (ppm)





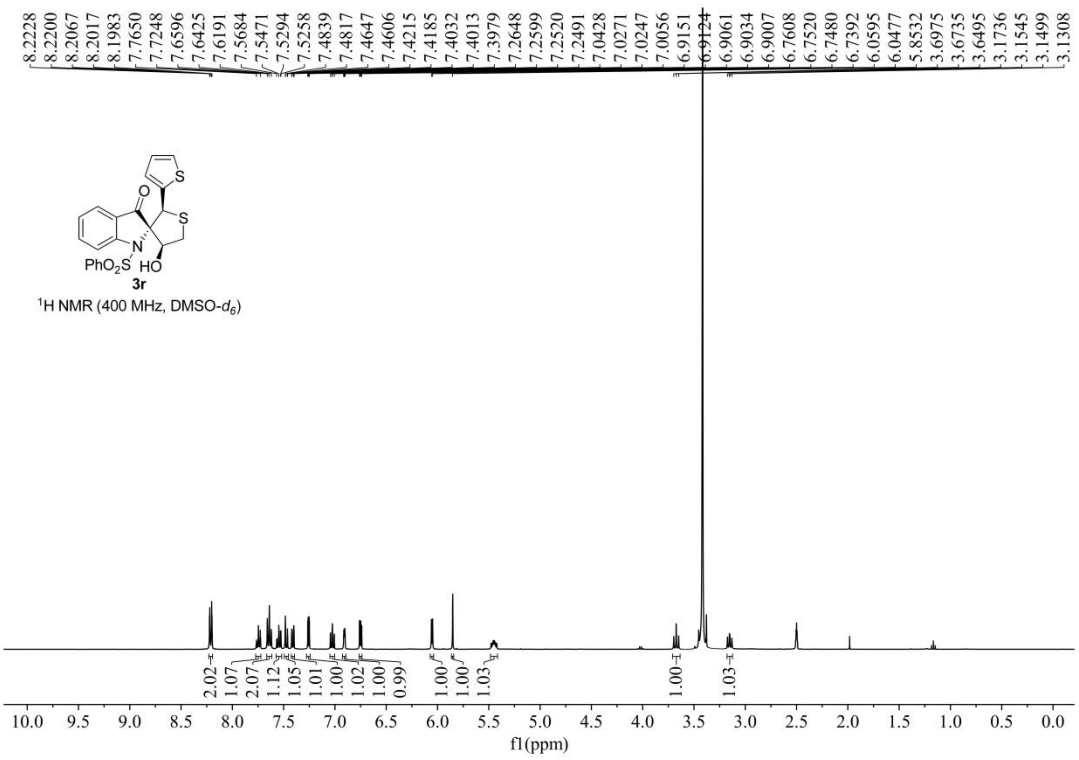
3q

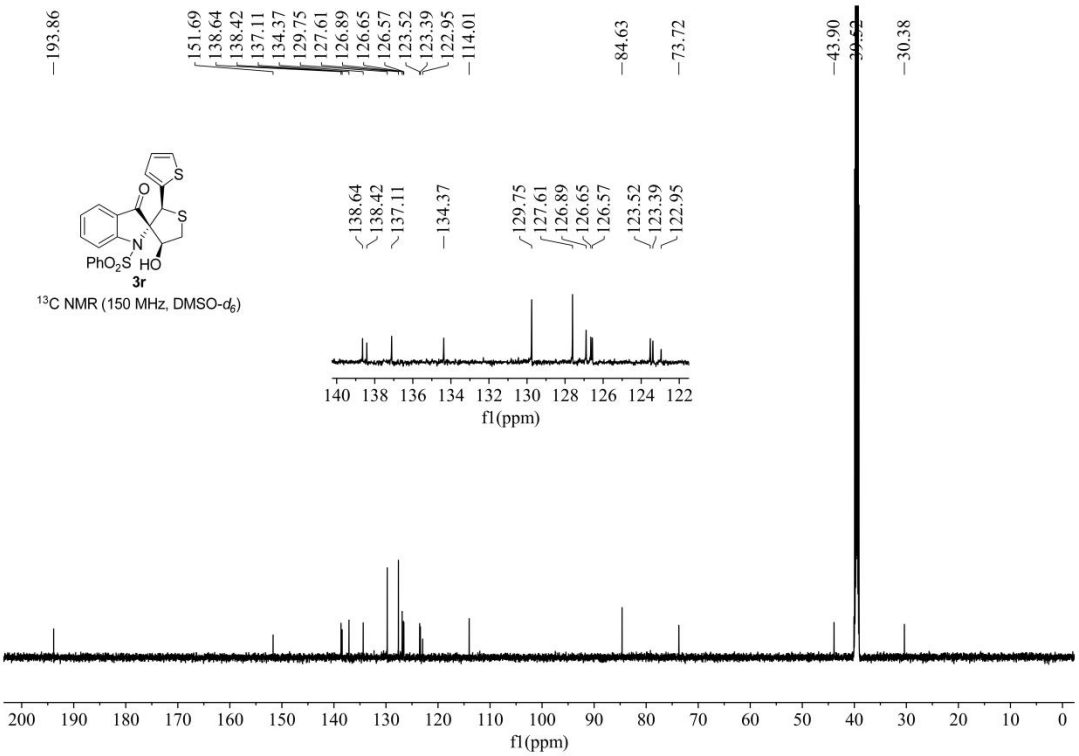
^{1}H NMR (400 MHz, DMSO-d_6)

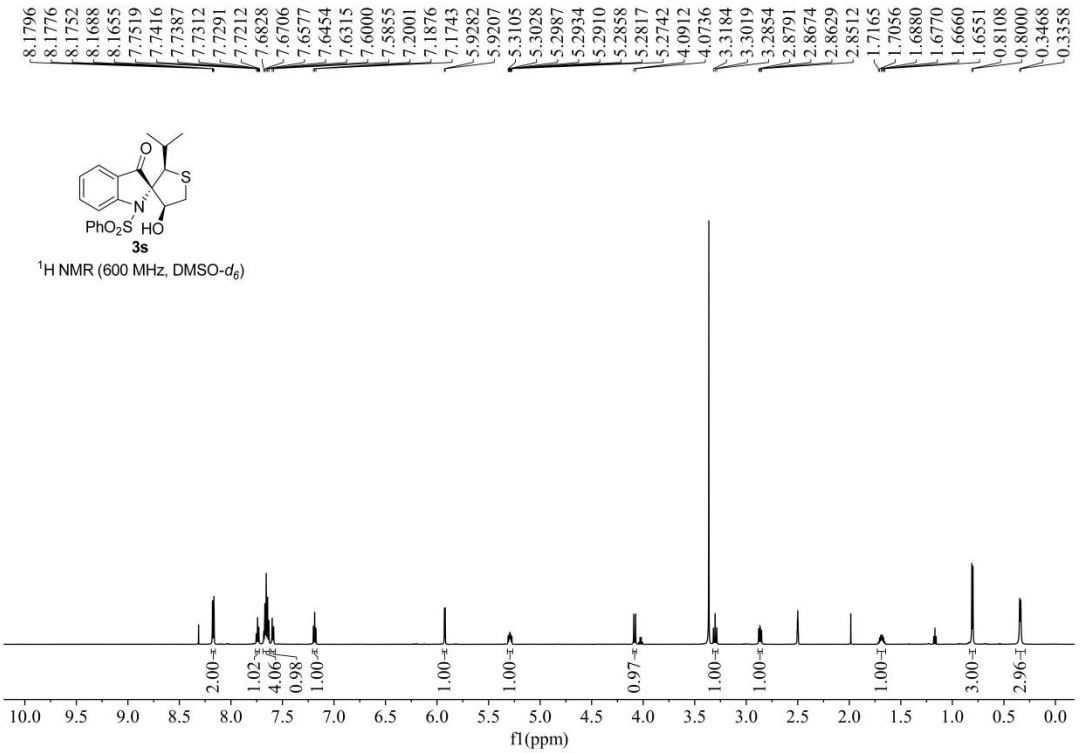


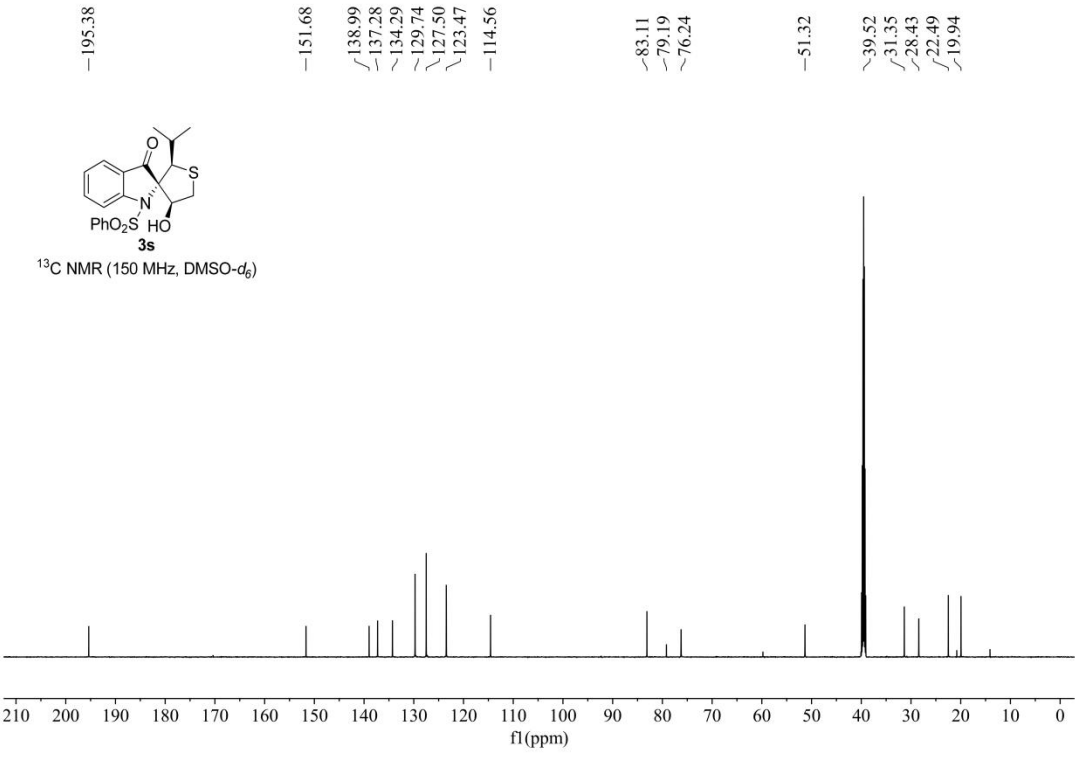
3q

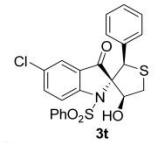
^{13}C NMR (100 MHz, DMSO-d_6)


3r
1H NMR (400 MHz, DMSO-d6)
fl (ppm)


3r
13C NMR (150 MHz, DMSO-d6)
fl (ppm)
fl (ppm)

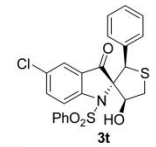

8.1796
8.1776
8.1752
8.1688
8.1655
7.7519
7.7416
7.7387
7.7312
7.7291
7.7212
7.6828
7.6706
7.6577
7.6454
7.6315
7.6000
7.5855
7.2001
7.1876
7.1743
5.9282
5.9207
5.3105
5.3028
5.2987
5.2934
5.2910
5.2858
5.2817
5.2742
4.0912
4.0736
3.3184
3.3019
3.2854
2.8791
2.8674
2.8629
2.8512
1.7165
1.7056
1.6880
1.6770
1.6660
1.6551
0.8108
0.8000
0.3468
0.3358
O
S
N
PhO2S HO
3s
1H NMR (600 MHz, DMSO-d6)
2.00
1.02
4.06
0.98
1.00
1.00
1.00
0.97
1.00
1.00
1.00
3.00
2.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


195.38
151.68
138.99
137.28
134.29
129.74
127.50
123.47
114.56
83.11
79.19
76.24
51.32
39.52
31.35
28.43
22.49
19.94
O
S
N
PhO2S HO
3s
13C NMR (150 MHz, DMSO-d6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



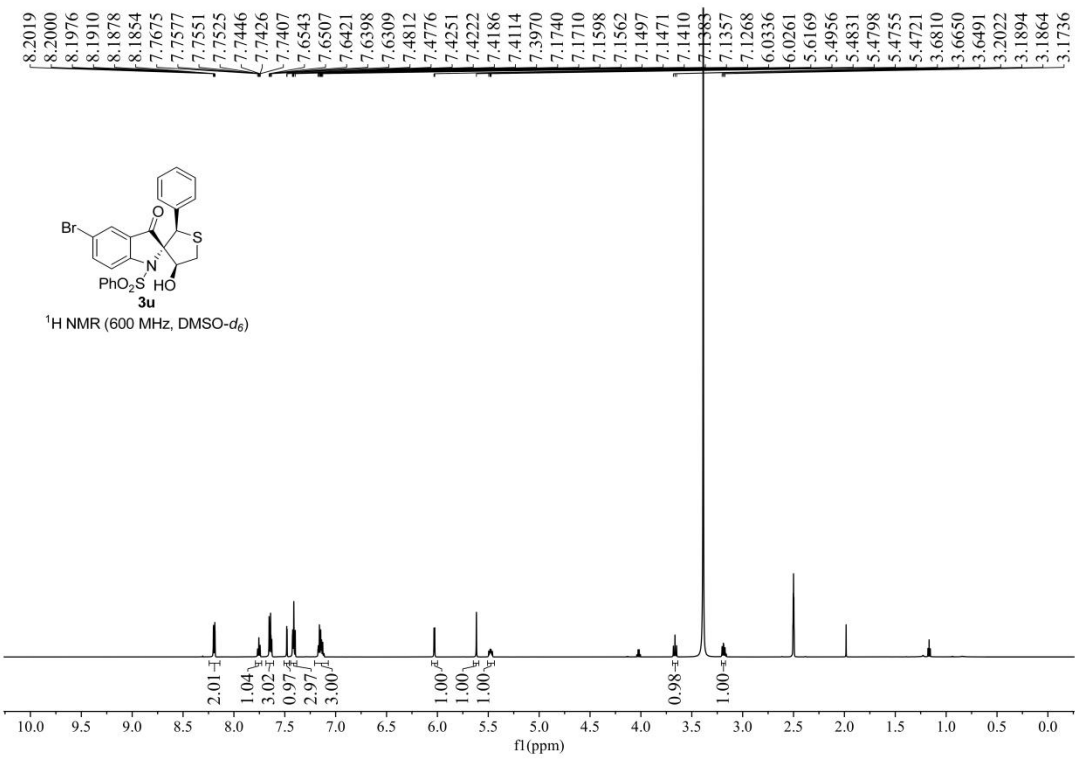
3t

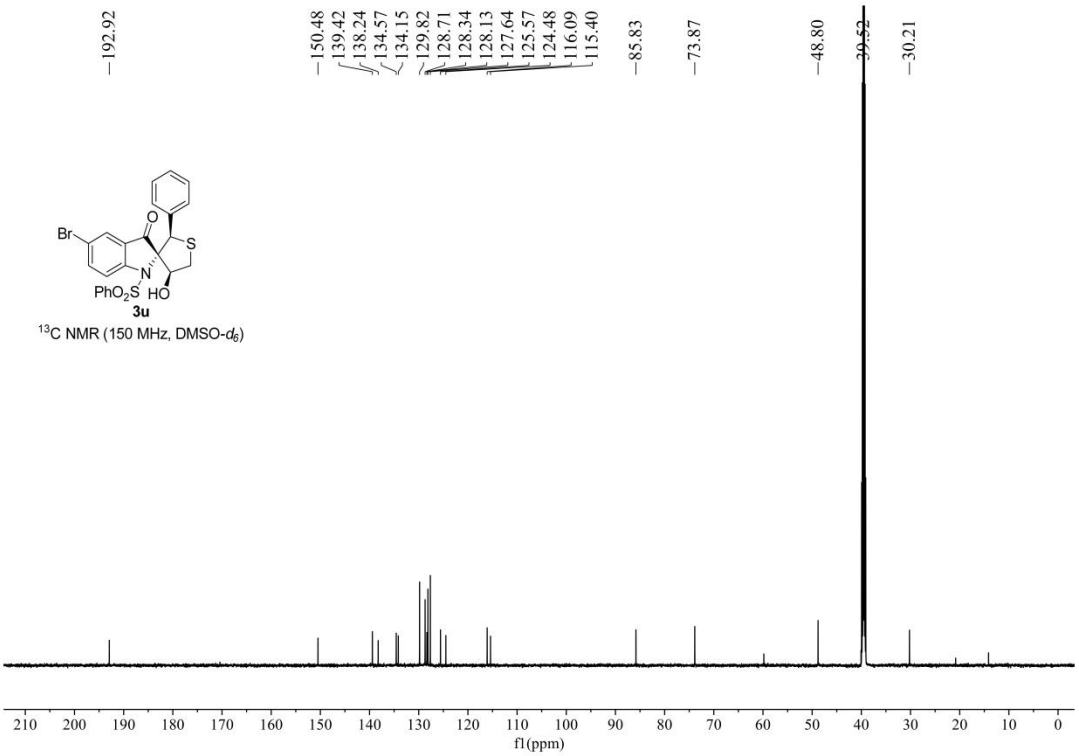
^{1}H NMR (400 MHz, DMSO-d_6)

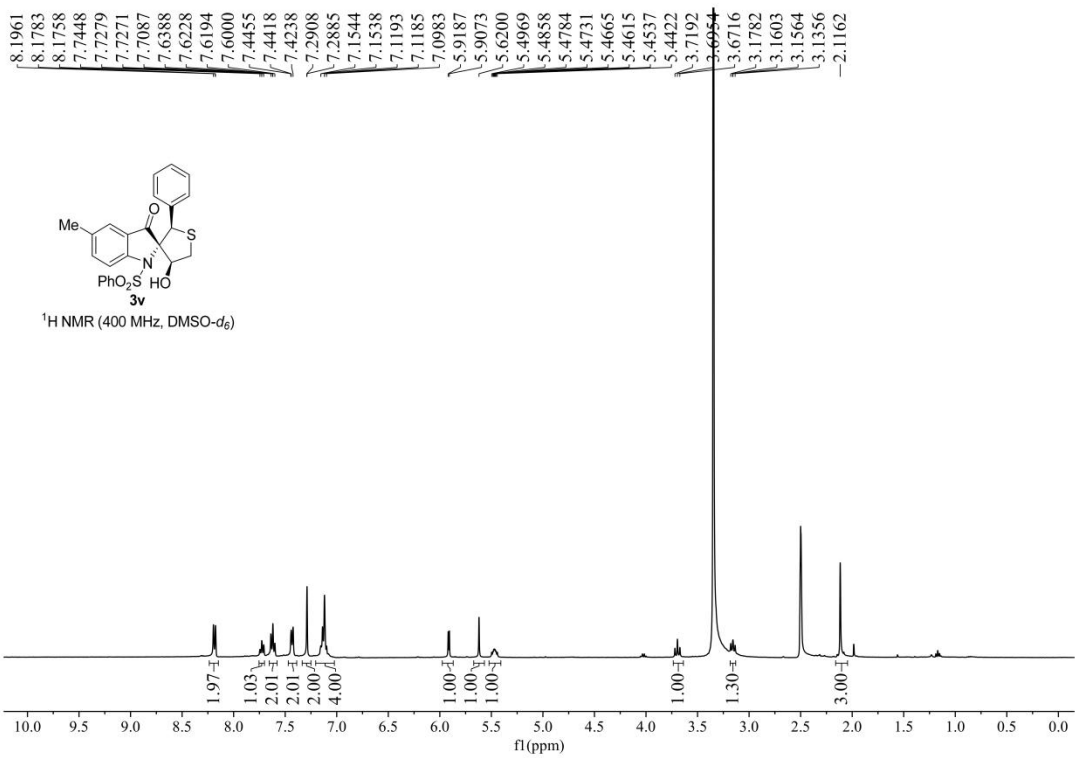


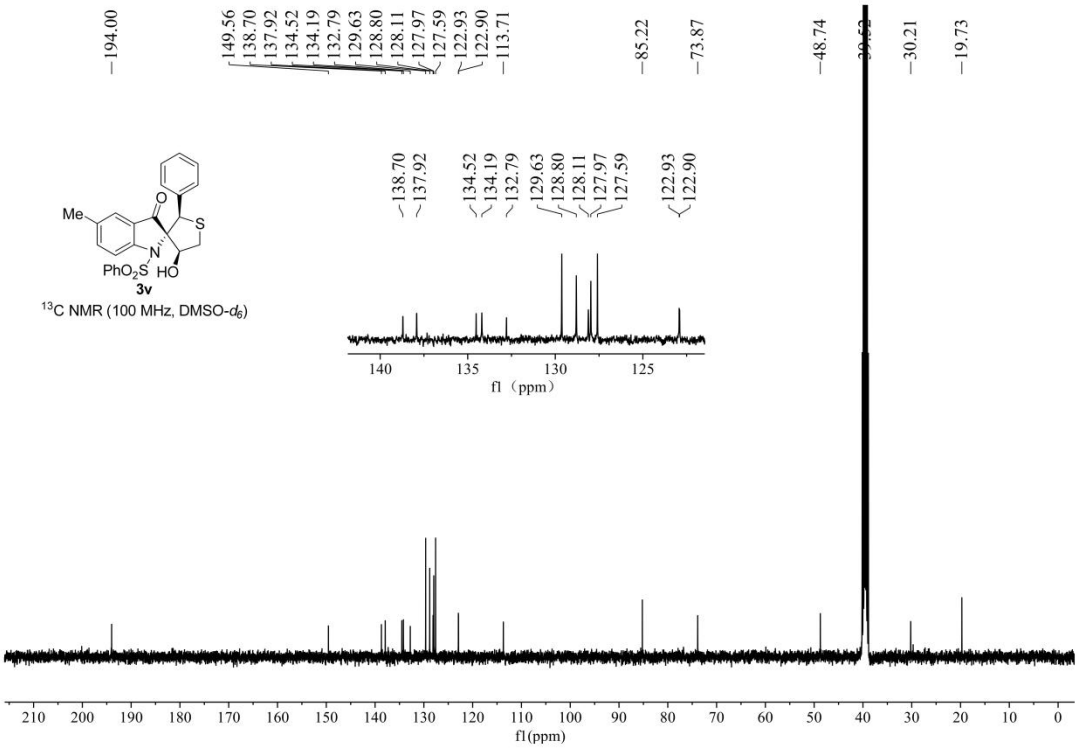
3t

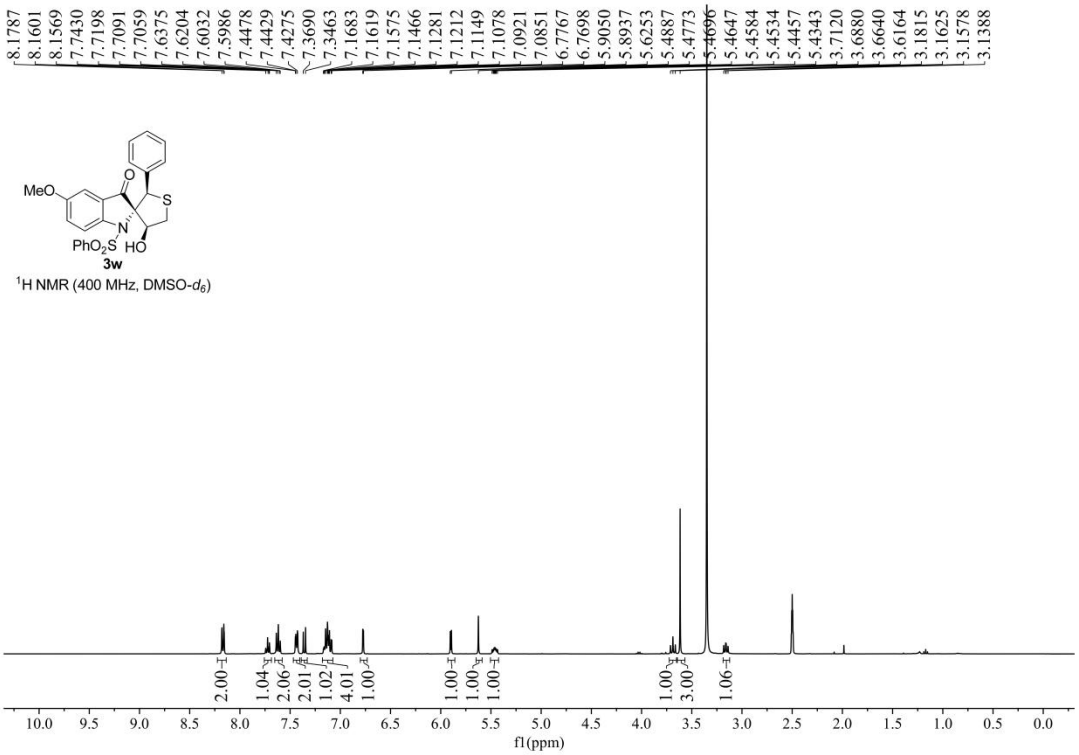
^{13}C NMR (100 MHz, DMSO-d_6)

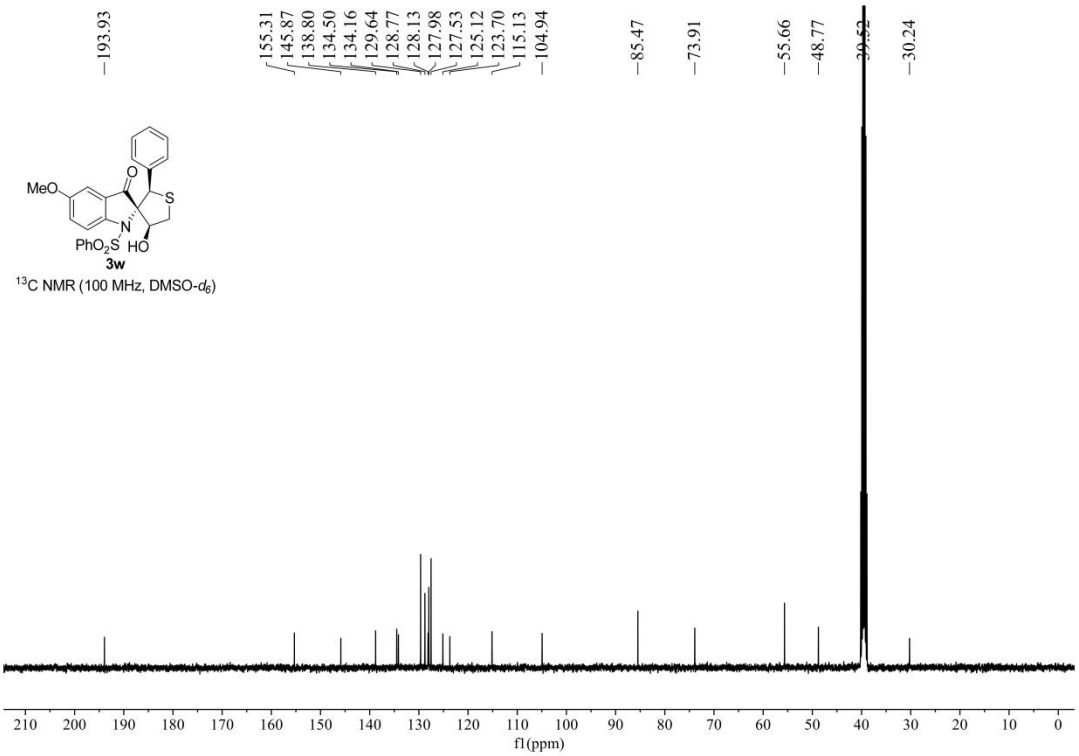

8.2019
8.2000
8.1976
8.1910
8.1878
8.1854
7.7675
7.7577
7.7551
7.7525
7.7446
7.7426
7.7407
7.6543
7.6507
7.6421
7.6398
7.6309
7.4812
7.4776
7.4251
7.4222
7.4186
7.4114
7.3970
7.1740
7.1710
7.1598
7.1562
7.1497
7.1471
7.1410
7.1383
7.1357
7.1268
6.0336
6.0261
5.6169
5.4956
5.4831
5.4798
5.4755
5.4721
3.6810
3.6650
3.6491
3.2022
3.1894
3.1864
3.1736
Br
O
S
N
PhO2S
HO
3u
1H NMR (600 MHz, DMSO-d6)
2.01
1.04
3.02
0.97
2.97
3.00
1.00
1.00
1.00
0.98
1.00
f1(ppm)

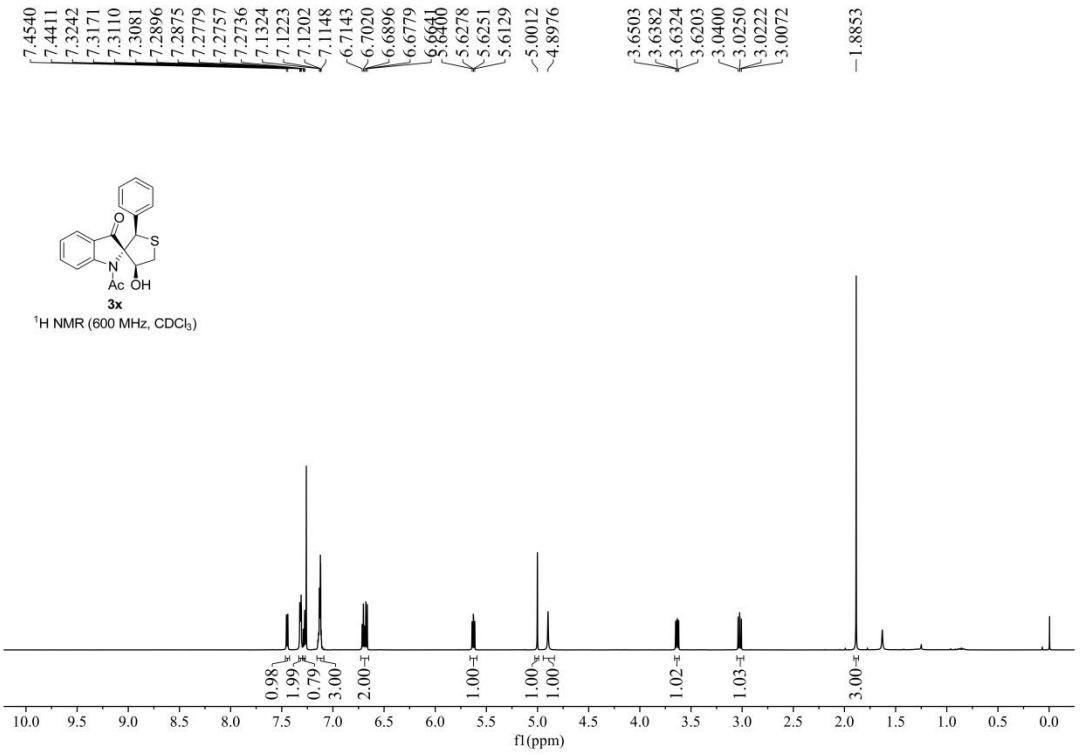

192.92
150.48
139.42
138.24
134.57
134.15
129.82
128.71
128.34
128.13
127.64
125.57
124.48
116.09
115.40
85.83
73.87
48.80
39.52
30.21
Br
O
S
N
PhO2S
HO
3u
13C NMR (150 MHz, DMSO-d6)
f1(ppm)

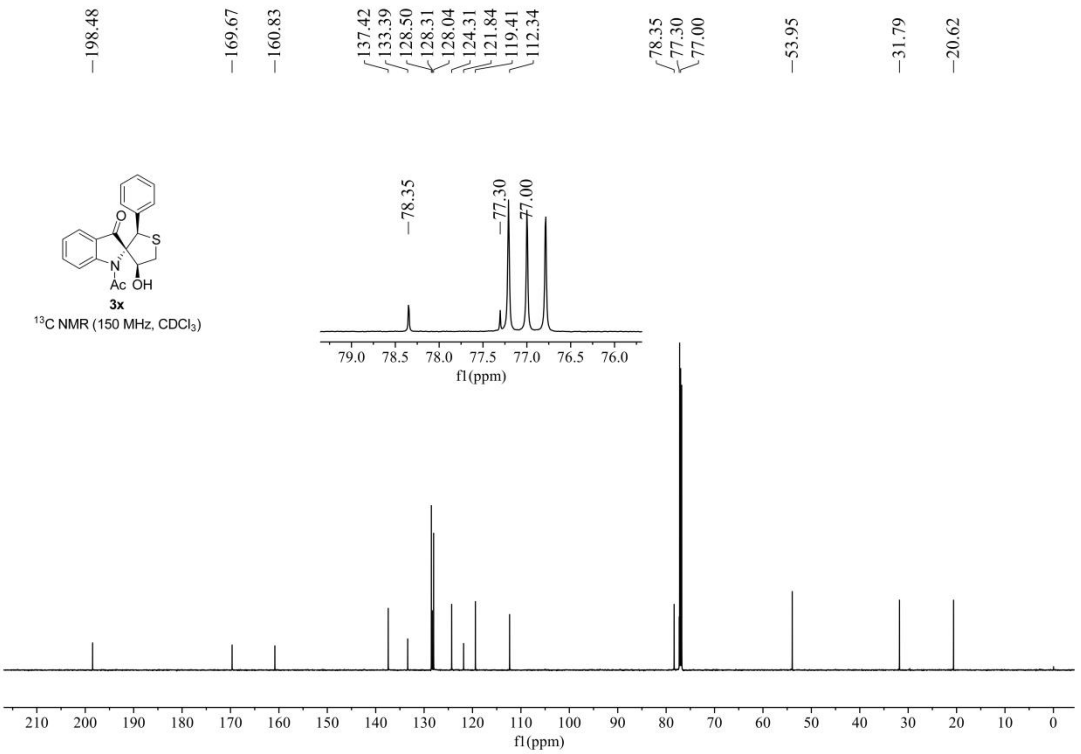

Me
O
N
S
PhO2S HO
3v
1H NMR (400 MHz, DMSO-d6)
f1(ppm)

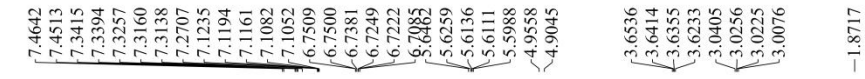

Me
O
N
S
PhO2S HO
3v
13C NMR (100 MHz, DMSO-d6)
f1(ppm)
f1 (ppm)

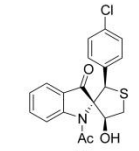

8.1787
8.1601
8.1569
7.7430
7.7198
7.7091
7.7059
7.6375
7.6204
7.6032
7.5986
7.4478
7.4429
7.4275
7.3690
7.3463
7.1683
7.1619
7.1575
7.1466
7.1281
7.1212
7.1149
7.1078
7.0921
7.0851
6.7767
6.7698
5.9050
5.8937
5.6253
5.4887
5.4773
5.4696
5.4647
5.4584
5.4534
5.4457
5.4343
3.7120
3.6880
3.6640
3.6164
3.1815
3.1625
3.1578
3.1388
MeO
O
S
N
PhO2S HO
3w
1H NMR (400 MHz, DMSO-d6)
2.00
1.04
2.06
2.01
1.02
4.01
1.00
1.00
1.00
1.00
1.00
3.00
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1(ppm)


193.93
155.31
145.87
138.80
134.50
134.16
129.64
128.77
128.13
127.98
127.53
125.12
123.70
115.13
104.94
85.47
73.91
55.66
48.77
39.52
30.24
MeO
O
S
N
PhO2S HO
3w
13C NMR (100 MHz, DMSO-d6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1(ppm)


7.4540
7.4411
7.3242
7.3171
7.3110
7.3081
7.2896
7.2875
7.2779
7.2757
7.2736
7.1324
7.1223
7.1202
7.1148
6.7143
6.7020
6.6896
6.6779
6.6641
6.6400
5.6278
5.6251
5.6129
5.0012
4.8976
3.6503
3.6382
3.6324
3.6203
3.0400
3.0250
3.0222
3.0072
1.8853
O
S
N
Ac
OH
3x
1H NMR (600 MHz, CDCl3)
0.98
1.99
0.79
3.00
2.00
1.00
1.00
1.00
1.02
1.03
3.00
f1 (ppm)

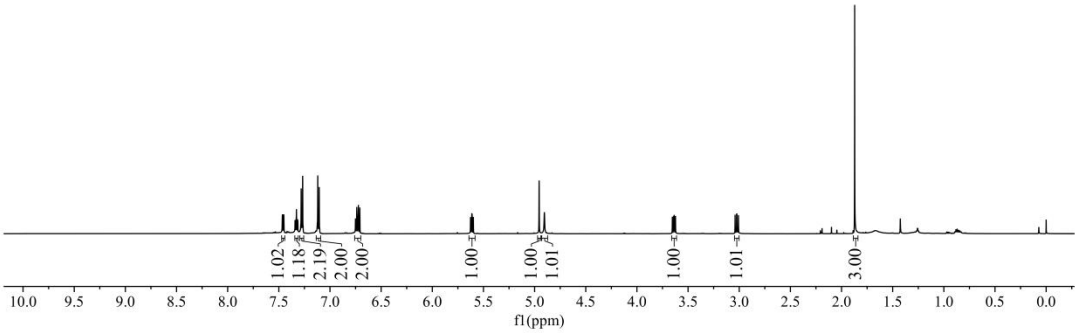

198.48
169.67
160.83
137.42
133.39
128.50
128.31
128.04
124.31
121.84
119.41
112.34
78.35
77.30
77.00
53.95
31.79
20.62
O
S
N
Ac
OH
3x
13C NMR (150 MHz, CDCl3)
78.35
77.30
77.00
f1 (ppm)

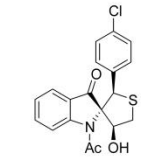




3y

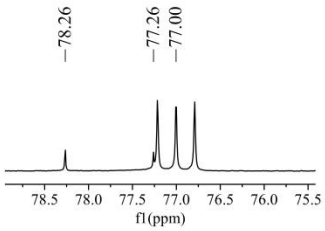
^{1}H NMR (600 MHz, $CDCl_3$)

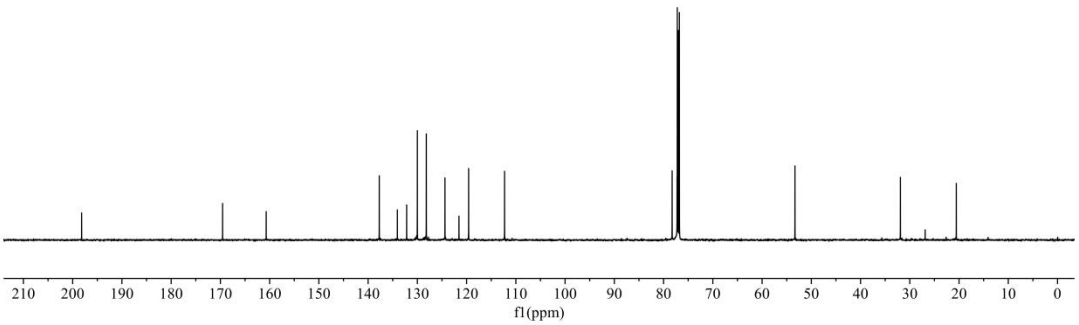


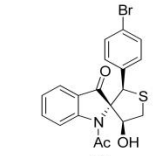


3y

^{13}C NMR (150 MHz, $CDCl_3$)

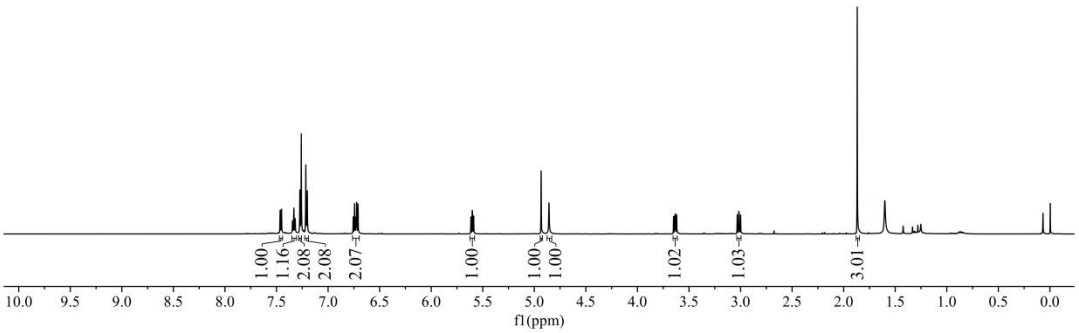


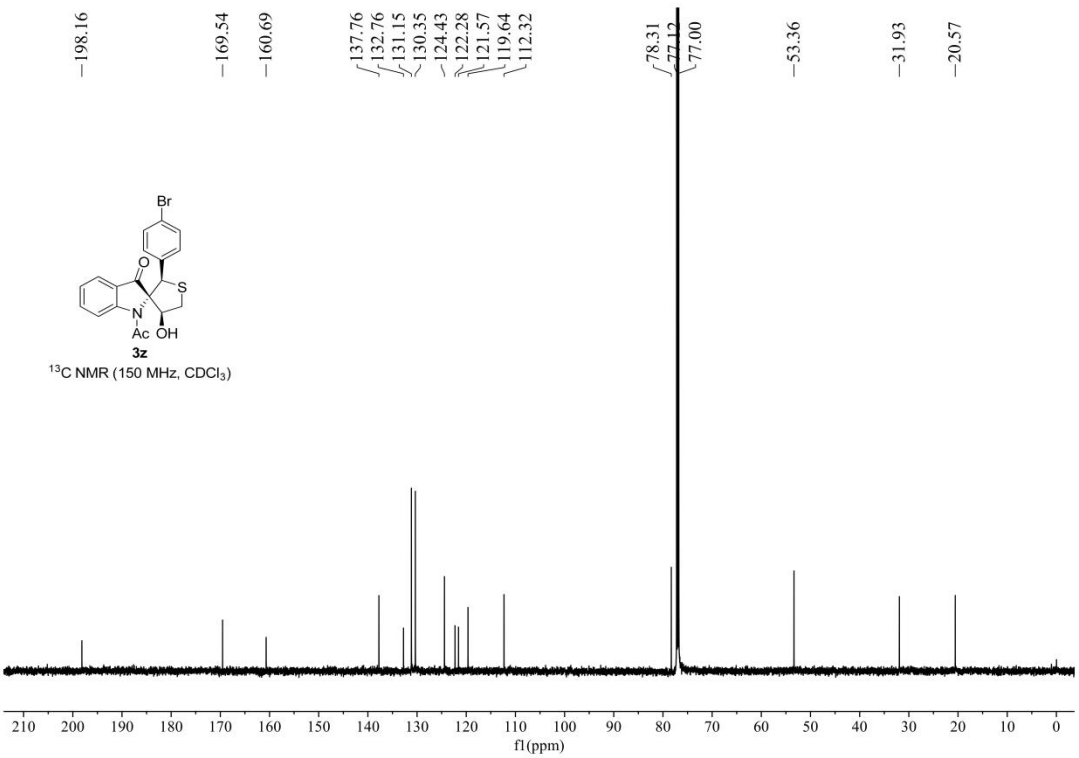




3z

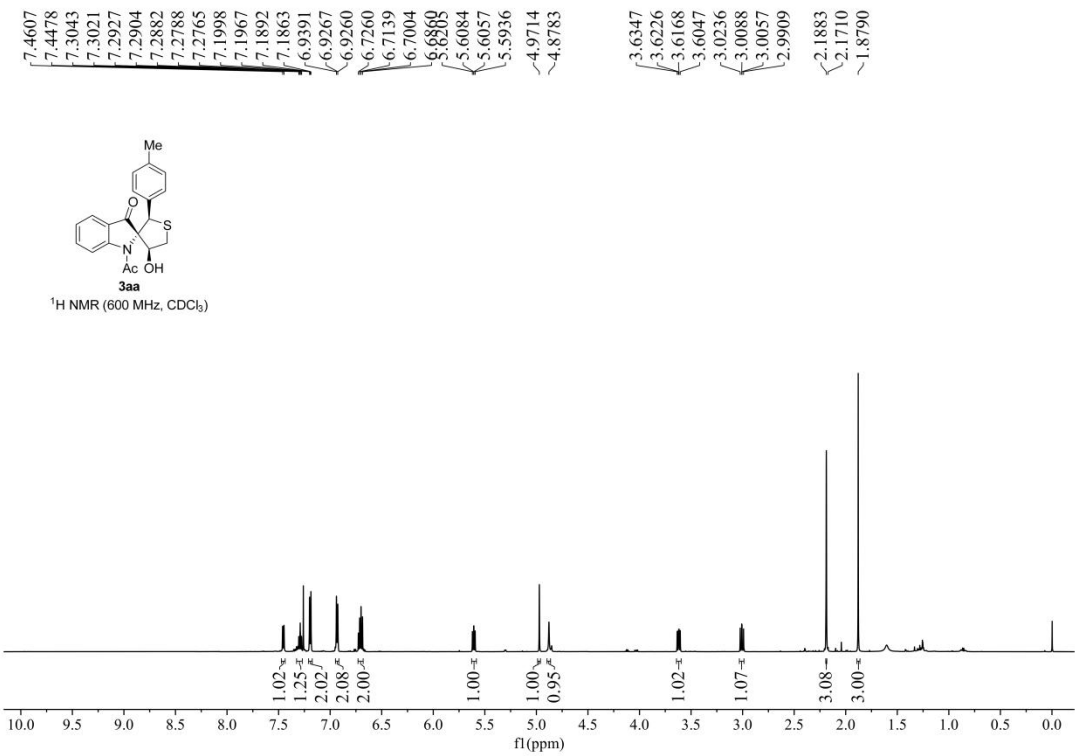
^{1}H NMR (600 MHz, $CDCl_3$)

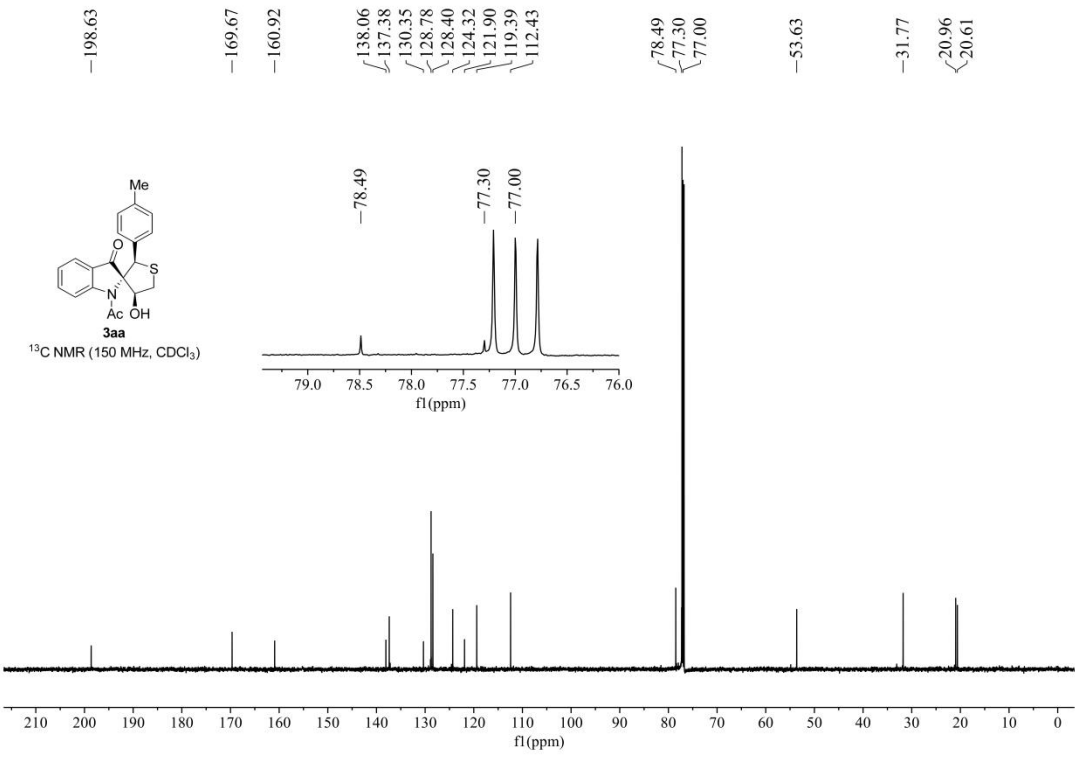


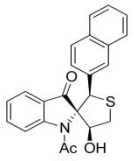


3z

^{13}C NMR (150 MHz, $CDCl_3$)

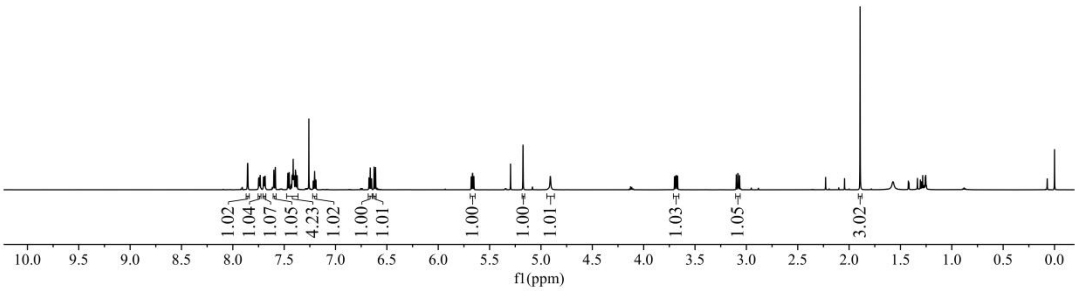

7.4607
7.4478
7.3043
7.3021
7.2927
7.2904
7.2882
7.2788
7.2765
7.1998
7.1967
7.1892
7.1863
6.9391
6.9267
6.9260
6.7260
6.7139
6.7004
5.6084
5.6057
5.5936
4.9714
4.8783
3.6347
3.6226
3.6168
3.6047
3.0236
3.0088
3.0057
2.9909
2.1883
2.1710
1.8790
Me
O
S
N
Ac OH
3aa
1H NMR (600 MHz, CDCl3)
1.02
1.25
2.02
2.08
2.00
1.00
1.00
0.95
1.02
1.07
3.08
3.00
f1(ppm)

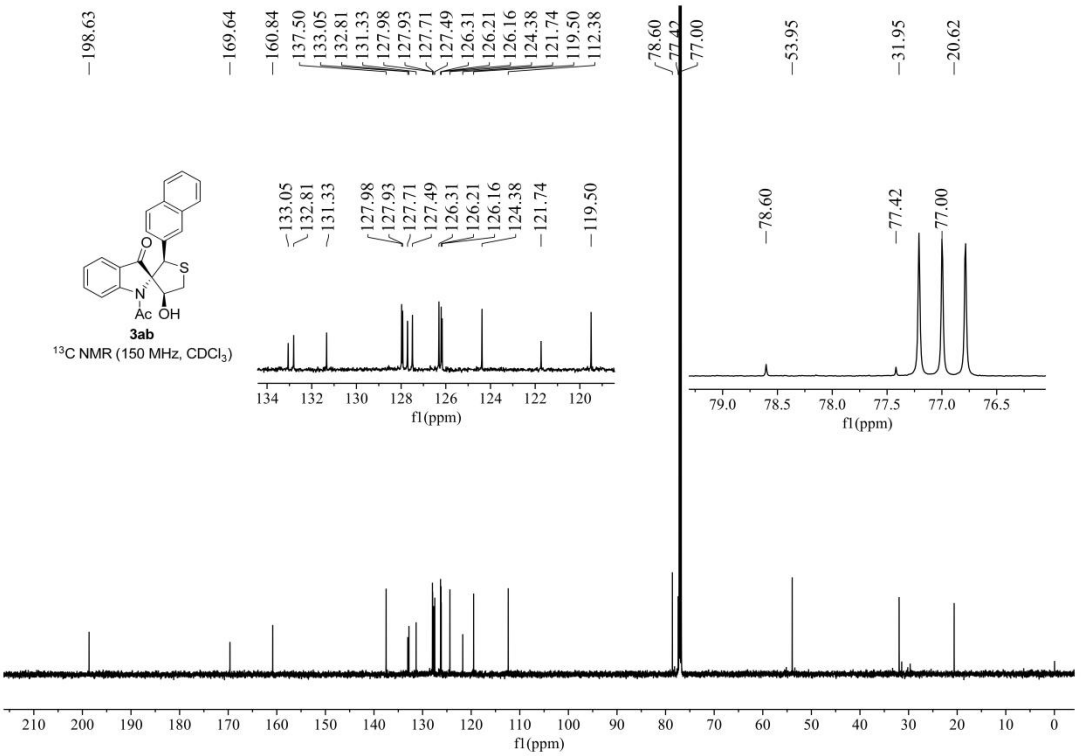

198.63
169.67
160.92
138.06
137.38
130.35
128.78
128.40
124.32
121.90
119.39
112.43
78.49
77.30
77.00
53.63
31.77
20.96
20.61
Me
O
S
N
Ac OH
3aa
13C NMR (150 MHz, CDCl3)
f1(ppm)



3ab

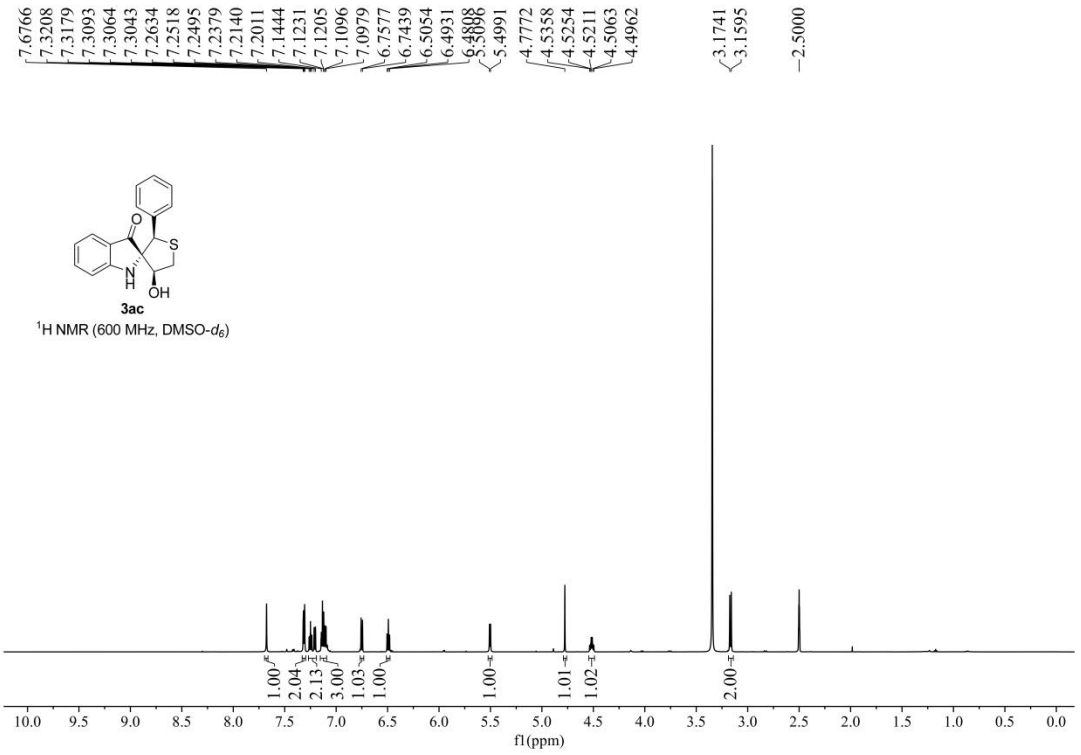
^{1}H NMR (600 MHz, $CDCl_3$)

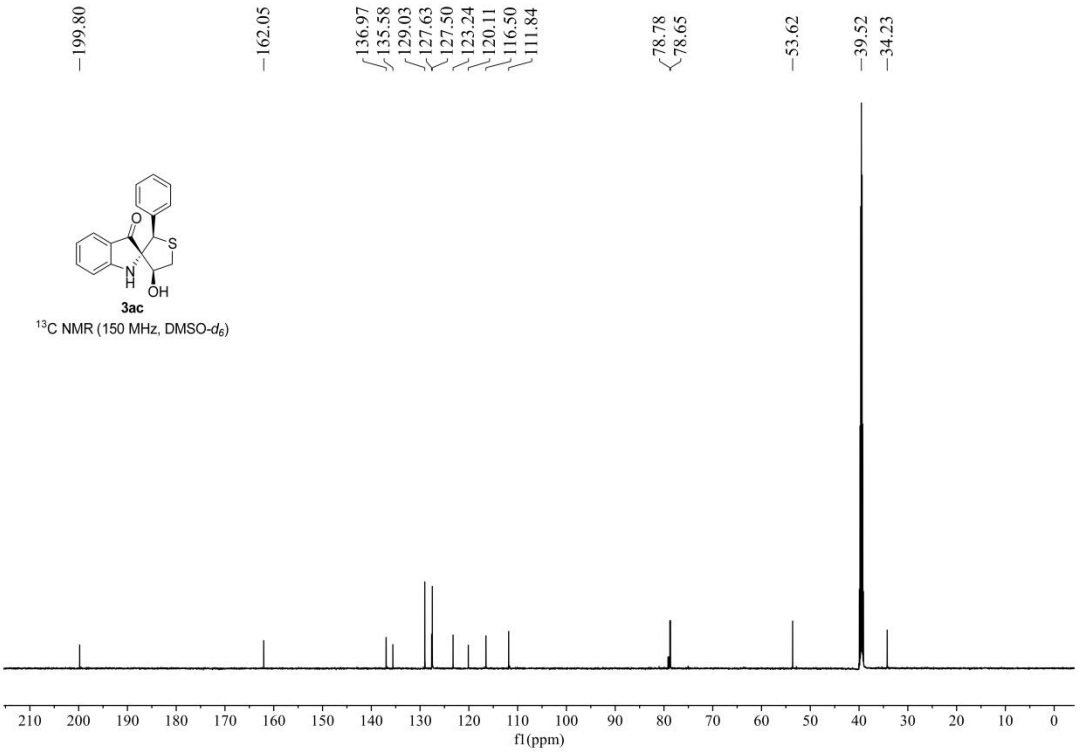


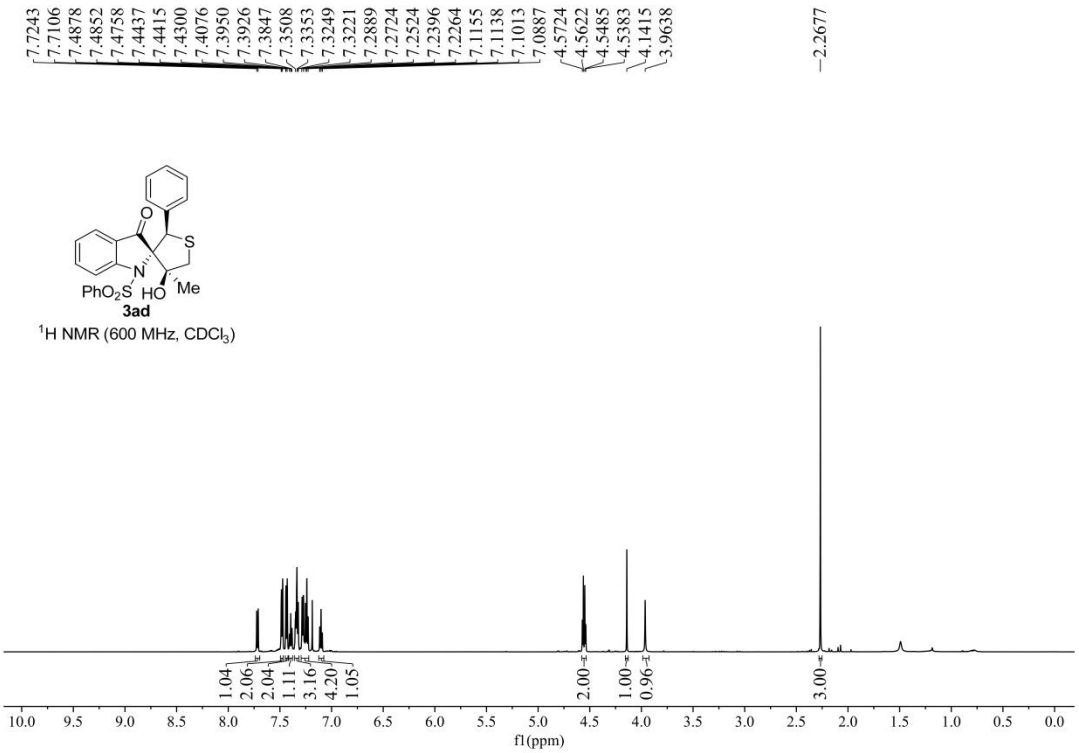


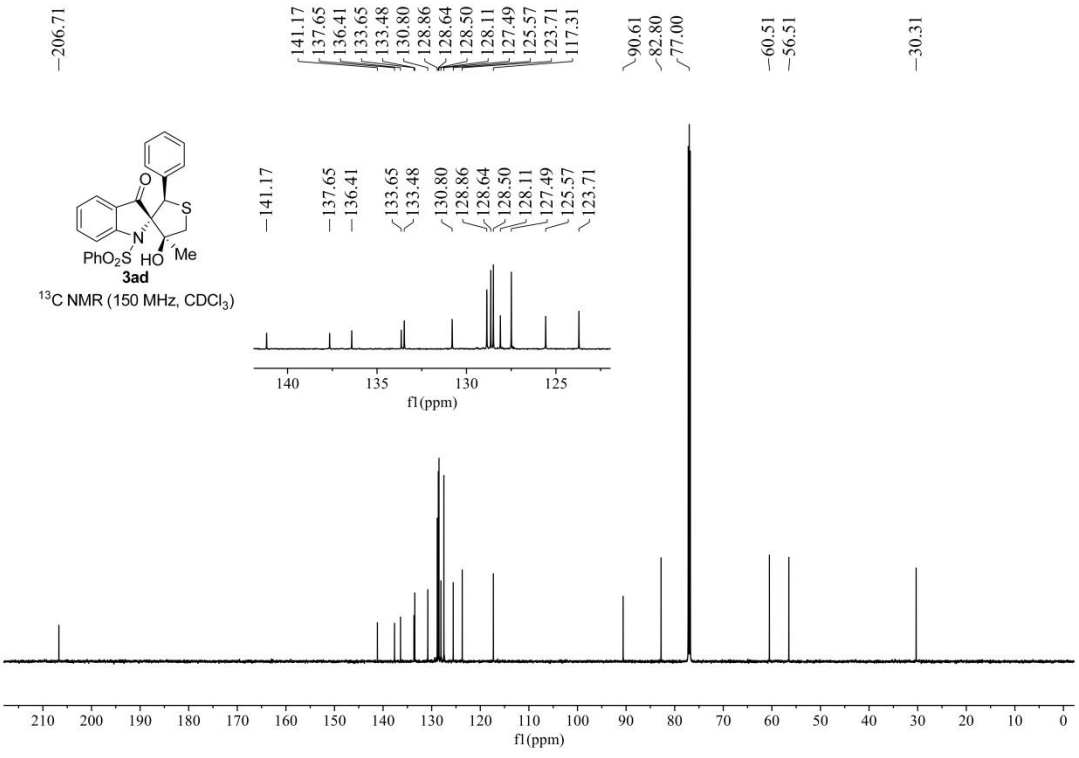
3ab

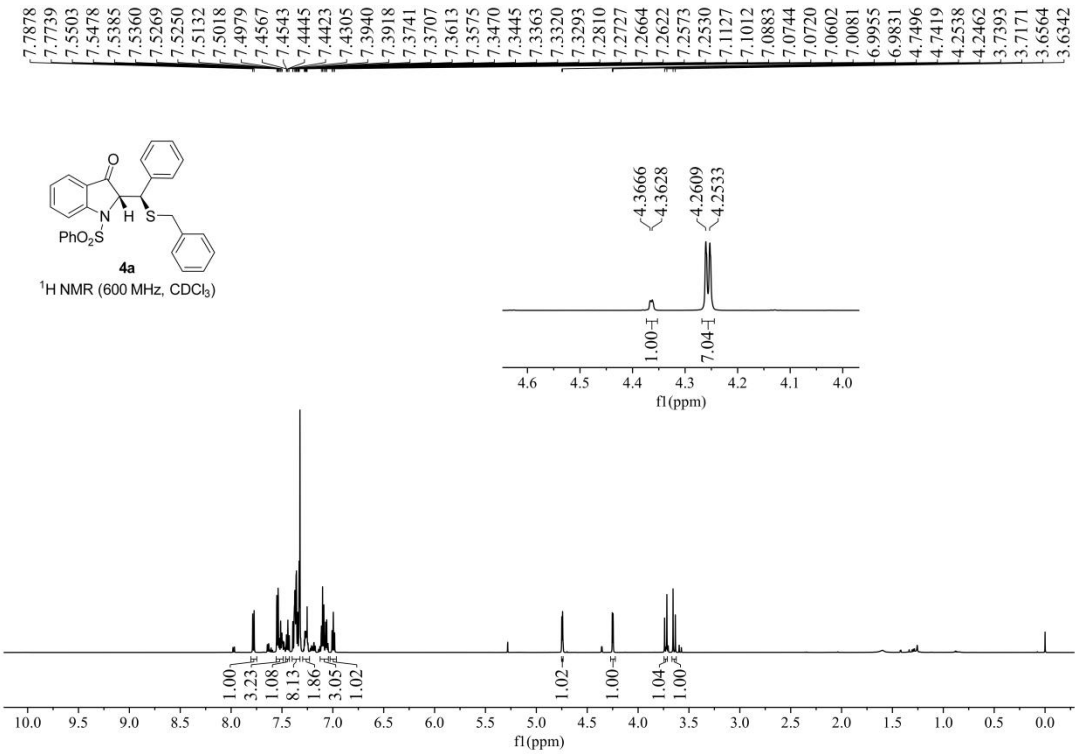
^{13}C NMR (150 MHz, $CDCl_3$)

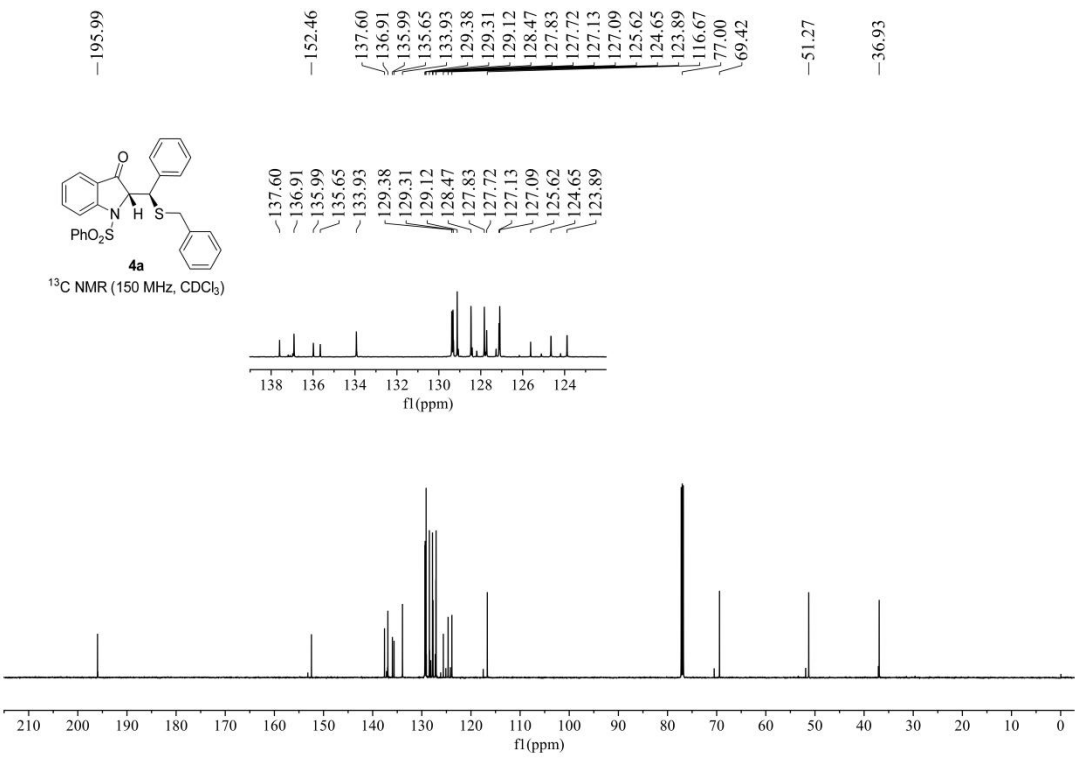

7.6766
7.3208
7.3179
7.3093
7.3064
7.3043
7.2634
7.2518
7.2495
7.2379
7.2140
7.2011
7.1444
7.1231
7.1205
7.1096
7.0979
6.7577
6.7439
6.5054
6.4931
5.4991
4.7772
4.5358
4.5254
4.5211
4.5063
4.4962
3.1741
3.1595
2.5000
O
S
N
H
OH
3ac
1H NMR (600 MHz, DMSO-d6)
1.00
2.04
2.13
3.00
1.03
1.00
1.00
1.01
1.02
2.00
f1(ppm)

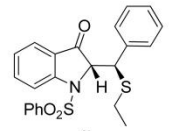

199.80
162.05
136.97
135.58
129.03
127.63
127.50
123.24
120.11
116.50
111.84
78.78
78.65
53.62
39.52
34.23
O
S
N
H
OH
3ac
13C NMR (150 MHz, DMSO-d6)
f1(ppm)


7.7243
7.7106
7.4878
7.4852
7.4758
7.4437
7.4415
7.4300
7.4076
7.3950
7.3926
7.3847
7.3508
7.3353
7.3249
7.3221
7.2889
7.2724
7.2524
7.2396
7.2264
7.1155
7.1138
7.1013
7.0887
4.5724
4.5622
4.5485
4.5383
4.1415
3.9638
2.2677
O
S
N
PhO2S HO
Me
3ad
1H NMR (600 MHz, CDCl3)
1.04
2.06
2.04
1.11
3.16
4.20
1.05
2.00
1.00
0.96
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


206.71
141.17
137.65
136.41
133.65
133.48
130.80
128.86
128.64
128.50
128.11
127.49
125.57
123.71
117.31
90.61
82.80
77.00
60.51
56.51
30.31
O
S
N
PhO2S HO
Me
3ad
13C NMR (150 MHz, CDCl3)
140 135 130 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

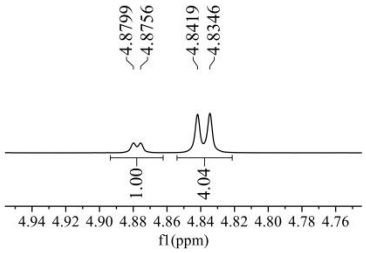

4a
1H NMR (600 MHz, CDCl3)
fl(ppm)

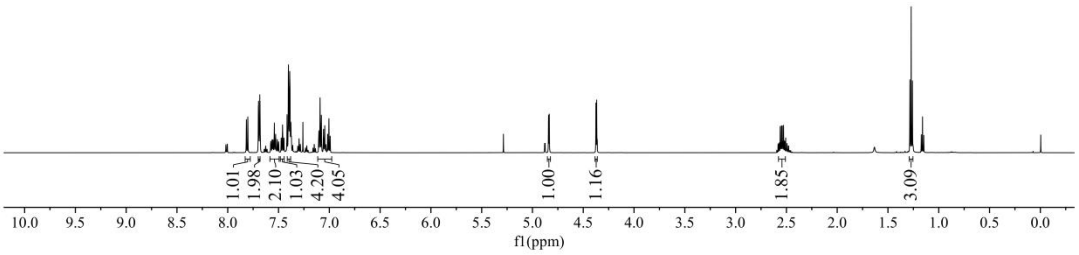

4a
13C NMR (150 MHz, CDCl3)
fl(ppm)

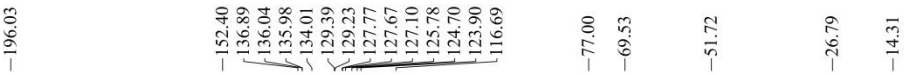


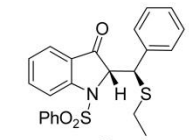
4b

^{1}H NMR (600 MHz, $CDCl_3$)



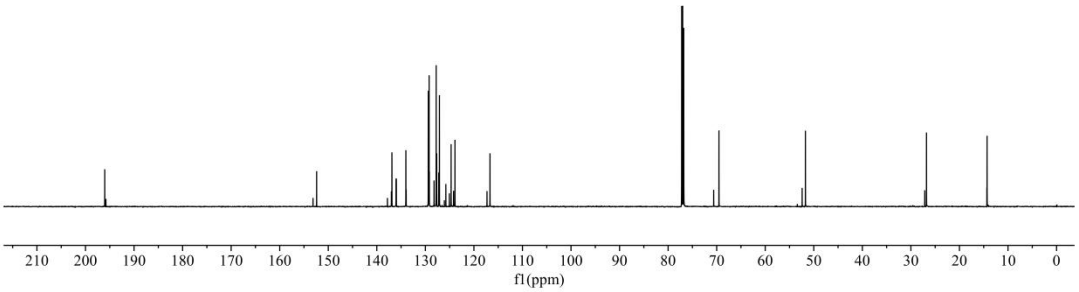


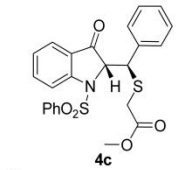




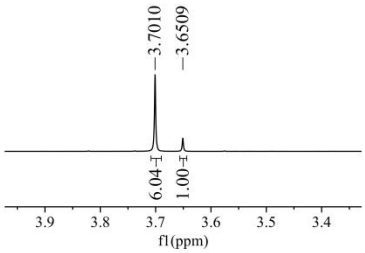
4b

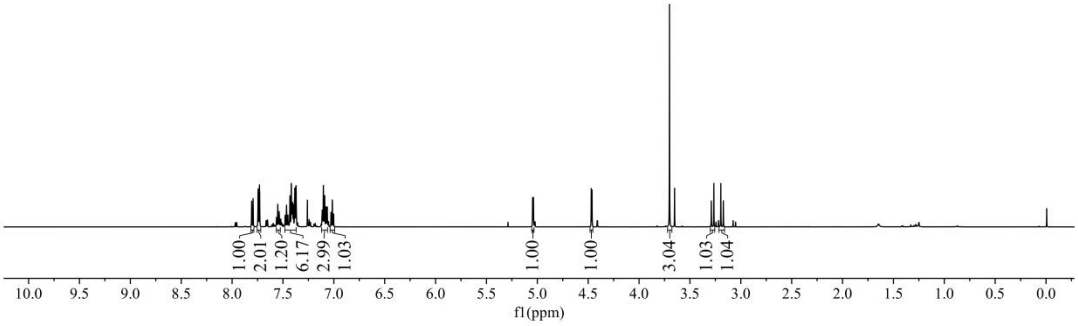
^{13}C NMR (150 MHz, $CDCl_3$)

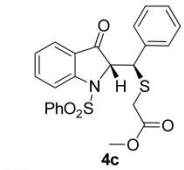




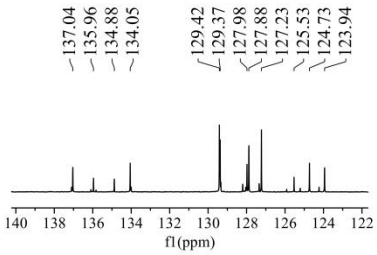
^{1}H NMR (600 MHz, $CDCl_3$)

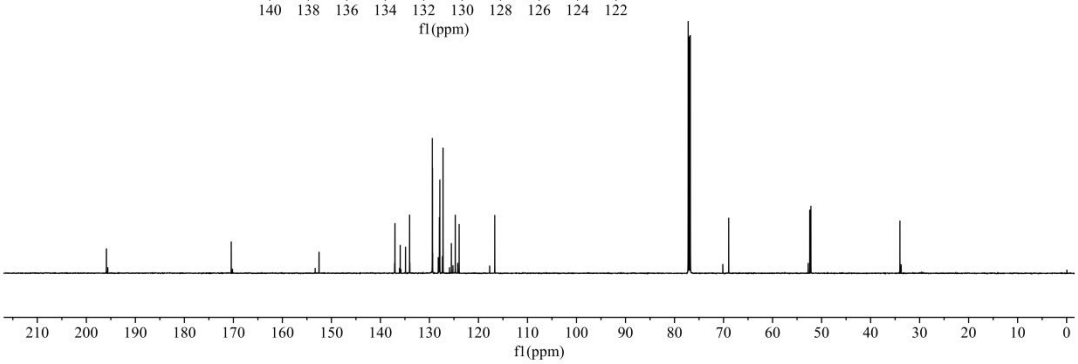


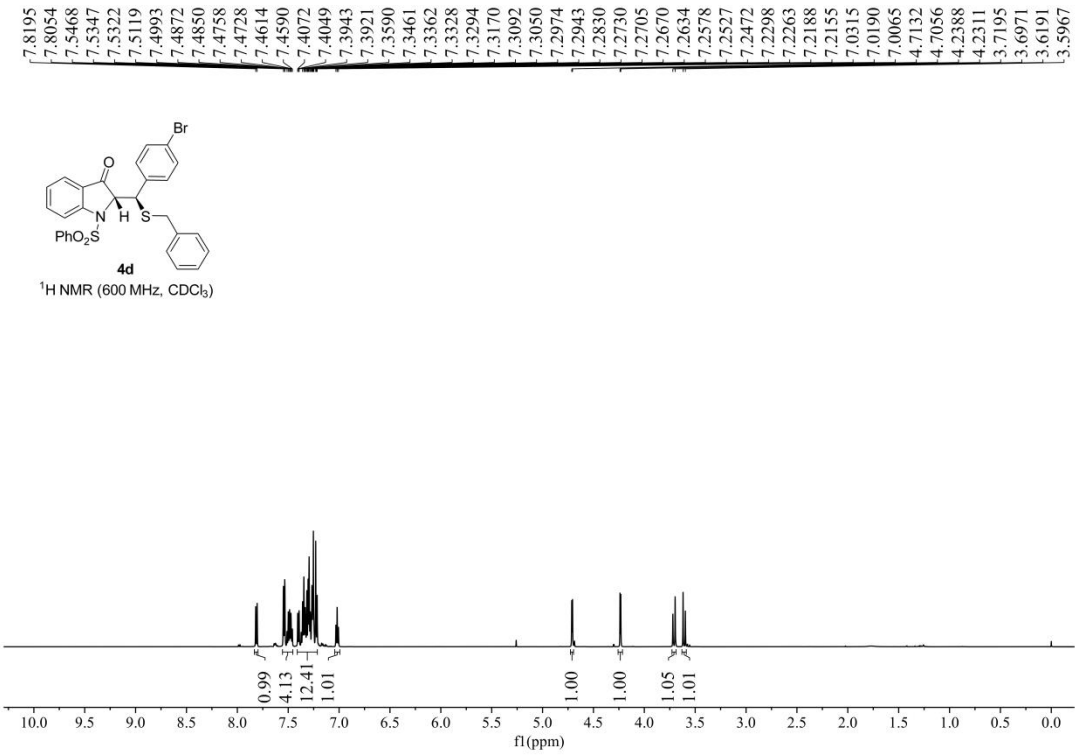


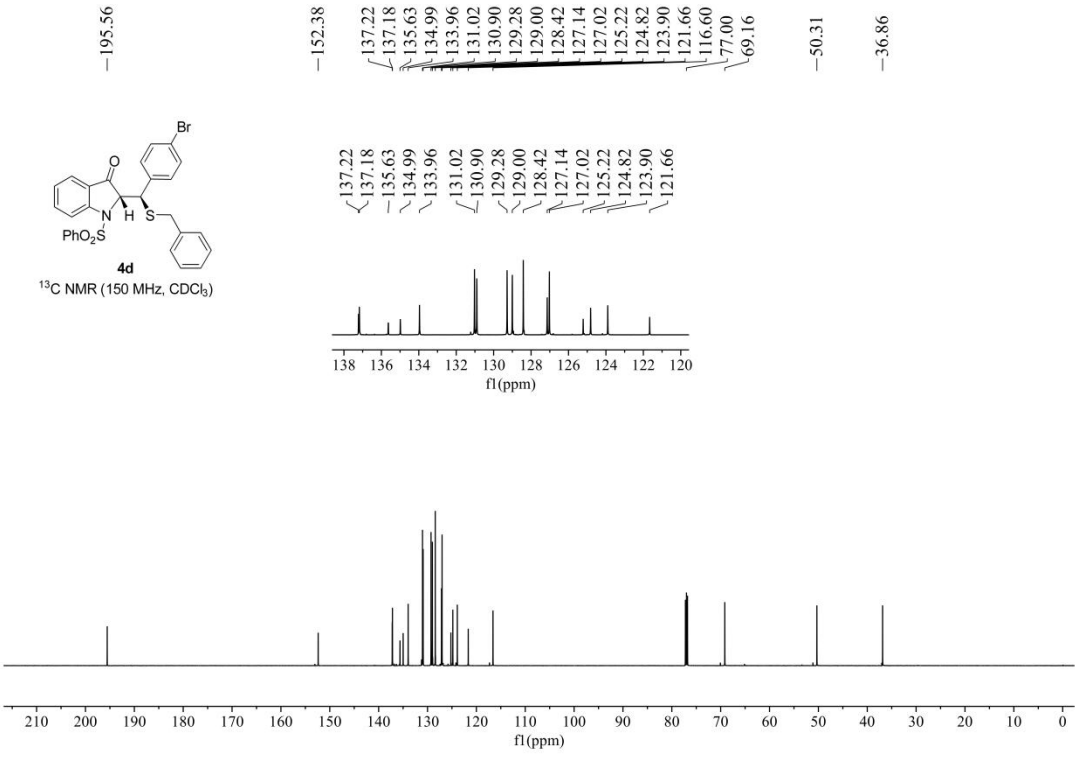


^{13}C NMR (150 MHz, $CDCl_3$)

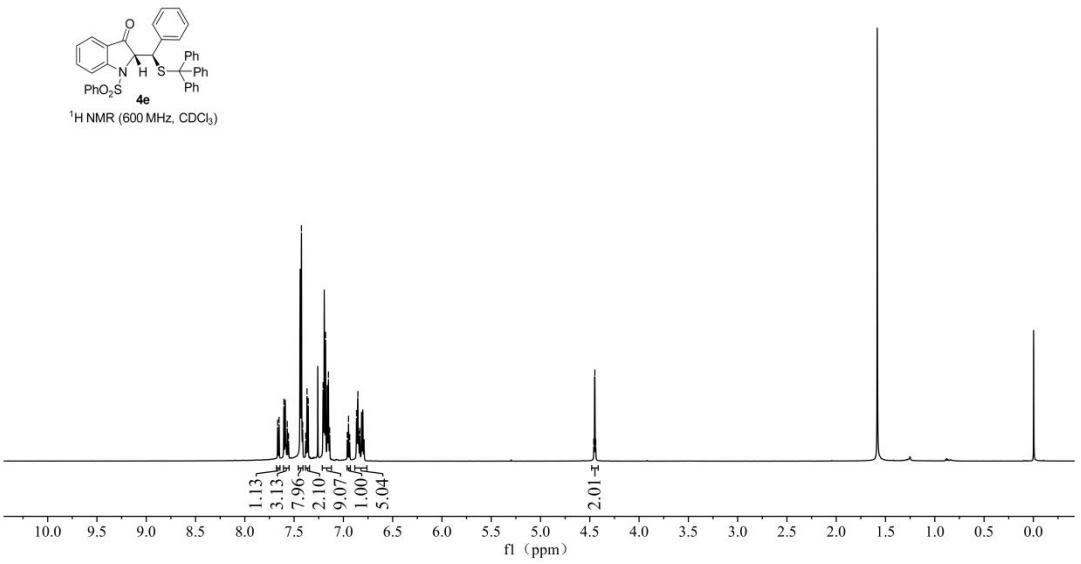


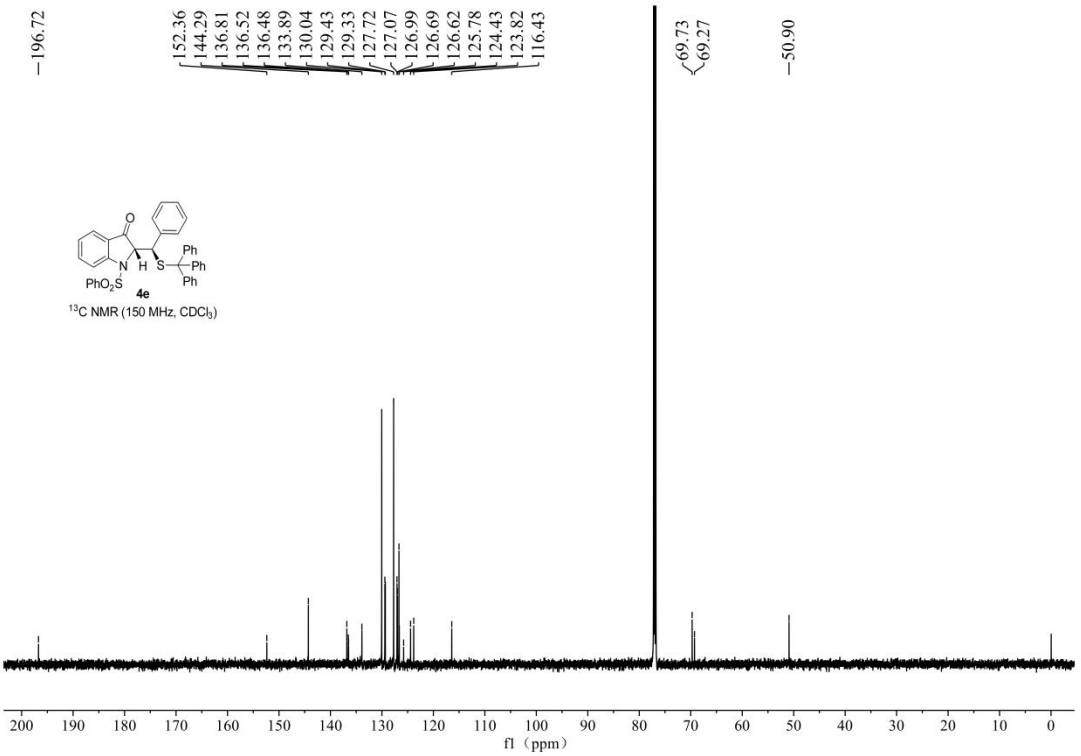


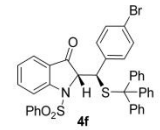

7.8195
7.8054
7.5468
7.5347
7.5322
7.5119
7.4993
7.4872
7.4850
7.4758
7.4728
7.4614
7.4590
7.4072
7.4049
7.3943
7.3921
7.3590
7.3461
7.3362
7.3328
7.3294
7.3170
7.3092
7.3050
7.2974
7.2943
7.2830
7.2730
7.2705
7.2670
7.2634
7.2578
7.2527
7.2472
7.2298
7.2263
7.2188
7.2155
7.0315
7.0190
7.0065
4.7132
4.7056
4.2388
4.2311
3.7195
3.6971
3.6191
3.5967
Br
O
N
H
S
PhO2S
4d
1H NMR (600 MHz, CDCl3)
0.99
4.13
12.41
1.01
1.00
1.00
1.05
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1(ppm)


195.56
152.38
137.22
137.18
135.63
134.99
133.96
131.02
130.90
129.28
129.00
128.42
127.14
127.02
125.22
124.82
123.90
121.66
116.60
77.00
69.16
50.31
36.86
Br
O
N
H
S
PhO2S
4d
13C NMR (150 MHz, CDCl3)
138 136 134 132 130 128 126 124 122 120
f1(ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1(ppm)

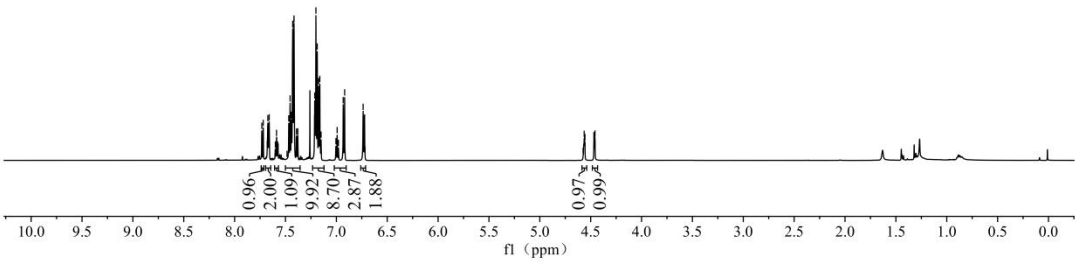

7.6666
7.6521
7.6031
7.5690
7.5565
7.4409
7.4314
7.4256
7.4132
7.3814
7.3694
7.3568
7.2057
7.1942
7.1809
7.1515
7.1393
6.9604
6.9479
6.9355
6.8664
6.8528
6.8337
6.8055
6.7892
4.4596
4.4517
4.4485
4.4398

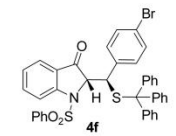

4e
1H NMR (600 MHz, CDCl3)
1.13
3.13
7.96
2.10
9.07
1.00
5.04
2.01
f1 (ppm)


196.72
152.36
144.29
136.81
136.52
136.48
133.89
130.04
129.43
129.33
127.72
127.07
126.99
126.69
126.62
125.78
124.43
123.82
116.43
69.73
69.27
50.90
4e
13C NMR (150 MHz, CDCl3)
f1 (ppm)

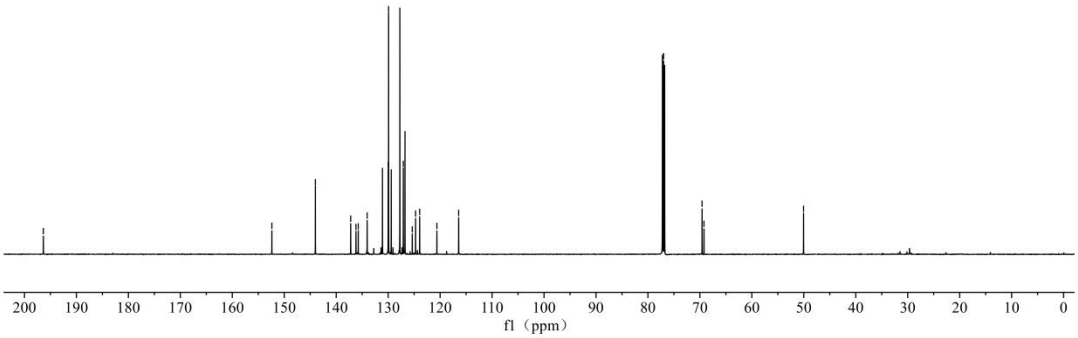


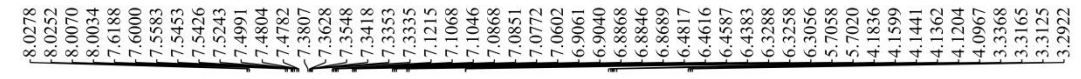
^{1}H NMR (600 MHz, $CDCl_3$)

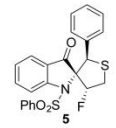




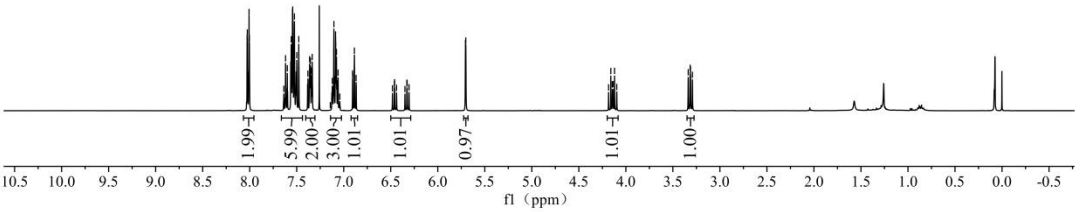
^{13}C NMR (150 MHz, $CDCl_3$)

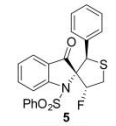




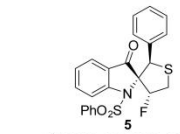


^{1}H NMR (400 MHz, $CDCl_3$)



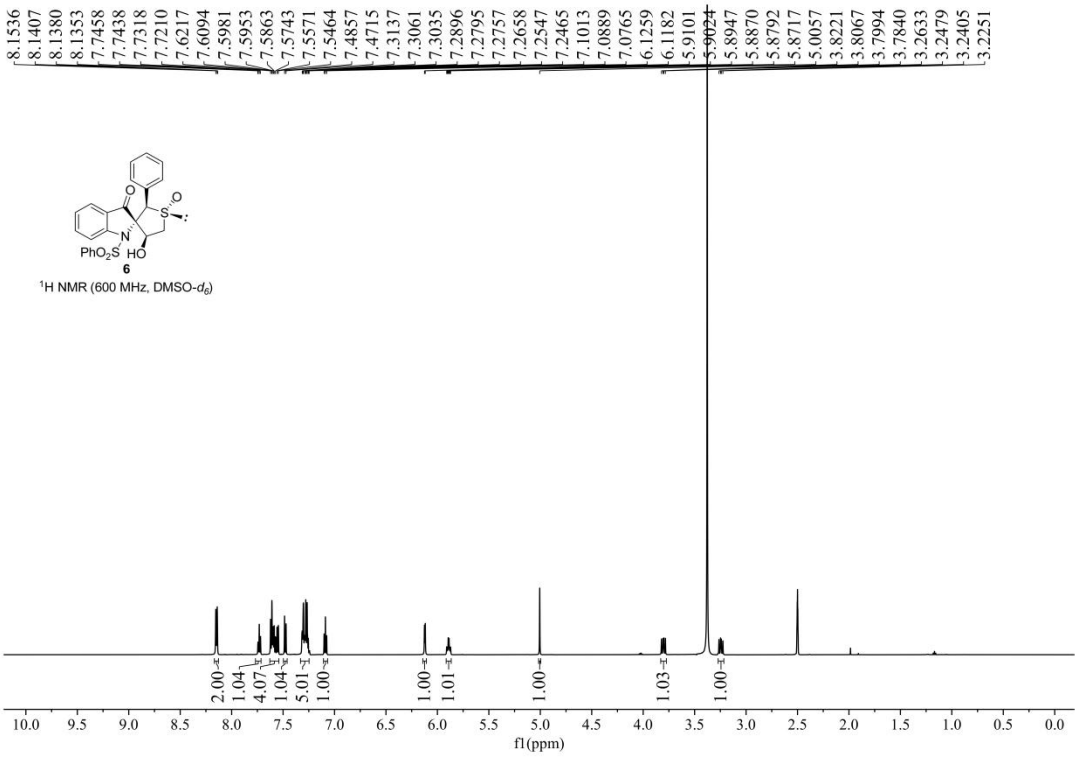


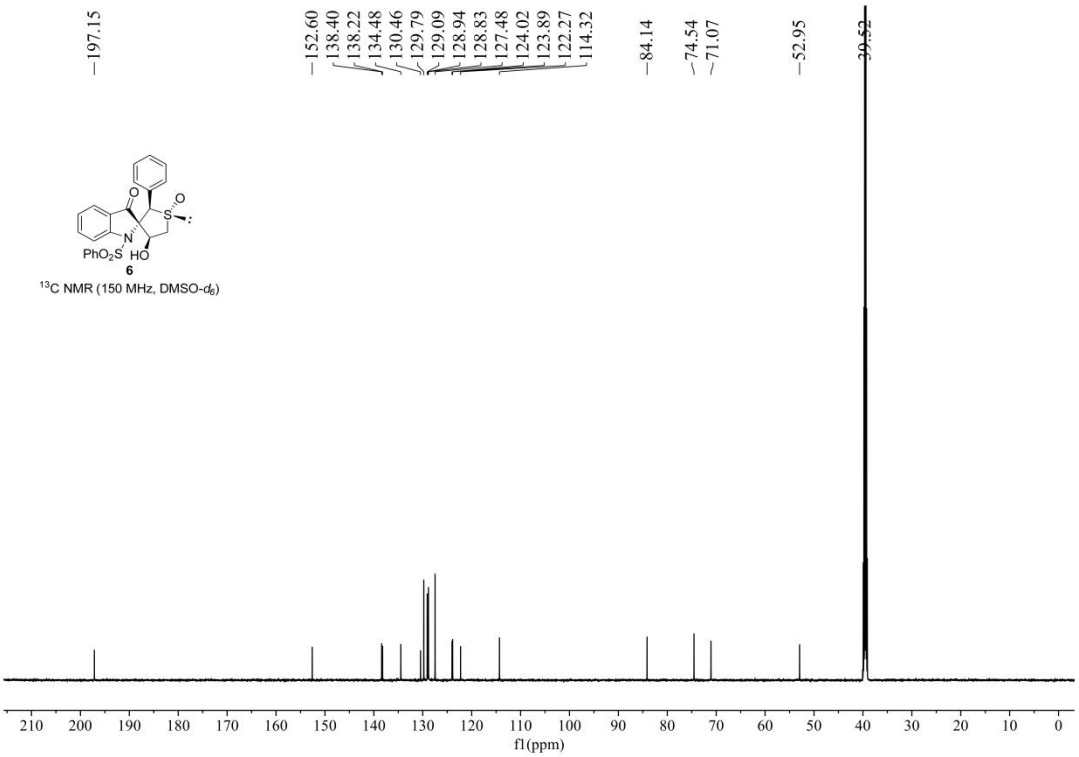
^{13}C NMR (100 MHz, $CDCl_3$)

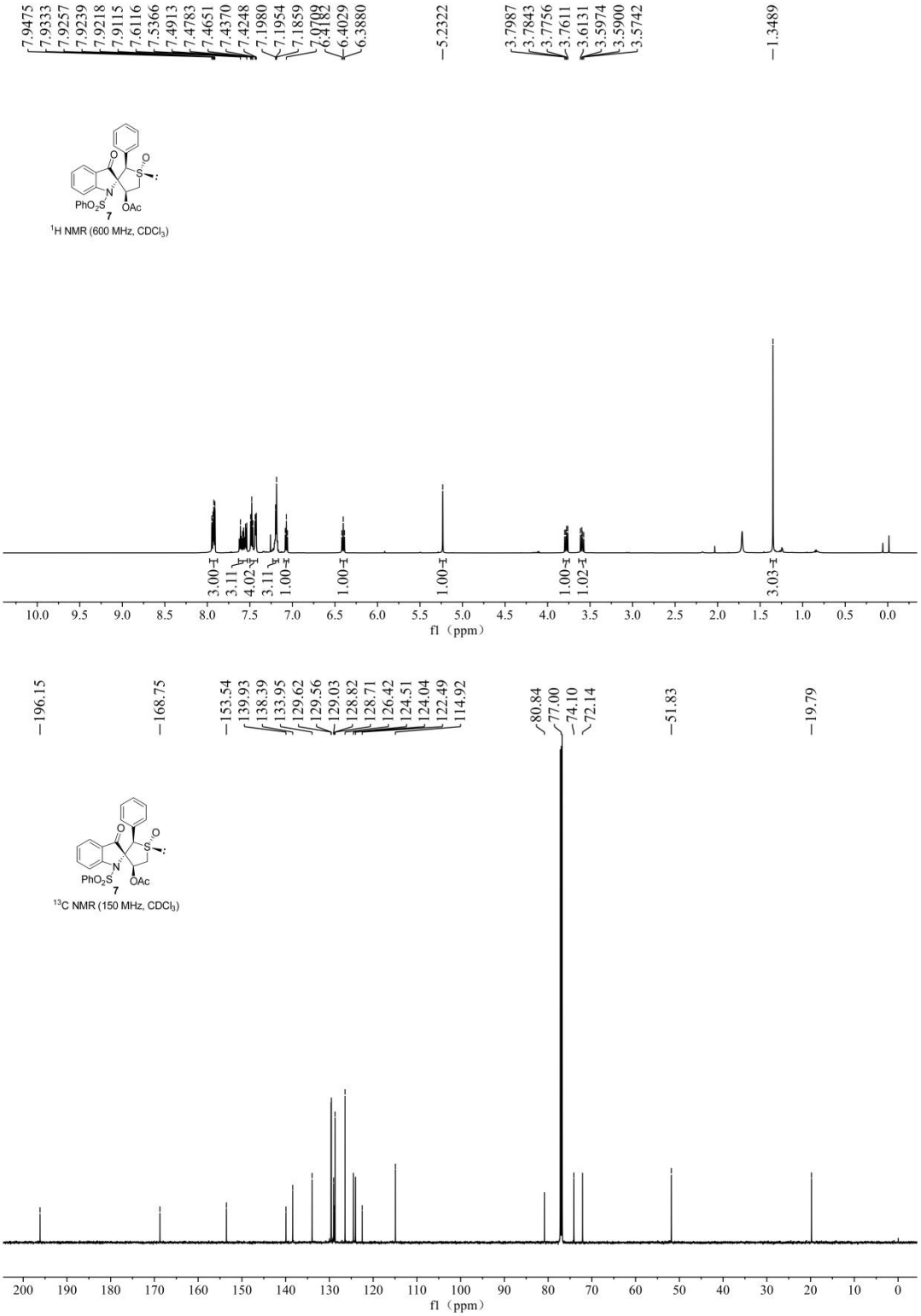


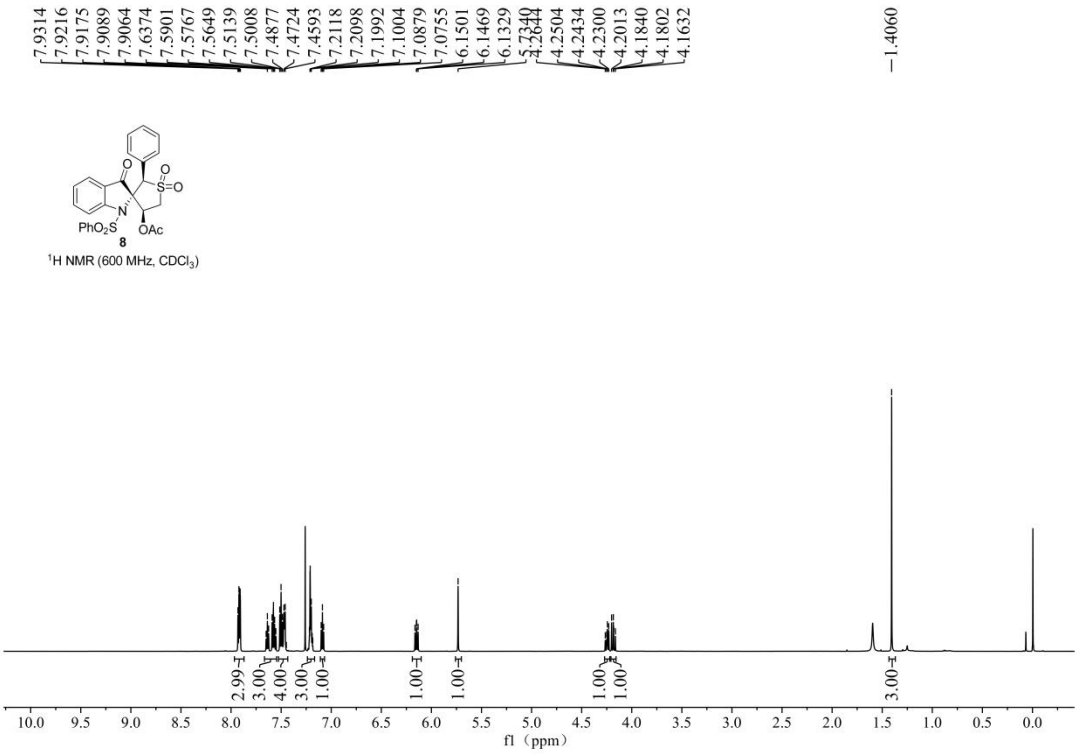
5

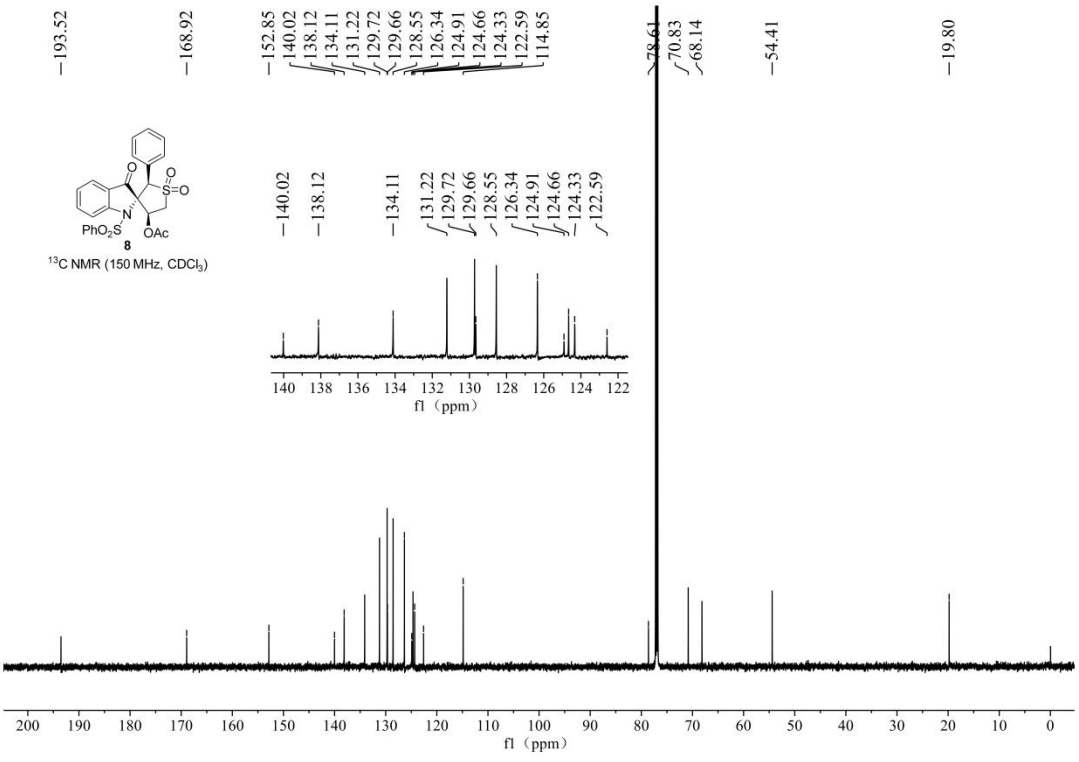
^{19}F NMR (377 MHz, $CDCl_3$)

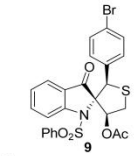

8.1536
8.1407
8.1380
8.1353
7.7458
7.7438
7.7318
7.7210
7.6217
7.6094
7.5981
7.5953
7.5863
7.5743
7.5571
7.5464
7.4857
7.4715
7.3137
7.3061
7.3035
7.2896
7.2795
7.2757
7.2658
7.2547
7.2465
7.1013
7.0889
7.0765
6.1259
6.1182
5.9101
5.9024
5.8947
5.8870
5.8792
5.8717
5.0057
3.8221
3.8067
3.7994
3.7840
3.2633
3.2479
3.2405
3.2251
PhO2S HO
6
1H NMR (600 MHz, DMSO-d6)
2.00
1.04
4.07
1.04
5.01
1.00
1.00
1.01
1.00
1.03
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1(ppm)


197.15
152.60
138.40
138.22
134.48
130.46
129.79
129.09
128.94
128.83
127.48
124.02
123.89
122.27
114.32
84.14
74.54
71.07
52.95
39.52
PhO2S HO
6
13C NMR (150 MHz, DMSO-d6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1(ppm)

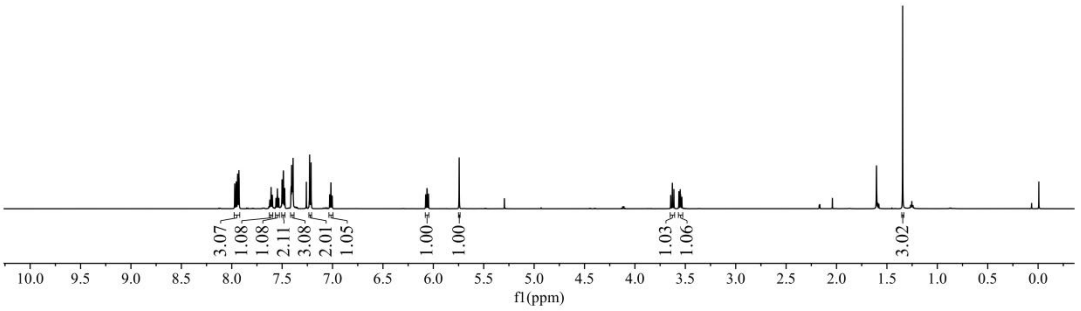

7.9475
7.9333
7.9257
7.9239
7.9218
7.9115
7.6116
7.5366
7.4913
7.4783
7.4651
7.4370
7.4248
7.1980
7.1954
7.1859
7.0709
6.4182
6.4029
6.3880
5.2322
3.7987
3.7843
3.7756
3.7611
3.6131
3.5974
3.5900
3.5742
1.3489
PhO2S
OAc
7
1H NMR (600 MHz, CDCl3)
3.00
3.11
4.02
3.11
1.00
1.00
1.00
1.00
1.02
3.03
f1 (ppm)
196.15
168.75
153.54
139.93
138.39
133.95
129.62
129.56
129.03
128.82
128.71
126.42
124.51
124.04
122.49
114.92
80.84
77.00
74.10
72.14
51.83
19.79
PhO2S
OAc
7
13C NMR (150 MHz, CDCl3)
f1 (ppm)

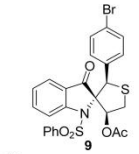

7.9314
7.9216
7.9175
7.9089
7.9064
7.6374
7.5901
7.5767
7.5649
7.5139
7.5008
7.4877
7.4724
7.4593
7.2118
7.2098
7.1992
7.1004
7.0879
7.0755
6.1501
6.1469
6.1329
5.7340
4.2644
4.2504
4.2434
4.2300
4.2013
4.1840
4.1802
4.1632
1.4060
PhO2S
OAc
8
1H NMR (600 MHz, CDCl3)
2.99
3.00
4.00
3.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)


193.52
168.92
152.85
140.02
138.12
134.11
131.22
129.72
129.66
128.55
126.34
124.91
124.66
124.33
122.59
114.85
78.61
70.83
68.14
54.41
19.80
PhO2S
OAc
8
13C NMR (150 MHz, CDCl3)
f1 (ppm)

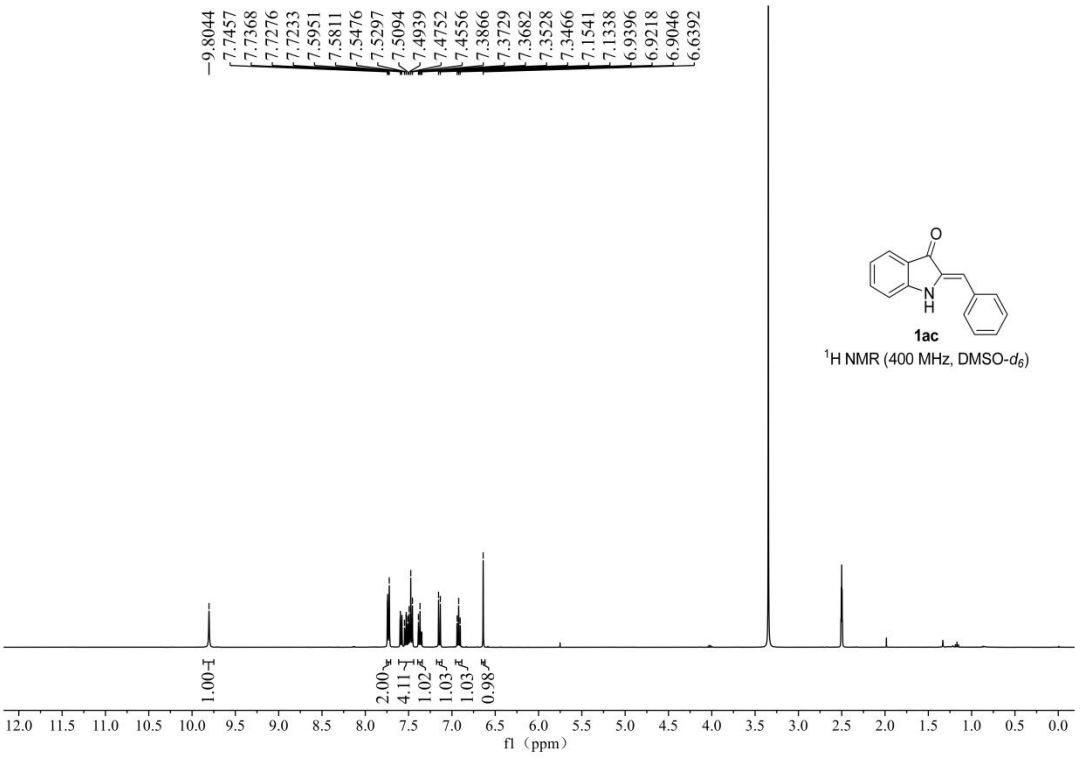


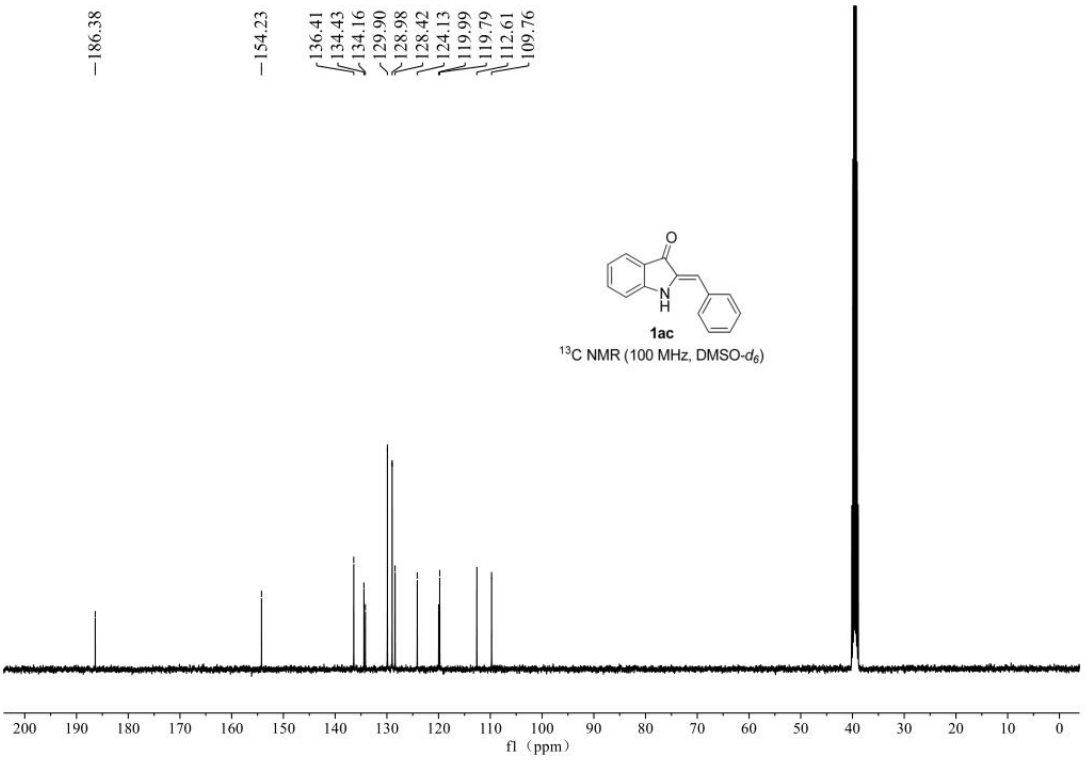
^{1}H NMR (600 MHz, $CDCl_3$)





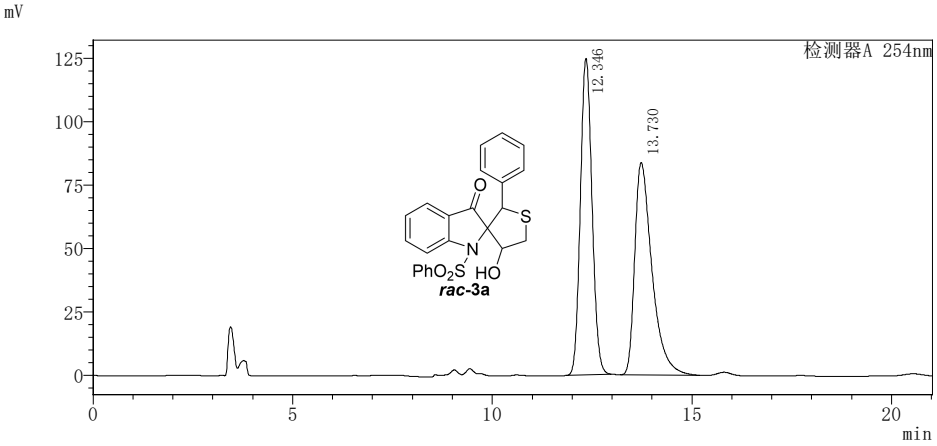
^{13}C NMR (150 MHz, $CDCl_3$)


9.8044
7.7457
7.7368
7.7276
7.7233
7.5951
7.5811
7.5476
7.5297
7.5094
7.4939
7.4752
7.4556
7.3866
7.3729
7.3682
7.3528
7.3466
7.1541
7.1338
6.9396
6.9218
6.9046
6.6392
1.00
2.00
4.11
1.02
1.03
1.03
0.98
f1 (ppm)
1ac
1H NMR (400 MHz, DMSO-d6)

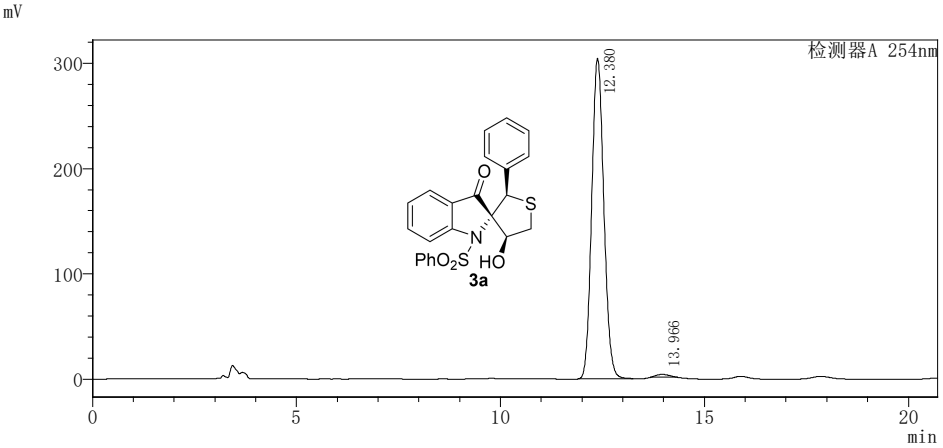

186.38
154.23
136.41
134.43
134.16
129.90
128.98
128.42
124.13
119.99
119.79
112.61
109.76
f1 (ppm)
1ac
13C NMR (100 MHz, DMSO-d6)

13. HPLC chromatograms

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 12.380 min (major), t_R = 13.966 min (minor), 98% ee.

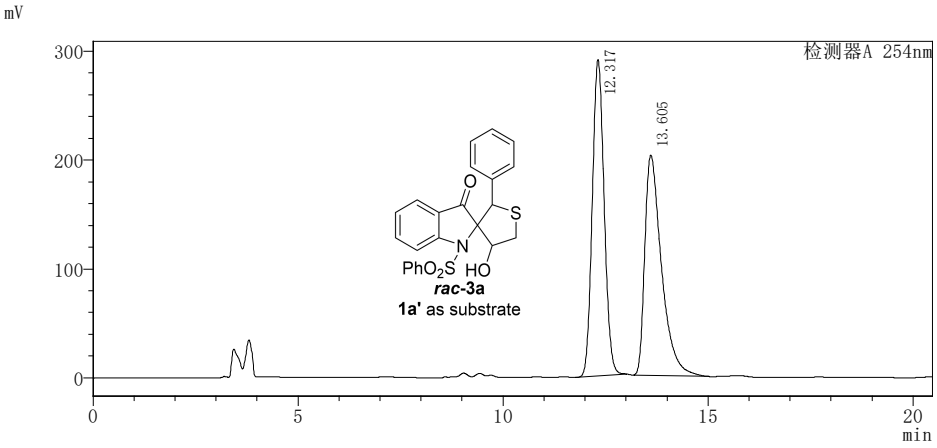


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	12.346	2518793	124841	50.042
2	PDA 254 nm	13.730	2514555	83752	49.958

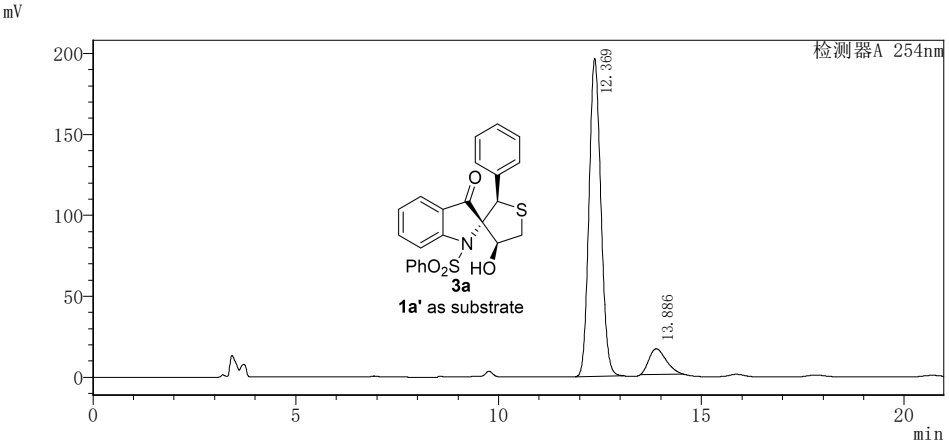


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	12.380	6281014	304712	99.023
2	PDA 254 nm	13.966	61963	2727	0.977

1a' (***E***) replaces **1a** (***Z***) to synthesize **3a** under standard conditions: the **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 12.369 min (major), t_R = 13.886 min (minor), 79% ee.

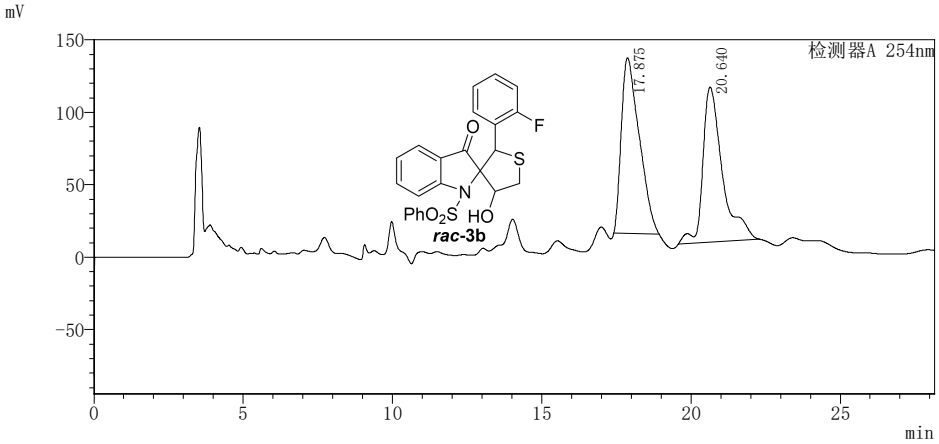


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	12.317	5836523	290657	50.434
2	PDA 254 nm	13.605	5736172	202180	49.566

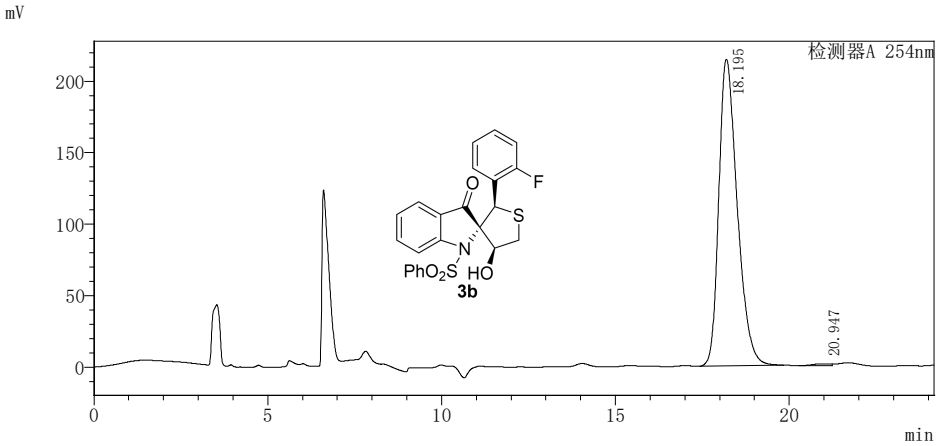


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	12.369	3993972	196454	89.603
2	PDA 254 nm	13.886	463431	15730	10.397

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.195 min (major), t_R = 20.947 min (minor), 99% ee.

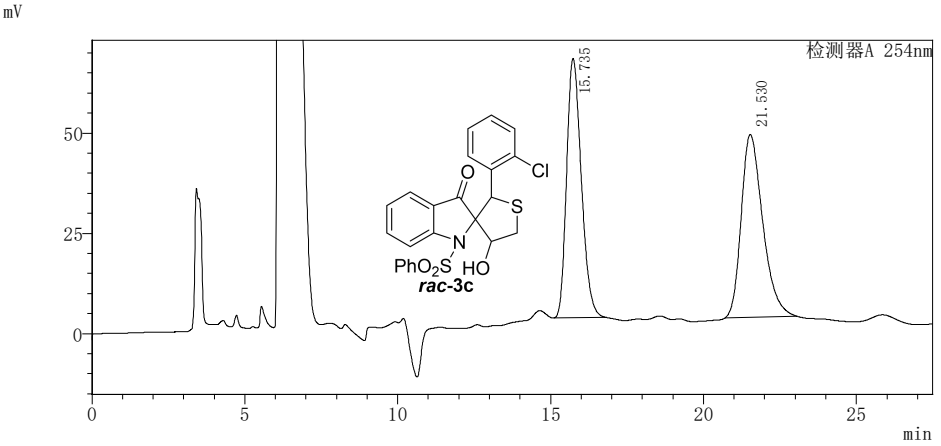


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	17.875	5058514	121150	50.752
2	PDA 254 nm	20.640	4908570	107131	49.248

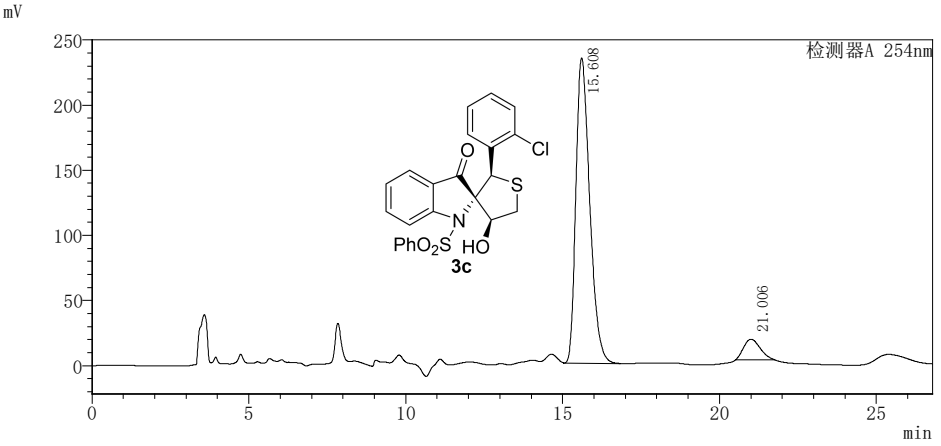


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	18.195	7921270	214558	99.380
2	PDA 254 nm	20.947	49406	1457	0.620

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 15.608 min (major), t_R = 21.006 min (minor), 85% ee.

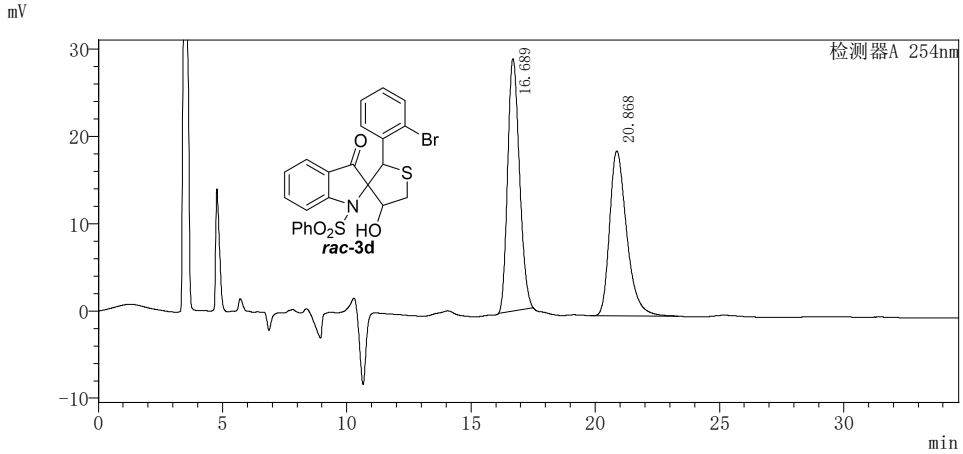


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	15.735	2156507	64721	49.186
2	PDA 254 nm	21.530	2227919	45576	50.814

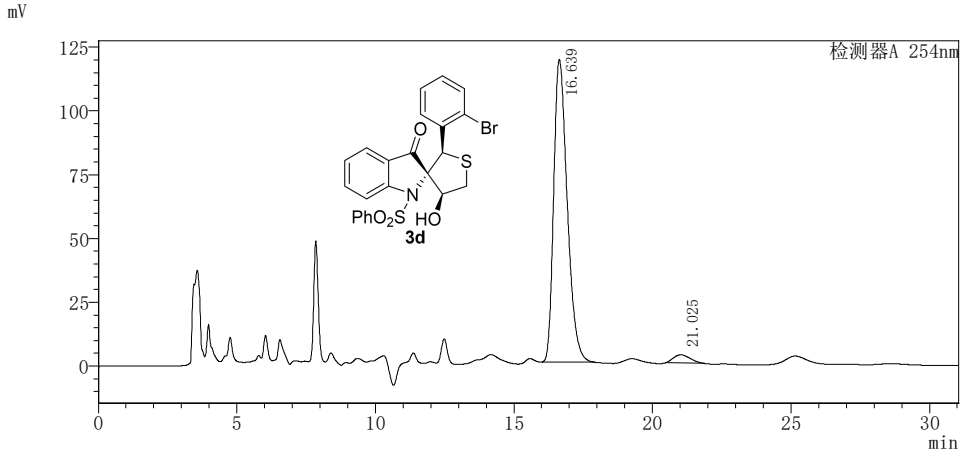


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	15.608	71.84051	234376	92.446
2	PDA 254 nm	21.006	587004	15907	7.554

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 16.639 min (major), t_R = 21.025 min (minor), 94% ee.

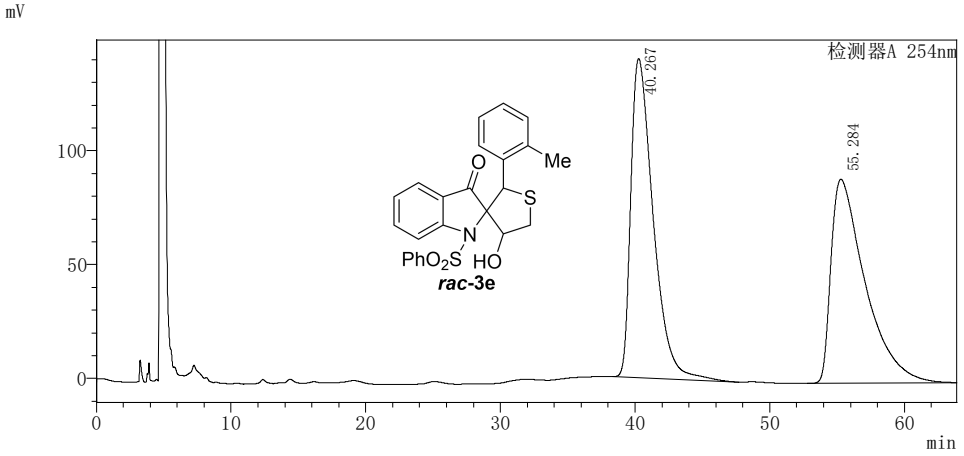


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	16.689	960257	28946	51.437
2	PDA 254 nm	20.868	906587	18912	48.563

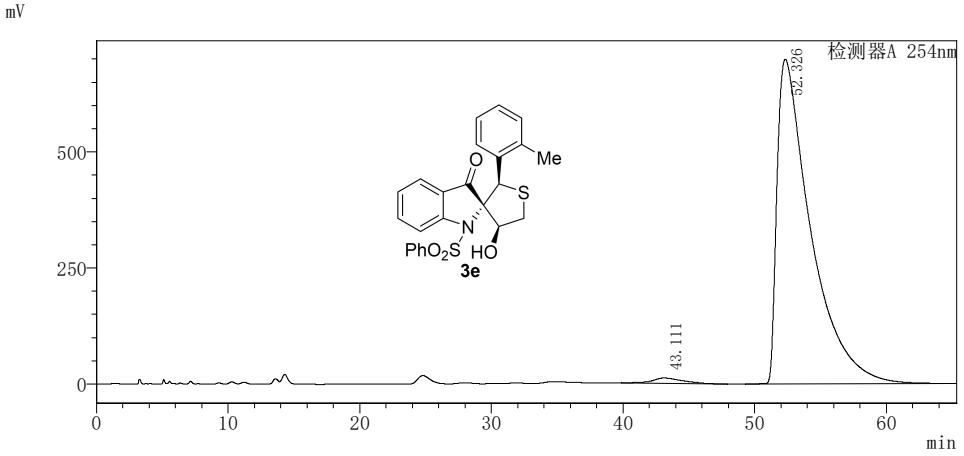


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	16.639	4023302	118680	96.814
2	PDA 254 nm	21.025	132389	3167	3.186

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 95/5, flow rate 1.0 mL/min, λ = 254 nm), t_R = 43.111 min (minor), t_R = 52.326 min (major), 97% ee.

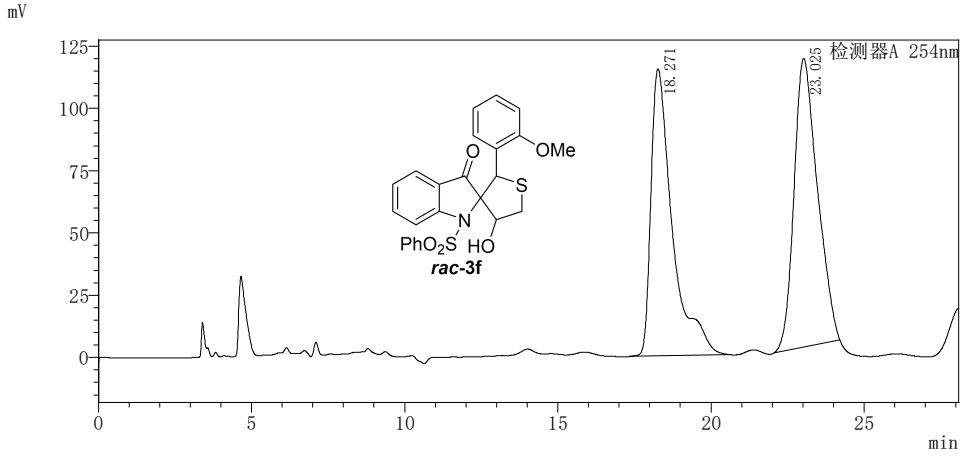


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	40.267	16206606	140223	50.646
2	PDA 254 nm	55.284	15793274	89690	49.354

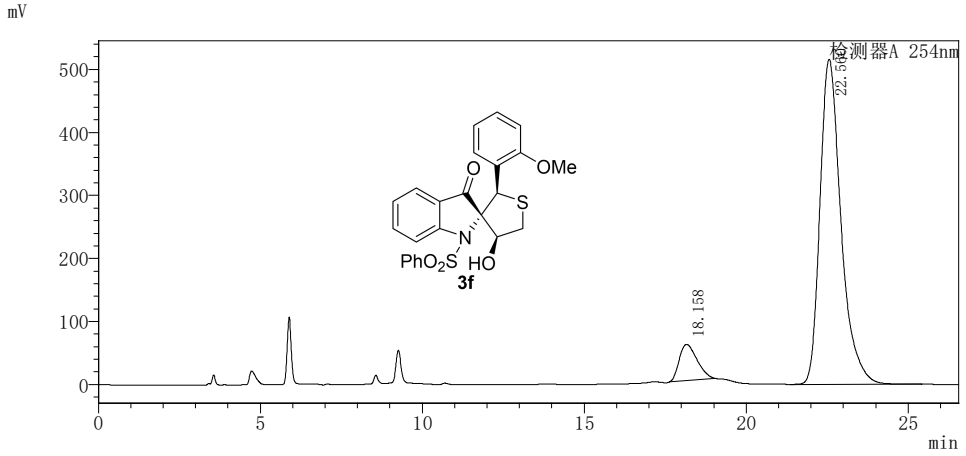


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	43.111	19.56709	11776	1.547
2	PDA 254 nm	52.326	124531533	699683	98.453

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 95/5, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.158 min (minor), t_R = 22.560 min (major), 83% ee.

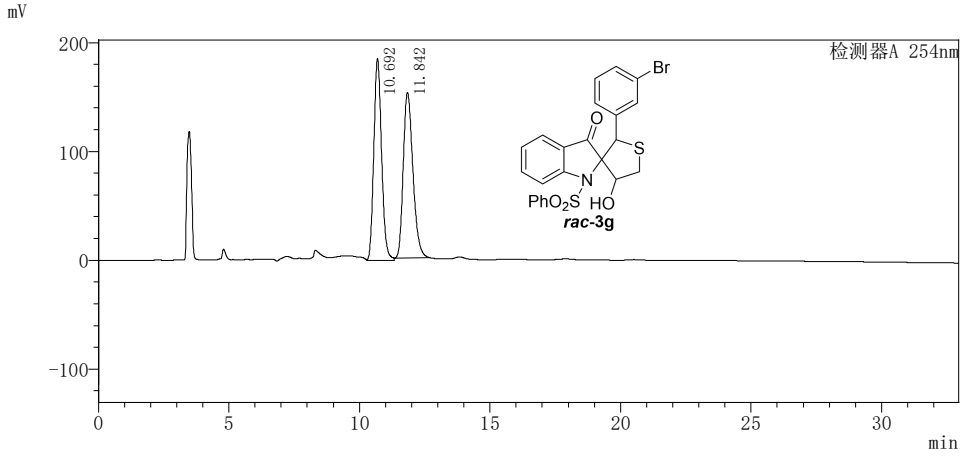


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	18.271	5607458	115208	47.724
2	PDA 254 nm	23.025	6142304	115858	52.276

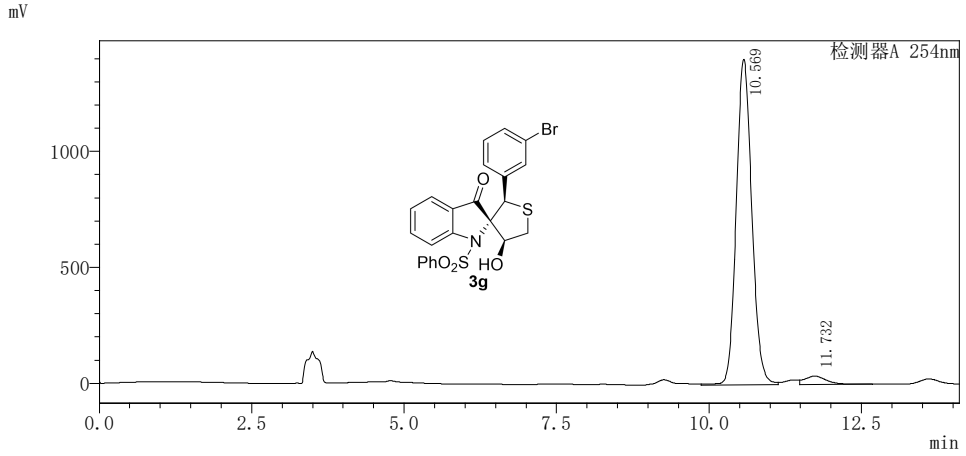


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	18.158	2182812	57428	8.569
2	PDA 254 nm	22.560	23289736	515954	91.431

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.569 min (major), t_R = 11.732 min (minor), 93% ee.

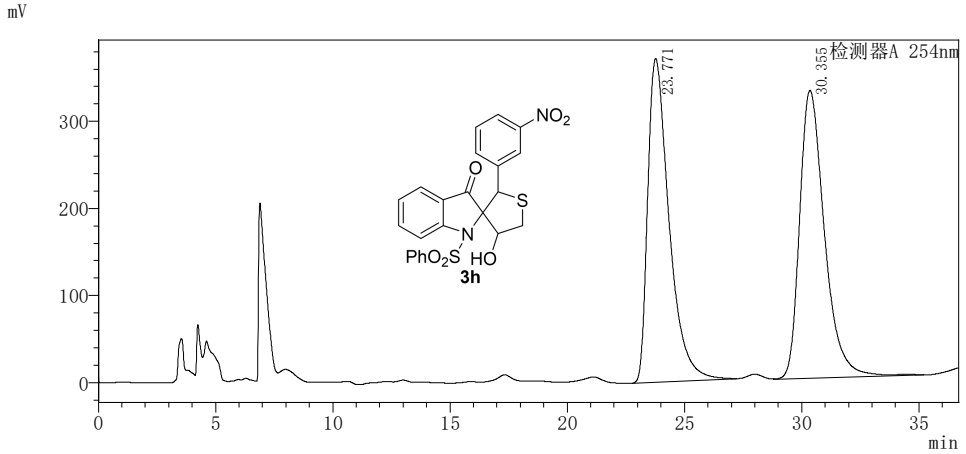


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	10.692	3847152	185607	49.647
2	PDA 254 nm	11.842	3901837	152271	50.353

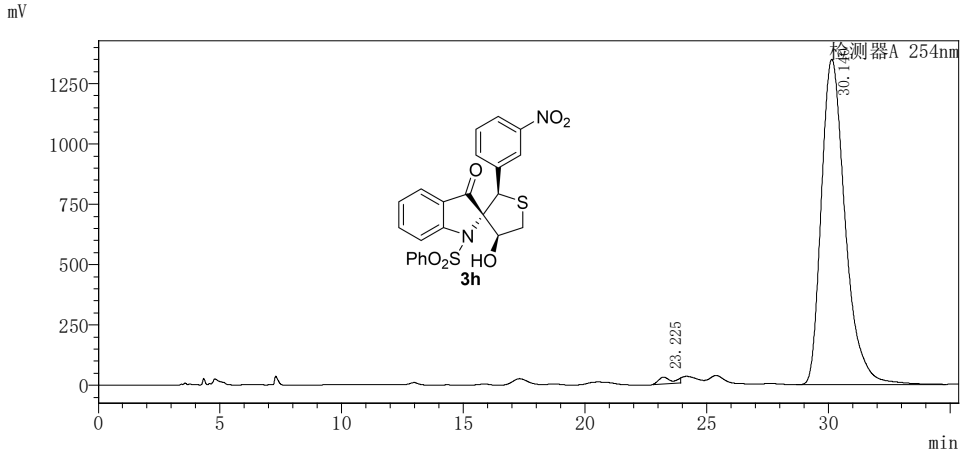


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	10.569	24926410	1404205	96.449
2	PDA 254 nm	11.732	917769	36502	3.551

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 23.225 min (minor), t_R = 30.140 min (major), 98% ee.

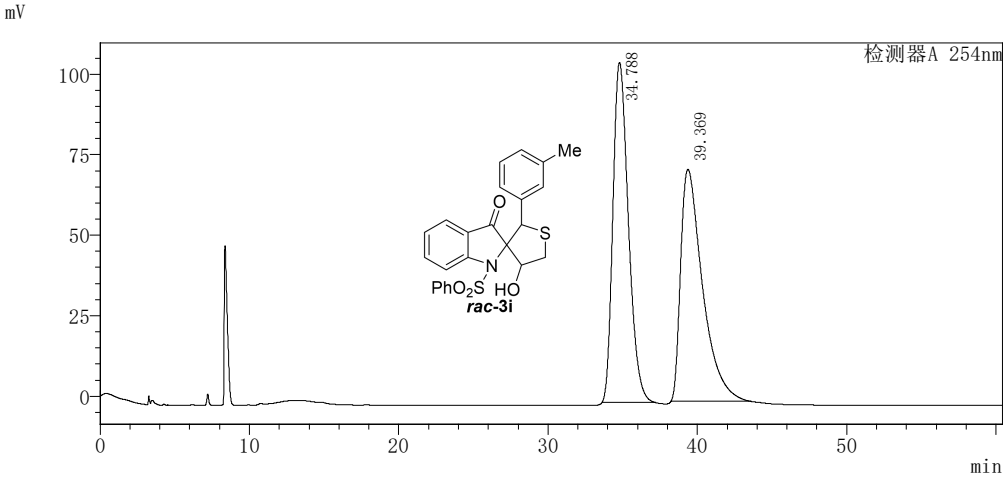


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	23.771	23543499	371758	49.072
2	PDA 254 nm	30.355	24433801	330745	50.928

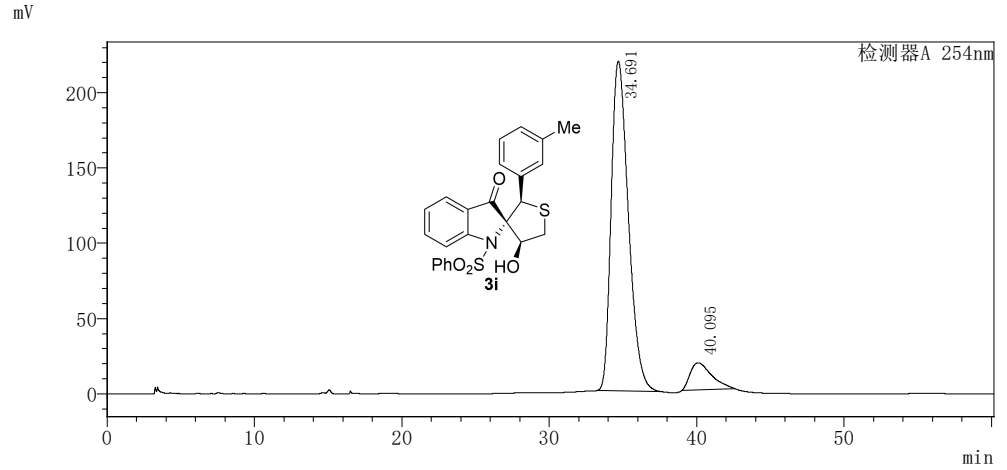


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	23.225	1076975	28235	1.156
2	PDA 254 nm	30.140	92110140	1348871	98.844

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 34.691 min (major), t_R = 40.095 min (minor), 82% ee (recrystallization up to 90% ee).

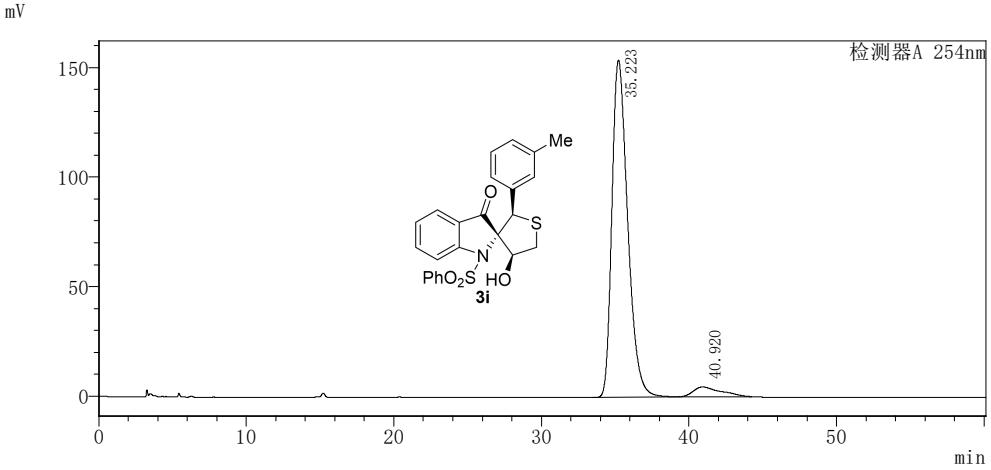


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	34.788	7620440	105674	50.929
2	PDA 254 nm	39.369	7342439	72053	49.071



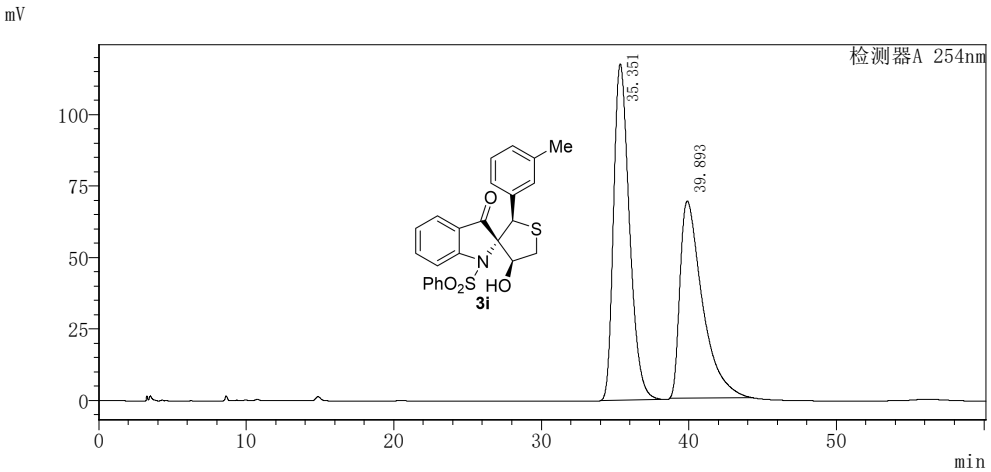
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	34.691	17793139	219168	90.757
2	PDA 254 nm	40.095	1812175	17975	9.243

Liquid phase of **3i**: the **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 35.223 min (major), t_R = 40.920 min (minor), 90% ee.



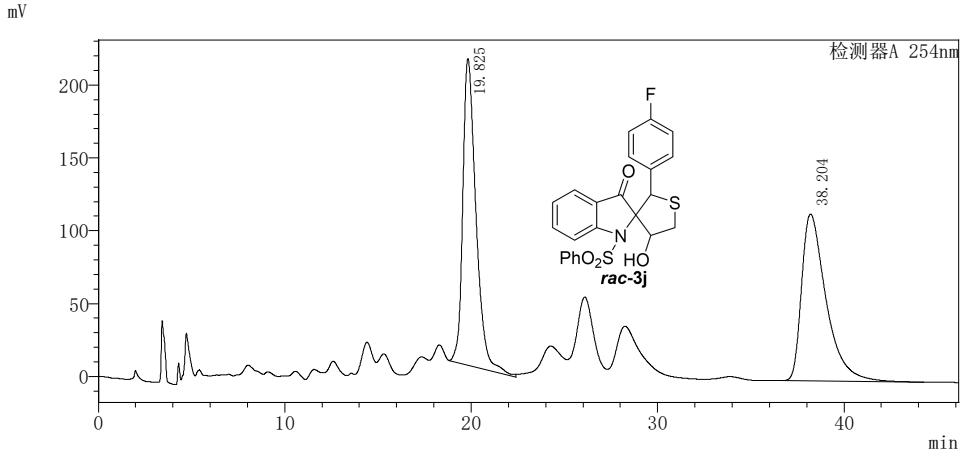
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	35.223	11459644	154046	95.205
2	PDA 254 nm	40.920	577209	4422	4.795

Solid phase of **3i**: the **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 35.351 min (major), t_R = 39.893 min (minor), 10% ee.

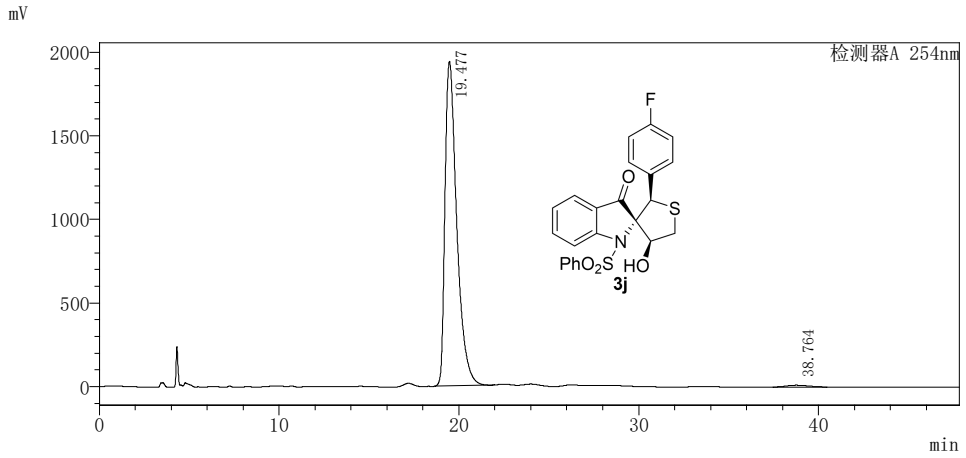


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	35.351	8794886	117669	54.557
2	PDA 254 nm	39.893	7325644	69068	45.443

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.477 min (major), t_R = 38.764 min (minor), 98% ee.

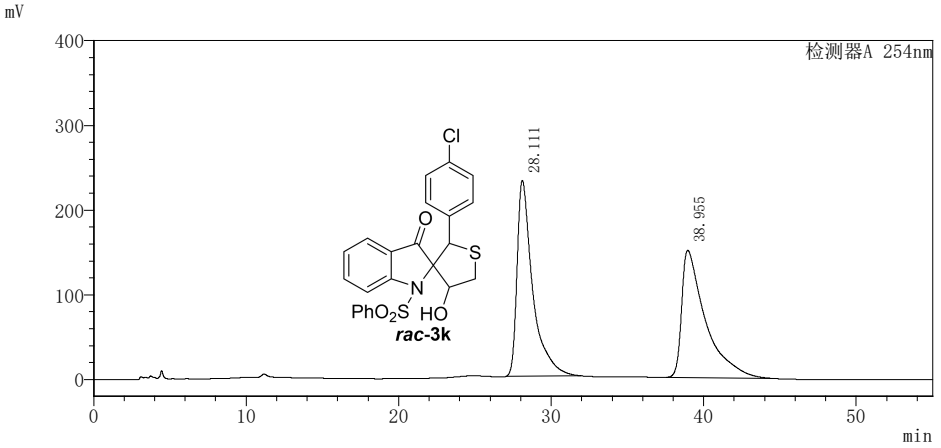


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.825	10340224	210621	49.613
2	PDA 254 nm	38.204	10501692	114614	50.387

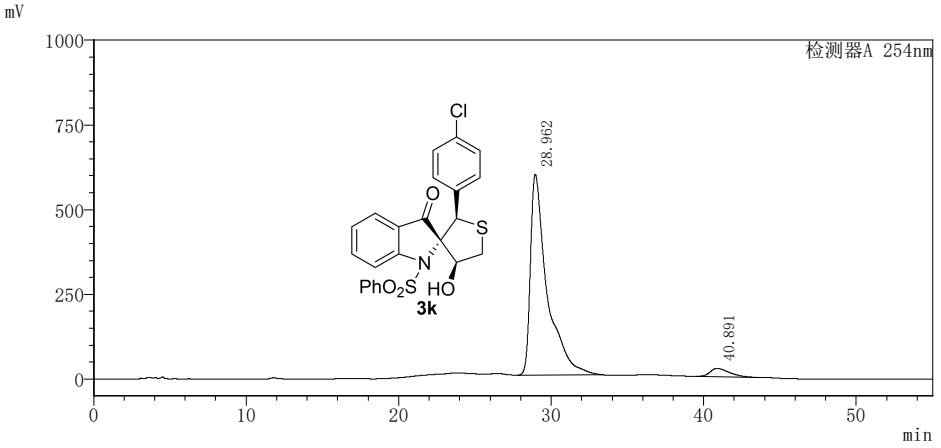


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.477	88228875	1940862	98.942
2	PDA 254 nm	38.764	943197	11131	1.058

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 17.648 min (major), t_R = 19.043 min (minor), 91% ee (recrystallization up to 98% ee).

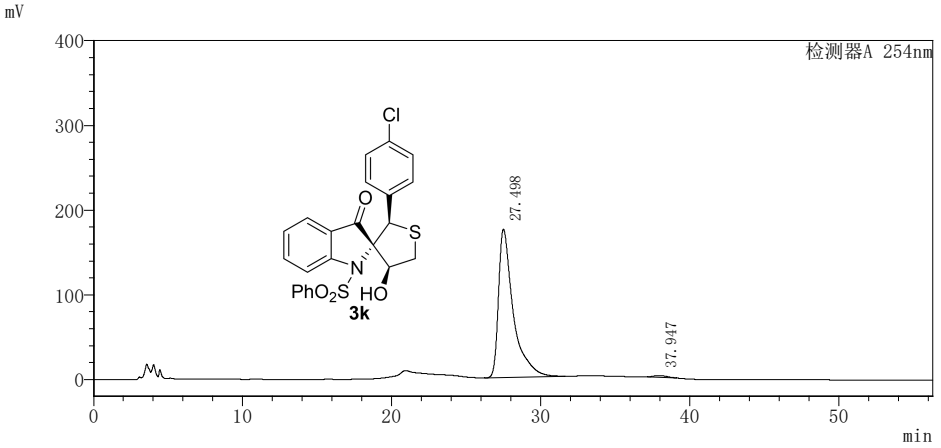


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	28.111	16467861	231286	50.209
2	PDA 254 nm	38.955	16330503	150315	49.791



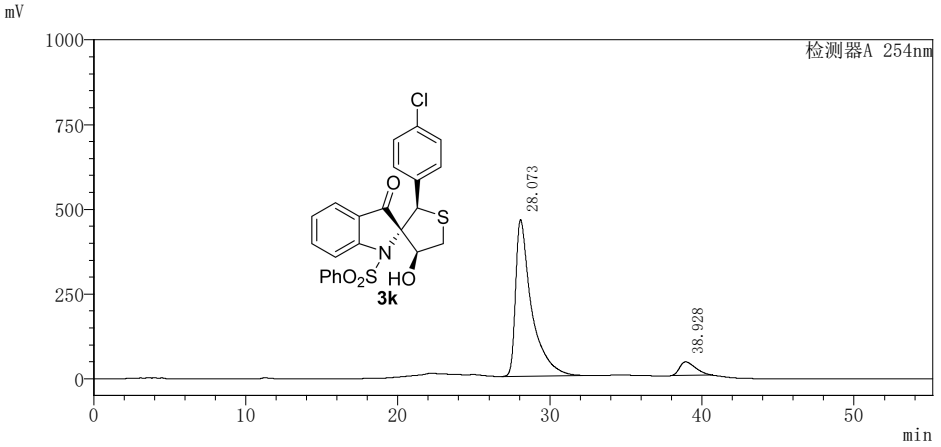
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	28.962	45411867	592904	95.478
2	PDA 254 nm	40.891	2150717	24482	4.522

Liquid phase of **3k**: the **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 27.498 min (major), t_R = 37.947 min (minor), 98% ee.



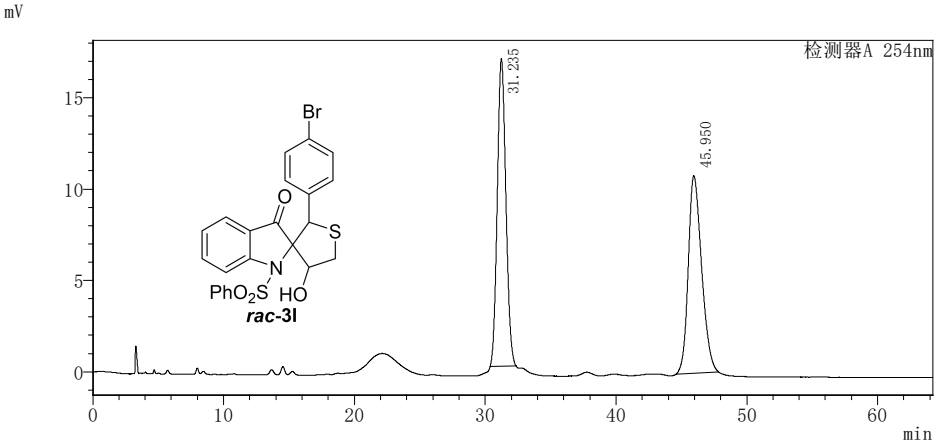
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	27.498	12022164	175245	98.886
2	PDA 254 nm	37.947	135468	2223	1.114

Solid phase of **3k**: the **enantiomeric excess** was determined by HPLC with an IA-H column (*n*–hexane/*i*–PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 28.073 min (major), t_R = 38.928 min (minor), 84% ee.

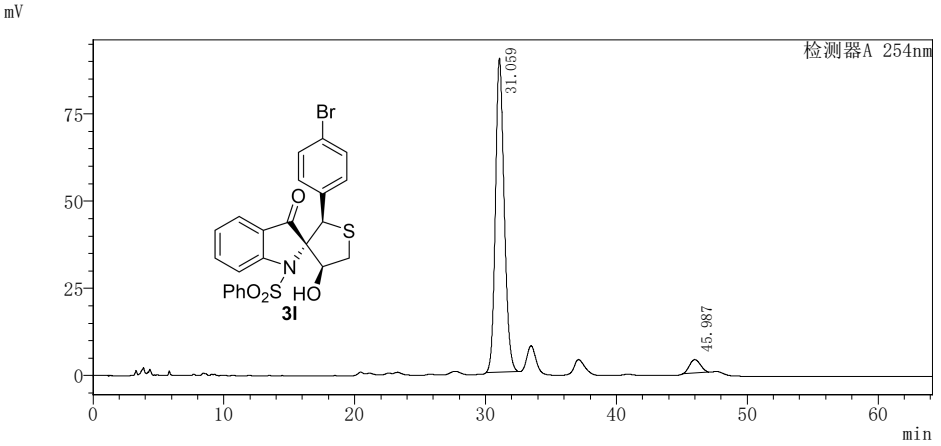


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	28.073	33603961	462212	92.045
2	PDA 254 nm	38.928	2904207	39932	7.955

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 31.059 min (major), t_R = 45.987 min (minor), 90% ee (recrystallization up to 98% ee).

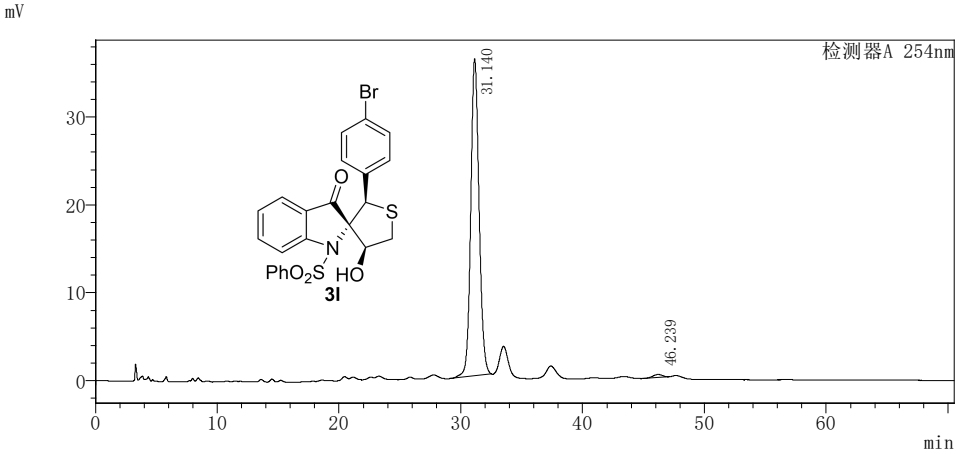


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	31.235	768098	16839	50.123
2	PDA 254 nm	45.950	764321	10810	49.877



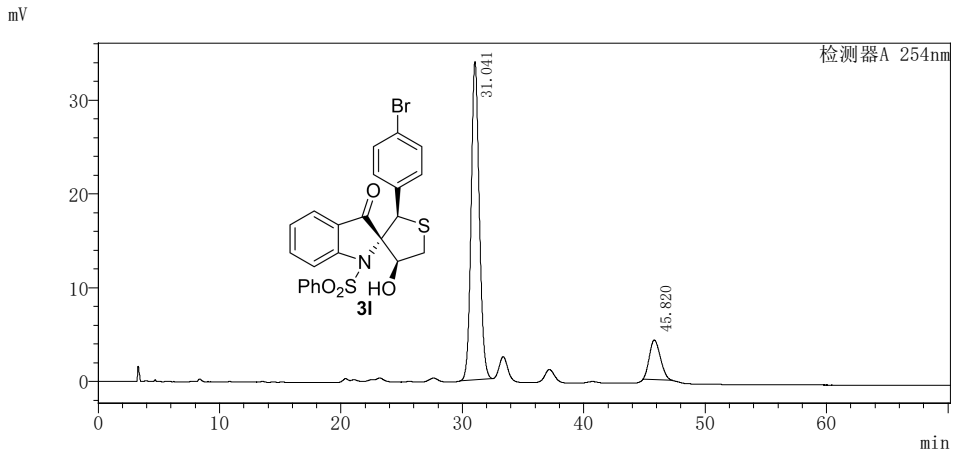
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	31.059	4194022	90078	94.936
2	PDA 254 nm	45.987	223717	3845	5.064

Liquid phase of **3l**: the **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 31.140 min (major), t_R = 46.239 min (minor), 98% ee.



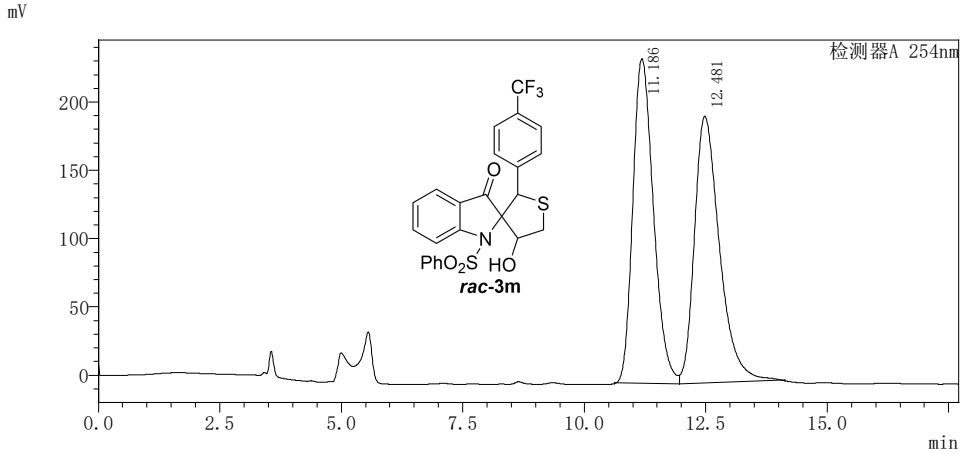
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	31.140	1714569	36107	98.885
2	PDA 254 nm	46.239	19342	348	1.115

Solid phase of **3l**: the **enantiomeric excess** was determined by HPLC with an IA-H column (*n*–hexane/*i*–PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 31.041 min (major), t_R = 45.820 min (minor), 72% ee.

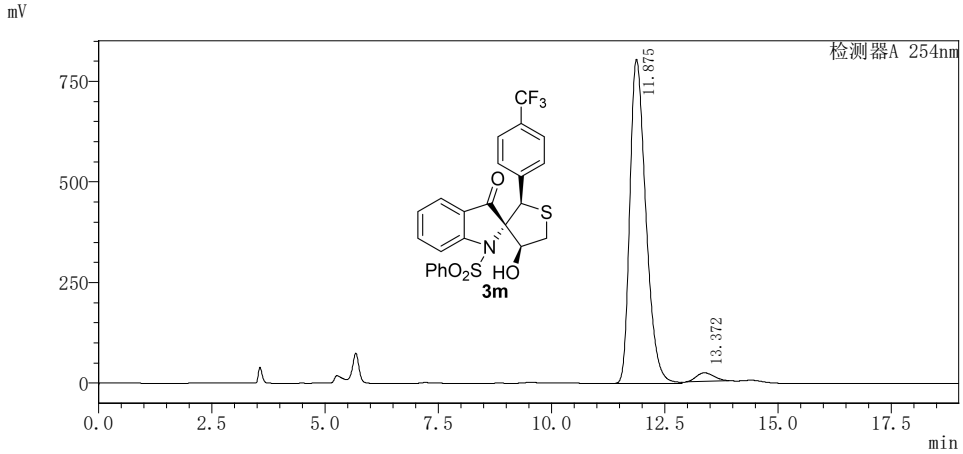


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	31.041	1596942	33968	85.600
2	PDA 254 nm	45.820	268634	4233	14.400

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*–hexane/*i*–PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 11.875 min (major), t_R = 13.372 min (minor), 94% ee.

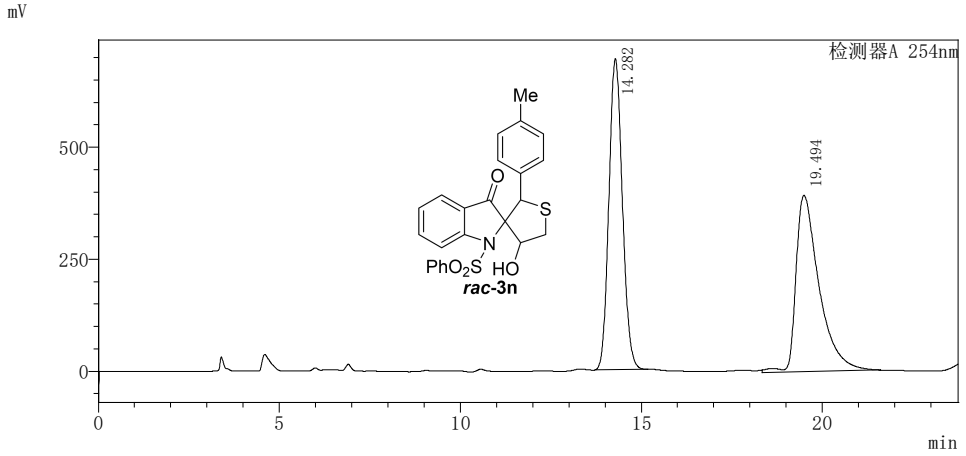


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	11.186	7027366	237870	50.056
2	PDA 254 nm	12.481	7011705	195295	49.944

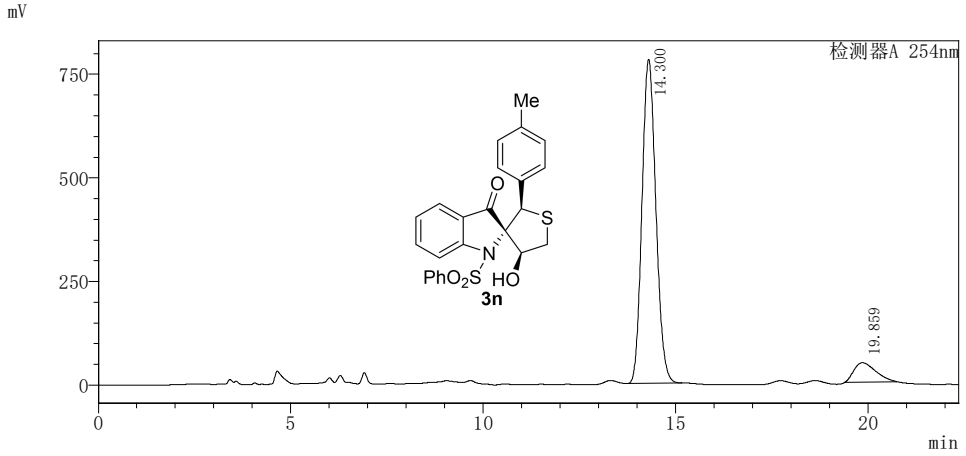


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	11.875	19823789	805739	97.185
2	PDA 254 nm	13.372	574212	21305	2.815

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 14.300 min (major), t_R = 19.859 min (minor), 83% ee.

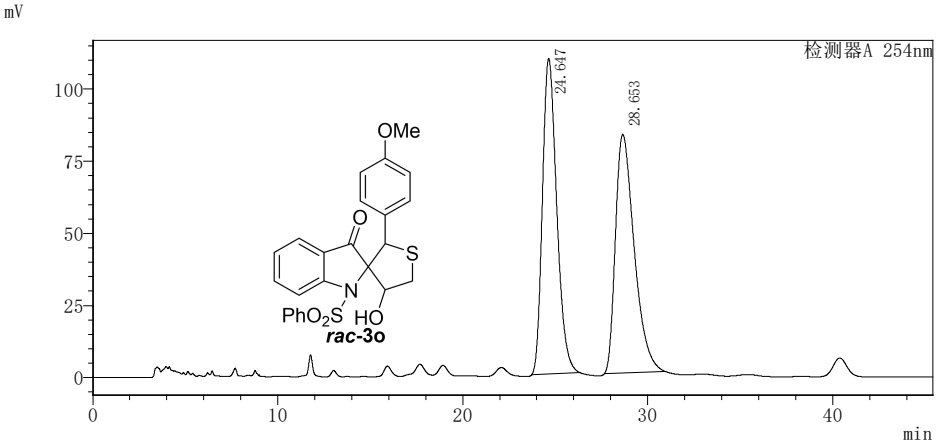


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	14.282	17960362	694297	50.788
2	PDA 254 nm	19.494	17402835	393384	49.212

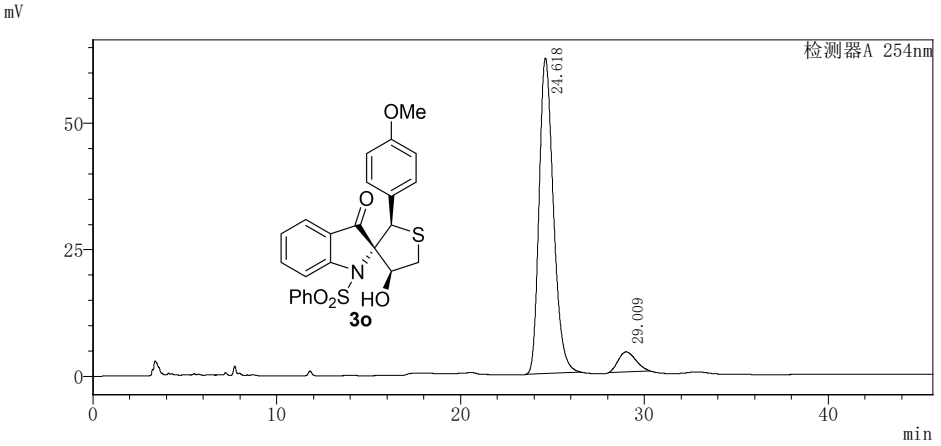


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	14.300	19630545	782098	91.534
2	PDA 254 nm	19.859	1862690	46937	8.466

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 24.618 min (major), t_R = 29.009 min (minor), 86% ee (recrystallization up to 99% ee).

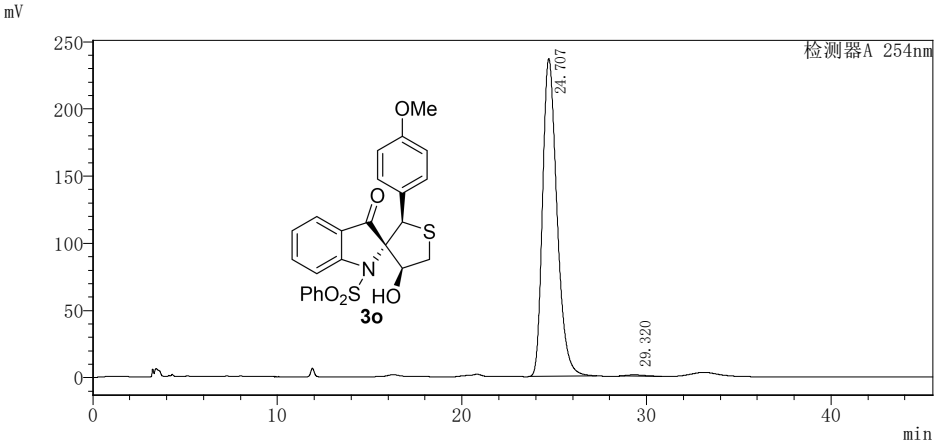


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	24.647	5868554	109366	50.056
2	PDA 254 nm	28.653	5855393	82782	49.944



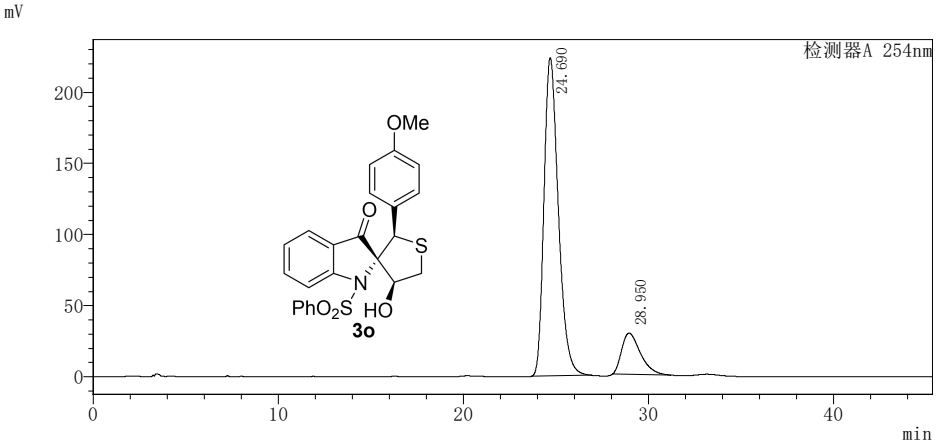
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	24.618	3373748	62419	92.729
2	PDA 254 nm	29.009	264554	3969	7.271

Liquid phase of **3o**: The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 24.707 min (major), t_R = 29.320 min (minor), 99% ee.



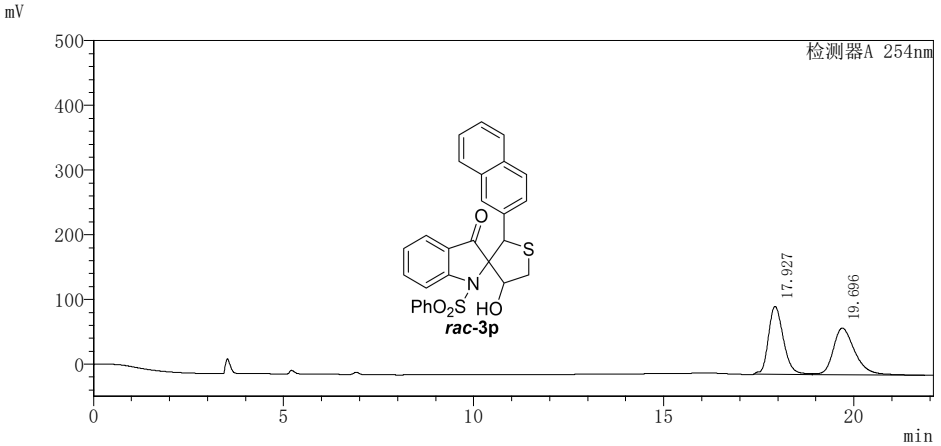
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	24.707	12825027	236582	99.503
2	PDA 254 nm	29.320	64030	971	0.497

Solid phase of **3o**: The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 24.690 min (major), t_R = 28.950 min (minor), 71% ee.

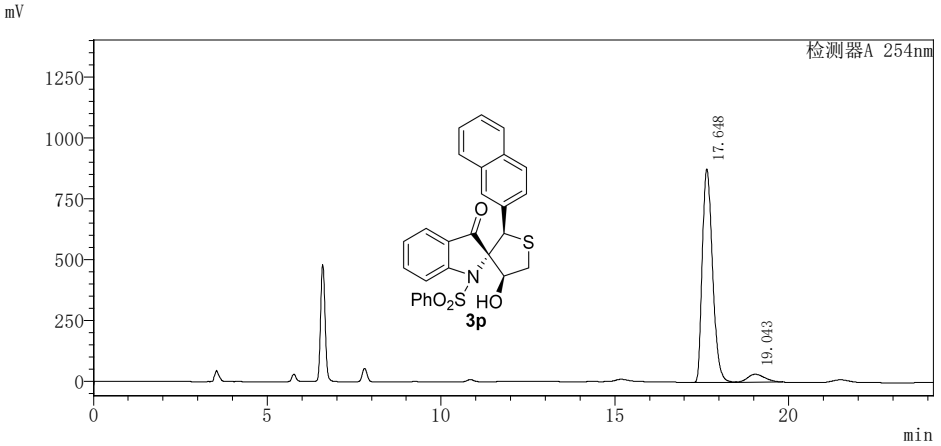


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	24.690	12062960	223779	85.451
2	PDA 254 nm	28.950	2053810	29136	14.549

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 0.8 mL/min, λ = 254 nm), t_R = 17.648 min (major), t_R = 19.043 min (minor), 88% ee.

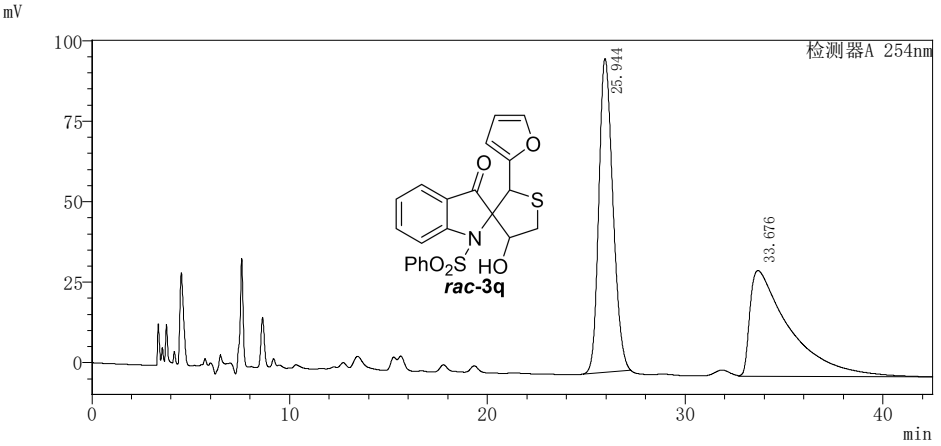


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	17.927	2888096	105300	50.079
2	PDA 254 nm	19.696	2878970	72411	49.921

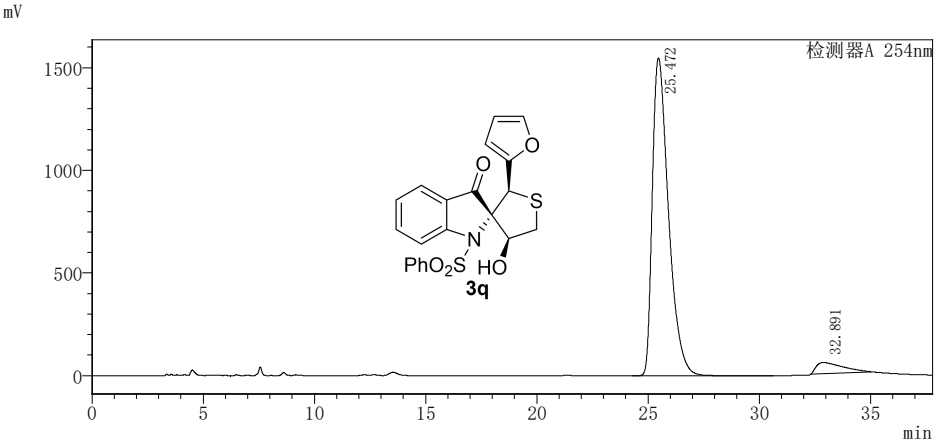


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	17.648	18027790	876428	94.128
2	PDA 254 nm	19.043	1124725	32338	5.872

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 85/15, flow rate 1.0 mL/min, λ = 254 nm), t_R = 25.472 min (major), t_R = 33.676 min (minor), 90% ee.

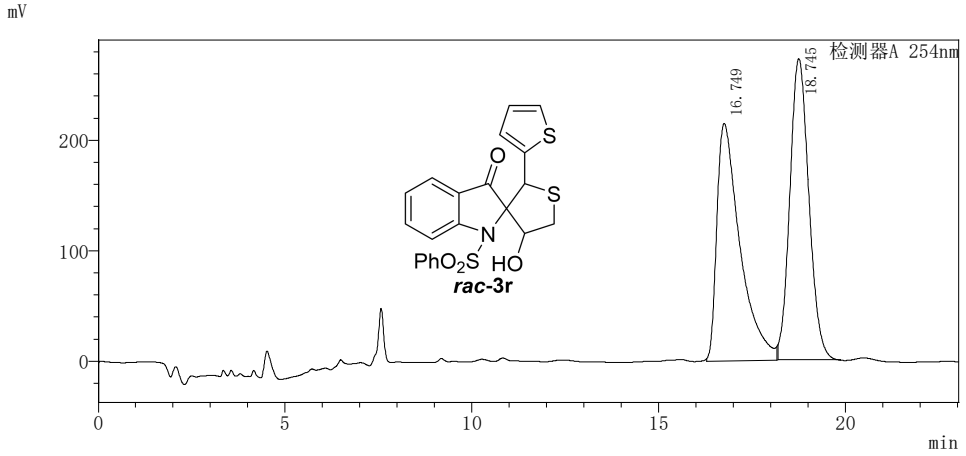


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	25.944	4817347	97457	51.124
2	PDA 254 nm	33.676	4605447	32790	48.876

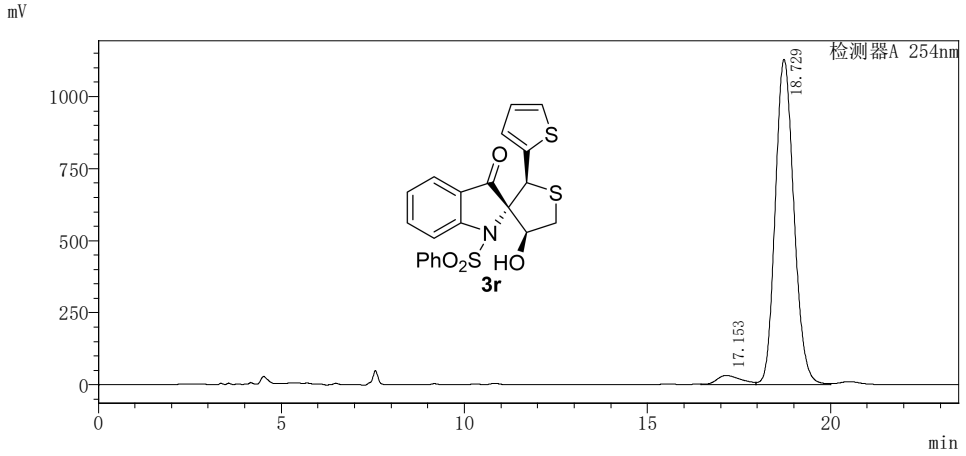


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	25.472	78661042	1549622	94.756
2	PDA 254 nm	33.676	4353399	53273	5.244

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 85/15, flow rate 1.0 mL/min, λ = 254 nm), t_R = 17.153 min (minor), t_R = 18.729 min (major), 93% ee.

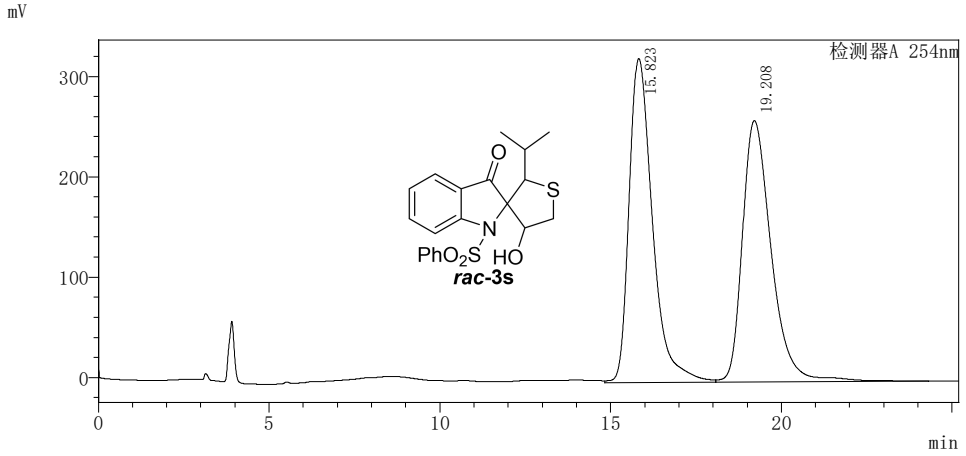


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	16.749	9298646	215146	49.171
2	PDA 254 nm	18.745	9612048	272437	50.829

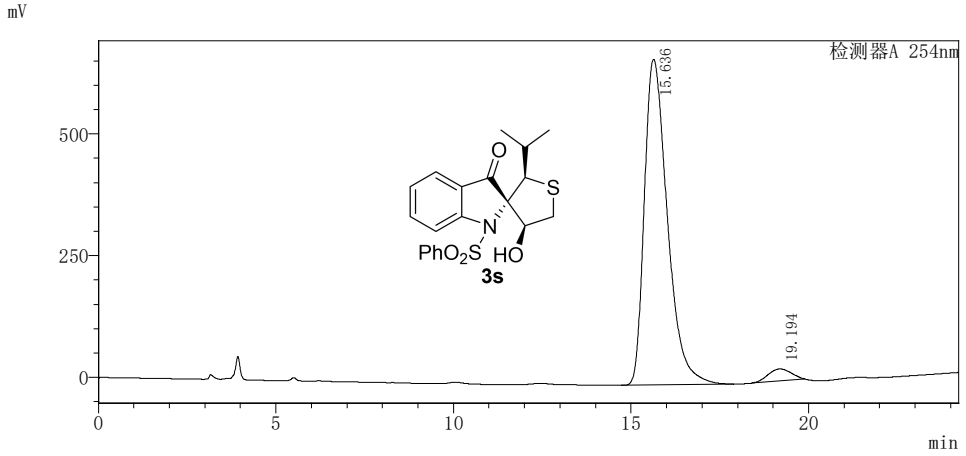


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	17.153	1478660	31763	3.560
2	PDA 254 nm	18.729	40052871	1129247	96.440

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 15.636 min (major), t_R = 19.194 min (minor), 93% ee.

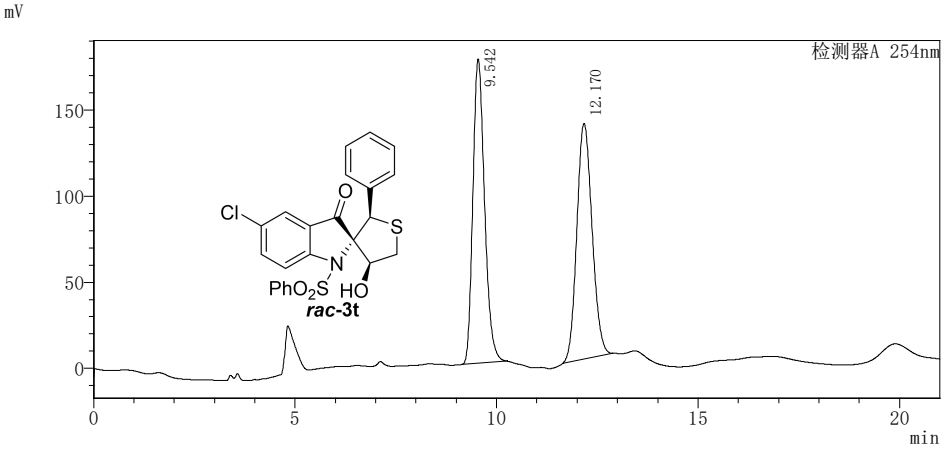


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	15.823	15389161	322920	50.159
2	PDA 254 nm	19.208	15291715	260483	49.841

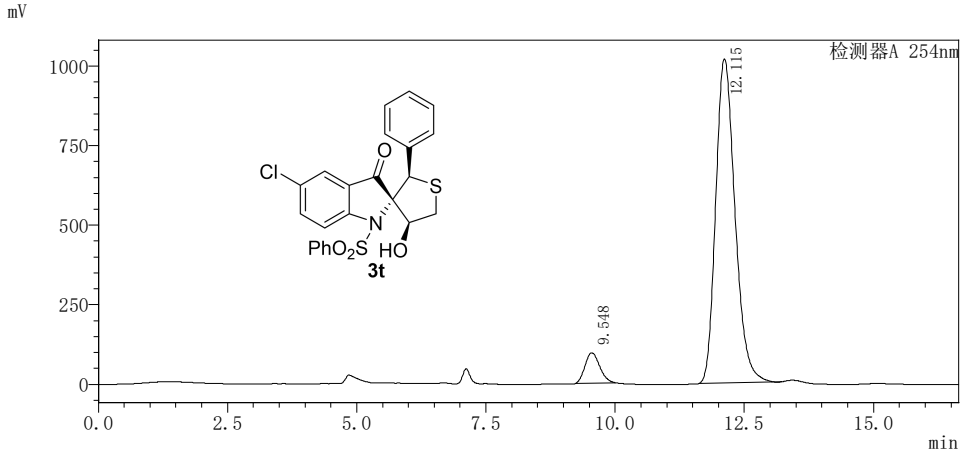


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	15.636	30168624	668874	96.528
2	PDA 254 nm	19.194	1085162	24269	3.472

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 9.548 min (minor), t_R = 12.115 min (major), 87% ee.

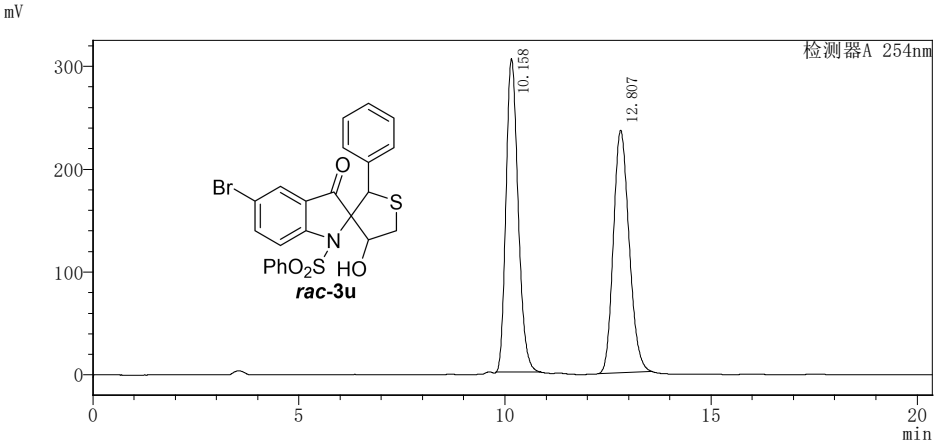


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	9.542	3554720	176626	49.754
2	PDA 254 nm	12.170	3589816	136693	50.246

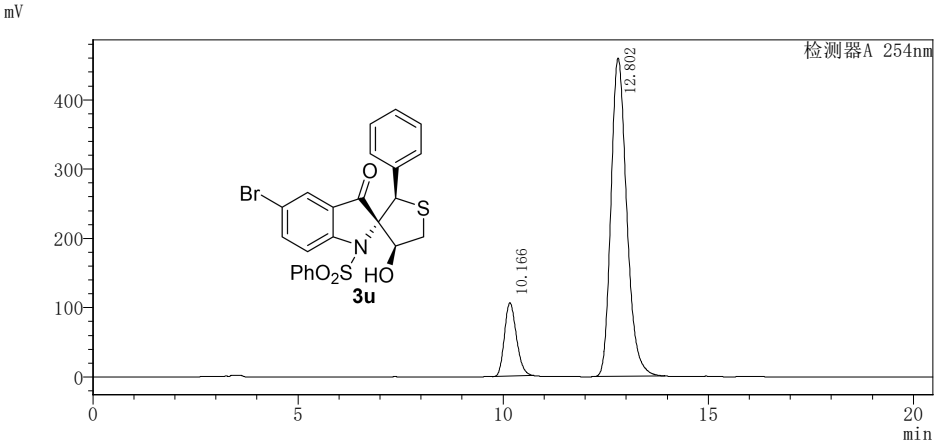


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	9.548	1884981	95581	6.654
2	PDA 254 nm	12.115	26444312	1019125	93.346

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.166 min (minor), t_R = 12.802 min (major), 70% ee.

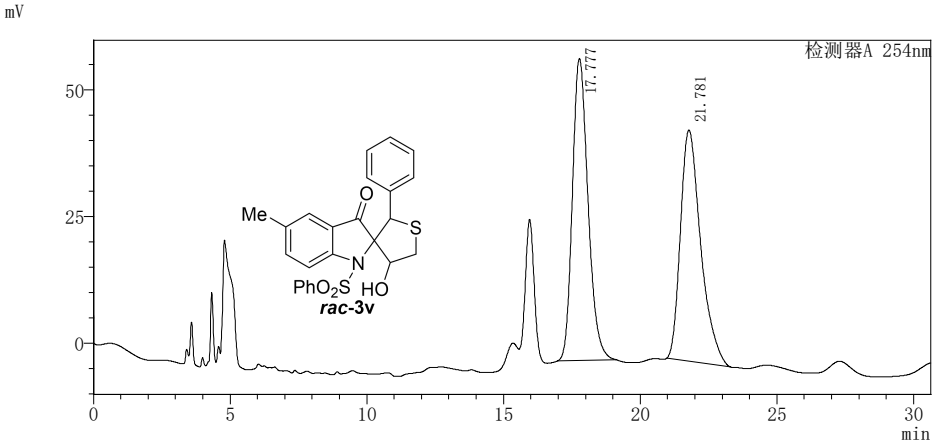


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	10.158	6246228	304947	50.00
2	PDA 254 nm	12.807	6246351	235651	50.00

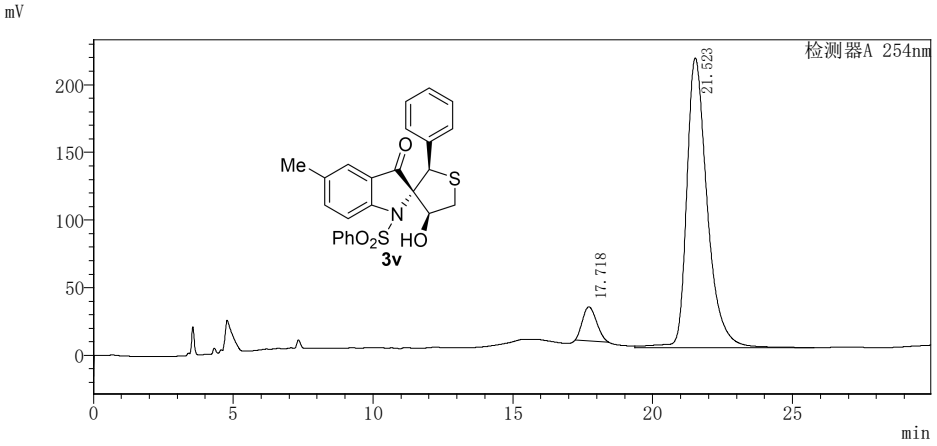


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	10.166	2159148	106038	14.952
2	PDA 254 nm	12.802	12281383	459647	85.048

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 17.718 min (minor), t_R = 21.523 min (major), 85% ee.

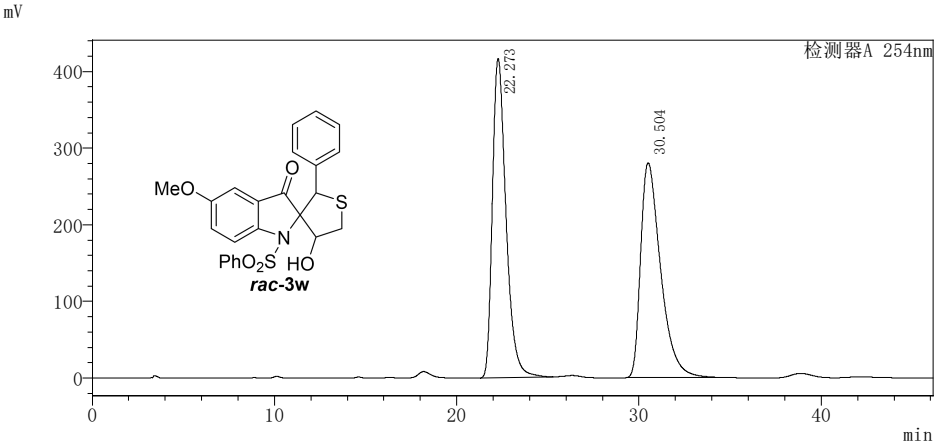


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	17.777	2367217	59600	50.130
2	PDA 254 nm	21.781	2354946	45623	49.870

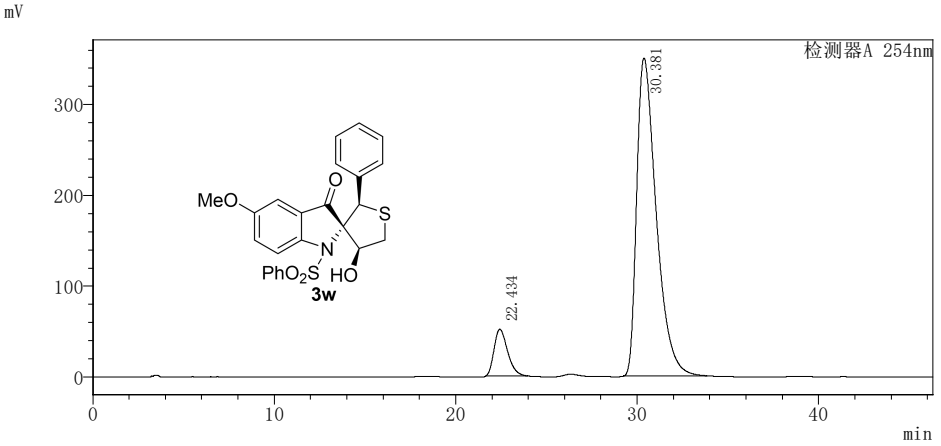


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	17.718	878742	25193	7.413
2	PDA 254 nm	21.523	10975252	214277	92.587

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 22.434 min (minor), t_R = 30.381 min (major), 82% ee (recrystallization up to 96% ee).

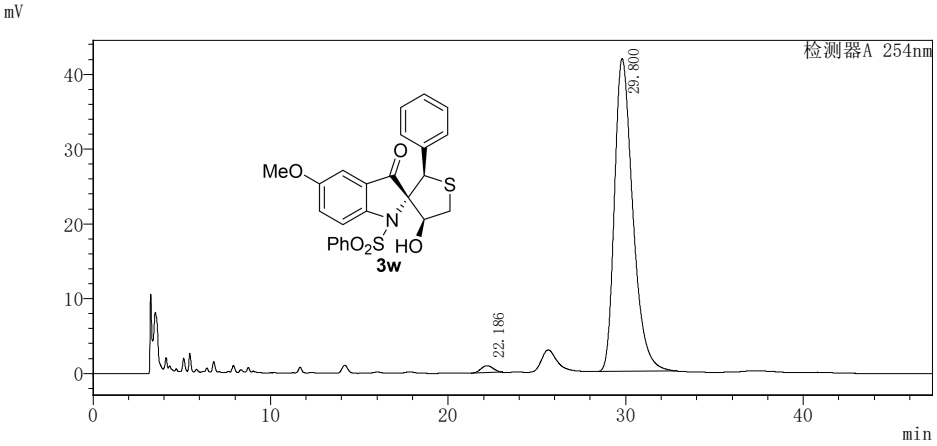


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	22.273	21632795	416744	50.411
2	PDA 254 nm	30.504	21279743	280193	49.589



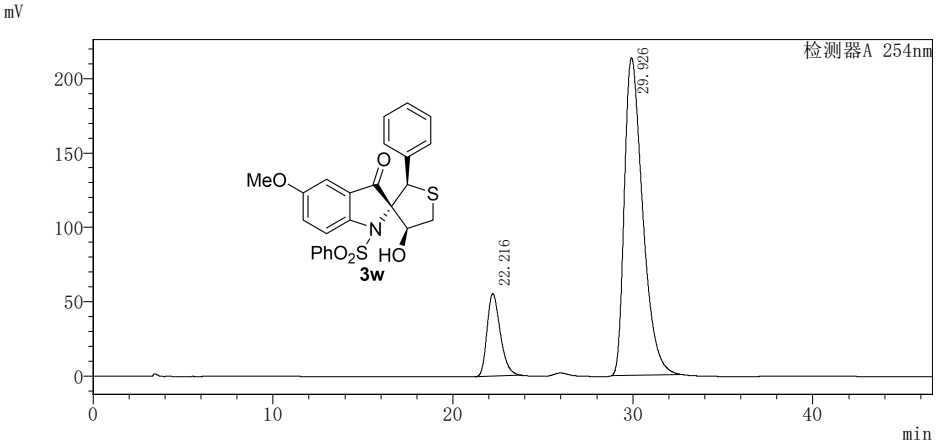
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	22.434	2660299	51408	9.213
2	PDA 254 nm	30.381	26215435	350406	90.787

Liquid phase of **3w**: the **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 22.186 min (minor), t_R = 29.800 min (major), 96% ee.



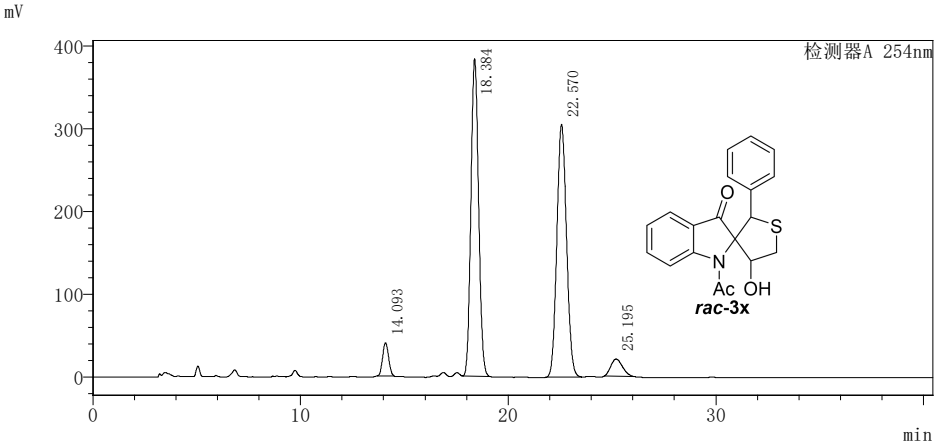
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	22.186	44127	932	1.449
2	PDA 254 nm	29.800	3000233	41854	98.551

Solid phase of **3w**: the **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 22.216 min (minor), t_R = 29.926 min (major), 68% ee.

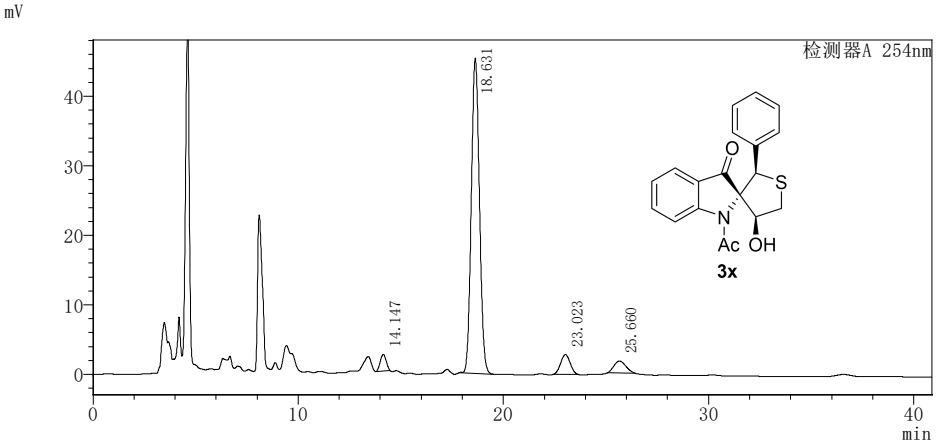


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	22.216	2846881	55563	15.802
2	PDA 254 nm	29.926	15169171	213770	84.198

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.631 min (major), t_R = 23.023 min (minor), 86% ee.

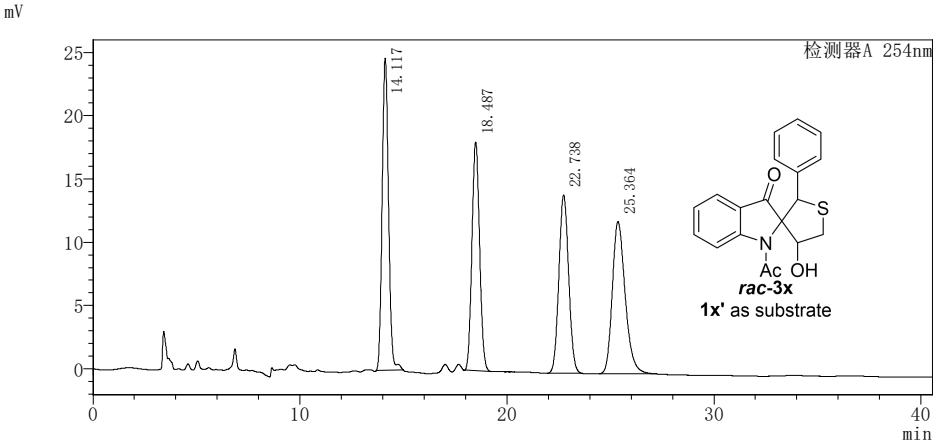


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	14.093	800184	40163	3.751
2	PDA 254 nm	18.384	9839368	384144	46.128
3	PDA 254 nm	22.570	9883945	305111	46.337
4	PDA 254 nm	25.195	807213	20743	3.784

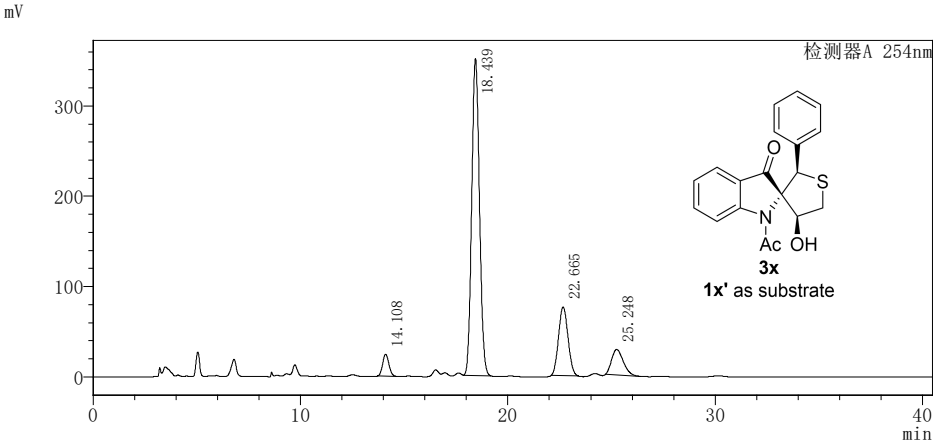


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	14.147	47313	2346	3.250
2	PDA 254 nm	18.631	1247332	45339	85.685
3	PDA 254 nm	23.023	91711	2840	6.300
4	PDA 254 nm	25.660	69354	1706	4.764

1x' (***E***) replaces **1x** (***Z***) to synthesize **3x** under standard conditions: the **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.439 min (major), t_R = 23.665 min (minor), 58% ee.

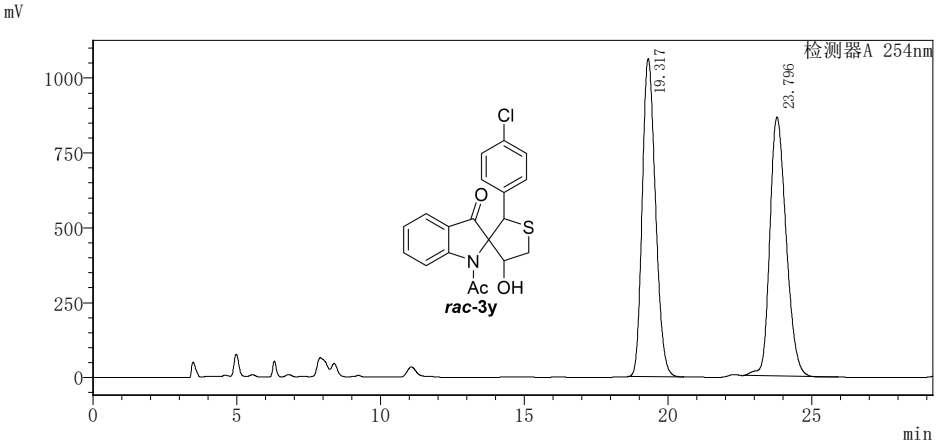


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	14.117	528189	24689	26.740
2	PDA 254 nm	18.487	463984	18081	23.489
3	PDA 254 nm	23.738	460823	14083	23.329
4	PDA 254 nm	25.364	522301	12028	26.442

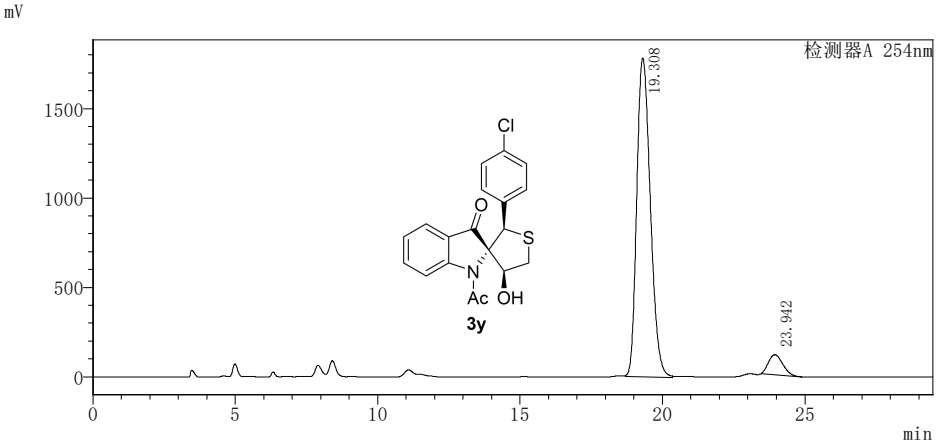


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	14.108	507881	24408	3.864
2	PDA 254 nm	18.439	9102437	350972	69.256
3	PDA 254 nm	23.665	2421065	76137	18.421
4	PDA 254 nm	25.248	1111782	28266	8.459

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.308 min (major), t_R = 23.942 min (minor), 88% ee.

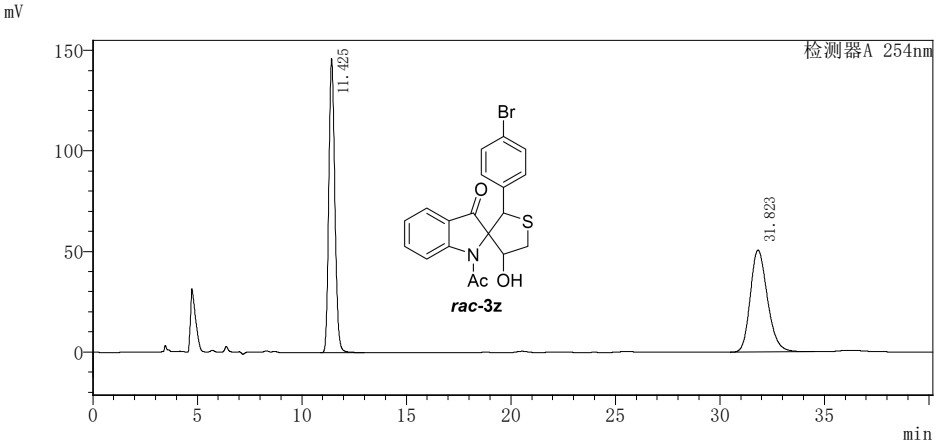


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.317	34165233	1062937	50.018
2	PDA 254 nm	23.796	34140084	865135	49.982

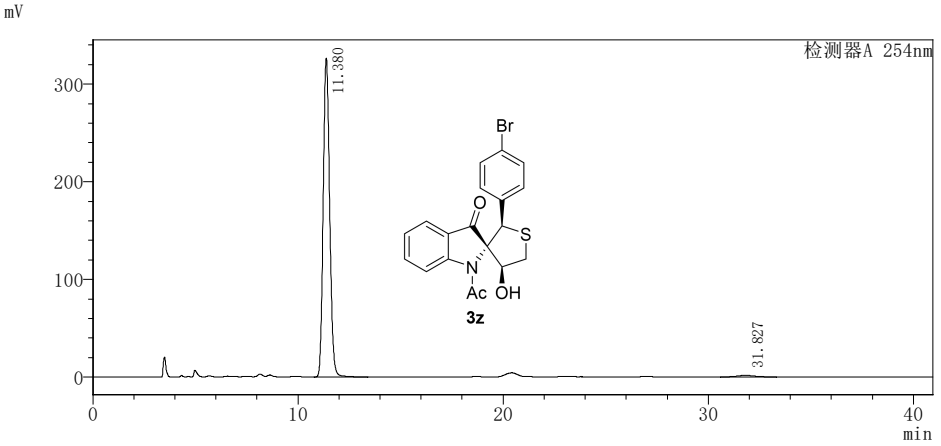


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.308	59233615	1784230	93.829
2	PDA 254 nm	23.942	3895594	111821	6.171

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 11.380 min (major), t_R = 31.827 min (minor), 98% ee.

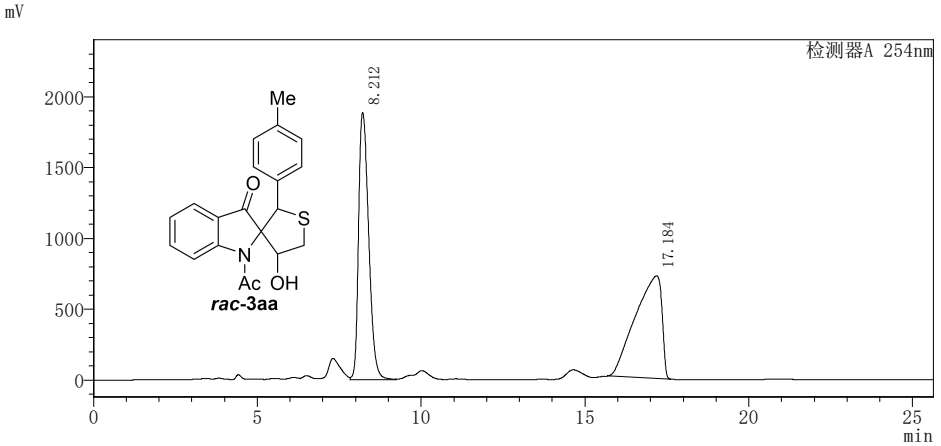


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	11.425	2940787	146406	50. 334
2	PDA 254 nm	31.823	2901764	50754	49.666

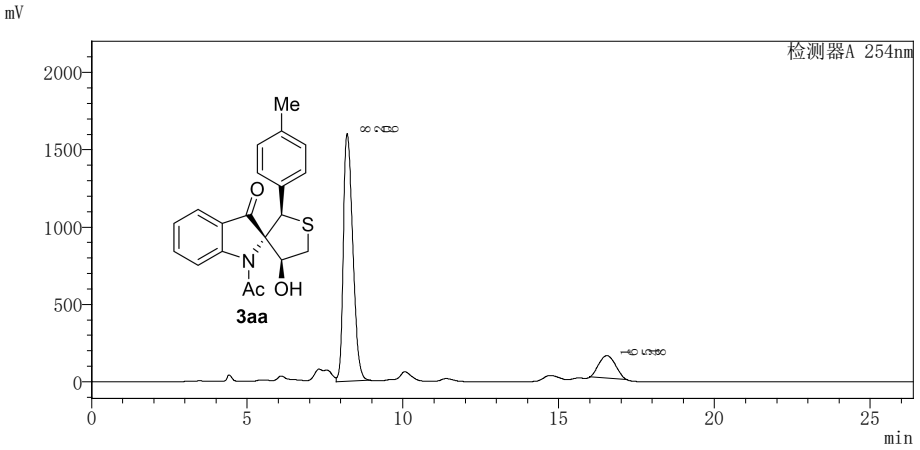


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	11.380	7158449	326738	98.697
2	PDA 254 nm	31.827	94494	1562	1.303

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.206 min (major), t_R = 16.548 min (minor), 72% ee.

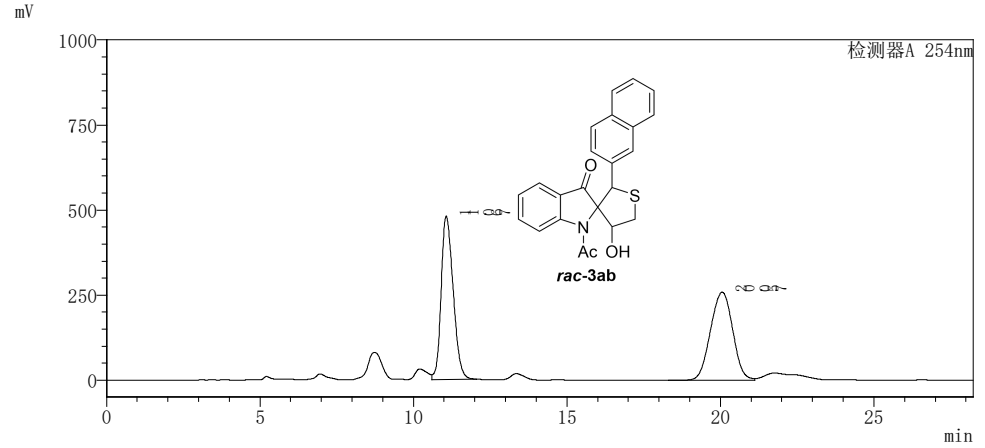


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.212	40861779	1886099	49.965
2	PDA 254 nm	17.184	40918999	724713	50.035

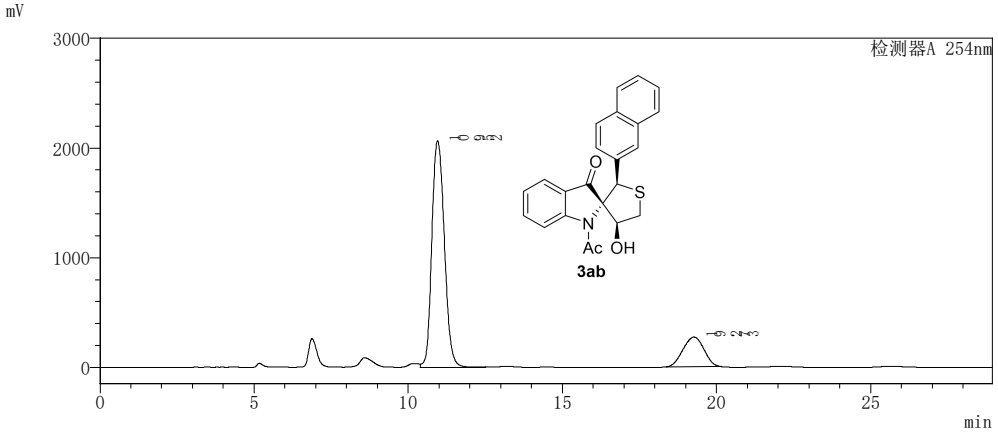


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.206	33870919	1601666	86.160
2	PDA 254 nm	16.548	5440742	145790	13.840

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.952 min (major), t_R = 19.273 min (minor), 64% ee.

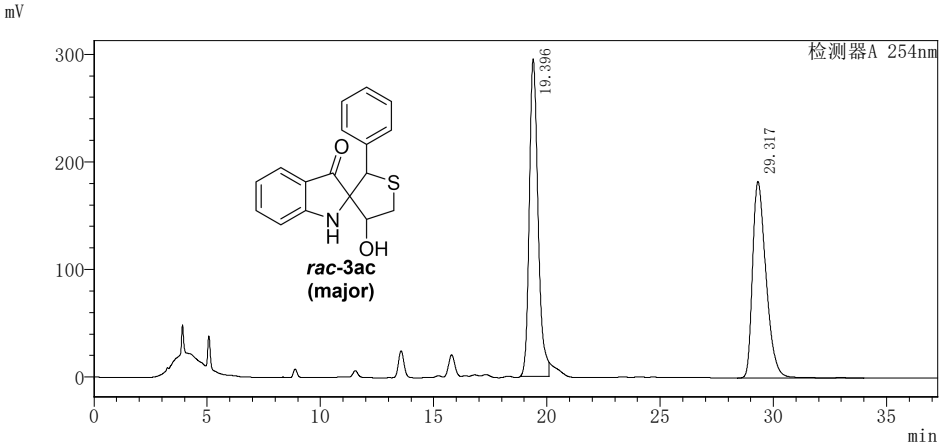


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	11.067	13077501	480618	50.055
2	PDA 254 nm	20.057	13048998	259256	49.945

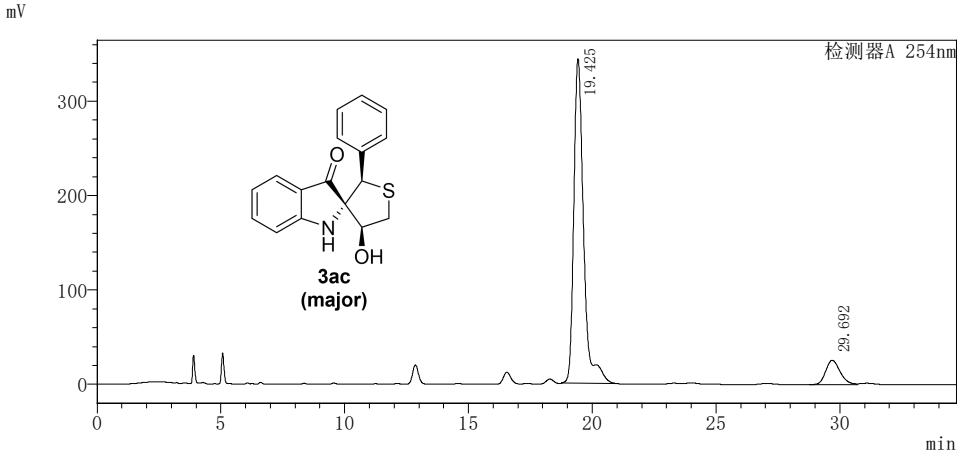


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	10.952	58598857	2066145	82.063
2	PDA 254 nm	19.273	12808721	270557	17.937

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.425 min (major), t_R = 29.692 min (minor), 80% ee.

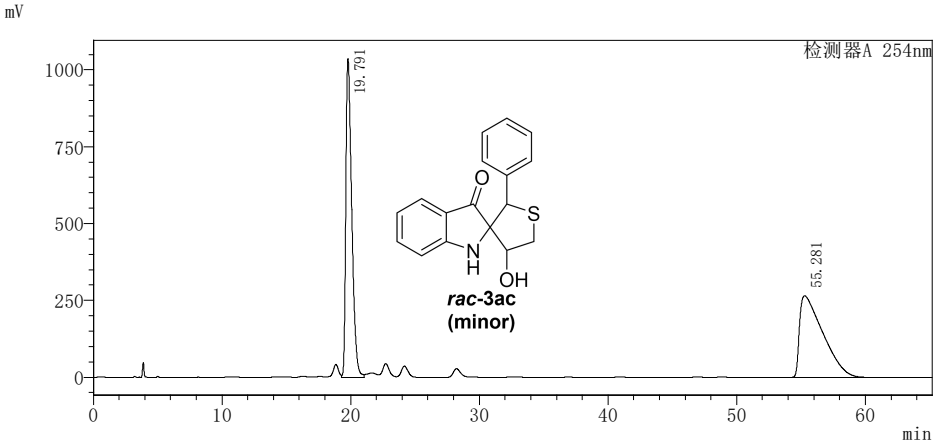


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.396	7950426	295495	51.322
2	PDA 254 nm	29.317	7540792	182559	48.678

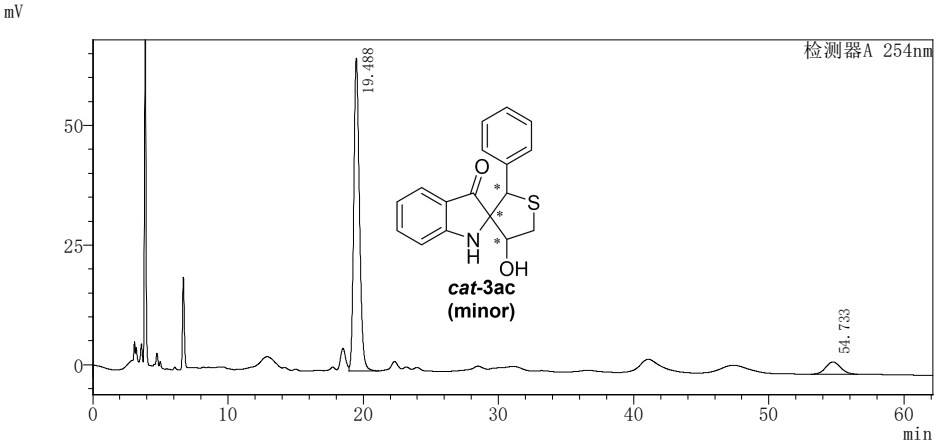


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.425	9467171	343940	90.103
2	PDA 254 nm	29.692	1039921	25754	9.897

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 19.488 min (major), t_R = 54.733 min (minor), 81% ee.

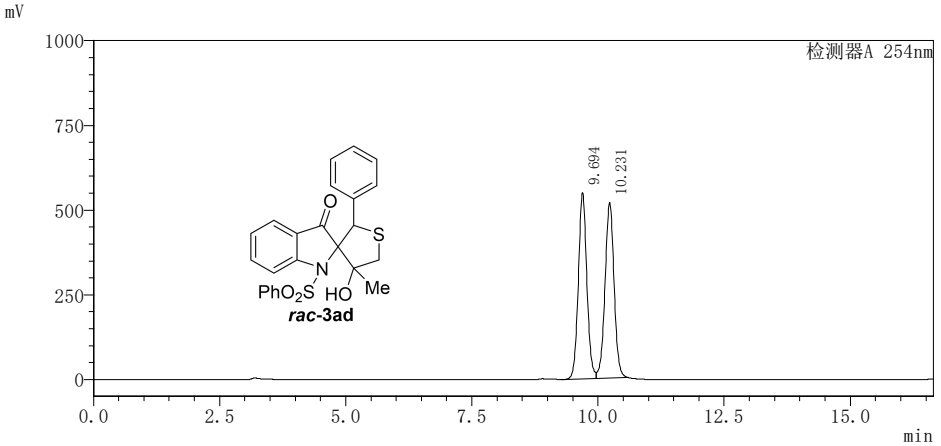


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.791	33244290	1037857	49.527
2	PDA 254 nm	55.281	33879845	266427	50.473

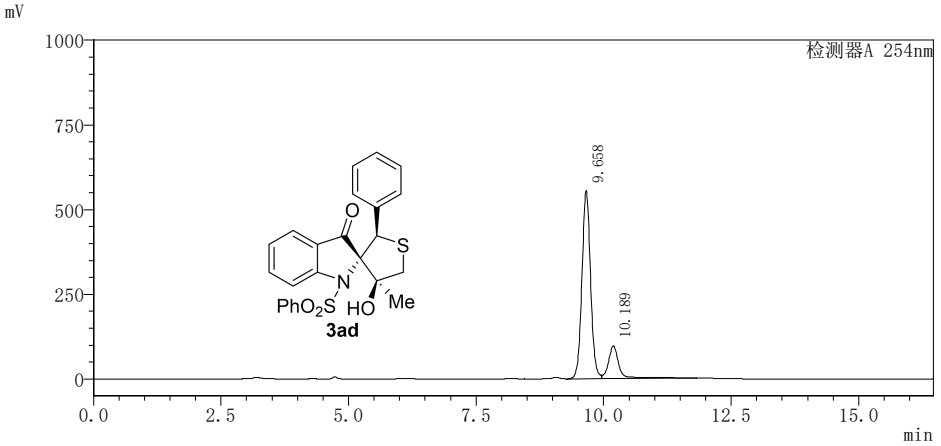


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.488	1911938	65394	90.742
2	PDA 254 nm	54.733	195076	2550	9.258

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 9.658 min (major), t_R = 10.189 min (minor), 64% ee.

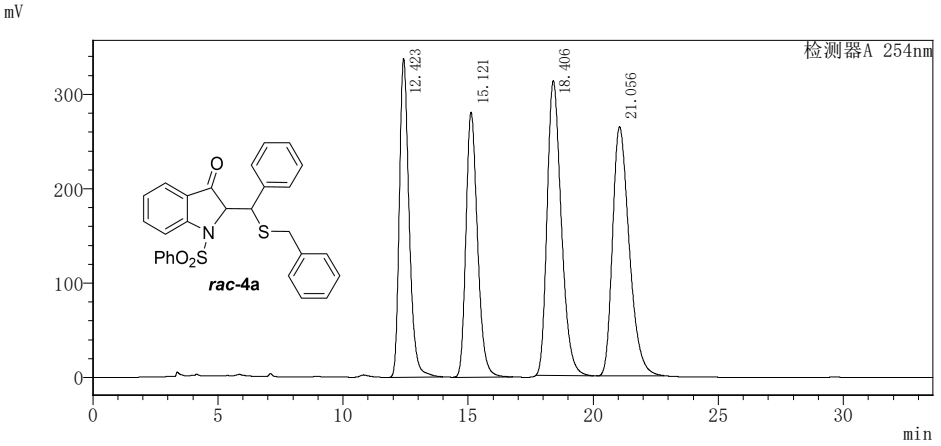


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	9.694	6505287	551082	50.063
2	PDA 254 nm	10.231	6488926	518760	49.937

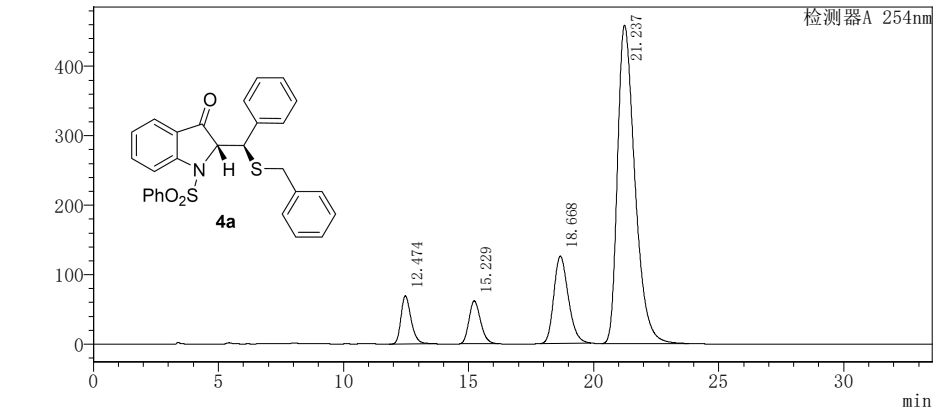


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	9.658	6543747	556586	81.992
2	PDA 254 nm	10.189	1437244	96965	18.008

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 18.668 min (minor), t_R = 21.237 min (major), 63% ee.

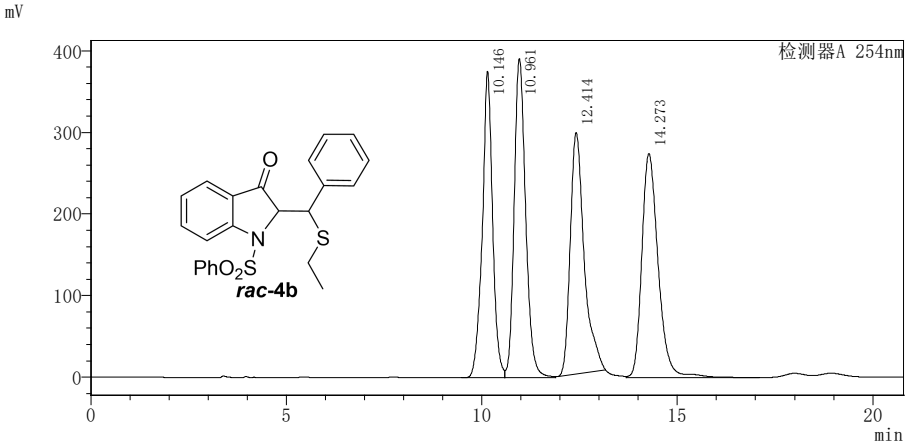


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	12.423	9125321	337753	21.372
2	PDA 254 nm	15.121	9007892	280736	21.097
3	PDA 254 nm	18.406	12304223	312388	28.817
4	PDA 254 nm	21.056	12260269	264122	28.714

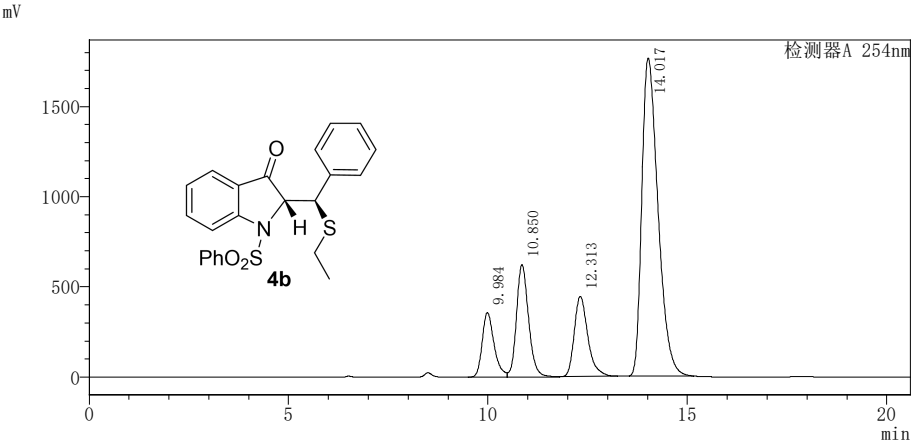


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	12.474	1953417	69353	6.275
2	PDA 254 nm	15.299	1982232	61730	6.368
3	PDA 254 nm	18.668	5042943	125449	16.200
4	PDA 254 nm	21.237	22150743	458390	71.157

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 10.850 min (minor), t_R = 14.017 min (major), 58% ee.

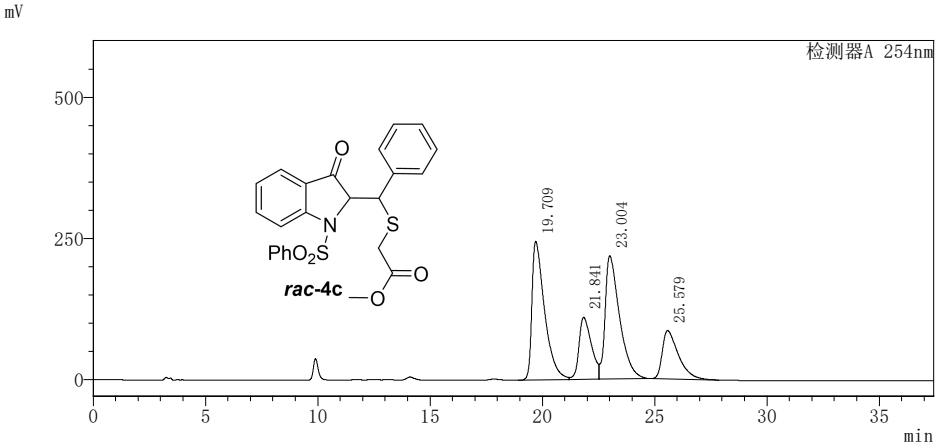


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	10.146	6885713	375764	22.803
2	PDA 254 nm	10.961	7989998	391316	26.459
3	PDA 254 nm	12.414	7329113	296009	24.271
4	PDA 254 nm	14.273	7992440	274785	26.467

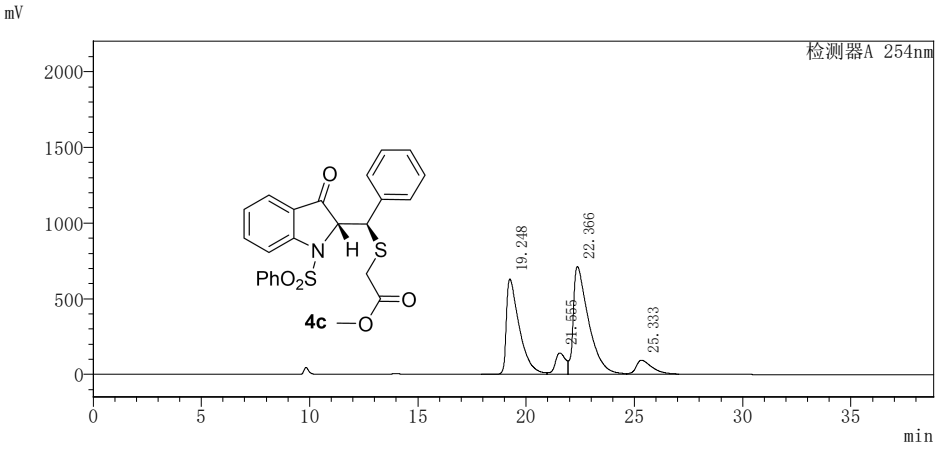


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	9.984	7479342	359695	9.240
2	PDA 254 nm	10.850	13277616	625266	16.403
3	PDA 254 nm	12.313	10472245	444262	12.937
4	PDA 254 nm	14.017	49717277	1762643	61.420

The **enantiomeric excess** was determined by HPLC with an IB-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 0.7 mL/min, λ = 254 nm), t_R = 19.248 min (minor), t_R = 22.366 min (major), 14% ee.

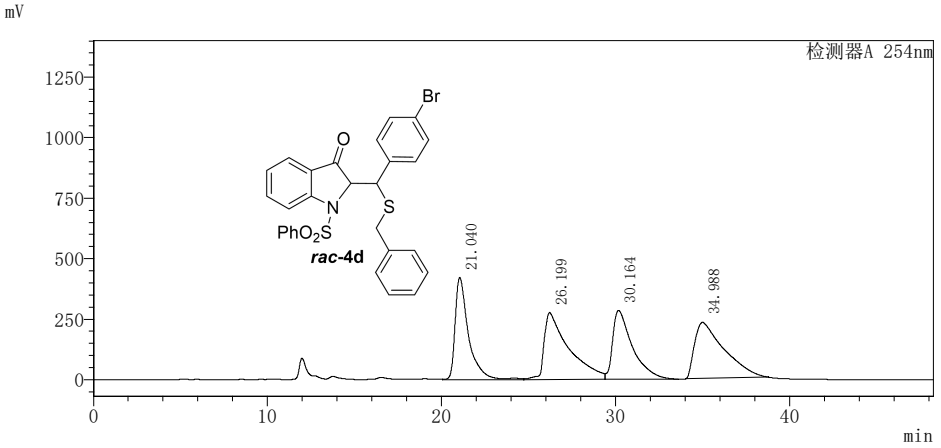


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.709	9677550	245743	34.498
2	PDA 254 nm	21.841	4287559	110201	15.284
3	PDA 254 nm	23.004	9783248	218736	34.874
4	PDA 254 nm	25.579	4304364	85925	15.344

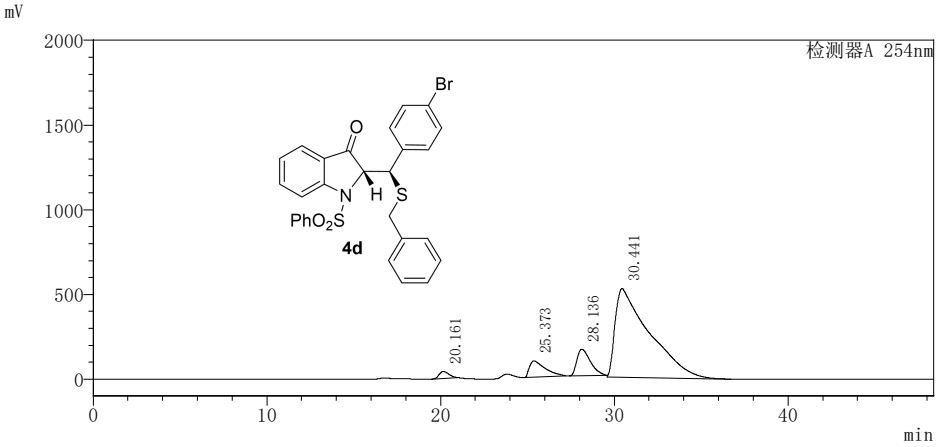


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	19.248	26187197	630271	37.121
2	PDA 254 nm	21.555	4658416	140720	6.603
3	PDA 254 nm	22.366	35072658	711453	49.717
4	PDA 254 nm	25.333	4626854	91699	6.559

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 0.7 mL/min, λ = 254 nm), t_R = 20.161 min (minor), t_R = 30.441 min (major), 84% ee.

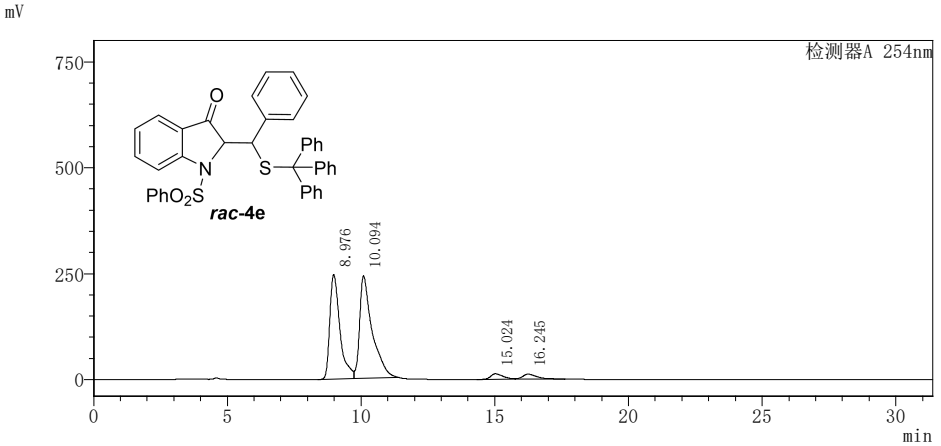


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	21.040	22599816	422912	22.653
2	PDA 254 nm	26.199	27245127	276781	27.309
3	PDA 254 nm	30.164	22497032	284823	22.550
4	PDA 254 nm	34.988	27423067	232320	27.488

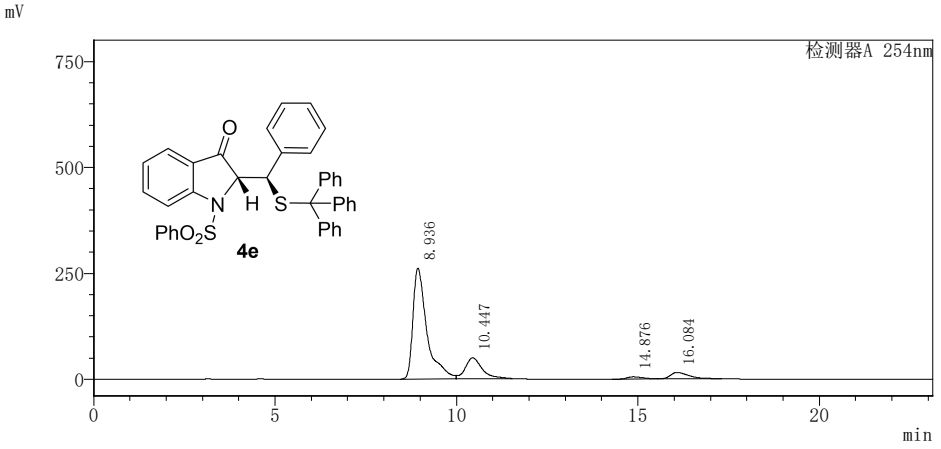


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	20.161	1605826	41159	1.820
2	PDA 254 nm	25.373	5981619	96595	6.781
3	PDA 254 nm	28.136	8492311	156946	9.627
4	PDA 254 nm	30.441	72132304	525039	81.772

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.936 min (major), t_R = 10.447 min (minor), 63% ee.

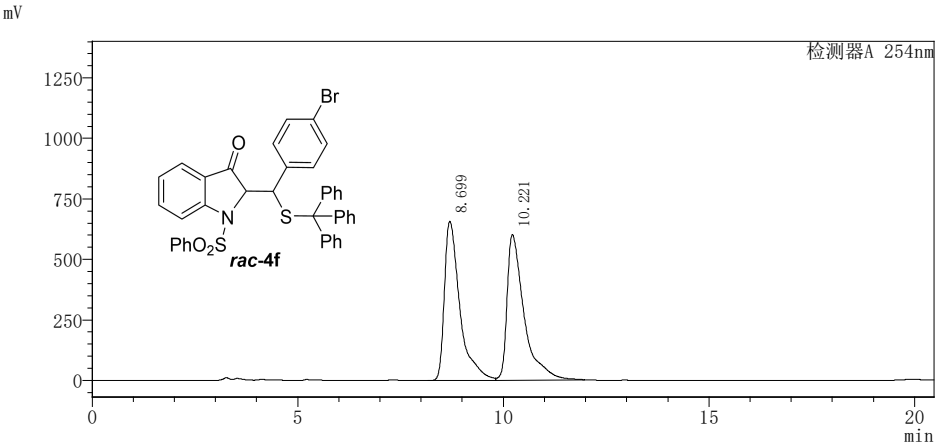


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.976	6372919	245096	47.303
2	PDA 254 nm	10.094	6292528	223431	46.705
3	PDA 254 nm	15.024	411651	13014	3.055
4	PDA 254 nm	16.245	11453	11453	2.937

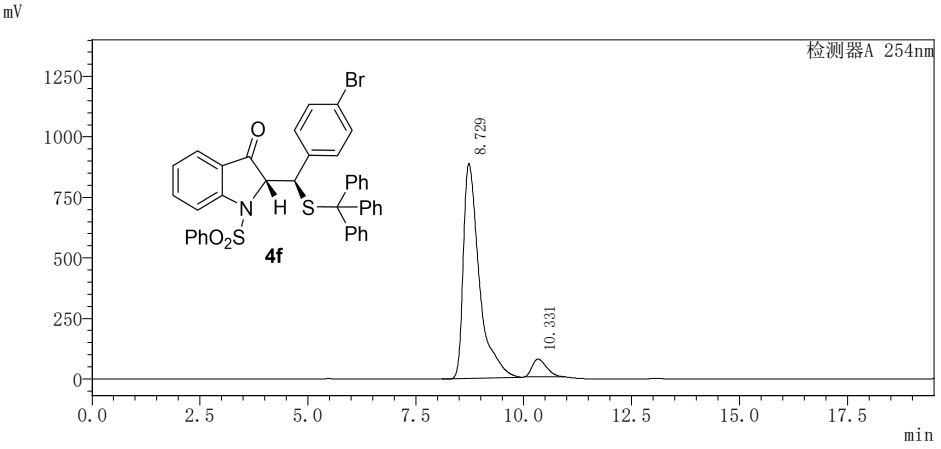


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.936	7013247	261446	75.437
2	PDA 254 nm	10.447	1593459	49431	17.140
3	PDA 254 nm	14.876	160806	5389	1.730
4	PDA 254 nm	16.084	529359	15185	5.693

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.729 min (major), t_R = 10.331 min (minor), 86% ee (By using mixed solvent with hexane and dichloromethane to control the recrystallization process, 96% ee was obtained in the liquid phase).

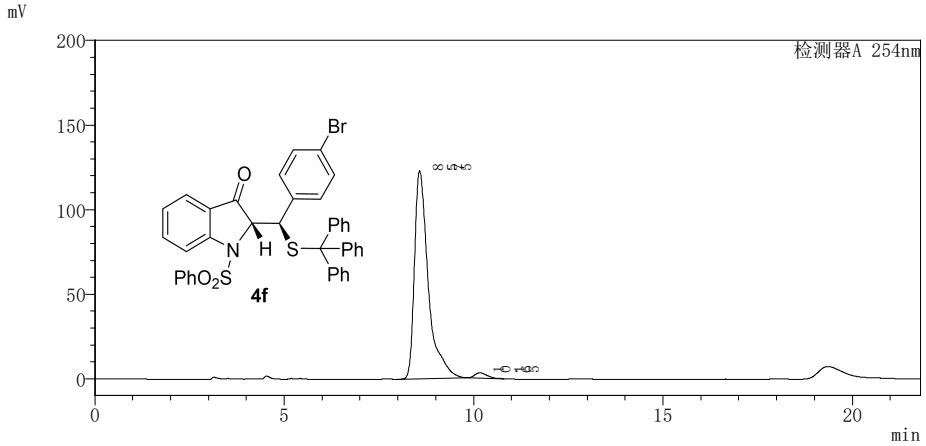


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.699	17251757	658412	49.922
2	PDA 254 nm	10.221	17305559	601911	50.078



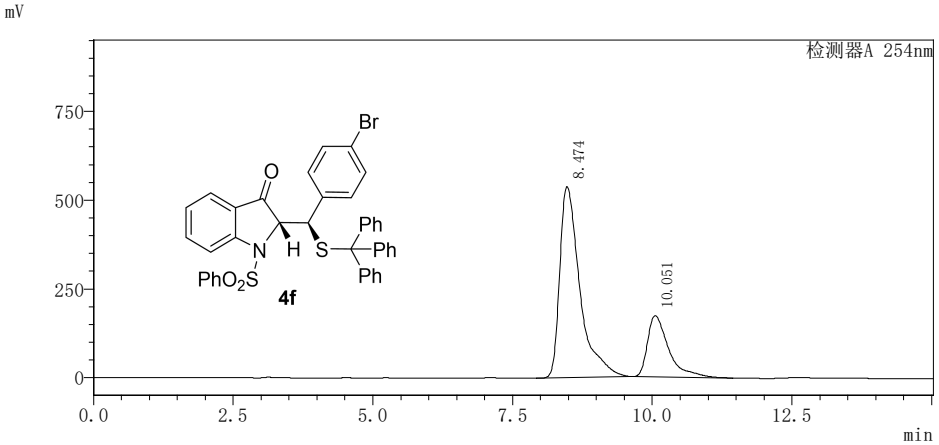
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.729	22921159	888754	93.100
2	PDA 254 nm	10.331	1698867	73715	6.900

Liquid phase of **4f**: the **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.575 min (major), t_R = 10.165 min (minor), 96% ee.



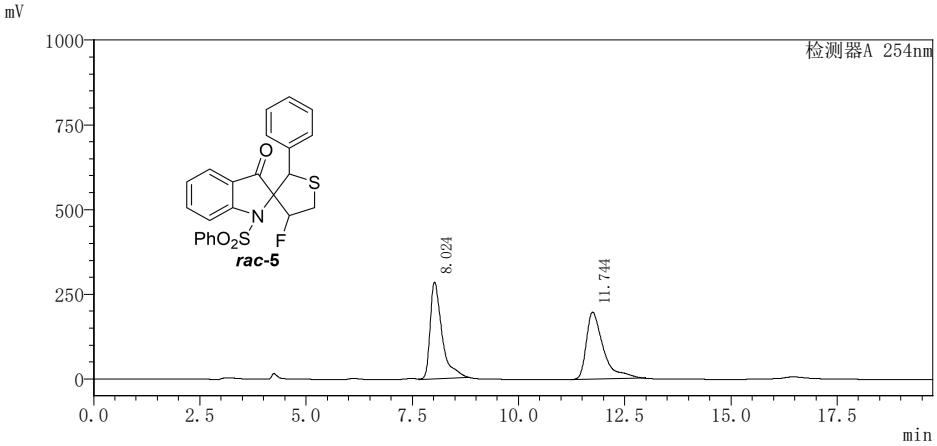
Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.575	3122249	122914	97.797
2	PDA 254 nm	10.165	70324	3155	2.203

Solid phase of **4f**: the **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.474 min (major), t_R = 10.051 min (minor), 50% ee.

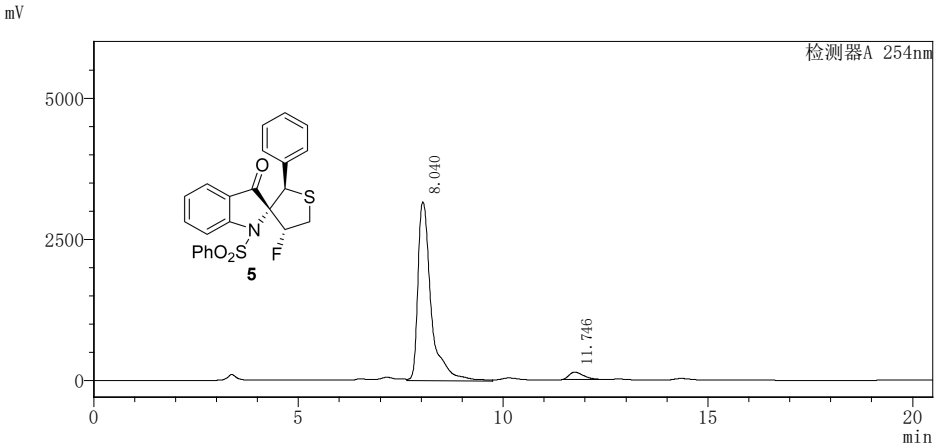


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.474	13530298	538026	74.845
2	PDA 254 nm	10.051	4547341	172629	25.155

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 8.040 min (major), t_R = 11.746 min (minor), 96% ee.

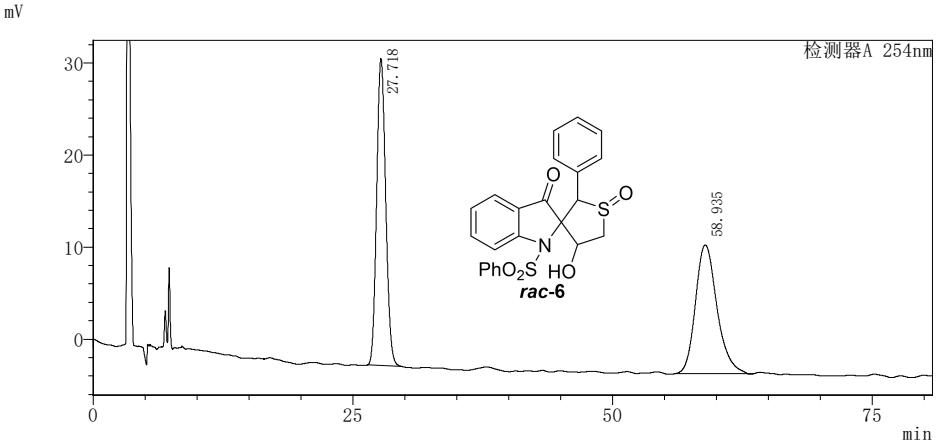


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.024	5558851	285661	50.038
2	PDA 254 nm	11.744	5550519	197881	49.962

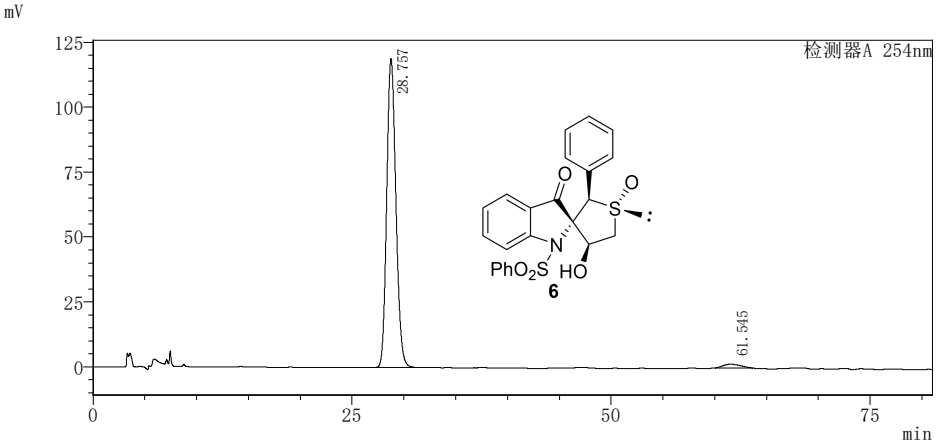


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	8.040	71458785	3163185	97.825
2	PDA 254 nm	11.746	1588730	93554	2.175

The **enantiomeric excess** was determined by HPLC with an IC-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 28.757 min (major), t_R = 61.545 min (minor), 96% ee.

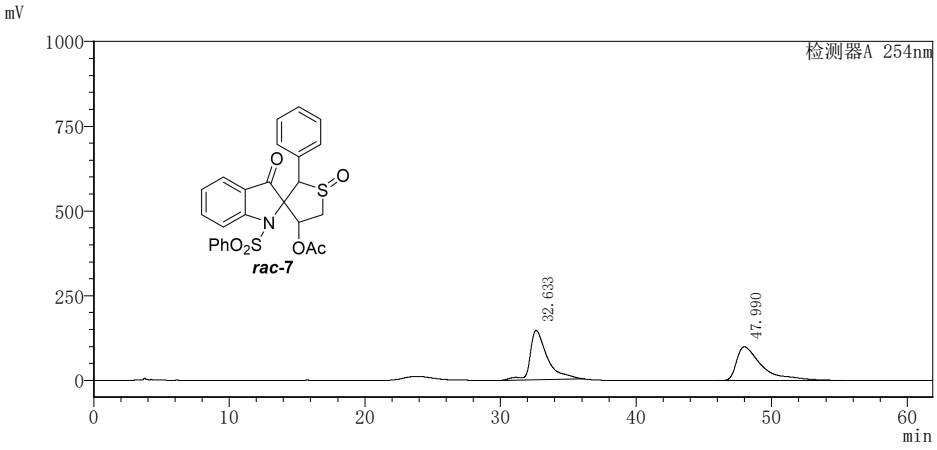


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	27.718	2021608	33382	50.037
2	PDA 254 nm	58.935	2018610	13996	49.963



Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	28.757	7337315	119135	97.865
2	PDA 254 nm	61.545	160043	1374	2.135

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 32.003 min (major), t_R = 47.945 min (minor), 99% ee.



Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
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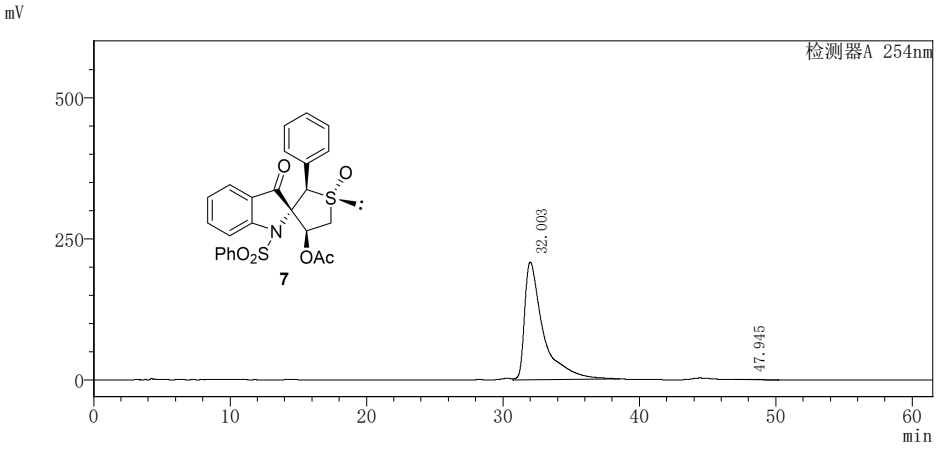
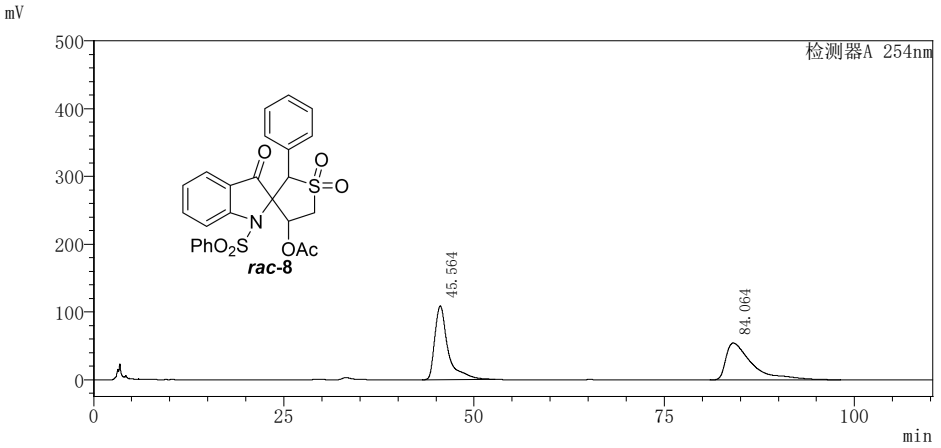
2	PDA 254 nm	47.990	13051046	99748	50.292

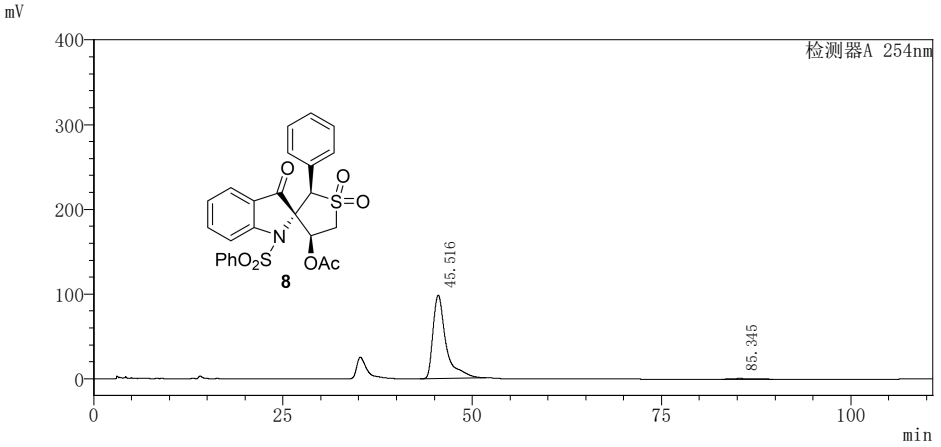


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	32.003	19907537	208503	99.792
2	PDA 254 nm	47.945	41486	456	0.208

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm), t_R = 45.516 min (major), t_R = 85.345 min (minor), 99% ee.

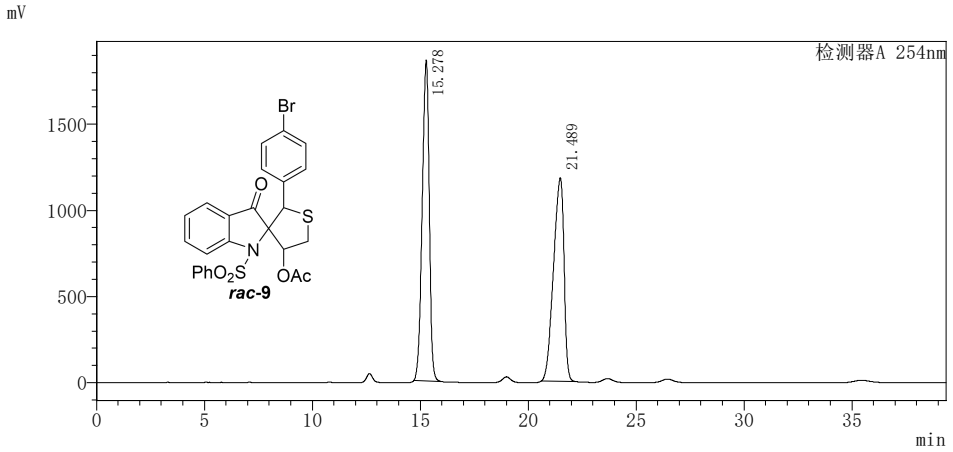


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	45.554	13183627	108871	50.123
2	PDA 254 nm	84.064	13118914	54610	49.877

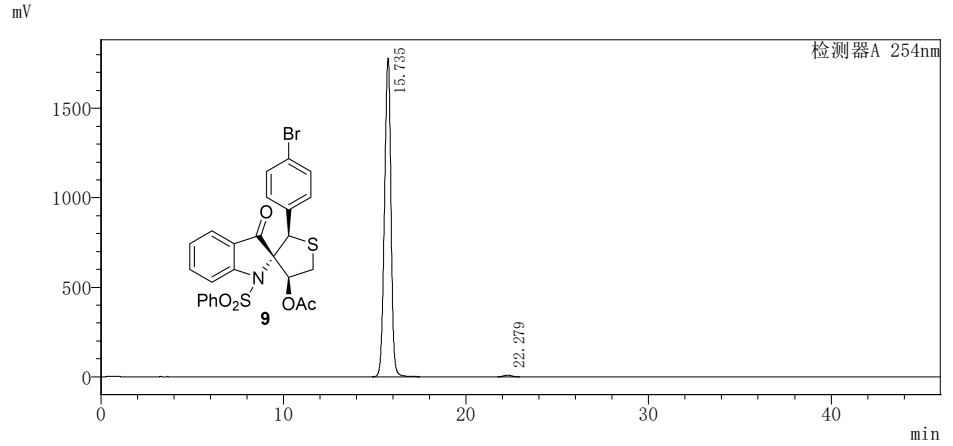


Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	45.516	11788032	98671	99.510
2	PDA 254 nm	85.345	58050	479	0.490

The **enantiomeric excess** was determined by HPLC with an IA-H column (*n*-hexane/*i*-PrOH = 90/10, flow rate 1 mL/min, λ = 254 nm), t_R = 15.735 min (major), t_R = 22.279 min (minor), 99% ee.



Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	15.278	42179636	1864109	51.263
2	PDA 254 nm	21.489	40101909	1181982	48.737



Peak	Processed Channel	Retention Time (min)	Peak Area (mAU*s)	Peak Hight (mAU)	Peak Area (%)
1	PDA 254 nm	15.735	43898320	1782473	99.365
2	PDA 254 nm	22.279	280661	9396	0.635

14. DFT calculations

All molecules were computed using density functional theory (DFT) at the WB97XD/6-31G* level of theory using the Gaussian 09 software package. The DFT method was chosen for its ability to accurately predict molecular properties and reaction pathways. The WB97XD functional was selected for its high accuracy in describing dispersion interactions, which can play a significant role in the behavior of molecules. The 6-31G* basis set was chosen for its balance between computational cost and accuracy in describing molecular electronic structure. This level of theory has been widely used in previous studies and has been shown to provide reliable results for a variety of molecular systems.

Based on the possible activation model of the cinchona-derived squaramide catalyzed asymmetric Michael addition reaction,[14] we performed DFT calculations using template substrates **1a** and **2a**. In computational studies, **1a** is the electrophile (**E**) in the reaction process, and the mercaptoglydehyde released by **2a** is the nucleophile (**Nu**). According to the relative position and reaction mode of substrate **1a**, we calculated the possible intermediates **Int3**-**Int10** and **In3'**, and the results showed that mode **A** catalytic mode had the lowest energy (**Figure S3**). In order to further investigate the effects of the configuration of substrate **1a** on the asymmetric sulfa-Michael/aldol cascade reaction, we replace **1a** (***Z***) in intermediate **Int3** with **1a'** (***E***) to optimize the intermediate **In3'**. Through the analysis visualization of optimized important intermediates **Int3**, **Int5**, and **Int3'**, it is not difficult to know that in the case of the intermediate **Int3**, the substrate induced mercaptoacetaldehyde to approach from the *Si* face (right side) of the (*Z*)-2-ylideneoxindole **1a** under the action of catalyst **B** hydrogen bonding. However, for the intermediate **Int5**, the binding situation is reversed, and mercaptoacetaldehyde is approached from the *Re* face (left side) of the (*Z*)-2-ylideneoxindole **1a**. It is worth noting that in the intermediate **Int3**, in addition to the hydrogen bonding of the squaramide catalyst **B**, there are also obvious π-π stacking interactions between the two pairs in the three benzene rings (2-ylideneoxindole **1a** (***Z***) phenyl ring of benzenesulfonyl group and its C2 double bond,

and benzene ring of catalyst **B** with trifluoromethyl substitution). The benzene ring π-π stacking interactions make the intermediate **Int3** more stable than the intermediate **Int5**. Therefore, nucleophilic addition from the right side in mode **A** is beneficial to Michael addition reaction. Although the energy of the intermediate **In3'** is only slightly less than that of the intermediate **In3** (ΔΔG = 0.3 kcal/mol), the (*E*)-2-ylideneoxindole **1a'** needs to overcome some steric hindrance in order to form the intermediate **In3'** by hydrogen bonding of the catalyst **B** due to the benzene ring facing up. It may be due to the above reasons that the intermediate **Int3** is the best intermediate to enter the subsequent reaction (**Figure S4**).

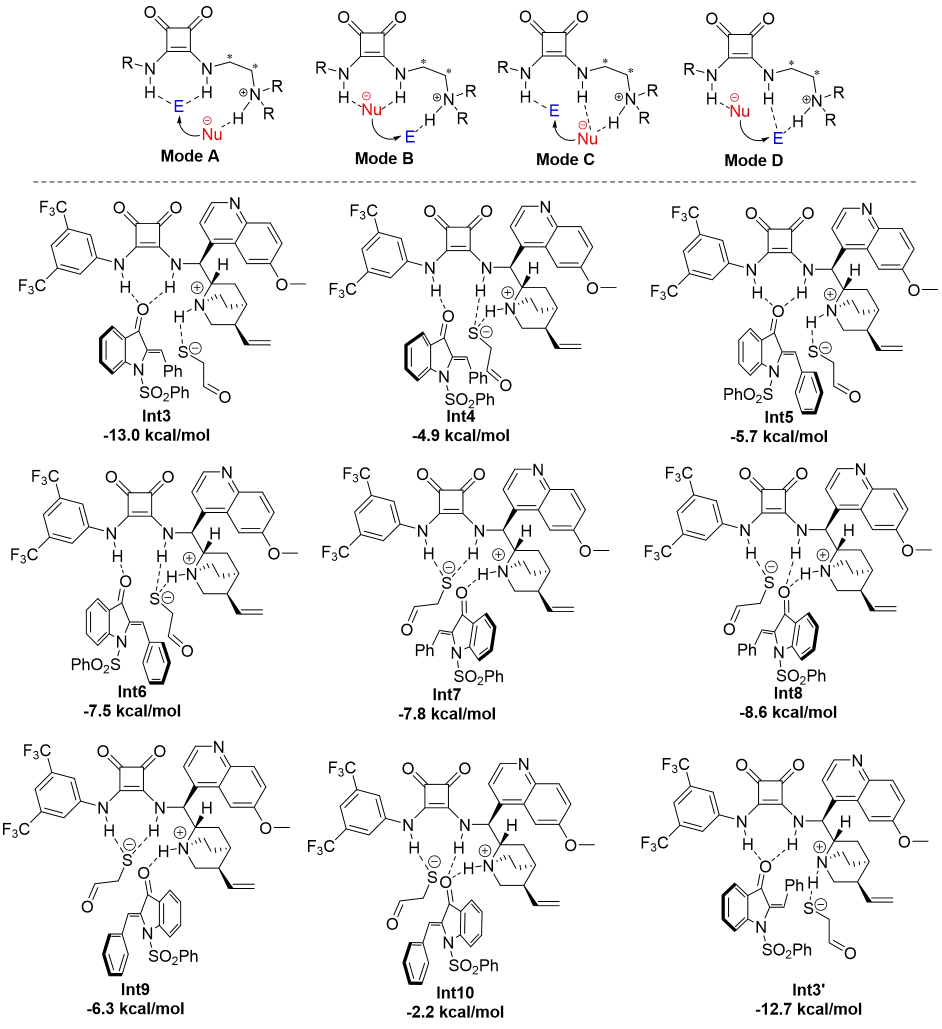


Figure S3. DFT-optimized structures and relative free energies (ΔG, kcal/mol) of **Int3-Int10** and **In3'** along four possible binding modes at the WB97XD/6-31G* level.

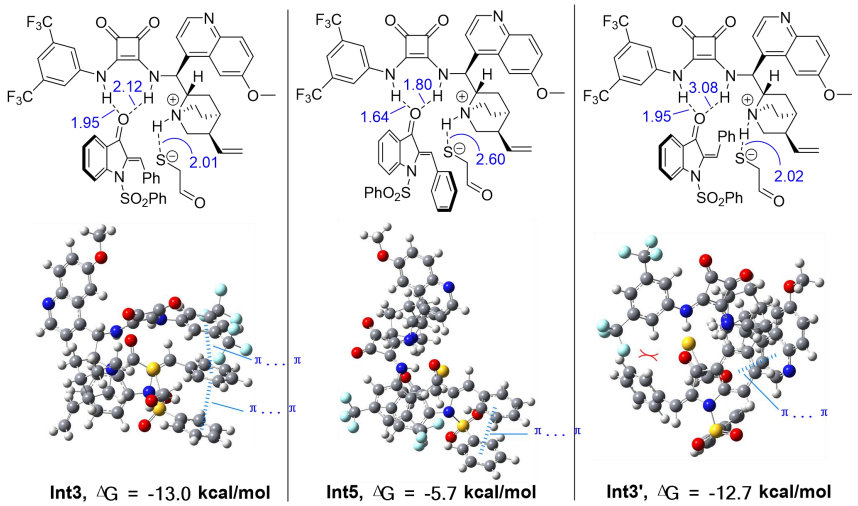


Figure S4. Analysis visualization of optimized key intermediates based on model **A**. All energies are in kcal/mol, and bond lengths are in angstroms (Å).

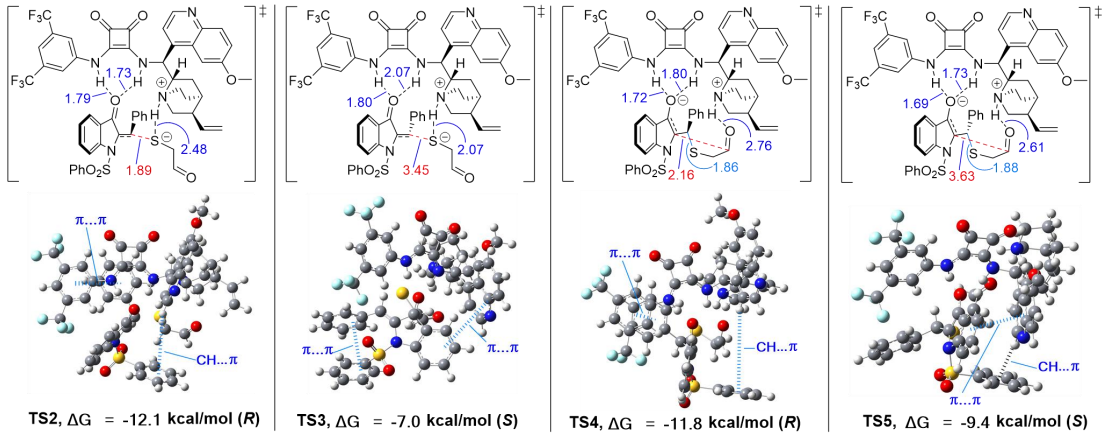


Figure S5. DFT-optimized structure of key transition states **TS2** and **TS3** for C−S bond formation, **TS4** and **TS5** for C−C bond formation in squaramide-catalyzed sulfa-Michael/aldol cascade reaction at the WB97XD/6-31G* level. The relative Gibbs energies are given in kcal/mol and intermolecular distances are in Å.

If the binding mode of catalyst **B** to substrate **1a** does not change during the subsequent reaction, it means that the stereoscopic configuration of the C2 carbon of indolin-3-one has been determined at this time (the subsequent aldol condensation reaction ring formation is cycloaddition to the right of indolin-3-one). We continue to explore the subsequent reaction based on the intermediate **Int3**, and then Michael addition forms the C-S bond. At the same time, with the generation of the chiral center, *R* configuration is generated through the transition state **TS2**, and *S*

configuration is generated through the transition state **TS3**. Through the analysis visualization of optimized transition state **TS2** and transition state **TS3**, we conclude that **TS2** has a lower energy. This may be due to the fact that in addition to the hydrogen bonding of catalyst **B**, the π-π stacking interaction of the benzene ring of the transition state **TS2** is stronger. Besides, the quinine ring of the catalyst and the benzene ring of the benzenesionyl group of the substrate are close to vertical, resulting in CH-π interaction.[15] These non-covalent interaction forces make the transition state **TS2** more stable. In addition, the distance between C-S in the transition state **TS2** ($d_{c\text{-}s}$ = 1.89 Å) is shorter than that between C-S in the transition state **TS3** ($d_{c\text{-}s}$ = 3.45 Å), indicating that C-S bonds are more easily formed in the transition state **TS2** in the subsequent transformation. In the subsequent transition states and intermediates, the subsequent transformation based on **TS2** basically continues the non-covalent interaction. Especially in the subsequent aldol condensation process, the transition state **TS4** has a similar interaction force to **TS2**. The C-C distance of transition state **TS4** ($d_{c\text{-}c}$ = 2.16 Å) to bond is also shorter than that of transition state **TS5** ($d_{c\text{-}c}$ = 3.63 Å) **(Figure S5)**.

According to the results of DFT calculations, the asymmetric reaction catalyzed by the cinchona-derived squaramide-catalyzed asymmetric sulfa-Michael/aldol cascade reaction is most likely to be the chiral sulfa-Michael addition through the transition **TS2**, and then the aldol condensation through the transition **TS4**, and finally the asymmetric construction of spiro[indoline-2,3'-thiophen]-3-one. The configuration of the final product selected by the theoretical calculation is consistent with the actual target compound.

Based on all the calculated intermediates and transition states, Gibbs free energy profiles for the overall catalytic pathways are shown in the **Figure S6**. A possible asymmetric catalytic cycle is shown in the **Figure S7**.

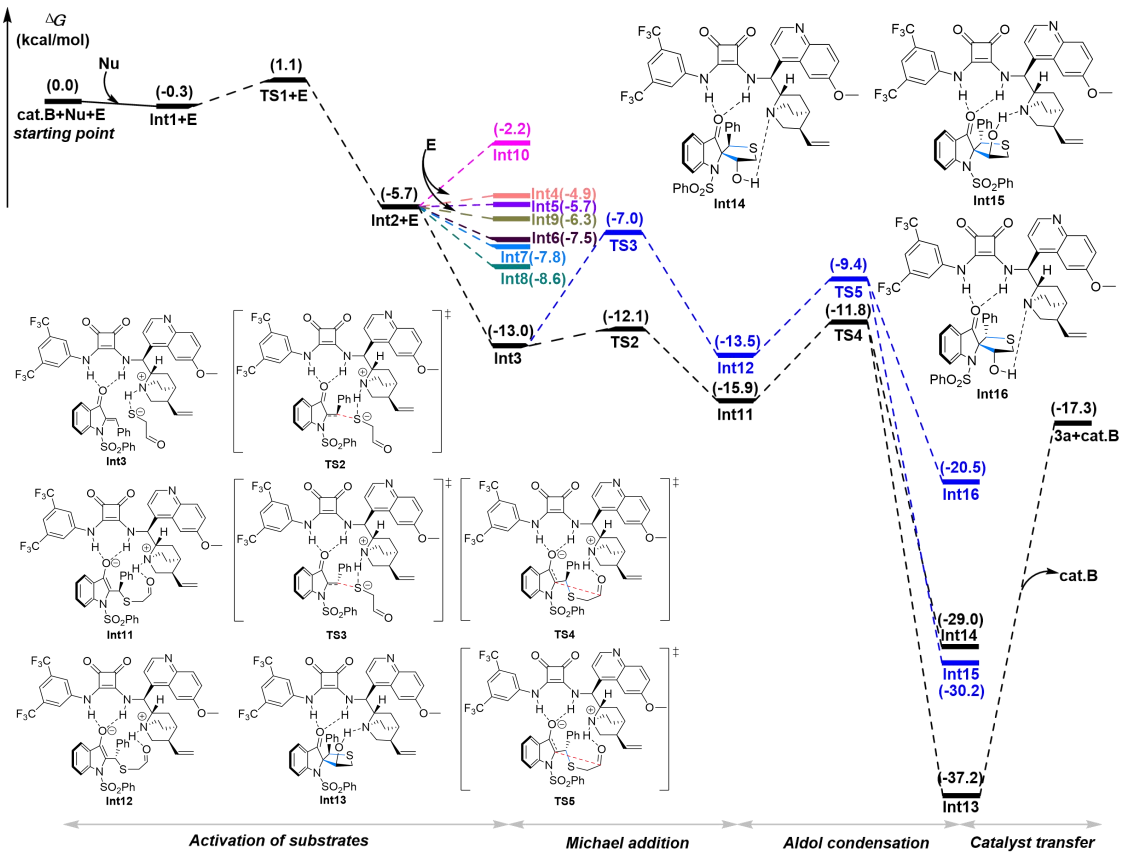


Figure S6. Gibbs free energy profiles for the overall catalytic pathways. The relative Gibbs energies are given in kcal/mol.

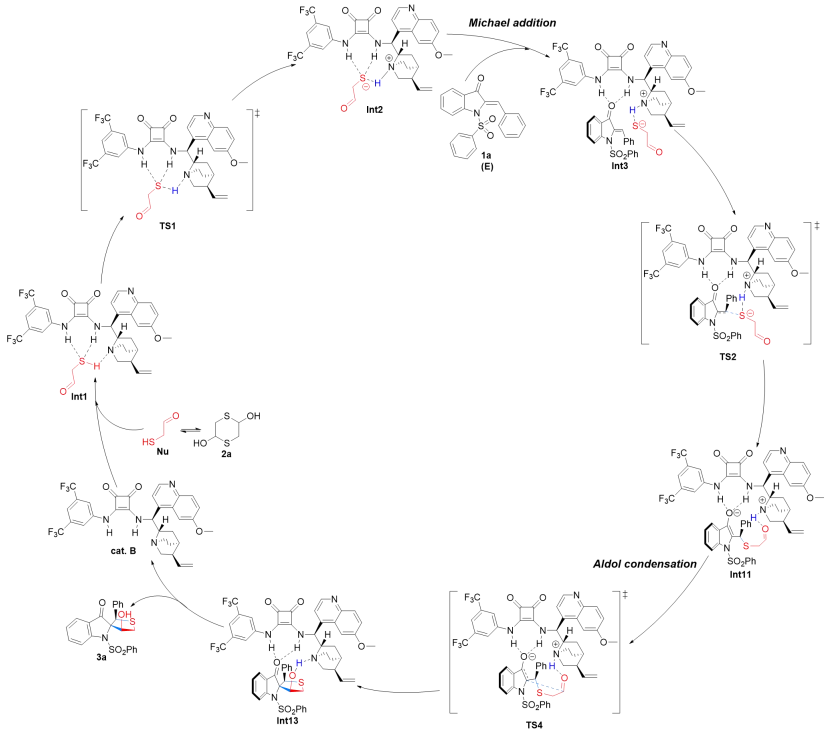
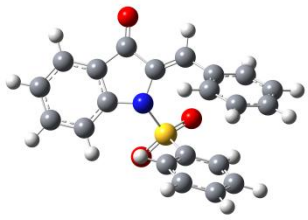


Figure S7. A proposed full catalytic cycle.

Cartesian coordinates of the optimized structures



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-933194.57 kcal/mol

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C	4.27583400	-1.84727400	-0.54586300
C	5.13357400	-0.74905400	-0.67296200
C	4.63114700	0.53880000	-0.54944400
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H	4.67880700	-2.85047500	-0.64749500
H	6.18766000	-0.90890500	-0.87462500
H	5.26181600	1.41617000	-0.65212200
C	2.47600700	1.92470200	-0.16728000
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C	-1.83982700	1.22937400	-1.37564800
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C	-3.19383700	0.98882000	-1.57876300
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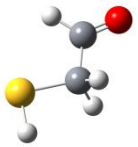

Nu

-346322.89 kcal/mol

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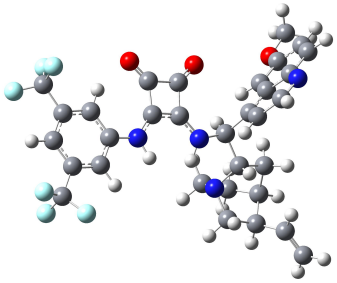

cat. B

-1429937.65 kcal/mol

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F	7.87364100	2.17361100	1.05364000
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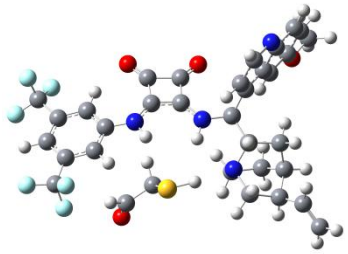

Int1

-1776260.85 kcal/mol

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H	-5.45306200	2.90334700	-1.39510100
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C	-2.47275000	3.84362500	0.07045600
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C	5.42815800	-1.67272000	-0.27790900
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C	6.42370200	1.69747900	1.11603000
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F	7.19044300	-2.55659300	-1.57506500
F	7.74147100	1.46463600	1.10620200
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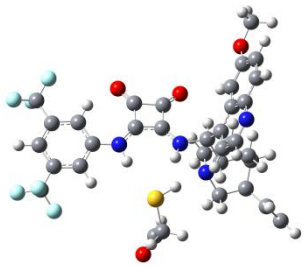
F	6.09440900	2.14434800	2.33909300
N	2.09029300	-0.49622300	0.82287100
C	1.08581100	-1.29523300	0.36573000
C	-0.27553900	-1.03505100	0.31891400
C	-0.58537200	-2.35286700	-0.28621800
C	0.92170000	-2.65683800	-0.21269300
O	1.64191000	-3.57393000	-0.52245800
O	-1.58331400	-2.89575300	-0.68654800
H	1.79440200	0.39969700	1.19806400
N	-1.03077500	0.02039400	0.65606900
H	-0.57699600	0.91219600	0.80324800
C	-6.51372700	-3.28162000	0.11938600
C	-6.13912300	-3.18952900	1.43370000
C	-5.04955600	-2.38077100	1.83647900
C	-4.33495900	-1.64415600	0.84673200
C	-4.73008100	-1.76478200	-0.50463400
C	-5.79346200	-2.56146500	-0.86639000
H	-7.35148600	-3.91181400	-0.15544000
H	-6.66590900	-3.73758500	2.20757300
C	-2.95619100	-0.83992900	2.64138500
C	-3.72601600	-1.61989300	3.53318100
H	-2.12302000	-0.25697800	3.02293300
H	-3.48376300	-1.61894000	4.59438500
N	-4.74255000	-2.35750700	3.16337000
O	-6.08677400	-2.59997900	-2.18945900
C	-7.10848700	-3.46788100	-2.63038400
H	-7.13674800	-3.36666100	-3.71574600
H	-8.08583800	-3.18598000	-2.21837600
H	-6.89050800	-4.51141000	-2.37190100
H	-4.19257100	-1.26713200	-1.30262600
C	-3.53215200	2.23595500	-2.16566700
H	-3.85837300	1.22752800	-2.44555200
H	-3.61836600	2.86148500	-3.06007300
C	-4.76629700	4.88461100	0.35222300
C	-5.30761500	6.07095700	0.09165400
H	-4.97812200	4.40494700	1.30913700
H	-5.96008100	6.56884600	0.80248500
H	-5.11784800	6.59018500	-0.84534100
C	-3.25358800	-0.82904400	1.30288600
C	-2.46063500	0.07572600	0.37082200
H	-2.62331200	-0.24174100	-0.66271900
C	-2.91642400	1.53893500	0.53557100
H	-2.79250300	1.78528700	1.59740700
C	3.08270900	2.64853800	-1.73697600
O	3.31837100	2.99618700	-2.86564300
H	3.86923900	2.64767100	-0.95664000
C	1.71168200	2.15988600	-1.30640400
H	0.98480200	2.46869700	-2.05922600
H	1.73203100	1.06430000	-1.25907800
S	1.27495800	2.85039000	0.33785600
H	-0.07990900	2.75980900	0.16873900

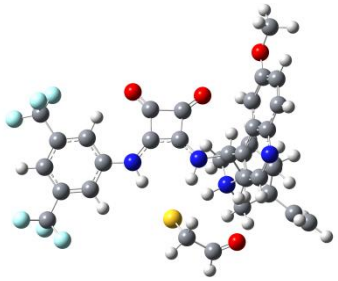


TS1

-1776259.404 kcal/mol

C	-4.55919200	1.29813700	-0.15716700
C	-4.79144800	1.99449800	-1.50566200
C	-2.41872700	1.57055500	-2.17013700
H	-4.88555200	0.25461000	-0.23273700
H	-5.84469000	1.91675900	-1.79052900
H	-1.83707000	0.64765700	-2.19917200
H	-1.93942300	2.26676800	-2.86537200
H	-5.16039300	1.75115200	0.63656600
N	-2.32160000	2.17460700	-0.82952600
C	-2.92552800	3.51389500	-0.87239200
H	-2.29154200	4.15872800	-1.49102500
H	-2.90599100	3.92115800	0.14629600
C	-4.38382600	3.48417900	-1.42137800
H	-4.39166300	3.88688200	-2.44199200
C	5.75778900	0.34122200	0.88809900
C	4.37717700	0.47168300	0.91828600
C	3.57369800	-0.42731400	0.21200900
C	4.16486000	-1.45263800	-0.52649000

C	5.55123400	-1.55993400	-0.54449900
C	6.36123300	-0.67599500	0.15736600
H	3.92429300	1.28022800	1.48440600
H	3.55746400	-2.14709000	-1.09943600
H	7.43939300	-0.77515800	0.13425000
C	6.18310100	-2.62936000	-1.40033100
C	6.60719400	1.27515300	1.70955600
F	6.32386900	-2.21391900	-2.66955200
F	5.44376600	-3.74656300	-1.42560600
F	7.40646100	-2.96157100	-0.95413800
F	7.80793000	1.47843400	1.14790700
F	6.02204000	2.47450200	1.86544800
F	6.82415500	0.78032900	2.94071600
N	2.18584700	-0.25611400	0.30480000
C	1.19722000	-0.86170200	-0.40047100
C	-0.18194400	-0.70663800	-0.29341400
C	-0.43941100	-1.58155900	-1.45354900
C	1.06717300	-1.83402400	-1.52149700
O	1.80251400	-2.52426600	-2.18411100
O	-1.42317600	-1.88481100	-2.09323700
H	1.90113500	0.54978500	0.84830100
N	-0.99598800	-0.00315900	0.50339600
H	-0.61724200	0.46107100	1.31866300
C	-5.28070500	-4.37836800	1.21180500
C	-5.14191100	-3.74126700	2.41670700
C	-4.40970500	-2.53653800	2.53243100
C	-3.81154600	-1.97794400	1.36298800
C	-3.95426100	-2.65685800	0.13086100
C	-4.67393200	-3.83106200	0.05339800
H	-5.84810900	-5.30012700	1.15730800
H	-5.58902500	-4.14287300	3.31983500
C	-3.02174500	-0.20974400	2.78542100
C	-3.63688400	-0.86193800	3.87821700
H	-2.49273100	0.72275300	2.96819500
H	-3.56431100	-0.42743900	4.87360600
N	-4.31587000	-1.97555100	3.77043800
O	-4.75206600	-4.40040800	-1.17166900
C	-5.41864200	-5.63680300	-1.30672800
H	-5.32393900	-5.91084400	-2.35767200
H	-6.48267400	-5.55357300	-1.05116600
H	-4.95451200	-6.41538700	-0.68858800
H	-3.47525100	-2.31205000	-0.77916900
C	-3.89842600	1.31291000	-2.55410000
H	-4.10724500	0.23726500	-2.57817800
H	-4.11337300	1.70448500	-3.55381900
C	-5.31246100	4.31805200	-0.58726300
C	-6.02925400	5.34111900	-1.04345300
H	-5.38254300	4.05262400	0.46897900
H	-6.68699100	5.91167100	-0.39472500
H	-5.98586100	5.64622500	-2.08679900
C	-3.10302700	-0.74630600	1.52462400
C	-2.44791200	-0.02986400	0.35229400
H	-2.63398400	-0.58754900	-0.56426600
C	-3.04223400	1.38027600	0.18305200
H	-2.90115900	1.92272400	1.12598400
C	0.65315300	5.30358700	-0.73446500
O	1.33863900	6.28346700	-0.87176200
H	0.18165900	4.79849100	-1.60523000
C	0.35839100	4.66613600	0.60948200
H	1.05029700	5.06491000	1.35374500
H	-0.66261800	4.91899100	0.91616800
S	0.54793100	2.85409500	0.54707200
H	-0.60826200	2.54713600	-0.14768800

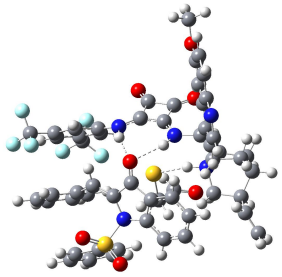


Int2

-1776266.27 kcal/mol

C	4.23961300	-1.42477700	-0.92904100
C	4.08488000	-1.89145000	-2.38377200
C	1.64125400	-1.36178400	-2.42829500
H	4.65141600	-0.41037900	-0.90852000
H	5.03630800	-1.79322600	-2.91235600
H	1.06548000	-0.46780300	-2.19955800
H	1.02447700	-2.00484100	-3.06009400
H	4.94240000	-2.05902800	-0.38281100
N	1.87597500	-2.12027500	-1.16233100
C	2.39603000	-3.48780100	-1.48673500
H	1.57158400	-4.04904200	-1.93119900
H	2.64939200	-3.95787000	-0.53346200
C	3.61928500	-3.36753800	-2.42439400
H	3.30825400	-3.58775300	-3.45289200
C	-5.72208300	-0.72183200	0.65668700
C	-4.33781300	-0.78671700	0.66878200

C	-3.58566700	0.26837800	0.13954100
C	-4.23233300	1.37573900	-0.40743900
C	-5.62407600	1.41490800	-0.40943400
C	-6.38218800	0.38104000	0.12154000
H	-3.83251100	-1.65522300	1.08111900
H	-3.66391400	2.18847300	-0.85092800
H	-7.46388500	0.42953500	0.11815800
C	-6.30004900	2.64456600	-0.96041900
C	-6.52727400	-1.88627900	1.16992200
F	-5.74979000	3.03246600	-2.11973800
F	-6.19618300	3.67877000	-0.10797600
F	-7.60968100	2.44183900	-1.18125600
F	-7.67634900	-1.48175100	1.73597800
F	-6.85497600	-2.73019700	0.17611500
F	-5.85331800	-2.59837600	2.08718100
N	-2.19277800	0.14854800	0.20986700
C	-1.24279200	0.92847000	-0.34643100
C	0.14432900	0.82393000	-0.24830400
C	0.36764300	1.85272100	-1.27205800
C	-1.14208500	2.08865700	-1.28209300
O	-1.90054600	2.85880400	-1.81883300
O	1.33534600	2.22849800	-1.90647200
H	-1.84944200	-0.74399500	0.58388200
N	0.97323600	0.03211800	0.45093000
H	0.54935600	-0.73416300	0.96779000
C	5.39906000	4.08337400	1.48223300
C	5.42160400	3.21245400	2.53965400
C	4.69418800	1.99987600	2.51036300
C	3.92889600	1.68162900	1.34829400
C	3.90606100	2.59921600	0.27260200
C	4.62599300	3.77441100	0.33521500
H	5.96705500	5.00486000	1.53608800
H	5.99743200	3.42772000	3.43350100
C	3.32059100	-0.35359300	2.48007500
C	4.09398700	0.07615100	3.58320200
H	2.82241900	-1.31798700	2.54364000
H	4.15700500	-0.55317100	4.46888400
N	4.76722900	1.19811000	3.60942800
O	4.53936200	4.58268800	-0.74723600
C	5.19027100	5.83391600	-0.71550400
H	4.94976200	6.31699700	-1.66287100
H	6.27922400	5.72289200	-0.63485400
H	4.82546700	6.45841100	0.10956900
H	3.29592700	2.44318300	-0.61108100
C	3.00574500	-1.03248000	-3.06267300
H	3.22808300	0.03222500	-2.93918300
H	2.97193100	-1.23409100	-4.13703700
C	4.69109700	-4.34962600	-2.04136800
C	5.20769100	-5.25262100	-2.86870900
H	5.04894900	-4.29936900	-1.01267800
H	5.98787100	-5.93597100	-2.54841700
H	4.86918600	-5.34397300	-3.89851000
C	3.23286300	0.43198500	1.35744800
C	2.39972900	-0.02750800	0.16663000
H	2.56633200	0.64527000	-0.67467000
C	2.85575800	-1.44101600	-0.24057200
H	2.86129400	-2.08742600	0.63788500
C	1.12771700	-4.11092000	1.94227000
O	2.30820200	-3.81928300	1.84191400
H	0.79196900	-5.14561900	1.73899000
C	0.03941700	-3.13277400	2.23071000
H	-0.72229800	-3.56828000	2.88300200
H	0.45326700	-2.23558900	2.70309100
S	-0.70570600	-2.81070600	0.57241800
H	0.96559500	-2.26963400	-0.62371300



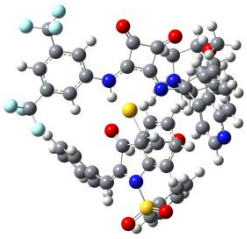
Int3

-2709468.13 kcal/mol

C	-5.08371300	-2.12889300	1.01442800
C	-4.82016500	-3.03885200	2.22152200
C	-3.20611000	-1.27683500	2.97483900
H	-5.79125600	-1.34134100	1.29988700
H	-5.72476600	-3.60078000	2.46946200
H	-3.46530700	-0.21927100	2.91217400
H	-2.34631700	-1.37533900	3.63897800
H	-5.54967100	-2.67923800	0.19380200
N	-2.73752700	-1.72195000	1.62538600
C	-2.39442100	-3.17964700	1.67041400
H	-1.67302100	-3.29721200	2.48184300
H	-1.89668300	-3.41468000	0.72564500
C	-3.67129200	-4.02406900	1.90597500
H	-3.51269000	-4.64532900	2.79453900

C	3.49311800	3.68446000	-0.71621000
C	2.15799500	3.39180500	-0.96975700
C	1.36928500	2.82805700	0.02967500
C	1.91186600	2.59363800	1.29258000
C	3.23574500	2.93129700	1.53837100
C	4.04085800	3.47001700	0.54162000
H	1.73138200	3.57314800	-1.95177900
H	1.32238000	2.09487500	2.05186200
H	5.08543000	3.67991400	0.73020200
C	3.80332500	2.65783800	2.90576700
C	4.32925400	4.25617400	-1.82723500
F	3.38777500	1.46853700	3.38176000
F	3.43029000	3.58799600	3.79571500
F	5.14855200	2.63222700	2.89729600
F	5.64393400	4.14483500	-1.58396800
F	4.08215500	3.62991400	-2.99563000
F	4.06964700	5.55929900	-2.02722400
N	0.06033700	2.42089900	-0.29531600
C	-0.93107200	2.31243200	0.60999600
C	-2.10195100	1.56716100	0.64360700
C	-2.51405800	2.14394300	1.93167300
C	-1.22671700	2.96707700	1.91087400
O	-0.67157600	3.76292700	2.62617700
O	-3.48306500	1.99841500	2.65597000
H	-0.04095800	1.87297000	-1.15012700
N	-2.63989900	0.61780800	-0.14323200
H	-2.17041000	0.38899200	-1.01574100
C	-6.76329900	3.92452800	-1.70973000
C	-6.91769300	2.88015000	-2.58369900
C	-6.30032600	1.62955400	-2.35129600
C	-5.49980200	1.46192700	-1.18377000
C	-5.36360200	2.54363700	-0.28771400
C	-5.97844600	3.75251000	-0.54240500
H	-7.24807800	4.87143000	-1.91697200
H	-7.51901300	2.98198400	-3.48083800
C	-5.11663100	-0.78591300	-1.93292800
C	-5.94226700	-0.51203200	-3.05056500
H	-4.68974300	-1.77978600	-1.84854800
H	-6.12165200	-1.29427300	-3.78624500
N	-6.51140700	0.64360000	-3.26981300
O	-5.78185300	4.72283200	0.37813700
C	-6.36920100	5.98921000	0.17119600
H	-6.06860900	6.59715600	1.02463000
H	-7.46433700	5.92679200	0.14078700
H	-6.00398100	6.45775700	-0.75127800
H	-4.79440800	2.46421100	0.63120700
C	-4.39315400	-2.16060400	3.40647600
H	-5.22853600	-1.53126100	3.72736400
H	-4.11127000	-2.78903300	4.25710000
C	-3.97471000	-4.93421000	0.74834900
C	-4.09804700	-6.25493200	0.83824700
H	-4.08993200	-4.45755300	-0.22509300
H	-4.32525800	-6.86715400	-0.02947100
H	-3.97783000	-6.77495900	1.78601700
C	-4.87582400	0.18541500	-0.99426900
C	-3.91221300	-0.01431000	0.16966800
H	-4.31006500	0.50702300	1.04429300
C	-3.75376000	-1.49652900	0.54663700
H	-3.33994900	-2.03612600	-0.30885800
C	-0.52894100	-2.01475100	-2.12227800
C	0.44404600	-2.92754000	-1.71319400
C	0.09695300	-4.25681200	-1.47627900
C	-1.21615100	-4.63741700	-1.73452800
C	-2.17506600	-3.73412200	-2.21508600
C	-1.83479700	-2.40253800	-2.39767700
H	0.82527800	-4.98197300	-1.13992800
H	-1.50297500	-5.66986000	-1.56044200
H	-3.17788300	-4.08282300	-2.44331200
H	-2.54783600	-1.66709600	-2.75933900
C	0.07708400	-0.69053300	-2.16361500
N	1.70332100	-2.28428000	-1.55795000
C	1.50981300	-0.89441500	-1.84123400
S	3.10816700	-3.07503100	-2.19322100
C	4.19029100	-3.15032700	-0.79165600
C	5.52371800	-2.80648400	-0.96910100
C	6.39268000	-2.93926900	0.10917200
C	5.92249700	-3.40088400	1.33429800
C	4.57926800	-3.74097700	1.49304100
C	3.70408900	-3.62695500	0.42144700
H	5.86147900	-2.41269300	-1.92085200
H	7.43496200	-2.66150600	-0.00668700
H	6.60346800	-3.49132100	2.17493800
H	4.21344900	-4.09574300	2.45131700
C	2.37328400	0.12507700	-1.77766200
H	1.98942500	1.05708900	-2.18712100
C	3.69350900	0.18536600	-1.13672400
C	3.78524700	-0.13122200	0.22260900
C	4.81428300	0.67708900	-1.81126800

C	4.98787500	0.04205900	0.89732400
C	6.01860600	0.83310400	-1.13555800
H	4.73733800	0.93959300	-2.86118200
C	6.10473000	0.52164800	0.22026000
H	5.04472600	-0.18039300	1.95729200
H	6.88458400	1.22061900	-1.66310300
H	7.04072600	0.66550200	0.75201900
O	-0.49766500	0.38563200	-2.32408700
H	2.88979100	-0.45574100	0.74535600
O	3.70030400	-2.22213200	-3.20380600
H	2.65475700	-3.88000700	0.53215700
O	2.68761500	-4.42617800	-2.51694000
C	0.51088100	-1.99675800	3.61389200
O	-0.37057600	-2.66339600	4.13045300
H	0.98393800	-1.16549300	4.17195000
C	0.97025000	-2.14332400	2.19978400
H	2.05909000	-2.03927000	2.13353600
H	0.67178600	-3.11676100	1.79517700
S	0.16264000	-0.73649600	1.34186500
H	-1.78759700	-1.23731100	1.42295000



Int3'

-2709467.81 kcal/mol

C	3.97591000	-2.77995000	2.09589300
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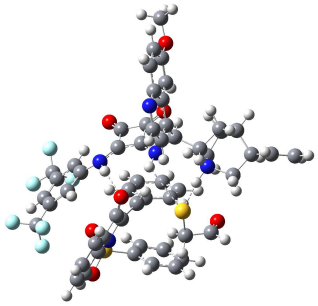
C	1.24581600	-3.35599800	3.20635100
H	4.14189500	-3.41648400	1.22057900
H	4.54105900	-4.37421800	3.45428300
H	0.51129300	-3.51699100	2.42212500
H	0.71904500	-3.35440900	4.16328000
H	4.87717600	-2.17288400	2.21669500
N	1.83355700	-1.99570500	3.04915900
C	2.60671700	-1.64672000	4.28269900
H	1.87974600	-1.49434600	5.08305700
H	3.09518700	-0.68961300	4.08697700
C	3.62234700	-2.76895700	4.59718500
H	3.23133300	-3.39569400	5.40806100
C	-5.66804400	0.60160300	0.20139300
C	-4.30336000	0.35575300	0.27036900
C	-3.82835600	-0.95442300	0.14843600
C	-4.73026400	-2.00464200	-0.02600300
C	-6.09221700	-1.73040400	-0.08384300
C	-6.57809900	-0.43481300	0.02305900
H	-3.59871100	1.16793100	0.42010700
H	-4.38136100	-3.02989200	-0.11276400
H	-7.64062700	-0.23580600	-0.03012200
C	-7.04034700	-2.87721100	-0.32459800
C	-6.17251200	2.00763500	0.37712000
F	-6.72808600	-3.94246900	0.42742200
F	-7.00675800	-3.27539400	-1.60781900
F	-8.31198400	-2.54367800	-0.04582700
F	-6.23565700	2.35004100	1.68039800
F	-5.36955800	2.90753000	-0.22000900
F	-7.40220900	2.17207700	-0.12926200
N	-2.43955700	-1.14070700	0.20600900
C	-1.74245000	-2.29129000	0.17442500
C	-0.36207800	-2.49957700	0.26792400
C	-0.50235300	-3.95740200	0.19447600
C	-1.99944400	-3.75784100	0.02562000
O	-2.95394400	-4.48273100	-0.12547200
O	0.26522100	-4.89898000	0.29236400
H	-1.89393100	-0.27820600	0.27399100
N	0.69079300	-1.67955200	0.42636800
H	0.48878200	-0.75993300	0.83004800
C	3.09408600	-3.74609900	-4.37270300
C	3.80889700	-2.59608500	-4.15809500
C	3.76014900	-1.91918100	-2.91822300
C	2.95995800	-2.45457300	-1.86629200
C	2.24809700	-3.65171500	-2.09868900
C	2.30462700	-4.28310300	-3.32544600
H	3.14602200	-4.23783600	-5.33716900
H	4.42797900	-2.16481200	-4.93791700
C	3.60995300	-0.53708100	-0.57592600
C	4.38750100	-0.11398400	-1.68086100
H	3.59835900	0.09032200	0.31008800
H	4.97187200	0.80210400	-1.60446100
N	4.47581600	-0.76528800	-2.81036600
O	1.57476300	-5.41520000	-3.44363400
C	1.56337200	-6.09322500	-4.68121100
H	0.90421000	-6.95024700	-4.54250800
H	2.56414400	-6.44894000	-4.95694500
H	1.16647500	-5.46020900	-5.48494900
H	1.63468000	-4.11902500	-1.33686600

C	2.38685900	-4.39026400	3.15566000
H	2.36048700	-4.92455800	2.20070000
H	2.24911300	-5.13332600	3.94638500
C	4.93890700	-2.19701100	5.04358100
C	5.54594600	-2.51577000	6.18240400
H	5.40362500	-1.47284300	4.37388100
H	6.50228500	-2.08217900	6.45781000
H	5.10853900	-3.22234700	6.88448400
C	2.90635300	-1.71409800	-0.64066000
C	2.04902400	-2.20426100	0.52675900
H	1.96014500	-3.29052700	0.46097000
C	2.74511200	-1.87364500	1.86130300
H	3.02681600	-0.82132600	1.88623100
C	0.15580400	1.26314000	-2.19994800
C	0.88923500	2.18627300	-2.94926400
C	1.63244200	1.76470800	-4.05060300
C	1.62074600	0.40512500	-4.34654900
C	0.87380000	-0.52102900	-3.60940500
C	0.12557600	-0.09018300	-2.52771000
H	2.20173900	2.45983600	-4.64986400
H	2.21263700	0.05464700	-5.18624500
H	0.89118300	-1.57110800	-3.88195100
H	-0.47432100	-0.77672700	-1.94088400
C	-0.54764700	1.96792800	-1.13515700
N	0.68324200	3.49702200	-2.43546700
C	-0.16716900	3.40784500	-1.27752700
S	1.87315900	4.70938900	-2.53617700
C	2.80167400	4.48391800	-1.03520400
C	2.81445400	5.49039400	-0.07724600
C	3.51948700	5.28087200	1.10567200
C	4.19094900	4.08047700	1.31252000
C	4.17544600	3.08491800	0.33578700
C	3.47851300	3.28059600	-0.84809800
H	2.28424600	6.41854400	-0.26187200
H	3.54013900	6.05722700	1.86388100
H	4.72570900	3.90744900	2.24071600
H	4.69879400	2.15236300	0.51551400
C	-0.44425000	4.42677000	-0.44587000
H	-0.02052800	5.39728300	-0.68634500
C	-1.19680800	4.37891100	0.81884300
C	-0.58934400	4.93963100	1.95014700
C	-2.48265600	3.84789200	0.93180000
C	-1.23100700	4.91220900	3.18217100
C	-3.13444200	3.84512900	2.15877900
H	-2.97623200	3.45232200	0.05300400
C	-2.50513200	4.36147900	3.28778900
H	-0.73986700	5.32668800	4.05735800
H	-4.13527800	3.43505600	2.23231200
H	-3.01150000	4.34192000	4.24783800
O	-1.29744400	1.48903400	-0.29642800
H	0.40470900	5.37232100	1.86195600
O	1.18653200	5.98400100	-2.46163200
H	3.45293400	2.51321400	-1.61574400
O	2.70696900	4.37718100	-3.67227900
C	2.26663600	1.74021900	2.81270900
O	3.34533000	1.16551800	2.72738800
H	2.04695100	2.37276100	3.69326000
C	1.14488400	1.59277700	1.85079900
H	0.63628500	2.54443000	1.67811900
H	1.50723000	1.19501100	0.89478800
S	-0.01747100	0.46776700	2.74061200
H	1.08458800	-1.21449500	2.94577300



Int4

-2709459.98 kcal/mol

C	-5.59227900	1.26662200	0.25013200
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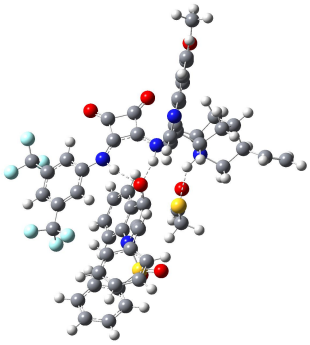
C	-3.22014200	1.99823400	-1.46447000
H	-5.95832600	0.26326100	0.01201800
H	-6.68191900	2.10903100	-1.42571300
H	-2.53308600	1.16800000	-1.61474500
H	-2.75942700	2.89215700	-1.88963700
H	-6.23265400	1.64702200	1.05035800
N	-3.34871800	2.26008700	-0.00227200
C	-4.03394700	3.57939600	0.20290100
H	-3.33033900	4.34923600	-0.11393700
H	-4.18596400	3.68476300	1.27980200
C	-5.35297700	3.62074100	-0.59797000
H	-5.19152400	4.19037800	-1.52120600
C	4.13271400	-2.68240400	0.76615800
C	2.78324300	-2.49321000	1.01052400

C	1.86553100	-2.56361400	-0.04412900
C	2.30960000	-2.89536300	-1.32068600
C	3.67236500	-3.07679500	-1.54098500
C	4.59687400	-2.96310600	-0.51597500
H	2.44337900	-2.27144500	2.01636700
H	1.60756100	-2.99399400	-2.14392200
H	5.65642400	-3.07749800	-0.70823600
C	4.12225900	-3.30268300	-2.95976500
C	5.13707300	-2.53259800	1.87624900
F	3.95821200	-2.18580900	-3.69662400
F	3.41179600	-4.27092500	-3.55694200
F	5.41721200	-3.64224400	-3.03569400
F	5.91548600	-3.62210700	1.98614500
F	5.95677300	-1.49153100	1.64531100
F	4.55588300	-2.33061900	3.06887600
N	0.53266800	-2.23161600	0.23931300
C	-0.45242700	-1.95696000	-0.64591100
C	-1.61046600	-1.19833000	-0.49079600
C	-2.09846500	-1.53816100	-1.83845000
C	-0.81968100	-2.34759500	-2.03777400
O	-0.32400900	-2.98184700	-2.93634100
O	-3.09594200	-1.27813800	-2.48085400
H	0.39739000	-1.79544100	1.15037300
N	-2.11862300	-0.36924700	0.44826800
H	-1.58023600	-0.20119000	1.29719300
C	-6.73511800	-4.43270000	0.70813900
C	-6.38473700	-4.12079400	1.99540500
C	-5.52466100	-3.03468200	2.28286300
C	-5.02276500	-2.24949600	1.20233900
C	-5.38644400	-2.59349800	-0.12062700
C	-6.22472700	-3.66078100	-0.36593900
H	-7.39474600	-5.27227400	0.52227700
H	-6.75482300	-4.70019500	2.83457600
C	-3.87165700	-0.94964500	2.86830700
C	-4.41519700	-1.80348800	3.85489000
H	-3.21072100	-0.14266000	3.17840700
H	-4.17172100	-1.63564800	4.90209700
N	-5.21906700	-2.80278400	3.58978900
O	-6.51143200	-3.90510000	-1.66599400
C	-7.30723500	-5.02513300	-1.98829700
H	-7.37129400	-5.03947700	-3.07655200
H	-8.31786400	-4.93801200	-1.56952400
H	-6.84798900	-5.95953000	-1.64253200
H	-4.99755300	-2.06462900	-0.98443200
C	-4.62859600	1.71469600	-2.02657900
H	-4.73133300	0.64966600	-2.25423600
H	-4.76684000	2.25850700	-2.96558700
C	-6.44400200	4.30139100	0.17934500
C	-7.11253800	5.36920600	-0.24495400
H	-6.68449900	3.87699800	1.15476900
H	-7.89875500	5.82231700	0.35095700
H	6.89682400	5.83268400	-1.20513700
C	-4.17292100	-1.15314100	1.54463900
C	-3.57318300	-0.23122300	0.49112900
H	-3.90801900	-0.53963600	-0.49736100
C	-4.11723200	1.19387900	0.71842600
H	-4.01456300	1.46461100	1.77220900
C	2.57779300	0.42489300	3.13899600
C	3.70185700	0.85693800	2.42397200
C	4.90882900	1.06446800	3.09092400
C	4.93287900	0.82588600	4.46095100
C	3.81169100	0.38958400	5.17706400
C	2.61859200	0.17870300	4.50882200
H	5.79872300	1.37913900	2.56897200
H	5.86922800	0.98037100	4.98883600
H	3.88442000	0.21504900	6.24512200
H	1.72132000	-0.16120800	5.01549600
C	1.48285100	0.23960700	2.20839000
N	3.36370500	1.00518900	1.05093600
C	1.97940000	0.72357500	0.88007000
S	4.45977200	1.36082500	-0.19378000
C	3.73172900	2.79959900	-0.93355800
C	3.75631500	2.91068300	-2.31958700
C	3.20868300	4.04484500	-2.90649600
C	2.64229900	5.03858600	-2.11277500
C	2.63638600	4.91645800	-0.72554700
C	3.19472300	3.79530000	-0.12394400
H	4.15995300	2.10544600	-2.92235700
H	3.20079400	4.13689800	-3.98722800
H	2.19194700	5.91017300	-2.57692100
H	2.18489800	5.68834900	-0.11115700
C	1.08070100	0.87103200	-0.10563900
H	0.07641100	0.72745900	0.28757100
C	1.09600100	1.16384800	-1.54866200
C	0.30561900	2.21461900	-2.02967000
C	1.73923200	0.31758300	-2.45586200
C	0.19259100	2.42920300	-3.39825300
C	1.60238000	0.52306800	-3.82434300

H	2.35282100	-0.49590500	-2.09253700
C	0.83291800	1.58101300	-4.29953800
H	-0.40223100	3.26366500	-3.75890500
H	2.09727600	-0.15478000	-4.51229600
H	0.72593800	1.73964400	-5.36863800
O	0.40275500	-0.31077000	2.40948600
H	-0.19489500	2.88899400	-1.33848000
O	4.44035100	0.27534000	-1.15348500
H	3.18838300	3.68384800	0.95596600
O	5.70126800	1.72856500	0.45847000
C	-0.87094500	4.82664600	0.78273300
O	-1.13116400	4.79927900	-0.41210800
H	-1.35484000	5.57942500	1.43688000
C	-0.02016500	3.83275300	1.49057000
H	0.65331600	3.32810100	0.79574500
H	0.55263600	4.29689200	2.29964700
S	-1.28056200	2.70000800	2.20072900
H	-2.41111200	2.34771700	0.52877100

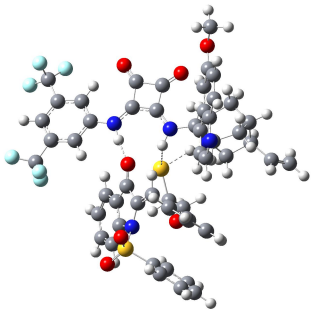


Int5

-2709460.80 kcal/mol

C	5.31673300	-2.19738400	-0.67359800
C	5.83000400	-2.11827500	-2.11907800
C	4.15811600	-0.36287800	-2.74681800
H	5.97984600	-1.62794300	-0.01689700
H	6.88110900	-2.41462300	-2.15902800
H	3.89898600	0.60339900	-2.31537100
H	3.79192900	-0.38551800	-3.77425500
H	5.32916200	-3.22793800	-0.30907400
N	3.39639900	-1.42776900	-2.01736100
C	3.50551200	-2.72724800	-2.75415200
H	2.91791400	-2.62404900	-3.66584100
H	3.02612400	-3.48050500	-2.12327900
C	4.99152700	-3.04576700	-3.02930300
H	5.22354900	-2.79029600	-4.07028000
C	-3.37481900	3.12969800	0.59561700
C	-2.18989200	2.45784400	0.84022900
C	-0.96634600	3.07822300	0.55500400
C	-0.94995000	4.38419300	0.06808700
C	-2.15697300	5.04077500	-0.15951300
C	-3.37534200	4.42751500	0.08844900
H	-2.19922500	1.44374800	1.22645300
H	-0.00760600	4.88882000	-0.12944200
H	-4.30673200	4.94791900	-0.09944600
C	-2.11568700	6.42301800	-0.75675800
C	-4.69699900	2.46243800	0.84440100
F	-1.84772300	6.37276500	-2.07475800
F	-1.16713800	7.18199200	-0.19114500
F	-3.28716100	7.06724900	-0.61738900
F	-5.50170000	3.21672800	1.61002500
F	-5.36710000	2.24188600	-0.30848000
F	-4.56776400	1.27100400	1.45033000
N	0.18744500	2.31319800	0.73290600
C	1.42346200	2.57367500	0.25330200
C	2.44595000	1.67036900	-0.02184300
C	3.37744900	2.71452900	-0.45206200
C	2.26930900	3.73723500	-0.14977600
O	2.12998400	4.93247600	-0.24984200
O	4.50921900	2.70654000	-0.89792200
H	0.02880700	1.30580400	0.91967600
N	2.51140600	0.32573300	-0.03653100
H	1.63871700	-0.15293200	0.29048500
C	7.68788000	0.30893100	3.67396500
C	6.67289400	-0.35787500	4.30854400
C	5.45650300	-0.65319300	3.64805400
C	5.29777300	-0.25454900	2.28839700
C	6.34968400	0.45025400	1.65648400
C	7.52036700	0.72660400	2.32970600
H	8.60569600	0.52155100	4.20971700
H	6.76962800	-0.67608100	5.34118800
C	3.09769800	-1.22605900	2.40193300
C	3.36084700	-1.55440700	3.75185000
H	2.11910000	-1.45305000	1.98282700
H	2.59334900	-2.05538700	4.33844900
N	4.49366600	-1.30248500	4.35972800
O	8.46353100	1.40418900	1.63170100
C	9.64225100	1.80379400	2.29716900
H	10.21944200	2.36900200	1.56488400
H	10.23206500	0.94047600	2.63072600
H	9.42120900	2.44862800	3.15660700

H	6.25610300	0.84109200	0.64901500
C	5.66107200	-0.67705900	-2.62697300
H	6.14094400	0.02775400	-1.94056100
H	6.14236600	-0.55512100	-3.60142900
C	5.27713800	-4.50860300	-2.83557300
C	5.77313500	-5.30509200	-3.77707500
H	5.05406000	-4.92088500	-1.85099700
H	5.97113100	-6.35524600	-3.58681900
H	6.00063000	-4.93680800	-4.77503500
C	4.06282000	-0.59626700	1.65605100
C	3.79909300	-0.30307500	0.18461100
H	4.55454100	0.38814000	-0.19199700
C	3.88564400	-1.61805100	-0.60433800
H	3.17887700	-2.32994800	-0.16895000
C	-1.27166800	-0.02803900	-1.16909900
C	-2.63535200	-0.25558300	-1.32817800
C	-3.40534100	0.52066800	-2.18336900
C	-2.76806900	1.54163500	-2.88501500
C	-1.39715900	1.76331400	-2.75511900
C	-0.63982000	0.96406900	-1.90301000
H	-4.46404800	0.33727700	-2.31513100
H	-3.35453800	2.17259500	-3.54535400
H	-0.92204700	2.56413300	-3.31239500
H	0.43141900	1.11044900	-1.81023500
C	-0.71349800	-0.95239100	-0.10623400
N	-3.07326000	-1.30247300	-0.45521400
C	-1.99280000	-1.58693300	0.44379200
S	-4.01029500	-2.57914000	-1.09169400
C	-5.55733800	-2.41580400	-0.23469300
C	-6.17926700	-3.56978300	0.22324200
C	-7.42485000	-3.45891800	0.83358900
C	-8.02246100	-2.21172400	0.98317900
C	-7.37779400	-1.06271700	0.52699800
C	-6.13917100	-1.16007200	-0.09174100
H	-5.68111600	-4.52775400	0.12767400
H	-7.91902100	-4.34991500	1.20712700
H	-8.99089500	-2.13082500	1.46760000
H	-7.83457200	-0.08687300	0.65737200
C	-2.05842700	-2.19544400	1.62383300
H	-1.09909800	-2.31140400	2.12415200
C	-3.25701800	-2.71777600	2.31316400
C	-4.27415300	-1.85203300	2.72408900
C	-3.36592000	-4.07879300	2.61364100
C	-5.37541800	-2.33486400	3.42266500
C	-4.47055300	-4.56299300	3.30590300
H	-2.58539800	-4.75817800	2.28417300
C	-5.47646300	-3.69118600	3.71624300
H	-6.15910600	-1.64897000	3.72982200
H	-4.54495100	-5.62389000	3.52769000
H	-6.33760600	-4.06897700	4.26007600
O	0.11931700	-0.49367900	0.79947300
H	-4.19538400	-0.79579000	2.49376200
O	-3.40328700	-3.84429500	-0.72180300
H	-5.62328200	-0.26759000	-0.42427500
O	-4.22184700	-2.26075000	-2.49754300
C	0.04224500	-1.46756400	-3.74365200
O	1.15511700	-0.98210100	-3.73166000
H	-0.65628000	-1.21453100	-4.56361600
C	-0.48360000	-2.46935100	-2.74498700
H	-1.57392800	-2.39256900	-2.70046700
H	-0.28299300	-3.46488200	-3.16774000
S	0.27314800	-2.40904300	-1.09948300
H	2.38911900	-1.18467600	-1.99530200



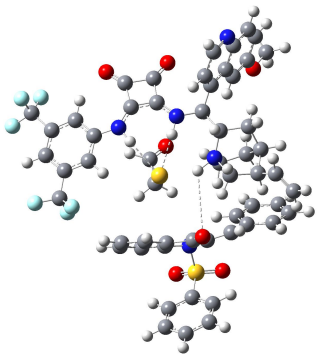
Int6

-2709462.63 kcal/mol

C	-1.66165100	4.49346800	1.77263100
C	-1.03735200	5.17689700	2.99963800
C	0.98779700	3.71478200	2.94362800
H	-1.49507000	5.11219900	0.88523900
H	-1.40898300	6.20118700	3.08554200
H	1.72494900	3.48169000	2.18062800
H	1.42865200	3.47855400	3.91468800
H	-2.74523500	4.39529200	1.88180200
N	-0.17935400	2.80143000	2.78538700
C	-1.04301200	2.90470300	3.99712500
H	-0.50458000	2.42449100	4.81754200
H	-1.94187600	2.31368000	3.80048400
C	-1.38633600	4.38482200	4.28232900
H	-0.74062000	4.75336400	5.08844500
C	4.90171400	-3.28224300	-0.71922200

C	3.89052400	-2.33328700	-0.68665800
C	4.19131200	-0.99413400	-0.42315400
C	5.52139700	-0.60824900	-0.24131800
C	6.51935200	-1.57410700	-0.30242200
C	6.22789000	-2.91575700	-0.52652600
H	2.86254300	-2.62956700	-0.86909500
H	5.77642800	0.43313400	-0.06773500
H	7.01669600	-3.65702600	-0.55247100
C	7.95787100	-1.14295200	-0.17030900
C	4.52394700	-4.72914600	-0.89059700
F	8.09235000	-0.09219900	0.65064200
F	8.47087000	-0.78731600	-1.36039800
F	8.73012900	-2.13348000	0.31054000
F	5.55356000	-5.47226800	-1.32348200
F	4.11166000	-5.26154500	0.27539800
F	3.51650600	-4.87957800	-1.76527300
N	3.10826300	-0.11707000	-0.33144900
C	3.09655500	1.22029800	-0.20423400
C	2.01203900	2.08488800	-0.02887200
C	2.87501600	3.27174900	0.00101700
C	4.06862800	2.34901100	-0.20126900
O	5.26762300	2.48127800	-0.27883400
O	2.68405900	4.46470000	0.17047400
H	2.18582100	-0.56235800	-0.35986500
N	0.68994300	1.92059800	0.13279300
H	0.31227600	0.97683800	0.16189400
C	-0.81321600	6.00060300	-4.04710200
C	-1.86175100	5.11925200	-4.01147500
C	-1.98638900	4.16420000	-2.97583900
C	-0.99807700	4.12926400	-1.94718500
C	0.07969600	5.04299900	-2.00282600
C	0.17297400	5.95900600	-3.03030700
H	-0.74503700	6.71880100	-4.85596800
H	-2.62825300	5.12557100	-4.77916500
C	-2.24943400	2.30582500	-1.00344300
C	-3.17031700	2.43204100	-2.07168600
H	-2.42457200	1.52418100	-0.26800200
H	-4.03088600	1.76861100	-2.11738300
N	-3.06057800	3.32700800	-3.02068700
O	1.24311800	6.78686800	-2.99283100
C	1.43382900	7.70036800	-4.05078900
H	2.36266000	8.22479400	-3.82525200
H	0.61491000	8.42871800	-4.11044200
H	1.53559400	7.18656300	-5.01491400
H	0.88453700	5.04002400	-1.27458700
C	0.49242900	5.17010400	2.84523100
H	0.78857800	5.59904000	1.88271100
H	0.96004800	5.77646500	3.62628500
C	-2.81444100	4.53872800	4.72354900
C	-3.18856000	5.06615300	5.88496300
H	-3.57743600	4.18715600	4.02779700
H	-4.23552300	5.16368700	6.15464800
H	-2.46086600	5.42241600	6.61073000
C	-1.17413100	3.15484600	-0.91380000
C	-0.20037100	3.06173500	0.25694800
H	0.44634800	3.93867100	0.24895300
C	-1.00445600	3.10424900	1.57333300
H	-1.75199000	2.30740600	1.56393700
C	0.02089100	-3.03189600	0.55918300
C	-1.13555400	-3.81695100	0.63924500
C	-1.20886200	-4.87972400	1.53324600
C	-0.09075900	-5.13068500	2.32173100
C	1.06849400	-4.34722400	2.25179800
C	1.12688200	-3.27992900	1.37124400
H	-2.09073900	-5.50171800	1.60330100
H	-0.12722200	-5.95971400	3.02224000
H	1.91208300	-4.56779600	2.89630600
H	1.98852300	-2.62356500	1.33740100
C	-0.21945200	-1.97248800	-0.40718700
N	-2.14167400	-3.30889800	-0.22561700
C	-1.63551300	-2.12981300	-0.83552700
S	-3.22087300	-4.34190400	-1.05442400
C	-4.79677400	-3.88429900	-0.37711300
C	-4.91385500	-3.60168100	0.98023300
C	-6.17308600	-3.31185700	1.49088300
C	-7.28735400	-3.31649100	0.65344600
C	-7.14821500	-3.59769900	-0.70265600
C	-5.89367300	-3.88279600	-1.23045600
H	-4.03370500	-3.55349400	1.61327500
H	-6.28188200	-3.07470500	2.54434300
H	-8.26846600	-3.08944600	1.05977400
H	-8.01450200	-3.58296900	-1.35597500
C	-2.24536400	-1.18490400	-1.55762800
H	-1.56645100	-0.42910400	-1.95273700
C	-3.68549500	-0.97526200	-1.78144600
C	-4.21824500	-0.89560200	-3.07039500
C	-4.50738700	-0.72960000	-0.67591600
C	-5.56009100	-0.58170700	-3.25165500

C	-5.84489100	-0.39566400	-0.86444600
H	-4.08854500	-0.80437600	0.32476600
C	-6.37334800	-0.32178300	-2.14983100
H	-5.96932200	-0.52716800	-4.25577700
H	-6.47701800	-0.20760200	-0.00207600
H	-7.41816300	-0.06355000	-2.29533700
O	0.51925700	-1.06816000	-0.78928000
H	-3.57939500	-1.08825200	-3.92638400
O	-2.90387800	-5.68984900	-0.62136200
H	-5.75862000	-4.07320200	-2.28933400
O	-3.19707200	-3.99214000	-2.46069500
C	-2.03223500	-0.72018100	2.80607900
O	-2.69135400	-1.45848700	2.10385300
H	-2.34000500	0.34485700	2.91974700
C	-0.76927400	-1.07327600	3.52158500
H	-0.84751500	-0.80290300	4.58123500
H	-0.58566900	-2.14760600	3.43215600
S	0.57053200	-0.12621700	2.69863400
H	0.13514600	1.73939300	2.74416200

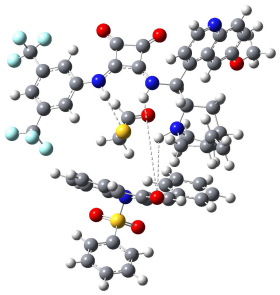


Int7

-2709462.95 kcal/mol

C	-1.80803600	-4.04980000	-1.53606400
C	-0.48612300	-4.57327500	-0.95753200
C	-0.01514400	-2.41425000	0.18161700
H	-2.62925500	-4.39751400	-0.90685700
H	-0.53412300	-5.66005000	-0.85206300
H	-0.55693100	-1.74654300	0.85352700
H	1.04576700	-2.16930600	0.26605100
H	-1.99194000	-4.45274900	-2.53581600
N	-0.39151600	-2.06127400	-1.22582700
C	0.57793500	-2.68517700	-2.17959600
H	1.52209400	-2.14189100	-2.09437900
H	0.19164400	-2.50539800	-3.18670300
C	0.70485700	-4.19197800	-1.86785400
H	1.62034800	-4.36193600	-1.29094400
C	-0.75650300	5.85007000	-0.45371200
C	-1.10428800	4.55839100	-0.82124100
C	-2.37575700	4.06036000	-0.50905100
C	-3.28717700	4.87038700	0.17186500
C	-2.91350000	6.16355400	0.52339100
C	-1.65539300	6.67010900	0.22011600
H	-0.39165500	3.92334300	-1.34162400
H	-4.27136600	4.49092200	0.43609100
H	-1.38143500	7.67771900	0.50574600
C	-3.93084900	7.04363500	1.20462800
C	0.64369100	6.32944100	-0.72036000
F	-4.63813600	6.36767200	2.11947200
F	-4.80615900	7.54955700	0.31907300
F	-3.35264600	8.08557500	1.82790300
F	0.72277100	7.66608800	-0.77646500
F	1.49444800	5.92685800	0.24875100
F	1.13070100	5.84662800	-1.87866500
N	-2.65160200	2.74594500	-0.89521800
C	-3.60406500	1.90711700	-0.40373800
C	-3.66310900	0.52258300	-0.48222700
C	-4.91311900	0.45376700	0.31277300
C	-4.87546100	1.99046700	0.36036100
O	-5.56743900	2.86503100	0.82478200
O	-5.61354600	-0.42258900	0.75312100
H	-1.84942900	2.27104600	-1.32080800
N	-2.84016500	-0.36735900	-1.07937900
H	-1.91624400	0.02021900	-1.30254600
C	-6.34551200	-5.24924700	1.16929100
C	-6.82359400	-4.82822800	-0.04387500
C	-6.12782800	-3.87270400	-0.82147500
C	-4.90434900	-3.34045100	-0.32422100
C	-4.43200200	-3.78203500	0.93177500
C	-5.13110100	-4.71466900	1.66631000
H	-6.90491600	-5.98110600	1.74014500
H	-7.75471000	-5.21445300	-0.44468700
C	-4.81197900	-2.03357600	-2.33822800
C	-6.03716300	-2.62190200	-2.72837100
H	-4.34614700	-1.28728300	-2.97456400
H	-6.49172300	-2.33562800	-3.67499800
N	-6.67720800	-3.51329500	-2.01549600
O	-4.58323400	-5.07003700	2.85491400
C	-5.30823400	-5.93750600	3.69974100
H	-4.71127400	-6.03700900	4.60688800
H	-5.44023700	-6.92836000	3.24660500

H	-6.28942600	-5.52101500	3.95828400
H	-3.52709100	-3.38194800	1.37419900
C	-0.27581000	-3.91061600	0.41041600
H	-1.16391900	-4.05997000	1.03353400
H	0.57268400	-4.35604600	0.93731200
C	0.78842000	-5.00627100	-3.12679700
C	1.80584200	-5.80460400	-3.43358300
H	-0.05114400	-4.92143400	-3.81812300
H	1.82225700	-6.38192500	-4.35262800
H	2.66463500	-5.90999400	-2.77400200
C	-4.23237700	-2.38683700	-1.14820000
C	-2.88475100	-1.79043600	-0.76692300
H	-2.70021100	-1.94263600	0.30179800
C	-1.78853900	-2.49989700	-1.59397100
H	-1.92001000	-2.15501500	-2.62448500
C	3.75883500	1.03444000	-0.90988600
C	3.96539200	1.02151000	0.46872200
C	3.92745000	2.19211300	1.21484000
C	3.66154900	3.37523200	0.52722800
C	3.43328100	3.39535900	-0.85406600
C	3.48105200	2.21657900	-1.58659600
H	4.08446600	2.17941600	2.28602800
H	3.60034200	4.30471800	1.08411600
H	3.18475100	4.33123300	-1.34067000
H	3.27510300	2.19283900	-2.65079700
C	3.77209100	-0.35207200	-1.39631200
N	4.15135700	-0.31828000	0.96195800
C	3.92694000	-1.18561800	-0.15626700
S	5.64625700	-0.55623700	1.80740900
C	6.86565800	-0.08009300	0.60643200
C	7.30435700	-1.03160800	-0.31221400
C	8.18929700	-0.63869000	-1.30983500
C	8.62073900	0.68402000	-1.37917900
C	8.17769500	1.62176700	-0.44949700
C	7.29111500	1.24493400	0.55288300
H	6.96489100	-2.05842300	-0.23360700
H	8.54320300	-1.36689100	-2.03218500
H	9.30982700	0.98541000	-2.16199800
H	8.52144400	2.64946400	-0.50405600
C	3.70285200	-2.50904700	-0.18630300
H	3.62663400	-2.88733600	-1.20695400
C	3.43987100	-3.48589400	0.87003600
C	3.51843800	-4.84834100	0.55481100
C	2.98253900	-3.11286700	2.14234300
C	3.16321400	-5.81806700	1.48583600
C	2.61060300	-4.08052500	3.06430600
H	2.90870300	-2.06166000	2.39936200
C	2.70353100	-5.43473100	2.74223600
H	3.23928900	-6.86980300	1.22801100
H	2.25025500	-3.77792900	4.04236700
H	2.41680400	-6.18741100	3.47014600
O	3.59927500	-0.78050500	-2.52120800
H	3.86759300	-5.14641700	-0.43124200
O	5.75711200	-1.97867500	2.05092300
H	6.93635600	1.95927200	1.28712600
O	5.63558200	0.40741800	2.89015500
C	-0.65463600	1.15088000	1.12448200
O	-1.20591500	0.17572700	1.59714000
H	-1.10452700	2.15414600	1.25751700
C	0.59799800	1.10630200	0.30177400
H	1.17194700	2.02634300	0.44169300
H	1.21085700	0.25465900	0.61230700
S	0.13886200	0.97367900	-1.48232900
H	-0.26870700	-0.99928000	-1.34113500



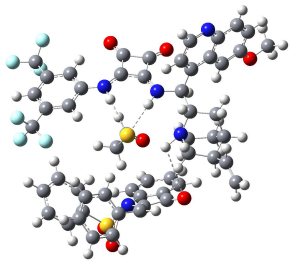
Int8

-2709463.72 kcal/mol

C	-3.23820700	-3.31716000	-1.20275200
C	-2.15800000	-4.39278800	-1.01645500
C	-1.11082200	-2.71323200	0.50173100
H	-3.89930200	-3.32367000	-0.33105300
H	-2.60567300	-5.38694100	-1.09195300
H	-1.76191800	-2.13864700	1.15661300
H	-0.09655600	-2.58368900	0.87784200
H	-3.86850000	-3.51625100	-2.07230100
N	-1.15525300	-2.07542100	-0.85086400
C	-0.35722900	-2.88424800	-1.82761300
H	0.63825400	-2.99953600	-1.39875300
H	-0.25131000	-2.28166000	-2.73261200
C	-1.04931800	-4.24417700	-2.08305500
H	-0.31071900	-5.03605200	-1.91539200

C	1.65758800	5.31317400	-0.18624000
C	0.85364100	4.27318100	-0.63494300
C	-0.53674800	4.36369000	-0.51339400
C	-1.10863600	5.51053700	0.04563100
C	-0.28056100	6.53990600	0.47644600
C	1.10458300	6.45801000	0.37200600
H	1.29941000	3.37838700	-1.06476000
H	-2.18689400	5.58872000	0.15926500
H	1.73464500	7.26324800	0.72691100
C	-0.90899000	7.79743400	1.02171300
C	3.14806000	5.14426600	-0.28203400
F	-2.02725600	7.53941300	1.71121200
F	-1.23762700	8.64443900	0.03054300
F	-0.06990800	8.45690400	1.84014800
F	3.82001100	6.21913900	0.14792300
F	3.56879200	4.09060400	0.45084900
F	3.54145700	4.90479600	-1.54893600
N	-1.28484200	3.26646300	-0.95136900
C	-2.54647000	2.91716800	-0.58145200
C	-3.16272600	1.67474500	-0.65460500
C	-4.40863200	2.16908100	-0.01852500
C	-3.74967400	3.55752500	0.01363400
O	-4.07056600	4.66458600	0.37417000
O	-5.44932900	1.68388500	0.34718200
H	-0.70485900	2.47964000	-1.26418000
N	-2.72376800	0.48845400	-1.13537100
H	-1.70426400	0.45905800	-1.25394800
C	-8.00306900	-2.46942600	1.03468200
C	-8.18543400	-2.03899800	-0.25325800
C	-7.11993600	-1.49429500	-1.00832600
C	-5.83159400	-1.39774100	-0.40972400
C	-5.66600000	-1.83932000	0.92202700
C	-6.72303400	-2.36372300	1.63306000
H	-8.84147800	-2.87871000	1.58610100
H	-9.15656900	-2.09933500	-0.73291900
C	-5.09112100	-0.43324800	-2.48283000
C	-6.41081200	-0.57029400	-2.97137200
H	-4.32832000	0.01957200	-3.10889400
H	-6.64598300	-0.23815600	-3.98090900
N	-7.39407300	-1.08751600	-2.27967500
O	-6.45102300	-2.76008900	2.90135500
C	-7.51671200	-3.20431200	3.71280100
H	-7.07969700	-3.41313800	4.68983900
H	-7.97079900	-4.12277400	3.31929000
H	-8.28925500	-2.43325000	3.82138500
H	-4.71693400	-1.75443400	1.43894900
C	-1.52010200	-4.18904500	0.36510200
H	-2.22690700	-4.44937400	1.15811400
H	-0.64776500	-4.83956900	0.48495200
C	-1.56050600	-4.37819100	-3.49197500
C	-1.24421400	-5.37805700	-4.30830300
H	-2.23306800	-3.59672800	-3.84803700
H	-1.64326400	-5.43835700	-5.31600800
H	-0.56800000	-6.17241800	-4.00034900
C	-4.78632100	-0.84922100	-1.21338900
C	-3.34691100	-0.76625500	-0.72652600
H	-3.31202100	-0.85233300	0.36460300
C	-2.56850400	-1.93542100	-1.36307000
H	-2.45564400	-1.68864700	-2.42443800
C	3.80687600	-1.04880100	-1.69944300
C	3.95534600	-0.42168700	-0.46428100
C	4.27816400	0.92345800	-0.37177000
C	4.46238400	1.61585200	-1.56694800
C	4.32634100	0.99140500	-2.81133100
C	3.98844500	-0.35275200	-2.88749000
H	4.37809400	1.41548700	0.58726300
H	4.69390900	2.67395400	-1.52573400
H	4.46315600	1.57145600	-3.71808600
H	3.84815800	-0.85749400	-3.83780600
C	3.34230000	-2.42116300	-1.46984800
N	3.69554500	-1.33013500	0.62371400
C	3.19965700	-2.53126400	0.02078200
S	5.04937700	-1.52934800	1.68838500
C	6.35373400	-2.03701800	0.59373800
C	6.46848600	-3.38875500	0.27576000
C	7.42815900	-3.77774900	-0.65197000
C	8.25230200	-2.82427400	-1.24536700
C	8.12886400	-1.47750600	-0.91212400
C	7.17263700	-1.07247400	0.01212500
H	5.82409200	-4.11586300	0.75742600
H	7.53317800	-4.82657000	-0.90953100
H	8.99845500	-3.13377200	-1.97065700
H	8.77718300	-0.73925500	-1.37261400
C	2.54402700	-3.56541800	0.57204800
H	2.33406200	-4.34725900	-0.15994700
C	1.98022900	-3.78946200	1.90212700
C	1.50811700	-5.07305300	2.20782500
C	1.76528000	-2.75592400	2.82663400

C	0.84626600	-5.32485000	3.40396300
C	1.08530800	-3.00336800	4.00972000
H	2.12146800	-1.75599700	2.60892100
C	0.62745100	-4.28704300	4.30469800
H	0.49552000	-6.32754100	3.62806800
H	0.91342100	-2.19033600	4.70759300
H	0.10117800	-4.47560100	5.23540600
O	3.02184800	-3.27290500	-2.27939400
H	1.66430500	-5.88029100	1.49577800
O	4.72077500	-2.63179700	2.56750000
H	7.06093700	-0.02937300	0.28543300
O	5.33864300	-0.20357200	2.19812200
C	-0.43230300	0.94612100	1.33308800
O	-1.17452300	0.05937600	1.70881900
H	-0.74888200	2.00445600	1.42312900
C	0.89139300	0.71412300	0.67079400
H	1.55358000	1.57249400	0.82056900
H	1.36749000	-0.18284300	1.07504900
S	0.57387900	0.50313300	-1.13560400
H	-0.64540200	-1.13538300	-0.82516400

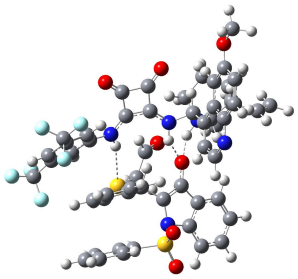


Int9

-2709461.39 kcal/mol

C	-4.46477300	-2.35565200	-1.31143800
C	-3.98738500	-3.57107000	-0.50170400
C	-2.25048500	-2.22596500	0.68356300
H	-5.37107400	-1.95044400	-0.85601300
H	-4.80788900	-4.28438800	-0.39013000
H	-2.25044700	-1.29148800	1.24227800
H	-1.34486200	-2.76166900	0.96165400
H	-4.73246000	-2.64286000	-2.33169100
N	-2.10522500	-1.90136700	-0.77015500
C	-1.77769400	-3.14195000	-1.54672100
H	-0.75623200	-3.42632300	-1.29177300
H	-1.80502500	-2.86363400	-2.60396800
C	-2.78715900	-4.25333000	-1.19670700
H	-2.30899100	-4.92508300	-0.47599600
C	3.13418800	4.21249200	-0.92871900
C	1.97599100	3.47740900	-1.11701000
C	0.78092700	3.88886700	-0.50902100
C	0.76260000	5.04251400	0.27469400
C	1.94251700	5.76281200	0.44590900
C	3.13401400	5.36323400	-0.14279200
H	1.98495500	2.58173900	-1.73215400
H	-0.16009700	5.37787900	0.74288600
H	4.04235700	5.93562400	0.00204900
C	1.91955200	6.97088300	1.34849000
C	4.41443500	3.79433300	-1.59804000
F	1.96345100	6.60782600	2.64181800
F	0.80680600	7.69630800	1.17703600
F	2.97026800	7.77924300	1.12804500
F	4.77703100	4.65112900	-2.56343400
F	5.43528100	3.75605900	-0.71244400
F	4.33045800	2.57403000	-2.15256400
N	-0.33886800	3.08735000	-0.72707100
C	-1.54512200	3.11049100	-0.10108000
C	-2.53374400	2.13710000	-0.12251300
C	-3.43456300	2.90936800	0.75795200
C	-2.34752200	4.00376800	0.77748400
O	-2.20276900	5.08490200	1.29539200
O	-4.52013900	2.71691400	1.24774500
H	-0.14005000	2.22114000	-1.23934900
N	-2.58403200	0.93493500	-0.71604500
H	-1.70640700	0.60729700	-1.13324500
C	-8.91317100	0.43077100	0.20076900
C	-8.65100300	1.00752400	-1.01371700
C	-7.33380400	1.08543100	-1.52588200
C	-6.26235300	0.54716900	-0.75522100
C	-6.55375900	-0.03421200	0.49922700
C	-7.84621300	-0.09474700	0.97190500
H	-9.93305500	0.38969400	0.56486700
H	-9.44717600	1.42578900	-1.62022400
C	-4.81044700	1.25834900	-2.53353700
C	-5.94553500	1.76496300	-3.20645100
H	-3.82626700	1.37821300	-2.97734900
H	-5.82415300	2.25321300	-4.17143400
N	-7.16566200	1.68018700	-2.73949500
O	-8.01057000	-0.67690200	2.18431900
C	-9.29751700	-0.67847600	2.76521500
H	-9.18139500	-1.14629700	3.74324000
H	-10.00980900	-1.26348500	2.16974900
H	-9.68086900	0.34065200	2.89666100

H	-5.77408000	-0.41693300	1.14698200
C	-3.51976600	-3.07391800	0.87363600
H	-4.31392200	-2.48779300	1.34867900
H	-3.29932800	-3.91817500	1.53306300
C	-3.16081000	-5.05032000	-2.41394600
C	-2.89051600	-6.34265800	-2.56836100
H	-3.67570700	-4.51277100	-3.21175100
H	-3.17816700	-6.88077400	-3.46634700
H	-2.36530500	-6.90794900	-1.80211300
C	-4.95351400	0.63741100	-1.31984800
C	-3.72581300	0.04387100	-0.63756300
H	-3.96016200	-0.15302000	0.41248500
C	-3.35406300	-1.27667000	-1.34255900
H	-3.08772400	-1.02221400	-2.37388800
C	0.87167500	-3.66669400	2.32238800
C	2.03516400	-2.93221000	2.55327500
C	2.18667700	-2.20415300	3.72901900
C	1.15049800	-2.25751700	4.65448900
C	-0.01291400	-3.00553000	4.43531900
C	-0.15877400	-3.71740400	3.25686300
H	3.08168600	-1.63206000	3.93243100
H	1.25048700	-1.69343500	5.57666400
H	-0.79669500	-3.01537700	5.18520000
H	-1.04819800	-4.30399700	3.04547500
C	0.93471000	-4.22456500	0.97549500
N	2.90096900	-2.99589200	1.42176200
C	2.23475500	-3.74528800	0.40418500
S	4.60264700	-3.13363600	1.64807700
C	5.21039100	-1.68563400	0.82564300
C	6.31831600	-1.80788900	-0.00102500
C	6.83577100	-0.65960900	-0.59311400
C	6.24519700	0.57688200	-0.35915100
C	5.13640800	0.68139300	0.48069100
C	4.61753200	-0.45287200	1.08808800
H	6.74144000	-2.78539500	-0.20167600
H	7.69161600	-0.73965000	-1.25514600
H	6.63749200	1.46845300	-0.83517700
H	4.68334100	1.65037800	0.66124000
C	2.53888100	-3.94002800	-0.88323200
H	1.82868900	-4.59182900	-1.39311900
C	3.63588900	-3.37616100	-1.70172300
C	3.56369600	-2.04645800	-2.12505800
C	4.69409500	-4.17921900	-2.13558200
C	4.54369500	-1.52364700	-2.96266800
C	5.67401800	-3.65137400	-2.96900000
H	4.75727700	-5.20918300	-1.79963100
C	5.60006600	-2.32362800	-3.38570700
H	4.47727800	-0.48641100	-3.27630500
H	6.49648200	-4.28077400	-3.29608000
H	6.36503100	-1.91559000	-4.04008500
O	0.07691600	-4.85586700	0.37483500
H	2.72016900	-1.42961600	-1.83267900
O	5.06179500	-4.31589900	0.94754700
H	3.75389900	-0.38535000	1.74257400
O	4.82625400	-2.98603900	3.07397900
C	0.38130300	0.29603200	1.13550500
O	-0.12755400	-0.50839600	1.88877000
H	0.12980900	1.37218100	1.21903500
C	1.31437800	-0.06730800	0.02237100
H	2.11520400	0.67591900	-0.05826300
H	1.75424900	-1.04766000	0.21933100
S	0.37214500	-0.08847800	-1.56365700
H	-1.26747400	-1.26173800	-0.91996600



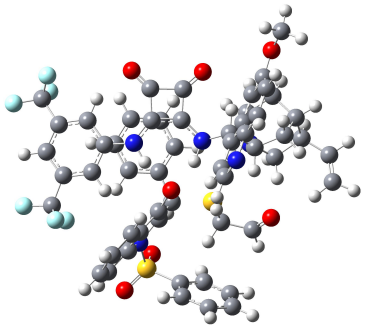
Int10

-2709457.29 kcal/mol

C	-5.60356300	0.13418200	-0.61497800
C	-6.12151300	0.26330500	-2.05718900
C	-3.83716200	0.02001900	-3.05418200
H	-5.80177500	-0.87172600	-0.23302400
H	-7.16457000	-0.05778000	-2.11166600
H	-3.04411900	-0.71651100	-2.94413100
H	-3.65352500	0.58159500	-3.97106900
H	-6.12711200	0.82579400	0.05056500
N	-3.70612000	1.00168100	-1.93335400
C	-4.56438100	2.19466100	-2.20872000
H	-4.09422800	2.74693700	-3.02403600
H	-4.52861400	2.81505200	-1.31044400
C	-6.00243700	1.73204300	-2.53276500
H	-6.14434100	1.74327700	-3.62012200
C	4.83234300	-2.15578400	-1.87517700
C	3.54270400	-1.69181100	-2.10178900

C	2.47226700	-2.26087700	-1.41768100
C	2.69390700	-3.31493700	-0.53052100
C	3.98433900	-3.78410800	-0.34252200
C	5.06640200	-3.20894700	-1.00314800
H	3.36952400	-0.86201900	-2.77867600
H	1.87300500	-3.74922600	0.02444800
H	6.07344600	-3.56974200	-0.82856600
C	4.25994000	-4.87386100	0.65872700
C	5.98529300	-1.41544600	-2.49152400
F	3.13948000	-5.41632700	1.14941500
F	4.96670400	-4.39661700	1.70360500
F	4.99251800	-5.86178300	0.11917100
F	7.08469300	-2.17596300	-2.59194600
F	5.69332500	-0.95417100	-3.71746100
F	6.31676600	-0.34111500	-1.74095000
N	1.19987000	-1.68747300	-1.57067300
C	0.02581100	-2.33537600	-1.38604900
C	-1.27078600	-1.93079500	-1.09407900
C	-1.81388300	-3.28963800	-1.32601200
C	-0.36978600	-3.76477900	-1.52540800
O	0.20690700	-4.80445700	-1.71830200
O	-2.93214200	-3.74723500	-1.42606900
H	1.19981200	-0.69023500	-1.76041900
N	-1.90279900	-0.77734100	-0.81269700
H	-1.40231700	0.09846600	-0.60944600
C	-5.36535500	-3.97984100	3.41705000
C	-4.61079200	-3.03805200	4.06524800
C	-3.89161100	-2.04926800	3.35204200
C	-3.96432000	-2.04030800	1.92636400
C	-4.73446700	-3.03223700	1.27511800
C	-5.42337600	-3.98004000	2.00037700
H	-5.90364900	-4.72303900	3.99369300
H	-4.54072400	-3.02158700	5.14770500
C	-2.51413500	-0.12094300	2.01038400
C	-2.49811700	-0.23993200	3.41786200
H	-1.95470100	0.68324000	1.53802300
H	-1.91448800	0.46484000	4.00703100
N	-3.16256000	-1.15724500	4.07756700
O	-6.13577200	-4.88026700	1.28030700
C	-6.77309000	-5.93955500	1.96038600
H	-7.22905000	-6.55765300	1.18641500
H	-7.55696300	-5.57476300	2.63650400
H	-6.05516800	-6.54490400	2.52749300
H	-4.76133400	-3.11900300	0.19514400
C	-5.24619600	-0.60052900	-2.98139600
H	-5.19136300	-1.62687400	-2.60391400
H	-5.68041400	-0.64784600	-3.98412100
C	-7.01946900	2.65474200	-1.92203000
C	-7.93518600	3.32340500	-2.61563900
H	-6.98341700	2.76819700	-0.83799600
H	-8.65475100	3.97348400	-2.12796800
H	-8.00019900	3.24624500	-3.69870500
C	-3.24090700	-1.00893900	1.25505500
C	-3.25413200	-0.84404900	-0.26218300
H	-3.72285200	-1.71077300	-0.72737500
C	-4.08478000	0.41436600	-0.59905600
H	-3.81891700	1.20175400	0.10648200
C	-1.21581900	4.10538300	0.33873300
C	-0.09768400	4.75000900	0.88152900
C	-0.15067800	6.09909200	1.23299700
C	-1.34821100	6.77262900	1.02485400
C	-2.46925000	6.13668900	0.47540400
C	-2.40480600	4.79807500	0.12348700
H	0.70659200	6.60471600	1.65321400
H	-1.40770300	7.82437800	1.28811100
H	-3.38441900	6.69977000	0.31871600
H	-3.25547600	4.28952500	-0.31925700
C	-0.83062400	2.73721600	0.02379400
N	0.99430100	3.83326100	0.90955200
C	0.49132000	2.58914000	0.38987200
S	1.93471700	3.81503200	2.34572800
C	3.53970400	3.35268000	1.74482000
C	4.35090600	2.61474200	2.60026300
C	5.65468300	2.33496900	2.20934900
C	6.12504500	2.77760200	0.97578000
C	5.29813900	3.51351600	0.12982100
C	3.99824800	3.81902200	0.51720600
H	3.95203500	2.23918400	3.53608200
H	6.29533100	1.74873300	2.85998200
H	7.13876200	2.54115300	0.66697500
H	5.66369100	3.84945300	-0.83517000
C	1.25068700	1.43539700	-0.14854100
H	0.44160900	0.74135800	-0.38595600
C	2.20775000	0.61723800	0.70473600
C	3.53289600	0.36181000	0.36651800
C	1.66784400	-0.01226400	1.83084300
C	4.30308600	-0.51430200	1.12810700
C	2.43388100	-0.88380800	2.59166000

H	0.63841100	0.19353900	2.11100300
C	3.75696300	-1.14641400	2.23634000
H	5.33111900	-0.70188200	0.83597900
H	1.99466600	-1.36605100	3.45966800
H	4.34999400	-1.84915200	2.81281900
O	-1.56706100	1.86097300	-0.59145600
H	3.99429000	0.84886700	-0.48642400
O	1.45366300	2.78344700	3.24953900
H	3.33923100	4.38567100	-0.13111900
O	2.01593100	5.19189500	2.80557100
C	-0.50285600	1.71729200	-3.06999800
O	-1.47669700	2.11269000	-3.67163400
H	-0.39261000	0.64270300	-2.81303400
C	0.65761200	2.61189500	-2.68222000
H	1.07544200	3.04609800	-3.59707400
H	0.27766900	3.44377000	-2.07946700
S	2.02395000	1.77828800	-1.83783500
H	-2.73773900	1.36144000	-1.80761600



TS2

-2709467.16 kcal/mol

C	5.23097600	1.01976500	0.57344900
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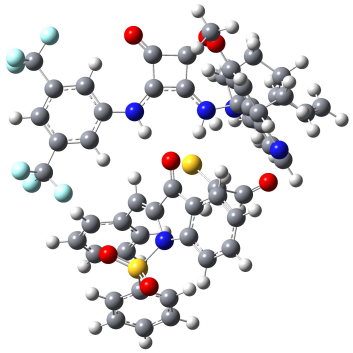
C	3.59481100	-0.15903600	2.81329500
H	5.70326400	0.24225000	-0.03118600
H	6.79856200	0.88199600	2.06066100
H	3.04399400	-1.04690300	2.50883500
H	3.29058700	0.10806700	3.82837300
H	5.52763300	1.98333400	0.15068300
N	3.18531500	0.99427200	1.94410100
C	3.68510000	2.27626700	2.54081200
H	3.10333000	2.46228800	3.44587400
H	3.45696000	3.05853200	1.82039500
C	5.19516400	2.14911300	2.82030500
H	5.33261000	1.92770700	3.88654900
C	-4.52210000	-2.51299700	-0.72633800
C	-3.21726600	-2.06209100	-0.86603100
C	-2.15743600	-2.82165200	-0.37025000
C	-2.41292200	-4.06473300	0.21063000
C	-3.72736200	-4.49661100	0.33561300
C	-4.79684500	-3.73075300	-0.11721500
H	-3.02841600	-1.09667800	-1.32393200
H	-1.60027700	-4.67249900	0.59901300
H	-5.81624200	-4.07356300	0.00408900
C	-3.98393100	-5.77004200	1.09564100
C	-5.62964600	-1.60637000	-1.19169700
F	-5.21122900	-6.26263100	0.86075000
F	-3.89150200	-5.55616300	2.42381100
F	-3.09745100	-6.72701200	0.78974400
F	-6.83919500	-2.17507900	-1.06827800
F	-5.64808900	-0.46655600	-0.47504700
F	-5.47623400	-1.25812900	-2.47838000
N	-0.88432300	-2.25018800	-0.42065400
C	0.22763300	-2.64757900	0.21626600
C	1.40619500	-1.93950800	0.43167800
C	2.06407000	-3.05238700	1.10351300
C	0.78036000	-3.85850900	0.90351300
O	0.38250600	-4.95604500	1.21143400
O	3.15569400	-3.20918900	1.62627900
H	-0.82259400	-1.28494200	-0.79032100
N	1.79326800	-0.65753000	0.22144700
H	1.07147300	-0.05899600	-0.21473100
C	6.80380600	-2.45680900	-3.34899100
C	5.95477300	-1.69118700	-4.10416700
C	4.84174400	-1.03357800	-3.52809800
C	4.61521500	-1.16206900	-2.12659100
C	5.49089600	-1.97510600	-1.36842800
C	6.56236500	-2.60858100	-1.96060500
H	7.64498300	-2.94940400	-3.82257500
H	6.10696300	-1.57081900	-5.17153600
C	2.67409700	0.22223900	-2.44898000
C	2.98834900	0.26383700	-3.82707000
H	1.75880700	0.70018200	-2.10760000
H	2.33824000	0.81357000	-4.50495000
N	4.03526800	-0.31597600	-4.35870400
O	7.33701900	-3.35994900	-1.14131100
C	8.39248700	-4.10851600	-1.70547700
H	8.83809400	-4.66282400	-0.87904200
H	9.15448300	-3.45924700	-2.15503000
H	8.02644900	-4.81728600	-2.45837700

H	5.32784900	-2.16712000	-0.31347900
C	5.11519600	-0.34440100	2.67788500
H	5.32987300	-1.23225900	2.07567000
H	5.55404800	-0.51223700	3.66540800
C	6.00021400	3.38799400	2.51581600
C	5.68647900	4.39532600	1.70464300
H	6.97099600	3.40425000	3.01039600
H	6.38808300	5.21058900	1.55582300
H	4.75314700	4.46572500	1.15184100
C	3.49203100	-0.46170900	-1.58507600
C	3.19938400	-0.44991900	-0.09089600
H	3.73435500	-1.27314000	0.38424200
C	3.69529100	0.86990000	0.52368700
H	3.23965200	1.71199200	-0.00609800
C	-2.46284200	1.26443200	-1.95267400
C	-3.56477700	1.94513700	-1.42695000
C	-4.69879400	2.18905500	-2.20447300
C	-4.67622000	1.74732500	-3.52089800
C	-3.57549200	1.06180500	-4.05562100
C	-2.46312800	0.80743000	-3.27026300
H	-5.56501400	2.69031500	-1.79560100
H	-5.54957200	1.91852700	-4.14276900
H	-3.60726400	0.71715600	-5.08461400
H	-1.60376600	0.26100000	-3.64726100
C	-1.46899100	1.09548700	-0.89718900
N	-3.30111300	2.22997100	-0.06252700
C	-1.97467700	1.71763700	0.22574600
S	-3.84356200	3.67958200	0.60840500
C	-2.67844200	4.90800000	0.03880300
C	-1.94226400	5.62056900	0.97956000
C	-1.04242800	6.58678500	0.53765500
C	-0.87208800	6.81212800	-0.82627500
C	-1.61223500	6.08486700	-1.75752500
C	-2.53256400	5.13467400	-1.32952800
H	-2.07862300	5.41392200	2.03512900
H	-0.47455000	7.16321600	1.26182500
H	-0.16446200	7.56211600	-1.16672000
H	-1.48171600	6.26549200	-2.81953400
C	-1.41570300	1.66556600	1.60159300
H	-2.06551300	2.23650300	2.26502200
C	-1.34597700	0.24926600	2.17869500
C	-0.27535400	-0.27929600	2.89629500
C	-2.50808700	-0.52255800	2.06196900
C	-0.33580000	-1.56331600	3.43621000
C	-2.57929100	-1.79347200	2.61700600
H	-3.36051700	-0.12815600	1.51581900
C	-1.48525900	-2.33073800	3.29138800
H	0.52372200	-1.96455100	3.96661300
H	-3.48542000	-2.38020200	2.49978500
H	-1.53060400	-3.33832000	3.69235500
O	-0.37132000	0.42534800	-1.04677200
H	0.62142900	0.31116600	3.04921800
O	-3.68813400	3.57039000	2.04894000
H	-3.12526800	4.57660000	-2.04701600
O	-5.14185000	3.96372900	0.03109900
C	1.61979200	4.24457500	0.18990100
O	2.77631300	4.06220800	-0.13499900
H	1.30208200	5.20983200	0.62379400
C	0.55320600	3.19861800	0.06826600
H	-0.36498900	3.64790300	-0.32065100
H	0.86227800	2.38377000	-0.58730500
S	0.22672900	2.59343100	1.75907500
H	2.15452600	1.04382600	1.88428000



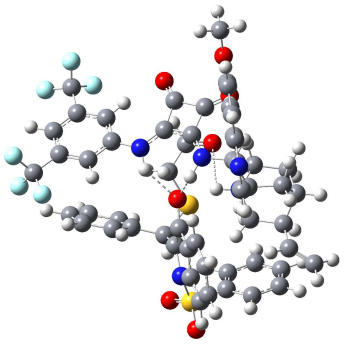
TS3

-2709462.12 kcal/mol

C	-5.23327200	-2.28752700	1.53356500
C	-5.71930100	-1.90521900	2.93923600
C	-4.02812400	-0.07548600	3.17893600
H	-5.89848500	-1.85120500	0.78109200
H	-6.76998000	-2.18034800	3.06183700
H	-3.77349400	0.79634100	2.58524200
H	-3.66361400	0.09130500	4.19507100
H	-5.26016300	-3.37087400	1.38710900
N	-3.28512700	-1.25632600	2.65586700
C	-3.38200100	-2.37002900	3.65476400
H	-2.78276300	-2.07650700	4.51860700
H	-2.90929100	-3.24238500	3.20073900
C	-4.86422000	-2.63070000	4.00585300
H	-5.09419200	-2.17633800	4.97744900

C	2.83689700	4.19568200	-0.09984300
C	1.83931900	3.23339600	-0.15033500
C	0.54580900	3.54041700	0.28336800
C	0.25669000	4.82747200	0.74469900
C	1.27090400	5.77630900	0.77408800
C	2.56574600	5.47726700	0.36300100
H	2.06251200	2.24509300	-0.53854500
H	-0.74991200	5.09116800	1.05544100
H	3.34410400	6.23146500	0.39413800
C	0.99329100	7.17031000	1.27654000
C	4.24280500	3.84094300	-0.50451500
F	1.35572000	8.09305900	0.36711800
F	1.69968400	7.42937800	2.39246400
F	-0.29802400	7.36711700	1.56155000
F	5.02463200	3.65156100	0.57924700
F	4.29473800	2.71125000	-1.22465600
F	4.81343800	4.81607300	-1.22765200
N	-0.39299700	2.50758000	0.23658400
C	-1.71967600	2.53547500	0.46524900
C	-2.64278900	1.48525000	0.44518400
C	-3.76669100	2.38089200	0.75444500
C	-2.77354100	3.53487300	0.79148800
O	-2.82576800	4.72074900	1.02055000
O	-4.96363000	2.22098400	0.91493000
H	-0.03723800	1.60769900	-0.09223500
N	-2.55396300	0.15717700	0.28393600
H	-1.64118300	-0.23806600	0.07521400
C	-4.74611000	0.80476900	-4.68250700
C	-4.34666100	-0.50462900	-4.75418400
C	-4.04427700	-1.24723500	-3.58991800
C	-4.14474500	-0.61018200	-2.31810700
C	-4.58308700	0.72937900	-2.26364900
C	-4.87481600	1.42833600	-3.41724000
H	-4.96927900	1.34692700	-5.59395900
H	-4.25500100	-1.01204300	-5.70871900
C	-3.41837700	-2.69053600	-1.36191800
C	-3.39239100	-3.22972500	-2.67212100
H	-3.11775500	-3.34820200	-0.55351800
H	-3.09608300	-4.26799600	-2.80793900
N	-3.67101400	-2.55059200	-3.75354500
O	-5.28067600	2.70694000	-3.24801400
C	-5.57808700	3.48411700	-4.38794000
H	-5.86885200	4.46428200	-4.00975400
H	-6.41027100	3.05731900	-4.96191000
H	-4.70285800	3.59480000	-5.04027000
H	-4.72948200	1.24802000	-1.32424500
C	-5.53547200	-0.39038000	3.13157900
H	-6.00135300	0.16572100	2.31208300
H	-6.01129600	-0.06046800	4.05957400
C	-5.14186900	-4.10544800	4.10108600
C	-5.71808300	-4.69181000	5.14571400
H	-4.83615300	-4.71057900	3.24714600
H	-5.90727600	-5.76059400	5.16475600
H	-6.02122000	-4.12514500	6.02360700
C	-3.78181000	-1.38103600	-1.16276600
C	-3.72668900	-0.70490500	0.20927000
H	-4.59194300	-0.04462700	0.31651300
C	-3.79610700	-1.75683200	1.33556500
H	-3.11200300	-2.57513400	1.12192200
C	0.77598100	-1.77065800	-2.39973000
C	1.94959400	-2.52845200	-2.42197900
C	2.06304400	-3.61407700	-3.28563600
C	0.97790100	-3.88965100	-4.11395400
C	-0.19790400	-3.12681700	-4.09737500
C	-0.30435700	-2.05194600	-3.23038200
H	2.96439300	-4.21032700	-3.33440000
H	1.05079800	-4.73199100	-4.79549900
H	-1.02848200	-3.37818600	-4.74868600
H	-1.19831300	-1.43848300	-3.18113600
C	0.90538300	-0.75320000	-1.37248500
N	2.85962600	-2.06222600	-1.42924300
C	2.21258800	-0.99875600	-0.71703100
S	4.53918500	-1.95603900	-1.78667700
C	5.26174800	-3.00274900	-0.54868200
C	6.43512000	-2.58111700	0.06188700
C	7.05919700	-3.43504100	0.96601900
C	6.50783900	-4.68027400	1.24745600
C	5.32614300	-5.08538700	0.62744700
C	4.69768500	-4.24770500	-0.28370000
H	6.83160300	-1.59401400	-0.14661800
H	7.96997100	-3.11577000	1.46168600
H	6.99595500	-5.33913400	1.95904300
H	4.89529900	-6.05539700	0.85401400
C	2.53804200	-0.41649400	0.44374300
H	1.83472200	0.34285600	0.77808900
C	3.65674900	-0.71655400	1.35813500
C	3.63463700	-1.89726900	2.10404200
C	4.68456900	0.20825800	1.55362700

C	4.63386600	-2.15018200	3.03696700
C	5.68773600	-0.05514100	2.47965200
H	4.70515100	1.12392200	0.97356600
C	5.66163300	-1.23096900	3.22556800
H	4.60788300	-3.06801500	3.61601300
H	6.48616600	0.66659100	2.62358800
H	6.44133200	-1.42936300	3.95534500
O	0.06642700	0.08474200	-1.05031000
H	2.81397100	-2.59506000	1.97310600
O	4.96783700	-0.59032000	-1.56510700
H	3.77316600	-4.54710600	-0.76770600
O	4.71336600	-2.59076300	-3.08000800
C	-0.79813000	-3.95936000	1.55622900
O	-1.93967700	-4.37758000	1.42236300
H	-0.10853800	-4.45478000	2.26631700
C	-0.25415500	-2.74213700	0.89352000
H	0.76659800	-2.92554400	0.53727000
H	-0.88052000	-2.46572100	0.03782600
S	-0.21089700	-1.48138300	2.23402900
H	-2.22868100	-1.09376100	2.51950900



Int11

-2709471.06 kcal/mol

C	3.99421100	2.43420700	-1.00633800
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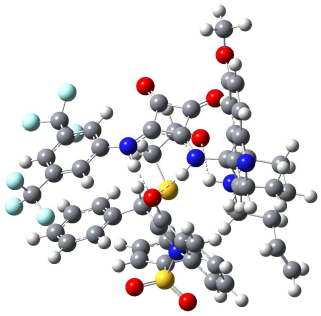
C	2.05986500	1.08171000	-2.62697200
H	3.75567500	3.41499400	-1.43261600
H	5.44465000	1.84581900	-2.49892800
H	1.38000100	1.93459100	-2.64661600
H	1.56603900	0.25009300	-3.13101700
H	4.76846000	2.59349100	-0.25218000
N	2.25825500	0.67432600	-1.19920000
C	3.26584600	-0.44680400	-1.13952000
H	2.90176500	-1.21856600	-1.81977200
H	3.23208800	-0.85233800	-0.12895800
C	4.66766800	0.08084900	-1.50721300
H	5.08372100	-0.56550400	-2.28632000
C	-5.31639500	-0.89681300	1.60440800
C	-4.04994000	-0.35232300	1.47312300
C	-3.67219100	0.25597200	0.27186700
C	-4.57553400	0.31378900	-0.78672300
C	-5.84094700	-0.24786000	-0.63495700
C	-6.22484400	-0.85697600	0.54965500
H	-3.35246200	-0.38570100	2.30252600
H	-4.31088000	0.81233700	-1.71471200
H	-7.21250700	-1.29001000	0.65492700
C	-6.81029100	-0.14321800	-1.78433800
C	-5.75871800	-1.51465000	2.90334100
F	-6.20661000	-0.38816100	-2.95814000
F	-7.34446700	1.08549100	-1.86224600
F	-7.82623400	-1.01359000	-1.66271000
F	-6.13387300	-2.79734800	2.73973500
F	-4.79015900	-1.49960400	3.83537700
F	-6.81657000	-0.86651500	3.41546000
N	-2.37666300	0.78976500	0.20041600
C	-1.90017700	1.70678900	-0.67114700
C	-0.66039000	2.34459700	-0.66194500
C	-0.92695500	3.04040300	-1.92932800
C	-2.30969400	2.38912300	-1.92996300
O	-3.26874000	2.38331300	-2.66704200
O	-0.26941100	3.74991400	-2.66468700
H	-1.64849400	0.31529800	0.74335600
N	0.36820700	2.30320000	0.19761300
H	0.38104400	1.46130500	0.78606800
C	0.31892700	7.72490700	1.33111700
C	1.21665900	7.27394000	2.26325000
C	1.81185100	5.99617200	2.15389200
C	1.46320600	5.16306400	1.05048400
C	0.54818900	5.65035900	0.09324800
C	-0.01692800	6.90223900	0.22769200
H	-0.12160000	8.70865000	1.44410600
H	1.49834400	7.88486700	3.11427000
C	2.96812300	3.53772300	1.97448500
C	3.24949500	4.45268300	3.01832800
H	3.47460200	2.57920300	2.00267400
H	3.96043100	4.17204900	3.79375300
N	2.69892700	5.63271500	3.12374500
O	-0.88360600	7.26843600	-0.74355900
C	-1.50419400	8.53322300	-0.66212700
H	-2.15188000	8.60135700	-1.53632800

H	-0.76889600	9.34714600	-0.69391400
H	-2.11342300	8.62657500	0.24565900
H	0.26843000	5.07825800	-0.78317400
C	3.43853800	1.42731700	-3.22657200
H	3.38086300	2.38761900	-3.74652000
H	3.72988300	0.67437300	-3.96582300
C	5.60811200	0.07864300	-0.32310300
C	6.93307700	0.02478500	-0.42416100
H	5.15418200	0.14566600	0.66761500
H	7.57313000	0.05456000	0.45190500
H	7.42830000	-0.05177500	-1.39070800
C	2.07389800	3.86718900	0.98733500
C	1.66022300	2.89417200	-0.11650400
H	1.53700900	3.45818500	-1.04515800
C	2.74083700	1.82422000	-0.34921700
H	2.98266400	1.33778800	0.59806100
C	1.93790200	-1.07505600	2.04462000
C	2.62754600	-2.27976500	2.25455400
C	3.68432800	-2.34916000	3.16838600
C	4.02866000	-1.18817100	3.84868700
C	3.32878600	0.01402000	3.66412100
C	2.27124200	0.07112900	2.77025000
H	4.21134400	-3.27528900	3.34966200
H	4.84702700	-1.22518600	4.56122200
H	3.60113100	0.89219000	4.24270600
H	1.69551800	0.98487700	2.64583800
C	0.94954400	-1.28310700	1.00120100
N	2.03411100	-3.25400500	1.42799100
C	1.02962800	-2.59953200	0.62270600
S	2.85155900	-4.65205300	0.94452200
C	3.75793700	-4.15933800	-0.51102800
C	3.23322400	-4.42745800	-1.77197200
C	3.94688700	-4.03212200	-2.89910100
C	5.18081200	-3.40321700	-2.75595400
C	5.70154100	-3.15536200	-1.48713200
C	4.98598000	-3.52103800	-0.35281800
H	2.29391100	-4.95918400	-1.87319900
H	3.54222800	-4.23128200	-3.88582900
H	5.74560500	-3.11445200	-3.63749800
H	6.66373000	-2.66779700	-1.37495200
C	0.17753300	-3.32124600	-0.37604100
H	0.61637600	-4.29784300	-0.57222300
C	-1.24792400	-3.61433300	0.07703400
C	-2.07857400	-4.38477200	-0.74474000
C	-1.73591900	-3.18894800	1.30942600
C	-3.37253700	-4.70100500	-0.35239900
C	-3.02683800	-3.52429100	1.71250200
H	-1.09544200	-2.61262100	1.96902900
C	-3.85446200	-4.26795100	0.88124900
H	-4.00429800	-5.29324000	-1.00786800
H	-3.38439700	-3.19730200	2.68287800
H	-4.86513400	-4.50852700	1.19298900
O	0.20803200	-0.32725000	0.48825200
H	-1.70426000	-4.72875500	-1.70609900
O	1.85074200	-5.62039800	0.54256600
H	5.38164700	-3.33438400	0.63995300
O	3.80582800	-4.95948700	1.99033100
C	-1.27590500	-0.57281000	-3.23275300
O	-0.37022200	-0.38933400	-4.01578000
H	-2.23418000	-0.02906500	-3.34928400
C	-1.22582700	-1.49270100	-2.05034600
H	-1.20230300	-0.88910200	-1.13487000
H	-2.14630400	-2.08736600	-2.02502600
S	0.25288400	-2.53849800	-2.06698800
H	1.36940600	0.30194800	-0.77183400



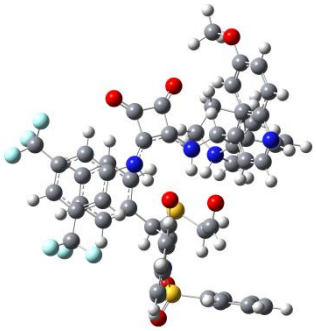
Int12

-2709468.64 kcal/mol

C	-4.49618800	1.96801700	-0.89055200
C	-4.18591900	2.85251800	-2.10404400
C	-2.63409300	1.04424200	-2.89071900
H	-5.27826000	1.24727400	-1.15426200
H	-5.05876900	3.46233200	-2.35072800
H	-2.88055400	-0.01850400	-2.87732300
H	-1.76747500	1.15960500	-3.54112600
H	-4.88402300	2.55832300	-0.05775800
N	-2.17130800	1.44035300	-1.51589000
C	-1.75501800	2.88173600	-1.53036800
H	-0.98691600	2.96792200	-2.30051200
H	-1.28425300	3.09118800	-0.56830500
C	-2.98541000	3.77927400	-1.80595700

H	-2.79162100	4.36819100	-2.70971800
C	3.88185900	-2.79473500	1.84265700
C	2.50696600	-2.62838000	1.79257200
C	1.81410100	-2.88426000	0.60473900
C	2.50863600	-3.33706000	-0.51614200
C	3.89491100	-3.44020400	-0.45635400
C	4.59645000	-3.17428200	0.71112700
H	1.96371700	-2.26882500	2.66061100
H	1.97956500	-3.59810500	-1.42915000
H	5.67554200	-3.25348600	0.74015900
C	4.63494700	-3.72919000	-1.73315300
C	4.59742600	-2.62395800	3.15648500
F	4.70817100	-2.61709300	-2.50053100
F	4.02370700	-4.66606800	-2.47079400
F	5.89397800	-4.13559300	-1.51538200
F	5.87470500	-2.24402100	2.99181100
F	3.99957600	-1.71626500	3.94432400
F	4.62007300	-3.78184100	3.84168500
N	0.44862300	-2.56551800	0.59999100
C	-0.40602500	-2.58520600	-0.44344000
C	-1.59159800	-1.85694200	-0.60528900
C	-1.84283900	-2.42761700	-1.93432600
C	-0.53765200	-3.20148400	-1.78600600
O	0.14668200	-3.89838100	-2.50627200
O	-2.70411600	-2.27145900	-2.78129900
H	0.19354100	-1.85250700	1.31432300
N	-2.17783900	-0.91570700	0.13849000
H	-1.71201700	-0.68681300	1.04212600
C	-6.56742500	-4.25679900	1.04729300
C	-6.75363500	-3.29189700	2.00264200
C	-6.06733200	-2.05703100	1.94505000
C	-5.16499700	-1.81946900	0.86760200
C	-4.99321300	-2.82022000	-0.11317600
C	-5.67580500	-4.01653500	-0.02750600
H	-7.10645200	-5.19401700	1.12163700
H	-7.43293800	-3.44778800	2.83395400
C	-4.74983200	0.32645800	1.86654000
C	-5.67311500	-0.01504700	2.88407200
H	-4.25535400	1.28909100	1.92994900
H	-5.87361800	0.69804300	3.68187500
N	-6.31152000	-1.15451900	2.93788700
O	-5.43655300	-4.90782500	-1.01643800
C	-6.08504800	-6.16062500	-0.97614800
H	-5.73351100	-6.70388500	-1.85351800
H	-7.17571500	-6.05345000	-1.03187900
H	-5.81908100	-6.72415700	-0.07312100
H	-4.33555200	-2.69033400	-0.96549100
C	-3.82251100	1.94203800	-3.28504900
H	-4.68180800	1.32235400	-3.55712100
H	-3.56638600	2.54439300	-4.16197800
C	-3.23057200	4.72986700	-0.66615800
C	-3.30938200	6.04995000	-0.79887100
H	-3.31872500	4.28912500	0.32691800
H	-3.47941100	6.69563200	0.05702400
H	-3.20154900	6.53654500	-1.76599100
C	-4.48188000	-0.56033600	0.85700100
C	-3.43729400	-0.28157700	-0.21291400
H	-3.78023900	-0.72610600	-1.15072000
C	-3.22030700	1.22110200	-0.45186200
H	-2.78092100	1.66690400	0.44671900
C	-0.95403800	1.90030900	2.40695200
C	-0.54148900	3.12618500	1.87846200
C	-1.22674800	4.30307500	2.19201000
C	-2.31275200	4.20643700	3.05633800
C	-2.72030700	2.98028400	3.60005100
C	-2.04013100	1.81512000	3.27508100
H	-0.92727200	5.25660900	1.78215900
H	-2.85304800	5.11208600	3.31646700
H	-3.56697400	2.94713500	4.27991400
H	-2.33045300	0.84639700	3.67053900
C	-0.12897000	0.83996400	1.83508400
N	0.53399800	2.88926500	0.97137600
C	0.76900500	1.45546800	0.98301900
S	1.82252800	4.03081800	1.02956000
C	2.46438900	3.96624100	-0.62207500
C	3.76297000	3.52835900	-0.83468100
C	4.26059700	3.52804400	-2.13576100
C	3.46727700	3.97056700	-3.18769400
C	2.17271000	4.43672600	-2.95167500
C	1.66613900	4.44380400	-1.66112100
H	4.36316900	3.18449500	0.00025700
H	5.26960400	3.17371400	-2.31995700
H	3.86000900	3.96425200	-4.19997500
H	1.56580200	4.79925500	-3.77536700
C	1.64624800	0.66670600	0.06062000
H	1.28718900	-0.35032800	0.23406800
C	3.14513300	0.62508500	0.35250300
C	4.10852300	0.39249200	-0.62844900

C	3.56143900	0.71003800	1.68261600
C	5.45297800	0.25354800	-0.29573400
C	4.90516900	0.59403500	2.01676200
H	2.82549500	0.89127200	2.45840700
C	5.85786600	0.35770800	1.03016500
H	6.18051200	0.06604100	-1.08015500
H	5.20451700	0.67314200	3.05633700
H	6.90520400	0.25146100	1.29555300
O	-0.35449300	-0.41515500	2.05640100
H	3.82889700	0.36656500	-1.67373600
O	2.84832600	3.59907900	1.96003400
H	0.67154900	4.82370900	-1.44882200
O	1.18850200	5.33051100	1.18350600
C	0.69913500	-0.82661200	-3.73483600
O	-0.02251600	0.00575300	-4.23420800
H	0.79919500	-1.83519300	-4.17662900
C	1.54317700	-0.59865500	-2.50827800
H	1.39318600	-1.42430200	-1.81049600
H	2.59011100	-0.68059300	-2.82604700
S	1.17779600	0.99184900	-1.71059700
H	-1.32050400	0.89962900	-1.28396500

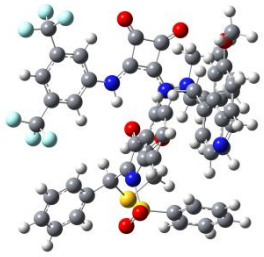


TS4

-2709466.96 kcal/mol

C	5.13668400	-1.38981500	-0.87722900
C	5.23123400	-1.36953700	-2.41043400
C	2.97768500	-0.30539400	-2.68035600
H	5.72072500	-0.56599000	-0.45454300
H	6.27819200	-1.34731800	-2.72306600
H	2.52503600	0.59490600	-2.27268300
H	2.41231300	-0.59802100	-3.56772100
H	5.56233000	-2.31143100	-0.47134900
N	2.79946900	-1.41164300	-1.69005900
C	3.14162300	-2.71440000	-2.34021800
H	2.35909800	-2.92526300	-3.07077800
H	3.09160700	-3.47305300	-1.55518600
C	4.54050000	-2.62594300	-2.99111300
H	4.41979200	-2.47092000	-4.06992500
C	-4.10644100	3.10178700	0.61359500
C	-2.87385800	2.50270300	0.80813500
C	-1.70208000	3.18107500	0.46155600
C	-1.77538300	4.47380800	-0.05319800
C	-3.02617800	5.05232600	-0.24586100
C	-4.19919100	4.38251700	0.07748600
H	-2.82116100	1.49332900	1.20137600
H	-0.87174400	5.01210200	-0.32667400
H	-5.16434500	4.84865200	-0.07934300
C	-3.09601100	6.39827900	-0.91617400
C	-5.36143400	2.32148100	0.89764900
F	-2.10378600	7.20841800	-0.52491200
F	-4.25688500	7.02656200	-0.66802500
F	-2.99708000	6.27199000	-2.25595000
F	-6.34237200	3.11287500	1.36313600
F	-5.83517600	1.73127700	-0.21756300
F	-5.15970100	1.35001500	1.79971800
N	-0.50528800	2.47760700	0.62888500
C	0.69573200	2.71828100	0.07659900
C	1.78879600	1.85782400	-0.07619800
C	2.60647100	2.89587900	-0.71025700
C	1.43806300	3.85788900	-0.53051800
O	1.20877900	5.01342200	-0.80278400
O	3.72634400	2.92738000	-1.19843600
H	-0.63458000	1.48841100	0.87291500
N	2.02056900	0.55144300	0.14654200
H	1.25449400	-0.03696900	0.48718400
C	6.93512700	2.36002900	3.38605600
C	6.31885600	1.39050600	4.11913600
C	5.27621000	0.59984700	3.55944200
C	4.89991400	0.82179200	2.20397300
C	5.54894300	1.84562100	1.45817200
C	6.53689700	2.60318200	2.04241800
H	7.72368000	2.97696100	3.80398400
H	6.59372400	1.19727400	5.15061400
C	3.26748500	-0.92131300	2.51585800
C	3.70984100	-1.03897500	3.84837300
H	2.45058700	-1.54735400	2.16056000
H	3.23823300	-1.76279900	4.51037000
N	4.68675500	-0.32525900	4.36017700
O	7.19294100	3.61241300	1.43208400
C	6.82132900	3.93318800	0.10406200
H	5.76296700	4.20728900	0.03345800

H	7.01424000	3.09225600	-0.57432700
H	7.44304700	4.78148900	-0.18238500
H	5.22606900	2.07262300	0.45023800
C	4.48636300	-0.13444300	-2.94562200
H	4.84568800	0.77785600	-2.45917300
H	4.66089000	-0.02011000	-4.01923500
C	5.31405100	-3.89858700	-2.78965800
C	5.78178300	-4.65423300	-3.77819700
H	5.48970900	-4.20264900	-1.75719800
H	6.34353800	-5.56227900	-3.58273000
H	5.62173300	-4.39264300	-4.82181500
C	3.86826100	-0.00715400	1.68062600
C	3.39787700	0.10071700	0.23700300
H	3.98342100	0.85425500	-0.28698000
C	3.65527200	-1.24520700	-0.46335500
H	3.32894500	-2.05930100	0.18315400
C	-2.35661600	-1.19919400	1.81752000
C	-3.34797300	-2.11542000	1.46854900
C	-4.40136000	-2.38510700	2.34889000
C	-4.40626500	-1.71421400	3.56556400
C	-3.40991500	-0.79326800	3.91984100
C	-2.37731500	-0.52561200	3.03755400
H	-5.19390400	-3.07287700	2.08774300
H	-5.22414800	-1.90099600	4.25503100
H	-3.45971300	-0.28630700	4.87782100
H	-1.59376800	0.18982200	3.27051300
C	-1.45950700	-1.04188600	0.68032400
N	-3.07599900	-2.60325800	0.16914300
C	-1.83345700	-1.98504000	-0.33057400
S	-3.65293400	-4.10149800	-0.32650400
C	-2.64647800	-5.33978500	0.48713400
C	-2.09671100	-6.35198900	-0.29419200
C	-1.31827900	-7.33179100	0.31418300
C	-1.09714200	-7.29460400	1.68750100
C	-1.66680400	-6.28582500	2.46182000
C	-2.45393200	-5.30631100	1.86765600
H	-2.27792300	-6.36417600	-1.36347700
H	-0.88597700	-8.12441300	-0.28818400
H	-0.48501400	-8.05731100	2.15886200
H	-1.50225000	-6.26177500	3.53419900
C	-1.84933400	-1.59653000	-1.80861800
H	-2.71902300	-2.09235200	-2.23734900
C	-1.98988300	-0.11130700	-2.10489100
C	-0.90474200	0.73841500	-2.32304000
C	-3.27982400	0.42084300	-2.18326000
C	-1.10448700	2.07467400	-2.65573600
C	-3.48130700	1.76081500	-2.49883900
H	-4.13617200	-0.22243500	-1.99639900
C	-2.39345100	2.59082500	-2.75085600
H	-0.24902400	2.72208700	-2.82984400
H	-4.49092900	2.15551700	-2.54220700
H	-2.54698500	3.63817000	-2.99028100
O	-0.52984100	-0.21379000	0.61091700
H	0.10274500	0.34718900	-2.22847700
O	-3.38646500	-4.20674000	-1.75094200
H	-2.90157800	-4.52687500	2.47395400
O	-5.00737200	-4.21088000	0.17971000
C	-0.00649000	-3.13349900	-0.17066000
O	0.97305200	-2.37812700	0.05709800
H	-0.37596700	-3.78046900	0.63954900
C	-0.18958300	-3.68698900	-1.57868200
H	0.71740300	-4.23282700	-1.86377600
H	-1.03559000	-4.36777700	-1.64873600
S	-0.41221400	-2.31998600	-2.73473400
H	1.81749300	-1.50721000	-1.33316000



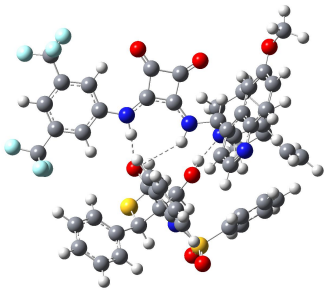
TS5

-2709464.53 kcal/mol

C	5.65282800	0.91112600	-1.26065300
C	6.38852500	1.40132800	-2.51673600
C	4.41174200	2.90856100	-2.84675100
H	5.79238000	1.62896400	-0.44405300
H	7.47016300	1.36186400	-2.36149300
H	3.98667200	3.40607600	-1.97126000
H	4.03239300	3.41226000	-3.73830200
H	6.04154500	-0.05148000	-0.92245400
N	3.89530900	1.50034600	-2.88945300
C	4.51121300	0.76518400	-4.04016800
H	4.38345800	1.40084900	-4.91908000
H	3.92790600	-0.14150400	-4.18407400
C	6.00366200	0.51350000	-3.73067900
H	6.58757500	0.87183000	-4.58757600

C	-4.80854900	1.96613600	-0.60537300
C	-3.46251200	1.67387500	-0.77843900
C	-2.51267600	2.69577300	-0.68928500
C	-2.92360400	4.00376600	-0.43056000
C	-4.27773400	4.26943300	-0.26031100
C	-5.23209600	3.26422100	-0.34385000
H	-3.14274600	0.65474900	-0.98045400
H	-2.19785400	4.80901100	-0.35439500
H	-6.28260200	3.48633200	-0.21111700
C	-4.68508100	5.69272000	0.02151100
C	-5.80475200	0.83979200	-0.68031200
F	-4.13365600	6.14253800	1.15999500
F	-6.01623800	5.82456900	0.14019000
F	-4.28585200	6.51797900	-0.96050200
F	-5.62903200	0.10284300	-1.78693500
F	-5.67787600	0.00802300	0.37228100
F	-7.07153500	1.28139600	-0.68432200
N	-1.17365200	2.33301700	-0.86949500
C	-0.07358900	3.07839000	-0.72241000
C	1.26389000	2.68023500	-0.79455000
C	1.77525300	4.01524200	-0.52079000
C	0.32885100	4.49433100	-0.42041100
O	-0.22984500	5.54168500	-0.20742100
O	2.89134300	4.50387300	-0.42402700
H	-0.97614700	1.31894100	-1.03386200
N	1.86949700	1.49595300	-1.07601700
H	1.21409200	0.68553900	-1.07835700
C	3.15792800	1.47921200	4.72341000
C	3.04493800	0.16025800	4.37027400
C	3.03522400	-0.24164300	3.01490200
C	3.17194500	0.75267700	2.00171100
C	3.28310700	2.10901400	2.38299000
C	3.27057500	2.46911300	3.71455400
H	3.15101200	1.75543300	5.77141400
H	2.93615400	-0.61534700	5.12065200
C	2.95385100	-1.03855000	0.41666800
C	2.80547500	-1.93205800	1.49951700
H	2.88173100	-1.43015600	-0.59297800
H	2.64162200	-2.98747300	1.29997800
N	2.85950400	-1.56662000	2.75498700
O	3.37480600	3.79370700	3.97312300
C	3.27555300	4.23534900	5.30981300
H	3.33795300	5.32293600	5.26782800
H	4.09844400	3.85113300	5.92585000
H	2.31732200	3.94677900	5.75965400
H	3.35867400	2.91223800	1.65713100
C	5.95199700	2.84618900	-2.80762900
H	6.32175900	3.51876600	-2.02920600
H	6.37674300	3.18278800	-3.75883900
C	6.38868000	-0.92901100	-3.50174900
C	5.59022200	-1.98122000	-3.34061800
H	7.46659900	-1.08292000	-3.44771800
H	6.01321300	-2.96617700	-3.16907000
H	4.50432100	-1.92538800	-3.36735500
C	3.14535400	0.29915300	0.64758800
C	3.20590400	1.26827700	-0.51722100
H	3.57939600	2.23420700	-0.17642200
C	4.16500500	0.75967000	-1.60217300
H	3.92504300	-0.27089500	-1.85287800
C	-0.58629800	-0.63320400	1.24654600
C	-1.15754200	-1.69803500	1.95903000
C	-1.27160200	-1.65721000	3.34905800
C	-0.79838500	-0.52540600	4.00095200
C	-0.24262700	0.55104200	3.29794300
C	-0.13816000	0.50399600	1.91770800
H	-1.73705500	-2.46746200	3.89548000
H	-0.88234200	-0.47048700	5.08229300
H	0.11508300	1.42302300	3.83670300
H	0.29231100	1.33462600	1.36870100
C	-0.64394000	-0.96879000	-0.16926400
N	-1.58475900	-2.67902400	1.03495700
C	-1.24386200	-2.20447200	-0.27368400
S	-1.54519300	-4.31521200	1.46712900
C	0.17811400	-4.72323700	1.70520700
C	0.87679200	-5.30713000	0.65105300
C	2.20128700	-5.68457600	0.85116000
C	2.80880400	-5.47947200	2.08896300
C	2.09918600	-4.88733300	3.13109100
C	0.77421600	-4.50798500	2.94513500
H	0.37522700	-5.47511400	-0.29663100
H	2.75377900	-6.15369500	0.04259500
H	3.84119700	-5.77958500	2.24187200
H	2.57774500	-4.71069400	4.08796300
C	-1.71858700	-2.71287000	-1.59066400
H	-1.70592600	-1.81473700	-2.21907300
C	-3.13386400	-3.26241000	-1.63770000
C	-3.50965000	-4.33427000	-2.44524100
C	-4.11823100	-2.60864700	-0.89321100

C	-4.83662100	-4.75012200	-2.49918100
C	-5.44364300	-3.02159300	-0.94739600
H	-3.84553700	-1.77578300	-0.25271600
C	-5.80909900	-4.09746300	-1.75018600
H	-5.10643300	-5.59405600	-3.12758800
H	-6.18812300	-2.49521100	-0.35963800
H	-6.84371300	-4.42529300	-1.78976400
O	-0.26923000	-0.21107000	-1.17067300
H	-2.76920100	-4.86752000	-3.03319300
O	-2.01724000	-5.06616900	0.32525900
H	0.20738900	-4.06141800	3.75309600
O	-2.19955200	-4.40219600	2.75972700
C	1.11157300	-1.59946100	-2.97343000
O	2.17419800	-1.01237000	-3.10635200
H	0.20737200	-1.24587300	-3.49015800
C	0.99475900	-2.86765900	-2.16450900
H	1.86426500	-3.49961100	-2.37260100
H	1.02904300	-2.60282600	-1.09850800
S	-0.49800100	-3.84041400	-2.46230400
H	2.86730300	1.49844100	-2.96581500

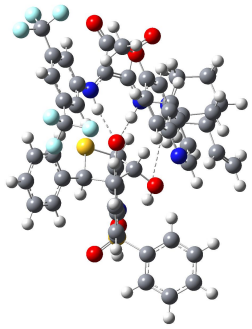


Int13

-2709492.28 kcal/mol

C	4.63022700	1.36342700	-1.26730000
C	4.90405000	1.67514900	-2.74697300
C	2.46078900	1.65530200	-3.27969800
H	4.70152100	2.28528900	-0.68057200
H	5.85208800	2.21143600	-2.85013500
H	1.61119600	2.20178900	-2.86835300
H	2.18305500	1.34461500	-4.29181600
H	5.38415000	0.68217300	-0.85998300
N	2.67313700	0.42350900	-2.49578800
C	3.65130600	-0.42112700	-3.20037300
H	3.17634400	-0.82180300	-4.10227500
H	3.88025900	-1.26931400	-2.54733900
C	4.94611700	0.36399700	-3.56519100
H	4.91369000	0.63121300	-4.62910600
C	-5.92326300	0.84163100	-0.28345100
C	-4.53927300	0.74098000	-0.27258700
C	-3.75285000	1.89331300	-0.37522400
C	-4.36965900	3.14179100	-0.48168800
C	-5.75829000	3.21409600	-0.48438700
C	-6.55132600	2.07671900	-0.38631600
H	-4.06406300	-0.23281500	-0.20016400
H	-3.77504100	4.04709700	-0.57345900
H	-7.63095700	2.15084000	-0.40184600
C	-6.40498600	4.57492100	-0.54570200
C	-6.73032400	-0.42129200	-0.15529900
F	-5.76328600	5.39261000	-1.39102600
F	-6.40130100	5.16796700	0.66071400
F	-7.68599100	4.50136100	-0.94614800
F	-8.02273400	-0.23572000	-0.45318200
F	-6.26348300	-1.38982800	-0.96761900
F	-6.67600400	-0.91538400	1.09759100
N	-2.36473600	1.71244900	-0.36500000
C	-1.37552700	2.61706900	-0.55567800
C	0.00678200	2.42798500	-0.61458100
C	0.25613600	3.85972800	-0.87355600
C	-1.24466100	4.08882900	-0.74100500
O	-1.98316300	5.04498000	-0.78426300
O	1.23919000	4.52561400	-1.12495200
H	-2.07885600	0.73456800	-0.32642700
N	0.85321800	1.39145300	-0.54724200
H	0.52251000	0.43507400	-0.47352900
C	4.56333600	4.56771400	3.41293400
C	4.26548200	3.35107100	3.96831700
C	3.61043000	2.34185300	3.22399500
C	3.26701800	2.60232200	1.86313900
C	3.56589600	3.87094500	1.31371200
C	4.20159900	4.83393000	2.06820500
H	5.06414600	5.32012200	4.01110600
H	4.52017300	3.12676800	4.99881500
C	2.35705800	0.37893400	1.81138200
C	2.71969700	0.24154300	3.16887100
H	1.87621800	-0.45221700	1.30200200
H	2.48954300	-0.68500700	3.69233100
N	3.33763900	1.16757000	3.85933600
O	4.44441100	6.01283700	1.44774900
C	5.01481000	7.06710800	2.19142500
H	5.07347700	7.91436300	1.50771000
H	6.02475600	6.81711700	2.54108800

H	4.38897900	7.34061700	3.05010100
H	3.26488100	4.14602300	0.30891200
C	3.74262200	2.52651800	-3.28567200
H	3.60293300	3.41565500	-2.66059600
H	3.96535200	2.87795900	-4.29859200
C	6.17963100	-0.45791600	-3.33334300
C	6.96710800	-0.94064300	-4.29084800
H	6.42214200	-0.67557900	-2.29288500
H	7.84562600	-1.53683100	-4.06206600
H	6.76568000	-0.75108400	-5.34297100
C	2.63532200	1.54361900	1.14088900
C	2.27716900	1.65041200	-0.33619300
H	2.42849200	2.67332300	-0.67745500
C	3.21485000	0.73209500	-1.15238500
H	3.28296400	-0.23100700	-0.63835000
C	-0.78452500	-1.71909000	1.55077300
C	0.08332500	-2.75974600	1.89375800
C	0.48542600	-2.91400900	3.22274400
C	0.01935000	-1.98463000	4.14706700
C	-0.82900700	-0.92520500	3.79781300
C	-1.24707200	-0.79450800	2.48571900
H	1.11650700	-3.73665200	3.53045100
H	0.32715200	-2.09237800	5.18295600
H	-1.16031100	-0.22395800	4.55523000
H	-1.91745600	0.00121400	2.17498000
C	-1.07695000	-1.80737800	0.13848900
N	0.39755200	-3.52331800	0.75461000
C	-0.33471300	-3.02551300	-0.43458300
S	1.68406900	-4.60289000	0.67715900
C	3.14902000	-3.61746100	0.42668000
C	3.84258200	-3.73509300	-0.77324700
C	5.01340700	-3.00300300	-0.94697500
C	5.46580900	-2.15851200	0.06404500
C	4.75814900	-2.04555500	1.25854600
C	3.60075800	-2.79002600	1.45134900
H	3.47853300	-4.40408900	-1.54541900
H	5.56902000	-3.08822400	-1.87589600
H	6.38235400	-1.59211500	-0.07256600
H	5.10551400	-1.38311700	2.04458700
C	-1.30650600	-4.09702900	-0.99664200
H	-0.72745900	-5.01782200	-1.07278300
C	-2.49168100	-4.34286000	-0.08704600
C	-3.67717100	-3.60749100	-0.15831600
C	-2.34193300	-5.29428100	0.92600500
C	-4.68555200	-3.81039600	0.77897700
C	-3.34830800	-5.49295000	1.86508200
H	-1.42727400	-5.87914300	0.98245100
C	-4.52150100	-4.74793000	1.79470700
H	-5.59887000	-3.23026900	0.71464800
H	-3.21536300	-6.23353400	2.64796600
H	-5.31024000	-4.90184600	2.52506500
O	-1.76585600	-1.05569700	-0.53446200
H	-3.81201200	-2.87693400	-0.94967400
O	1.46851900	-5.39727200	-0.51802200
H	3.06290900	-2.72879600	2.39069100
O	1.77559500	-5.21795000	1.98659600
C	0.54622600	-2.53446900	-1.59558200
O	1.23119300	-1.39764000	-1.14410200
H	1.24631700	-3.33366100	-1.86677000
C	-0.39211600	-2.28099000	-2.77904100
H	-0.84143700	-1.29050700	-2.69294600
H	0.14718100	-2.35832600	-3.72626400
S	-1.69738000	-3.55954500	-2.71236600
H	1.56929500	-0.82431700	-1.88474600



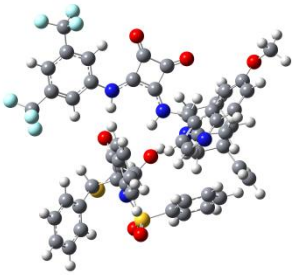
Int14

-2709484.13 kcal/mol

C	2.76269000	4.62465700	1.28590700
C	3.40616400	5.81192500	0.55615600
C	1.44748400	5.70416300	-0.99661700
H	2.01368800	4.99862400	1.99617500
H	3.98396000	6.41881400	1.26020100
H	0.42370900	5.60288400	-0.62893100
H	1.37238900	6.10177800	-2.01358600
H	3.50486500	4.07876300	1.87694700
N	2.05802200	4.37136900	-1.09018700
C	3.43324500	4.51418600	-1.57302600
H	3.39590400	5.02381600	-2.54103000
H	3.84530700	3.51302600	-1.74994600
C	4.33875200	5.29923600	-0.56825700

H	4.76924500	6.17655000	-1.06691400
C	-4.57209400	-1.90493200	0.26877800
C	-3.48145600	-1.12364300	-0.08937000
C	-3.67637400	0.10326700	-0.72592000
C	-4.97435800	0.54730600	-0.99294700
C	-6.04903500	-0.25234500	-0.62474900
C	-5.86845300	-1.48400400	0.00180100
H	-2.47203800	-1.44940500	0.14259800
H	-5.13704200	1.51737000	-1.45471900
H	-6.71917900	-2.09220100	0.28218500
C	-7.44871500	0.26804300	-0.82505500
C	-4.30044600	-3.18720900	1.00536800
F	-7.54017500	1.07868100	-1.88463900
F	-7.85858200	0.96907200	0.25151900
F	-8.33041600	-0.73149000	-0.99629600
F	-3.47873000	-3.99637600	0.31622400
F	-3.68940700	-2.94443800	2.18773400
F	-5.41810500	-3.87480400	1.27162900
N	-2.53260800	0.83419500	-1.05980400
C	-2.41384000	2.19172300	-1.03852400
C	-1.29067600	2.93756200	-0.71803600
C	-2.06314200	4.19800900	-0.68123300
C	-3.28620200	3.38238500	-1.14198600
O	-4.44231000	3.60627700	-1.41037800
O	-1.84546000	5.32554100	-0.30011500
H	-1.67258500	0.35373700	-0.80995500
N	-0.03528300	2.56752600	-0.40497200
H	0.11285800	1.56553400	-0.47465600
C	-2.69207500	0.20228100	3.16366200
C	-1.45180100	-0.29267000	3.47455700
C	-0.26865200	0.38005400	3.08839900
C	-0.37627100	1.60585200	2.37105500
C	-1.65823500	2.15040600	2.16162500
C	-2.79680000	1.45063100	2.50121000
H	-3.57744600	-0.35930000	3.43554400
H	-1.34182000	-1.22861500	4.01286800
C	2.00445600	1.54746500	2.15164600
C	2.00307700	0.38447100	2.96026500
H	2.95874400	1.88144800	1.76347800
H	2.95254100	-0.08552200	3.21385000
N	0.92115900	-0.21342500	3.38730400
O	-3.96844200	2.02330800	2.14683800
C	-5.17348200	1.34338100	2.43966400
H	-5.96594400	1.92266200	1.96780400
H	-5.34565500	1.29082200	3.52192700
H	-5.17679100	0.33249700	2.01732000
H	-1.78884200	3.12632400	1.71310100
C	2.28659900	6.64382600	-0.08615900
H	1.65898800	7.09052900	0.69307900
H	2.72059200	7.46981300	-0.66180000
C	5.46849600	4.45212500	-0.05275400
C	6.74311900	4.82915800	-0.00352700
H	5.20082900	3.45032300	0.29021100
H	7.51965300	4.17358000	0.37983300
H	7.05880500	5.81165400	-0.34852300
C	0.82313000	2.15967200	1.80865600
C	0.72513600	3.20420000	0.68303900
H	0.13847000	4.06498100	1.02136600
C	2.10446200	3.70829000	0.21654700
H	2.74464900	2.83606100	0.04892600
C	0.88701500	-2.49456200	0.70504600
C	2.11554700	-3.06763800	0.37292200
C	2.50009000	-4.28324500	0.93055800
C	1.61458400	-4.87944900	1.82389800
C	0.38289200	-4.30576400	2.16337700
C	0.00825700	-3.09719800	1.60078900
H	3.43259200	-4.76914900	0.67402200
H	1.89251400	-5.83142000	2.26624500
H	-0.27590300	-4.81344100	2.85900200
H	-0.94045700	-2.62575800	1.83377200
C	0.74329100	-1.26996300	-0.04662400
N	2.80150600	-2.24023300	-0.53874900
C	1.92586000	-1.15660400	-1.02543100
S	4.24539300	-2.69202000	-1.24552200
C	5.34378200	-2.78483500	0.15150700
C	6.23540500	-3.85277100	0.20485400
C	7.11887400	-3.93193200	1.27621700
C	7.09800400	-2.95806000	2.27115500
C	6.19809500	-1.89642900	2.20093600
C	5.31137500	-1.79870000	1.13537400
H	6.22337600	-4.60973200	-0.57186200
H	7.81954000	-4.75836600	1.33451400
H	7.78519100	-3.02786700	3.10858900
H	6.18355000	-1.14153700	2.98041900
C	1.38950000	-1.44766500	-2.47849600
H	2.25781000	-1.76122300	-3.06569600
C	0.33295100	-2.52864400	-2.54234000
C	-1.03390200	-2.24362000	-2.49499900

C	0.74559900	-3.86378400	-2.56615600
C	-1.96771000	-3.27291900	-2.44238400
C	-0.18924900	-4.89155800	-2.50326900
H	1.80471600	-4.10204100	-2.61709800
C	-1.54796400	-4.59926000	-2.43353400
H	-3.02543400	-3.03374100	-2.39849000
H	0.14832100	-5.92346500	-2.50988200
H	-2.27835200	-5.40043100	-2.37772000
O	-0.15459500	-0.44526600	0.02922700
H	-1.37512200	-1.21263500	-2.49948900
O	4.60662100	-1.57623000	-2.11945300
H	4.60713500	-0.97568800	1.06076500
O	4.14464800	-4.02509800	-1.81488000
C	2.50399100	0.31021600	-0.98929800
O	3.79997300	0.46327400	-0.48482600
H	1.88144000	0.84378600	-0.27754400
C	2.31898300	0.95220000	-2.37214800
H	2.14031500	2.02817700	-2.28347300
H	3.20249400	0.77132500	-2.99354600
S	0.86168600	0.17669800	-3.11691800
H	4.41100800	0.06177900	-1.12561900



Int15

-2709485.27 kcal/mol

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C	-5.23295600	-1.67710400	-2.33632200
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H	-4.60895600	-2.52580300	-0.44567600
H	-6.17954900	-2.22511000	-2.30926900
H	-2.03036400	-2.08663200	-3.18041400
H	-2.88321100	-1.08755200	-4.34987800
H	-5.31482100	-0.93184300	-0.28380200
N	-3.00357600	-0.40118300	-2.39257200
C	-4.10956900	0.49428200	-2.76791900
H	-3.83432000	1.01710600	-3.69018700
H	-4.20160200	1.24872200	-1.97934800
C	-5.44955200	-0.27773500	-2.95565800
H	-5.63742600	-0.40954700	-4.02883000
C	5.85417600	-0.70634200	-0.33191400
C	4.48946000	-0.66644000	-0.55804200
C	3.77895300	-1.85206300	-0.79050200
C	4.45685100	-3.07034300	-0.80488400
C	5.83164800	-3.08216200	-0.57890500
C	6.54452800	-1.91594100	-0.33804000
H	3.96615100	0.28344900	-0.56703900
H	3.92451600	-3.99808300	-0.99984200
H	7.61378200	-1.94460200	-0.16800100
C	6.53449300	-4.41614000	-0.55188100
C	6.59537300	0.56472300	-0.01415100
F	6.13346900	-5.20657400	-1.55714800
F	6.28216300	-5.07229600	0.59358300
F	7.86809200	-4.28304300	-0.64777900
F	7.78151100	0.61681500	-0.63910000
F	5.90075000	1.65988300	-0.36995200
F	6.84196000	0.66702800	1.30455800
N	2.39971800	-1.72361800	-0.97948800
C	1.45133300	-2.68078900	-1.11677200
C	0.06446400	-2.55651100	-1.11325000
C	-0.13655800	-3.99977900	-1.34891600
C	1.38400800	-4.15827200	-1.29355200
O	2.16856700	-5.07444400	-1.36454500
O	-1.10124300	-4.70887300	-1.53671100
H	2.07307500	-0.75757200	-0.99100800
N	-0.81844800	-1.55123700	-0.99667100
H	-0.49906300	-0.59348000	-0.88412400
C	-3.66912300	-5.19254000	3.29411500
C	-3.22865300	-4.04458300	3.89874900
C	-2.72693100	-2.95909000	3.14271600
C	-2.69266300	-3.06835000	1.71949800
C	-3.13350200	-4.26876800	1.11594500
C	-3.61404800	-5.30897400	1.88222000
H	-4.04569900	-6.00623600	3.90300000
H	-3.24787900	-3.93565400	4.97803300
C	-1.76854900	-0.85116500	1.71143500
C	-1.82107500	-0.86469500	3.12180400
H	-1.39514200	0.03383200	1.20300400
H	-1.45977000	-0.00097700	3.67807200
N	-2.29432300	-1.86250000	3.82658900
O	-4.01562700	-6.41145800	1.20600400
C	-4.42572900	-7.54532600	1.93825200
H	-4.65076100	-8.31200900	1.19639400
H	-5.32781200	-7.34220300	2.52968500

H	-3.62960800	-7.90814400	2.60023600
H	-3.05962000	-4.43136400	0.04687500
C	-4.20554400	-2.42181900	-3.20451800
H	-3.94396400	-3.37882500	-2.73866300
H	-4.63164900	-2.65013000	-4.18712200
C	-6.61252500	0.46898600	-2.37149000
C	-7.57563700	1.05567700	-3.07726000
H	-6.64342100	0.53358000	-1.28341000
H	-8.39130500	1.58919800	-2.59808900
H	-7.58796300	1.01863700	-4.16443900
C	-2.20825800	-1.93628400	0.99521000
C	-2.16721000	-1.87393700	-0.52889300
H	-2.38229400	-2.85794000	-0.94537600
C	-3.25224700	-0.88854900	-1.01693700
H	-3.21156500	0.00170400	-0.38250400
C	1.11857000	1.47047200	1.20862900
C	0.36624900	2.49258000	1.79989600
C	0.26992300	2.55892600	3.19360000
C	0.90721500	1.56805000	3.93134300
C	1.63871800	0.52897200	3.33738100
C	1.75743300	0.48265900	1.96102900
H	-0.26421400	3.36239700	3.68194600
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H	2.32931800	-0.29644000	1.46620700
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N	-0.17558000	3.33923000	0.81591900
C	0.29375300	2.93557100	-0.52801900
S	-1.50836900	4.33589300	1.10029500
C	-2.93734500	3.26095700	1.08597700
C	-3.90035300	3.45279800	0.09966300
C	-5.04412600	2.66031200	0.10968800
C	-5.20856700	1.68391200	1.08910800
C	-4.23685600	1.50010100	2.07007300
C	-3.10091200	2.30149600	2.08185200
H	-3.75810400	4.22388100	-0.64984700
H	-5.80404800	2.80511400	-0.65207700
H	-6.10403400	1.06929900	1.09761200
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C	1.26215800	3.94928400	-1.25128600
H	2.12906400	3.35387500	-1.55032000
C	1.76575300	5.07947400	-0.39128200
C	2.86218200	4.82154100	0.43730800
C	1.17707000	6.34252700	-0.36553200
C	3.34942200	5.80168400	1.29349000
C	1.67106100	7.32666600	0.48579400
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H	1.20268600	8.30599400	0.49898400
H	3.13159800	7.82895100	1.98461300
O	1.69725000	1.04156300	-1.08956200
H	3.34366400	3.84568900	0.40863400
O	-1.61532100	5.21228700	-0.04716300
H	-2.35763700	2.17989200	2.86176100
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C	-0.83296100	2.53489800	-1.51149100
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H	0.46294600	1.99552400	-3.17344700
H	-1.08228900	2.74464500	-3.66683300
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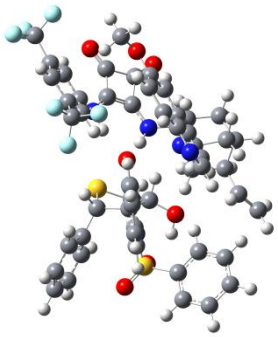

Int16

-2709475.66 kcal/mol

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H	-0.92652100	5.18127500	-1.94121000
H	-2.74515000	6.83687800	-1.33048300
H	0.47697200	5.50864700	0.86926400
H	-0.54608800	6.09546700	2.16314700
H	-2.52810400	4.46262000	-1.98027600
N	-1.34195800	4.49098200	1.11110200
C	-2.72872200	4.80027800	1.46461300
H	-2.72595900	5.26685000	2.45489000
H	-3.28316000	3.85782500	1.55226700
C	-3.41900300	5.73272000	0.41559400

H	-3.77018600	6.64761000	0.90896900
C	4.47126500	-2.50594900	-0.22721500
C	3.48090900	-1.61207400	0.15519500
C	3.80439200	-0.48991600	0.91869400
C	5.13269600	-0.26124200	1.28707800
C	6.10671700	-1.17051600	0.89268400
C	5.79503500	-2.30141900	0.14021600
H	2.45439900	-1.75803800	-0.16716000
H	5.39933100	0.62917200	1.84936700
H	6.56823600	-3.00022000	-0.15390400
C	7.55076200	-0.88240900	1.21178700
C	4.07250600	-3.65565000	-1.11002700
F	7.68887800	-0.17027900	2.33512500
F	8.13166600	-0.17929200	0.21841100
F	8.26243600	-2.01346600	1.35336800
F	2.98269700	-4.28868200	-0.63979800
F	3.75232600	-3.22839700	-2.35228500
F	5.04589900	-4.56464300	-1.24381600
N	2.75425800	0.36443700	1.27319800
C	2.82377300	1.72520100	1.31678900
C	1.84278900	2.63552100	0.96246000
C	2.77871700	3.77646700	1.05369500
C	3.84355500	2.77385900	1.54244400
O	4.99813600	2.81737200	1.89334400
O	2.74260200	4.94135200	0.72922200
H	1.84729700	0.01705800	0.97478200
N	0.57631800	2.45634500	0.54123900
H	0.29712800	1.48082200	0.54283700
C	3.31565800	0.02996200	-2.96111600
C	2.06211100	-0.33594700	-3.37915300
C	0.91910000	0.42728200	-3.04447800
C	1.08265000	1.60361600	-2.25793000
C	2.38856400	2.01602200	-1.92987200
C	3.48239800	1.23173400	-2.22990400
H	4.16485400	-0.59880200	-3.19863400
H	1.91096000	-1.23399700	-3.96944500
C	-1.30338900	1.76822400	-2.22050200
C	-1.34521400	0.64826700	-3.08698300
H	-2.24945900	2.17691100	-1.88818800
H	-2.31050900	0.28458600	-3.43797700
N	-0.29381500	-0.03336100	-3.46180300
O	4.67091300	1.67764000	-1.76800600
C	5.83021600	0.90722000	-2.01715900
H	6.63574900	1.39673000	-1.47169600
H	6.06755100	0.88361200	-3.08807600
H	5.72157100	-0.11611300	-1.64165900
H	2.57223800	2.95288500	-1.42026100
C	-1.16880300	6.79632000	0.17187200
H	-0.41262600	7.16388900	-0.53086500
H	-1.53945400	7.66529200	0.72817000
C	-4.60039200	5.06635000	-0.23197900
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H	-4.43700600	4.05097100	-0.59958100
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H	-6.01794500	6.61657900	-0.00378200
C	-0.10050500	2.24553700	-1.75933000
C	0.00655300	3.22483900	-0.57856100
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C	-1.00086700	-2.40199000	-0.95483900
C	-2.30682400	-2.81633700	-0.67911200
C	-2.82723900	-3.95378000	-1.29268000
C	-2.00465400	-4.62097600	-2.19501900
C	-0.70144500	-4.19711000	-2.48853100
C	-0.18546800	-3.07514400	-1.86286700
H	-3.82016500	-4.32297400	-1.07105700
H	-2.39136400	-5.51057800	-2.68313400
H	-0.09954500	-4.75402500	-3.19785700
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C	-6.41294900	-2.71663900	-1.23928000
C	-7.06694900	-2.58900700	-2.46024500
C	-6.63235000	-1.64857300	-3.39022400
C	-5.54444400	-0.82685300	-3.10349800
C	-4.88401300	-0.93750000	-1.88570600
H	-6.72504500	-3.45635600	-0.51026200
H	-7.91275400	-3.23034600	-2.68557000
H	-7.14138200	-1.55720500	-4.34466000
H	-5.20542600	-0.09678000	-3.83161000
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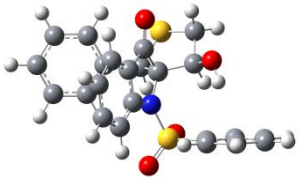
H	-0.38969300	-1.93584000	2.05163200
C	-2.21423900	-2.43622200	2.96913400
C	-3.18173900	-2.05812400	3.89796500

C	-2.01851200	-3.79516600	2.70997900
C	-3.94941900	-3.02108700	4.54346200
C	-2.78464200	-4.75865400	3.35399700
H	-1.25938900	-4.10155000	1.99305700
C	-3.75525400	-4.37171100	4.27222200
H	-4.70182100	-2.71233400	5.26253700
H	-2.62120400	-5.81034300	3.13990200
H	-4.35635900	-5.12079100	4.77853900
O	0.30092600	-0.57002000	-0.10591300
H	-3.33268700	-1.00854100	4.12615300
O	-4.83024800	-0.91078900	1.47337400
H	-4.04162200	-0.29745400	-1.64519300
O	-4.85132700	-3.39824900	1.09877100
C	-2.28100300	0.53183900	0.81801100
O	-3.41711000	0.92829100	0.10763300
H	-1.46042600	1.00541000	0.28768100
C	-2.25387100	1.04184700	2.25772500
H	-1.98620300	2.10251800	2.27791400
H	-3.22183600	0.88843800	2.74506000
S	-0.93690500	0.11129800	3.07558400
H	-4.19292700	0.61523100	0.60440700



3a

-1279534.77 kcal/mol

C	-0.82506000	1.32141400	-1.42003600
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C	0.10071900	2.90204900	0.15402800
C	-0.37620800	3.91467800	-0.67431000
C	-1.07309000	3.65274300	-1.85843100
C	-1.30743400	2.33892100	-2.23450800
H	0.60847500	3.13603800	1.07930200
H	-0.20742200	4.94510700	-0.37521900
H	-1.43456800	4.47386400	-2.46822900
H	-1.85330900	2.08250700	-3.13674800
C	-0.96593800	-0.12167600	-1.59343500
N	0.22752100	0.36572400	0.38671300
C	-0.31754900	-0.80049900	-0.36022700
S	1.35632000	0.24106100	1.61175600
C	2.92831300	0.15031900	0.76897200
C	3.69061900	-1.00899300	0.88233100
C	4.90032900	-1.09040900	0.19742400
C	5.33240700	-0.02391600	-0.58550100
C	4.56430900	1.13623000	-0.68152100
C	3.35814700	1.23407100	0.00175500
H	3.33339800	-1.82908800	1.49577600
H	5.50156500	-1.99019300	0.27539900
H	6.27229900	-0.09431500	-1.12363700
H	4.90557100	1.96775400	-1.28923100
C	-1.36256900	-1.56458100	0.49787400
H	-0.89014700	-1.73659500	1.46561600
C	-2.64060500	-0.78808000	0.72489000
C	-3.71210200	-0.80739700	-0.17037900
C	-2.71044600	0.03915600	1.84917100
C	-4.82589100	-0.00445900	0.05297100
C	-3.82197000	0.84581200	2.06849500
H	-1.88442500	0.05246600	2.55593700
C	-4.88356300	0.82594600	1.16892800
H	-5.65331700	-0.02951700	-0.65004700
H	-3.85916500	1.48514000	2.94546800
H	-5.75514600	1.45111700	1.33948200
O	-1.50342300	-0.70330900	-2.50836800
H	-3.66613900	-1.44878000	-1.04438100
O	1.13538800	-1.03693300	2.26346800
H	2.75781500	2.13539700	-0.06631000
O	1.31679600	1.48071900	2.36160500
C	0.72222700	-1.84954100	-0.81978100
O	1.58974300	-1.37260300	-1.81789900
H	1.27661200	-2.18968800	0.06333000
C	-0.08155000	-3.02292100	-1.37271500
H	-0.38730300	-2.80299500	-2.39629000
H	0.50992400	-3.93988900	-1.35094100
S	-1.55490500	-3.20743500	-0.30816600
H	2.30476400	-0.88220700	-1.39367000

15. References

1. (a) J. P. Malerich, K. Hagihara and V. H. Rawal, Chiral Squaramide Derivatives are Excellent Hydrogen Bond Donor Catalysts, *J. Am. Chem. Soc.*, 2008, **130**, 14416−14417; (b) S. Del Pozo, S. Vera, M. Oiarbide and C. Palomo, Catalytic Asymmetric Synthesis of Quaternary Barbituric Acids, *J. Am. Chem. Soc.*, 2017, **139**, 15308−15311.

2. X.-H. Fei, Y.-L. Zhao, F.-F. Yang, X. Guan, Z.-Q. Li, D.-P. Wang, M. Zhou, Y.-Y. Yang and B. He, Construction of Oxepino[3,2-b]indoles via [4+3] Annulation of 2-Ylideneoxindoles with Crotonate-Derived Sulfur Ylides, *Adv. Synth. Catal.*, 2021, **363**, 3018−3024.

3. C. Guo, M. Schedler, C. G. Daniliuc and F. Glorius, N-Heterocyclic Carbene Catalyzed Formal [3+2] Annulation Reaction of Enals: An Efficient Enantioselective Access to Spiro-Heterocycles, *Angew. Chem., Int. Ed.*, 2014, **53**, 10232−10236.

4. L.-J. Zhang, Y. Wang, X.-Q. Hu and P.-F. Xu, Hydrogen-Bonding Network Promoted [3+2] Cycloaddition: Asymmetric Catalytic Construction of Spiro-pseudoindoxyl Derivatives, *Chem. Asian J.*, 2016, **11**, 834−838.

5. L. Yang, W. Huang, X.-H. He, M.-C. Yang, X. Li, G. He, C. Peng and B. Han, Stereoselective Synthesis of Hydropyrano[3,2-b]indoles via Organocatalytic Asymmetric Inverse-Electron-Demand Oxa-Diels–Alder Reaction, *Adv. Synth. Catal.*, 2016, **358**, 2970−2975.

6. M. Kondo, N. Matsuyama, T. Z. Aye, I. Mattan, T. Sato, Y. Makita, M. Ishibashi, M. A. Arai, S. Takizawa and H. Sasai, Practical Stereoselective Synthesis of C3-Spirooxindole- and C2-Spiropseudoindoxyl-Pyrrolidines via Organocatalyzed Pictet-Spengler Reaction/Oxidative Rearrangement Sequence, *Adv. Synth. Catal.*, 2021, **363**, 2648−2663.

7. E. Brambilla, C. Pozza, S. Rizzato, G. Abbiati and V. Pirovano, Phosphine-Catalyzed [3+2] Cycloaddition of Aza-Aurones and Allenoates: Enantioselective Synthesis of 2-Spirocyclopentyl-Indolin-3-Ones, *Eur. J. Org. Chem.*, 2023, **26**, e202201385.

8. J.-X. Zhu, F. Pi, T. Sun, W.-Y. Huang, L. Gao, Z.-C. Chen, W. Du and Y.-C. Chen, Asymmetric 2,4-Dienylation/[4+2] Annulation Cascade to Construct Fused Frameworks via Auto-Tandem Palladium Catalysis, *Org. Lett.*, 2023, **25**, 3682−3686.

9. Q. Ren, M. Lang, H. Liu, X. Li, D. Wu, J. Wu, M. Yang, J. Wei, Z. Ren, L. Wang, Stereocontrol of C−N Axial and Spiro-Central Chirality via Rh(II)-Catalyzed Enantioselective N−H Bond Insertion of Indolinone-Spiroacetal, *Org. Lett.*, 2023, **25**, 7745−7750.

10. Q. Yin and S. L. You, Enantioselective Chlorocyclization of Indole Derived Benzamides for the Synthesis of Spiro-indolines, *Org. Lett.*, 2013, **15**, 4266−4269.

11. Y. Zhu, W. He, W. Wang, C. E. Pitsch, X. Wang and X. Wang, Enantioselective Tandem Cyclization of Alkyne-Tethered Indoles Using Cooperative Silver(I)/Chiral Phosphoric Acid Catalysis, *Angew. Chem. Int. Ed.*, 2017, **129**, 12374−12377.

12. J. Luo, Y.-B. Fang, X.-Y. Mao, M. Yang, Y.-L. Zhao, Y.-L. Liu, G.-S. Chen, Y.-F. Ji, Organocatalytic Asymmetric Cyclization Reaction of 2-Alkynyl-3,3-Difluoro-3*H*-Indoles and 2-Mercaptoimidazoles: Access to *gem*-Difluorinated C2-Spiro Indolines, *Adv. Synth. Catal.*, 2019, **361**, 1408−1413.

13. P. Sah, A. K. Gond, G. Saini and M. A. Kapur, Sequential Transition Metal and Organocatalytic Approach to the Enantioselective Synthesis of C2-Spiroindoline Systems, *Org. Lett.*, 2023, **25**, 9170−9175.

14. (a) J. Guo and M. W. Wong, Cinchona Alkaloid-Squaramide Catalyzed Sulfa-Michael Addition Reaction: Mode of Bifunctional Activation and Origin of Stereoinduction, *J. Org. Chem.*, 2017, **82**, 4362−4368; (b) M. N. Grayson, Mechanism and Origins of Stereoselectivity in the Cinchona Thiourea- and Squaramide-Catalyzed Asymmetric Michael Addition of Nitroalkanes to Enones, *J. Org. Chem.*, 2017, **82**, 4396−4401; (c) C. Trujillo, I. Rozas, A. Botte and S. J. Connon, A DFT mechanistic study of the organocatalytic asymmetric reaction of aldehydes and homophthalic anhydride, *Chem. Commun.*, 2017, **53**, 8874−8877; (d) P. Wang, Y. Gao, Y. Zhao, W. Liu and Y. Wang, Unveiling Mechanism of a Quinine-Squaramide Catalyzed Enantioselective Aza-Friedel−Crafts Reaction between Cyclic Trifluoromethyl Ketimine and Naphthol: A DFT Study, *J. Org. Chem.*, 2017, **82**, 13109−13114; (e) S. Ričko, J. A. Izzo and K. A. Jørgensen, Insights on the Pseudo-Enantiomeric Properties of Bifunctional Cinchona Alkaloid Squaramide-derived Organocatalyst, *Chem. Eur. J.*, 2020, **26**, 15727−15732; (f) A. Biswas, A. Ghosh, R. Shankhdhar and I. Chatterjee, Squaramide Catalyzed Asymmetric Synthesis of Five- and Six-Membered Rings, *Asian J. Org. Chem.*, 2021, **10**, 1345–1376.

15. (a) G. Tanriver, B. Dedeoglu, S. Catak and V. Aviyente, Computational Studies on Cinchona Alkaloid-Catalyzed Asymmetric Organic Reactions, *Acc. Chem. Res.*, 2016, **49**, 1250−1262; (b) S. Grimme, Do Special Noncovalent π-π Stacking Interactions Really Exist? *Angew. Chem., Int. Ed.*, 2008, **47**, 3430−3434; (c) J. E. Antoline, E. H. Krenske, A. G. Lohse, K. N. Houk and R. P. Hsung, Stereoselectivities and Regioselectivities of (4+3) Cycloadditions Between Allenamide-Derived Chiral Oxazolidinone-Stabilized Oxyallyls and Furans: Experiment and Theory, *J. Am. Chem. Soc.*, 2011, **133**, 14443–14451; (d) X. Xu, B. Pooi, H. Hirao and S. H. Hong, CH-π and CF-π Interactions Lead to Structural Changes of N-Heterocyclic Carbene Palladium Complexes, *Angew. Chem. Int. Ed.*, 2014, **53**, 1283–1287; (e) J. Li and R. Q. Zhang, Strong orbital interaction in a weak CH-π hydrogen bonding system, *Sci. Rep.*, 2016, **6**, 22304; (f) O. Manuel, C. J. AS and T. F. Dean, Parametrization of Non-covalent Interactions for Transition State Interrogation Applied to Asymmetric Catalysis, *J. Am. Chem. Soc.*, 2017, **139**, 6803−6806; (g) J. Wang, X. Gu, P. Zhang, X. Huang, X. Zheng, M. Chen, H. Feng, R. T. K. Kwok, J. W. Y. Lam and B. Z. Tang, Ionization and Anion-π^+ Interaction: A New Strategy for Structural Design of Aggregation-Induced Emission Luminogens, *J. Am. Chem. Soc.*, 2017, **139**, 16974−16979; (h) C. Liu, M. Wang, S. Liu, Y. Wang, Y. Peng, Y. Lan and Q. Liu, Manganese-Catalyzed Asymmetric Hydrogenation of Quinolines Enabled by π-π Interaction, *Angew. Chem. Int. Ed.*, 2021, **60**, 5108–5113; (i) R. Maji, S. C. Mallojjala and S. E. Wheeler, Electrostatic Interactions in Asymmetric Organocatalysis, *Acc. Chem. Res.*, 2023, 56, 1990−2000.

16. T. Wei, M.-S. Xie and H.-M. Guo, Construction of thioglycoside bonds via an asymmetric organocatalyzed sulfa-Michael/aldol reaction: access to 4'-thionucleosides. *Chem. Commun.*, 2024, **60**, 5018−5021.