Supporting Information

Catalytic enantioselective divergent reaction of thioimidates with naphthols: construction of *N*,*S*-acetal-containing tetrasubstituted carbon centers

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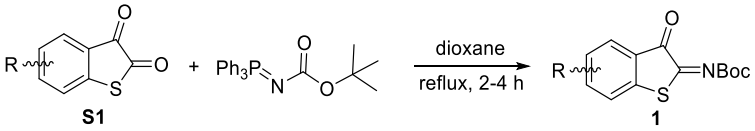
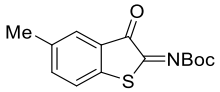
1. General information

Unless otherwise noted, all commercial available reagents were used as received without further purification. Reactions were monitored by thin layer chromatography (TLC) with 0.2 mm silica gel-coated HSGF 254 plates visualized by UV light at 254 or 365 nm. Products were isolated and purified by column chromatography on silica gel (200−300 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer using $CDCl_3$ or DMSO-d_6.as the solvent. The chemical shifts (δ) were reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$, ^{1}H: δ = 7.26 ppm, ^{13}C: δ = 77.16 ppm; DMSO-d_6: δ = 2.50 ppm, ^{13}C: δ = 39.51 ppm). Coupling constants (J) were given in Hertz (Hz). Splitting patterns of apparent multiplets associated with an averaged coupling constants were designated as s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). All ^{13}C spectra were recorded with broadband proton decoupling. HRMS were performed on Agilent 6545 LC/Q-TOF mass spectrometer. Melting points were recorded on a OptiMelt MPA 1000. The enantiomeric excesses were determined by chiral high-performance liquid chromatography (HPLC) analysis. HPLC analysis was performed on Agilent 1260 II, and Chiral columns were manufactured by Daicel Chemical Industries. Optical rotations were measured with a Rudolph Autopol-III polarimeter.

2. The procedure for the preparation of cyclic α-carbonyl thioimidates 1



A mixture of benzothiophene-2,3-dione **S1** (5 mmol, 1.0 equiv) and *N*-Boc-imino-(triphenyl)phosphorane (7.5 mmol, 1.5 equiv) in dioxane (10 mL) was heated to reflux for 2-4 hours. After the mixture was cooled to room temperature, the solvent was concentrated in vacuo. The residue was subjected to flash chromatograph on silica gel (PE: EA = 20:1) to afford the desired product **1**.



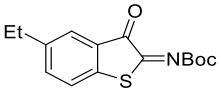
***tert*-butyl 5-methyl-3-oxobenzo[b]thiophen-2(3*H*)-ylidenecarbamate (1a)**

The product **1a** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 63% yield; m.p. 140.8-141.3 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.47 (d, J= 8.0Hz, 1H), 7.31 (d,J= 8.0Hz, 1H), 2.40 (s, 3H), 1.60 (s, 9H);

^{13}C NMR (101MHz, $CDCl_3$) δ 186.3, 169.0, 161.0, 141.6, 137.8, 126.8, 124.8, 83.8, 28.2, 27.8, 15.2.

HRMS (ESI) *m/z*: Calcd for $[M+H]^+$ $C_{15}H_{18}NO_3S$ 292.1002, found 292.1010..



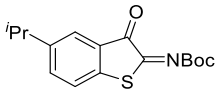
***tert*-butyl 5-ethyl-3-oxobenzo[b]thiophen-2(3*H*)-ylidenecarbamate (1b)**

The product **1b** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 57% yield; m.p. 85.4-86.3 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.49 (d, *J* = 1.9 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 2.69 (q, *J* = 7.5 Hz, 2H), 1.60 (s, 9H), 1.26 (t, *J* = 7.6 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 186.3, 169.0, 161.0, 141.6, 137.8, 126.8, 124.8, 83.8, 28.2, 27.8, 15.2;

HRMS(ESI) *m/z:* Calcd for $[M+H]^+$ $C_{15}H_{18}NO_3S$ 292.1002, found 292.1010.



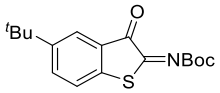
***tert*-butyl5-isopropyl-3-oxobenzo[b]thiophen-2(3*H*)-ylidenecarbamate (1c)**

The product **1c** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 61% yield; m.p. 97.0-97.5 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 2.95 (h, *J* = 7.0 Hz, 1H), 1.60 (s, 9H), 1.27 (d, *J* = 6.9 Hz, 7H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 186.3, 169.2, 161.1, 148.9, 141.7, 136.8, 126.5, 125.5, 124.8, 83.8, 33.7, 27.8, 23.7;

HRMS(ESI) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{20}NO_3S$ 306.1158, found 306.1164.



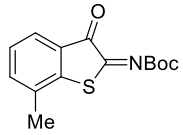
***tert*-butyl 5-tert-butyl-3-oxobenzo[b]thiophen-2(3*H*)-ylidenecarbamate (1d)**

The product **1d** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 64% yield; m.p. 136.8-137.5 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.93 (s, 1H), 7.71 (d, *J*= 8.2 Hz, 1H), 7.36 (d, *J*= 8.2Hz, 1H), 1.60 (s, 9H), 1.34 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 186.4, 169.4, 161.0, 151.4, 141.5, 135.5, 126.2, 124.6, 83.8, 34.9, 31.1, 28.3, 27.8;

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd. for $C_{17}H_{22}NO_3S$ 320.1315, found 320.1319.



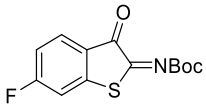
***tert*-butyl7-methyl-3-oxobenzo[b]thiophen-2(3*H*)-ylidenecarbamate (1e)**

The product **1e** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 65% yield; m.p. 126.9-127.5 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.73 (d, *J*= 7.5 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.27 (t, *J*= 7.6 Hz, 1H), 2.35 (s, 3H), 1.61 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 186.5, 168.4, 161.1, 143.8, 138.6, 134.2, 127.3, 126.3, 125.1, 83.9, 27.8, 18.6;

HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd. for $C_{14}H_{15}NO_3SNa$ 300.0665, found 300.0671.



tert-butyl 6-fluoro-3-oxobenzo[b]thiophen-2(3*H*)-ylidenecarbamate (1f)

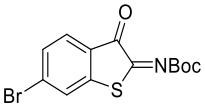
The product **1f** was purified by flash column chromatography (petroleum ether / ethyl acetate =

10:1); yellow solid; 41% yield; m.p. 102.6-103.1 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J*= 8.5, 5.4 Hz, 1H), 7.16 (dt, *J*= 7.8, 1.6 Hz, 1H), 7.05 (ddd, *J*= 10.5, 7.8, 1.9 Hz, 1H), 1.61 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.2, 169.8, 167.2, 160.9, 148.0 (d, *J*= 11.0Hz), 130.3 (d, *J*= 11.0 Hz), 123.1, 115.4 (d, *J*= 23.3 Hz), 112.8 (d, *J*= 25.8 Hz), 84.3, 27.9;

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd. for $C_{13}H_{13}FNO_3S$ 282.0595, found 282.0587.



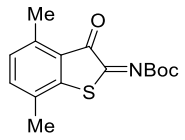
***tert*-butyl 6-bromo-3-oxobenzo[*b*]thiophen-2(3*H*)-ylidenecarbamate (1g)**

The product **1g** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 31% yield; m.p. 134.6-137.3 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.48 – 7.42 (m, 1H), 7.38 (dd, *J* = 7.7, 1.1 Hz, 1H), 1.59 (s, 9H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 182.9, 167.8, 161.1, 147.6, 137.3, 133.1, 124.9, 124.0, 123.9, 84.1, 27.8.

HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd. for $C_{13}H_{12}{}^{79}BrNO_3SNa$ 363.9613, found 363.9628; $C_{13}H_{12}{}^{81}BrNO_3SNa$ 365.9593, found 365.9609.



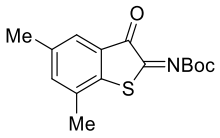
***tert*-butyl 4,7-dimethyl-3-oxobenzo[*b*]thiophen-2(3*H*)-ylidenecarbamate (1h)**

The product **1h** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 68% yield; m.p.118.7-119.5 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J*= 7.7 Hz, 1H), 7.03 (d, *J*= 7.7 Hz, 1H), 2.63 (s, 3H), 2.31 (s, 3H), 1.61 (s, 9H);

^{13}C NMR (101 MHz, CDCl3) δ 186.9, 168.6, 161.4, 144.0, 140.5, 137.6, 131.3, 129.8, 129.7, 123.9, 83.7, 27.9, 18.7, 18.2;

HRMS (ESI) *m/z*: $[M+H]^+$Calcd. for $C_{15}H_{18}NO_3S$ 292.1002, found 292.1014.



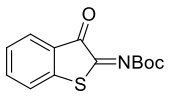
***tert*-butyl (5,7-dimethyl-3-oxobenzo[b]thiophen-2(3H)-ylidene)carbamate (1i)**

The product **1i** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid; 60% yield; m.p. 129.2-130.2 ℃;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54(s, 1H), 7.30 (s, 1H), 2.36 (s, 3H), 2.31 (s, 3H), 1.61 (s, 9H);

^{13}C NMR (101 MHz, CDCl3) δ 186.7, 169.1, 161.2, 140.7, 139.7, 137.5, 133.84, 126.4, 125.5, 83.8, 27.9, 20.8, 18.4.

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd. for $C_{15}H_{18}NO_3S$ 292.1002, found 292.1010.



***tert*-butyl (3-oxobenzo[*b*]thiophen-2(3*H*)-ylidene)carbamate (1j)**

The product **1j** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); Yellow solid; 59% yield; m.p. 91.0-91.8 °C;

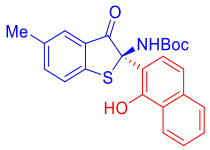
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J*= 7.6 Hz, 1H), 7.67 (t, *J*= 7.6 Hz, 1H), 7.43 (d, *J*= 7.9 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 1.60 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 186.0, 168.4, 161.0, 144.58, 137.8, 127.7, 127.5, 126.4, 125.0, 83.95, 27.8;

HRMS (ESI) *m/z*: $[M+H]^+$ Calcd. for $C_{13}H_{14}NO_3S$ 264.0689, found 264.0693.

3. The general procedure for asymmetric synthesis of 3, 5 and 7.

In an ordinary vial equipped with a magnetic stirring bar, cyclic α-carbonyl thioimidates **1** (0.15 mmol, 1.5 equiv.) was added to a solution of 1-naphthols **2** or phenols **4** or 2-naphthols **6** (0.1 mmol, 1.0 equiv.), 5Å MS (50 mg) and catalyst **C** (0.01 mmol, 6.4 mg) in $CHCl_3$ (1.0 mL) at 0 °C. And then, the mixture was stirred at the same temperature for the specified time. After completion, the reaction mixture was directly purified by flash chromatography on silica gel to afford the desired product **3** or **5** or **7**.



***tert*-butyl (S)-(2-(1-hydroxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate. (3a)**

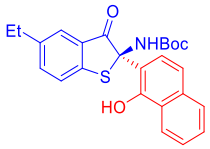
The product **3a** was purified by flash column chromatography (petroleum ether / ethyl acetate = 12:1); yellow solid, 40.0 mg, 95% yield, m.p. 111.3-112.8 °C; 93% ee; $[\alpha]_D^{20}$ = +364.2 (*c* 0.48, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 11.5 min (minor), t_R = 12.6 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.3 Hz, 1H), 7.76 (d, *J* = 8.9 Hz, 1H), 7.62 – 7.48 (m, 2H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.14 (t, *J* = 7.9 Hz, 2H), 6.99 (d, *J* = 7.9 Hz, 1H), 5.90 (s, 2H), 2.38 (s, 3H), 1.29 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.0, 155.3, 135.9, 135.7, 134.3, 132.0, 131.6, 130.1, 129.5, 129.4, 127.7, 126.3, 123.7, 121.6, 120.8, 120.0, 117.3, 112.8, 82.1, 80.4, 28.0, 21.0;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{23}NO_4SNa$ 444.1240, found 444.1244.

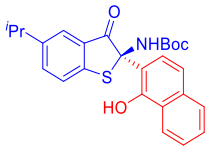


***tert*-butyl (S)-(5-ethyl-2-(1-hydroxynaphthalen-2-yl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate. (3b)**

The product **3b** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 37.8 mg, 86% yield; 93% ee; $[\alpha]_D^{20}$ = +276.0 (*c* 0.51, CH_2Cl_2);

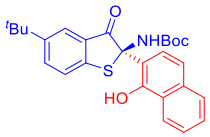
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 8.7 min (minor), t_R = 10.8 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.41 – 8.22 (m, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.67 – 7.58 (m, 1H), 7.54 (d, *J* = 1.8 Hz, 1H), 7.45 – 7.35 (m, 4H), 7.24 (s, 1H), 7.19 (d, *J* = 5.7 Hz, 1H), 5.62 (s, 1H), 2.78 (h, *J* = 6.9 Hz, 1H), 1.33 (d, *J* = 7.1 Hz, 9H), 1.12 (dd, *J* = 7.0, 5.2 Hz, 7H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 201.4, 153.6, 153.5, 147.7, 142.0, 137.6, 135.4, 127.7, 127.4, 127.3, 127.2, 126.9, 125.9, 125.8, 123.8, 123.2, 119.8, 112.7, 82.0, 79.9, 28.3, 15.3；
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1404.



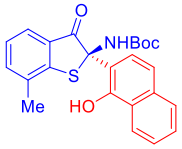
***tert*-butyl (S)-(2-(1-hydroxynaphthalen-2-yl)-5-isopropyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3c)**

The product **3c** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 38.2 mg, 85% yield; 94% ee; $[\alpha]_D^{20}$ = +242.2 (*c* 0.72, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 7.4 min (minor), t_R = 8.5 min (major);
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.42 – 8.37 (m, 1H), 8.13 (d, *J* = 8.9 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.62 (d, *J* = 1.9 Hz, 1H), 7.52 – 7.46 (m, 3H), 7.34 – 7.29 (m, 2H), 5.65 (s, 1H), 2.87 (p, *J* = 6.9 Hz, 1H), 1.41 (s, 9H), 1.20 (dd, *J* = 6.9, 5.0 Hz, 6H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 201.3, 153.5, 147.7, 146.6, 136.4, 135.3, 127.6, 127.1, 127.0, 126.8, 126.0, 125.8, 125.7, 123.7, 123.1, 119.7, 112.5, 81.9, 79.9, 33.5, 31.6, 29.7, 28.1, 23.7, 23.6;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{27}NO_4SNa$ 472.1553, found 472.1559.



***tert*-butyl (S)-(5-(*tert*-butyl)-2-(1-hydroxynaphthalen-2-yl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3d)**

The product **3d** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 45.9 mg, 99% yield; 94% ee; $[\alpha]_D^{20}$ = +161.1 (*c* 0.51, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 6.1 min (minor), t_R = 7.6 min (major);
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.44 – 8.33 (m, 1H), 8.12 (d, *J* = 8.9 Hz, 1H), 7.76 (d, *J* = 2.1 Hz, 1H), 7.73 – 7.69 (m, 1H), 7.65 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.29 (dd, *J* = 9.0, 0.8 Hz, 1H), 5.70 (s, 1H), 1.42 (s, 9H), 1.27 (s, 9H);
^{13}C NMR (400 MHz, $CDCl_3$) δ 201.4, 153.5, 153.4, 149.0, 147.5, 135.3, 135.2, 127.6, 127.0, 126.8, 126.8, 125.8, 125.7, 125.0, 123.6, 123.1, 119.7, 112.5, 81.9, 80.0, 77.3, 77.0, 76.7, 34.6, 31.1, 28.2;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{27}H_{29}NO_4SNa$ 486.1710, found 486.1715.



***tert*-butyl (S)-(2-(1-hydroxynaphthalen-2-yl)-7-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3e)**

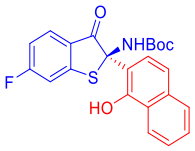
The product **3e** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 29.5 mg, 70% yield; 91% ee; $[\alpha]_D^{20}$ = +362.6 (*c* 0.62, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 13.2 min (minor), t_R = 8.3 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.46 – 8.32 (m, 1H), 8.10 (d, *J* = 8.9 Hz, 1H), 7.75 – 7.69 (m, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.50 (dd, *J* = 5.9, 3.3 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 9.1 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 5.66 (s, 1H), 2.40 (s, 3H), 1.41 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ201.8, 153.6, 153.5, 150.2, 137.4, 135.4, 133.1, 128.1, 127.7, 127.2, 127.1, 126.9, 126.0, 125.8, 125.8, 125.7, 123.2, 119.8, 112.7, 82.0, 79.7, 28.3, 19.1;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{23}NO_4SNa$ 444.1240, found 444.1244.



***tert*-butyl (S)-(6-fluoro-2-(1-hydroxynaphthalen-2-yl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3f)**

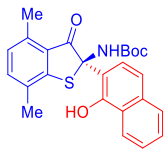
The product **3a** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 34.4 mg, 81% yield; 92% ee; $[\alpha]_D^{20}$ = +362.5 (*c* 0.49, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 10/90, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 21.9 min (minor), t_R = 17.0 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (s, 1H), 8.34 – 8.26 (m, 1H), 7.94 (d, *J* = 8.9 Hz, 1H), 7.68 (t, *J* = 7.1 Hz, 1H), 7.63 (d, *J* = 6.8 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.21 (d, *J* = 9.0 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.80 (t, *J* = 8.6 Hz, 1H), 5.70 (s, 1H), 1.34 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 199.3, 168.4 (d, *J* = 260 Hz), 153.4, 153.2, 135.3, 130.8 (d, *J* = 11.1 Hz), 127.7, 127.1, 126.7, 125.8, 125.5, 123.7 (d, *J* = 10.1 Hz), 123.0, 119.9, 113.8 (d, *J* = 23.2 Hz), 112.4, 110.9 (d, *J* = 26.3 Hz), 82.1, 80.2, 28.1;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{20}FNO_4SNa$ 448.0989, found 448.1003.



***tert*-butyl (S)-(2-(1-hydroxynaphthalen-2-yl)-4,7-dimethyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3g)**

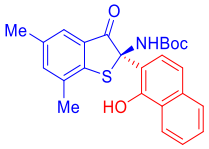
The product **3g** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 42.2 mg, 97% yield; 94% ee; $[\alpha]_D^{20}$ = +39.8 (*c* 0.67, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 11.4 min (minor), t_R = 7.3 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 8.45 – 8.28 (m, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.71 – 7.60 (m, 1H), 7.43 (d, *J* = 2.5 Hz, 2H), 7.25 – 7.13 (m, 2H), 6.79 (d, *J* = 7.5 Hz, 1H), 5.60 (s, 1H), 2.45 (s, 3H), 2.29 (s, 3H), 1.50 (s, 1H), 1.38 – 1.23 (m, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 202.5, 153.6, 153.6, 150.6, 140.8, 136.5, 135.3, 130.3, 128.1, 127.7, 127.2, 126.9, 125.8, 124.3, 123.3, 119.6, 113.0, 81.8, 78.5, 28.3, 19.0, 18.7.

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1405.



tert-butyl (S)-(2-(1-hydroxynaphthalen-2-yl)-5,7-dimethyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3h)

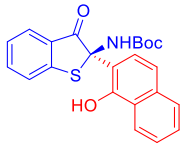
The product **3h** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 41.0 mg, 94% yield; 91% ee; $[\alpha]_D^{20}$ = +354.3 (*c* 0.57, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 13.7 min (minor), t_R = 8.1 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.38 – 8.27 (m, 1H), 8.01 (d, *J* = 8.9 Hz, 1H), 7.70 – 7.58 (m, 1H), 7.47 – 7.38 (m, 2H), 7.34 (d, *J* = 1.8 Hz, 1H), 7.20 (d, *J* = 8.9 Hz, 1H), 7.16 (d, *J* = 1.7 Hz, 1H), 5.62 (s, 1H), 2.29 (s, 3H), 2.20 (s, 3H), 1.33 (s, 9H);

^{13}C NMR (400 MHz, $CDCl_3$) δ 201.8, 153.6, 153.5, 153.4, 147.2, 138.9, 135.8, 135.4, 132.8, 127.7, 127.2, 127.1, 126.9, 126.0, 125.9, 125.8, 123.2, 119.7, 112.9, 81.9, 79.9, 28.3, 20.8, 19.0.

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1404.



tert-butyl (S)-(2-(1-hydroxynaphthalen-2-yl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3i)

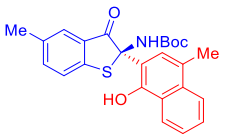
The product **3i** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 38.3 mg, 94% yield; 92% ee; $[\alpha]_D^{20}$ = +225.1 (*c* 0.30, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 12.4 min (minor), t_R = 10.8 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.40 – 8.28 (m, 1H), 8.04 (d, *J* = 8.9 Hz, 1H), 7.68 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.67 – 7.63 (m, 1H), 7.51 (td, *J* = 7.7, 1.4 Hz, 1H), 7.43 (dd, *J* = 6.0, 2.2 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.25 (s, 1H), 7.15 – 7.08 (m, 1H), 5.58 (s, 1H), 1.34 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.3, 153.5, 150.1, 149.0, 137.2, 135.4, 128.6, 127.8, 127.3, 127.2, 126.9, 125.9, 125.8, 125.6, 124.0, 123.2, 119.9, 112.5, 82.2, 79.6, 28.3;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{21}NO_4SNa$ 430.1083, found 430.1089.



tert-butyl (S)-(2-(1-hydroxy-4-methylnaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3j)

The product **3j** was purified by flash column chromatography (petroleum ether / ethyl acetate = 12:1); yellow oil, 41.8 mg, 96% yield; 95% ee; $[\alpha]_D^{20}$ = +303.2 (*c* 0.73, CH_2Cl_2);

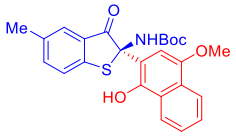
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 8.7 min (minor), t_R = 6.7 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (s, 1H), 8.48 – 8.35 (m, 1H), 7.90 (d, *J* = 1.1 Hz, 1H), 7.85 – 7.79 (m, 1H), 7.56 (d, *J* = 1.8 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.40 (dd, *J* = 8.2, 1.9 Hz, 1H), 7.31 (d,

J = 8.1 Hz, 1H), 5.78 (s, 1H), 2.53 (s, 3H), 2.30 (s, 3H), 1.42 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.4, 153.6, 151.8, 147.5, 138.4, 135.6, 134.3, 128.6, 127.5, 127.4, 127.1, 126.0, 125.5, 123.8, 123.7, 123.7, 112.0, 81.9, 79.8, 28.3, 20.9, 19.1;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1395.



***tert*-butyl (S)-(2-(1-hydroxy-4-methoxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3k)**

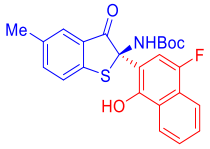
The product **3k** was purified by flash column chromatography (petroleum ether / ethyl acetate = 12:1); yellow oil, 43.3 mg, 96% yield; 86% ee; $[\alpha]_D^{20}$ = +181.6 (*c* 0.82, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 8.3 min (minor), t_R = 6.4 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.40 – 8.27 (m, 1H), 8.15 – 8.03 (m, 1H), 7.57 (d, J = 1.9 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.47 (d, J = 3.5 Hz, 1H), 7.41 (dd, J = 8.1, 1.9 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 5.78 (s, 1H), 3.90 (s, 3H), 2.31 (s, 3H), 1.54 – 1.36 (m, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.2, 153.6, 149.0, 147.2, 147.0, 138.4, 135.7, 128.6, 127.8, 127.5, 127.2, 127.1, 126.5, 123.7, 123.0, 121.6, 111.9, 104.0, 81.9, 80.1, 55.9, 28.3, 20.9.

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_5S$ 474.1346, found 474.1352.



***tert*-butyl (S)-(2-(4-fluoro-1-hydroxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3l)**

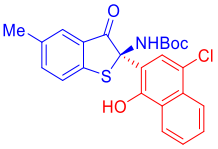
The product **3l** was purified by flash column chromatography (petroleum ether / ethyl acetate = 12:1); yellow oil, 43.0 mg, 98% yield; 94% ee; $[\alpha]_D^{20}$ = +312.3 (*c* 0.77, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, EtOH/hexane = 15/85, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.4 min (minor), t_R = 6.5 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (s, 1H), 8.33 (d, J = 7.8 Hz, 1H), 7.91 (d, J = 7.7 Hz, 1H), 7.82 (d, J = 12.6 Hz, 1H), 7.58 – 7.50 (m, 3H), 7.41 (d, J = 8.2 Hz, 1H), 7.29 (d, J = 8.1 Hz, 1H), 5.85 (s, 1H), 2.30 (s, 3H), 1.41 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.9, 153.5, 151.7 (d, J = 242.0 Hz), 149.3 (d, J = 3.0 Hz), 147.1, 138.5, 135.7, 128.5, 127.8, 127.6 (d, J = 5.0 Hz) 127.0, 126.7, 125.0 (d, J = 18.0 Hz), 123.7, 123.3, 123.2, 120.0 (d, J = 3.0 Hz), 112.1 (d, J = 3.0 Hz), 109.3 (d, J = 26.0 Hz), 82.0, 79.1, 28.2, 20.7.

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{22}FNO_4S$ 462.1146, found 462.1153.



***tert*-butyl (S)-(2-(4-chloro-1-hydroxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3m)**

The product **3m** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2);

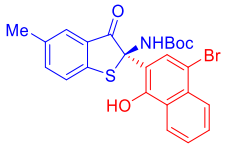
yellow oil, 42.0 mg, 92% yield; 93% ee; $[\alpha]_D^{20}$ = +192.7 (*c* 0.31, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, EtOH/hexane = 15/85, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.4 min (minor), t_R = 6.5 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.28 (dd, *J* = 9.4, 5.2 Hz, 1H), 8.12 (dd, *J* = 7.8, 3.5 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.43 (m, 3H), 7.33 (t, *J* = 6.1 Hz, 1H), 7.26 – 7.19 (m, 1H), 5.72 (s 1H), 2.22 (s, 3H), 1.32 (s, 9H);

^{13}C NMR (101 MHz, CDCl_3) δ 201.2, 153.5, 152.7, 152.7, 147.3, 138.8, 135.9, 132.3, 128.8, 128.6, 127.9, 127.0, 126.6, 125.8, 124.0, 123.9, 123.7, 122.9, 113.0, 82.2, 79.2, 28.3, 20.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{22}{}^{35}ClNO_4S$ 478.0850, found 478.0860; Calcd. for $[M+Na]^+$ $C_{24}H_{22}{}^{37}ClNO_4S$ 480.0829, found 480.0838;



***tert*-butyl (S)-(2-(4-bromo-1-hydroxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3n)**

The product **3n** was purified by flash column chromatography (petroleum ether / ethyl acetate = 12:1); yellow oil, 38.1 mg, 99% yield; 86% ee; $[\alpha]_D^{20}$ = +212.6 (*c* 0.98, CH_2Cl_2);

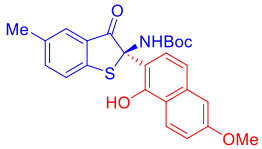
The ee was determined by HPLC: Chiralpak IC, EtOH/hexane = 15/85, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.9 min (minor), t_R = 6.7 min (major);

^{1}H NMR (101 MHz, $CDCl_3$) δ 9.92 (s, 1H), 8.18 (d, *J* = 9.0 Hz, 1H), 8.06 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 2.0 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.34 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 5.58 (s, 1H), 2.24 (s, 3H), 1.34 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.4, 153.6, 153.5, 147.7, 142.0, 137.6, 135.4, 127.7, 127.4, 127.3, 127.2, 126.9, 125.9, 125.8, 123.8, 123.2, 119.8, 112.7, 82.0, 79.9, 28.3, 15.3;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{22}BrNO_4S$ 478.0850, found 478.0860;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{22}{}^{79}BrNO_4S$ 522.0345, found 522.0351; Calcd. for $[M+Na]^+$ $C_{24}H_{22}{}^{81}BrNO_4S$ 524.0327, found 524.0351.



***tert*-butyl (S)-(2-(1-hydroxy-6-methoxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3o)**

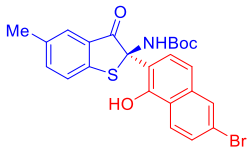
The product **3o** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:3); yellow oil, 31.9 mg, 71% yield; 94% ee; $[\alpha]_D^{20}$ = +319.3 (*c* 0.50, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 15/85, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 36.6 min (minor), t_R = 21.8 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.72 (s, 1H), 8.19 (d, *J* = 9.2 Hz, 1H), 7.96 (d, *J* = 8.9 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.30 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 1H), 7.07 (d, *J* = 8.9 Hz, 1H), 7.03 (dd, *J* = 9.3, 2.5 Hz, 1H), 6.89 (d, *J* = 2.5 Hz, 1H), 5.62 (s, 1H), 3.80 (s, 3H), 2.21 (s, 3H), 1.33 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.4, 159.2, 153.7, 153.6, 147.5, 138.4, 137.1, 135.6, 128.6, 127.3, 126.8, 125.1, 123.7, 122.1, 118.7, 118.3, 110.7, 105.2, 81.9, 79.9, 55.4, 28.3, 20.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_5S$ 474.1346, found 474.1359.



***tert*-butyl (S)-(2-(6-bromo-1-hydroxynaphthalen-2-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (3p)**

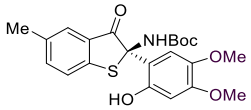
The product **3p** was purified by flash column chromatography (petroleum ether / CH_2Cl_2 = 1:2); yellow oil, 45.5 mg, 91% yield; 89% ee; $[\alpha]_D^{20}$ = +176.2 (*c* 0.61, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 13.4 min (minor), t_R = 23.7 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 8.27 (d, *J* = 9.0 Hz, 1H), 8.14 (d, *J* = 8.9 Hz, 1H), 7.87 (s, 1H), 7.61 – 7.50 (m, 2H), 7.42 (d, *J* = 8.3 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.20 (d, *J* = 9.1 Hz, 1H), 5.60 (s, 1H), 2.31 (s, 3H), 1.41 (s, 10H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.3, 153.7, 153.6, 147.4, 138.6, 136.5, 135.8, 129.2, 129.1, 128.6, 127.4, 127.2, 125.4, 125.3, 123.7, 122.3, 118.8, 113.2, 82.1, 79.8, 28.3, 20.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{22}{}^{79}BrNO_4S$ 522.0345, found 522.0350; Calcd. for $[M+Na]^+$ $C_{24}H_{22}{}^{81}BrNO_4S$ 524.0327, found 524.0334.



***tert*-butyl (S)-(2-(2-hydroxy-4,5-dimethoxyphenyl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5a)**

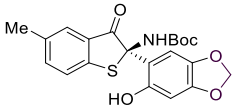
The product **5a** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 42.8 mg, 99% yield; 92% ee; $[\alpha]_D^{20}$ = +229.9 (*c* 0.71, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 9.4 min (minor), t_R = 12.0 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 7.59 (s, 1H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.26 (d, *J* = 7.7 Hz, 1H), 6.54 (s, 1H), 5.80 (s, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 2.32 (s, 3H), 1.39 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.8, 153.7, 151.4, 151.0, 147.3, 142.3, 138.3, 135.5, 128.4, 127.5, 123.6, 112.5, 110.7, 103.6, 81.9, 78.8, 56.7, 56.1, 28.2, 20.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{22}H_{25}NO_6SNa$ 454.1295, found 454.1304.



***tert*-butyl (S)-(2-(6-hydroxybenzo[*d*][1,3]dioxol-5-yl)-5-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5b)**

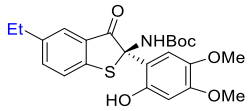
The product **5b** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 34.0 mg, 82% yield; 82% ee; $[\alpha]_D^{20}$ = +93.0 (*c* 0.71, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 10.1 min (minor), t_R = 16.7 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.26 (s, 1H), 7.62 (d, *J* = 19.3 Hz, 2H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 6.50 (s, 1H), 6.31 (s, 1H), 5.91 (s, 1H), 5.83 (s, 1H), 2.33 (s, 3H), 1.28 (s, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 198.3, 153.5, 152.0, 148.2, 147.6, 139.2, 137.2, 134.0, 129.4, 126.4, 123.5, 115.7, 105.3, 101.2, 98.4, 79.6, 75.8, 28.0, 20.3;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{21}H_{21}NO_6SNa$ 438.0982, found 438.0986.



tert-butyl (S)-(5-ethyl-2-(2-hydroxy-4,5-dimethoxyphenyl)-3-oxo-2,3-dihydrobenzo[b]thiophen-2-yl)carbamate (5c)

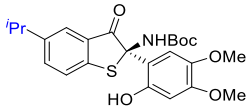
The product **5c** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 42.7 mg, 96% yield; 90% ee; $[\alpha]_D^{20}$ = +186.8 (*c* 1.08, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 9.3 min (minor), t_R = 7.3 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ8.89 (s, 1H), 7.68 – 7.59 (m, 1H), 7.50 – 7.34 (m, 2H), 7.28 (d, *J* = 7.8 Hz, 1H), 6.53 (d, *J* = 3.3 Hz, 1H), 5.90 (s, 1H), 3.81 (s, 3H), 3.75 (d, *J* = 5.7 Hz, 3H), 2.75 – 2.56 (m, 2H), 1.40 – 1.25 (m, 10H), 1.21 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.8, 153.8, 151.4, 151.0, 142.3, 141.8, 138.7, 137.3, 135.4, 125.8, 123.7, 112.6, 103.5, 78.7, 78.3, 56.8, 56.0, 28.2, 26.4, 15.3, 13.4.

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{27}NO_6SNa$ 468.1451, found 468.1457.



tert-butyl (S)-(2-(2-hydroxy-4,5-dimethoxyphenyl)-5-isopropyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5d)

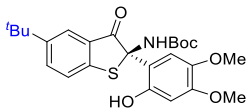
The product **5d** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 45.7 mg, 99% yield; 88% ee; $[\alpha]_D^{20}$ = +177.9 (*c* 1.33, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 6.8 min (minor), t_R = 5.8 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.64 (s, 1H), 7.45 (d, *J* = 10.1 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 1H), 6.51 (s, 1H), 5.90 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 2.88 (p, *J* = 6.9 Hz, 1H), 1.37 (s, 9H), 1.22 (d, *J* = 1.9 Hz, 3H), 1.20 (d, *J* = 1.9 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.8, 153.8, 151.4, 151.0, 147.8, 146.5, 142.3, 136.2, 127.5, 125.8, 123.7, 112.6, 103.6, 81.8, 78.8, 56.8, 56.0, 33.6, 29.8, 28.2, 23.8, 23.8;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{29}NO_6SNa$ 482.1608, found 482.1615.



tert-butyl (S)-(5-(*tert*-butyl)-2-(2-hydroxy-4,5-dimethoxyphenyl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5e)

The product **5e** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 47.0 mg, 99% yield; 87% ee; $[\alpha]_D^{20}$ = +188.2 (*c* 0.84, CH_2Cl_2);

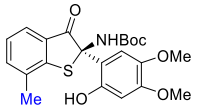
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.5 min (minor), t_R = 5.0 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 7.78 (d, *J* = 2.1 Hz, 1H), 7.63 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.42 (s, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 6.53 (s, 1H), 5.83 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 1.37 (s,

9H), 1.28 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.9, 153.7, 151.5, 151.1, 148.9, 147.5, 142.3, 135.1, 127.3, 124.9, 123.5, 112.7, 103.6, 79.9, 78.9, 77.5, 77.4, 77.2, 76.8, 56.8, 56.0, 34.7, 31.2, 28.3, 28.2;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{31}NO_6SNa$ 496.1764, found 496.1766.



***tert*-butyl (S)-(2-(2-hydroxy-4,5-dimethoxyphenyl)-7-methyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5f)**

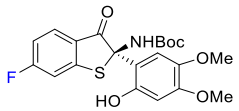
The product **5f** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 43.0 mg, 99% yield; 88% ee; $[\alpha]_D^{20}$ = +248.9 (*c* 1.11, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 13.6 min (minor), t_R = 6.6 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.27 (s, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 6.54 (s, 1H), 5.96 (s, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 2.32 (s, 3H), 1.34 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.9, 154.0, 151.4, 151.0, 150.3, 142.3, 137.1, 132.9, 127.7, 125.6, 125.5, 116.0, 112.5, 111.3, 103.3, 78.2, 56.9, 56.0, 28.2, 19.0.

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{22}H_{25}NO_6SNa$ 454.1295, found 454.1300.



***tert*-butyl (S)-(6-fluoro-2-(2-hydroxy-4,5-dimethoxyphenyl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5g)**

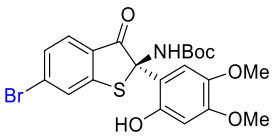
The product **5g** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 42.6 mg, 98% yield; 88% ee; $[\alpha]_D^{20}$ = +43.9 (*c* 0.1.16, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 11.4 min (minor), t_R = 8.1 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 7.80 (dd, *J* = 8.5, 5.4 Hz, 1H), 7.27 (s, 1H), 7.04 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.89 (td, *J* = 8.6, 2.2 Hz, 1H), 6.53 (s, 1H), 5.95 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 1.37 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.6, 168.4 (d, *J* = 261.6 Hz), 153.8, 153.4 (d, *J* = 10.1 Hz), 151.5, 150.8, 142.4, 130.6 (d, *J* = 11.1 Hz), 124.3, 116.0, 113.8 (d, *J* = 23.2 Hz), 110.9 (d, *J* = 26.3 Hz), 110.8, 103.5, 82.2, 78.9, 56.8, 56.1, 28.2;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{21}H_{22}FNO_6SNa$ 458.1044, found 458.1048.



***tert*-butyl (S)-(6-bromo-2-(2-hydroxy-4,5-dimethoxyphenyl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5h)**

The product **5h** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 44.6 mg, 90% yield; 92% ee; $[\alpha]_D^{20}$ = +105.8 (*c* 0.63, CH_2Cl_2);

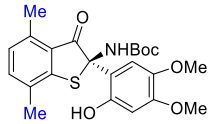
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min,

l = 254 nm, t_R= 14.4 min (minor), t_R = 8.4 min (major);

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.01 (s, 1H), 7.90 (s, 1H), 7.51 – 7.43 (m, 2H), 7.40 (dd, *J* = 7.0, 1.9 Hz, 1H), 6.52 (s, 1H), 6.48 (s, 1H), 3.70 (s, 3H), 3.58 (s, 3H), 1.30 (s, 9H);

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 196.5, 154.8, 154.1, 151.0, 150.5, 140.9, 136.5, 129.8, 126.4, 123.6, 121.8, 115.2, 112.1, 101.7, 80.0, 75.8, 57.1, 55.9, 28.3;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{21}H_{22}{}^{79}BrNO_6SNa$ 518.0243, found 518.0242; $C_{21}H_{22}{}^{81}BrNO_6SNa$ 520.0225, found 520.0223.



***tert*-butyl (S)-(2-(2-hydroxy-4,5-dimethoxyphenyl)-4,7-dimethyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5i)**

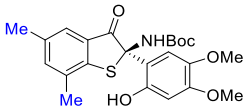
The product **5i** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 43.2 mg, 97% yield; 89% ee; $[\alpha]_D^{20}$ = +266.1 (*c* 0.98, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 10.6 min (minor), t_R = 9.1 min (major);

^{1}H NMR (400 MHz, CDCl$_3$) δ 9.03 (s, 1H), 7.44 (s, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 6.55 (s, 1H), 5.76 (s, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 2.55 (s, 3H), 2.30 (s, 3H), 1.36 (s, 9H);

^{13}C NMR (101 MHz, CDCl$_3$) δ 201.9, 153.7, 151.5, 151.2, 150.5, 142.2, 140.6, 136.3, 130.2, 128.0, 124.6, 112.9, 111.1, 103.7, 81.8, 56.8, 56.0, 28.2, 19.0, 18.6;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{27}NO_6SNa$ 468.1451, found 468.1457.



***tert*-butyl (S)-(2-(2-hydroxy-4,5-dimethoxyphenyl)-5,7-dimethyl-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5j)**

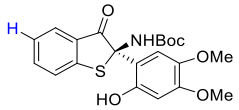
The product **5j** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 44.6 mg, 99% yield; 90% ee; $[\alpha]_D^{20}$ = +193.9 (*c* 1.17, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 8.9 min (minor), t_R = 11.1 min (major);

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.90 (s, 1H), 7.46 (s, 1H), 7.33 (s, 1H), 7.22 (s, 1H), 6.51 (s, 1H), 5.96 (d, *J* = 7.6 Hz, 1H), 3.79 (s, 3H), 3.73 (s, 3H), 2.29 (s, 6H), 1.36 (s, 9H);

^{13}C NMR (101 MHz, CDCl$_3$) δ 200.9, 153.8, 151.2, 150.9, 147.2, 142.1, 138.5, 135.5, 132.5, 127.5, 125.6, 112.5, 103.3, 81.7, 78.5, 76.8, 56.7, 55.9, 28.1, 20.7, 18.8;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{27}NO_6SNa$ 468.1451, found 468.1459.



***tert*-butyl (S)-(2-(2-hydroxy-4,5-dimethoxyphenyl)-3-oxo-2,3-dihydrobenzo[*b*]thiophen-2-yl)carbamate (5k)**

The product **5k** was purified by flash column chromatography (petroleum ether / ethyl acetate = 3:1); yellow oil, 41.5 mg, 99% yield; 91% ee; $[\alpha]_D^{20}$ = +259.3 (*c* 0.88, CH_2Cl_2);

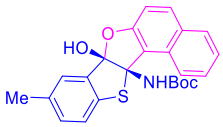
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min,

l = 254 nm, t_R= 13.2 min (minor), t_R = 9.1 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.55 (t, J = 8.2 Hz, 1H), 7.34 (d, J = 8.0 Hz, 2H), 7.19 (t, J = 7.2 Hz, 1H), 6.51 (s, 1H), 5.97 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 1.36 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.4, 153.8, 151.3, 150.8, 150.5, 150.5, 142.2, 136.8, 128.2, 127.7, 125.3, 123.8, 112.3, 103.3, 81.8, 78.2, 56.7, 55.9, 29.7, 28.1;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{21}H_{23}NO_6SNa$ 440.1138, found 440.1149.



***tert*-butyl ((7aS,12aS)-7a-hydroxy-9-methylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7a)**

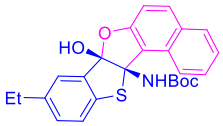
The product **7a** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow solid, 41.7 mg, 99% yield; m.p. 104.9-105.6; 94% ee; $[\alpha]_D^{20}$ = -513.0 (*c* 0.75, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, l = 254 nm, t_R= 8.5 min (minor), t_R = 7.3 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.4 Hz, 1H), 7.84 (d, J = 8.2 Hz, 1H), 7.76 (d, J = 8.8 Hz, 1H), 7.55 (dd, J = 15.4, 7.7 Hz, 2H), 7.38 (t, J = 7.6 Hz, 1H), 7.20 – 7.10 (m, 2H), 6.99 (d, J = 8.0 Hz, 1H), 5.96 (s, 1H), 5.91 (s, 1H), 2.38 (s, 3H), 1.29 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.1, 155.3, 135.9, 135.7, 134.3, 132.0, 131.6, 130.1, 129.5, 129.4, 127.7, 126.3, 123.8, 121.6, 120.8, 120.0, 117.4, 112.8, 82.1, 80.4, 28.0, 21.0;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{23}NO_4SNa$ 444.1240, found 444.1247.



***tert*-butyl ((7aS,12aS)-9-ethyl-7a-hydroxybenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7b)**

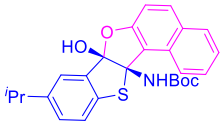
The product **7b** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 43.2 mg, 99% yield; 90% ee; $[\alpha]_D^{20}$ = -453.8 (*c* 0.68, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, l = 254 nm, t_R= 3.7min (minor), t_R = 4.1 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 (s, 1H), 7.95 (d, J = 8.3 Hz, 1H), 7.90 (d, J = 8.2 Hz, 1H), 7.82 (d, J = 8.8 Hz, 1H), 7.57 (q, J = 14.4, 10.9 Hz, 2H), 7.39 (dd, J = 15.5, 7.7 Hz, 2H), 7.13 (dd, J = 16.1, 8.4 Hz, 2H), 7.03 (d, J = 7.9 Hz, 1H), 2.62 (q, J = 7.7 Hz, 2H), 1.35 – 1.10 (m, 12H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.3, 154.2, 140.3, 137.7, 135.5, 130.9, 129.9, 129.4, 129.4, 129.0, 127.2, 124.2, 123.3, 122.1, 121.3, 120.1, 118.8, 112.3, 79.8, 78.7, 27.7, 18.6, 15.8;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1406.



***tert*-butyl ((7aS,12aS)-7a-hydroxy-9-isopropylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7c).**

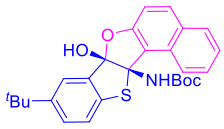
The product **7c** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 44.5 mg, 99% yield; 90% ee; $[\alpha]_D^{20}$ = -435.1 (*c* 0.79, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, l = 254 nm, t_R= 5.4 min (minor), t_R = 6.8 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.08 (s, 1H), 7.92 (dd, J = 16.2, 8.3 Hz, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 7.46 (s, 1H), 7.38 (t, J = 7.5 Hz, 1H), 7.18 (d, J = 8.0 Hz, 1H), 7.11 (d, J = 8.8 Hz, 1H), 7.03 (d, J = 8.0 Hz, 1H), 2.91 (hept, J = 6.6 Hz, 1H), 1.23 (s, 6H), 1.19 (d, J = 18.6 Hz, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.3, 154.2, 145.1, 137.6, 135.7, 130.9, 129.5, 129.4, 129.0, 128.6, 127.2, 123.4, 122.6, 122.1, 121.3, 120.1, 118.8, 112.3, 80.0, 78.7, 33.1, 27.7, 24.1, 24.0;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{27}NO_4SNa$ 472.1553, found 472.1559.



***tert*-butyl ((7aS,12aS)-9-(*tert*-butyl)-7a-hydroxybenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7d)**

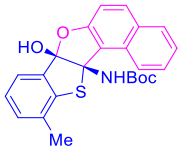
The product **7d** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 44.9 mg, 97% yield; 89% ee; $[\alpha]_D^{20}$ = -367.5 (*c* 0.76, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, l = 254 nm, t_R= 5.2 min (minor), t_R = 7.4 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.10 (s, 1H), 7.92 (dd, J = 15.9, 8.3 Hz, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.67 – 7.43 (m, 3H), 7.36 (dd, J = 19.5, 7.9 Hz, 2H), 7.12 (d, J = 8.8 Hz, 1H), 7.05 (d, J = 8.2 Hz, 1H), 1.30 (s, 9H), 1.16 (s, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.8, 154.7, 147.8, 137.8, 136.0, 131.4, 129.9, 129.8, 129.4, 128.0, 127.7, 123.8, 122.5, 121.9, 121.5, 120.5, 119.4, 112.8, 80.6, 79.2, 34.8, 31.7, 28.1;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{27}H_{29}NO_4SNa$ 486.1710, found 486.1717.



***tert*-butyl ((7aS,12aS)-7a-hydroxy-11-methylbenzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-12a(7aH)-yl)carbamate (7e)**

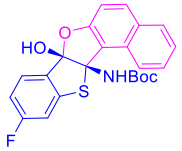
The product **7e** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 42.0 mg, 99% yield; 98% ee; $[\alpha]_D^{20}$ = -238.8 (*c* 0.97, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, l = 254 nm, t_R= 6.4 min (minor), t_R = 8.2 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (s, 1H), 7.97 (d, J = 8.2 Hz, 1H), 7.90 (d, J = 8.2 Hz, 1H), 7.82 (d, J = 8.8 Hz, 1H), 7.60 (t, J = 7.6 Hz, 2H), 7.45 – 7.36 (m, 2H), 7.12 (q, J = 10.0, 8.6 Hz, 3H), 2.05 (s, 3H), 1.14 (s, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.8, 154.7, 138.1, 131.4, 131.0, 130.6, 129.9, 129.8, 129.4, 127.7, 125.4, 123.8, 122.7, 122.6, 120.5, 119.7, 112.7, 79.9, 79.2, 28.1, 19.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{23}NO_4SNa$ 444.1240, found 444.1248.



tert-butyl ((7aS,12aS)-10-fluoro-7a-hydroxybenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7f)

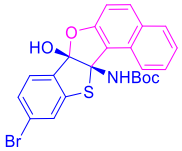
The product **7f** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 42.1 mg, 99% yield; 93% ee; $[\alpha]_D^{20}$ = -465.8 (*c* 0.67, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.2 min (minor), t_R = 5.5 min (major);

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.23 (s, 1H), 7.92 (t, *J* = 7.4 Hz, 2H), 7.84 (d, *J* = 8.9 Hz, 1H), 7.78 – 7.50 (m, 3H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.10 (dd, *J* = 12.6, 8.6 Hz, 2H), 7.00 (t, *J* = 8.9 Hz, 1H), 1.20 (s, 9H);

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 163.3 (d, *J* = 247.3 Hz), 162.1, 154.3, 154.1, 141.4 (d, *J* = 10.1 Hz), 134.3, 131.2, 129.4, 129.4, 129.0, 127.4, 126.4 (d, *J* = 10.1 Hz), 123.5, 122.1, 119.7, 117.8, 112.3, 111.6 (d, *J* = 23.2 Hz), 108.6 (d, *J* = 25.3 Hz), 80.6, 78.8, 27.7;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{20}FNO_4SNa$ 448.0989, found 448.0996.



tert-butyl ((7aS,12aS)-10-bromo-7a-hydroxybenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7g)

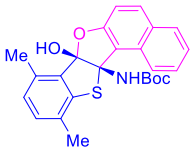
The product **7g** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 48.3 mg, 99% yield; 94% ee; $[\alpha]_D^{20}$ = -97.7 (*c* 0.92, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.2 min (minor), t_R = 5.5 min (major);

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.07 (s, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 8.9 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.49 (s, 1H), 7.43 – 7.31 (m, 2H), 7.23 – 7.07 (m, 3H), 1.20 (s, 9H);

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 154.6, 154.5, 142.5, 135.3, 132.1, 131.8, 130.0, 129.7, 129.5, 127.9, 124.0, 122.7, 121.5, 120.4, 120.1, 119.9, 112.8, 79.9, 79.4, 28.2;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{20}{}^{79}BrNO_4S$ 508.0189, found 508.0189; Calcd. for $[M+Na]^+$ $C_{23}H_{20}{}^{81}BrNO_4S$ 510.0170, found 510.0174.



tert-butyl ((7aS,12aS)-7a-hydroxy-8,11-dimethylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7h)

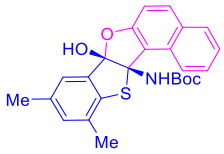
The product **7c** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 43.2 mg, 99% yield; 84% ee; $[\alpha]_D^{20}$ = -381.2 (*c* 0.63, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.7 min (minor), t_R = 5.8 min (major);

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.02 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.49 (s, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.23 (s, 1H), 7.09 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.97 (s, 1H), 2.29 (s, 3H), 2.02 (s, 3H), 1.16 (s, 9H);

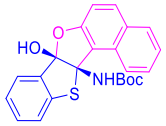
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 154.7, 154.7, 138.1, 135.3, 134.6, 131.9, 131.4, 130.3, 129.9,

129.8, 129.4, 127.7, 123.8, 123.3, 122.7, 120.6, 119.6, 112.7, 80.0, 79.1, 28.1, 21.0, 19.8;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1401.



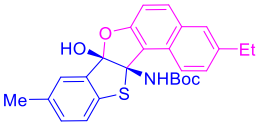
***tert*-butyl ((7aS,12aS)-7a-hydroxy-9,11-dimethylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7i)**

The product **7i** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 43.3 mg, 99% yield; 91% ee; $[\alpha]_D^{20}$ = -481.1 (*c* 0.69, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 6.6 min (minor), t_R = 7.5 min (major);
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.02 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 27.1 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.23 (s, 1H), 7.09 (d, *J* = 8.8 Hz, 1H), 6.97 (s, 1H), 2.29 (s, 3H), 2.01 (s, 3H), 1.16 (s, 9H);
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 154.7, 154.7, 138.1, 135.3, 134.6, 131.9, 131.4, 130.3, 129.9, 129.8, 129.4, 127.7, 123.8, 123.2, 122.7, 120.6, 119.6, 112.7, 80.0, 79.1, 28.1, 21.0, 19.8;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_4SNa$ 458.1397, found 458.1404.



***tert*-butyl ((7aS,12aS)-7a-hydroxybenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7j)**

The product **7j** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 40.5 mg, 99% yield; 92% ee; $[\alpha]_D^{20}$ = +7.4 (*c* 0.71, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.2 min (minor), t_R = 3.9 min (major);
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.14 (s, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.58 (dd, *J* = 7.4, 4.1 Hz, 3H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.12 (t, *J* = 9.0 Hz, 2H), 1.17 (s, 9H);
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 154.8, 154.7, 139.2, 138.2, 131.5, 130.7, 129.9, 129.8, 129.5, 127.7, 125.4, 125.0, 123.8, 122.6, 121.9, 120.5, 119.2, 112.8, 80.1, 79.2, 28.2;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{23}H_{21}NO_4SNa$ 430.1083, found 430.1090.



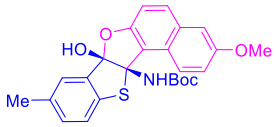
***tert*-butyl ((7aS,12aS)-3-ethyl-7a-hydroxy-9-methylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7k)**

The product **7k** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 44.5 mg, 99% yield; 91% ee; $[\alpha]_D^{20}$ = -492.6 (*c* 0.72, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 10.3 min (minor), t_R = 5.2 min (major);
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.88 (d, *J* = 8.5 Hz, 1H), 7.69 (d, *J* = 8.9 Hz, 1H), 7.62 (s, 1H), 7.51 (s, 1H), 7.43 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.18 – 7.07 (m, 2H), 6.98 (d, *J* = 8.0 Hz, 1H), 5.90 (d, *J* =

5.8 Hz, 2H), 2.79 (q, *J* = 7.6 Hz, 2H), 2.38 (s, 3H), 1.33 (d, *J* = 7.6 Hz, 3H), 1.29 (d, *J* = 2.1 Hz, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.0, 154.7, 139.6, 135.8, 134.3, 131.9, 131.1, 130.4, 128.9, 127.7, 127.3, 126.2, 121.6, 120.7, 119.9, 117.3, 112.7, 82.0, 80.5, 28.8, 28.0, 21.0, 15.6;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{27}NO_4SNa$ 472.1553, found 472.1560.



***tert*-butyl ((7aS,12aS)-7a-hydroxy-3-methoxy-9-methylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7l)**

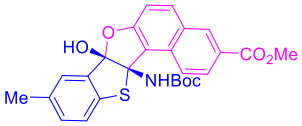
The product **7l** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 44.5 mg, 98% yield; 86% ee; $[\alpha]_D^{20}$ = -433.2 (*c* 0.61, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 14.3 min (minor), t_R = 7.4 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 (s, 1H), 7.89 (d, *J* = 9.1 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.52 (s, 1H), 7.40 – 7.31 (m, 2H), 7.27 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.99 (d, *J* = 7.9 Hz, 1H), 3.84 (s, 3H), 2.31 (s, 3H), 1.19 (s, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 155.5, 154.3, 152.7, 137.9, 135.3, 133.8, 131.0, 130.6, 129.7, 125.4, 124.7, 123.7, 121.2, 120.4, 119.6, 118.5, 112.5, 107.7, 79.9, 78.8, 55.2, 27.8, 20.6;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_5SNa$ 474.1346, found 474.1351.



methyl (7aS,12aS)-12a-((*tert*-butoxycarbonyl)amino)-7a-hydroxy-9-methyl-7a,12a-dihydrobenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-3-carboxylate (7m)

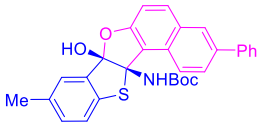
The product **7m** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 47.5 mg, 99% yield; 88% ee; $[\alpha]_D^{20}$ = +6.33 (*c* 0.55, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 17.1 min (minor), t_R = 8.1 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 (s, 1H), 7.89 (d, *J* = 9.1 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.52 (s, 1H), 7.40 – 7.31 (m, 2H), 7.27 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.99 (d, *J* = 7.9 Hz, 1H), 3.84 (s, 3H), 2.31 (s, 3H), 1.19 (s, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 155.5, 154.3, 152.7, 137.9, 135.3, 133.8, 131.0, 130.6, 129.7, 125.4, 124.7, 123.7, 121.2, 120.4, 119.6, 118.5, 112.5, 107.7, 79.9, 78.8, 55.2, 27.8, 20.6;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{25}NO_6SNa$ 502.1295, found 502.1298.

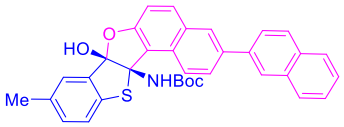


***tert*-butyl ((7aS,12aS)-7a-hydroxy-9-methyl-3-phenylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7n)**

The product **7n** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 47.7 mg, 96% yield; 90% ee; $[\alpha]_D^{20}$ = -443.5 (*c* 0.68, CH_2Cl_2);

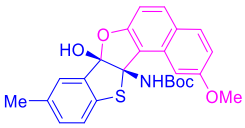
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 16.3 min (minor), t_R = 6.9 min (major);

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (s, 1H), 8.12 (s, 1H), 8.04 (d, J = 8.7 Hz, 1H), 7.98 – 7.87 (m, 2H), 7.80 (d, J = 7.4 Hz, 2H), 7.59 (s, 1H), 7.51 (t, J = 7.7 Hz, 2H), 7.39 (d, J = 7.0 Hz, 2H), 7.17 – 7.08 (m, 2H), 7.01 (d, J = 7.9 Hz, 1H), 2.32 (s, 3H), 1.21 (s, 9H);
^{13}C NMR (101 MHz, DMSO-d_6) δ 154.4, 154.2, 140.0, 137.7, 135.3, 135.0, 133.8, 131.5, 131.0, 129.7, 129.0, 128.7, 127.3, 126.7, 126.4, 126.3, 125.4, 122.9, 121.2, 120.2, 118.9, 112.7, 79.7, 78.8, 27.8, 20.6;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{30}H_{27}NO_4SNa$ 520.1553, found 520.1562.



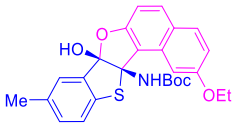
***tert*-butyl ((7aS,12aS)-7a-hydroxy-9-methyl-3-(naphthalen-2-yl)benzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7o)**

The product **7o** was purified by flash column chromatography (petroleum ether / ethyl acetate = 10:1); yellow oil, 50.1 mg, 94% yield; 96% ee; $[\alpha]_D^{20}$ = -461.8 (*c* 0.63, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak IC, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.0 min (minor), t_R = 7.5 min (major);
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.18 – 8.14 (m, 2H), 8.09 (d, J = 8.7 Hz, 1H), 8.01 – 7.97 (m, 1H), 7.97 – 7.93 (m, 2H), 7.91 – 7.88 (m, 1H), 7.88 – 7.83 (m, 2H), 7.56 (s, 1H), 7.55 – 7.49 (m, 2H), 7.22 – 7.14 (m, 2H), 7.02 (d, J = 8.0 Hz, 1H), 6.03 (s, 1H), 6.00 (s, 1H), 2.40 (s, 3H), 1.33 (s, 9H);
^{13}C NMR (101 MHz, CDCl$_3$) δ 156.2, 155.6, 138.3, 136.5, 136.0, 135.8, 134.4, 133.9, 132.7, 132.1, 132.1, 130.5, 128.7, 128.7, 128.3, 127.8, 127.7, 127.6, 126.5, 126.4, 126.1, 125.9, 125.7, 121.7, 121.5, 120.2, 117.6, 113.4, 82.2, 80.5, 28.1, 21.1;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{34}H_{29}NO_4SNa$ 570.1710, found 570.1720.



***tert*-butyl ((7aS,12aS)-7a-hydroxy-2-methoxy-9-methylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7p)**

The product **7p** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); yellow solid 41.5 mg, 92% yield; m.p. 148.6-149.1 °C; 86% ee; $[\alpha]_D^{20}$ = -492.6 (*c* 0.68, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 6.2 min (minor), t_R = 10.0 min (major);
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.72 (d, J = 9.0 Hz, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.52 (s, 1H), 7.23 (s, 1H), 7.15 (d, J = 8.0 Hz, 1H), 7.06 – 7.01 (m, 1H), 6.99 (dd, J = 8.2, 5.4 Hz, 2H), 5.98 (s, 1H), 5.90 (s, 1H), 3.97 (s, 3H), 2.38 (s, 3H), 1.29 (s, 9H);
^{13}C NMR (101 MHz, CDCl$_3$) δ 159.2, 156.1, 136.0, 135.7, 134.4, 132.1, 131.4, 131.1, 130.9, 126.4, 125.5, 121.7, 119.9, 116.4, 116.0, 110.3, 100.0, 82.2, 80.7, 55.5, 28.1, 21.1;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{25}NO_5SNa$ 474.1346, found 474.1351.



***tert*-butyl ((7aS,12aS)-2-ethoxy-7a-hydroxy-9-methylbenzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-12a(7aH)-yl)carbamate (7q)**

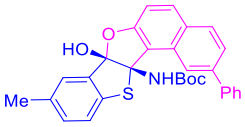
The product **7q** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); yellow solid, 46.2 mg, 99% yield; m.p. 143.2-143.7 °C; 96% ee; $[\alpha]_D^{20}$ = -555.2 (*c* 0.71, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.2 min (minor), t_R = 6.9 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 9.0 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.51 (s, 1H), 7.22 – 7.19 (m, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.05 – 7.00 (m, 1H), 6.98 (dd, *J* = 10.4, 8.8 Hz, 2H), 5.91 (s, 1H), 5.86 (s, 1H), 4.19 (dt, *J* = 14.3, 7.2 Hz, 2H), 2.38 (s, 3H), 1.52 (t, *J* = 7.0 Hz, 3H), 1.29 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4, 155.9, 135.9, 135.6, 134.2, 132.0, 131.3, 131.0, 130.8, 126.3, 125.3, 121.6, 119.8, 116.2, 116.1, 110.1, 100.7, 82.1, 80.6, 63.6, 28.0, 21.0, 14.8;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{27}NO_5SNa$ 488.1502, found 488.1509.



***tert*-butyl ((7aS,12aS)-7a-hydroxy-9-methyl-2-phenylbenzo[4,5]thieno[3,2-*b*]naphtho[1,2-*d*]furan-12a(7a*H*)-yl)carbamate (7r)**

The product **7r** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); yellow oil, 47.1 mg, 96% yield; 83% ee; $[\alpha]_D^{20}$ = -433.5 (*c* 0.68, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, ^{i}PrOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 5.4 min (minor), t_R = 6.6 min (major);

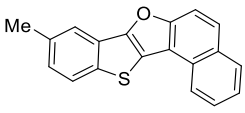
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28 (s, 1H), 8.11 (s, 1H), 7.98 (d, *J* = 8.6 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.79 (t, *J* = 8.6 Hz, 3H), 7.69 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 2H), 7.44 (d, *J* = 7.4 Hz, 1H), 7.41 (s, 1H), 7.15 – 7.06 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 1H), 2.31 (s, 3H), 1.18 (s, 9H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.7, 154.5, 140.3, 138.7, 137.6, 135.1, 134.0, 131.2, 130.8, 129.8, 129.7, 129.1, 128.6, 127.8, 127.1, 125.5, 122.6, 121.3, 120.6, 119.9, 118.8, 112.4, 79.4, 78.9, 27.7, 20.6;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{30}H_{27}NO_4SNa$ 520.1553, found 520.1558.

4. The general procedure for synthesis of compound 8.

In an ordinary vial equipped with a magnetic stirring bar, the solution of compound **5a** (0.1 mmol, 42.2 mg) in CH_2Cl_2 (1.0 mL) was cooled at 0 °C. Then TFA (1.0 mmol, 10 equiv) was added slowly into the solution at 0 °C, and the mixture was stirred at room temperature for 19 h. After completion, the reaction was quenched by saturated $NaHCO_3$ (aq). The mixture was extracted with CH_2Cl_2 (5 mL × 3), and the combined organic layer was dried over Na_2SO_4 and concentrated. The residue was purified using flash column chromatography on silica gel to give the desired product **8** in 42% yield.



9-methylbenzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan (8)

The product **8** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); yellow oil, 12.2 mg, 42% yield;

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.29 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* =

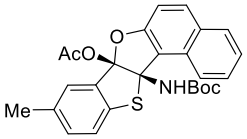
8.8 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.41 – 7.35 (m, 2H), 7.15 – 7.09 (m, 2H), 7.00 (d, *J* = 7.9 Hz, 1H), 2.31 (s, 3H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 154.5, 138.0, 135.0, 134.6, 131.8, 131.5, 130.1, 130.0, 129.3, 127.5, 126.7, 123.8, 123.1, 121.9, 121.8, 118.3, 112.7, 83.6, 21.0;

HRMS (ESI) *m/z*: Calcd. for $[M+H]^+$ $C_{19}H_{13}OS$ 289.0682, found 289.0678.

5. The general procedure for synthesis of compound 9.

In an ordinary vial equipped with a magnetic stirring bar, the solution of compound **5a** (0.1 mmol, 42.2 mg), Et_3N (0.2 mmol, 2.0 equiv) and DMAP (0.02 mmol, 0.2 equiv) in CH_2Cl_2 (1.0 mL) was cooled at 0 °C. Then AcCl (0.12 mmol, 1.2 equiv) was added slowly into the solution at 0 °C, and the mixture was stirred at room temperature for 12 h. After completion, the reaction was quenched by saturated H_2O. The mixture was extracted with CH_2Cl_2 (5 mL × 3), and the combined organic layer was dried over Na_2SO_4 and concentrated. The residue was purified using flash column chromatography on silica gel to give the desired product **9** in 64% yield with 90% ee.



(7a*R*,12a*S*)-12a-((*tert*-butoxycarbonyl)amino)-9-methylbenzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-7a(12a*H*)-yl acetate (9)

The product **9** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); yellow oil, 29.6 mg, 64% yield; 90% ee; $[\alpha]_D^{20}$ = -492.2 (*c* 1.50, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 10/90, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 12.2 min (minor), t_R = 10.3 min (major);

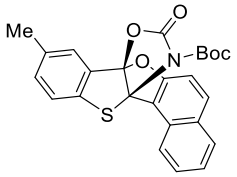
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.62 – 7.53 (m, 1H), 7.44 – 7.33 (m, 2H), 7.15 – 7.09 (m, 1H), 7.06 (d, *J* = 8.8 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 5.51 (s, 1H), 2.37 (s, 3H), 2.19 (s, 3H), 1.47 – 1.09 (m, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 154.4, 135.3, 135.1, 134.9, 132.2, 131.6, 130.3, 129.4, 128.6, 127.9, 125.4, 124.0, 121.6, 121.5, 120.2, 111.9, 80.7, 80.3, 27.8, 26.9, 21.6, 21.1;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{25}NO_5SNa$ 486.1346, found 486.1345.

6. The general procedure for synthesis of compound 10a.

In an ordinary vial equipped with a magnetic stirring bar, the solution of compound **5a** (0.1 mmol, 42.2 mg) in CH_2Cl_2 (1.0 mL) was added CDI (0.15 mmol, 1.5 equiv), and the mixture was stirred at room temperature for 12 h. After completion, the reaction mixture was directly purified by flash chromatography on silica gel to afford the desired product **10a** in 51% yield and 90% ee.



***tert*-butyl (7a*R*,12a*S*)-9-methyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10a)**

The product **10a** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 129.1-131.0 °C; 22.8 mg, 51% yield; 90% ee; $[\alpha]_D^{20}$ = -169.6 (*c* 0.91, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.3 min (minor), t_R = 5.0 min (major);

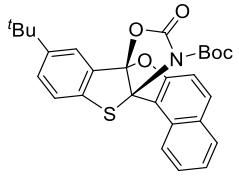
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.6 Hz, 1H), 7.86 – 7.75 (m, 2H), 7.65 – 7.56 (m, 1H), 7.51 – 7.46 (m, 1H), 7.45 – 7.36 (m, 1H), 7.21 – 7.16 (m, 1H), 7.12 (d, *J* = 8.9 Hz, 1H), 7.00 (d, *J* = 8.1 Hz, 1H), 2.36 (s, 3H), 1.54 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 149.8, 149.2, 136.8, 136.1, 133.9, 133.5, 131.4, 130.7, 129.4, 128.9, 127.7, 125.9, 124.9, 124.4, 122.2, 121.2, 119.1, 112.2, 86.0, 83.6, 27.9, 21.0;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{21}NO_5SNa$ 470.1033, found 470.1033.

7. The general procedure for synthesis of compound 10 by the one-pot two steps.

In an ordinary vial equipped with a magnetic stirring bar, cyclic α-carbonyl thioimidates **1** (0.15 mmol, 1.5 equiv.) was added to a solution of 2-naphthols **6** (0.1 mmol, 1.0 equiv.), 5Å MS (50 mg) and catalyst **C** (0.01 mmol, 6.4 mg) in $CHCl_3$ (1.0 mL) at 0 °C for 5-10 min monitored by TLC. After completion, the CDI (0.21 mmol, 2.1 equiv) was added to the mixture and the reaction mixture was kept stirring at room temperature for 14 h. Ultimately, the mixture was directly purified by flash chromatography on silica gel to afford the desired products **10**.



***tert*-butyl (7a*R*,12a*S*)-9-(tert-butyl)-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10b)**

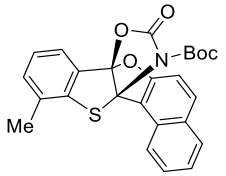
The product **10a** was purified by flash column chromatography (petroleum ether / DCM = 1:2); white solid, m.p. 137.8-138.2 °C; 28.5 mg, 58% yield; 92% ee; $[\alpha]_D^{20}$ = -216.7 (*c* 1.20, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IF, ^{i}PrOH/hexane = 1/99, flow rate = 0.8 mL/min, *l* = 254 nm, t_R= 8.6 min (minor), t_R = 9.0 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.5 Hz, 1H), 7.81 (dd, *J* = 15.2, 8.5 Hz, 2H), 7.68 (d, *J* = 2.0 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.46 – 7.37 (m, 2H), 7.15 (d, *J* = 8.9 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 1.54 (s, 9H), 1.33 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 149.8, 149.7, 149.3, 136.9, 133.9, 131.2, 130.7, 130.1, 129.4, 128.9, 127.7, 124.9, 124.4, 122.2, 122.0, 121.4, 119.1, 112.2, 86.0, 83.7, 34.8, 31.3, 27.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{28}H_{27}NO_5SNa$ 512.1502, found 512.1502.



***tert*-butyl (7a*R*,12a*S*)-11-methyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10c)**

The product **10c** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 132.5-133.2 °C; 33.3 mg, 74% yield; 93% ee; $[\alpha]_D^{20}$ = -189.2 (*c* 1.21, CH_2Cl_2);

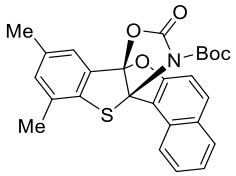
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 3.8 min (minor), t_R = 4.2 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.7 Hz, 1H), 7.87 – 7.76 (m, 2H), 7.65 – 7.58 (m, 1H),

7.55 – 7.48 (m, 1H), 7.44 – 7.36 (m, 1H), 7.18 (d, *J* = 6.2 Hz, 2H), 7.13 (d, *J* = 8.9 Hz, 1H), 2.19 (s, 3H), 1.54 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 149.9, 149.2, 140.0, 134.0, 132.9, 132.2, 131.3, 130.7, 129.4, 128.9, 127.7, 126.5, 125.0, 124.4, 122.8, 121.7, 119.1, 112.2, 86.0, 83.0, 27.9, 19.8;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{25}H_{21}NO_5SNa$ 470.1033, found 470.1034.



***tert*-butyl (7a*R*,12a*S*)-9,11-dimethyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10d)**

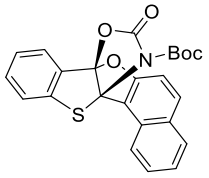
The product **10d** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 128.0-129.0 °C; 23.4 mg, 51% yield; 88% ee; $[\alpha]_D^{20}$ = -115.7 (*c* 1.10, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak IC, ^{i}PrOH/hexane = 15/85, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.9 min (minor), t_R = 5.5 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.86 – 7.75 (m, 2H), 7.65 – 7.56 (m, 1H), 7.45 – 7.36 (m, 1H), 7.32 (d, *J* = 1.6 Hz, 1H), 7.12 (d, *J* = 8.9 Hz, 1H), 7.02 (d, *J* = 1.6 Hz, 1H), 2.33 (s, 3H), 2.15 (s, 3H), 1.54 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 149.9, 149.2, 136.6, 136.5, 134.0, 133.9, 131.8, 131.2, 130.7, 129.4, 128.9, 127.7, 125.0, 124.4, 123.2, 121.6, 119.2, 112.2, 86.0, 83.2, 27.9, 20.9, 19.7;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{23}NO_5SNa$ 484.1189, found 484.1192.



***tert*-butyl (7a*R*,12a*S*)-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10e)**

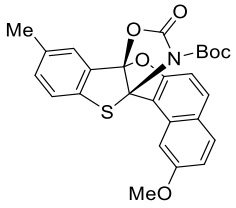
The product **10e** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 100.8-101.7 °C; 32.8 mg, 76% yield; 94% ee; $[\alpha]_D^{20}$ = -206.2 (*c* 1.50, CH_2Cl_2);

The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.6 min (minor), t_R = 6.0 min (major);

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 8.7, 1.1 Hz, 1H), 7.87 – 7.77 (m, 2H), 7.67 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.46 – 7.34 (m, 2H), 7.29 – 7.24 (m, 1H), 7.17 – 7.09 (m, 2H), 1.54 (s, 9H);

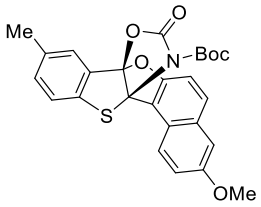
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 149.8, 149.2, 140.3, 134.0, 132.5, 131.4, 130.7, 129.4, 128.9, 127.7, 126.0, 125.6, 124.9, 124.5, 122.4, 121.2, 119.0, 112.2, 86.1, 83.3, 27.9;

HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{24}H_{19}NO_5SNa$ 456.0876, found 456.0878.



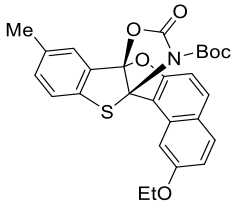
***tert*-butyl (7a*R*,12a*S*)-2-methoxy-9-methyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylat*e* (10f)**

The product **10f** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 149.9-151.7 °C; 34.5 mg, 72% yield; 90% ee; $[\alpha]_D^{20}$ = -294.6 (*c* 1.29, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 3.9 min (minor), t_R = 4.5 min (major);
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 2.4 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 9.0 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.19 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.08 – 6.98 (m, 2H), 6.95 (d, *J* = 8.8 Hz, 1H), 4.04 (s, 3H), 2.36 (s, 3H), 1.54 (s, 9H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 157.1, 150.3, 149.1, 136.8, 136.2, 133.5, 133.4, 131.6, 131.1, 130.3, 126.0, 125.9, 122.1, 121.1, 118.4, 117.3, 109.3, 103.8, 85.8, 83.6, 55.6, 28.0, 21.0;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{23}NO_6SNa$ 500.1138, found 500.1140.



***tert*-butyl (7a*R*,12a*S*)-3-methoxy-9-methyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10g)**

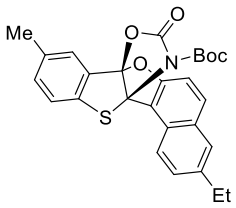
The product **10g** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 148.2-149.7 °C; 22.2 mg, 46% yield; 93% ee; $[\alpha]_D^{20}$ = -169.6 (*c* 0.91, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 4.5 min (minor), t_R = 6.4 min (major);
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 9.3 Hz, 1H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.30 – 7.25 (m, 1H), 7.21 – 7.16 (m, 1H), 7.14 – 7.05 (m, 2H), 7.01 (d, *J* = 8.1 Hz, 1H), 3.90 (s, 3H), 2.36 (s, 3H), 1.53 (s, 9H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 154.9, 149.8, 149.2, 136.8, 136.1, 133.4, 132.4, 132.0, 131.5, 126.5, 125.9, 124.6, 122.1, 121.1, 120.0, 119.3, 112.5, 107.2, 86.0, 83.7, 55.3, 27.9, 21.0;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{26}H_{23}NO_6SNa$ 500.1138, found 500.1140.



***tert*-butyl (7aR,12aS)-2-ethoxy-9-methyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10h)**

The product **10h** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 142.7-143.5 °C; 29.5 mg, 60% yield; 87% ee; $[\alpha]_D^{20}$ = -176.7 (*c* 2.20, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 3.6 min (minor), t_R = 4.6 min (major);
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 2.4 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.48 (d, *J* = 1.6 Hz, 1H), 7.23 – 7.15 (m, 1H), 7.07 – 6.98 (m, 2H), 6.95 (d, *J* = 8.7 Hz, 1H), 4.45 – 4.19 (m, 2H), 2.36 (s, 3H), 1.60 – 1.54 (m, 3H), 1.54 (s, 9H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 157.0, 150.3, 149.2, 136.8, 136.1, 133.4, 133.3, 131.6, 131.1, 130.3, 125.9, 122.1, 121.1, 118.3, 117.5, 109.2, 104.4, 85.8, 83.6, 63.8, 28.0, 21.0, 14.8;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{27}H_{25}NO_6SNa$ 514.1295, found 514.1295.



***tert*-butyl (7a*R*,12a*S*)-3-ethyl-9-methyl-14-oxo-7a,12a-(epoxymethanoimino)benzo[4,5]thieno[3,2-b]naphtho[1,2-d]furan-13-carboxylate (10i)**

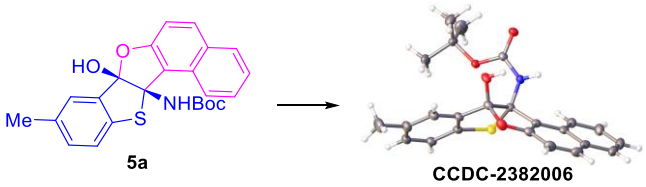
The product **10i** was purified by flash column chromatography (petroleum ether / ethyl acetate = 8:1); white solid, m.p. 130.7-132.1 °C; 30.8 mg, 65% yield; 93% ee; $[\alpha]_D^{20}$ = -272.1 (*c* 1.19, CH_2Cl_2);
The ee was determined by HPLC: Chiralpak AD-H, EtOH/hexane = 20/80, flow rate = 1.0 mL/min, *l* = 254 nm, t_R= 3.8 min (minor), t_R = 4.3 min (major);
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 8.9 Hz, 1H), 7.57 (d, *J* = 1.7 Hz, 1H), 7.51 – 7.44 (m, 2H), 7.21 – 7.14 (m, 1H), 7.09 (d, *J* = 8.9 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 2.78 (q, *J* = 7.6 Hz, 2H), 2.35 (s, 3H), 1.54 (s, 9H), 1.30 (t, *J* = 7.6 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9, 149.8, 149.2, 140.3, 136.8, 136.1, 133.4, 131.5, 131.1, 128.9, 127.7, 126.7, 125.9, 124.8, 122.1, 121.1, 119.0, 112.0, 85.9, 83.7, 28.7, 27.9, 21.0, 15.4;
HRMS (ESI) *m/z*: Calcd. for $[M+Na]^+$ $C_{27}H_{25}NO_5SNa$ 498.1346, found 498.1348.

8. X-ray crystal structure of 5a, 5r and 10a

A suitable crystal was selected for structure determination on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 150.00(10) K during data collection. Using Olex2[1], the structure was solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the SHELXL[3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Single crystal of·compound **5a**·was obtained from the·solvent of·EtOH at room temperature by slow evaporation of solvent.



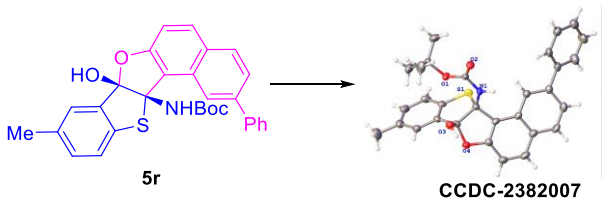
ORTEP of **5a** (at 50% level)

Crystal data and structure refinement for 5a

Identification code	**5a**
Empirical formula	$C_{24}H_{23}NO_4S$
Formula weight	421.49
Temperature/K	170.00(10)
Crystal system	triclinic

Space group	P-1
a/Å	12.6164(6)
b/Å	12.7840(8)
c/Å	15.2354(8)
α/°	79.875(5)
β/°	87.455(4)
γ/°	72.020(5)
Volume/Å^3	2300.8(2)
Z	4
ρ_{calc}g/cm^3	1.217
μ/mm^{-1}	1.483
F(000)	888.0
Crystal size/mm^3	0.15 × 0.13 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.894 to 147.498
Index ranges	-14 ≤ h ≤ 15, -15 ≤ k ≤ 12, -14 ≤ l ≤ 18
Reflections collected	16302
Independent reflections	9041 [R_{int} = 0.0255, R_{sigma} = 0.0358]
Data/restraints/parameters	9041/0/558
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0456, wR_2 = 0.1237
Final R indexes [all data]	R_1 = 0.0534, wR_2 = 0.1317
Largest diff. peak/hole / e Å^{-3}	0.39/-0.41

Single crystal of·compound **5r**·was obtained from the··solvent of·EtOH at room temperature by slow evaporation of solvent.



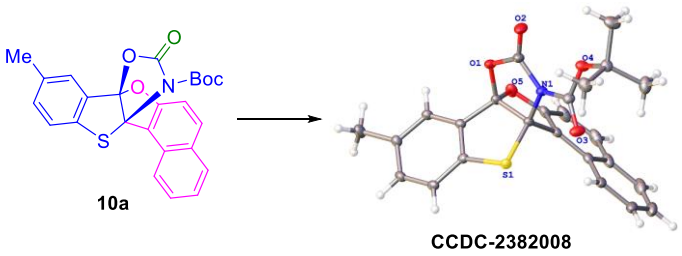
ORTEP of **5r** (at 50% level)

Table 1 Crystal data and structure refinement for 5r

Identification code	**5r**
Empirical formula	$C_{30}H_{27}NO_4S$
Formula weight	497.58
Temperature/K	169.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.9249(7)

b/Å	11.4332(7)
c/Å	13.6054(9)
α/°	95.386(5)
β/°	91.498(5)
γ/°	107.747(6)
Volume/Å^3	1608.69(19)
Z	2
ρ_{calc}g/cm^3	1.027
μ/mm^{-1}	0.130
F(000)	524.0
Crystal size/mm^3	0.15 × 0.12 × 0.09
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.52 to 50
Index ranges	-11 ≤ h ≤ 12, -12 ≤ k ≤ 13, -13 ≤ l ≤ 16
Reflections collected	10281
Independent reflections	5656 [R_{int} = 0.0466, R_{sigma} = 0.0837]
Data/restraints/parameters	5656/0/329
Goodness-of-fit on F^2	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0613, wR_2 = 0.1834
Final R indexes [all data]	R_1 = 0.0805, wR_2 = 0.1979
Largest diff. peak/hole / e Å^{-3}	0.41/-0.43

Single crystal of·compound **10a**·was obtained from the·solvent of·EtOH at room temperature by slow evaporation of solvent.



ORTEP of **10a** (at 50% level)

Table 1 Crystal data and structure refinement for 10a.

Identification code	**10a**
Empirical formula	$C_{25}H_{21}NO_5S$
Formula weight	447.49
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.04640(10)

b/Å	13.51470(10)
c/Å	16.2197(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2202.21(4)
Z	4
ρ_{calc}g/cm^3	1.350
μ/mm^{-1}	1.621
F(000)	936.0
Crystal size/mm^3	0.17 × 0.14 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.516 to 152.604
Index ranges	-11 ≤ h ≤ 12, -15 ≤ k ≤ 16, -20 ≤ l ≤ 20
Reflections collected	13215
Independent reflections	4462 [R_{int} = 0.0168, R_{sigma} = 0.0166]
Data/restraints/parameters	4462/0/294
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0238, wR_2 = 0.0631
Final R indexes [all data]	R_1 = 0.0240, wR_2 = 0.0634
Largest diff. peak/hole / e Å^{-3}	0.20/-0.14
Flack/Hooft parameter	0.009(3)/0.000(3)

9. Determination of the absolute configuration of 3a and 5a by ECD spectrum

Computational details

Based on the experimental crystal structure of enantiomers, there are only two possible configurations (*R*,*S*)-**3ga** and (*S*,*R*)-**3ga**. To further determine the precise configuration of our chiral product, theoretical calculation of the ECD spectrum has been performed and compared with the experimental spectrum. For the ECD spectrum calculations, all structures were optimized at B3LYP[1] level of theory with 6-311+g(d,p)[2] basis set for all atoms. Empirical dispersion correction has been considered by using Grimme's DFT empirical dispersion correction with the Becke-Jonson (D3BJ) damping function.[3] Optimized minima were verified at the same level of theory by harmonic vibrational analysis to have no imaginary frequency. CD spectra were calculated by TDDFT at the CAM-B3LYP[4]/Def2SVP[5] level. All DFT geometry optimizations and TDDFT calculations were performed with Gaussian 16 program.[6]

1. Becke, A. D. Phys. Rev. 1988, A38, 3098. (b) Becke, A. D. J.Chem. Phys. 1993, 98, 5648.(c) Lee, C.; Yang, W.; Parr, R. G. Phys. Rev. 1988, B37, 785
2. (a) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. J. Chem. Phys. 1980, 72, 650−654. (b) McLean, A. D.; Chandler, G. S. J. Chem. Phys. 1980, 72, 5639−5648.
3. Grimme, S.; Ehrlich, S.; Georigk, L. *J. Compt. Chem*. **2011**, *32*, 1456-1465.
4. Yanai, T. V.; Tew, D. P.; Handy, N. C. *Chem. Phys. Lett*. **2004**, *393*, 51-57.
5. Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

6. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E. *et al*. Gaussian, Inc., Wallingford CT, 2019.

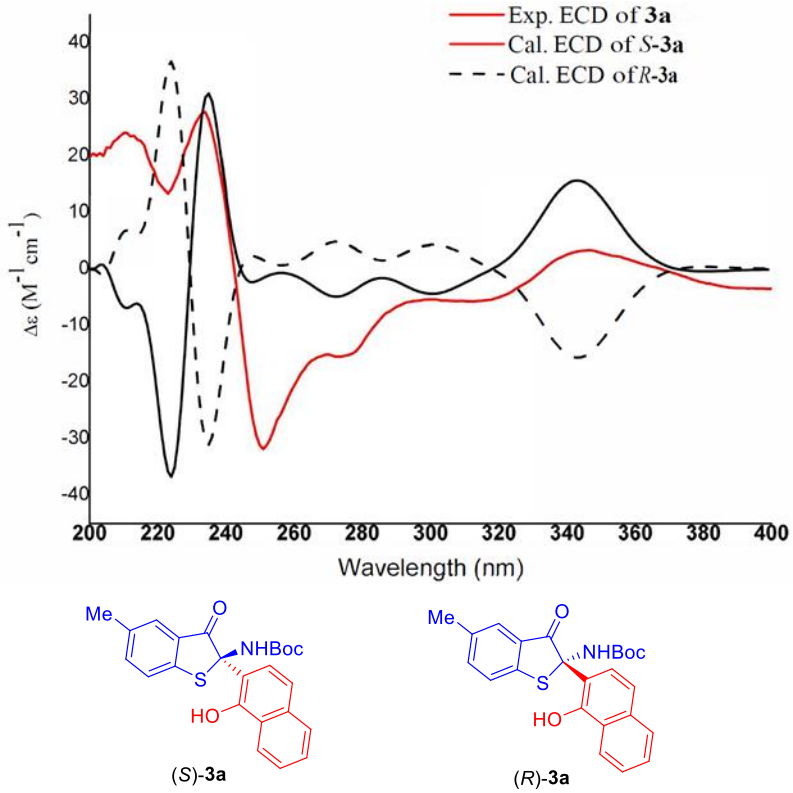


Figure S1. Experimental ECD spectra (200-400 nm) of **3a** in methanol and the calculated ECD spectra of the model molecules of **3a** at the CAM-B3LYP/def2-TZVP level.

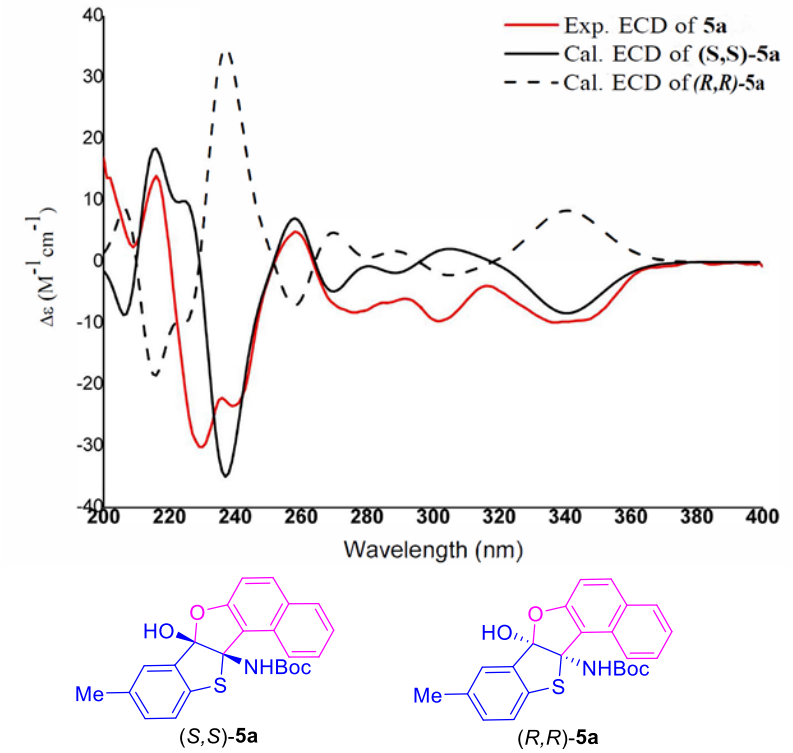


Figure S2. Experimental ECD spectra (200-400 nm) of **5a** in methanol and the calculated ECD

spectra of the model molecules of **3a** at the CAM-B3LYP/def2-TZVP level.

10. DFT calculations

Geometry optimizations without symmetry restriction were carried out with the Gaussian 16 program[1]. Specifically, geometry optimizations were firstly performed at the M06-2X[2-4]/ 6-31G(d,p)[5] level. The solvation effects of the experimentally used solvent (i.e., chloroform) were taken into consideration by using the SMD[6] solvation model. Frequency calculations were performed at the same level to evaluate enthalpy and entropy corrections and to identify the stationary points whether they are local minimum (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC)[7] calculations were also conducted to verify the critical steps involved in the proposed reaction pathway. The energetic results were further improved by the single-point calculations at the /M06-2X[2-4]/6-311++G(2d,p)[8] level with the solvation effects included. Unless otherwise statement, the M06-2X/6-311++G(2d,p)/SMD(chloroform)//M06-2X/6-31G(d,p)/SMD(chloroform) Gibbs free energies (in kcal/mol) are used in the following discussion, while the electronic energies are also given in the related figures for reference. Visualization of noncovalent interaction states was carried out using the NCI plot.[9,10] The data of NCI isosurfaces were produced toward the Multiwfn program[11] and were shown by the VMD program.[12] The strength of noncovalent interactions was indicated by the color of the isosurface. The blue, green, and red represented strong, weak, and repulsive interaction, respectively. Optimized structures were generated using the CYLview program[13].

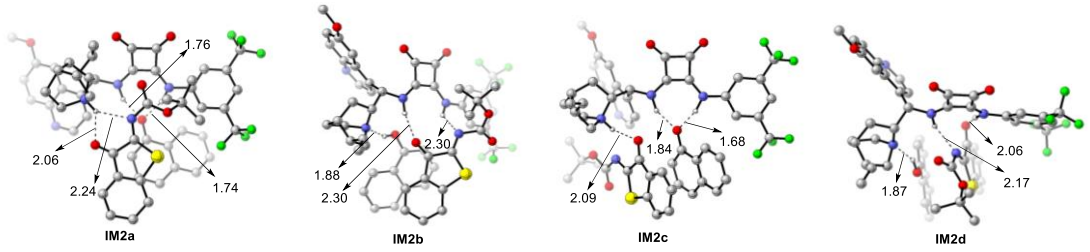


Figure S3. Optimized geometries along with the key bond distances in Å, part of the hydrogen atoms are omitted for clarity. (color code, C: grey, O: red, H: white, N: blue, F: green, S: yellow). (for 1-naphthol)

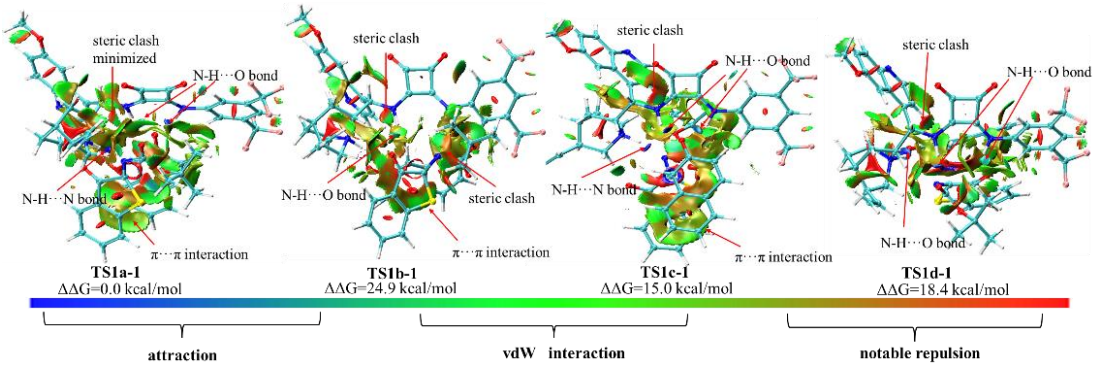


Figure S4. Noncovalent interaction analysis of the transition state **TS1a-1**—**TS1d-1** (for 2-naphthol).

Table S1 Coordinates and energies (in hatree) of the calculated structures at the M06-2X/6-311++G(2d,p)/SMD(chloroform)//M06-2X/6-31G(d,p)/SMD(chloroform) level of theory.

C

Free Energy = -2279.321635 Hartree

Energy = -2279.811680 Hartree

C	-2.274869	0.196585	-0.325757
C	-2.713759	-0.645967	0.866083
C	-5.747102	-2.480747	-0.394616
H	-4.443722	-1.087059	-1.288473
C	-5.320566	-3.121881	1.888359
H	-1.850045	-1.451443	4.049737
C	-6.087484	-3.233188	0.758312
H	-5.549265	-3.688911	2.784160
H	-6.942696	-3.897856	0.751851
N	-3.478022	-2.232220	3.093345
N	-0.837732	0.450878	-0.317647
N	2.366665	0.261061	-0.172789
C	3.755495	0.134532	-0.122625
C	4.499046	1.264576	0.233291
C	4.415795	-1.064575	-0.410602
C	5.882795	1.192515	0.301201
H	4.001383	2.204674	0.453010
C	5.802244	-1.102113	-0.335892
H	3.861210	-1.957315	-0.685925
C	6.556395	0.011204	0.018046
H	7.637480	-0.040673	0.071498
C	6.520086	-2.371391	-0.709964
C	6.658269	2.399226	0.751710
F	5.752753	-3.451044	-0.534574
F	6.899227	-2.354303	-1.996427
F	7.632854	-2.535668	0.021516
F	7.879116	2.433588	0.203569
F	6.031755	3.539861	0.426996
F	6.823064	2.408315	2.082346
C	-1.996092	-0.661771	2.035352
C	-4.658282	-1.635806	-0.379064
C	-4.193204	-2.267203	1.934294
C	-2.421742	-1.462379	3.123834
C	-3.859729	-1.501514	0.778803
H	-1.099301	-0.059148	2.139757
H	-2.494505	-0.390858	-1.222920
O	-6.446870	-2.533841	-1.555264
C	-7.551325	-3.409641	-1.630413
H	-7.947682	-3.306844	-2.640524
H	-7.252601	-4.451982	-1.468685
H	-8.333512	-3.138140	-0.911512
C	1.422731	-0.667663	-0.500877
C	0.040488	-0.527447	-0.541872
C	1.362261	-2.096417	-0.919742
C	-0.160164	-1.929356	-0.977713
O	2.140807	-2.993807	-1.128070
O	-1.119264	-2.598851	-1.263212
C	-2.493147	3.919709	-0.345312
C	-4.807639	3.097178	0.098799
C	-4.002503	4.168673	-0.674635
H	-2.107848	4.702375	0.315428
H	-1.890532	3.939693	-1.259580
H	-4.297148	5.149818	-0.283718
C	-2.917577	2.694580	1.660830
H	-2.867452	1.703876	2.113047
H	-2.310797	3.363282	2.278528
C	-4.385935	3.181517	1.570638
H	-5.035070	2.556970	2.191831
H	-4.484942	4.211458	1.930044
H	-5.877532	3.289914	-0.015806
C	-4.464146	1.680193	-0.400055
H	-4.851853	0.952058	0.319702
H	-4.938299	1.461784	-1.362002
C	-2.929753	1.592941	-0.518841
H	-2.641962	1.862366	-1.542453
N	-2.289324	2.625585	0.325861
C	-4.288202	4.162948	-2.150017
H	-3.969841	3.282908	-2.711184
C	-4.896347	5.149474	-2.800229
H	-5.226857	6.047918	-2.284807
H	-5.086495	5.098382	-3.867214
H	-0.590323	1.369353	0.042303
H	2.016565	1.180775	0.056082

2a

Free Energy = -460.942602 Hartree

Energy = -461.063792 Hartree

C	0.787635	-3.154722	1.844155
C	0.681744	-2.685118	0.558402
C	1.725517	-2.907365	-0.388471
C	2.878197	-3.626242	0.029312

C	2.964041	-4.101912	1.365757
C	1.941262	-3.868308	2.244762
H	0.747132	-1.885074	-2.017835
H	-0.015685	-2.978003	2.554655
C	1.635252	-2.431065	-1.720215
C	3.914029	-3.845048	-0.916104
H	3.848963	-4.649781	1.674260
H	2.004651	-4.230632	3.265691
C	3.807092	-3.375774	-2.199846
C	2.656121	-2.661416	-2.606801
H	4.797056	-4.394069	-0.601103
H	4.608335	-3.551644	-2.910608
H	2.583954	-2.295409	-3.625815
O	-0.396402	-1.992475	0.104317
H	-1.038060	-1.897369	0.817046

1j

Free Energy = -1181.565628 Hartree

Energy = -1181.762305 Hartree

C	-2.706303	-0.736434	-0.000181
C	-2.911804	0.641772	0.000096
C	-4.194327	1.180239	0.000290
C	-5.281881	0.314966	0.000202
C	-5.072371	-1.065962	-0.000076
C	-3.787100	-1.607729	-0.000271
H	-4.315538	2.259096	0.000504
H	-6.292505	0.707677	0.000349
H	-5.926505	-1.735644	-0.000143
H	-3.639369	-2.682603	-0.000487
C	-0.454817	0.440003	-0.000090
C	-1.655885	1.409521	0.000152
O	-1.525535	2.605509	0.000371
N	0.720598	0.920227	-0.000043
C	1.802569	0.008761	-0.000272
O	2.936482	0.691049	0.000122
C	4.219717	-0.007059	0.000178
C	5.220429	1.141044	0.000898
H	6.240688	0.749102	0.000994
H	5.085223	1.766180	-0.885351
H	5.084780	1.765459	0.887588
C	4.357866	-0.843687	-1.267500
H	4.176970	-0.222572	-2.149521
H	5.377236	-1.235136	-1.330506
H	3.661458	-1.682465	-1.272072
C	4.357187	-0.844694	1.267265
H	3.660787	-1.683485	1.270787
H	5.376528	-1.236176	1.330519
H	4.175796	-0.224283	2.149681
O	1.691867	-1.199624	-0.000449
S	-0.993245	-1.246666	-0.000409

IM1a

Free Energy = -2740.269280 Hartree

Energy = -2740.906021 Hartree

C	2.805559	-0.441661	-0.344481
C	3.603733	0.514627	-1.210097
C	6.864390	-1.276502	-1.801201
H	5.138622	-1.785376	-0.709084
C	6.901344	0.844733	-2.941474
H	3.418989	3.549602	-2.722111
C	7.530901	-0.328205	-2.618740
H	7.381679	1.591298	-3.564477
H	8.529826	-0.522790	-2.989422
N	5.050678	2.325863	-2.848390
N	1.410415	-0.479233	-0.789846
N	-1.790332	-0.679287	-0.412634
C	-3.165256	-0.941135	-0.416024
C	-4.047262	0.136425	-0.297404
C	-3.671453	-2.237323	-0.559556
C	-5.417631	-0.087539	-0.320740
H	-3.667966	1.145709	-0.169778
C	-5.046397	-2.429255	-0.569549
H	-3.008223	-3.090175	-0.639047
C	-5.938356	-1.367641	-0.456751
H	-7.008442	-1.535774	-0.472812
C	-5.591484	-3.828590	-0.658422
C	-6.340353	1.095704	-0.225144
F	-4.745302	-4.655757	-1.283640
F	-5.827540	-4.343472	0.556172
F	-6.755479	-3.856994	-1.326039
F	-7.574333	0.734254	0.151156
F	-5.895160	1.998697	0.661675
F	-6.459723	1.731993	-1.401518
C	3.082750	1.723552	-1.603955
C	5.592014	-1.024228	-1.333341
C	5.596158	1.135074	-2.476460
C	3.844589	2.594585	-2.421010
C	4.924554	0.180358	-1.655371

H	2.098472	2.052400	-1.279124
H	3.192746	-1.454546	-0.487004
O	7.412380	-2.459234	-1.431628
C	8.709052	-2.771810	-1.895706
H	8.943056	-3.755792	-1.489898
H	8.746066	-2.819109	-2.990311
H	9.452473	-2.051133	-1.535268
C	-0.790117	-1.563590	-0.175580
C	0.589090	-1.420630	-0.298950
C	-0.665288	-2.935286	0.397488
C	0.851783	-2.730574	0.330381
O	-1.412558	-3.809690	0.755741
O	1.846847	-3.302860	0.714472
C	1.786569	0.682142	3.091668
C	4.261397	0.382994	3.148020
C	2.959940	0.078903	3.927695
H	1.430491	1.606485	3.556889
H	0.939798	-0.010490	3.039627
H	3.015114	0.612296	4.883933
C	3.164064	2.145498	1.779874
H	3.594748	2.286811	0.788829
H	2.584720	3.045444	2.011872
C	4.266937	1.884325	2.831482
H	5.240788	2.191942	2.439774
H	4.087605	2.461327	3.745013
H	5.126182	0.105492	3.755835
C	4.272388	-0.373162	1.808172
H	5.046625	0.053406	1.159409
H	4.503960	-1.435315	1.936340
C	2.872991	-0.224521	1.187337
H	2.261558	-1.045575	1.570492
N	2.212970	1.006439	1.707983
C	2.780811	-1.383791	4.235384
H	2.611685	-2.060249	3.395811
C	2.820334	-1.888141	5.464201
H	2.980965	-1.254962	6.333574
H	2.693771	-2.949938	5.647278
H	0.982707	0.406293	-1.027658
H	-1.519028	0.293098	-0.520485
C	-0.884621	3.076472	1.881682
C	-0.792402	2.628596	0.586299
C	-1.820233	2.934527	-0.359450
C	-2.966072	3.652011	0.083264
C	-3.039021	4.092712	1.431867
C	-2.014488	3.818937	2.297827
H	-0.851176	1.985860	-2.049629
H	-0.096334	2.839746	2.588939
C	-1.747004	2.495563	-1.707942
C	-4.024962	3.865362	-0.838391
H	-3.917772	4.637968	1.760765
H	-2.068224	4.155468	3.328009
C	-3.947553	3.399396	-2.126528
C	-2.791473	2.717469	-2.570754
H	-4.914862	4.384604	-0.495442
H	-4.777905	3.550095	-2.807773
H	-2.732084	2.370075	-3.596777
O	0.217140	1.850557	0.130639
H	0.901057	1.562382	0.832167

IM2a

Free Energy = -3921.818019 Hartree

Energy = -3922.682828 Hartree

C	3.086770	-1.204908	-0.633161
C	3.843109	-0.089426	-1.322789
C	7.146616	-1.581008	-2.351120
H	5.409752	-2.417221	-1.499686
C	7.142255	0.778119	-2.841338
H	3.553280	3.219382	-2.013364
C	7.799332	-0.424301	-2.848539
H	7.609484	1.679345	-3.223122
H	8.807319	-0.484394	-3.240304
N	5.242326	2.128947	-2.389207
N	1.680593	-1.141775	-0.990702
N	-1.464732	-1.480866	-1.002517
C	-2.837023	-1.713424	-0.927832
C	-3.674526	-0.608023	-0.732140
C	-3.393080	-2.991273	-1.029676
C	-5.046708	-0.785893	-0.661282
H	-3.245813	0.382233	-0.624403
C	-4.771857	-3.142368	-0.918988
H	-2.761348	-3.863822	-1.149861
C	-5.617123	-2.053650	-0.742212
H	-6.690406	-2.188384	-0.670470
C	-5.353294	-4.528411	-0.924684
C	-5.945258	0.409830	-0.526253
F	-4.645738	-5.365057	-1.693948
F	-5.381669	-5.053512	0.308828
F	-6.617154	-4.532293	-1.378490

F	-6.921718	0.187567	0.370074	O	-1.134496	-4.594344	0.234907
F	-5.277425	1.500815	-0.127915	O	2.106683	-4.016505	0.417176
F	-6.549374	0.709228	-1.686218	S	-1.719138	2.759278	1.545945
C	3.270450	1.154545	-1.418272	C	0.963850	3.052855	1.234294
C	5.863816	-1.497778	-1.850949	O	2.140565	2.741145	1.151976
C	5.822449	0.896400	-2.343385	C	2.718683	-0.147518	3.019843
C	4.011902	2.234200	-1.957579	C	4.882755	-1.366363	2.799158
C	5.172025	-0.264589	-1.827473	C	3.613674	-1.234996	3.671673
H	2.257003	1.336061	-1.069966	H	2.781036	0.812693	3.537871
H	3.468036	-2.179800	-0.955016	H	1.677746	-0.461514	2.960141
O	7.715594	-2.810232	-2.332646	H	3.921674	-0.870357	4.657961
C	9.016100	-2.955606	-2.864762	C	4.502449	0.822258	1.660407
H	9.263814	-4.012111	-2.764879	H	4.888244	0.880648	0.645588
H	9.051749	-2.678775	-3.924767	H	4.285405	1.836317	1.997817
H	9.750153	-2.362807	-2.306508	C	5.449836	0.045837	2.593538
C	-4.545494	2.417400	-3.394833	H	6.442650	-0.000552	2.139024
C	-3.910890	3.499213	-2.828673	H	5.554304	0.555653	3.556296
C	-2.580917	3.400350	-2.355089	H	5.609228	-2.007183	3.303551
C	-1.931034	2.139922	-2.421058	C	4.524877	-1.936211	1.416707
C	-2.581732	1.061995	-3.054930	H	5.363582	-1.766002	0.732169
C	-3.867222	1.190977	-3.534523	H	4.323331	-3.010386	1.438099
H	-2.362610	5.500361	-1.827639	C	3.257209	-1.239219	0.911839
H	-5.567564	2.510515	-3.748032	H	2.378353	-1.769018	1.282653
H	-4.421082	4.455687	-2.751358	N	3.180834	0.103711	1.608378
C	-1.867090	4.534932	-1.862958	C	2.888914	-2.542017	3.867879
C	-0.586499	1.967714	-1.870714	H	2.460756	-3.022882	2.987013
H	-2.040524	0.125717	-3.158401	C	2.759176	-3.128445	5.052908
H	-4.361082	0.348938	-4.009182	H	3.167593	-2.684103	5.957652
C	-0.546042	4.405380	-1.527513	H	2.240303	-4.074763	5.161611
H	0.016484	5.285172	-1.223978	C	-0.147459	2.005619	1.277089
C	-0.980164	4.376498	1.584831	N	0.223471	0.779985	1.253373
C	0.407610	4.387972	1.436860	C	-0.593397	-0.287126	1.676624
C	1.124563	5.582443	1.454048	O	-0.085561	-1.356437	1.945035
C	0.430526	6.773522	1.616610	O	-1.878220	0.018301	1.843882
C	-0.961097	6.757094	1.761069	C	-2.684475	-0.721278	2.840422
C	-1.680778	5.564377	1.748417	C	-3.935906	0.136068	2.963013
H	2.202955	5.556688	1.331853	H	-3.705276	1.107079	3.409482
H	0.962596	7.718095	1.631608	H	-4.384856	0.301637	1.980487
H	-1.495361	7.693628	1.884241	H	-4.667558	-0.374424	3.595183
H	-2.760360	5.566369	1.853966	C	-1.921067	-0.749967	4.162028
C	-0.492099	-2.377244	-0.739024	H	-2.604456	-1.059122	4.957533
C	0.886722	-2.177357	-0.707212	H	-1.084176	-1.449553	4.136731
C	-0.375054	-3.725968	-0.128854	H	-1.551556	0.251810	4.406727
C	1.128926	-3.479711	-0.072143	C	-3.027864	-2.121832	2.349172

H	-3.765916	-2.085047	1.545978
H	-2.144454	-2.665650	2.009309
H	-3.470463	-2.680176	3.180023
C	0.096448	3.147295	-1.501709
H	-1.130436	-0.530140	-1.268122
H	1.245790	-0.284235	-1.355858
H	2.465546	0.711142	1.166922
O	-0.092455	0.788425	-1.745757
H	1.151352	3.083792	-1.261077

IM2b

Free Energy = -3921.818218 Hartree

Energy = -3922.678104 Hartree

C	3.086703	-0.715411	0.366228
C	3.648898	-1.275149	-0.936186
C	6.855880	-3.001582	0.027750
H	5.344861	-2.069644	1.158060
C	6.585991	-3.094216	-2.362809
H	2.960453	-1.431725	-4.254974
C	7.330444	-3.388456	-1.251176
H	6.910523	-3.389445	-3.354708
H	8.266539	-3.923339	-1.355711
N	4.667343	-2.185432	-3.422307
N	1.627081	-0.816474	0.414817
N	-1.397277	-1.738961	0.072056
C	-2.669588	-2.146713	-0.331258
C	-2.957924	-3.470564	-0.682200
C	-3.678418	-1.178890	-0.407912
C	-4.242022	-3.791852	-1.103707
H	-2.197573	-4.243779	-0.616141
C	-4.948670	-1.532598	-0.839041
H	-3.482872	-0.147643	-0.127177
C	-5.252050	-2.840045	-1.195266
H	-6.244767	-3.109994	-1.534713
C	-5.981308	-0.453562	-1.003422
C	-4.564711	-5.228250	-1.414674
F	-5.838121	0.524429	-0.104059
F	-5.883990	0.124442	-2.218607
F	-7.226454	-0.933147	-0.901787
F	-5.533089	-5.324464	-2.339116
F	-3.498223	-5.892173	-1.873393
F	-4.999837	-5.879837	-0.326145
C	2.955463	-1.116216	-2.111020
C	5.666293	-2.318089	0.153835
C	5.354211	-2.402871	-2.266193
C	3.509830	-1.582934	-3.327768
C	4.892432	-1.986132	-0.982190
H	1.996865	-0.606416	-2.124699
H	3.464929	-1.332490	1.188231
O	7.518295	-3.267950	1.182469
C	8.715228	-4.011061	1.108431
H	9.059004	-4.130496	2.135960
H	8.549909	-5.002373	0.670129
H	9.486444	-3.482988	0.534715
C	-0.095347	5.951462	-3.072774
C	-1.326963	5.357529	-2.961170
C	-1.455445	4.002148	-2.559446
C	-0.270335	3.267051	-2.266807
C	0.989285	3.899788	-2.405456
C	1.078181	5.213698	-2.793491
H	-3.616828	3.945283	-2.681048
H	-0.016326	6.987487	-3.386190
H	-2.230768	5.918267	-3.183530
C	-2.723517	3.371193	-2.454990
C	-0.396400	1.908616	-1.848210
H	1.890585	3.320002	-2.234817
H	2.050256	5.682539	-2.908691
C	-1.639545	1.316406	-1.792335
C	-2.807216	2.048639	-2.102322
H	-1.690782	0.261284	-1.546024
H	-3.772111	1.551984	-2.054875
O	0.678853	1.146482	-1.536447
C	-2.672876	3.960851	0.926756
C	-1.296851	3.732884	0.890953
C	-0.408358	4.757345	0.566608
C	-0.915684	6.015971	0.278477
C	-2.296303	6.233553	0.300175
C	-3.189444	5.212573	0.620980
H	0.657161	4.556441	0.538035
H	-0.244246	6.826898	0.020570
H	-2.684949	7.219340	0.064946
H	-4.258512	5.395997	0.640698
C	-0.249300	-2.471519	0.136186
C	1.050933	-2.017231	0.311121
C	0.164298	-3.900176	0.178091
C	1.594871	-3.391969	0.408525
O	-0.368107	-4.979439	0.084855
O	2.680442	-3.862527	0.636571

S	-3.667034	2.554085	1.404453
C	-0.949538	2.347389	1.213351
O	0.137703	1.812470	1.202432
C	3.045927	3.059338	0.457566
C	5.396262	2.329581	0.849388
C	4.324490	3.341879	1.307664
H	2.891699	3.858824	-0.275746
H	2.158601	3.009013	1.093470
H	4.694480	4.346715	1.071362
C	4.212620	1.921989	-1.300983
H	4.370832	0.953462	-1.771071
H	3.851087	2.597300	-2.082910
C	5.522752	2.454620	-0.672283
H	6.376355	1.873904	-1.034307
H	5.699229	3.499622	-0.949215
H	6.346547	2.548772	1.343252
C	4.948285	0.892496	1.155259
H	5.592357	0.201975	0.601086
H	5.053193	0.647216	2.217040
C	3.475166	0.737695	0.723277
H	2.828499	0.967734	1.578975
N	3.133027	1.780643	-0.288942
C	4.061654	3.290217	2.786816
H	3.580498	2.389722	3.171356
C	4.377203	4.261435	3.637066
H	4.851843	5.179044	3.298046
H	4.175556	4.177973	4.699857
H	1.468769	1.614286	-1.155430
C	-2.217806	1.593983	1.656960
N	-2.079043	0.444016	2.188189
C	-3.248122	-0.194113	2.691192
O	-4.363373	0.090665	2.322078
O	-3.045179	-1.149441	3.582282
C	-1.788971	-1.427915	4.286781
C	-2.231400	-2.478125	5.299384
H	-3.008873	-2.074726	5.952831
H	-2.632382	-3.355014	4.785242
H	-1.382286	-2.789493	5.912707
C	-1.290825	-0.175024	4.998701
H	-0.491396	-0.451535	5.691924
H	-0.889554	0.557134	4.295525
H	-2.098919	0.281263	5.577948
C	-0.749043	-2.008440	3.336654
H	-1.190735	-2.817450	2.746946
H	-0.345028	-1.245917	2.668652
H	0.076187	-2.426042	3.921499
H	1.090434	0.004029	0.144839
H	-1.317750	-0.777607	0.389644

IM2c

Free Energy = -3921.824832 Hartree

Energy = -3922.686251 Hartree

C	1.627664	1.956374	-0.917391
C	2.166064	1.823154	0.498247
C	4.336545	4.851932	1.030215
H	2.909611	4.358925	-0.448580
C	4.638609	3.313663	2.863170
H	2.275560	-0.422119	3.033828
C	4.967925	4.494656	2.248309
H	5.090433	3.024005	3.806149
H	5.695784	5.153176	2.706293
N	3.410598	1.277199	2.976726
N	0.231212	1.551650	-1.010860
N	-2.842292	1.561088	-0.109148
C	-4.200353	1.597523	0.187773
C	-4.761634	0.440276	0.744999
C	-5.018082	2.706382	-0.059999
C	-6.119229	0.388862	1.019195
H	-4.133696	-0.421481	0.949467
C	-6.373449	2.626312	0.239372
H	-4.602124	3.626491	-0.460442
C	-6.948192	1.477535	0.771108
H	-8.008909	1.432215	0.986957
C	-7.258738	3.794558	-0.094448
C	-6.687005	-0.852835	1.646692
F	-6.608009	4.959911	-0.008898
F	-7.741584	3.704699	-1.344961
F	-8.320569	3.860720	0.725136
F	-7.977704	-1.024554	1.319605
F	-6.022059	-1.951234	1.268473
F	-6.630751	-0.800999	2.987489
C	1.843253	0.714710	1.237824
C	3.412679	4.007691	0.446864
C	3.687593	2.430981	2.299848
C	2.501971	0.483614	2.471217
C	3.078522	2.776631	1.056466
H	1.103245	-0.000076	0.883740
H	1.644980	3.006614	-1.219224

O	4.584615	6.010282	0.373911	C	4.581936	0.321548	-0.862589
C	5.466445	6.941467	0.965183	H	4.390475	0.990066	-0.026625
H	5.486958	7.800949	0.295524	H	4.941742	-0.619563	-0.446992
H	5.111041	7.264309	1.950582	C	5.525578	0.938093	-1.910615
H	6.481462	6.536889	1.056767	H	5.989926	1.837260	-1.497413
C	-4.548974	-3.982449	-1.037627	H	6.329441	0.241544	-2.167380
C	-3.786460	-4.524576	-0.026861	H	5.310675	1.846790	-3.876095
C	-2.719787	-3.797817	0.553352	C	3.500329	2.123408	-2.703431
C	-2.459259	-2.483740	0.080752	H	3.849050	2.911556	-2.026920
C	-3.231682	-1.962880	-0.975850	H	2.998694	2.617252	-3.539575
C	-4.263976	-2.693940	-1.527081	C	2.487079	1.218414	-1.981954
H	-2.118759	-5.355532	1.944542	H	1.764801	0.807154	-2.691980
H	-5.367965	-4.552988	-1.464915	N	3.260468	0.002976	-1.508329
H	-3.995337	-5.525542	0.341952	C	3.381771	0.178075	-5.023486
C	-1.899304	-4.356975	1.578620	H	2.391710	0.606459	-4.864711
H	-2.985460	-0.972838	-1.350674	C	3.770062	-0.112770	-6.259752
H	-4.857677	-2.276805	-2.334327	H	4.745980	-0.547365	-6.461341
C	-0.860336	-3.625669	2.094107	H	3.129124	0.071739	-7.115085
H	-0.237422	-4.049041	2.876771	H	2.699490	-0.558489	-0.838555
C	0.380233	-4.906001	-0.750160	C	1.897697	-3.060625	0.054685
C	0.069315	-3.725205	-1.424644	N	2.795070	-2.218278	0.430980
C	-0.919745	-3.699265	-2.409906	C	3.701676	-2.620497	1.428240
C	-1.606715	-4.868460	-2.692049	O	3.640408	-3.662332	2.044997
C	-1.302563	-6.046677	-1.999503	O	4.617553	-1.666983	1.587181
C	-0.304366	-6.082185	-1.028868	C	5.654612	-1.781811	2.616249
H	-1.143450	-2.765058	-2.914167	C	6.478397	-0.519414	2.397480
H	-2.394249	-4.869662	-3.437225	H	6.937235	-0.520792	1.403481
H	-1.852776	-6.954727	-2.224329	H	5.844047	0.365336	2.502904
H	-0.072567	-7.002417	-0.502925	H	7.277867	-0.464833	3.140955
C	-2.045622	2.564344	-0.529927	C	6.496779	-3.030214	2.376560
C	-0.692002	2.521005	-0.870345	H	7.377742	-2.995429	3.023649
C	-2.109503	4.037382	-0.762644	H	5.939218	-3.941341	2.591836
C	-0.619350	3.973575	-1.083336	H	6.842419	-3.060146	1.338548
O	-2.951980	4.903010	-0.735536	C	5.006525	-1.763033	3.995539
O	0.265667	4.755096	-1.367198	H	4.463481	-0.824281	4.141835
S	1.714551	-4.760101	0.429210	H	4.333782	-2.611991	4.128411
C	0.880259	-2.596802	-0.985778	H	5.789018	-1.825495	4.757592
O	0.882299	-1.450736	-1.413939	H	-0.041596	0.601370	-0.729693
C	3.516806	-0.864379	-2.708730	H	-2.333330	0.668880	0.079911
C	4.706232	1.287639	-3.158495	C	-0.557491	-2.337349	1.609581
C	4.239146	-0.036863	-3.805279	C	-1.362034	-1.700373	0.643195
H	4.116824	-1.707101	-2.357257	O	-1.142160	-0.497975	0.250906
H	2.548712	-1.240424	-3.040936	H	0.243221	-1.758744	2.061507
H	5.133113	-0.587323	-4.117516				

IM2d

Free Energy = -3921.834335 Hartree

Energy = -3922.690678 Hartree

C	2.930996	0.718922	-0.801364
C	3.442192	1.462185	0.431490
C	6.684508	3.073070	-0.604076
H	5.184111	2.060416	-1.683767
C	6.348126	3.400061	1.758945
H	2.637306	1.980047	3.688683
C	7.127111	3.576474	0.645994
H	6.647058	3.790416	2.725653
H	8.065424	4.111811	0.725220
N	4.385381	2.619642	2.842677
N	1.471698	0.752161	-0.866604
N	-1.622797	1.818914	-1.020487
C	-2.855766	2.462158	-0.876550
C	-2.959841	3.777008	-0.403011
C	-4.023825	1.751584	-1.174882
C	-4.214149	4.350861	-0.252494
H	-2.075930	4.360894	-0.181533
C	-5.265140	2.347216	-0.991597
H	-3.958107	0.732050	-1.535981
C	-5.384438	3.652673	-0.535284
H	-6.355828	4.113758	-0.401804
C	-6.489119	1.559989	-1.363404
C	-4.325049	5.741343	0.308362
F	-6.704349	1.567683	-2.687210
F	-6.375854	0.270078	-1.000193
F	-7.593872	2.045123	-0.780810
F	-5.332337	6.420869	-0.262039
F	-4.577278	5.717245	1.628345
F	-3.204956	6.448506	0.133425
C	2.704123	1.445299	1.588754
C	5.492138	2.388509	-0.698184
C	5.111517	2.713561	1.693268
C	3.219963	2.029392	2.770786
C	4.686344	2.172633	0.442972
H	1.741517	0.946186	1.614196
H	3.316929	1.232701	-1.689120
O	7.380040	3.225061	-1.758498
C	8.573909	3.977213	-1.725631
H	8.942408	4.000245	-2.751137
H	8.395248	5.004474	-1.387118
H	9.331435	3.508532	-1.086037
C	-0.992234	-2.028513	6.622252
C	-1.970160	-1.643172	5.714124
C	-1.641541	-1.401426	4.377677
C	-0.303784	-1.553261	3.971807
C	0.675359	-1.936344	4.891287
C	0.334628	-2.175620	6.214340
H	-3.658805	-0.806211	3.780745
H	-1.262934	-2.213276	7.656877
H	-2.999945	-1.524657	6.037547
C	-2.650026	-0.969674	3.412887
C	0.083380	-1.310603	2.565056
H	1.697978	-2.040470	4.545503
H	1.094283	-2.473997	6.928532
C	-0.987234	-0.939361	1.542843
C	-2.358582	-0.746668	2.130014
H	-3.129255	-0.381037	1.457742
O	1.257251	-1.410892	2.224324
C	-2.613001	-4.020361	0.638647
C	-3.222621	-2.997925	-0.093134
C	-4.542314	-3.100068	-0.531883
C	-5.257099	-4.250956	-0.237815
C	-4.644696	-5.281003	0.487267
C	-3.332093	-5.179369	0.934474
H	-4.980409	-2.276052	-1.087921
H	-6.285679	-4.356784	-0.563798
H	-5.208678	-6.181039	0.712226
H	-2.876050	-5.984724	1.500272
C	-0.414415	2.432812	-1.140458
C	0.885526	1.930246	-1.092328
C	0.051864	3.813469	-1.433839
C	1.473703	3.256139	-1.401312
O	-0.456647	4.893458	-1.619600
O	2.596129	3.659480	-1.596962
S	-0.944150	-3.709457	1.091980
C	-2.334572	-1.869835	-0.370494
O	-2.611709	-0.898326	-1.049403
C	3.069934	-3.074704	-0.272301
C	5.377626	-2.268108	-0.745774
C	4.360563	-3.386021	-1.067128
H	2.964489	-3.694865	0.620762
H	2.181420	-3.180606	-0.888616
H	4.778819	-4.327838	-0.694813
C	4.142807	-1.560167	1.303987
H	4.240304	-0.516199	1.587456

H	3.731270	-2.103496	2.155465
C	5.467886	-2.146183	0.781249
H	6.291822	-1.486707	1.065580
H	5.663797	-3.126539	1.226331
H	6.349313	-2.526574	-1.172931
C	4.894093	-0.919520	-1.301865
H	5.497528	-0.120142	-0.861933
H	5.019600	-0.866742	-2.386821
C	3.405131	-0.740700	-0.966602
H	2.773627	-1.148557	-1.762465
N	3.110447	-1.648486	0.213914
C	4.098951	-3.538284	-2.544571
H	3.378671	-2.853656	-2.992983
C	4.686903	-4.463351	-3.295968
H	5.385031	-5.182832	-2.873726
H	4.489851	-4.538974	-4.360119
C	-0.961797	-1.962653	0.345856
N	0.135847	-1.676191	-0.505382
C	0.169422	-2.282006	-1.707686
O	1.077138	-2.117702	-2.531890
O	-0.867196	-3.127766	-1.947121
C	-0.926018	-3.947467	-3.143182
C	-2.226021	-4.723719	-2.959013
H	-2.203342	-5.298422	-2.027779
H	-3.078653	-4.039987	-2.919825
H	-2.372828	-5.414520	-3.793969
C	0.263670	-4.902735	-3.173654
H	0.129996	-5.632120	-3.978392
H	1.199508	-4.367310	-3.337767
H	0.324766	-5.447254	-2.225558
C	-1.003087	-3.068426	-4.387462
H	-1.815275	-2.343398	-4.277056
H	-0.069028	-2.530845	-4.547070
H	-1.215240	-3.690479	-5.262600
H	-1.662668	0.803665	-1.120813
H	0.917603	-0.128672	-0.721853
H	2.168998	-1.442842	0.603857
H	-0.673801	0.011951	1.083322

TS1b

Free Energy = -3921.777729 Hartree

Energy = -3922.638876 Hartree

C	-2.633826	-0.702481	-1.363868
C	-2.889606	-1.668715	-0.206728
C	-5.624708	-3.988289	-1.364684
H	-4.424350	-2.582755	-2.378249
C	-5.184004	-4.371140	0.972643
H	-1.912784	-2.202199	2.999749
C	-5.910837	-4.664218	-0.150377
H	-5.359504	-4.886269	1.910721
H	-6.683683	-5.421946	-0.108685
N	-3.461500	-3.198046	2.107945
N	-1.205764	-0.395557	-1.491738
N	2.004795	-1.244357	-1.000168
C	3.168908	-1.921900	-0.586315
C	4.414424	-1.299165	-0.698029
C	3.079062	-3.199253	-0.022772
C	5.549644	-1.962240	-0.244343
H	4.507386	-0.315496	-1.145791
C	4.232611	-3.845609	0.396342
H	2.119978	-3.688130	0.091280
C	5.479792	-3.237755	0.299228
H	6.373530	-3.746380	0.641796
C	4.149296	-5.242360	0.944372
C	6.875525	-1.255693	-0.310866
F	2.920874	-5.535373	1.390410
F	4.465852	-6.158001	0.018303
F	5.002813	-5.416573	1.966641
F	7.895615	-2.129264	-0.353869
F	6.968500	-0.473476	-1.392217
F	7.075392	-0.477098	0.761029
C	-2.156799	-1.547088	0.948184
C	-4.644107	-3.020638	-1.411977
C	-4.159487	-3.393359	0.954505
C	-2.481427	-2.331182	2.081411
C	-3.904018	-2.679855	-0.255823
H	-1.364099	-0.810926	1.027334
H	-2.931791	-1.198369	-2.293404
O	-6.272440	-4.239557	-2.528037
C	-7.228526	-5.278634	-2.551873
H	-7.585881	-5.333269	-3.579997
H	-6.784319	-6.241993	-2.276144
H	-8.077045	-5.064203	-1.891287
C	0.678276	3.512400	5.849888
C	1.579361	2.683482	5.205299
C	1.238820	2.053961	3.995699
C	-0.054049	2.277091	3.470027
C	-0.965419	3.104240	4.140929

C	-0.600500	3.730889	5.317522
H	3.126337	0.974277	3.763191
H	0.964592	3.997734	6.777885
H	2.567101	2.517545	5.625350
C	2.173422	1.194273	3.293094
C	-0.442262	1.632682	2.210746
H	-1.945548	3.250891	3.698678
H	-1.295950	4.389426	5.827088
C	0.645175	1.096213	1.398227
C	1.879441	0.717163	2.067380
H	0.306637	0.458506	0.585397
H	2.604205	0.126672	1.514377
O	-1.640847	1.610735	1.844142
C	0.895384	4.684708	1.398147
C	-0.284054	4.322549	0.739525
C	-1.457002	5.053584	0.927473
C	-1.448765	6.140199	1.789376
C	-0.271190	6.485013	2.462735
C	0.903583	5.767325	2.276596
H	-2.355204	4.780007	0.388187
H	-2.350162	6.722878	1.943347
H	-0.274461	7.329075	3.145333
H	1.809623	6.037612	2.808611
C	0.903275	-1.865003	-1.473640
C	-0.409942	-1.471562	-1.698400
C	0.655820	-3.235209	-2.017898
C	-0.786983	-2.791369	-2.255066
O	1.313531	-4.228654	-2.188784
O	-1.799746	-3.258564	-2.722346
S	2.295319	3.679606	1.041474
C	-0.122856	3.107815	-0.069669
O	-0.973226	2.571968	-0.766011
C	-3.907784	2.736587	-0.259971
C	-5.847184	1.378933	-1.032445
C	-5.240134	2.796495	-1.049081
H	-3.977029	3.217453	0.718480
H	-3.077979	3.176291	-0.810518
H	-5.929804	3.460851	-0.517134
C	-4.523474	0.743078	0.987647
H	-4.283734	-0.301780	1.153135
H	-4.343542	1.276920	1.922494
C	-5.946899	0.929797	0.430276
H	-6.490322	-0.016088	0.500218
H	-6.500542	1.670392	1.014791
H	-6.835034	1.398805	-1.498128
C	-4.932871	0.393023	-1.773857
H	-5.266442	-0.624675	-1.554450
H	-4.987895	0.525156	-2.857679
C	-3.473759	0.588352	-1.318793
H	-2.960261	1.295870	-1.978659
N	-3.522997	1.307833	0.011323
C	-5.055267	3.340283	-2.440319
H	-4.275529	2.883777	-3.051168
C	-5.785411	4.324253	-2.952605
H	-6.565613	4.812853	-2.374199
H	-5.631483	4.678607	-3.966073
H	-2.586374	1.326861	0.501421
C	1.263089	2.512740	0.107803
N	1.738090	1.869084	-0.976786
C	3.089286	1.735316	-1.061795
O	3.897322	1.835469	-0.147793
O	3.571274	1.357502	-2.274323
C	2.904449	1.601141	-3.542028
C	4.020937	1.333185	-4.547356
H	4.848887	2.028735	-4.388522
H	4.400946	0.315057	-4.426335
H	3.651733	1.450146	-5.569876
C	2.440544	3.051781	-3.642574
H	2.161141	3.272260	-4.677293
H	1.579446	3.240065	-3.000229
H	3.253476	3.726343	-3.356985
C	1.756197	0.620694	-3.763502
H	2.112364	-0.408397	-3.655000
H	0.942080	0.803809	-3.059436
H	1.367953	0.739278	-4.779994
H	-0.833884	0.508629	-1.201347
H	1.976698	-0.225967	-0.959782

TS1c

Free Energy = -3921.791538 Hartree

Energy = -3922.655635 Hartree

C	-3.058633	-0.170577	-0.727439
C	-3.904369	-0.961181	0.273224
C	-7.123029	-1.791907	-1.508432
H	-5.337223	-0.882367	-2.148403
C	-7.247615	-2.562387	0.767970
H	-3.729537	-2.249135	3.412898
C	-7.843567	-2.411551	-0.455332

H	-7.758003	-3.054152	1.588833	C	1.532493	1.182474	-1.992314
H	-8.849008	-2.781201	-0.615035	H	2.537508	-1.291486	-1.958721
N	-5.400812	-2.357557	2.240181	H	4.900114	-1.978075	-2.323729
N	-1.645340	-0.480472	-0.540731	C	1.200927	2.575062	-2.148411
N	1.111022	-2.061938	-0.091409	C	2.140505	3.478444	-2.744959
C	2.244576	-2.796770	0.258802	H	0.142741	2.816433	-2.159113
C	3.388764	-2.066307	0.612189	H	1.814194	4.488971	-2.974139
C	2.283395	-4.194023	0.274725	O	0.689825	0.351448	-1.571914
C	4.556553	-2.735642	0.944386	C	3.166661	4.583250	0.156781
H	3.352638	-0.981177	0.624998	C	2.015789	5.259111	-0.243020
C	3.468141	-4.831991	0.628161	C	2.045566	6.613766	-0.569732
H	1.409726	-4.781674	0.009132	C	3.251982	7.292713	-0.488920
C	4.617265	-4.125309	0.960045	C	4.408967	6.611254	-0.089911
H	5.529243	-4.640682	1.236714	C	4.383231	5.258881	0.232443
C	3.515332	-6.334428	0.586621	H	1.127162	7.102077	-0.881348
C	5.800599	-1.937433	1.212859	H	3.305340	8.347187	-0.735909
F	2.342196	-6.880391	0.928317	H	5.350044	7.149314	-0.031984
F	3.815631	-6.784314	-0.641554	H	5.288359	4.742511	0.534491
F	4.448276	-6.823330	1.418875	C	-0.108049	-2.500017	-0.469901
F	6.624399	-2.573995	2.059983	C	-1.283260	-1.785572	-0.685352
F	6.496429	-1.723561	0.083425	C	-0.776556	-3.800825	-0.797918
F	5.525952	-0.737650	1.738046	C	-2.039651	-2.987302	-1.085078
C	-3.372703	-1.313806	1.488244	O	-0.473082	-4.967100	-0.834018
C	-5.847158	-1.316097	-1.296278	O	-3.153981	-3.207989	-1.495034
C	-5.929766	-2.103354	1.011112	S	2.925687	2.876923	0.539773
C	-4.159041	-2.000799	2.443495	C	0.831648	4.396436	-0.312961
C	-5.223560	-1.433535	-0.032870	O	-0.288732	4.752260	-0.619770
H	-2.343866	-1.053186	1.715999	C	-2.811649	3.634839	0.052684
H	-3.385351	-0.484096	-1.729629	C	-5.090429	2.713609	0.332204
O	-7.620897	-1.628649	-2.758410	C	-4.282574	4.026273	0.297020
C	-8.899644	-2.155551	-3.043732	H	-2.109445	4.184230	0.677304
H	-9.083024	-1.943360	-4.096894	H	-2.501238	3.800541	-0.980204
H	-8.933630	-3.239750	-2.886241	H	-4.372315	4.506306	1.279025
H	-9.679721	-1.673655	-2.442527	C	-3.179084	1.890808	1.703820
C	5.558197	0.029768	-2.782808	H	-2.805687	0.928199	2.033488
C	5.184049	1.350053	-2.941095	H	-2.753311	2.653024	2.361119
C	3.855877	1.757778	-2.711109	C	-4.711917	1.967852	1.618807
C	2.914284	0.787300	-2.295632	H	-5.145387	0.963398	1.616515
C	3.297851	-0.558342	-2.202735	H	-5.100924	2.493033	2.495044
C	4.607280	-0.938327	-2.427388	H	-6.160893	2.930497	0.311890
H	4.160272	3.830370	-3.319239	C	-4.715966	1.840978	-0.875100
H	6.589802	-0.264266	-2.949578	H	-5.384833	0.982498	-0.908295
H	5.914638	2.093347	-3.248275	H	-4.863795	2.392775	-1.807388
C	3.434309	3.118324	-2.938337	C	-3.242789	1.370945	-0.769606

H	-2.678689	1.693306	-1.651476
N	-2.603090	2.170473	0.348584
C	-4.760383	5.003733	-0.739067
H	-4.679184	4.690326	-1.780269
C	-5.265575	6.199165	-0.457647
H	-5.351293	6.553419	0.566392
H	-5.609894	6.868448	-1.238659
H	-1.548735	2.050141	0.383504
C	1.194167	2.959901	0.053559
N	0.242886	2.197202	0.586802
C	0.644392	1.117548	1.335002
O	1.727662	0.552831	1.287718
O	-0.333243	0.769632	2.203622
C	0.018247	0.018838	3.410134
C	0.354226	-1.428711	3.073263
H	-0.429646	-1.878998	2.454575
H	1.304047	-1.497308	2.543044
H	0.428172	-2.007695	3.998906
C	-1.248004	0.101688	4.256389
H	-1.086493	-0.398977	5.214345
H	-1.510250	1.144855	4.454722
H	-2.094801	-0.385191	3.764717
C	1.164901	0.712356	4.143829
H	2.104301	0.628303	3.598152
H	0.931865	1.771486	4.291661
H	1.291045	0.251529	5.127542
H	-0.936499	0.183437	-0.885807
H	1.230418	-1.048034	-0.125881

TS1d

Free Energy = -3921.792747 Hartree

Energy = -3922.654842 Hartree

C	2.988776	0.852987	-0.059582
C	3.633399	1.479468	1.172484
C	6.721027	3.127739	-0.234851
H	5.156677	2.047337	-1.133018
C	6.633594	3.497254	2.142005
H	3.225438	1.984773	4.503083
C	7.282138	3.671897	0.948268
H	7.027468	3.908534	3.065084
H	8.210332	4.229113	0.915234
N	4.833454	2.679583	3.451373
N	1.535609	0.985395	-0.078864
N	-1.577455	1.375552	-1.202493
C	-2.742486	2.025115	-1.619426
C	-2.711538	3.325214	-2.139490
C	-3.977672	1.385165	-1.463577
C	-3.897122	3.941595	-2.516121
H	-1.774874	3.853584	-2.260737
C	-5.146589	2.032831	-1.837244
H	-4.019207	0.380231	-1.061841
C	-5.130282	3.314762	-2.372402
H	-6.047202	3.813054	-2.664088
C	-6.459538	1.346199	-1.590911
C	-3.846309	5.309193	-3.138373
F	-6.348563	0.008852	-1.667087
F	-6.943122	1.623492	-0.369657
F	-7.393750	1.723573	-2.474741
F	-4.935125	6.030745	-2.825748
F	-2.773925	6.003895	-2.735322
F	-3.796248	5.244453	-4.475917
C	3.051078	1.435344	2.414578
C	5.540217	2.416822	-0.187830
C	5.416517	2.778932	2.224521
C	3.693102	2.043828	3.522082
C	4.860823	2.214300	1.037536
H	2.105401	0.926377	2.569244
H	3.332562	1.446591	-0.907740
O	7.288415	3.261009	-1.458569
C	8.475495	4.017003	-1.568047
H	8.737318	4.011996	-2.625979
H	8.326590	5.053077	-1.242089
H	9.296135	3.568437	-0.995590
C	0.367349	-3.205784	6.412564
C	-0.902825	-3.063219	5.888397
C	-1.112117	-2.373148	4.679490
C	0.010553	-1.843793	4.002082
C	1.289505	-1.967002	4.566548
C	1.473389	-2.646488	5.755437
H	-3.287509	-2.521569	4.729032
H	0.508471	-3.739156	7.347337
H	-1.760070	-3.475847	6.412739
C	-2.440888	-2.153236	4.157609
C	-0.174225	-1.117712	2.739147
H	2.123585	-1.497880	4.055249
H	2.465004	-2.741077	6.185248
C	-1.511390	-1.031739	2.212600
C	-2.626709	-1.443065	3.018262

H	-1.660918	-0.287262	1.437770
H	-3.630679	-1.230567	2.662424
O	0.804108	-0.634403	2.117584
C	-2.939856	-4.274754	1.418491
C	-3.535112	-3.275106	0.643168
C	-4.910223	-3.259624	0.408910
C	-5.689399	-4.269730	0.951797
C	-5.091054	-5.270608	1.727525
C	-3.722280	-5.284153	1.974531
H	-5.337270	-2.457843	-0.187434
H	-6.760253	-4.285856	0.783435
H	-5.709471	-6.055333	2.151888
H	-3.276472	-6.062438	2.584451
C	-0.330588	1.708007	-1.654458
C	0.957298	1.490265	-1.171557
C	0.149778	2.311102	-2.917941
C	1.565851	2.042358	-2.413401
O	-0.355338	2.774151	-3.911220
O	2.696640	2.124938	-2.837646
S	-1.190678	-4.117264	1.591518
C	-2.589054	-2.260269	0.182477
O	-2.854728	-1.255325	-0.453818
C	2.862501	-2.962295	-0.578649
C	5.207690	-2.306733	-0.067835
C	4.341948	-3.242384	-0.936100
H	2.409309	-3.759964	0.013173
H	2.252127	-2.796114	-1.465271
H	4.579857	-4.274606	-0.656387
C	3.374555	-1.962103	1.595152
H	3.360914	-1.014453	2.129484
H	2.708233	-2.651111	2.118188
C	4.799560	-2.511574	1.397142
H	5.488630	-1.984433	2.062037
H	4.844945	-3.574102	1.654726
H	6.263334	-2.548124	-0.212387
C	4.947038	-0.838871	-0.436330
H	5.425873	-0.201978	0.312044
H	5.389166	-0.583703	-1.402901
C	3.428480	-0.577297	-0.483999
H	3.040021	-0.681142	-1.501705
N	2.757232	-1.712632	0.254081
C	4.609638	-3.085680	-2.409272
H	4.240308	-2.175398	-2.883310
C	5.263242	-3.980622	-3.141190
H	5.635305	-4.905822	-2.707833
H	5.449347	-3.824328	-4.198285
C	-1.178805	-2.574369	0.666920
N	-0.093427	-2.209599	0.009813
C	-0.130866	-1.954362	-1.333366
O	0.698123	-1.250071	-1.903051
O	-1.062672	-2.673923	-1.985246
C	-1.331745	-2.454825	-3.400707
C	-2.541513	-3.349868	-3.642425
H	-2.304281	-4.389154	-3.399110
H	-3.378793	-3.028506	-3.016202
H	-2.848516	-3.296452	-4.690191
C	-0.138748	-2.917311	-4.230769
H	-0.404741	-2.907562	-5.291951
H	0.720612	-2.263591	-4.079180
H	0.135356	-3.940923	-3.957126
C	-1.690202	-0.995658	-3.661962
H	-2.498471	-0.683560	-2.993139
H	-0.830073	-0.339218	-3.522504
H	-2.039819	-0.887700	-4.692832
H	-1.705760	0.464601	-0.765672
H	0.985224	0.527600	0.653363
H	1.734535	-1.535542	0.384281

TS1a

Free Energy = -3921.807873 Hartree

Energy = -3922.672530 Hartree

C	2.422656	-1.907754	-0.204366
C	3.286917	-1.403503	-1.338792
C	5.586551	-4.246924	-2.242533
H	4.009482	-4.079787	-0.855250
C	6.121660	-2.320357	-3.586922
H	3.833282	1.431730	-3.119403
C	6.371913	-3.623523	-3.245479
H	6.701161	-1.815733	-4.352343
H	7.163243	-4.168402	-3.745527
N	4.917287	-0.286628	-3.364655
N	1.028645	-1.544534	-0.429022
N	-2.237095	-1.389166	-0.222531
C	-3.609094	-1.663053	-0.225416
C	-4.526035	-0.609607	-0.154903
C	-4.088753	-2.976577	-0.304129
C	-5.890407	-0.868443	-0.176470
H	-4.174286	0.411179	-0.058802

C	-5.456807	-3.208552	-0.303485	C	1.156408	6.707945	0.414065
H	-3.402247	-3.811921	-0.355778	H	4.504860	5.101847	-0.790511
C	-6.377511	-2.166558	-0.247888	H	4.267067	7.599502	-0.666301
H	-7.443202	-2.364080	-0.256868	H	2.133071	8.585264	0.097839
C	-5.967611	-4.623150	-0.327361	H	0.224160	7.153846	0.744578
C	-6.848918	0.287236	-0.157239	C	-1.305382	-2.240748	0.269156
F	-5.079065	-5.467269	-0.865608	C	0.084719	-2.251806	0.195659
F	-6.246949	-5.068534	0.904364	C	-1.344180	-3.404632	1.186343
F	-7.101208	-4.718363	-1.041031	C	0.180114	-3.383498	1.141717
F	-8.002919	-0.030063	0.441437	O	-2.201060	-4.056828	1.733179
F	-6.336063	1.351950	0.476513	O	1.101794	-3.951818	1.694359
F	-7.157447	0.692703	-1.404268	S	0.062853	4.145172	0.785703
C	3.114550	-0.120767	-1.787602	C	2.480499	3.303994	-0.122851
C	4.580889	-3.548301	-1.607917	O	3.424141	2.569242	-0.350082
C	5.094704	-1.575660	-2.958832	C	3.054213	0.191929	2.928666
C	3.959249	0.399996	-2.796881	C	4.823099	-1.562141	2.801107
C	4.309739	-2.201691	-1.943916	C	3.826421	-0.869296	3.757705
H	2.368321	0.521901	-1.332119	H	3.426380	1.203805	3.107685
H	2.453863	-3.000537	-0.181180	H	1.980076	0.166774	3.113366
O	5.761449	-5.531687	-1.848411	H	4.407774	-0.342404	4.522753
C	6.764585	-6.296839	-2.482837	C	4.665355	0.257768	1.098141
H	6.721632	-7.285054	-2.025387	H	4.828231	-0.050497	0.068520
H	6.579440	-6.393183	-3.559026	H	4.751672	1.343191	1.130434
H	7.761838	-5.871412	-2.319900	C	5.610799	-0.462214	2.078206
C	-4.273721	3.893776	-2.230913	H	6.448261	-0.891724	1.522287
C	-3.094449	4.604224	-2.351188	H	6.028846	0.242023	2.804533
C	-1.847567	3.963025	-2.227005	H	5.491261	-2.209142	3.374051
C	-1.827272	2.582189	-1.930849	C	4.063823	-2.370280	1.737798
C	-3.029821	1.867465	-1.882769	H	4.750619	-2.623006	0.921101
C	-4.247661	2.507021	-2.020129	H	3.653480	-3.305799	2.127240
H	-0.658975	5.700613	-2.801665	C	2.892979	-1.525469	1.221632
H	-5.225568	4.405314	-2.332629	H	2.016447	-1.684595	1.851350
H	-3.117572	5.669450	-2.563338	N	3.242451	-0.072551	1.457423
C	-0.609293	4.663393	-2.483804	C	2.917351	-1.843590	4.460831
C	-0.548007	1.879178	-1.748765	H	2.218741	-2.415087	3.847958
H	-2.978665	0.790254	-1.778312	C	2.941482	-2.045810	5.773557
H	-5.174059	1.943350	-1.980192	H	3.621114	-1.498039	6.422191
C	0.574111	4.010388	-2.420602	H	2.282867	-2.765112	6.248416
H	1.493269	4.519976	-2.693803	C	1.086032	2.775459	0.195781
C	1.301485	5.323396	0.346876	N	1.070583	1.539321	0.694928
C	2.505072	4.769349	-0.091956	C	0.008986	1.020875	1.385385
C	3.585013	5.572304	-0.456670	O	0.106372	-0.013153	2.035347
C	3.445433	6.950049	-0.385751	O	-1.132390	1.742033	1.320064
C	2.234877	7.505693	0.047712	C	-2.061906	1.747948	2.452950

C	-3.148304	2.710482	1.988418
H	-2.723379	3.688959	1.749769
H	-3.646925	2.332787	1.090689
H	-3.899023	2.835137	2.773468
C	-1.330630	2.288640	3.677202
H	-2.022695	2.347657	4.522195
H	-0.511723	1.621245	3.959301
H	-0.930336	3.287370	3.484277
C	-2.650628	0.369936	2.737164
H	-3.007860	-0.094070	1.818290
H	-1.922487	-0.296946	3.195889
H	-3.505406	0.486725	3.410871
C	0.658894	2.670552	-1.898027
H	-1.891129	-0.499733	-0.592870
H	0.763583	-0.690817	-0.923978
H	2.543725	0.562502	0.960576
O	-0.503484	0.669464	-1.430506
H	1.556877	2.101295	-2.108272

IM3b

Free Energy = -3921.787407 Hartree

Energy = -3922.649447 Hartree

C	-2.818414	-0.879564	-1.185194
C	-3.105760	-1.728028	0.051373
C	-6.041628	-3.907628	-0.846556
H	-4.777160	-2.672060	-1.995758
C	-5.563661	-4.134699	1.504991
H	-2.080011	-2.066577	3.270659
C	-6.340397	-4.461588	0.425220
H	-5.751128	-4.558684	2.485421
H	-7.164688	-5.153838	0.545666
N	-3.727831	-3.005202	2.501754
N	-1.387351	-0.634205	-1.329444
N	1.873096	-1.234016	-1.132406
C	3.116497	-1.788674	-0.770018
C	4.280525	-1.069466	-1.037867
C	3.201725	-3.011472	-0.093735
C	5.511795	-1.571613	-0.633615
H	4.236951	-0.117923	-1.558433
C	4.446707	-3.501647	0.273891
H	2.312512	-3.579160	0.146982
C	5.616729	-2.791500	0.018281
H	6.580777	-3.178008	0.327059
C	4.548002	-4.843607	0.942246
C	6.731328	-0.730471	-0.892242
F	3.403259	-5.194740	1.543496
F	4.850074	-5.812825	0.066891
F	5.513300	-4.853360	1.876241
F	7.861822	-1.445617	-0.757672
F	6.723679	-0.226356	-2.135822
F	6.810093	0.300801	-0.048696
C	-2.330923	-1.572118	1.174123
C	-4.994160	-3.023325	-0.993968
C	-4.470787	-3.242267	1.384144
C	-2.683726	-2.226307	2.379539
C	-4.197709	-2.652348	0.113271
H	-1.464623	-0.919381	1.157693
H	-3.161413	-1.428935	-2.069212
O	-6.739456	-4.199371	-1.969873
C	-7.770053	-5.162350	-1.888779
H	-8.159906	-5.269267	-2.900764
H	-7.389497	-6.131885	-1.547660
H	-8.580594	-4.833285	-1.227863
C	0.323855	1.266093	6.425036
C	1.285600	0.798514	5.541720
C	1.075324	0.859377	4.158751
C	-0.137922	1.402820	3.691201
C	-1.106166	1.866601	4.589232
C	-0.877614	1.804487	5.953105
H	2.990007	-0.046617	3.623818
H	0.506380	1.212265	7.493715
H	2.215097	0.381170	5.916849
C	2.074745	0.370695	3.215816
C	-0.407072	1.446666	2.248131
H	-2.026366	2.279031	4.189490
H	-1.622807	2.169480	6.651335
C	0.677608	1.038919	1.271733
C	1.900896	0.441818	1.892214
H	0.222308	0.311154	0.581837
H	2.682548	0.113340	1.217379
O	-1.515286	1.792421	1.822629
C	0.579797	4.783589	0.679791
C	-0.279708	4.256057	-0.289988
C	-1.154294	5.075878	-1.011326
C	-1.196445	6.429579	-0.727116
C	-0.360090	6.953099	0.270421
C	0.530895	6.151662	0.968809
H	-1.769632	4.647021	-1.797713

H	-1.861551	7.086407	-1.276213
H	-0.398196	8.015497	0.491071
H	1.189036	6.578231	1.718183
C	0.777241	-1.980087	-1.392840
C	-0.580848	-1.701668	-1.491874
C	0.561502	-3.422788	-1.731296
C	-0.930818	-3.097113	-1.820675
O	1.260926	-4.392362	-1.874193
O	-1.964352	-3.670939	-2.078065
S	1.706272	3.648037	1.391669
C	-0.160892	2.807185	-0.417807
O	-0.912011	2.104874	-1.087774
C	-3.738208	2.733718	-0.316082
C	-5.830007	1.531691	-0.938200
C	-5.066965	2.864365	-1.102122
H	-3.740905	3.289053	0.624303
H	-2.875957	3.045174	-0.899622
H	-5.667062	3.651456	-0.633162
C	-4.516535	0.900910	1.088523
H	-4.401632	-0.158358	1.295303
H	-4.239053	1.453760	1.987684
C	-5.925115	1.237537	0.564809
H	-6.588925	0.388772	0.747023
H	-6.342426	2.100117	1.092318
H	-6.825754	1.622590	-1.377283
C	-5.062289	0.374356	-1.599646
H	-5.486999	-0.573019	-1.255230
H	-5.155575	0.393930	-2.688641
C	-3.573832	0.467561	-1.225107
H	-3.038372	1.079258	-1.958003
N	-3.499709	1.290730	0.045450
C	-4.840361	3.253505	-2.538524
H	-4.185680	2.613341	-3.131063
C	-5.385811	4.321731	-3.109788
H	-6.038699	4.991265	-2.555428
H	-5.203155	4.565004	-4.150931
H	-2.551618	1.258596	0.473716
C	1.070084	2.231760	0.316446
N	1.887231	1.865964	-0.778943
C	3.223896	1.955093	-0.621648
O	3.870917	2.011859	0.415789
O	3.953919	1.899814	-1.788122
C	3.453186	2.280602	-3.089079
C	4.717770	2.233349	-3.944498
H	5.469555	2.916579	-3.541464
H	5.140280	1.224546	-3.940091
H	4.496760	2.517575	-4.977361
C	2.895319	3.700737	-3.050120
H	2.673521	4.041728	-4.066312
H	1.979924	3.744845	-2.457950
H	3.633060	4.378825	-2.610994
C	2.426613	1.286828	-3.635691
H	2.808553	0.262476	-3.558816
H	1.480970	1.358060	-3.097293
H	2.249086	1.495083	-4.696045
H	-1.013037	0.312642	-1.244037
H	1.806951	-0.205092	-1.154386

IM3c

Free Energy = -3921.808978 Hartree

Energy = -3922.673219 Hartree

C	-2.919523	-0.750880	-0.691010
C	-3.490124	-1.722091	0.346117
C	-6.540140	-3.277881	-1.236721
H	-5.054150	-1.987474	-1.980213
C	-6.332817	-4.053695	1.031650
H	-2.812976	-2.936046	3.446030
C	-7.027952	-4.044911	-0.147822
H	-6.660807	-4.648720	1.876969
H	-7.930296	-4.635755	-0.246767
N	-4.488131	-3.428159	2.382951
N	-1.463309	-0.761892	-0.617515
N	1.550525	-1.828091	-0.148746
C	2.819113	-2.353030	0.099516
C	3.790013	-1.453720	0.569207
C	3.160417	-3.692824	-0.105823
C	5.079174	-1.899363	0.815494
H	3.522916	-0.411800	0.729168
C	4.462890	-4.105357	0.158157
H	2.426648	-4.407977	-0.466224
C	5.438310	-3.228991	0.615714
H	6.444733	-3.572317	0.822412
C	4.828077	-5.537164	-0.122144
C	6.127855	-0.904689	1.224805
F	3.827700	-6.374219	0.176827
F	5.122391	-5.723789	-1.418108
F	5.903765	-5.922234	0.582014
F	7.087770	-1.473947	1.969056

F	6.735711	-0.367429	0.152747	C	0.052112	-3.807873	-1.101098
F	5.612316	0.108121	1.931275	C	-1.350131	-3.239728	-1.321341
C	-2.809101	-1.942331	1.517888	O	0.584148	-4.878910	-1.258243
C	-5.396631	-2.521156	-1.101665	O	-2.413374	-3.645039	-1.727536
C	-5.142392	-3.303479	1.195026	S	2.115346	3.557823	0.477340
C	-3.351271	-2.793504	2.510098	C	-0.290727	4.451473	-0.459606
C	-4.680415	-2.489232	0.117258	O	-1.380025	4.491951	-0.994636
H	-1.857625	-1.444982	1.684802	C	-3.525564	3.001815	0.138780
H	-3.242982	-1.119273	-1.674893	C	-5.507409	1.575669	0.506234
O	-7.144059	-3.236253	-2.450124	C	-5.032594	3.041941	0.461751
C	-8.282167	-4.045034	-2.658699	H	-2.944278	3.706597	0.734083
H	-8.578541	-3.884257	-3.695162	H	-3.320895	3.231886	-0.907435
H	-8.054964	-5.107448	-2.512750	H	-5.182949	3.477621	1.457087
H	-9.111526	-3.755099	-2.002573	C	-3.395034	1.219799	1.779433
C	5.555997	1.317254	-2.897310	H	-2.793216	0.370968	2.082301
C	4.840320	2.497131	-3.066961	H	-3.133385	2.056957	2.432157
C	3.472396	2.543794	-2.786774	C	-4.906050	0.933550	1.763009
C	2.836758	1.368984	-2.343060	H	-5.090681	-0.144869	1.763092
C	3.547996	0.175771	-2.230261	H	-5.368968	1.346506	2.663352
C	4.912360	0.149700	-2.484746	H	-6.598831	1.533443	0.532774
H	3.172141	4.595982	-3.489859	C	-4.989081	0.824161	-0.729528
H	6.622301	1.302443	-3.099328	H	-5.439958	-0.166884	-0.750942
H	5.342673	3.394728	-3.415749	H	-5.300964	1.332199	-1.646413
C	2.684335	3.759198	-2.997728	C	-3.442000	0.712765	-0.687875
C	1.393016	1.389986	-2.025943	H	-3.008747	1.159409	-1.589915
H	3.007682	-0.717560	-1.937826	N	-2.958384	1.633931	0.409987
H	5.473323	-0.770297	-2.360036	C	-5.775400	3.890378	-0.530474
C	0.716629	2.732516	-1.884904	H	-5.678500	3.610949	-1.580066
C	1.403967	3.842464	-2.625743	C	-6.526273	4.935854	-0.203405
H	-0.314081	2.613012	-2.241450	H	-6.638758	5.253618	0.830024
H	0.832543	4.747299	-2.812799	H	-7.054703	5.513287	-0.954371
O	0.744280	0.363950	-1.880718	H	-1.868196	1.795491	0.389163
C	1.724243	5.270241	0.516340	C	0.499624	3.116632	-0.357812
C	0.451404	5.602975	0.052050	N	-0.288375	2.191014	0.409202
C	-0.007895	6.921240	0.047546	C	0.382709	1.233722	1.049795
C	0.825080	7.919041	0.525376	O	1.565849	0.889990	0.887940
C	2.104830	7.587771	0.993368	O	-0.408485	0.597552	1.976113
C	2.566572	6.277924	0.993330	C	0.201005	0.180466	3.233450
H	-1.002716	7.131642	-0.333413	C	0.944661	-1.139507	3.063611
H	0.496979	8.952372	0.535053	H	0.303845	-1.886956	2.583192
H	2.754386	8.375039	1.363809	H	1.843769	-1.005216	2.461723
H	3.560710	6.041147	1.357533	H	1.240189	-1.525927	4.044049
C	0.449236	-2.440869	-0.632190	C	-0.990332	0.003293	4.170565
C	-0.837603	-1.946778	-0.835793	H	-0.645672	-0.317586	5.157111

H	-1.531830	0.946445	4.286790
H	-1.684438	-0.755039	3.795889
C	1.115689	1.277278	3.775936
H	2.017338	1.382623	3.172000
H	0.587280	2.235949	3.788114
H	1.407035	1.032755	4.801534
H	-0.935288	0.075061	-0.862695
H	1.450088	-0.835383	0.085018

IM3a

Free Energy = -3921.6245441 Hartree

Energy = -3922.682856 Hartree

C	1.957167	-2.156254	-0.113918
C	2.788227	-1.943464	-1.361097
C	4.413143	-5.262323	-2.098310
H	3.067450	-4.639899	-0.602327
C	5.131455	-3.636373	-3.723832
H	3.638946	0.519458	-3.530896
C	5.177402	-4.918419	-3.241950
H	5.700856	-3.341220	-4.598511
H	5.792655	-5.658511	-3.738815
N	4.352500	-1.395030	-3.656908
N	0.620975	-1.595335	-0.300708
N	-2.623533	-1.089908	-0.094421
C	-4.009191	-1.275058	-0.131364
C	-4.860047	-0.178095	-0.275725
C	-4.572957	-2.558194	-0.060600
C	-6.234665	-0.360478	-0.376012
H	-4.466428	0.830397	-0.281242
C	-5.948611	-2.710257	-0.132514
H	-3.944826	-3.431735	0.054382
C	-6.802453	-1.622388	-0.304013
H	-7.874356	-1.760397	-0.380094
C	-6.550784	-4.082159	0.003469
C	-7.082945	0.856492	-0.608505
F	-5.677266	-5.047295	-0.306824
F	-6.974347	-4.311735	1.253207
F	-7.616808	-4.226011	-0.800256
F	-8.379496	0.624054	-0.382724
F	-6.705333	1.877986	0.178786
F	-6.969245	1.298248	-1.874067
C	2.802303	-0.710046	-1.955544
C	3.632672	-4.315510	-1.468847
C	4.337944	-2.641341	-3.104716
C	3.609032	-0.476995	-3.095287
C	3.574905	-2.986486	-1.948856
H	2.246440	0.114375	-1.521319
H	1.801812	-3.228693	0.026463
O	4.394564	-6.506105	-1.558622
C	5.162418	-7.515959	-2.177903
H	4.994316	-8.420799	-1.594105
H	4.840568	-7.692730	-3.210932
H	6.232379	-7.276724	-2.164680
C	-3.731380	4.809655	-2.165247
C	-2.436183	5.247060	-2.410177
C	-1.343673	4.392145	-2.223416
C	-1.588415	3.083911	-1.768074
C	-2.895574	2.641910	-1.573646
C	-3.972486	3.494687	-1.757180
H	0.150857	5.778147	-3.020383
H	-4.564257	5.489447	-2.313117
H	-2.261545	6.260108	-2.760331
C	0.018522	4.806553	-2.553463
C	-0.466748	2.146968	-1.550336
H	-3.036272	1.607640	-1.289250
H	-4.987018	3.143793	-1.596698
C	1.068377	4.016636	-2.314325
H	2.070381	4.341251	-2.583227
C	2.788558	5.014588	0.459048
C	3.708060	4.185285	-0.185396
C	5.005677	4.611589	-0.475103
C	5.382734	5.893520	-0.110977
C	4.460955	6.729604	0.535064
C	3.169173	6.308143	0.824250
H	5.683752	3.931138	-0.981435
H	6.382123	6.255021	-0.325343
H	4.762138	7.734211	0.815874
H	2.470322	6.969973	1.324833
C	-1.759390	-1.953467	0.499196
C	-0.380083	-2.114199	0.414105
C	-1.901306	-3.009221	1.529359
C	-0.387280	-3.177885	1.446633
O	-2.809324	-3.503112	2.153651
O	0.472984	-3.828800	2.001842
S	1.224003	4.281698	0.782907
C	3.160859	2.871529	-0.523059
O	3.772118	1.967539	-1.057454
C	3.176796	0.027170	2.777509

C	4.637198	-1.988927	2.650227
C	3.859457	-1.078713	3.627157
H	3.704395	0.982028	2.849177
H	2.132146	0.181539	3.052254
H	4.587925	-0.600229	4.291799
C	4.596656	-0.282724	0.828736
H	4.615554	-0.666212	-0.188928
H	4.863016	0.773830	0.778690
C	5.513746	-1.086655	1.772630
H	6.210340	-1.686893	1.181156
H	6.111504	-0.417097	2.399563
H	5.247950	-2.697185	3.215295
C	3.660198	-2.730927	1.726187
H	4.219839	-3.152703	0.882591
H	3.146284	-3.556275	2.226550
C	2.598519	-1.736790	1.231931
H	1.760935	-1.710678	1.931546
N	3.184568	-0.353125	1.323955
C	2.887151	-1.843970	4.485851
H	2.044509	-2.323083	3.985118
C	3.015211	-1.971579	5.801986
H	3.838391	-1.508631	6.341197
H	2.302761	-2.541180	6.389163
C	1.652650	2.721956	-0.173063
N	1.486904	1.514692	0.548855
C	0.382848	1.295320	1.284778
O	0.206523	0.281238	1.964913
O	-0.541699	2.298469	1.231366
C	-1.535580	2.449197	2.284030
C	-2.155569	3.811098	1.989242
H	-1.414558	4.607040	2.098711
H	-2.548669	3.841359	0.968673
H	-2.978152	4.003700	2.683839
C	-0.864621	2.456793	3.654356
H	-1.592436	2.763365	4.411622
H	-0.482448	1.469500	3.914133
H	-0.039517	3.176096	3.661655
C	-2.584561	1.352767	2.162240
H	-3.009383	1.381014	1.155036
H	-2.149423	0.369234	2.341318
H	-3.395400	1.526191	2.876295
C	0.941787	2.698038	-1.616711
H	-2.216061	-0.276476	-0.551526
H	0.488023	-0.699213	-0.765520
H	2.519413	0.420563	0.836948
O	-0.654442	0.950456	-1.346734
H	1.531679	1.938700	-2.144825

IM3d

Free Energy = -3921.823647 Hartree

Energy = -3922.683810 Hartree

C	2.930896	0.719312	-0.801980
C	3.442130	1.462039	0.431175
C	6.684476	3.073258	-0.603765
H	5.183894	2.061348	-1.683897
C	6.348352	3.398892	1.759482
H	2.637495	1.978230	3.688688
C	7.127242	3.575890	0.646556
H	6.647410	3.788661	2.726387
H	8.065606	4.111104	0.726005
N	4.385615	2.618041	2.842935
N	1.471620	0.752523	-0.867224
N	-1.622942	1.819101	-1.020211
C	-2.855947	2.462271	-0.876128
C	-2.960051	3.776877	-0.401897
C	-4.023983	1.751916	-1.175041
C	-4.214349	4.350710	-0.251280
H	-2.076139	4.360591	-0.179964
C	-5.265313	2.347481	-0.991566
H	-3.958235	0.732565	-1.536654
C	-5.384623	3.652695	-0.534585
H	-6.356022	4.113723	-0.400984
C	-6.489217	1.560339	-1.363793
C	-4.325265	5.740900	0.310292
F	-6.703435	1.567232	-2.687774
F	-6.376527	0.270629	-0.999698
F	-7.594291	2.046089	-0.782329
F	-5.332620	6.420680	-0.259681
F	-4.577374	5.716129	1.630283
F	-3.205206	6.448194	0.135622
C	2.704105	1.444653	1.588456
C	5.492041	2.388846	-0.698155
C	5.111674	2.712545	1.693523
C	3.220096	2.028018	2.770779
C	4.686344	2.172370	0.442956
H	1.741436	0.945655	1.613688
H	3.316823	1.233410	-1.689552
O	7.379911	3.225860	-1.758163

C	8.573712	3.978115	-1.725018
H	8.942045	4.001822	-2.750568
H	8.394993	5.005144	-1.385834
H	9.331390	3.509114	-1.085839
C	-0.989714	-2.031052	6.622214
C	-1.967908	-1.645086	5.714635
C	-1.639760	-1.402820	4.378169
C	-0.302189	-1.554739	3.971709
C	0.677220	-1.938451	4.890637
C	0.336949	-2.178272	6.213715
H	-3.657167	-0.807089	3.782249
H	-1.260065	-2.216218	7.656857
H	-2.997538	-1.526487	6.038522
C	-2.648544	-0.970509	3.413948
C	0.084501	-1.311414	2.564934
H	1.699691	-2.042624	4.544432
H	1.096822	-2.477157	6.927462
C	-0.986460	-0.939661	1.543277
C	-2.357558	-0.747039	2.131051
H	-0.673105	0.011798	1.084001
H	-3.128455	-0.381096	1.459209
O	1.258246	-1.411627	2.223742
C	-2.612713	-4.020305	0.638895
C	-3.222667	-2.997626	-0.092266
C	-4.542563	-3.099604	-0.530442
C	-5.257232	-4.250570	-0.236413
C	-4.644509	-5.280855	0.488067
C	-3.331698	-5.179391	0.934698
H	-4.980877	-2.275383	-1.086004
H	-6.285963	-4.356291	-0.561954
H	-5.208398	-6.180957	0.712996
H	-2.875416	-5.984943	1.500023
C	-0.414641	2.433139	-1.140150
C	0.885343	1.930677	-1.092356
C	0.051472	3.813958	-1.433026
C	1.473379	3.256718	-1.400928
O	-0.457208	4.893952	-1.618263
O	2.595766	3.660179	-1.596562
S	-0.943628	-3.709602	1.091471
C	-2.334725	-1.869486	-0.369750
O	-2.612213	-0.897776	-1.048229
C	3.069840	-3.074315	-0.273474
C	5.377401	-2.267885	-0.747974
C	4.360073	-3.385658	-1.068961
H	2.964736	-3.694603	0.619540
H	2.181007	-3.180004	-0.889376
H	4.778424	-4.327552	-0.696951
C	4.143675	-1.560119	1.302500
H	4.241426	-0.516216	1.586111
H	3.732495	-2.103557	2.154080
C	5.468448	-2.146165	0.779017
H	6.292571	-1.486775	1.063012
H	5.664519	-3.126588	1.223876
H	6.348842	-2.526384	-1.175668
C	4.893736	-0.919163	-1.303631
H	5.497465	-0.119917	-0.863859
H	5.018715	-0.866215	-2.388639
C	3.404954	-0.740280	-0.967636
H	2.773069	-1.148029	-1.763258
N	3.110758	-1.648169	0.212926
C	4.097776	-3.537730	-2.546295
H	3.377632	-2.852756	-2.994390
C	4.685009	-4.463027	-3.297969
H	5.382983	-5.182841	-2.876044
H	4.487491	-4.538513	-4.362045
C	-0.961593	-1.962481	0.345903
N	0.135658	-1.675738	-0.505705
C	0.168729	-2.281271	-1.708165
O	1.076179	-2.116886	-2.532640
O	-0.868080	-3.126845	-1.947412
C	-0.927590	-3.946110	-3.143726
C	-2.227627	-4.722226	-2.959258
H	-2.204678	-5.297201	-2.028196
H	-3.080145	-4.038383	-2.919543
H	-2.374857	-5.412759	-3.794358
C	0.261945	-4.901549	-3.175057
H	0.127818	-5.630657	-3.979969
H	1.197774	-4.366181	-3.339381
H	0.323395	-5.446370	-2.227156
C	-1.005090	-3.066669	-4.387700
H	-1.817177	-2.341607	-4.276765
H	-0.071047	-2.529129	-4.547530
H	-1.217646	-3.688450	-5.262933
H	-1.662705	0.803829	-1.120462
H	0.917564	-0.128220	-0.722158
H	2.169538	-1.442480	0.603406

TS2a

Free Energy = -3921.820578 Hartree

Energy = -3922.682037 Hartree

C	2.350920	-1.808187	-0.165640
C	3.139608	-1.408750	-1.394733
C	5.393024	-4.328355	-2.166025
H	3.931582	-4.013483	-0.682562
C	5.802253	-2.557826	-3.746985
H	3.514553	1.216289	-3.508798
C	6.091434	-3.816526	-3.288783
H	6.314863	-2.137877	-4.605627
H	6.846470	-4.411065	-3.788428
N	4.596443	-0.515248	-3.653631
N	0.936237	-1.501532	-0.363610
N	-2.334596	-1.517128	-0.176917
C	-3.681975	-1.879318	-0.223583
C	-4.661499	-0.895416	-0.391602
C	-4.081347	-3.220795	-0.134180
C	-6.001909	-1.249241	-0.487251
H	-4.389100	0.153187	-0.425164
C	-5.428173	-3.542456	-0.207086
H	-3.351422	-4.007641	0.003382
C	-6.408923	-2.571944	-0.394133
H	-7.455882	-2.842357	-0.464215
C	-5.855915	-4.976076	-0.048007
C	-7.009534	-0.167290	-0.748896
F	-4.874075	-5.830599	-0.358266
F	-6.234482	-5.239934	1.209400
F	-6.905086	-5.259673	-0.836842
F	-8.231301	-0.501146	-0.320688
F	-6.666844	0.987245	-0.158064
F	-7.114225	0.097357	-2.066581
C	2.916292	-0.185589	-1.969398
C	4.434211	-3.566151	-1.532649
C	4.820472	-1.751065	-3.123770
C	3.677137	0.225387	-3.090189
C	4.124300	-2.263538	-1.987959
H	2.198084	0.503193	-1.536510
H	2.400347	-2.894029	-0.050939
O	5.609967	-5.563885	-1.650882
C	6.569470	-6.390057	-2.274872
H	6.573457	-7.323103	-1.711611
H	6.303526	-6.603391	-3.316892
H	7.571613	-5.946703	-2.237407
C	-4.513196	3.735488	-2.661525
C	-3.362362	4.511980	-2.656304
C	-2.120128	3.948205	-2.343290
C	-2.067417	2.581359	-2.012828
C	-3.218983	1.796982	-2.089709
C	-4.446110	2.364743	-2.396706
H	-0.961508	5.750042	-2.786201
H	-5.468192	4.191873	-2.900952
H	-3.416184	5.567198	-2.907256
C	-0.887721	4.728230	-2.425938
C	-0.785012	1.950060	-1.639315
H	-3.121372	0.728747	-1.936554
H	-5.339400	1.750773	-2.443365
C	0.295812	4.206474	-2.096490
H	1.200338	4.804607	-2.181753
C	1.827359	5.207298	0.925861
C	2.900618	4.607403	0.265414
C	4.149272	5.227730	0.178819
C	4.320141	6.467017	0.772018
C	3.243213	7.071433	1.436705
C	1.999035	6.459679	1.520572
H	4.951187	4.726124	-0.354719
H	5.277101	6.973928	0.721663
H	3.383016	8.044601	1.897233
H	1.178109	6.943839	2.038736
C	-1.355909	-2.265800	0.398594
C	0.031857	-2.202485	0.320206
C	-1.331249	-3.355481	1.401899
C	0.191280	-3.276218	1.329099
O	-2.148590	-4.004063	2.010445
O	1.142568	-3.786511	1.881970
S	0.348928	4.259595	0.962014
C	2.561628	3.317290	-0.331779
O	3.308746	2.623935	-0.992234
C	3.076757	0.485622	2.803547
C	4.924117	-1.179033	2.629714
C	3.976711	-0.476134	3.626978
H	3.390845	1.527889	2.911317
H	2.024537	0.407839	3.081445
H	4.591959	0.123925	4.307424
C	4.529546	0.543956	0.866106
H	4.631690	0.221935	-0.167855
H	4.578393	1.634053	0.867944
C	5.596351	-0.091880	1.782687
H	6.395542	-0.521644	1.172483

H	6.052194	0.662851	2.431882
H	5.667420	-1.763092	3.178030
C	4.121210	-2.077796	1.678470
H	4.759119	-2.354656	0.830614
H	3.784591	-3.003833	2.153332
C	2.882352	-1.304277	1.199738
H	2.052975	-1.479542	1.887890
N	3.161458	0.166277	1.339972
C	3.185285	-1.449311	4.460146
H	2.449855	-2.068360	3.944034
C	3.347778	-1.595392	5.770604
H	4.066956	-0.996781	6.324853
H	2.768708	-2.316287	6.337933
C	1.087814	2.878583	-0.074604
N	1.138804	1.625694	0.595354
C	0.081894	1.162415	1.294340
O	0.125421	0.146005	1.987552
O	-1.054185	1.908565	1.176012
C	-2.036013	1.923004	2.258288
C	-2.995342	3.028552	1.832413
H	-2.480504	3.990984	1.771181
H	-3.424611	2.803849	0.850440
H	-3.811885	3.114606	2.554644
C	-1.353310	2.269930	3.577975
H	-2.113339	2.409404	4.352354
H	-0.684865	1.466483	3.892459
H	-0.782170	3.197122	3.483528
C	-2.774262	0.594156	2.353257
H	-3.267005	0.370581	1.405890
H	-2.096594	-0.221453	2.604401
H	-3.550350	0.667530	3.121495
C	0.447833	2.825723	-1.536917
H	-2.047896	-0.628476	-0.583273
H	0.647312	-0.657104	-0.852544
H	2.300177	0.831393	0.864658
O	-0.698042	0.738165	-1.460052
H	1.221540	2.285976	-2.100663

IM4a

Free Energy = -3921.827343 Hartree

Energy = -3922.691078 Hartree

C	2.411775	-1.918114	-0.139009
C	3.148081	-1.518294	-1.397648
C	5.295596	-4.471116	-2.317772
H	3.913190	-4.144084	-0.761144
C	5.673745	-2.684745	-3.889221
H	3.510011	1.144835	-3.470660
C	5.952906	-3.957188	-3.464370
H	6.157977	-2.262116	-4.762907
H	6.670573	-4.560332	-4.007016
N	4.529295	-0.613711	-3.703140
N	0.995030	-1.560928	-0.272427
N	-2.252154	-1.430724	0.000079
C	-3.621623	-1.678366	-0.015024
C	-4.492296	-0.607173	-0.252270
C	-4.157914	-2.957711	0.179699
C	-5.861544	-0.817923	-0.321989
H	-4.096579	0.396877	-0.360635
C	-5.534458	-3.134194	0.127485
H	-3.515091	-3.802839	0.391456
C	-6.406432	-2.081862	-0.132735
H	-7.476910	-2.243412	-0.182340
C	-6.107998	-4.498371	0.401279
C	-6.762886	0.334825	-0.657774
F	-5.248428	-5.474400	0.086884
F	-6.426167	-4.647699	1.693834
F	-7.232098	-4.704827	-0.303373
F	-7.940496	0.249195	-0.029513
F	-6.210787	1.514949	-0.338500
F	-7.031118	0.379198	-1.978147
C	2.942510	-0.273531	-1.933767
C	4.383829	-3.698894	-1.630189
C	4.741629	-1.865679	-3.208227
C	3.660926	0.140326	-3.079234
C	4.083029	-2.382906	-2.051930
H	2.276200	0.429186	-1.445951
H	2.434357	-3.006052	-0.035970
O	5.509393	-5.719581	-1.831632
C	6.428469	-6.551148	-2.506041
H	6.441352	-7.492161	-1.956191
H	6.116424	-6.746069	-3.538979
H	7.438377	-6.123908	-2.504891
C	-4.325625	3.485831	-3.337330
C	-3.183370	4.273225	-3.270044
C	-1.987566	3.752778	-2.765494
C	-1.971188	2.418137	-2.316821
C	-3.105194	1.615298	-2.455625
C	-4.289454	2.145769	-2.944287

H	-0.793951	5.530067	-3.212545
H	-5.247668	3.909568	-3.721812
H	-3.209097	5.301718	-3.617363
C	-0.756808	4.540906	-2.765859
C	-0.740077	1.839253	-1.747388
H	-3.030347	0.565702	-2.194390
H	-5.175468	1.525494	-3.022838
C	0.385782	4.065330	-2.267136
H	1.290961	4.666791	-2.302051
C	1.549476	5.280282	0.789198
C	2.700053	4.690351	0.266292
C	3.919090	5.370201	0.228085
C	3.975645	6.660593	0.727988
C	2.819271	7.253919	1.252728
C	1.603490	6.581120	1.289531
H	4.788035	4.874432	-0.193619
H	4.907009	7.214948	0.712230
H	2.871350	8.266554	1.640222
H	0.719369	7.057038	1.699897
C	-1.301827	-2.236337	0.550645
C	0.085608	-2.230204	0.431162
C	-1.295560	-3.324366	1.552622
C	0.228177	-3.310608	1.438959
O	-2.121004	-3.943071	2.182825
O	1.168233	-3.863958	1.963702
S	0.117167	4.252772	0.791279
C	2.471651	3.343132	-0.250711
O	3.283244	2.620356	-0.784856
C	3.281879	0.412423	2.698522
C	5.056137	-1.341080	2.599297
C	4.150518	-0.550437	3.571749
H	3.645025	1.442839	2.784361
H	2.237703	0.393179	3.020366
H	4.800928	0.049024	4.220575
C	4.706635	0.326816	0.784752
H	4.804765	-0.044469	-0.234137
H	4.820446	1.412527	0.732369
C	5.769147	-0.316482	1.709814
H	6.546515	-0.802957	1.112216
H	6.263009	0.439105	2.331220
H	5.773586	-1.939857	3.167250
C	4.205349	-2.234183	1.681311
H	4.825168	-2.562664	0.836819
H	3.835678	-3.132415	2.185283
C	3.005814	-1.398387	1.195819
H	2.182802	-1.533027	1.903844
N	3.330205	0.046839	1.262488
C	3.325037	-1.445695	4.454848
H	2.578921	-2.075757	3.967610
C	3.458777	-1.512710	5.775536
H	4.187672	-0.902385	6.303897
H	2.846974	-2.176783	6.377312
C	0.985087	2.882478	-0.105340
N	1.015285	1.656815	0.640052
C	-0.001191	1.126289	1.384434
O	0.151720	0.151680	2.096508
O	-1.165095	1.795007	1.243877
C	-2.081065	1.865797	2.396581
C	-3.126844	2.872537	1.936513
H	-2.672336	3.845398	1.732459
H	-3.626694	2.525561	1.026731
H	-3.885096	2.998894	2.713816
C	-1.321282	2.379055	3.615764
H	-2.026048	2.534845	4.437236
H	-0.572243	1.654963	3.943551
H	-0.830771	3.330508	3.396954
C	-2.728596	0.517530	2.684653
H	-3.303960	0.171260	1.825756
H	-1.987598	-0.236182	2.948954
H	-3.424939	0.637985	3.520347
C	0.483616	2.725366	-1.601936
H	-1.923299	-0.573518	-0.439260
H	0.703523	-0.784031	-0.857077
O	-0.672001	0.655283	-1.430212
H	1.299099	2.151443	-2.065000
H	1.911090	1.117235	0.701329

IM5a

Free Energy = -3921.837196 Hartree

Energy = -3922.697525 Hartree

C	-2.589101	1.742165	-0.584107
C	-3.576586	0.675293	-0.999290
C	-6.637042	2.580422	-2.087206
H	-4.732491	3.193534	-1.425831
C	-7.081426	0.216643	-2.219669
H	-3.943864	-2.694941	-1.117477
C	-7.514576	1.506274	-2.382429
H	-7.726450	-0.627430	-2.438616

H	-8.520445	1.695385	-2.737033	H	3.037786	0.525042	2.954482
N	-5.430702	-1.384751	-1.630997	H	3.707362	0.966992	5.322132
N	-1.226995	1.363369	-0.969153	C	-0.322928	-1.647294	1.777714
N	2.018267	1.297438	-1.071278	C	-1.014193	-2.224876	2.982663
C	3.405542	1.409143	-1.184510	H	-1.906979	-2.824844	2.828021
C	4.197517	0.390986	-0.636406	O	1.672112	-0.500190	1.181993
C	4.015747	2.469241	-1.861292	C	2.356023	-3.569430	0.090852
C	5.574919	0.431512	-0.792507	C	1.932570	-2.627903	-0.847460
H	3.732391	-0.418380	-0.083278	C	2.749222	-2.235260	-1.905793
C	5.401018	2.493289	-1.977324	C	4.023421	-2.774817	-2.000643
H	3.424665	3.279141	-2.272552	C	4.458221	-3.698006	-1.042794
C	6.199134	1.480443	-1.460307	C	3.635601	-4.111006	0.001257
H	7.276642	1.507650	-1.573889	H	2.377801	-1.502652	-2.617306
C	6.050699	3.673370	-2.646221	H	4.692294	-2.468181	-2.796455
C	6.416679	-0.701485	-0.278846	H	5.466383	-4.094141	-1.108742
F	5.288209	4.170088	-3.628595	H	3.987990	-4.831040	0.731745
F	6.276859	4.669739	-1.779245	C	1.119556	2.315460	-1.098019
F	7.237094	3.344289	-3.181694	C	-0.273078	2.294878	-1.002543
F	6.760897	-1.547821	-1.268571	C	1.171994	3.799396	-1.102562
F	7.563168	-0.260783	0.258971	C	-0.342094	3.770311	-0.901940
F	5.782881	-1.425666	0.651926	O	2.019505	4.653093	-1.210338
C	-3.254259	-0.655760	-0.905982	O	-1.222674	4.564767	-0.654265
C	-5.357871	2.333474	-1.636202	S	1.170351	-3.957585	1.340402
C	-5.773843	-0.072189	-1.760811	C	0.602614	-2.091114	-0.582246
C	-4.214301	-1.645810	-1.222953	O	0.026958	-1.237345	-1.225635
C	-4.892212	1.009679	-1.459133	C	-1.666596	1.510358	3.002995
H	-2.274403	-0.985285	-0.577699	C	-3.864429	2.704171	2.953818
H	-2.812233	2.675972	-1.107699	C	-2.451966	2.735366	3.590193
O	-6.981834	3.885059	-2.223241	H	-1.582384	0.713396	3.750622
C	-8.277882	4.189211	-2.691780	H	-0.649081	1.805468	2.720530
H	-8.335898	5.276959	-2.728577	H	-2.572856	2.588719	4.670420
H	-8.449273	3.788676	-3.697974	C	-3.606077	0.332068	2.278482
H	-9.052785	3.813757	-2.012877	H	-4.185340	0.037591	1.403151
C	2.077174	-0.179530	6.141340	H	-3.343537	-0.585673	2.816878
C	0.956723	-0.955363	5.869182	C	-4.424931	1.294041	3.174939
C	0.571337	-1.200249	4.549037	H	-5.485537	1.253577	2.908120
C	1.338285	-0.650240	3.506654	H	-4.344459	1.019292	4.232663
C	2.467239	0.122684	3.785163	H	-4.496605	3.460578	3.426546
C	2.834942	0.361841	5.101614	C	-3.787801	2.928938	1.429979
H	-1.155346	-2.436895	5.069901	H	-4.732971	2.607077	0.976197
H	2.364084	0.005353	7.171443	H	-3.638619	3.980559	1.165028
H	0.373278	-1.376959	6.682254	C	-2.598040	2.097993	0.922339
C	-0.604458	-2.010241	4.236434	H	-1.714439	2.735172	1.016214
C	0.971237	-0.903332	2.098520	N	-2.344924	0.952634	1.819043

C	-1.746372	4.048799	3.389895
H	-1.535521	4.355816	2.363896
C	-1.374572	4.849380	4.383718
H	-1.563037	4.589623	5.422800
H	-0.869708	5.791591	4.197487
C	-0.062644	-2.718304	0.686524
N	-1.316722	-3.290438	0.292475
C	-1.389884	-4.138244	-0.786942
O	-0.445689	-4.357392	-1.514004
O	-2.627642	-4.631938	-0.888795
C	-2.999674	-5.466347	-2.035961
C	-4.482542	-5.717692	-1.796813
H	-4.638945	-6.201445	-0.829067
H	-5.045032	-4.779136	-1.815107
H	-4.878055	-6.370596	-2.579075
C	-2.206292	-6.766484	-1.992365
H	-2.570205	-7.439299	-2.774063
H	-1.143143	-6.584693	-2.153272
H	-2.342955	-7.260364	-1.026059
C	-2.786737	-4.696479	-3.334521
H	-3.315143	-3.738786	-3.301163
H	-1.728640	-4.515931	-3.524167
H	-3.197491	-5.278772	-4.164335
H	-0.987491	-0.871496	1.341741
H	-0.970763	0.386290	-1.057129
H	1.677657	0.416863	-0.695196
H	-2.120189	-3.242826	0.900044

TS3a

Free Energy = -3921.809447 Hartree

Energy = -3922.669039 Hartree

C	-2.453741	1.615395	-0.440353
C	-3.461720	0.686263	-1.082917
C	-6.269344	2.928000	-2.219978
H	-4.426712	3.322856	-1.282301
C	-6.822436	0.637262	-2.717430
H	-4.005792	-2.606632	-1.671101
C	-7.163602	1.963536	-2.750733
H	-7.482576	-0.126049	-3.114809
H	-8.110211	2.265489	-3.181858
N	-5.343602	-1.136218	-2.171567
N	-1.085871	1.291435	-0.822694
N	2.118729	1.330979	-1.174514
C	3.504833	1.468009	-1.282228
C	4.298568	0.398405	-0.850960
C	4.104848	2.599960	-1.840858
C	5.674418	0.452340	-1.022527
H	3.834388	-0.459021	-0.372575
C	5.488083	2.634608	-1.971586
H	3.506139	3.449948	-2.148636
C	6.289509	1.566742	-1.582893
H	7.365119	1.604369	-1.709904
C	6.141349	3.877522	-2.509865
C	6.510370	-0.739148	-0.649527
F	5.339091	4.539002	-3.353002
F	6.470350	4.727712	-1.526934
F	7.274401	3.589834	-3.170384
F	6.695646	-1.560842	-1.700603
F	7.730894	-0.375862	-0.229708
F	5.946376	-1.469614	0.319493
C	-3.226507	-0.663229	-1.133783
C	-5.065424	2.538310	-1.672103
C	-5.593664	0.203027	-2.164490
C	-4.200258	-1.536384	-1.676284
C	-4.693640	1.174204	-1.629708
H	-2.302316	-1.087783	-0.757321
H	-2.640939	2.634451	-0.789343
O	-6.526094	4.258563	-2.211402
C	-7.738468	4.711081	-2.776541
H	-7.731173	5.795816	-2.671696
H	-7.808802	4.455644	-3.840308
H	-8.608271	4.307160	-2.245165
C	2.119135	0.561300	5.795530
C	1.141169	-0.411592	5.669535
C	0.709135	-0.827878	4.400955
C	1.294882	-0.239143	3.261812
C	2.297771	0.727278	3.399658
C	2.700748	1.136666	4.659464
H	-0.704755	-2.338994	5.114936
H	2.438569	0.877648	6.783468
H	0.699613	-0.861744	6.554115
C	-0.316134	-1.841181	4.231596
C	0.906484	-0.689065	1.905648
H	2.738527	1.141413	2.498261
H	3.465432	1.898289	4.767570
C	-0.309088	-1.504088	1.760936
C	-0.770772	-2.158976	3.004310
H	-1.509803	-2.954952	2.919835

O	1.592032	-0.362919	0.928271
C	2.233706	-3.503847	-0.046531
C	1.799680	-2.569665	-0.985545
C	2.591659	-2.202213	-2.070682
C	3.859362	-2.753812	-2.190504
C	4.308962	-3.667313	-1.230231
C	3.506375	-4.059909	-0.162972
H	2.207663	-1.477407	-2.783702
H	4.511596	-2.463115	-3.005921
H	5.312804	-4.071553	-1.313624
H	3.869453	-4.773540	0.568653
C	1.219920	2.325972	-0.987077
C	-0.158947	2.253993	-0.791921
C	1.242172	3.799685	-0.803523
C	-0.248133	3.693482	-0.476602
O	2.060655	4.683735	-0.878489
O	-1.124082	4.414279	-0.042924
S	1.074858	-3.846167	1.230685
C	0.481710	-2.007433	-0.703032
O	-0.113222	-1.239832	-1.435056
C	-1.769911	1.079875	3.241634
C	-4.064323	2.023502	3.040671
C	-2.734373	2.161091	3.810902
H	-1.693595	0.233823	3.923971
H	-0.764844	1.480544	3.085477
H	-2.926641	1.915314	4.861645
C	-3.494244	-0.251688	2.194938
H	-3.939072	-0.504094	1.233162
H	-3.180306	-1.180012	2.681270
C	-4.475639	0.546218	3.080397
H	-5.494554	0.420226	2.704242
H	-4.460358	0.177994	4.111360
H	-4.827789	2.655406	3.500744
C	-3.849185	2.404768	1.571388
H	-4.701974	2.059067	0.976175
H	-3.769929	3.487133	1.430333
C	-2.541337	1.755310	1.090238
H	-1.719545	2.437661	1.321626
N	-2.254686	0.537466	1.930332
C	-2.166354	3.555351	3.769275
H	-1.842977	3.943758	2.802284
C	-2.048658	4.329182	4.842900
H	-2.353734	3.985550	5.828456
H	-1.642807	5.333059	4.777274
C	-0.158058	-2.536784	0.622470
N	-1.438694	-3.103668	0.302923
C	-1.563257	-4.044645	-0.689482
O	-0.648983	-4.354079	-1.421233
O	-2.817386	-4.516885	-0.715392
C	-3.179733	-5.584027	-1.651201
C	-4.655196	-5.806042	-1.346358
H	-4.792976	-6.090452	-0.299861
H	-5.231904	-4.896704	-1.539388
H	-5.049876	-6.605287	-1.978803
C	-2.362754	-6.831659	-1.335113
H	-2.727274	-7.666743	-1.940010
H	-1.305426	-6.677034	-1.552730
H	-2.475287	-7.099651	-0.280542
C	-2.990106	-5.121210	-3.091799
H	-3.555871	-4.204321	-3.281979
H	-1.938883	-4.945957	-3.318897
H	-3.371838	-5.894072	-3.765418
H	-1.310557	-0.389869	1.607918
H	-0.835165	0.342651	-1.093840
H	1.808342	0.424314	-0.831399
H	-2.215223	-2.982668	0.936043

IM7b

Free Energy = -3921.855039 Hartree

Energy = -3922.719147 Hartree

C	-2.341120	1.747415	0.380893
C	-2.766433	2.070916	-1.049953
C	-5.498460	4.645863	-0.732806
H	-4.242741	3.725189	0.682264
C	-5.203523	4.071595	-3.052855
H	-2.053131	1.220859	-4.255896
C	-5.865717	4.792572	-2.094988
H	-5.447379	4.171593	-4.104886
H	-6.653634	5.477092	-2.384453
N	-3.541022	2.522607	-3.736409
N	-0.909246	1.523583	0.484469
N	2.238462	1.659132	0.506145
C	3.612353	1.659385	0.309656
C	4.282561	0.460709	0.596130
C	4.326472	2.754459	-0.182599
C	5.644243	0.365745	0.375810
H	3.718238	-0.396474	0.954440
C	5.699112	2.626710	-0.381863

H	3.822803	3.690256	-0.412262	H	-4.645991	1.327577	2.330690
C	6.376920	1.445633	-0.114129	C	-3.068698	0.575122	1.070260
H	7.443244	1.362890	-0.290459	H	-2.518858	0.417463	2.005952
C	6.467217	3.829531	-0.855416	N	-2.974119	-0.769461	0.370781
C	6.358414	-0.935815	0.597003	C	-4.238894	-1.174183	3.604883
F	5.768319	4.548503	-1.742432	H	-3.441091	-0.450807	3.785930
F	6.773125	4.650363	0.160779	C	-4.914506	-1.655963	4.641858
F	7.625203	3.481726	-1.439025	H	-5.701757	-2.395732	4.517148
F	7.426417	-0.786112	1.393794	H	-4.700775	-1.329870	5.654278
F	5.570350	-1.868478	1.145176	H	-0.489307	0.612229	0.726917
F	6.821496	-1.441376	-0.564258	H	1.837955	0.778774	0.852604
C	-2.124381	1.467682	-2.103127	H	-2.030173	-0.930433	-0.063178
C	-4.497050	3.771239	-0.369996	C	-1.292285	-0.339289	5.853082
C	-4.162962	3.172833	-2.714108	C	-1.330875	-1.654095	5.460194
C	-2.553628	1.720871	-3.429158	C	-0.835021	-2.051996	4.190305
C	-3.813880	3.003446	-1.340867	C	-0.273650	-1.058450	3.342460
H	-1.315938	0.765075	-1.923051	C	-0.235062	0.290116	3.773950
H	-2.588777	2.615556	1.004521	C	-0.745445	0.647680	4.999214
O	-6.087586	5.331477	0.277527	H	-1.300632	-4.163236	4.397575
C	-7.072618	6.289235	-0.048583	H	-1.680528	-0.051882	6.825370
H	-7.379683	6.737145	0.896369	H	-1.755595	-2.412192	6.112642
H	-6.672674	7.072958	-0.702263	C	-0.907962	-3.397915	3.736500
H	-7.946004	5.826852	-0.523677	C	0.220926	-1.413578	2.026879
C	1.333491	2.621608	0.216469	H	0.209350	1.025602	3.110090
C	-0.055115	2.524742	0.232996	H	-0.715830	1.683127	5.322486
C	1.288259	4.057173	-0.179547	C	0.031610	-2.731891	1.591650
C	-0.240844	3.947498	-0.105799	C	-0.479114	-3.713984	2.472126
O	2.086370	4.924621	-0.442892	H	-0.525239	-4.755020	2.156534
O	-1.197828	4.675940	-0.224396	O	0.749052	-0.529267	1.242653
C	-3.184901	-1.846891	1.404120	C	2.674826	-2.368656	-1.016706
C	-5.297758	-0.530420	1.375619	C	1.671179	-1.452454	-1.337317
C	-4.498643	-1.581313	2.176983	C	1.933591	-0.353222	-2.151817
H	-3.191664	-2.793634	0.858641	C	3.217766	-0.172167	-2.646603
H	-2.319355	-1.840850	2.063160	C	4.219461	-1.096467	-2.330352
H	-5.085729	-2.505939	2.189633	C	3.963796	-2.196832	-1.517875
C	-4.001772	-0.945484	-0.715167	H	1.133255	0.345389	-2.378755
H	-3.907542	-0.103557	-1.395974	H	3.449252	0.685858	-3.267887
H	-3.716653	-1.852093	-1.253850	H	5.227128	-0.945106	-2.704747
C	-5.399183	-1.026340	-0.073659	H	4.756303	-2.892876	-1.266827
H	-6.094890	-0.406344	-0.644311	S	2.173408	-3.666979	0.059217
H	-5.780280	-2.051665	-0.094859	C	0.371194	-1.776587	-0.754637
H	-6.290476	-0.412688	1.815345	O	-0.691634	-1.237743	-1.040241
C	-4.557157	0.815536	1.368689	C	0.403244	-3.047764	0.160494
H	-5.001543	1.465932	0.609194	N	-0.547934	-3.988588	-0.373544

C	-0.522429	-4.360950	-1.691871
O	0.180183	-3.827065	-2.522550
O	-1.396997	-5.357712	-1.892882
C	-1.565122	-5.919386	-3.230325
C	-2.613589	-7.001843	-3.009260
H	-2.253294	-7.743847	-2.291926
H	-3.539402	-6.567069	-2.622967
H	-2.834669	-7.508066	-3.952267
C	-0.252150	-6.529262	-3.709092
H	-0.424435	-7.072103	-4.642972
H	0.502059	-5.761536	-3.881861
H	0.124974	-7.238981	-2.967035
C	-2.086739	-4.847477	-4.181315
H	-2.993032	-4.390306	-3.772046
H	-1.340101	-4.071434	-4.350133
H	-2.342840	-5.305895	-5.140768
H	-1.070125	-4.572698	0.260320

IM6a

Free Energy = -3921.849538 Hartree

Energy = -3922.716986 Hartree

C	-2.868120	1.189796	-1.193460
C	-3.602166	-0.125888	-1.391116
C	-7.054365	0.877017	-2.521251
H	-5.320630	1.986996	-2.081714
C	-6.951397	-1.518724	-2.297002
H	-3.178085	-3.477374	-1.078693
C	-7.673784	-0.396061	-2.604719
H	-7.392818	-2.507723	-2.354528
H	-8.708245	-0.488531	-2.911982
N	-4.956440	-2.612118	-1.621706
N	-1.468676	1.057904	-1.581258
N	1.653627	1.280134	-1.682431
C	3.013023	1.344067	-1.355646
C	3.720509	0.140979	-1.350619
C	3.643969	2.527112	-0.963102
C	5.037799	0.114859	-0.920990
H	3.230198	-0.785004	-1.628519
C	4.962162	2.465644	-0.530603
H	3.110314	3.471644	-0.952906
C	5.676797	1.273073	-0.497270
H	6.692397	1.242752	-0.117552
C	5.638781	3.713431	-0.035787
C	5.785771	-1.186893	-0.885298
F	4.769202	4.697806	0.216036
F	6.319421	3.476856	1.100156
F	6.529451	4.182953	-0.923336
F	6.679785	-1.271611	-1.883500
F	6.475513	-1.324379	0.258747
F	4.970125	-2.244502	-0.995414
C	-2.975589	-1.326695	-1.174586
C	-5.737494	0.987443	-2.127314
C	-5.595729	-1.440531	-1.896493
C	-3.693884	-2.542436	-1.288115
C	-4.974831	-0.158670	-1.804789
H	-1.924897	-1.388699	-0.919072
H	-3.309422	1.940514	-1.858116
O	-7.690280	2.037923	-2.809622
C	-9.035558	1.977506	-3.236641
H	-9.338077	3.008324	-3.419506
H	-9.138844	1.404738	-4.165525
H	-9.685287	1.546198	-2.466179
C	3.481074	2.930048	2.519385
C	3.986126	1.654052	2.545012
C	3.229474	0.552159	2.064724
C	1.913667	0.785879	1.584383
C	1.431902	2.115247	1.545043
C	2.190927	3.168967	1.994676
H	4.776066	-0.941304	2.356462
H	4.086664	3.762143	2.863440
H	4.994118	1.470604	2.907755
C	3.766418	-0.759241	2.002764
C	1.115777	-0.296926	1.051016
H	0.463891	2.291480	1.093015
H	1.814495	4.184686	1.921403
C	1.707342	-1.574312	0.978874
C	3.027371	-1.772777	1.454728
H	3.458959	-2.764781	1.384297
O	-0.104132	-0.061038	0.610243
C	2.523275	-4.160570	-1.113719
C	2.071979	-3.084452	-1.877253
C	2.588087	-2.820735	-3.146339
C	3.597391	-3.634785	-3.636219
C	4.058978	-4.708754	-2.864674
C	3.529383	-4.988120	-1.609697
H	2.195336	-1.984628	-3.718470
H	4.030727	-3.444543	-4.611538
H	4.850815	-5.340574	-3.254787

H	3.895967	-5.827168	-1.027890
C	0.727678	2.257678	-1.610162
C	-0.661061	2.134258	-1.580916
C	0.656918	3.744626	-1.512857
C	-0.863321	3.589668	-1.492156
O	1.431272	4.665418	-1.424390
O	-1.825701	4.320421	-1.372548
S	1.677470	-4.378991	0.420288
C	1.002177	-2.333678	-1.212842
O	0.308473	-1.483242	-1.749440
C	-1.901196	2.318242	2.311777
C	-4.377126	2.037223	2.288551
C	-3.236949	2.958849	2.772472
H	-1.341722	1.865144	3.134234
H	-1.257988	3.063115	1.838925
H	-3.258663	2.967626	3.867768
C	-2.844420	0.092082	1.995517
H	-3.119637	-0.633831	1.230245
H	-2.096876	-0.383961	2.634307
C	-4.070426	0.614275	2.770831
H	-4.927173	-0.039845	2.588853
H	-3.880360	0.613619	3.849297
H	-5.327039	2.389933	2.696855
C	-4.433608	2.005657	0.753731
H	-5.075322	1.176823	0.441225
H	-4.865897	2.923970	0.346183
C	-3.002444	1.842006	0.214444
H	-2.578442	2.837505	0.076566
N	-2.158161	1.234850	1.307868
C	-3.387859	4.379631	2.292775
H	-3.164918	4.580650	1.243252
C	-3.776235	5.379731	3.075963
H	-3.993406	5.225504	4.130265
H	-3.889309	6.388614	2.694033
C	0.908432	-2.700959	0.290293
N	-0.483165	-2.735719	0.694687
C	-0.872532	-3.414562	1.822548
O	-0.227862	-4.268613	2.391812
O	-2.112193	-3.010962	2.170660
C	-2.854565	-3.756187	3.181543
C	-4.183638	-3.013695	3.238280
H	-4.037756	-1.999940	3.622901
H	-4.635333	-2.956660	2.243241
H	-4.876542	-3.531835	3.906240
C	-2.148810	-3.684755	4.532162
H	-2.813166	-4.077109	5.307953
H	-1.224261	-4.260423	4.530878
H	-1.916783	-2.644228	4.780451
C	-3.061948	-5.191412	2.709907
H	-3.548032	-5.199207	1.729668
H	-2.112793	-5.724035	2.643563
H	-3.709787	-5.717834	3.416619
H	-0.998807	0.183045	-1.353605
H	1.274310	0.337569	-1.755092
H	-0.866426	-1.791170	0.633621
H	-1.164199	0.806040	0.970946

TS4b

Free Energy = -3921.850862 Hartree

Energy = -3922.715134 Hartree

C	-2.221854	1.852785	0.371545
C	-2.701401	2.119672	-1.052838
C	-5.205797	4.917438	-0.744622
H	-3.957971	3.968016	0.657955
C	-5.070591	4.212298	-3.043588
H	-2.237743	1.040991	-4.235252
C	-5.625805	5.029322	-2.094865
H	-5.358395	4.280612	-4.087017
H	-6.371028	5.760590	-2.383081
N	-3.577257	2.496548	-3.719395
N	-0.799884	1.554763	0.437795
N	2.346921	1.504496	0.265073
C	3.710073	1.435227	0.001081
C	4.315079	0.182933	0.183775
C	4.469172	2.516298	-0.449605
C	5.660767	0.023875	-0.090608
H	3.715319	-0.660859	0.516044
C	5.824570	2.322284	-0.708702
H	4.014995	3.492856	-0.599446
C	6.439353	1.090137	-0.538448
H	7.493846	0.959768	-0.752105
C	6.641706	3.509671	-1.137000
C	6.302230	-1.327600	0.039501
F	5.977131	4.280732	-2.006899
F	6.964828	4.287317	-0.092626
F	7.791717	3.139129	-1.721206
F	7.457134	-1.259741	0.718932
F	5.514472	-2.210113	0.665799

F	6.602626	-1.849660	-1.165121	H	1.916116	0.628634	0.576876
C	-2.172606	1.404783	-2.099378	H	-2.059210	-0.877222	0.084430
C	-4.258318	3.984201	-0.382935	C	-0.711079	0.246860	5.784269
C	-4.089699	3.248299	-2.706294	C	-0.926500	-1.087241	5.548495
C	-2.648787	1.625950	-3.414991	C	-0.585825	-1.673514	4.299662
C	-3.685113	3.119438	-1.343640	C	0.002611	-0.840395	3.304550
H	-1.421371	0.640208	-1.920541	C	0.228146	0.533071	3.575623
H	-2.372813	2.772789	0.947588	C	-0.130849	1.068832	4.787373
O	-5.691558	5.693773	0.255054	H	-1.275814	-3.668988	4.791262
C	-6.618087	6.706958	-0.074416	H	-0.981830	0.678852	6.742532
H	-6.845527	7.220505	0.859607	H	-1.373103	-1.717402	6.312681
H	-6.193683	7.426870	-0.783735	C	-0.848506	-3.042350	4.015391
H	-7.544943	6.290380	-0.486395	C	0.310051	-1.409599	2.024366
C	1.487364	2.533571	0.085675	H	0.687609	1.144350	2.804771
C	0.100283	2.514446	0.180840	H	0.039930	2.120875	4.990402
C	1.505048	3.991987	-0.224792	C	-0.027894	-2.731502	1.765825
C	-0.023740	3.960120	-0.072796	C	-0.571623	-3.555879	2.771266
O	2.337798	4.826022	-0.484519	H	-0.775411	-4.606139	2.571413
O	-0.946398	4.739724	-0.105766	O	0.823568	-0.723769	1.029029
C	-3.176459	-1.595658	1.701774	C	2.399418	-2.636969	-1.096316
C	-5.229325	-0.185914	1.692150	C	1.456198	-1.637496	-1.327624
C	-4.428933	-1.210519	2.527325	C	1.708574	-0.610128	-2.227546
H	-3.254449	-2.583953	1.241890	C	2.928901	-0.579191	-2.894540
H	-2.273427	-1.574964	2.309165	C	3.874712	-1.578554	-2.657317
H	-5.054156	-2.102171	2.645571	C	3.622963	-2.614765	-1.760654
C	-4.082468	-0.822194	-0.428137	H	0.954591	0.155330	-2.389707
H	-3.994653	-0.036112	-1.174421	H	3.150488	0.222679	-3.590278
H	-3.871957	-1.777036	-0.915977	H	4.833203	-1.544402	-3.165033
C	-5.440951	-0.790331	0.296809	H	4.371466	-3.377700	-1.576500
H	-6.146623	-0.187725	-0.280300	S	1.910037	-3.844019	0.095026
H	-5.862753	-1.796290	0.382297	C	0.222756	-1.775866	-0.526190
H	-6.186736	0.014705	2.177827	O	-0.854624	-1.227039	-0.836111
C	-4.431107	1.116956	1.527737	C	0.206675	-3.102091	0.327390
H	-4.887188	1.721811	0.737279	N	-0.859348	-3.950575	-0.128337
H	-4.442121	1.715300	2.442949	C	-0.971960	-4.325648	-1.443088
C	-2.975498	0.773769	1.174125	O	-0.288152	-3.872892	-2.332800
H	-2.384748	0.658148	2.090276	O	-1.958226	-5.230340	-1.561908
N	-2.982556	-0.619177	0.575147	C	-2.277842	-5.786579	-2.872515
C	-4.063819	-0.714923	3.902703	C	-3.404469	-6.762154	-2.557471
H	-3.258115	0.018026	3.975698	H	-3.062641	-7.529891	-1.858353
C	-4.652361	-1.130833	5.018455	H	-4.252688	-6.237921	-2.108937
H	-5.444725	-1.875292	5.002666	H	-3.744118	-7.252033	-3.473534
H	-4.361562	-0.741874	5.988663	C	-1.068753	-6.524507	-3.437783
H	-0.456489	0.594140	0.488855	H	-1.363088	-7.060460	-4.344821

H	-0.261312	-5.834354	-3.682165
H	-0.703767	-7.257499	-2.712383
C	-2.765658	-4.679519	-3.801006
H	-3.596818	-4.138886	-3.337494
H	-1.965495	-3.975762	-4.030366
H	-3.127709	-5.119974	-4.734456
H	-1.360964	-4.506778	0.547173

TS4a

Free Energy = -3921.6936894 Hartree

Energy = -3922.716302 Hartree

C	2.923576	-1.174516	-1.066426
C	3.678597	0.090929	-1.443143
C	7.086024	-1.133632	-2.487636
H	5.353299	-2.125889	-1.806116
C	7.010828	1.267260	-2.673442
H	3.293662	3.455627	-1.682174
C	7.713330	0.098310	-2.807891
H	7.464404	2.223037	-2.914852
H	8.737616	0.122216	-3.159656
N	5.044269	2.486129	-2.130776
N	1.531544	-1.064993	-1.498311
N	-1.588328	-1.372503	-1.683634
C	-2.939548	-1.473925	-1.342147
C	-3.705891	-0.306779	-1.391557
C	-3.513507	-2.663164	-0.885685
C	-5.019493	-0.324396	-0.949285
H	-3.265911	0.622569	-1.736000
C	-4.831205	-2.645158	-0.446634
H	-2.936681	-3.580069	-0.839675
C	-5.603682	-1.488540	-0.462735
H	-6.620935	-1.489631	-0.084996
C	-5.441351	-3.903944	0.101230
C	-5.825086	0.942436	-0.962223
F	-4.520577	-4.830368	0.396804
F	-6.138725	-3.661462	1.224972
F	-6.301050	-4.463588	-0.766843
F	-6.784629	0.913371	-1.903005
F	-6.449638	1.142120	0.210469
F	-5.070805	2.024046	-1.202564
C	3.071156	1.321272	-1.405155
C	5.780775	-1.157529	-2.041039
C	5.668202	1.276771	-2.221626
C	3.793317	2.490996	-1.744028
C	5.039260	0.038162	-1.894310
H	2.028300	1.435824	-1.130034
H	3.352299	-2.005804	-1.634885
O	7.705449	-2.333402	-2.592757
C	9.046799	-2.358569	-3.053805
H	9.339713	-3.408198	-3.061665
H	9.128469	-1.953810	-4.068393
H	9.711134	-1.803687	-2.382166
C	-3.263445	-2.948586	2.638159
C	-3.834631	-1.700104	2.628316
C	-3.142887	-0.581507	2.089644
C	-1.824539	-0.765777	1.592521
C	-1.274526	-2.071074	1.585971
C	-1.972201	-3.141279	2.093333
H	-4.760524	0.838530	2.352886
H	-3.814679	-3.797140	3.031118
H	-4.842088	-1.551253	3.008453
C	-3.748996	0.696783	1.985550
C	-1.101635	0.341010	1.015243
H	-0.304149	-2.222753	1.127638
H	-1.543632	-4.138429	2.056679
C	-1.751809	1.579157	0.895697
C	-3.075801	1.726181	1.382994
H	-3.564613	2.688307	1.280505
O	0.128998	0.166040	0.553150
C	-2.669033	4.028007	-1.361261
C	-2.131280	2.947517	-2.060504
C	-2.585614	2.603327	-3.334945
C	-3.615700	3.344651	-3.894650
C	-4.158804	4.426654	-3.188654
C	-3.694027	4.784353	-1.926424
H	-2.133120	1.765396	-3.858313
H	-4.001044	3.092366	-4.876296
H	-4.963515	5.002161	-3.635723
H	-4.123832	5.627967	-1.396348
C	-0.630859	-2.322556	-1.586603
C	0.753074	-2.152855	-1.523853
C	-0.515162	-3.799033	-1.494678
C	0.996312	-3.602040	-1.445590
O	-1.260885	-4.751476	-1.427533
O	1.976552	-4.309200	-1.335018
S	-1.908570	4.337846	0.203391
C	-1.037999	2.293471	-1.335601
O	-0.255718	1.491625	-1.819158

C	1.956433	-1.879677	2.564383
C	4.420853	-1.532115	2.487977
C	3.310622	-2.387205	3.131655
H	1.376920	-1.336136	3.315534
H	1.350746	-2.717122	2.213150
H	3.330159	-2.203467	4.211446
C	2.816705	0.294511	1.933608
H	3.048635	0.930029	1.078501
H	2.067249	0.817662	2.532969
C	4.082902	-0.058806	2.741770
H	4.914809	0.577356	2.426891
H	3.920506	0.109506	3.811677
H	5.386238	-1.789977	2.930356
C	4.460045	-1.745971	0.967791
H	5.096164	-0.970769	0.530821
H	4.895854	-2.713621	0.703228
C	3.023937	-1.660881	0.413349
H	2.603648	-2.671353	0.376839
N	2.163154	-0.946321	1.415235
C	3.508540	-3.862255	2.906228
H	3.360931	-4.230965	1.889368
C	3.853860	-4.718903	3.862923
H	4.000673	-4.390794	4.889684
H	4.000160	-5.774503	3.656026
C	-1.015171	2.716429	0.157736
N	0.358335	2.905453	0.575883
C	0.618139	3.534212	1.769236
O	-0.201776	4.172014	2.401209
O	1.909537	3.374691	2.088603
C	2.481312	4.087303	3.231496
C	3.946400	3.675825	3.182694
H	4.046203	2.597314	3.333278
H	4.386551	3.938452	2.216452
H	4.502370	4.187333	3.972712
C	1.832471	3.610304	4.525564
H	2.367339	4.042897	5.376173
H	0.785290	3.908370	4.579971
H	1.898372	2.519944	4.601159
C	2.342541	5.592051	3.028644
H	2.759443	5.880084	2.058920
H	1.300021	5.906909	3.077365
H	2.903424	6.111543	3.810853
H	1.038529	-0.201414	-1.274622
H	-1.242616	-0.421858	-1.802859
H	0.924311	2.078290	0.405105
H	1.036992	-0.523006	1.006404

IM8b

Free Energy = -3921.851329 Hartree

Energy = -3922.717993 Hartree

C	-2.042112	2.019090	0.354794
C	-2.266922	2.712245	-0.984459
C	-4.592475	5.572937	-0.221762
H	-3.690483	4.107950	0.991718
C	-4.100580	5.550373	-2.579780
H	-1.347240	2.526896	-4.246712
C	-4.756210	6.119585	-1.520401
H	-4.195745	5.949142	-3.583868
H	-5.386714	6.985726	-1.680110
N	-2.638853	3.932892	-3.516918
N	-0.668009	1.548785	0.497679
N	2.484219	1.186048	0.614536
C	3.868676	1.062599	0.518783
C	4.379201	-0.236771	0.390040
C	4.739185	2.153635	0.524046
C	5.742547	-0.431120	0.258405
H	3.703478	-1.087891	0.382924
C	6.106866	1.921562	0.398713
H	4.363243	3.168375	0.627517
C	6.629497	0.643426	0.262369
H	7.696976	0.486082	0.160884
C	7.037021	3.102278	0.466705
C	6.292302	-1.815276	0.061823
F	6.541831	4.159593	-0.187626
F	7.248565	3.487165	1.733388
F	8.235868	2.820137	-0.065126
F	7.351877	-2.038420	0.851107
F	5.385019	-2.766622	0.320754
F	6.713126	-2.004000	-1.203003
C	-1.624067	2.265219	-2.112665
C	-3.790500	4.469992	-0.024513
C	-3.264917	4.420002	-2.410289
C	-1.848252	2.902587	-3.356680
C	-3.115621	3.859136	-1.106480
H	-0.969230	1.398993	-2.068149
H	-2.192302	2.763977	1.142715
O	-5.195883	6.079235	0.882662
C	-5.990992	7.236265	0.738548

H	-6.351451	7.479214	1.738103
H	-5.408739	8.081850	0.353984
H	-6.852065	7.057886	0.083342
C	1.722690	2.307027	0.717915
C	0.338567	2.415776	0.663071
C	1.896296	3.770239	0.940882
C	0.363629	3.871590	0.919535
O	2.816184	4.539294	1.072833
O	-0.477288	4.722075	1.071026
C	-3.283480	-1.524344	0.633498
C	-5.293790	-0.040372	0.513890
C	-4.730318	-1.317177	1.177577
H	-3.207690	-2.410473	-0.001949
H	-2.589019	-1.669028	1.464401
H	-5.361595	-2.156820	0.856822
C	-3.688392	-0.292909	-1.375583
H	-3.391769	0.575632	-1.960325
H	-3.459399	-1.179397	-1.978254
C	-5.189783	-0.228814	-1.003111
H	-5.670945	0.606783	-1.520171
H	-5.714149	-1.140512	-1.308111
H	-6.333579	0.104880	0.818475
C	-4.453138	1.194570	0.875615
H	-4.735022	2.015662	0.207736
H	-4.642619	1.534440	1.898739
C	-2.964028	0.832679	0.710679
H	-2.574258	0.498848	1.681058
N	-2.823489	-0.365446	-0.166185
C	-4.748131	-1.283665	2.679804
H	-4.095863	-0.552318	3.161587
C	-5.469570	-2.101704	3.439204
H	-6.120851	-2.854218	3.000668
H	-5.439224	-2.049933	4.522583
H	-0.456793	0.610162	0.179702
H	1.971335	0.312731	0.536251
H	-1.366863	-0.836196	-0.947627
C	-0.978288	-1.328204	5.212804
C	-1.260308	-2.541275	4.637744
C	-0.910234	-2.804857	3.288379
C	-0.259005	-1.772381	2.553417
C	0.034419	-0.528688	3.167327
C	-0.323939	-0.313505	4.473728
H	-1.670813	-4.829560	3.249269
H	-1.254305	-1.141272	6.245307
H	-1.760708	-3.318841	5.207302
C	-1.197894	-4.050284	2.659616
C	0.019753	-2.058214	1.199118
H	0.537735	0.243047	2.593546
H	-0.102572	0.637199	4.946782
C	-0.304279	-3.239699	0.583894
C	-0.889348	-4.277411	1.342649
H	-1.105502	-5.229169	0.874671
O	0.644938	-1.155199	0.374857
C	2.601833	-2.503166	-1.728487
C	1.745526	-1.402858	-1.752057
C	2.120942	-0.219464	-2.374162
C	3.383688	-0.132721	-2.955316
C	4.244792	-1.229369	-2.915748
C	3.863196	-2.426283	-2.312357
H	1.432469	0.620544	-2.392208
H	3.698959	0.787571	-3.434127
H	5.233506	-1.154858	-3.356084
H	4.541865	-3.271526	-2.286401
S	1.946009	-3.911759	-0.879639
C	0.465200	-1.613636	-1.002050
O	-0.571021	-0.930319	-1.565959
C	0.218032	-3.169834	-0.825203
N	-0.538401	-3.681420	-1.930964
C	-1.818037	-4.146873	-2.113223
O	-2.258155	-4.330167	-3.227917
O	-2.465157	-4.397687	-0.966918
C	-3.770916	-5.061340	-1.005662
C	-4.119278	-5.230200	0.469633
H	-3.428818	-5.922492	0.959433
H	-4.078598	-4.273800	1.000696
H	-5.130083	-5.636410	0.563162
C	-3.643614	-6.422635	-1.681190
H	-4.571119	-6.984016	-1.536312
H	-3.454266	-6.322027	-2.749476
H	-2.828571	-6.993366	-1.225638
C	-4.796742	-4.170237	-1.697840
H	-4.868754	-3.207079	-1.183177
H	-4.535053	-4.002285	-2.742387
H	-5.779674	-4.648066	-1.651456
H	-0.109259	-3.503568	-2.830901

IM7a

Free Energy = -3921.856357 Hartree

Energy = -3922.724090 Hartree

C	2.841805	-1.308337	-1.009401
C	3.559944	0.024823	-1.143340
C	6.982374	-0.902264	-2.418586
H	5.304954	-2.049607	-1.869053
C	6.816518	1.493684	-2.248963
H	3.035116	3.367045	-0.923769
C	7.559190	0.384695	-2.560514
H	7.223848	2.493516	-2.353090
H	8.575955	0.499559	-2.915761
N	4.813737	2.544334	-1.526550
N	1.448579	-1.127648	-1.406506
N	-1.642731	-1.151129	-1.701570
C	-3.017492	-1.154575	-1.461800
C	-3.655175	0.086361	-1.376538
C	-3.741040	-2.329020	-1.236321
C	-4.993531	0.150273	-1.022760
H	-3.095288	1.001891	-1.540915
C	-5.081912	-2.229408	-0.890285
H	-3.262442	-3.301940	-1.293310
C	-5.726753	-1.002975	-0.768923
H	-6.764316	-0.946807	-0.456840
C	-5.867066	-3.476987	-0.593441
C	-5.662122	1.485028	-0.853410
F	-5.084333	-4.551888	-0.457167
F	-6.572558	-3.345543	0.545628
F	-6.755463	-3.745521	-1.562173
F	-6.573378	1.712220	-1.810087
F	-6.312139	1.556953	0.321136
F	-4.786117	2.499451	-0.886511
C	2.922386	1.209563	-0.874866
C	5.687318	-1.040170	-1.965776
C	5.484300	1.385847	-1.784235
C	3.580264	2.443678	-1.103695
C	4.907172	0.090755	-1.632720
H	1.905129	1.243806	-0.489570
H	3.285578	-1.994804	-1.738772
O	7.640715	-2.053104	-2.705285
C	8.966482	-1.963546	-3.181635
H	9.295144	-2.989147	-3.349078
H	9.020160	-1.412745	-4.128097
H	9.629863	-1.492021	-2.446915
C	-3.650323	-3.439649	2.091555
C	-4.176932	-2.184915	2.259099
C	-3.401056	-1.025953	1.995047
C	-2.049908	-1.181900	1.585269
C	-1.528791	-2.491736	1.427916
C	-2.311004	-3.595215	1.664066
H	-4.991273	0.396916	2.362273
H	-4.266570	-4.316138	2.261530
H	-5.212751	-2.057365	2.560049
C	-3.951968	0.276728	2.074031
C	-1.279181	-0.021421	1.254019
H	-0.509121	-2.622963	1.082999
H	-1.906195	-4.588880	1.502447
C	-1.842594	1.249040	1.342030
C	-3.198577	1.369783	1.746081
H	-3.647037	2.354160	1.787882
O	-0.019288	-0.136554	0.789051
C	-2.396491	4.374302	-0.228761
C	-1.885337	3.496621	-1.186945
C	-2.235271	3.605783	-2.533184
C	-3.119798	4.601277	-2.915445
C	-3.633995	5.478393	-1.952579
C	-3.282288	5.379863	-0.611086
H	-1.808042	2.907840	-3.247412
H	-3.417340	4.702824	-3.952879
H	-4.328464	6.254786	-2.257917
H	-3.693320	6.066509	0.120916
C	-0.784489	-2.198589	-1.648248
C	0.602228	-2.155158	-1.523898
C	-0.806265	-3.685294	-1.641002
C	0.718525	-3.628486	-1.529963
O	-1.634975	-4.564121	-1.649397
O	1.624313	-4.425233	-1.427700
S	-1.826661	4.080530	1.408365
C	-0.986315	2.481621	-0.639490
O	-0.362499	1.663691	-1.291069
C	1.876903	-2.810150	2.331337
C	4.316779	-2.310730	2.424007
C	3.251682	-3.357781	2.820851
H	1.251087	-2.492642	3.172162
H	1.329234	-3.590827	1.792105
H	3.243315	-3.425848	3.915084
C	2.600140	-0.520803	2.211261
H	2.804909	0.305273	1.526548
H	1.819297	-0.183089	2.902858
C	3.872385	-0.952138	2.979073

H	4.664791	-0.209423	2.848234
H	3.674761	-1.031705	4.053360
H	5.286243	-2.603066	2.836086
C	4.402019	-2.181098	0.895358
H	4.990440	-1.290178	0.652548
H	4.914711	-3.038056	0.447677
C	2.962882	-2.075728	0.344277
H	2.626072	-3.082901	0.085020
N	2.037309	-1.647859	1.427683
C	3.550442	-4.727580	2.273566
H	3.388802	-4.878314	1.204524
C	3.988184	-5.742929	3.010402
H	4.148057	-5.639433	4.081076
H	4.200830	-6.713295	2.574275
C	-1.010508	2.474896	0.924102
N	0.299876	2.429492	1.502246
C	1.276471	3.300426	1.124780
O	1.109686	4.178837	0.302398
O	2.423698	3.025236	1.780037
C	3.234971	4.136261	2.287492
C	4.265308	3.424340	3.152114
H	3.775771	2.848707	3.942630
H	4.860260	2.742590	2.537550
H	4.938735	4.151397	3.613312
C	2.331499	5.037956	3.121990
H	2.927417	5.811999	3.612739
H	1.584220	5.530144	2.493186
H	1.818568	4.456506	3.894054
C	3.918220	4.911057	1.166431
H	4.570635	4.263048	0.575469
H	3.185924	5.380412	0.508429
H	4.537466	5.695073	1.613875
H	1.023065	-0.224611	-1.217686
H	-1.208669	-0.230298	-1.675375
H	0.549622	1.649968	2.090415
H	0.551458	-0.928851	1.052361

7i'

Free Energy = -1642.4895898 Hartree

Energy = -1642.8694653 Hartree

C	-6.272696	-1.232595	-0.403573
C	-5.400686	-1.954930	0.370211
C	-4.028532	-1.599975	0.446379
C	-3.592119	-0.470732	-0.305290
C	-4.506170	0.262419	-1.099831
C	-5.823603	-0.114298	-1.146282
H	-3.465582	-3.187213	1.806663
H	-7.318667	-1.518244	-0.449452
H	-5.749421	-2.812624	0.938333
C	-3.102557	-2.335417	1.240448
C	-2.219872	-0.141462	-0.211781
H	-4.140052	1.116513	-1.659736
H	-6.528702	0.444116	-1.753004
C	-1.342205	-0.861750	0.553930
C	-1.779493	-1.974557	1.300023
H	-1.083309	-2.528294	1.924702
C	0.639812	2.274766	1.014012
C	0.310753	2.163981	-0.333968
C	0.457742	3.242552	-1.192121
C	0.923667	4.453437	-0.686208
C	1.240165	4.566372	0.666201
C	1.105293	3.480367	1.527967
H	0.210451	3.125525	-2.242353
H	1.042696	5.307292	-1.344317
H	1.606044	5.510621	1.057090
H	1.369018	3.570288	2.576405
S	0.416007	0.791896	1.951286
C	-0.216833	0.822421	-0.737809
O	0.318020	0.427447	-1.937988
C	0.010500	-0.223314	0.439080
N	1.001506	-1.208309	0.111032
C	2.327298	-0.873926	-0.067224
O	2.728408	0.261477	-0.155694
O	3.053500	-2.000650	-0.142607
C	4.491490	-1.922475	-0.375681
C	4.907416	-3.387700	-0.398703
H	4.668624	-3.868974	0.553437
H	4.385979	-3.921792	-1.197479
H	5.983824	-3.469743	-0.569852
C	5.167470	-1.187728	0.777131
H	6.253374	-1.260422	0.666352
H	4.884378	-0.135352	0.795400
H	4.890473	-1.648149	1.730066
C	4.765697	-1.262226	-1.722744
H	4.213782	-1.778615	-2.513759
H	4.475885	-0.211441	-1.714467
H	5.833218	-1.333106	-1.950844
O	-1.663424	0.903520	-0.869882

H	0.804357	-2.172886	0.336371
H	0.129717	-0.513404	-2.062979

3i

Free Energy = -1642.526311 Hartree

Energy = -1642.869285 Hartree

C	-3.203586	-4.678715	-0.424791
C	-2.331617	-4.150957	-1.341244
C	-1.498005	-3.054316	-1.000957
C	-1.585056	-2.510990	0.306187
C	-2.488286	-3.078908	1.240887
C	-3.281376	-4.137879	0.880197
H	-0.504822	-2.897415	-2.919762
H	-3.836809	-5.517253	-0.696905
H	-2.264873	-4.563396	-2.344055
C	-0.577807	-2.486079	-1.917801
C	-0.751605	-1.406548	0.667216
H	-2.534182	-2.656258	2.237485
H	-3.972022	-4.567928	1.598335
C	0.116881	-0.841808	-0.259542
C	0.194712	-1.419082	-1.554182
H	0.870138	-0.978909	-2.276500
C	3.412537	0.509909	-0.599093
C	3.305768	-0.038648	0.680630
C	4.418429	-0.529837	1.364857
C	5.654232	-0.483227	0.740663
C	5.762254	0.061146	-0.546047
C	4.657273	0.561276	-1.225612
H	4.290196	-0.936292	2.363123
H	6.536682	-0.864880	1.241294
H	6.734518	0.094239	-1.027838
H	4.762305	0.981785	-2.219907
S	1.903207	1.128790	-1.268748
C	1.948749	0.029735	1.207840
O	1.615744	-0.184831	2.362918
C	0.911048	0.424557	0.130120
N	0.071394	1.456943	0.689600
C	-0.918156	1.987696	-0.097339
O	-0.945015	1.852792	-1.303668
O	-1.780974	2.676632	0.657146
C	-2.916692	3.349653	0.036018
C	-3.624968	3.978222	1.229075
H	-3.937007	3.207083	1.938243
H	-2.959751	4.675432	1.745343
H	-4.510863	4.524178	0.894600
C	-3.816068	2.325371	-0.648004
H	-4.738646	2.813968	-0.975014
H	-3.324639	1.883316	-1.514818
H	-4.080297	1.529641	0.054639
C	-2.423463	4.424022	-0.927214
H	-1.729363	5.097571	-0.416022
H	-1.921774	3.981762	-1.788027
H	-3.274706	5.014321	-1.278959
O	-0.914239	-0.953543	1.936118
H	-0.058753	-0.653498	2.298704
H	-0.091718	1.437323	1.687517

4a

Free Energy = -460.942688 Hartree

Energy = -461.063518 Hartree

C	3.188225	6.818653	1.448611
C	3.537680	5.853289	0.539939
C	2.688353	4.744803	0.294858
C	1.459892	4.639794	1.004653
C	1.124879	5.654597	1.939238
C	1.966664	6.715135	2.154982
H	3.959829	3.805182	-1.184274
H	3.844717	7.663295	1.629444
H	4.473593	5.923027	-0.008009
C	3.022323	3.727843	-0.640643
C	0.608426	3.531098	0.760927
H	0.187125	5.576470	2.482406
H	1.696744	7.483286	2.872742
C	0.965506	2.569073	-0.150419
C	2.189286	2.667678	-0.861802
H	2.431843	1.885254	-1.572368
O	0.201897	1.481743	-0.434978
H	-0.603515	1.507716	0.093986
H	-0.330366	3.453431	1.305306

IM1a-1

Free Energy = -2740.264846 Hartree

Energy = -2740.898344 Hartree

C	-2.699475	-0.640439	-0.883999
C	-2.915779	-1.013655	0.575946
C	-6.370586	-2.503789	0.704267
H	-5.177616	-1.806400	-0.884852
C	-5.454500	-2.415012	2.930803

H	-1.365192	-0.883771	3.593268	H	4.474029	5.926664	0.009919
C	-6.493832	-2.735834	2.098153	C	3.036417	3.724769	-0.621799
H	-5.512342	-2.589398	3.999667	C	0.653516	3.478600	0.830501
H	-7.396945	-3.171196	2.508026	H	0.233433	5.507926	2.570537
N	-3.268983	-1.579510	3.330755	H	1.728033	7.428410	2.951066
N	-1.299973	-0.799478	-1.278573	C	1.002449	2.532473	-0.100586
N	1.704065	-1.312689	-0.532339	C	2.202903	2.662126	-0.845536
C	3.063823	-1.561204	-0.355530	H	2.432000	1.911797	-1.596836
C	3.892285	-0.472877	-0.064792	C	0.699028	-2.205531	-0.731319
C	3.618657	-2.840219	-0.474961	C	-0.629160	-1.934033	-1.012582
C	5.259020	-0.660816	0.080637	C	0.446255	-3.677098	-0.647515
H	3.471358	0.523086	0.042905	C	-1.040358	-3.345430	-0.891354
C	4.989723	-2.995527	-0.314087	O	1.101235	-4.674336	-0.483501
H	2.991025	-3.706344	-0.664695	O	-2.090453	-3.933545	-0.923853
C	5.830577	-1.920897	-0.042374	C	-2.323302	3.059117	-1.338687
H	6.898486	-2.063316	0.071981	C	-4.772146	2.626553	-1.117270
C	5.595323	-4.359244	-0.509505	C	-3.723218	3.428131	-1.924851
C	6.113858	0.525069	0.430905	H	-1.920661	3.879262	-0.735940
F	4.733468	-5.336647	-0.212793	H	-1.599850	2.859611	-2.136672
F	5.982417	-4.543038	-1.781413	H	-3.908961	4.492280	-1.738966
F	6.684230	-4.526398	0.256185	C	-3.178505	2.228034	0.743888
F	7.384218	0.352758	0.043473	H	-3.353273	1.325503	1.326447
F	5.659264	1.646837	-0.151200	H	-2.550009	2.886593	1.350894
F	6.130157	0.751396	1.751736	C	-4.512993	2.911243	0.366018
C	-1.925380	-0.787887	1.501075	H	-5.324937	2.515265	0.982723
C	-5.219627	-1.947615	0.188619	H	-4.469114	3.991595	0.539299
C	-4.256217	-1.849103	2.432360	H	-5.777392	2.939534	-1.409936
C	-2.151227	-1.081715	2.867386	C	-4.594351	1.111449	-1.329950
C	-4.139957	-1.598634	1.032388	H	-5.140043	0.577027	-0.544587
H	-0.973620	-0.358234	1.199973	H	-5.002204	0.779310	-2.289716
H	-3.298882	-1.310533	-1.509876	C	-3.088821	0.804680	-1.267095
O	-7.344257	-2.800766	-0.191164	H	-2.679159	0.912203	-2.278809
C	-8.525901	-3.411043	0.283113	N	-2.397295	1.859685	-0.466840
H	-9.149987	-3.578380	-0.594591	C	-3.824704	3.206238	-3.408643
H	-8.318393	-4.374683	0.762673	H	-3.598704	2.206242	-3.781103
H	-9.063840	-2.761916	0.984157	C	-4.175851	4.146504	-4.279288
C	3.201315	6.794041	1.494196	H	-4.407030	5.158971	-3.957662
C	3.547703	5.841982	0.571275	H	-4.245079	3.942055	-5.342488
C	2.706002	4.725918	0.330045	H	-0.744037	0.044966	-1.332782
C	1.489618	4.602390	1.058918	H	1.406226	-0.342527	-0.444160
C	1.159230	5.603193	2.010021	O	0.244550	1.420431	-0.331556
C	1.992970	6.670519	2.220873	H	-0.744465	1.596659	-0.182114
H	3.962821	3.816162	-1.181291	H	-0.252514	3.354279	1.418650
H	3.851068	7.644229	1.672608				

IM2b-1

Free Energy = -3921.811321 Hartree

Energy = -3922.671070 Hartree

C	3.241277	-0.644095	0.086159
C	3.728473	-1.724691	-0.876658
C	6.667979	-3.336258	0.839529
H	5.316379	-1.834717	1.432982
C	6.362285	-4.340415	-1.327735
H	3.005104	-3.084058	-3.904800
C	7.068036	-4.263469	-0.156557
H	6.631998	-5.046966	-2.105103
H	7.917254	-4.916355	0.004277
N	4.587045	-3.675569	-2.753587
N	1.778624	-0.557224	0.039290
N	-1.402432	-1.469824	0.069214
C	-2.628337	-2.132764	-0.050052
C	-3.779356	-1.374996	-0.298430
C	-2.735466	-3.525992	0.031209
C	-5.011298	-2.002149	-0.423635
H	-3.724206	-0.296181	-0.399416
C	-3.983587	-4.124382	-0.090281
H	-1.866738	-4.146224	0.204456
C	-5.136197	-3.382088	-0.314289
H	-6.102130	-3.864407	-0.405173
C	-4.091104	-5.615567	0.075401
C	-6.231071	-1.172790	-0.717572
F	-2.987725	-6.244208	-0.349970
F	-4.272359	-5.958190	1.357952
F	-5.131175	-6.111876	-0.612527
F	-6.454744	-1.077484	-2.045605
F	-7.334604	-1.720419	-0.186909
F	-6.118344	0.069255	-0.248723
C	3.063235	-1.954021	-2.055418
C	5.588998	-2.506512	0.628288
C	5.243551	-3.507449	-1.572374
C	3.532842	-2.930479	-2.965486
C	4.857519	-2.556608	-0.580611
H	2.181089	-1.372855	-2.303313
H	3.522224	-0.962931	1.095689
O	7.300444	-3.203781	2.033075
C	8.379706	-4.067227	2.316013
H	8.715489	-3.809390	3.320491
H	8.071033	-5.119183	2.302229
H	9.210681	-3.922041	1.615181
C	-5.200509	1.894791	-2.677123
C	-4.191944	0.968678	-2.699363
C	-2.840262	1.367026	-2.538402
C	-2.529762	2.747166	-2.383654
C	-3.596318	3.685009	-2.384843
C	-4.894935	3.267589	-2.518857
H	-2.011535	-0.629467	-2.635145
H	-6.231788	1.572658	-2.772234
H	-4.417169	-0.086149	-2.828113
C	-1.778261	0.426477	-2.512838
H	-3.363029	4.739882	-2.271112
H	-5.700092	3.995241	-2.504282
C	-0.475191	0.825866	-2.348926
H	0.333437	0.098332	-2.344825
C	-0.904116	5.253515	1.043111
C	0.288401	4.524724	1.006504
C	1.519194	5.163975	1.145228
C	1.546846	6.544619	1.288299
C	0.352809	7.269250	1.295859
C	-0.883336	6.634815	1.177768
H	2.437588	4.586243	1.158367
H	2.496175	7.057075	1.398559
H	0.382035	8.348539	1.405934
H	-1.804162	7.207669	1.200973
C	-0.255962	-2.000214	0.570851
C	1.069165	-1.575962	0.550211
C	0.059132	-3.165107	1.441767
C	1.526515	-2.753612	1.335906
O	-0.572226	-4.009153	2.030025
O	2.590688	-3.141268	1.749749
S	-2.389447	4.281040	0.906036
C	0.068925	3.084034	0.840695
O	0.901402	2.210917	0.732206
C	3.658873	2.937737	-1.029496
C	5.932046	2.002757	-0.660362
C	5.067283	3.262417	-0.445023
H	3.491730	3.477406	-1.965678
H	2.859892	3.232615	-0.347742
H	5.510406	4.081221	-1.024225
C	4.394213	1.154520	-2.433277
H	4.366569	0.078164	-2.591061
H	3.986406	1.625208	-3.333049
C	5.840307	1.633451	-2.147027
H	6.555796	0.840774	-2.385420

H	6.098646	2.500654	-2.764185
H	6.966936	2.203923	-0.370893
C	5.371065	0.818900	0.143694
H	5.848023	-0.097848	-0.215877
H	5.603247	0.899485	1.210579
C	3.841913	0.769691	-0.069647
H	3.350565	1.344244	0.725819
N	3.483041	1.492997	-1.314323
C	4.998575	3.704893	0.989674
H	4.595263	2.988722	1.708051
C	5.370058	4.905446	1.427579
H	5.777414	5.653484	0.751647
H	5.293056	5.179415	2.475116
C	-1.436952	2.788374	0.894126
N	-1.844466	1.596878	1.059194
C	-3.249483	1.417321	1.206821
O	-4.044375	1.940620	0.465824
O	-3.634666	0.559784	2.143004
C	-2.922078	0.284638	3.396739
C	-3.985978	-0.448711	4.204064
H	-4.852532	0.195531	4.372047
H	-4.315250	-1.340118	3.664210
H	-3.579148	-0.755358	5.170954
C	-2.547083	1.600235	4.071700
H	-2.258656	1.406121	5.108279
H	-1.700826	2.086321	3.580741
H	-3.400717	2.284546	4.077845
C	-1.712752	-0.613092	3.172149
H	-2.012961	-1.556771	2.707852
H	-0.958678	-0.124893	2.551911
H	-1.264348	-0.846770	4.142659
H	1.341364	0.340418	-0.141508
H	-1.381455	-0.491545	-0.205326
C	-0.164082	2.206167	-2.224995
O	1.106466	2.635626	-2.112358
C	-1.177540	3.141694	-2.226951
H	-0.919255	4.193400	-2.133718
H	1.748478	1.921060	-1.886672

IM2c-1

Free Energy = -3921.818471 Hartree

Energy = -3922.680246 Hartree

C	-2.677475	-0.838309	-0.766152
C	-3.032990	-1.783735	0.383947
C	-5.591729	-4.159017	-1.039813
H	-4.421366	-2.642387	-1.912354
C	-5.252835	-4.654558	1.292506
H	-2.139447	-2.520934	3.577783
C	-5.907211	-4.915466	0.118381
H	-5.447785	-5.232372	2.189365
H	-6.643000	-5.709191	0.076706
N	-3.629687	-3.490705	2.571346
N	-1.237043	-0.599241	-0.824180
N	1.584609	-1.926991	-0.115722
C	2.889715	-2.375145	0.058622
C	3.619049	-1.798624	1.105068
C	3.489472	-3.344918	-0.751344
C	4.933910	-2.176824	1.324018
H	3.156189	-1.040001	1.728653
C	4.808277	-3.706931	-0.500094
H	2.935876	-3.817439	-1.558294
C	5.550493	-3.135247	0.527332
H	6.579223	-3.427248	0.700909
C	5.473897	-4.699752	-1.412393
C	5.679551	-1.570703	2.478569
F	4.604330	-5.588329	-1.906660
F	6.056708	-4.094278	-2.459059
F	6.437505	-5.385411	-0.776174
F	7.001568	-1.544080	2.257182
F	5.282537	-0.313239	2.722672
F	5.487986	-2.265351	3.611897
C	-2.346121	-1.717224	1.574006
C	-4.660661	-3.143597	-0.981167
C	-4.277222	-3.631850	1.382921
C	-2.683814	-2.588744	2.637554
C	-4.000652	-2.831885	0.232010
H	-1.537116	-1.000356	1.716750
H	-2.913706	-1.363390	-1.698021
O	-6.163510	-4.375064	-2.248493
C	-7.065710	-5.453181	-2.381016
H	-7.365507	-5.465397	-3.428697
H	-6.590730	-6.409710	-2.134094
H	-7.956881	-5.315085	-1.757285
C	5.008767	3.479238	-2.287892
C	4.912298	3.234779	-0.938239
C	3.827167	2.499385	-0.408052
C	2.816569	2.012157	-1.284931
C	2.954578	2.263330	-2.676771

C	4.020554	2.976971	-3.164587
H	4.499608	2.554317	1.653975
H	5.846110	4.044935	-2.683781
H	5.674688	3.602279	-0.255771
C	3.712076	2.211448	0.987186
C	1.696828	1.326413	-0.750440
H	2.192746	1.881584	-3.351789
H	4.103673	3.163498	-4.231142
C	2.646794	1.525761	1.483914
H	2.555817	1.315245	2.545605
C	1.342736	4.892465	-1.247542
C	0.434540	4.236022	-2.081778
C	0.450274	4.432410	-3.459996
C	1.390300	5.301260	-3.999209
C	2.303739	5.946479	-3.161169
C	2.294313	5.749803	-1.780780
H	-0.264873	3.901461	-4.080906
H	1.425143	5.472613	-5.069317
H	3.045884	6.610870	-3.592483
H	3.021320	6.243838	-1.145230
C	0.704000	-2.221375	-1.089861
C	-0.534637	-1.639125	-1.341476
C	0.512224	-3.230762	-2.176827
C	-0.874215	-2.614474	-2.387858
O	1.150626	-4.127842	-2.668662
O	-1.852443	-2.840826	-3.066230
S	1.177651	4.516430	0.484784
C	-0.454388	3.341163	-1.344971
O	-1.362432	2.658674	-1.780522
C	-3.953300	2.782644	-0.340492
C	-5.777892	1.106550	-0.098354
C	-5.487920	2.616908	-0.257243
H	-3.579383	3.598245	0.282723
H	-3.612740	2.954140	-1.362072
H	-5.862337	3.126558	0.638748
C	-3.859933	1.177655	1.478674
H	-3.205080	0.459896	1.961103
H	-3.808573	2.099761	2.061689
C	-5.295317	0.671064	1.290488
H	-5.326922	-0.420564	1.371832
H	-5.934917	1.080257	2.076995
H	-6.848888	0.923861	-0.212838
C	-4.994731	0.291590	-1.135992
H	-5.268793	-0.758750	-1.023956
H	-5.266709	0.582511	-2.154324
C	-3.469258	0.474474	-0.933211
H	-3.012329	0.939629	-1.808941
N	-3.280217	1.525087	0.136928
C	-6.157068	3.230172	-1.454632
H	-5.852178	2.847911	-2.429408
C	-7.076946	4.185649	-1.387001
H	-7.399138	4.598205	-0.434319
H	-7.542068	4.590721	-2.279248
H	-2.263114	1.777042	0.269922
C	-0.121604	3.388428	0.143516
N	-0.869612	2.711700	0.943713
C	-0.503942	2.670063	2.300129
O	0.445271	3.253269	2.775538
O	-1.384525	1.930672	2.974130
C	-1.137928	1.626125	4.382582
C	-2.278912	0.676689	4.724108
H	-3.248213	1.157632	4.559939
H	-2.226965	-0.226056	4.108900
H	-2.219732	0.380327	5.774248
C	-1.236707	2.899070	5.215826
H	-1.155790	2.642641	6.276206
H	-0.439281	3.598460	4.964848
H	-2.204127	3.385020	5.056478
C	0.211635	0.927842	4.531213
H	0.346464	0.204497	3.720785
H	1.032601	1.644619	4.492937
H	0.246865	0.406601	5.492293
H	-0.757386	-0.096923	-0.057033
H	1.262296	-1.186297	0.525682
H	0.935785	0.934426	-1.423468
C	1.587009	1.049576	0.624654
O	0.597317	0.374869	1.131013

IM2d-1

Free Energy = -3921.830086 Hartree

Energy = -3922.686301 Hartree

C	-3.020991	0.950618	0.242457
C	-3.164458	1.623034	-1.120563
C	-6.120032	3.935781	-0.793594
H	-5.115606	2.698322	0.582873
C	-5.285875	4.023646	-3.050040
H	-1.713782	1.691121	-4.190014
C	-6.200038	4.437293	-2.117552

H	-5.308105	4.397526	-4.067935	C	0.422454	-1.278915	-1.788411
H	-6.967204	5.150135	-2.394519	H	1.767613	1.047124	-2.002643
N	-3.385013	2.768740	-3.711824	H	3.685463	1.488776	-3.496462
N	-1.600006	0.743385	0.548993	C	0.309201	-3.537744	-2.657703
N	1.647710	1.462319	0.877518	H	-0.154522	-4.517155	-2.599606
C	2.917555	2.075006	0.970293	C	2.680520	-4.516459	-0.435210
C	3.927755	1.693642	0.087656	C	3.239624	-3.264992	-0.697023
C	3.176213	3.061251	1.925284	C	4.246348	-3.100915	-1.642252
C	5.177424	2.296088	0.162780	C	4.697430	-4.223239	-2.328092
H	3.739586	0.928688	-0.656021	C	4.141306	-5.475178	-2.057512
C	4.428510	3.659913	1.970087	C	3.128585	-5.640889	-1.109585
H	2.401576	3.372974	2.614898	H	4.640647	-2.105881	-1.832358
C	5.445656	3.288305	1.095721	H	5.475913	-4.127655	-3.076638
H	6.418218	3.764148	1.141004	H	4.499798	-6.345504	-2.598063
C	4.714722	4.679349	3.036642	H	2.704708	-6.620548	-0.917284
C	6.204148	1.896233	-0.857150	C	0.494095	2.164299	0.919278
F	3.613008	5.340558	3.405724	C	-0.855094	1.848853	0.779198
F	5.217305	4.103977	4.142342	C	0.209998	3.625906	1.015843
F	5.618196	5.582034	2.626309	C	-1.269063	3.269400	0.880827
F	5.931056	2.424366	-2.063518	O	0.865846	4.628862	1.150174
F	7.435764	2.299192	-0.520158	O	-2.323305	3.858020	0.863411
F	6.242647	0.564849	-1.025217	S	1.385654	-4.508109	0.795490
C	-2.269642	1.348288	-2.124715	C	2.613666	-2.194527	0.073477
C	-5.144070	3.027517	-0.448597	O	2.933252	-1.030627	0.125773
C	-4.265413	3.097415	-2.725223	C	-3.733625	-2.756442	0.339461
C	-2.423669	1.937192	-3.402386	C	-5.888759	-1.598419	-0.106967
C	-4.202611	2.571880	-1.400098	C	-5.252438	-2.755001	0.693108
H	-1.454236	0.654245	-1.953579	H	-3.481886	-3.600006	-0.309427
H	-3.437389	1.638773	0.987489	H	-3.120795	-2.839629	1.238560
O	-6.974045	4.303425	0.197216	H	-5.699386	-3.693279	0.343202
C	-7.953175	5.275063	-0.094740	C	-3.975451	-1.546852	-1.704013
H	-8.499421	5.440721	0.834080	H	-3.773550	-0.603281	-2.206580
H	-7.502175	6.221341	-0.416577	H	-3.483024	-2.335528	-2.281438
H	-8.655419	4.927585	-0.862376	C	-5.499571	-1.792790	-1.578486
C	3.610281	-0.459809	-4.447311	H	-6.049209	-1.090510	-2.212430
C	2.986783	-1.681773	-4.486132	H	-5.766104	-2.803664	-1.905600
C	1.912193	-1.977110	-3.609063	H	-6.975135	-1.613077	0.015766
C	1.459842	-0.974818	-2.706804	C	-5.317064	-0.244473	0.346053
C	2.115244	0.284785	-2.697081	H	-5.596662	0.511784	-0.393654
C	3.173740	0.532185	-3.535775	H	-5.736897	0.077856	1.304391
H	1.655774	-4.036152	-4.233008	C	-3.781804	-0.376550	0.452694
H	4.441428	-0.248518	-5.111872	H	-3.522308	-0.662634	1.479344
H	3.321668	-2.451425	-5.176951	N	-3.323738	-1.521266	-0.371929
C	1.304032	-3.262885	-3.555089	C	-5.492508	-2.660534	2.173451

H	-5.099361	-1.777475	2.680463
C	-6.123983	-3.582671	2.893892
H	-6.528275	-4.481446	2.434631
H	-6.264643	-3.473062	3.964441
H	-1.713172	-2.121566	-0.639654
C	1.439851	-2.748658	0.892108
N	0.682104	-1.921331	1.486050
C	-0.394033	-2.338048	2.287839
O	-1.417598	-1.689426	2.340554
O	-0.115261	-3.428641	2.984481
C	-0.991170	-3.908914	4.065260
C	-0.279967	-5.174669	4.521557
H	-0.267388	-5.919131	3.720836
H	0.751201	-4.953774	4.807927
H	-0.798807	-5.601329	5.383520
C	-2.384042	-4.224252	3.535244
H	-2.919137	-4.827199	4.274822
H	-2.962880	-3.319557	3.353264
H	-2.320323	-4.803990	2.609103
C	-1.017264	-2.857607	5.166645
H	-0.003920	-2.644906	5.517777
H	-1.478203	-1.931890	4.817071
H	-1.601161	-3.234174	6.010973
H	-1.331712	-0.146115	0.965185
H	1.638345	0.459854	0.697410
C	-0.150958	-2.531283	-1.761538
O	-1.107724	-2.883727	-0.877899
H	0.108459	-0.531113	-1.061763

IM2a-1

Free Energy = -3921.830769 Hartree

Energy = -3922.693555 Hartree

C	2.258734	-2.169385	-0.311703
C	3.125646	-1.425430	-1.305433
C	5.639386	-3.939989	-2.554483
H	3.963129	-4.110490	-1.289776
C	6.147397	-1.771231	-3.472101
H	3.596063	1.707903	-2.514692
C	6.451604	-3.102846	-3.360536
H	6.743843	-1.105402	-4.086306
H	7.304050	-3.506606	-3.892886
N	4.808579	0.125562	-2.972578
N	0.870826	-1.774977	-0.475618
N	-2.269244	-1.602897	-0.630096
C	-3.651944	-1.578009	-0.733996
C	-4.213136	-0.552830	-1.503491
C	-4.496996	-2.489628	-0.082779
C	-5.592866	-0.413203	-1.582008
H	-3.563895	0.141804	-2.029731
C	-5.870911	-2.334496	-0.200637
H	-4.085153	-3.302236	0.510768
C	-6.443831	-1.298268	-0.936092
H	-7.519490	-1.189830	-1.004084
C	-6.785700	-3.261683	0.550836
C	-6.132153	0.728903	-2.394962
F	-6.188629	-4.412274	0.874538
F	-7.216895	-2.700626	1.693033
F	-7.880931	-3.558077	-0.167693
F	-7.463202	0.837611	-2.293865
F	-5.600040	1.897657	-1.999459
F	-5.837777	0.594090	-3.696153
C	2.893216	-0.093366	-1.535563
C	4.556248	-3.419168	-1.877275
C	5.039105	-1.206814	-2.796757
C	3.769483	0.643021	-2.371090
C	4.229909	-2.046818	-1.974481
H	2.066451	0.426448	-1.057474
H	2.312709	-3.246578	-0.500987
O	5.859261	-5.267526	-2.396719
C	6.937934	-5.855909	-3.093589
H	6.918125	-6.914797	-2.836816
H	6.823946	-5.748989	-4.178558
H	7.899809	-5.431401	-2.782913
C	-0.600995	6.699672	-2.344931
C	-1.577200	5.881530	-1.826433
C	-1.340059	4.502542	-1.626051
C	-0.069343	3.951259	-1.959610
C	0.913047	4.819807	-2.508534
C	0.654372	6.154366	-2.697222
H	-3.326926	4.031188	-0.888291
H	-0.793911	7.756879	-2.495880
H	-2.552837	6.284852	-1.566036
C	-2.344307	3.622971	-1.115338
C	0.188943	2.580062	-1.713847
H	1.882890	4.406242	-2.774919
H	1.422204	6.799627	-3.113646
C	-2.090004	2.302700	-0.909002
H	-2.855786	1.647391	-0.502465

C	1.094880	4.936418	0.903734
C	2.289993	4.378102	0.444098
C	3.306170	5.177837	-0.072993
C	3.110540	6.551393	-0.128956
C	1.907575	7.102806	0.321215
C	0.887289	6.306844	0.839877
H	4.222925	4.712387	-0.422319
H	3.884205	7.197461	-0.528588
H	1.756664	8.175929	0.259593
H	-0.046772	6.748181	1.170150
C	-1.488563	-2.514292	-0.013090
C	-0.093466	-2.542029	0.038485
C	-1.602242	-3.739644	0.822134
C	-0.079423	-3.735038	0.894244
O	-2.489789	-4.426755	1.274220
O	0.793119	-4.379141	1.448725
S	-0.080010	3.763450	1.538329
C	2.313449	2.924296	0.570917
O	3.241840	2.169276	0.351090
C	2.893988	-0.579720	3.096053
C	4.574032	-2.398499	2.783963
C	3.577140	-1.786892	3.794759
H	3.303647	0.377954	3.426976
H	1.812868	-0.577637	3.238919
H	4.153547	-1.401124	4.642961
C	4.585396	-0.361792	1.341181
H	4.767073	-0.544702	0.284503
H	4.723999	0.704033	1.520414
C	5.449489	-1.258567	2.246192
H	6.285284	-1.657026	1.665502
H	5.872728	-0.682785	3.075211
H	5.183094	-3.154408	3.284494
C	3.817809	-3.010057	1.594003
H	4.522966	-3.183656	0.773067
H	3.342555	-3.964414	1.835517
C	2.710719	-2.040673	1.167514
H	1.811136	-2.236333	1.752422
N	3.134024	-0.655407	1.611270
C	2.589234	-2.793047	4.327063
H	1.898814	-3.251241	3.616679
C	2.537281	-3.152629	5.604892
H	3.206774	-2.723291	6.346651
H	1.823591	-3.890056	5.956269
C	0.979971	2.418124	1.124714
N	0.883228	1.153371	1.315197
C	-0.247468	0.539839	1.883055
O	-0.213515	-0.625930	2.220238
O	-1.263165	1.375101	2.065808
C	-2.429741	1.005188	2.876385
C	-3.233713	2.298256	2.901367
H	-2.684128	3.086898	3.422780
H	-3.439230	2.634289	1.881120
H	-4.183517	2.136586	3.417604
C	-1.972673	0.618023	4.278011
H	-2.849059	0.523812	4.925298
H	-1.437648	-0.332201	4.278165
H	-1.326788	1.397694	4.693670
C	-3.209043	-0.106363	2.190728
H	-3.512355	0.209022	1.189237
H	-2.618506	-1.021669	2.118416
H	-4.115162	-0.320331	2.765459
C	-0.797972	1.718988	-1.200276
O	-0.583607	0.470419	-0.952874
H	-1.755947	-0.736116	-0.910569
H	0.599204	-0.869972	-0.878618
H	2.520417	0.069541	1.177507
H	1.140852	2.153901	-2.020963

TS1b-1

Free Energy = -3921.778126 Hartree

Energy = -3922.638316 Hartree

C	2.868425	0.949435	-0.649365
C	3.137678	1.570497	0.718725
C	5.930198	4.047382	0.199256
H	4.672098	3.015167	-1.141218
C	5.523104	3.780382	2.558492
H	2.214722	1.212282	3.964740
C	6.248404	4.352923	1.547391
H	5.723844	4.010544	3.599128
H	7.044680	5.048257	1.783349
N	3.780256	2.380538	3.356610
N	1.440344	0.689224	-0.848600
N	-1.830968	1.325621	-0.873332
C	-3.140061	1.848237	-0.923675
C	-4.138359	1.247395	-0.153190
C	-3.463847	2.931491	-1.741536
C	-5.429596	1.751721	-0.179995
H	-3.922699	0.375683	0.456532

C	-4.765331	3.422973	-1.744766	H	2.516720	-4.777142	-1.083740
H	-2.710688	3.405661	-2.357717	H	2.692130	-7.150465	-0.375826
C	-5.762586	2.848563	-0.966905	H	0.883531	-8.173368	0.967539
H	-6.772684	3.240788	-0.977742	H	-1.130588	-6.873566	1.580133
C	-5.109196	4.551755	-2.674942	C	-0.714652	2.072816	-0.987106
C	-6.449068	1.131238	0.732116	C	0.646511	1.774311	-0.970295
F	-4.077755	5.384451	-2.852486	C	-0.449163	3.541474	-1.070584
F	-5.458836	4.096775	-3.890376	C	1.032911	3.193086	-1.122926
F	-6.144462	5.272507	-2.218321	O	-1.112613	4.547537	-1.084680
F	-7.701576	1.356673	0.308980	O	2.081764	3.785160	-1.242302
F	-6.280235	-0.187093	0.846132	S	-1.836607	-4.061135	0.878547
F	-6.361248	1.644893	1.976071	C	0.369689	-3.065162	-0.384381
C	2.418649	1.147152	1.807942	O	1.122870	-2.295372	-0.963980
C	4.918520	3.158747	-0.096205	C	4.124305	-2.650784	-0.444245
C	4.469458	2.873672	2.288926	C	6.060778	-1.179010	-0.986213
C	2.776648	1.578879	3.108332	C	5.419704	-2.550380	-1.288635
C	4.179378	2.531869	0.933439	H	4.197867	-3.364067	0.379435
H	1.602491	0.443438	1.693406	H	3.256956	-2.907258	-1.048898
H	3.171150	1.669433	-1.416040	H	6.118253	-3.324470	-0.952606
O	6.574994	4.592570	-0.861157	C	4.861518	-1.015587	1.197112
C	7.561011	5.572393	-0.613469	H	4.656087	-0.037274	1.620369
H	7.911222	5.899337	-1.592379	H	4.719846	-1.756488	1.986069
H	7.148049	6.433612	-0.075584	C	6.249820	-1.078576	0.532274
H	8.408481	5.162206	-0.051351	H	6.815063	-0.177402	0.784405
C	-3.604944	-1.008310	4.147555	H	6.819367	-1.937245	0.899613
C	-2.724885	-2.040143	4.425917	H	7.021357	-1.102496	-1.500752
C	-1.562293	-2.208602	3.661007	C	5.133498	-0.034115	-1.422187
C	-1.299608	-1.329478	2.587987	H	5.503128	0.898472	-0.986942
C	-2.178629	-0.267071	2.344735	H	5.127915	0.095691	-2.507775
C	-3.321955	-0.110347	3.112705	C	3.696311	-0.318466	-0.944012
H	-0.812247	-3.921099	4.775644	H	3.144984	-0.852737	-1.724869
H	-4.506232	-0.886471	4.738385	N	3.798929	-1.323139	0.176214
H	-2.924372	-2.727580	5.243628	C	5.155030	-2.771400	-2.753253
C	-0.584938	-3.231211	3.965668	H	4.388134	-2.148755	-3.216075
H	-1.942347	0.441852	1.555739	C	5.793811	-3.668736	-3.495685
H	-4.006574	0.707714	2.908151	H	6.558655	-4.314815	-3.071950
C	0.607783	-3.312243	3.328486	H	5.578653	-3.790547	-4.551806
H	1.367894	-4.031705	3.613540	H	2.888317	-1.492338	0.716676
C	-0.427407	-5.079531	0.608335	C	-0.976399	-2.623178	0.177263
C	0.617959	-4.484294	-0.105952	N	-1.628005	-1.727942	-0.579298
C	1.740970	-5.228139	-0.475890	C	-2.997815	-1.743785	-0.542438
C	1.831029	-6.556478	-0.090957	O	-3.708563	-2.176170	0.345839
C	0.802503	-7.134731	0.662512	O	-3.583379	-1.126390	-1.608959
C	-0.329499	-6.410565	1.013491	C	-3.226609	-1.465015	-2.977194

C	-4.452176	-1.006560	-3.760577
H	-5.338533	-1.555107	-3.432506
H	-4.626779	0.060089	-3.591129
H	-4.307886	-1.171466	-4.832103
C	-3.039708	-2.974317	-3.105348
H	-2.966000	-3.251703	-4.160859
H	-2.127269	-3.304854	-2.601909
H	-3.893523	-3.499167	-2.666717
C	-1.988635	-0.706275	-3.448827
H	-2.146825	0.372721	-3.359059
H	-1.107339	-0.991731	-2.870882
H	-1.805925	-0.933991	-4.503956
H	1.077812	-0.262671	-0.900773
H	-1.721434	0.311285	-0.771116
C	0.942382	-2.377530	2.267152
O	2.116429	-2.317226	1.817537
C	-0.152964	-1.587736	1.732450
H	0.143544	-0.786998	1.058254

TS1d-1

Free Energy = -3921.788584 Hartree

Energy = -3922.652937 Hartree

C	-3.149846	0.808676	0.407302
C	-3.631688	0.787581	-1.036820
C	-6.864357	2.721952	-1.050416
H	-5.396451	2.408209	0.427736
C	-6.500967	1.753077	-3.224710
H	-2.811845	-0.533681	-4.050115
C	-7.287021	2.497840	-2.384919
H	-6.786008	1.576018	-4.256094
H	-8.215926	2.919257	-2.749282
N	-4.547546	0.490611	-3.702126
N	-1.685166	0.810485	0.470559
N	1.448324	1.755486	0.303026
C	2.708940	2.372536	0.269943
C	3.840470	1.570119	0.094304
C	2.866657	3.753434	0.432352
C	5.102032	2.149614	0.061408
H	3.727385	0.497121	-0.018176
C	4.140519	4.304357	0.382403
H	2.010578	4.398741	0.578931
C	5.275141	3.520152	0.198572
H	6.262033	3.966240	0.169228
C	4.296665	5.796534	0.488111
C	6.288351	1.241504	-0.090067
F	5.459547	6.126046	1.073174
F	4.289217	6.381206	-0.717288
F	3.311904	6.352070	1.205224
F	7.375968	1.898492	-0.510568
F	6.607211	0.639654	1.064667
F	6.043237	0.257680	-0.977881
C	-2.891427	0.141557	-1.992909
C	-5.683002	2.179523	-0.592000
C	-5.277022	1.192160	-2.788005
C	-3.395879	0.010740	-3.310688
C	-4.868127	1.392199	-1.436552
H	-1.939701	-0.308909	-1.739562
H	-3.535307	1.716776	0.888727
O	-7.569125	3.461854	-0.157240
C	-8.753257	4.090133	-0.598568
H	-9.133064	4.649757	0.256238
H	-8.558589	4.786019	-1.423009
H	-9.509257	3.358973	-0.909244
C	3.802958	-1.804684	-3.974696
C	2.908369	-2.861889	-4.048473
C	1.739860	-2.863916	-3.276677
C	1.480352	-1.790281	-2.392860
C	2.374364	-0.708015	-2.362944
C	3.524699	-0.718309	-3.139181
H	0.955359	-4.728798	-4.084694
H	4.707276	-1.813270	-4.573783
H	3.101441	-3.698137	-4.715354
C	0.746269	-3.913314	-3.395587
C	0.338567	-1.866559	-1.498763
H	2.149482	0.144494	-1.728960
H	4.211475	0.120856	-3.089635
C	-0.425139	-3.878775	-2.725635
H	-1.185772	-4.641450	-2.854142
C	2.422127	-4.474417	-0.274907
C	3.009404	-3.210688	-0.146069
C	4.318176	-2.976983	-0.561174
C	5.042541	-4.030316	-1.102984
C	4.455543	-5.293454	-1.224965
C	3.144951	-5.531100	-0.817908
H	4.741629	-1.980900	-0.471268
H	6.060410	-3.873675	-1.442222
H	5.029713	-6.108811	-1.653965
H	2.697848	-6.513073	-0.929776

C	0.274341	2.351654	-0.021662
C	-1.047173	1.921844	0.045612
C	-0.112611	3.645869	-0.659558
C	-1.565814	3.181241	-0.536017
O	0.458694	4.625894	-1.066716
O	-2.662745	3.623612	-0.773853
S	0.749522	-4.547585	0.294584
C	2.084845	-2.194658	0.357998
O	2.348864	-1.021687	0.582515
C	-3.269309	-2.675388	1.898259
C	-5.583525	-1.752634	2.001773
C	-4.493138	-2.471836	2.825385
H	-3.210545	-3.679824	1.473974
H	-2.328101	-2.454868	2.396345
H	-4.870721	-3.469177	3.084905
C	-4.475150	-2.231103	-0.173311
H	-4.650109	-1.462885	-0.923387
H	-4.071224	-3.107047	-0.679250
C	-5.726500	-2.511598	0.674709
H	-6.613205	-2.175350	0.131534
H	-5.843805	-3.583795	0.861057
H	-6.532992	-1.746024	2.541933
C	-5.140519	-0.317436	1.659532
H	-5.750048	0.057858	0.831821
H	-5.267500	0.365893	2.502183
C	-3.654045	-0.352020	1.285614
H	-3.057936	-0.309719	2.203224
N	-3.375189	-1.734866	0.732214
C	-4.115124	-1.775355	4.114199
H	-3.096324	-1.948101	4.461302
C	-4.919379	-1.008964	4.844223
H	-5.947401	-0.801496	4.558940
H	-4.577536	-0.567755	5.774250
H	-2.478012	-1.798800	0.193506
C	0.693549	-2.760577	0.477167
N	-0.282230	-2.220140	1.190824
C	-0.013706	-1.487053	2.287295
O	-0.788280	-0.622414	2.730836
O	1.104144	-1.852705	2.940489
C	1.646106	-1.051919	4.028043
C	2.956298	-1.766926	4.337109
H	2.765644	-2.799349	4.642307
H	3.595947	-1.779782	3.450182
H	3.486431	-1.254975	5.144584
C	0.710407	-1.094724	5.232176
H	1.210822	-0.655329	6.100396
H	-0.208720	-0.542865	5.035920
H	0.460232	-2.132494	5.472952
C	1.919844	0.373164	3.556311
H	2.590610	0.358488	2.691916
H	0.994803	0.888624	3.292316
H	2.408914	0.933033	4.359091
H	-1.269951	0.280554	1.248977
H	1.449512	0.758708	0.522613
C	-0.738170	-2.793232	-1.796946
O	-1.854438	-2.731192	-1.243879
H	0.065453	-0.964204	-0.956143

TS1c-1

Free Energy = -3921.794000 Hartree

Energy = -3922.657331 Hartree

C	-3.010862	-0.605049	-0.664640
C	-3.762022	-1.540455	0.285288
C	-6.947411	-2.490093	-1.496100
H	-5.261519	-1.381425	-2.091156
C	-6.948170	-3.451958	0.709805
H	-3.398903	-3.060436	3.302500
C	-7.586305	-3.252670	-0.484996
H	-7.394586	-4.050447	1.496367
H	-8.561567	-3.691747	-0.655754
N	-5.086531	-3.212711	2.158224
N	-1.574037	-0.806503	-0.529515
N	1.328170	-2.147815	-0.273309
C	2.545562	-2.786827	-0.046832
C	3.575704	-2.012891	0.502973
C	2.775731	-4.138178	-0.333093
C	4.825240	-2.578313	0.720424
H	3.385849	-0.974788	0.766672
C	4.032570	-4.674816	-0.083968
H	1.986435	-4.764931	-0.738579
C	5.076719	-3.912692	0.432683
H	6.050223	-4.350248	0.615418
C	4.288804	-6.110688	-0.451226
C	5.904672	-1.686149	1.263633
F	3.194522	-6.866399	-0.307281
F	4.684613	-6.229056	-1.728377
F	5.257341	-6.648679	0.306966
F	7.038625	-2.355676	1.509517

F	6.200929	-0.700464	0.399929	O	-2.851803	-3.568159	-1.683666
F	5.528608	-1.094911	2.406737	S	2.663566	3.096297	0.935459
C	-3.170383	-1.946815	1.454984	C	0.424412	4.265185	-0.089483
C	-5.710415	-1.926599	-1.269232	O	-0.700494	4.431889	-0.521439
C	-5.666785	-2.904723	0.965135	C	-3.051991	3.143532	0.385779
C	-3.872824	-2.771526	2.365645	C	-5.226733	2.008011	0.680281
C	-5.045937	-2.094740	-0.032614	C	-4.535539	3.385357	0.724671
H	-2.159096	-1.624365	1.681920	H	-2.367473	3.707376	1.018463
H	-3.334714	-0.869642	-1.681702	H	-2.810750	3.406283	-0.644472
O	-7.489742	-2.267658	-2.718244	H	-4.618310	3.773656	1.747050
C	-8.727309	-2.876103	-3.022141	C	-3.194665	1.251173	1.908827
H	-8.954896	-2.595236	-4.050324	H	-2.729195	0.299927	2.139178
H	-8.667183	-3.968499	-2.954943	H	-2.802284	1.989349	2.612690
H	-9.528871	-2.512701	-2.368189	C	-4.731170	1.202306	1.888211
C	4.425037	5.168721	-3.058356	H	-5.079708	0.167427	1.823266
C	4.719457	3.887975	-2.634481	H	-5.123333	1.624595	2.817115
C	3.692363	2.993342	-2.284783	H	-6.311728	2.130102	0.715498
C	2.342590	3.416242	-2.349203	C	-4.830202	1.268435	-0.607046
C	2.063807	4.713168	-2.824506	H	-5.428507	0.362560	-0.690040
C	3.085478	5.575607	-3.168516	H	-5.058462	1.879046	-1.484940
H	5.012851	1.304531	-1.902502	C	-3.320644	0.916218	-0.589031
H	5.223692	5.854333	-3.321689	H	-2.819025	1.345206	-1.463143
H	5.751386	3.552888	-2.570620	N	-2.703675	1.686348	0.561934
C	3.973664	1.625450	-1.918468	C	-5.142243	4.398228	-0.204292
C	1.307178	2.533240	-1.866535	H	-5.084766	4.178466	-1.270724
H	1.026730	5.034877	-2.889608	C	-5.732415	5.517775	0.198017
H	2.851647	6.576425	-3.517677	H	-5.798988	5.778564	1.251156
C	2.991954	0.740259	-1.636466	H	-6.168947	6.215421	-0.508557
H	3.214912	-0.301404	-1.432293	H	-1.641016	1.665043	0.552056
C	2.656637	4.817917	0.544644	C	0.987850	2.899839	0.286578
C	1.430932	5.310594	0.097962	N	0.125706	2.000911	0.768943
C	1.264723	6.652356	-0.238488	C	0.659914	0.936799	1.450960
C	2.350854	7.507219	-0.127802	O	1.811720	0.529211	1.384794
C	3.588049	7.006578	0.295306	O	-0.269607	0.394846	2.273822
C	3.757270	5.666936	0.631561	C	0.169579	-0.408727	3.414724
H	0.296072	6.990930	-0.594132	C	-1.089031	-0.528418	4.268654
H	2.251888	8.556808	-0.381889	H	-1.451252	0.461485	4.560821
H	4.439464	7.677061	0.359585	H	-1.889290	-1.052286	3.738858
H	4.725057	5.292529	0.948103	H	-0.866948	-1.093412	5.177446
C	0.151078	-2.664359	-0.684257	C	1.246358	0.331003	4.208013
C	-1.093337	-2.049395	-0.802630	H	1.399201	-0.179981	5.162810
C	-0.400336	-3.985363	-1.123174	H	2.195599	0.363799	3.674848
C	-1.746383	-3.277758	-1.292896	H	0.921721	1.354870	4.419034
O	0.015617	-5.105129	-1.289907	C	0.645489	-1.780283	2.953611

H	-0.102362	-2.257677	2.311244
H	1.583836	-1.703780	2.403917
H	0.804554	-2.422734	3.825062
H	-0.933381	-0.044553	-0.784880
H	1.334023	-1.126382	-0.225277
H	0.270319	2.769900	-2.088937
C	1.594172	1.142268	-1.637477
O	0.679364	0.321403	-1.380607

TS1a-1

Free Energy = -3921.818102 Hartree

Energy = -3922.682378 Hartree

C	2.247178	-2.167677	-0.316582
C	3.113339	-1.503330	-1.366065
C	5.545701	-4.138554	-2.521232
H	3.931079	-4.187903	-1.169283
C	6.033315	-2.054185	-3.626385
H	3.580362	1.530225	-2.808303
C	6.328461	-3.377267	-3.425945
H	6.609098	-1.445293	-4.314896
H	7.152446	-3.832084	-3.961971
N	4.741412	-0.105474	-3.212984
N	0.850931	-1.819969	-0.539239
N	-2.310923	-1.737008	-0.692192
C	-3.696947	-1.727570	-0.754363
C	-4.288367	-0.717084	-1.518893
C	-4.512436	-2.638767	-0.067539
C	-5.670762	-0.589268	-1.559573
H	-3.659967	-0.026627	-2.075419
C	-5.890278	-2.496515	-0.148366
H	-4.075697	-3.440494	0.522788
C	-6.493947	-1.474039	-0.878988
H	-7.572153	-1.375931	-0.916574
C	-6.777194	-3.425197	0.635113
C	-6.241167	0.539884	-2.368908
F	-6.151647	-4.554149	0.979226
F	-7.209443	-2.845398	1.766717
F	-7.871889	-3.761620	-0.066145
F	-7.568616	0.640036	-2.234481
F	-5.706702	1.717208	-1.997558
F	-5.977057	0.396483	-3.675504
C	2.895047	-0.186413	-1.677713
C	4.498906	-3.553393	-1.840190
C	4.963051	-1.424027	-2.947567
C	3.742147	0.474406	-2.600000
C	4.181835	-2.188380	-2.029516
H	2.112166	0.380241	-1.181913
H	2.311058	-3.254811	-0.422917
O	5.761701	-5.452509	-2.268766
C	6.808696	-6.103915	-2.957030
H	6.794462	-7.138280	-2.614155
H	6.652390	-6.085100	-4.041922
H	7.784282	-5.663123	-2.720456
C	-0.424074	6.747486	-2.219176
C	-1.456424	5.942467	-1.775654
C	-1.244428	4.574527	-1.534707
C	0.042600	4.021974	-1.723234
C	1.068499	4.849610	-2.213379
C	0.841534	6.190979	-2.456565
H	-3.313386	4.135323	-1.013031
H	-0.595842	7.803019	-2.401950
H	-2.448129	6.357479	-1.616884
C	-2.327933	3.695674	-1.151252
C	0.276092	2.636060	-1.361167
H	2.053113	4.421362	-2.385956
H	1.647998	6.816190	-2.826022
C	-2.161045	2.362710	-1.004393
H	-2.993700	1.711091	-0.757046
C	1.131650	4.985728	1.098325
C	2.312885	4.474803	0.557679
C	3.367707	5.310301	0.196180
C	3.223633	6.679065	0.369513
C	2.031518	7.191941	0.895053
C	0.978691	6.359956	1.263576
H	4.267846	4.873576	-0.226343
H	4.025364	7.354415	0.092010
H	1.921586	8.265321	1.014642
H	0.057233	6.773442	1.659591
C	-1.492815	-2.611720	-0.062957
C	-0.100233	-2.597066	-0.015906
C	-1.574374	-3.830864	0.781816
C	-0.050920	-3.783004	0.853698
O	-2.442722	-4.537975	1.238754
O	0.838856	-4.397739	1.408605
S	-0.077573	3.767096	1.510919
C	2.264221	3.027043	0.348694
O	3.181211	2.320065	-0.027904
C	2.771262	-0.431334	3.051301

C	4.582607	-2.118885	2.756417
C	3.556756	-1.561727	3.768557
H	3.112357	0.562278	3.352549
H	1.695586	-0.503704	3.213842
H	4.114464	-1.112908	4.598258
C	4.407746	-0.119025	1.270076
H	4.593114	-0.300250	0.214236
H	4.468290	0.957342	1.429424
C	5.355865	-0.927508	2.176100
H	6.209830	-1.273953	1.588199
H	5.748754	-0.303182	2.984900
H	5.257420	-2.812906	3.262750
C	3.856911	-2.816481	1.596057
H	4.562896	-2.963934	0.770299
H	3.459970	-3.797103	1.872752
C	2.677334	-1.941067	1.155103
H	1.792693	-2.191364	1.742227
N	2.988848	-0.519463	1.563296
C	2.659574	-2.628665	4.340425
H	1.975640	-3.133692	3.656371
C	2.676102	-2.985732	5.619901
H	3.340353	-2.508109	6.336417
H	2.026539	-3.767648	5.998552
C	0.875466	2.473449	0.662458
N	0.874833	1.180302	1.007093
C	-0.193102	0.573224	1.610662
O	-0.145756	-0.580453	2.023025
O	-1.273016	1.365932	1.752328
C	-2.351605	1.020116	2.673117
C	-3.200506	2.286161	2.691460
H	-2.646950	3.118677	3.134021
H	-3.487754	2.565270	1.673968
H	-4.107369	2.119168	3.278987
C	-1.790816	0.736463	4.063416
H	-2.615169	0.702112	4.781726
H	-1.258299	-0.213907	4.096144
H	-1.112135	1.541179	4.364457
C	-3.148955	-0.152053	2.119804
H	-3.544389	0.100257	1.131659
H	-2.527886	-1.046657	2.044906
H	-3.997191	-0.365162	2.777586
C	-0.856784	1.747754	-1.209757
O	-0.700733	0.504728	-1.175217
H	-1.846547	-0.884156	-1.027018
H	0.587579	-0.907457	-0.911902
H	2.282429	0.165361	1.134917
H	1.169986	2.165544	-1.763293

IM3b-1

Free Energy = -3921.785527 Hartree

Energy = -3922.647570 Hartree

C	2.880813	0.977051	-0.581337
C	3.155268	1.642887	0.764901
C	5.984884	4.057716	0.170142
H	4.711565	3.000827	-1.137302
C	5.574366	3.870974	2.537216
H	2.212959	1.417694	4.019106
C	6.307921	4.399981	1.508509
H	5.778523	4.131528	3.569960
H	7.114615	5.090361	1.722598
N	3.806069	2.527283	3.376876
N	1.453512	0.715214	-0.760180
N	-1.816543	1.278425	-0.894988
C	-3.130906	1.785733	-0.980470
C	-4.139820	1.206078	-0.206576
C	-3.444510	2.843725	-1.834516
C	-5.429234	1.714269	-0.263708
H	-3.937474	0.344661	0.422404
C	-4.744559	3.336837	-1.870489
H	-2.682253	3.296345	-2.455724
C	-5.751179	2.787867	-1.086448
H	-6.760145	3.181598	-1.119588
C	-5.076120	4.437771	-2.836977
C	-6.459665	1.123333	0.655079
F	-4.037535	5.256448	-3.038438
F	-5.427383	3.949008	-4.038965
F	-6.106550	5.181932	-2.406374
F	-7.708928	1.380290	0.238639
F	-6.326451	-0.198040	0.773684
F	-6.352089	1.639065	1.897536
C	2.422363	1.273722	1.865107
C	4.960090	3.175064	-0.097393
C	4.506193	2.973376	2.295609
C	2.785551	1.740457	3.152116
C	4.212139	2.593015	0.951492
H	1.580851	0.597103	1.764218
H	3.190270	1.668092	-1.372563
O	6.636946	4.559684	-0.906129

C	7.637521	5.532808	-0.689927
H	7.991559	5.823071	-1.678889
H	7.237065	6.416434	-0.179829
H	8.479162	5.128145	-0.115338
C	-3.569521	-0.717666	4.255531
C	-2.721165	-1.762474	4.592227
C	-1.603594	-2.049448	3.801090
C	-1.353564	-1.291348	2.643030
C	-2.175889	-0.210027	2.349985
C	-3.283980	0.071899	3.143810
H	-0.872777	-3.626968	5.114112
H	-4.440630	-0.504497	4.865349
H	-2.909471	-2.359459	5.480333
C	-0.636935	-3.052149	4.221069
H	-1.947960	0.409354	1.487786
H	-3.935737	0.901663	2.887170
C	0.548897	-3.232565	3.605190
H	1.305446	-3.913228	3.978436
C	-0.329126	-5.087383	0.234986
C	0.622067	-4.382912	-0.512264
C	1.588284	-5.048636	-1.275689
C	1.626781	-6.431137	-1.254004
C	0.695749	-7.137488	-0.476589
C	-0.282727	-6.486208	0.259089
H	2.278823	-4.478371	-1.891079
H	2.364109	-6.970033	-1.838106
H	0.732512	-8.222538	-0.461157
H	-1.009451	-7.049541	0.834760
C	-0.717103	2.051720	-0.980276
C	0.650581	1.788466	-0.916331
C	-0.478449	3.526826	-1.070840
C	1.012394	3.209015	-1.071189
O	-1.162361	4.518321	-1.116355
O	2.056213	3.818003	-1.159276
S	-1.570868	-4.115821	0.995923
C	0.477904	-2.938772	-0.378587
O	1.234541	-2.110467	-0.872880
C	4.109864	-2.644859	-0.215463
C	6.050342	-1.213606	-0.833296
C	5.377272	-2.577167	-1.102287
H	4.228381	-3.295671	0.652835
H	3.229323	-2.962399	-0.767291
H	6.068271	-3.361308	-0.774580
C	4.852917	-0.932310	1.341575
H	4.675973	0.078618	1.694755
H	4.689985	-1.616894	2.176118
C	6.238578	-1.080685	0.684169
H	6.843376	-0.200514	0.916704
H	6.765284	-1.954933	1.077614
H	7.013783	-1.171310	-1.345953
C	5.150355	-0.057675	-1.299589
H	5.534034	0.876229	-0.879531
H	5.156635	0.050447	-2.387422
C	3.705312	-0.307836	-0.832725
H	3.155771	-0.867809	-1.594687
N	3.791715	-1.276070	0.328337
C	5.063710	-2.817351	-2.554813
H	4.325213	-2.162826	-3.019354
C	5.624770	-3.775491	-3.284687
H	6.359891	-4.455215	-2.861072
H	5.374148	-3.913613	-4.330972
H	2.880380	-1.388349	0.822048
C	-0.752655	-2.510866	0.456175
N	-1.513251	-1.723548	-0.437782
C	-2.854395	-1.792986	-0.344034
O	-3.546493	-2.201807	0.579500
O	-3.506911	-1.227744	-1.424970
C	-3.222627	-1.657804	-2.775694
C	-4.485122	-1.253075	-3.531387
H	-5.353563	-1.775053	-3.121641
H	-4.652912	-0.176610	-3.427869
H	-4.394718	-1.491952	-4.595261
C	-3.036960	-3.172769	-2.818034
H	-3.012807	-3.519116	-3.855716
H	-2.101960	-3.466768	-2.334263
H	-3.866301	-3.666436	-2.302835
C	-2.010667	-0.933531	-3.360358
H	-2.170903	0.149405	-3.341878
H	-1.107465	-1.171756	-2.795035
H	-1.869168	-1.236212	-4.403323
H	1.099552	-0.240138	-0.821999
H	-1.690805	0.262585	-0.768094
C	0.886830	-2.433395	2.437202
O	2.045230	-2.395936	2.006662
C	-0.223091	-1.683592	1.734605
H	0.216032	-0.804894	1.248701

IM3c-1

Free Energy = -3921.809207 Hartree

Energy = -3922.673611 Hartree

C	-2.941298	-0.551926	-0.677986
C	-3.678348	-1.446607	0.321554
C	-6.897983	-2.464900	-1.358910
H	-5.216694	-1.396789	-2.035961
C	-6.861462	-3.326444	0.887558
H	-3.264519	-2.834246	3.394962
C	-7.521213	-3.177764	-0.302837
H	-7.295253	-3.886966	1.708428
H	-8.501263	-3.619350	-0.435477
N	-4.972395	-3.031263	2.288995
N	-1.505937	-0.784831	-0.571625
N	1.317663	-2.271294	-0.112792
C	2.542363	-2.924228	0.003565
C	3.607207	-2.174566	0.521905
C	2.755075	-4.255829	-0.373222
C	4.869895	-2.742577	0.619342
H	3.437212	-1.145141	0.831287
C	4.027960	-4.797046	-0.241486
H	1.940524	-4.863574	-0.757327
C	5.103739	-4.058362	0.242307
H	6.089413	-4.498073	0.328924
C	4.258642	-6.209058	-0.705888
C	5.991806	-1.864247	1.093715
F	3.190594	-6.985740	-0.491872
F	4.523112	-6.256810	-2.020857
F	5.303130	-6.771770	-0.078025
F	7.125401	-2.550530	1.287412
F	6.259011	-0.897132	0.197632
F	5.688916	-1.247809	2.244264
C	-3.065248	-1.802243	1.497487
C	-5.654917	-1.897827	-1.181008
C	-5.573538	-2.774063	1.094345
C	-3.753969	-2.584696	2.454671
C	-4.968268	-2.011885	0.050013
H	-2.051117	-1.466013	1.694115
H	-3.292606	-0.845816	-1.677474
O	-7.462284	-2.295966	-2.580324
C	-8.705301	-2.915263	-2.834044
H	-8.950446	-2.682431	-3.870227
H	-8.645690	-4.003514	-2.716741
H	-9.495384	-2.520305	-2.184294
C	4.446327	4.880446	-3.332943
C	4.768290	3.608264	-2.876975
C	3.777412	2.760614	-2.376450
C	2.442451	3.203459	-2.312409
C	2.126528	4.469011	-2.802756
C	3.121509	5.303916	-3.307629
H	5.154421	1.106167	-1.991235
H	5.222205	5.532348	-3.720129
H	5.795221	3.255694	-2.915596
C	4.104818	1.391512	-1.985222
C	1.396804	2.308711	-1.686549
H	1.093949	4.805120	-2.796055
H	2.856299	6.286625	-3.683477
C	3.166549	0.474583	-1.695855
H	3.410025	-0.564464	-1.504369
C	2.286110	4.800145	0.880765
C	1.103220	5.224942	0.274583
C	0.725938	6.569077	0.261135
C	1.546901	7.498056	0.877412
C	2.734994	7.073616	1.490184
C	3.116645	5.738531	1.498833
H	-0.197300	6.852544	-0.235428
H	1.280915	8.549121	0.884695
H	3.376741	7.807457	1.968241
H	4.041772	5.430123	1.974114
C	0.150790	-2.713505	-0.624289
C	-1.056902	-2.044605	-0.812250
C	-0.425309	-4.001662	-1.125343
C	-1.739236	-3.243587	-1.329441
O	-0.038222	-5.128537	-1.312692
O	-2.846834	-3.491662	-1.742959
S	2.587353	3.071062	0.814320
C	0.373339	4.140820	-0.376733
O	-0.631268	4.264115	-1.049814
C	-2.966732	3.230415	0.232400
C	-5.148298	2.122631	0.552282
C	-4.450700	3.497739	0.552741
H	-2.286764	3.822305	0.847271
H	-2.725185	3.448533	-0.808163
H	-4.539006	3.922557	1.560136
C	-3.129926	1.408919	1.827209
H	-2.671482	0.468009	2.107804
H	-2.746027	2.175761	2.505385
C	-4.667103	1.363036	1.795137
H	-5.018329	0.327197	1.766376

H	-5.068487	1.821087	2.703171
H	-6.233244	2.250183	0.570773
C	-4.740210	1.331268	-0.700556
H	-5.341850	0.425019	-0.752749
H	-4.957316	1.906226	-1.605208
C	-3.230524	0.975970	-0.650187
H	-2.719682	1.367848	-1.537177
N	-2.620842	1.785363	0.472442
C	-5.043341	4.480207	-0.416549
H	-4.985379	4.217715	-1.473342
C	-5.621059	5.622136	-0.061419
H	-5.688697	5.924748	0.980454
H	-6.046724	6.296620	-0.796609
H	-1.517105	1.776554	0.460609
C	1.042947	2.751227	-0.196793
N	0.097600	1.926944	0.508082
C	0.615881	0.895162	1.177874
O	1.754265	0.411432	1.060226
O	-0.280994	0.366606	2.070878
C	0.225603	-0.196550	3.317342
C	-1.003423	-0.231493	4.221567
H	-1.399093	0.777024	4.371884
H	-1.794405	-0.858481	3.799564
H	-0.736295	-0.643368	5.198269
C	1.280141	0.721230	3.933764
H	1.497039	0.389221	4.953243
H	2.205922	0.713623	3.358658
H	0.903860	1.748186	3.980100
C	0.762805	-1.606368	3.097550
H	0.028335	-2.223253	2.568331
H	1.688533	-1.587249	2.521650
H	0.967619	-2.077308	4.064048
H	-0.860087	-0.034001	-0.815907
H	1.342222	-1.286618	0.159541
H	0.435287	2.412962	-2.202233
C	1.748916	0.842565	-1.716785
O	0.854385	0.007969	-1.746199

IM3d-1

Free Energy = -3921.819245 Hartree

Energy = -3922.682637 Hartree

C	3.181515	0.508508	-0.483629
C	3.681195	1.314067	0.714885
C	6.998056	2.755976	-0.337413
H	5.515389	1.680475	-1.378129
C	6.587616	3.297888	1.973266
H	2.790193	2.113779	3.890796
C	7.408388	3.360418	0.878383
H	6.861909	3.765172	2.912786
H	8.355497	3.881830	0.944617
N	4.573998	2.652069	3.050516
N	1.725464	0.596962	-0.606018
N	-1.306684	1.816576	-0.953710
C	-2.501893	2.537012	-0.894345
C	-3.703941	1.859336	-1.149300
C	-2.546640	3.888958	-0.535665
C	-4.913843	2.525039	-1.025978
H	-3.682492	0.814139	-1.434914
C	-3.775050	4.534796	-0.451631
H	-1.637970	4.444325	-0.341657
C	-4.973427	3.871937	-0.683040
H	-5.922792	4.386895	-0.594142
C	-3.796405	6.004786	-0.133248
C	-6.195422	1.763292	-1.200762
F	-2.805742	6.347096	0.700473
F	-3.660081	6.752100	-1.236654
F	-4.953486	6.366654	0.444077
F	-7.124854	2.488837	-1.835300
F	-6.023879	0.626811	-1.892054
F	-6.726409	1.417817	-0.010914
C	2.909061	1.402487	1.846586
C	5.793841	2.090674	-0.414809
C	5.338982	2.632180	1.923217
C	3.401405	2.074832	2.991350
C	4.942796	1.993905	0.709975
H	1.937693	0.920341	1.885734
H	3.613252	0.954549	-1.386424
O	7.737744	2.788751	-1.474211
C	8.945988	3.517905	-1.464191
H	9.350673	3.442260	-2.473425
H	8.778482	4.574575	-1.224982
H	9.670184	3.094156	-0.758033
C	-4.932047	-0.818033	3.543748
C	-3.943942	-1.563551	4.172108
C	-2.649762	-1.619790	3.643862
C	-2.348972	-0.942747	2.448805
C	-3.332475	-0.144364	1.868294
C	-4.617175	-0.086539	2.401589

H	-1.852177	-2.773000	5.315436
H	-5.934533	-0.784527	3.956507
H	-4.161925	-2.097297	5.092975
C	-1.579717	-2.267682	4.391619
C	-0.980052	-1.076209	1.811226
H	-3.094181	0.438483	0.984907
H	-5.367354	0.528536	1.915722
C	-0.290338	-2.194062	4.022714
H	0.513206	-2.611207	4.619213
C	-2.771209	-3.991268	0.624809
C	-3.243866	-2.887169	-0.087823
C	-4.539196	-2.849708	-0.602183
C	-5.368016	-3.943512	-0.405418
C	-4.891588	-5.056694	0.298288
C	-3.603709	-5.094176	0.820835
H	-4.872035	-1.965572	-1.138920
H	-6.381502	-3.940541	-0.790483
H	-5.544456	-5.911397	0.446790
H	-3.253564	-5.962174	1.369229
C	-0.059886	2.349798	-1.074326
C	1.206442	1.780761	-0.941684
C	0.492639	3.673697	-1.460062
C	1.878017	3.044501	-1.337319
O	0.053399	4.761149	-1.749943
O	3.024716	3.370054	-1.533992
S	-1.113051	-3.847684	1.184920
C	-2.244262	-1.834612	-0.258999
O	-2.375538	-0.843632	-0.953639
C	3.121650	-3.255620	0.211620
C	5.489201	-2.566371	-0.132860
C	4.445863	-3.651338	-0.483473
H	2.935423	-3.830710	1.121603
H	2.269151	-3.352117	-0.455320
H	4.796124	-4.595548	-0.051795
C	4.151416	-1.714297	1.793772
H	4.278398	-0.661414	2.029602
H	3.656181	-2.189453	2.641009
C	5.478007	-2.385133	1.391201
H	6.312885	-1.755490	1.709166
H	5.591493	-3.354357	1.886634
H	6.475121	-2.884242	-0.479837
C	5.108008	-1.221962	-0.772689
H	5.713258	-0.430975	-0.320143
H	5.312915	-1.218697	-1.846845
C	3.608074	-0.971066	-0.553380
H	3.016108	-1.388094	-1.373051
N	3.193265	-1.812546	0.638981
C	4.275450	-3.846898	-1.969495
H	3.602341	-3.161132	-2.484690
C	4.889582	-4.807214	-2.652454
H	5.542737	-5.526855	-2.163743
H	4.759753	-4.913090	-3.724316
H	2.238783	-1.545741	0.950059
C	-0.946189	-2.062073	0.563055
N	0.236824	-1.817245	-0.182206
C	0.324410	-2.380654	-1.402776
O	1.305276	-2.255562	-2.147619
O	-0.747151	-3.133835	-1.764537
C	-0.771281	-3.891389	-3.001082
C	-2.136170	-4.570822	-2.953995
H	-2.226482	-5.191110	-2.056873
H	-2.935415	-3.824390	-2.936940
H	-2.271330	-5.205414	-3.834325
C	0.342094	-4.934995	-2.991672
H	0.219986	-5.611429	-3.843176
H	1.325091	-4.466923	-3.052729
H	0.285449	-5.527576	-2.072776
C	-0.685502	-2.954009	-4.201512
H	-1.447005	-2.172957	-4.114269
H	0.295760	-2.485073	-4.264407
H	-0.875329	-3.517270	-5.120503
H	1.126022	-0.234696	-0.416905
H	-1.400090	0.800157	-0.992527
C	0.104114	-1.513791	2.788854
O	1.292300	-1.340446	2.535513
H	-0.676962	-0.112685	1.381513

IM3a-1

Free Energy = -3921.828161 Hartree

Energy = -3922.691649 Hartree

C	2.237639	-2.108212	-0.332723
C	3.086477	-1.516690	-1.439142
C	5.472905	-4.238709	-2.483468
H	3.917295	-4.178710	-1.064581
C	5.915466	-2.246735	-3.763655
H	3.506198	1.401818	-3.114150
C	6.217978	-3.551711	-3.475224
H	6.463475	-1.693708	-4.518808

H	7.019568	-4.048891	-4.007611	H	2.047834	4.391661	-2.099085
N	4.644229	-0.267235	-3.447449	H	1.704605	6.749456	-2.747592
N	0.830388	-1.814613	-0.583805	C	-2.360937	2.401549	-1.180999
N	-2.335961	-1.860103	-0.747964	H	-3.231786	1.773327	-1.023158
C	-3.723296	-1.866429	-0.769333	C	1.307864	4.861701	1.459914
C	-4.345066	-0.885867	-1.547874	C	2.443326	4.370154	0.815327
C	-4.508747	-2.762615	-0.030582	C	3.631967	5.100510	0.761403
C	-5.729001	-0.771742	-1.553881	C	3.677760	6.343853	1.369184
H	-3.737592	-0.206234	-2.140205	C	2.537942	6.840239	2.018168
C	-5.889637	-2.635008	-0.077322	C	1.353757	6.116309	2.071989
H	-4.046676	-3.540313	0.572502	H	4.486089	4.680465	0.238417
C	-6.523810	-1.641966	-0.822855	H	4.584943	6.936960	1.341863
H	-7.603621	-1.555652	-0.833297	H	2.579027	7.817873	2.488621
C	-6.746224	-3.547447	0.757782	H	0.481383	6.518779	2.575776
C	-6.330198	0.333648	-2.372991	C	-1.484424	-2.672581	-0.077974
F	-6.099983	-4.658829	1.119846	C	-0.095441	-2.604458	-0.030965
F	-7.155284	-2.936655	1.881253	C	-1.526388	-3.859842	0.812223
F	-7.854558	-3.915961	0.095203	C	-0.003639	-3.760637	0.877430
F	-7.659745	0.395870	-2.246012	O	-2.371811	-4.574237	1.298758
F	-5.833068	1.530442	-2.005312	O	0.906048	-4.331418	1.443386
F	-6.052704	0.192591	-3.676807	S	-0.078343	3.781732	1.453304
C	2.862865	-0.224527	-1.836781	C	2.226059	3.075542	0.174097
C	4.454218	-3.600322	-1.807922	O	3.057437	2.449608	-0.455255
C	4.874096	-1.562785	-3.091902	C	2.720839	-0.209167	2.955699
C	3.674049	0.363158	-2.837104	C	4.612097	-1.809505	2.686782
C	4.129161	-2.252903	-2.088798	C	3.582173	-1.263701	3.700795
H	2.108048	0.383486	-1.347560	H	3.010039	0.812995	3.214119
H	2.316495	-3.198522	-0.363768	H	1.653581	-0.332043	3.144222
O	5.700338	-5.530171	-2.139260	H	4.134983	-0.753589	4.497970
C	6.722050	-6.233079	-2.813999	C	4.297113	0.121728	1.134818
H	6.723745	-7.237838	-2.391760	H	4.472907	-0.077449	0.080474
H	6.525010	-6.298664	-3.890468	H	4.311330	1.204777	1.264918
H	7.704824	-5.775540	-2.649719	C	5.310668	-0.605708	2.041289
C	-0.422123	6.702286	-2.420181	H	6.164968	-0.933559	1.442976
C	-1.506572	5.915986	-2.053699	H	5.694001	0.066418	2.815779
C	-1.321644	4.580941	-1.684038	H	5.332731	-2.448609	3.202621
C	-0.026417	4.032790	-1.665586	C	3.896245	-2.588040	1.573302
C	1.049533	4.820459	-2.068784	H	4.592622	-2.739058	0.739665
C	0.855252	6.148762	-2.439613	H	3.553794	-3.574012	1.900275
H	-3.445330	4.199746	-1.349267	C	2.668716	-1.784411	1.119628
H	-0.572885	7.738056	-2.704794	H	1.802800	-2.056122	1.725516
H	-2.510958	6.330086	-2.059601	N	2.910245	-0.338400	1.469309
C	-2.464664	3.729479	-1.372090	C	2.756788	-2.351664	4.336603
C	0.175208	2.621417	-1.179877	H	2.072020	-2.905349	3.692330

C	2.833855	-2.670557	5.623959
H	3.499978	-2.142726	6.302507
H	2.233976	-3.469011	6.047531
C	0.770247	2.547745	0.319769
N	0.855705	1.221896	0.814706
C	-0.188950	0.624950	1.416213
O	-0.137022	-0.509726	1.899337
O	-1.327662	1.373267	1.467585
C	-2.358950	1.081412	2.455457
C	-3.251726	2.316999	2.409281
H	-2.705871	3.203645	2.741953
H	-3.610514	2.494458	1.391980
H	-4.117555	2.174437	3.061958
C	-1.747176	0.932585	3.846372
H	-2.545965	0.955765	4.593737
H	-1.199829	-0.004359	3.945234
H	-1.069229	1.768775	4.046569
C	-3.141415	-0.154558	2.033377
H	-3.585736	0.009015	1.047009
H	-2.490829	-1.030524	1.999119
H	-3.954440	-0.342430	2.741743
C	-1.054034	1.752378	-1.270130
O	-0.927000	0.536356	-1.404968
H	-1.907762	-1.034153	-1.166233
H	0.551864	-0.894394	-0.918786
H	2.126111	0.330807	1.036089
H	0.954005	2.123533	-1.767864

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Free Energy = -3921.829412 Hartree

Energy = -3922.690648 Hartree

C	2.235485	-2.092326	-0.338989
C	3.075673	-1.525398	-1.464675
C	5.480721	-4.256171	-2.441669
H	3.931178	-4.167781	-1.017485
C	5.900935	-2.298497	-3.780572
H	3.458943	1.344284	-3.231016
C	6.215990	-3.591923	-3.455882
H	6.440855	-1.762884	-4.553888
H	7.019659	-4.097475	-3.977162
N	4.612902	-0.322335	-3.517959
N	0.824812	-1.815606	-0.596103
N	-2.338982	-1.880926	-0.772264
C	-3.725992	-1.886229	-0.788746
C	-4.350378	-0.913771	-1.575495
C	-4.509305	-2.772959	-0.036153
C	-5.734094	-0.796607	-1.574720
H	-3.745077	-0.242233	-2.179247
C	-5.890147	-2.642922	-0.076684
H	-4.045277	-3.544916	0.572918
C	-6.526611	-1.656635	-0.829300
H	-7.606270	-1.568121	-0.834484
C	-6.743830	-3.544080	0.773565
C	-6.336872	0.303918	-2.399098
F	-6.098719	-4.653772	1.142472
F	-7.142848	-2.920297	1.893593
F	-7.857984	-3.915476	0.122567
F	-7.667413	0.358515	-2.280915
F	-5.849476	1.504400	-2.029040
F	-6.049375	0.163631	-3.700729
C	2.837773	-0.248768	-1.901866
C	4.459625	-3.607118	-1.780199
C	4.856415	-1.604333	-3.124400
C	3.638785	0.316475	-2.922906
C	4.122131	-2.270888	-2.097824
H	2.077448	0.366251	-1.430808
H	2.320868	-3.182569	-0.343351
O	5.720374	-5.535620	-2.061618
C	6.746020	-6.248259	-2.719556
H	6.758739	-7.240323	-2.268415
H	6.545872	-6.346964	-3.792962
H	7.725135	-5.777133	-2.572543
C	-0.491128	6.719883	-2.369620
C	-1.569423	5.916228	-2.023096
C	-1.372482	4.578089	-1.671926
C	-0.071717	4.043200	-1.652141
C	0.998749	4.848728	-2.034099
C	0.791979	6.180434	-2.386759
H	-3.494890	4.172328	-1.360726
H	-0.651205	7.757862	-2.640636
H	-2.578308	6.319162	-2.030828
C	-2.509584	3.711637	-1.380714
C	0.141786	2.623770	-1.190885
H	2.001563	4.431764	-2.067950
H	1.636814	6.794455	-2.680504
C	-2.395622	2.382589	-1.204564
H	-3.262500	1.745217	-1.062230
C	1.397845	4.767602	1.539657

C	2.506827	4.270823	0.854524
C	3.730401	4.944114	0.849648
C	3.838777	6.132358	1.551910
C	2.725434	6.633341	2.242334
C	1.506306	5.967922	2.245600
H	4.561780	4.523960	0.291267
H	4.774678	6.679359	1.567170
H	2.816115	7.567869	2.787448
H	0.656075	6.372936	2.783925
C	-1.485187	-2.682434	-0.089493
C	-0.096901	-2.605871	-0.039893
C	-1.524591	-3.857058	0.816001
C	-0.001623	-3.751303	0.883381
O	-2.368671	-4.567673	1.310814
O	0.908921	-4.311476	1.456702
S	-0.040374	3.761495	1.459953
C	2.226689	3.039635	0.121459
O	3.012006	2.442966	-0.588836
C	2.706513	-0.131470	2.910985
C	4.624576	-1.700722	2.652436
C	3.599084	-1.152158	3.668773
H	2.974002	0.900866	3.154853
H	1.646731	-0.276437	3.124705
H	4.153031	-0.615928	4.448062
C	4.250472	0.202713	1.079021
H	4.421069	0.008409	0.022614
H	4.255472	1.286237	1.209607
C	5.294091	-0.499325	1.974347
H	6.140351	-0.827101	1.364221
H	5.685307	0.189253	2.730490
H	5.362116	-2.318661	3.170611
C	3.908264	-2.509602	1.562244
H	4.600144	-2.667070	0.726117
H	3.583578	-3.494398	1.910942
C	2.666368	-1.727640	1.104215
H	1.808685	-2.011640	1.717166
N	2.875707	-0.274025	1.426816
C	2.802053	-2.241255	4.337087
H	2.116244	-2.815790	3.712363
C	2.901886	-2.536833	5.628515
H	3.569500	-1.987195	6.288032
H	2.320540	-3.336791	6.074599
C	0.763127	2.536532	0.288585
N	0.840152	1.203824	0.784949
C	-0.213262	0.612981	1.392057
O	-0.163502	-0.514472	1.882077
O	-1.340701	1.370942	1.430965
C	-2.382497	1.089576	2.414762
C	-3.266149	2.330789	2.356871
H	-2.713550	3.216907	2.679813
H	-3.626937	2.500384	1.339153
H	-4.130979	2.200378	3.013231
C	-1.779186	0.943593	3.809506
H	-2.582835	0.974253	4.551224
H	-1.237587	0.004306	3.917069
H	-1.098374	1.777166	4.010619
C	-3.168314	-0.143514	1.991494
H	-3.603053	0.017230	1.000473
H	-2.524233	-1.024691	1.967717
H	-3.988594	-0.322085	2.693780
C	-1.082762	1.745453	-1.288651
O	-0.944844	0.531900	-1.431518
H	-1.912601	-1.061002	-1.202569
H	0.539285	-0.909084	-0.959514
H	1.999688	0.428627	0.987793
H	0.914468	2.140803	-1.799598

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Free Energy = -3921.837283 Hartree

Energy = -3922.699783 Hartree

C	2.292000	-2.143852	-0.307189
C	3.092915	-1.558947	-1.449519
C	5.449736	-4.279530	-2.556024
H	3.944182	-4.209363	-1.083317
C	5.845555	-2.295666	-3.863815
H	3.455933	1.353109	-3.153240
C	6.159782	-3.598239	-3.576857
H	6.367894	-1.746688	-4.639847
H	6.944498	-4.097393	-4.132146
N	4.583330	-0.315557	-3.517127
N	0.874156	-1.827296	-0.506089
N	-2.291009	-1.886621	-0.731661
C	-3.676520	-1.890203	-0.770555
C	-4.287936	-0.935835	-1.589791
C	-4.473523	-2.754625	-0.005925
C	-5.670909	-0.811322	-1.606786
H	-3.673298	-0.283063	-2.204723
C	-5.853077	-2.617493	-0.064065

H	-4.020011	-3.512932	0.628124	H	4.510112	4.582513	0.485065
C	-6.476456	-1.646970	-0.847505	H	4.654758	6.779763	1.696133
H	-7.555392	-1.552631	-0.865992	H	2.638872	7.701851	2.789890
C	-6.717803	-3.489123	0.805788	H	0.483219	6.499626	2.723945
C	-6.257948	0.274384	-2.461495	C	-1.446818	-2.670989	-0.011762
F	-6.093083	-4.607822	1.181989	C	-0.057893	-2.598414	0.051159
F	-7.089625	-2.842326	1.922374	C	-1.506568	-3.818031	0.922833
F	-7.846866	-3.843519	0.171714	C	0.018338	-3.735244	0.993897
F	-7.590857	0.324878	-2.377874	O	-2.362601	-4.507136	1.429064
F	-5.785543	1.482990	-2.094828	O	0.915783	-4.310949	1.567371
F	-5.935565	0.118895	-3.752895	S	-0.145142	3.843302	1.456925
C	2.859519	-0.267235	-1.845587	C	2.184262	3.088669	0.248845
C	4.452585	-3.638865	-1.851950	O	2.985660	2.451838	-0.400299
C	4.825960	-1.608967	-3.162223	C	2.867604	-0.162076	2.852956
C	3.634154	0.315899	-2.875442	C	4.715075	-1.829579	2.666563
C	4.115108	-2.294258	-2.131366	C	3.714127	-1.198011	3.661301
H	2.125744	0.345348	-1.332803	H	3.177899	0.861442	3.092076
H	2.356774	-3.235224	-0.338502	H	1.805554	-0.258498	3.093259
O	5.691835	-5.569080	-2.210883	H	4.293392	-0.664244	4.424743
C	6.699471	-6.269664	-2.907347	C	4.421538	0.041954	1.050424
H	6.721418	-7.270708	-2.476687	H	4.602511	-0.193657	0.002867
H	6.473631	-6.346900	-3.977551	H	4.493862	1.129196	1.141515
H	7.682971	-5.803134	-2.775100	C	5.444355	-0.679179	1.962936
C	-0.457330	6.699570	-2.469243	H	6.278829	-1.062088	1.367038
C	-1.543881	5.899532	-2.139008	H	5.864733	0.007377	2.706439
C	-1.352268	4.574149	-1.740400	H	5.416844	-2.471340	3.206411
C	-0.049608	4.050762	-1.658301	C	3.964544	-2.627933	1.588070
C	1.030666	4.851013	-2.020220	H	4.652968	-2.831334	0.757572
C	0.829037	6.170307	-2.420651	H	3.595770	-3.591649	1.952975
H	-3.481855	4.164335	-1.488129	C	2.768774	-1.775967	1.121840
H	-0.613388	7.727425	-2.778194	H	1.905596	-2.023897	1.745846
H	-2.553753	6.295550	-2.196690	N	3.029555	-0.341589	1.389757
C	-2.494262	3.709025	-1.461352	C	2.867150	-2.223957	4.363710
C	0.153394	2.646134	-1.148180	H	2.178678	-2.807200	3.749570
H	2.036558	4.439961	-2.002653	C	2.917056	-2.456411	5.671417
H	1.680312	6.781869	-2.700193	H	3.586081	-1.898027	6.322266
C	-2.381520	2.385456	-1.243412	H	2.293140	-3.210359	6.140142
H	-3.250134	1.747402	-1.115869	C	0.700111	2.617377	0.351164
C	1.290203	4.858978	1.569719	N	0.735091	1.290666	0.896388
C	2.429461	4.343090	0.953261	C	-0.311849	0.648028	1.499154
C	3.650819	5.018825	0.985315	O	-0.218894	-0.462605	1.986723
C	3.721455	6.230040	1.652875	O	-1.428608	1.397782	1.492218
C	2.576120	6.749905	2.271996	C	-2.509275	1.112876	2.442348
C	1.358636	6.080428	2.239776	C	-3.398122	2.345261	2.332216

H	-2.866370	3.239668	2.667172
H	-3.718675	2.498514	1.298439
H	-4.287419	2.215134	2.954546
C	-1.950349	0.987214	3.855896
H	-2.781773	0.988339	4.566548
H	-1.380761	0.067304	3.985635
H	-1.307399	1.843441	4.083253
C	-3.257811	-0.133307	1.995165
H	-3.652466	0.015279	0.986147
H	-2.604299	-1.008292	2.004875
H	-4.103846	-0.318065	2.664128
C	-1.063761	1.754640	-1.270612
O	-0.908747	0.540954	-1.378431
H	-1.858144	-1.082914	-1.181425
H	0.596984	-0.987957	-1.004622
H	1.632650	0.748546	0.894738
H	0.952475	2.148430	-1.709767

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Free Energy = -3921.828534 Hartree

Energy = -3922.690250 Hartree

C	-2.129241	1.908644	0.690166
C	-2.316565	2.563716	-0.681412
C	-4.516270	5.556594	-0.032816
H	-3.637177	4.129693	1.240468
C	-4.066821	5.396785	-2.391789
H	-1.339988	2.283216	-3.922339
C	-4.687826	6.040521	-1.354537
H	-4.159798	5.749623	-3.413160
H	-5.291373	6.918699	-1.549069
N	-2.646862	3.709583	-3.263564
N	-0.772058	1.374126	0.849500
N	2.474827	1.288961	0.462781
C	3.868707	1.338450	0.384824
C	4.561667	0.121428	0.471700
C	4.579534	2.525679	0.195057
C	5.941965	0.107811	0.350889
H	4.015934	-0.804644	0.630420
C	5.966818	2.477370	0.098338
H	4.066549	3.480319	0.138704
C	6.667403	1.281840	0.166393
H	7.747255	1.261903	0.077036
C	6.719461	3.772584	-0.036344
C	6.688254	-1.195008	0.353300
F	6.066989	4.647344	-0.811623
F	6.901791	4.361399	1.154201
F	7.935962	3.585037	-0.571629
F	7.816897	-1.115668	1.072851
F	5.961137	-2.203529	0.847877
F	7.057236	-1.546331	-0.894187
C	-1.645137	2.096852	-1.785712
C	-3.752907	4.435154	0.207581
C	-3.262869	4.251357	-2.176275
C	-1.854399	2.690509	-3.053949
C	-3.122115	3.740376	-0.851005
H	-0.950489	1.265286	-1.707821
H	-2.218000	2.711529	1.426960
O	-5.075614	6.144272	1.055639
C	-5.822140	7.325775	0.865438
H	-6.149693	7.637461	1.857337
H	-5.212777	8.123404	0.424181
H	-6.704798	7.152363	0.237949
C	-2.592858	-5.028164	4.146285
C	-2.123021	-3.787188	4.555777
C	-1.386699	-2.980872	3.684241
C	-1.146015	-3.403901	2.359085
C	-1.591659	-4.667957	1.973301
C	-2.303974	-5.473582	2.861901
H	-1.049793	-1.420281	5.173550
H	-3.160486	-5.650331	4.829219
H	-2.305161	-3.439260	5.568638
C	-0.782815	-1.743205	4.170007
C	-0.469071	-2.410080	1.432251
H	-1.379157	-5.051032	0.980668
H	-2.632114	-6.456110	2.539630
C	0.545243	-1.542822	2.142856
C	0.145954	-1.067166	3.472112
C	2.455163	-3.402344	-0.728619
C	2.050478	-2.144896	-1.177110
C	2.891443	-1.338556	-1.939580
C	4.167275	-1.798952	-2.236853
C	4.576907	-3.053822	-1.774556
C	3.733188	-3.866415	-1.021774
H	2.538146	-0.365066	-2.267804
H	4.854486	-1.184624	-2.807801
H	5.582641	-3.397172	-1.991890
H	4.069021	-4.835751	-0.669672
C	1.606922	2.301753	0.711600

C	0.223013	2.286605	0.874984
C	1.675976	3.778888	0.923140
C	0.167997	3.738587	1.148987
O	2.521910	4.639320	0.906739
O	-0.700573	4.523450	1.446420
S	1.247749	-4.282575	0.212403
C	0.703211	-1.781836	-0.749214
O	0.127028	-0.733177	-0.960717
C	-3.847855	-1.423536	1.308280
C	-5.399452	0.196384	0.233859
C	-5.346869	-1.160042	0.972960
H	-3.586623	-2.462987	1.072306
H	-3.662018	-1.295433	2.381497
H	-5.704908	-1.933043	0.280682
C	-3.309844	-0.600101	-0.854499
H	-2.521375	-0.151332	-1.456922
H	-3.325836	-1.664063	-1.114492
C	-4.692329	0.037669	-1.119435
H	-4.582650	1.020393	-1.592687
H	-5.281864	-0.588316	-1.797386
H	-6.440251	0.502619	0.096751
C	-4.636011	1.267318	1.024157
H	-4.736072	2.216040	0.495006
H	-5.073813	1.415251	2.016475
C	-3.146628	0.835006	1.151455
H	-2.899396	0.703681	2.211433
N	-2.946659	-0.516798	0.575201
C	-6.206615	-1.206019	2.201175
H	-5.951967	-0.502232	2.995250
C	-7.228152	-2.037140	2.378735
H	-7.510830	-2.758490	1.616062
H	-7.820083	-2.028030	3.288013
C	-0.007472	-2.923205	0.058401
N	-1.194555	-3.299748	-0.662786
C	-1.205176	-3.448421	-2.022652
O	-0.212726	-3.338246	-2.710520
O	-2.451570	-3.720726	-2.431274
C	-2.746653	-3.825630	-3.859803
C	-4.241908	-4.113300	-3.870813
H	-4.458090	-5.044402	-3.340468
H	-4.793199	-3.301900	-3.387258
H	-4.597227	-4.208217	-4.899907
C	-1.967958	-4.985993	-4.469341
H	-2.311665	-5.152315	-5.494321
H	-0.897605	-4.781180	-4.485357
H	-2.147939	-5.900971	-3.897549
C	-2.444220	-2.497449	-4.544399
H	-2.989744	-1.685219	-4.053472
H	-1.376853	-2.275174	-4.522814
H	-2.771756	-2.543750	-5.586895
H	-0.598643	0.485427	0.382632
H	2.089301	0.353497	0.544019
H	-2.079355	-3.337106	-0.178687
O	1.574918	-1.171694	1.600214
H	-1.249261	-1.646649	1.183910
H	0.680352	-0.213194	3.872664

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Free Energy = -3921.811258 Hartree

Energy = -3922.673144 Hartree

C	-1.966655	1.795268	0.685347
C	-2.227317	2.476428	-0.662652
C	-4.355584	5.485584	0.151761
H	-3.371329	4.073021	1.359210
C	-4.084293	5.323276	-2.233447
H	-1.467434	2.220868	-3.962035
C	-4.626108	5.968213	-1.153881
H	-4.250046	5.676509	-3.245380
H	-5.240175	6.847854	-1.303345
N	-2.731722	3.638248	-3.207149
N	-0.587403	1.328877	0.805899
N	2.643285	1.355973	0.641658
C	4.022744	1.451653	0.476054
C	4.742676	0.249343	0.420645
C	4.696775	2.668223	0.336234
C	6.112861	0.277242	0.213370
H	4.224490	-0.699210	0.534852
C	6.074219	2.659939	0.143800
H	4.162734	3.611442	0.394465
C	6.801075	1.479009	0.073284
H	7.872829	1.492253	-0.085879
C	6.798336	3.975972	0.065432
C	6.873330	-1.009300	0.068092
F	6.055848	4.918090	-0.528118
F	7.117690	4.435025	1.284258
F	7.944889	3.868388	-0.624366
F	8.096496	-0.924934	0.609534
F	6.244143	-2.041177	0.643473

F	7.051694	-1.330595	-1.228702	S	1.105167	-4.211588	0.225065
C	-1.628901	2.018486	-1.811549	C	0.529156	-1.774571	-0.873079
C	-3.579934	4.361343	0.335994	O	-0.083074	-0.779253	-1.211597
C	-3.268451	4.176351	-2.077359	C	-3.869133	-1.511954	1.332273
C	-1.922212	2.621741	-3.058334	C	-5.253184	0.229797	0.264721
C	-3.033820	3.661399	-0.766213	C	-5.315914	-1.169104	0.907467
H	-0.934935	1.184668	-1.790128	H	-3.645085	-2.564900	1.144670
H	-2.065670	2.578163	1.442772	H	-3.721662	-1.347195	2.404036
O	-4.826092	6.077137	1.277901	H	-5.648472	-1.882719	0.143142
C	-5.569472	7.269277	1.145851	C	-3.219272	-0.693605	-0.839855
H	-5.812436	7.585415	2.160282	H	-2.377191	-0.313725	-1.412710
H	-4.985812	8.057764	0.656421	H	-3.341620	-1.743386	-1.118600
H	-6.501493	7.107363	0.591056	C	-4.525412	0.091400	-1.077496
C	-2.907161	-4.703993	4.111646	H	-4.316019	1.081112	-1.494721
C	-2.429151	-3.453072	4.459842	H	-5.148387	-0.443768	-1.800791
C	-1.646262	-2.705836	3.568594	H	-6.261162	0.628380	0.124867
C	-1.372994	-3.197452	2.266413	C	-4.433971	1.168323	1.159852
C	-1.810726	-4.499748	1.961875	H	-4.510702	2.182221	0.767806
C	-2.563846	-5.235165	2.867578	H	-4.845141	1.193737	2.173625
H	-1.308162	-1.080107	4.979246	C	-2.949673	0.707060	1.202397
H	-3.509536	-5.276865	4.807630	H	-2.632205	0.554886	2.239069
H	-2.636570	-3.040924	5.443820	N	-2.859582	-0.676359	0.609387
C	-1.050517	-1.454130	3.990853	C	-6.258345	-1.266512	2.071687
C	-0.671131	-2.298978	1.316596	H	-6.052277	-0.612602	2.919996
H	-1.539732	-4.967005	1.020585	C	-7.301039	-2.087839	2.124720
H	-2.879403	-6.238706	2.600974	H	-7.536081	-2.760619	1.303883
C	0.250803	-1.347529	1.932621	H	-7.958372	-2.118410	2.987163
C	-0.139974	-0.806910	3.236026	C	-0.182572	-2.875166	-0.013449
C	2.325131	-3.340205	-0.703538	N	-1.334287	-3.319579	-0.754131
C	1.906633	-2.114018	-1.219774	C	-1.303144	-3.560692	-2.098982
C	2.761086	-1.308896	-1.967633	O	-0.307828	-3.439276	-2.779711
C	4.062093	-1.740741	-2.190778	O	-2.531027	-3.914821	-2.511163
C	4.484268	-2.967712	-1.667323	C	-2.784372	-4.154428	-3.930304
C	3.629036	-3.776113	-0.923573	C	-4.267251	-4.500733	-3.949903
H	2.396137	-0.359170	-2.347692	H	-4.462807	-5.387416	-3.341196
H	4.758268	-1.126787	-2.751151	H	-4.860300	-3.670579	-3.555498
H	5.507685	-3.288889	-1.828862	H	-4.591981	-4.702702	-4.973622
H	3.974460	-4.722319	-0.521104	C	-1.946125	-5.330747	-4.417789
C	1.749333	2.337571	0.902393	H	-2.246437	-5.591666	-5.436685
C	0.360005	2.276944	0.983803	H	-0.883603	-5.087352	-4.415340
C	1.761912	3.795773	1.227600	H	-2.114356	-6.202883	-3.779346
C	0.245031	3.692437	1.385996	C	-2.515668	-2.880703	-4.724305
O	2.581997	4.676757	1.305664	H	-3.088003	-2.046699	-4.305668
O	-0.661148	4.417717	1.724653	H	-1.456018	-2.624950	-4.716403

H	-2.835631	-3.024394	-5.760264
H	-0.325467	0.517416	0.249047
H	2.268099	0.412165	0.744462
H	-2.191228	-3.524825	-0.264514
O	1.265638	-0.946435	1.343540
H	-1.684457	-1.370944	0.918002
H	0.387812	0.075265	3.582127

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Free Energy = -3921.849419 Hartree

Energy = -3922.710242 Hartree

C	2.195875	1.999308	-0.726706
C	2.484424	2.575743	0.658193
C	5.129680	5.203854	0.111978
H	4.042082	3.986511	-1.214616
C	4.655064	5.021297	2.465558
H	1.529908	2.249981	3.897118
C	5.369708	5.602276	1.451836
H	4.801487	5.313244	3.499761
H	6.101372	6.368029	1.678509
N	3.003011	3.524050	3.276707
N	0.788760	1.684735	-0.922109
N	-2.361635	1.623028	-0.962347
C	-3.735160	1.557948	-0.774546
C	-4.312831	0.282008	-0.873672
C	-4.533368	2.660494	-0.464820
C	-5.669188	0.123696	-0.661241
H	-3.679812	-0.576609	-1.083915
C	-5.898062	2.464433	-0.259603
H	-4.100484	3.654605	-0.381123
C	-6.485849	1.211137	-0.351455
H	-7.548057	1.080605	-0.180021
C	-6.750646	3.669679	0.025484
C	-6.290435	-1.242394	-0.715604
F	-6.153313	4.505918	0.884606
F	-7.002919	4.370763	-1.089910
F	-7.937004	3.329095	0.552550
F	-7.326739	-1.277778	-1.567293
F	-5.422299	-2.186971	-1.096080
F	-6.777216	-1.610646	0.485607
C	1.778606	2.127574	1.747124
C	4.199402	4.226752	-0.169827
C	3.685086	4.022251	2.208382
C	2.080190	2.627974	3.037888
C	3.464295	3.600855	0.863089
H	1.017737	1.361435	1.632396
H	2.456966	2.770034	-1.462044
O	5.777964	5.736184	-0.953179
C	6.693842	6.785957	-0.722537
H	7.065781	7.080384	-1.703771
H	6.208804	7.648265	-0.250718
H	7.538721	6.458309	-0.105207
C	2.027716	-5.704743	-3.743322
C	1.879406	-4.422745	-4.210518
C	1.212544	-3.435048	-3.447133
C	0.721081	-3.755856	-2.143448
C	0.842415	-5.110620	-1.714414
C	1.476874	-6.050186	-2.491226
H	1.387114	-1.893226	-4.955396
H	2.535246	-6.454739	-4.339906
H	2.260914	-4.144863	-5.189787
C	1.002411	-2.124404	-3.965059
C	0.127454	-2.718368	-1.367563
H	0.380971	-5.423725	-0.781861
H	1.539229	-7.076069	-2.142017
C	-0.174337	-1.477537	-1.936385
C	0.310345	-1.184382	-3.255514
C	-2.593392	-2.277053	1.147288
C	-1.728136	-1.195202	1.308314
C	-2.141440	-0.028316	1.944103
C	-3.444435	0.056234	2.415987
C	-4.314254	-1.025179	2.245650
C	-3.905049	-2.194867	1.611050
H	-1.442226	0.796030	2.051926
H	-3.793797	0.961342	2.900483
H	-5.338799	-0.949342	2.595254
H	-4.598281	-3.017499	1.473264
C	-1.521735	2.674038	-0.843179
C	-0.130257	2.661891	-0.846068
C	-1.566731	4.155942	-0.690043
C	-0.031469	4.128046	-0.744973
O	-2.420555	5.000259	-0.565094
O	0.880820	4.920768	-0.740305
S	-1.892108	-3.667228	0.319788
C	-0.388838	-1.423160	0.762587
O	0.602726	-0.741680	1.029584
C	3.256374	-1.652980	-1.108950
C	5.318832	-0.257402	-1.099732

C	4.633403	-1.453712	-1.793488
H	3.243881	-2.512449	-0.434639
H	2.456004	-1.773162	-1.836575
H	5.238153	-2.346724	-1.602598
C	3.852752	-0.420677	0.912935
H	3.666825	0.504986	1.452632
H	3.550263	-1.254235	1.551601
C	5.304997	-0.528795	0.411862
H	5.925432	0.200798	0.937925
H	5.717024	-1.520625	0.620259
H	6.343552	-0.154688	-1.463196
C	4.533507	1.041635	-1.349010
H	4.880748	1.806960	-0.648201
H	4.698001	1.431656	-2.357079
C	3.032221	0.774887	-1.152863
H	2.581000	0.446714	-2.096662
N	2.920801	-0.451963	-0.267086
C	4.497396	-1.304874	-3.285332
H	3.953840	-0.434128	-3.653191
C	4.969345	-2.184825	-4.161447
H	5.503200	-3.076189	-3.842061
H	4.839178	-2.047518	-5.229922
C	-0.223116	-2.838471	0.098241
N	0.854962	-3.494703	0.796361
C	0.868544	-3.605249	2.161636
O	0.039488	-3.100615	2.886058
O	1.941473	-4.321541	2.538779
C	2.142540	-4.637844	3.949870
C	3.409378	-5.483129	3.926849
H	3.259571	-6.382902	3.324417
H	4.241917	-4.916040	3.501532
H	3.678170	-5.784528	4.942393
C	0.963020	-5.448659	4.476233
H	1.191157	-5.807750	5.483894
H	0.053975	-4.848319	4.514246
H	0.789553	-6.318715	3.836158
C	2.362172	-3.356090	4.746447
H	3.188685	-2.781209	4.317337
H	1.464021	-2.738505	4.756158
H	2.628364	-3.609704	5.776662
H	0.425558	0.725411	-0.895626
H	-1.898804	0.728460	-1.172934
H	1.488969	-4.082389	0.276260
O	-0.818170	-0.597314	-1.229803
H	1.944170	-0.593172	0.125967
H	0.107544	-0.195900	-3.657470

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Free Energy = -3921.844873 Hartree

Energy = -3922.710143 Hartree

C	2.116827	2.056646	-0.812855
C	2.427643	2.670253	0.550978
C	4.964166	5.372835	-0.129978
H	3.878901	4.091991	-1.397314
C	4.568080	5.224289	2.240459
H	1.584675	2.380275	3.824004
C	5.231116	5.807433	1.193434
H	4.735928	5.542834	3.263491
H	5.942622	6.602090	1.381609
N	2.993685	3.689762	3.132566
N	0.715680	1.692731	-0.960543
N	-2.431439	1.532110	-0.904343
C	-3.796598	1.429764	-0.675801
C	-4.336623	0.134698	-0.726629
C	-4.620032	2.515355	-0.371873
C	-5.681223	-0.059246	-0.472678
H	-3.683616	-0.709631	-0.933593
C	-5.971740	2.283259	-0.123757
H	-4.216308	3.524047	-0.325633
C	-6.522446	1.010493	-0.167598
H	-7.575103	0.852211	0.036452
C	-6.856141	3.467810	0.150896
C	-6.261577	-1.444282	-0.477953
F	-6.255299	4.360758	0.947908
F	-7.183794	4.111520	-0.979596
F	-8.004824	3.105970	0.743476
F	-7.319138	-1.530687	-1.299297
F	-5.375709	-2.371227	-0.861131
F	-6.703774	-1.798174	0.744422
C	1.771178	2.221470	1.670085
C	4.059757	4.359279	-0.362967
C	3.625456	4.188045	2.033777
C	2.095061	2.758496	2.940591
C	3.378142	3.731299	0.704737
H	1.033680	1.428086	1.594473
H	2.329547	2.820560	-1.570431
O	5.561069	5.903892	-1.225370
C	6.443031	6.991894	-1.045354

H	6.772792	7.278922	-2.043715
H	5.940388	7.845336	-0.575853
H	7.318679	6.709555	-0.448857
C	2.114192	-5.702501	-3.674173
C	1.904823	-4.436369	-4.160822
C	1.226424	-3.457993	-3.395457
C	0.788556	-3.770227	-2.070771
C	0.972874	-5.110523	-1.619587
C	1.616206	-6.042230	-2.398478
H	1.297432	-1.941698	-4.937395
H	2.629735	-6.445750	-4.272342
H	2.245296	-4.164785	-5.156850
C	0.952987	-2.166227	-3.930867
C	0.182633	-2.739082	-1.296589
H	0.552949	-5.420597	-0.666632
H	1.727301	-7.057913	-2.032010
C	-0.179094	-1.520838	-1.877836
C	0.251399	-1.236318	-3.216937
C	-2.472448	-2.327493	1.293333
C	-1.639002	-1.214730	1.401993
C	-2.070372	-0.048094	2.025787
C	-3.360196	0.004955	2.537247
C	-4.198646	-1.107578	2.418953
C	-3.770662	-2.277728	1.797650
H	-1.395838	0.800671	2.093974
H	-3.723749	0.909076	3.013085
H	-5.213517	-1.057019	2.799889
H	-4.438953	-3.126525	1.702164
C	-1.622120	2.611282	-0.837228
C	-0.231734	2.642309	-0.881282
C	-1.709656	4.094830	-0.721355
C	-0.176454	4.112851	-0.820651
O	-2.585818	4.915403	-0.593425
O	0.710365	4.932939	-0.862687
S	-1.751673	-3.712941	0.474073
C	-0.311403	-1.410248	0.814705
C	3.279817	-1.566254	-1.160648
C	5.297683	-0.108701	-1.238629
C	4.629026	-1.337806	-1.890242
H	3.314177	-2.413367	-0.471650
H	2.462324	-1.723991	-1.861607
H	5.266299	-2.208501	-1.702134
C	3.898061	-0.279796	0.820226
H	3.699836	0.649548	1.349255
H	3.640670	-1.110469	1.482031
C	5.337379	-0.352836	0.277124
H	5.950443	0.404706	0.771379
H	5.785973	-1.327712	0.490048
H	6.307459	0.018484	-1.634722
C	4.465465	1.161250	-1.485823
H	4.808922	1.949011	-0.808337
H	4.588025	1.538640	-2.504609
C	2.979753	0.851642	-1.240740
H	2.512422	0.491771	-2.164870
N	2.932618	-0.360992	-0.330083
C	4.443692	-1.221236	-3.379644
H	3.867918	-0.371093	-3.746632
C	4.909111	-2.107078	-4.253335
H	5.474175	-2.979022	-3.934062
H	4.742168	-1.994221	-5.319562
C	-0.118792	-2.836799	0.181414
N	1.001303	-3.440372	0.860190
C	1.062256	-3.515909	2.226565
O	0.238621	-3.024029	2.965663
O	2.172781	-4.183109	2.585183
C	2.428790	-4.459428	3.995738
C	3.725033	-5.258010	3.951130
H	3.590524	-6.176488	3.373821
H	4.522184	-4.670724	3.487145
H	4.036280	-5.525657	4.964011
C	1.297077	-5.300798	4.576325
H	1.569299	-5.628523	5.583730
H	0.367831	-4.733488	4.630141
H	1.136620	-6.190776	3.960733
C	2.624719	-3.152783	4.757226
H	3.417528	-2.559041	4.291787
H	1.705481	-2.567408	4.779457
H	2.929011	-3.373190	5.784514
H	0.385639	0.724066	-0.892446
H	-1.947129	0.646718	-1.104342
H	1.639467	-4.018018	0.334028
O	-0.829328	-0.650607	-1.163421
H	1.972562	-0.524610	0.096152
H	0.001726	-0.263511	-3.630424
O	0.666623	-0.693302	1.039788

IM6a-1

Free Energy = -3921.846878 Hartree

Energy = -3922.710519 Hartree

C	-2.520145	-1.424085	0.649335
C	-3.071572	-0.261845	1.461119
C	-5.405727	-1.854222	3.956098
H	-4.245074	-2.642602	2.386062
C	-5.317780	0.521054	4.342873
H	-2.677000	3.080956	1.881374
C	-5.817266	-0.708674	4.683225
H	-5.604907	1.416339	4.883560
H	-6.516366	-0.797336	5.505687
N	-3.934611	1.937435	3.034605
N	-1.136917	-1.124999	0.265363
N	1.916603	-1.342554	0.801906
C	3.292296	-1.404788	1.021634
C	3.872097	-0.316465	1.685788
C	4.086525	-2.473646	0.610627
C	5.234795	-0.298689	1.919580
H	3.252434	0.522000	1.991234
C	5.455801	-2.423183	0.857429
H	3.656289	-3.320071	0.081697
C	6.050320	-1.349480	1.503863
H	7.119022	-1.329611	1.683541
C	6.311383	-3.521199	0.292920
C	5.869322	0.911194	2.541576
F	5.742864	-4.723722	0.436227
F	6.517527	-3.341888	-1.024695
F	7.518036	-3.567800	0.874766
F	6.814737	0.572518	3.428882
F	6.468745	1.678885	1.614428
F	4.974925	1.684185	3.172680
C	-2.626444	1.016678	1.243486
C	-4.516699	-1.732745	2.908729
C	-4.400015	0.679403	3.276733
C	-3.073458	2.083810	2.061007
C	-3.996549	-0.472238	2.536553
H	-1.918063	1.227902	0.450730
H	-2.519901	-2.300016	1.312573
O	-5.842257	-3.108248	4.225598
C	-6.745773	-3.287488	5.296795
H	-6.954234	-4.356375	5.337016
H	-6.307943	-2.972751	6.251132
H	-7.684397	-2.746785	5.128450
C	5.155138	-0.485405	-1.854244
C	4.209186	-1.287573	-2.444819
C	2.851024	-0.899657	-2.506663
C	2.413761	0.331579	-1.928784
C	3.422656	1.119218	-1.312836
C	4.744673	0.731665	-1.285470
H	2.242019	-2.671126	-3.599243
H	6.192294	-0.798679	-1.804528
H	4.488621	-2.247023	-2.872791
C	1.904328	-1.734862	-3.162996
C	1.017689	0.705486	-1.977365
H	3.179025	2.064838	-0.853236
H	5.470001	1.368567	-0.788238
C	0.116282	-0.144779	-2.646568
C	0.602034	-1.364248	-3.231075
C	1.919652	4.198178	-0.654854
C	1.680064	3.394482	0.466577
C	2.107829	3.770975	1.739593
C	2.786768	4.969247	1.890950
C	3.028197	5.773363	0.770219
C	2.606334	5.402127	-0.501523
H	1.893705	3.122160	2.583679
H	3.131070	5.285570	2.868947
H	3.560998	6.711192	0.893936
H	2.806100	6.037112	-1.357834
C	1.114908	-2.200133	0.143253
C	-0.258287	-2.106529	-0.058719
C	1.197751	-3.491193	-0.598849
C	-0.309894	-3.364748	-0.822390
O	2.054615	-4.274513	-0.921843
O	-1.158458	-4.012206	-1.401060
S	1.353884	3.534993	-2.179305
C	0.964491	2.160498	0.157597
O	0.663176	1.292282	0.964451
C	-3.409561	-1.912697	-3.004281
C	-5.543639	-1.895852	-1.721469
C	-4.787008	-2.607374	-2.868275
H	-3.342171	-1.260157	-3.876973
H	-2.590266	-2.635655	-3.049105
H	-5.358182	-2.443281	-3.788797
C	-4.083754	0.120884	-1.833622
H	-3.942591	0.673800	-0.904705
H	-3.751585	0.768478	-2.648200
C	-5.529000	-0.386972	-2.005964
H	-6.192780	0.137700	-1.313267
H	-5.893642	-0.190823	-3.019248

H	-6.567479	-2.274705	-1.674641
C	-4.828643	-2.129096	-0.380188
H	-5.238204	-1.439307	0.364227
H	-4.997229	-3.145432	-0.012801
C	-3.320131	-1.898574	-0.589197
H	-2.849240	-2.843698	-0.869411
N	-3.152056	-1.047289	-1.809928
C	-4.666998	-4.094845	-2.649974
H	-3.842278	-4.440294	-2.024843
C	-5.504648	-4.981704	-3.176022
H	-6.323337	-4.676171	-3.823676
H	-5.401946	-6.044427	-2.984440
C	0.558712	2.028594	-1.345814
N	-0.872102	2.134202	-1.428702
C	-1.574749	3.185103	-0.940982
O	-1.134271	4.051590	-0.208418
O	-2.863923	3.085216	-1.346997
C	-3.705323	4.274842	-1.388997
C	-4.952050	3.776969	-2.110476
H	-4.699107	3.412744	-3.110196
H	-5.419737	2.964016	-1.546094
H	-5.680121	4.586272	-2.209866
C	-3.007944	5.361089	-2.202195
H	-3.693022	6.198833	-2.360273
H	-2.119958	5.729449	-1.685831
H	-2.712331	4.969288	-3.180117
C	-4.057393	4.753443	0.014694
H	-4.531452	3.951029	0.587468
H	-3.168439	5.098442	0.543767
H	-4.767938	5.582860	-0.055819
H	-0.720207	-0.308391	0.704895
H	1.483358	-0.461716	1.068497
H	-1.296358	1.453671	-2.099833
O	-1.179510	0.076133	-2.798353
H	-0.138452	-1.975087	-3.738914
H	-2.125435	-0.630149	-2.022837

TS4b-1

Free Energy = -3921.6763539 Hartree

Energy = -3922.6976905 Hartree

C	-3.258565	1.033538	-1.059822
C	-3.805303	-0.348379	-1.377727
C	-7.319469	0.311153	-2.565908
H	-5.767199	1.580281	-1.909835
C	-6.895551	-2.060261	-2.607535
H	-2.948580	-3.632950	-1.366636
C	-7.754096	-1.014362	-2.825765
H	-7.201052	-3.083620	-2.799606
H	-8.754013	-1.206345	-3.195615
N	-4.794668	-2.950239	-1.941117
N	-1.841371	1.097136	-1.414196
N	1.229521	1.586265	-1.592137
C	2.596387	1.750167	-1.351435
C	3.469256	0.796190	-1.879736
C	3.095548	2.780880	-0.551919
C	4.824024	0.862583	-1.585711
H	3.083840	-0.007182	-2.501997
C	4.457683	2.821129	-0.279756
H	2.430532	3.521916	-0.122919
C	5.339966	1.872360	-0.782931
H	6.392083	1.898765	-0.527833
C	4.969193	3.902446	0.628541
C	5.730813	-0.187277	-2.160419
F	4.121708	4.132143	1.646935
F	6.157130	3.588826	1.165872
F	5.124487	5.071809	-0.012111
F	5.951775	0.012201	-3.471999
F	6.928467	-0.207247	-1.559807
F	5.205329	-1.418760	-2.049941
C	-3.037187	-1.475469	-1.223241
C	-6.043847	0.548779	-2.096170
C	-5.580042	-1.850395	-2.126222
C	-3.574167	-2.754319	-1.509983
C	-5.143925	-0.517280	-1.863952
H	-2.009180	-1.425049	-0.879603
H	-3.775379	1.761401	-1.693267
O	-8.101252	1.401256	-2.752077
C	-9.418853	1.207404	-3.240735
H	-9.859039	2.201618	-3.314061
H	-9.412727	0.741795	-4.232175
H	-10.014861	0.598411	-2.552330
C	2.327243	1.490732	2.406599
C	1.082882	1.249079	1.915826
C	3.400108	0.610837	2.106538
C	0.782346	0.067236	1.162706
C	1.797574	-0.890308	0.946679
C	3.154624	-0.556185	1.314030
O	-0.444883	-0.068292	0.700776

C	2.929331	-3.631602	-1.195182
C	2.238019	-2.701823	-1.974057
C	2.493653	-2.560176	-3.340405
C	3.481842	-3.342133	-3.917462
C	4.189243	-4.262096	-3.130456
C	3.923925	-4.420957	-1.773953
H	1.917208	-1.845286	-3.921187
H	3.710910	-3.246035	-4.972990
H	4.964271	-4.868260	-3.589430
H	4.476619	-5.143406	-1.182011
C	0.238253	2.459944	-1.333562
C	-1.137687	2.232615	-1.288792
C	0.073954	3.911089	-1.086805
C	-1.431322	3.661742	-1.068829
O	0.793998	4.871992	-0.930739
O	-2.430213	4.335709	-0.924670
S	2.414457	-3.714066	0.489452
C	1.203888	-1.987892	-1.224862
O	0.341719	-1.278468	-1.721979
C	-2.423333	2.032387	2.481883
C	-4.860586	1.507887	2.458614
C	-3.819588	2.544525	2.931510
H	-1.865176	1.578228	3.304353
H	-1.818666	2.837874	2.053771
H	-3.821730	2.543687	4.029028
C	-3.146089	-0.248215	2.070715
H	-3.402039	-0.942878	1.269610
H	-2.335920	-0.698153	2.649242
C	-4.372872	0.126712	2.922478
H	-5.157897	-0.621959	2.787026
H	-4.117174	0.153111	3.987146
H	-5.841154	1.730225	2.885868
C	-4.933585	1.469086	0.919120
H	-5.420922	0.537312	0.612981
H	-5.513698	2.298305	0.508635
C	-3.497882	1.554015	0.384127
H	-3.229202	2.612654	0.332783
N	-2.581990	0.983300	1.431633
C	-4.080350	3.962829	2.480019
H	-3.207730	4.616934	2.473351
C	-5.261283	4.469917	2.135973
H	-6.171740	3.876183	2.130979
H	-5.357114	5.512948	1.851309
C	1.319123	-2.225342	0.304701
N	0.006684	-2.637567	0.783294
C	-0.105783	-3.083717	2.079248
O	0.823062	-3.459017	2.767678
O	-1.399690	-3.082106	2.439495
C	-1.811244	-3.674792	3.710975
C	-3.327484	-3.530779	3.678256
H	-3.615882	-2.475565	3.672143
H	-3.739571	-4.013793	2.787786
H	-3.763176	-3.999393	4.564586
C	-1.223257	-2.884110	4.874129
H	-1.654735	-3.247866	5.811358
H	-0.139374	-2.990556	4.920376
H	-1.473459	-1.822569	4.773856
C	-1.419968	-5.148275	3.750849
H	-1.806435	-5.662824	2.865913
H	-0.337807	-5.272328	3.791882
H	-1.861261	-5.612344	4.637586
H	-1.285655	0.259610	-1.246863
H	0.939168	0.641900	-1.839181
H	-0.694210	-1.933816	0.556913
H	-1.520199	0.641786	1.065643
C	4.320516	-1.262672	0.893532
C	5.583973	-0.910302	1.308546
C	5.793171	0.186307	2.169098
C	4.709504	0.943040	2.535471
H	0.270342	1.948741	2.089398
H	2.529584	2.382313	2.994130
H	4.834225	1.835009	3.144649
H	6.794081	0.451070	2.494457
H	6.433504	-1.476618	0.938216
H	4.240715	-2.064783	0.179578

IM7b-1

Free Energy = -3921.846734 Hartree

Energy = -3922.713728 Hartree

C	-2.653569	-1.662532	0.514399
C	-3.323930	-0.464942	1.160923
C	-5.502430	-1.900756	3.881050
H	-4.249490	-2.790525	2.442690
C	-5.681986	0.500419	3.894947
H	-3.370037	2.917561	1.006687
C	-6.044201	-0.709262	4.426432
H	-6.074252	1.431156	4.290146
H	-6.737329	-0.746582	5.257885

N	-4.465579	1.838810	2.358774	H	5.345138	0.934710	-1.127304
N	-1.256856	-1.304306	0.223870	C	-0.269597	0.047462	-2.476638
N	1.787944	-1.264875	0.896952	C	0.000181	-1.204386	-3.102949
C	3.164662	-1.196985	1.106138	C	2.271795	4.077156	-0.649499
C	3.666197	0.000677	1.625592	C	1.945399	3.305047	0.472323
C	4.038798	-2.245333	0.812572	C	2.495509	3.573808	1.723888
C	5.029539	0.157880	1.810341	C	3.396839	4.620182	1.851030
H	2.985792	0.820166	1.842966	C	3.729789	5.384979	0.729048
C	5.401193	-2.060624	1.022984	C	3.178842	5.125631	-0.522900
H	3.672838	-3.179645	0.396624	H	2.205214	2.965885	2.575885
C	5.920857	-0.866683	1.509178	H	3.849742	4.836788	2.811643
H	6.986371	-0.740457	1.657184	H	4.438502	6.200775	0.831898
C	6.334887	-3.171337	0.629273	H	3.450797	5.729116	-1.382133
C	5.534881	1.510402	2.218743	C	1.073074	-2.202023	0.239574
F	5.831720	-4.373679	0.930335	C	-0.296134	-2.223402	-0.017474
F	6.571258	-3.168248	-0.694634	C	1.298463	-3.481756	-0.480602
F	7.524532	-3.062264	1.237603	C	-0.205420	-3.514064	-0.737046
F	6.789238	1.464944	2.682305	O	2.235623	-4.175250	-0.793786
F	5.526646	2.359410	1.175038	O	-0.961778	-4.263591	-1.314711
F	4.768787	2.065011	3.172209	S	1.510558	3.568460	-2.153341
C	-3.028798	0.804459	0.730963	C	1.004040	2.224101	0.184606
C	-4.621185	-1.845972	2.822115	O	0.597493	1.387842	0.973007
C	-4.777721	0.591691	2.809550	C	-3.430983	-2.372946	-3.094464
C	-3.621874	1.923757	1.362597	C	-5.522518	-2.804297	-1.802333
C	-4.236659	-0.607939	2.256915	C	-4.634167	-3.353089	-2.943215
H	-2.346353	0.969938	-0.098825	H	-3.508363	-1.778511	-4.010818
H	-2.650814	-2.479763	1.247546	H	-2.494526	-2.938013	-3.127072
O	-5.802758	-3.139059	4.344215	H	-5.233688	-3.331438	-3.860895
C	-6.694986	-3.248079	5.433332	C	-4.538627	-0.533216	-2.014322
H	-6.787587	-4.314260	5.639354	H	-4.541913	0.083759	-1.116530
H	-6.306517	-2.744470	6.326253	H	-4.390237	0.137881	-2.866119
H	-7.684478	-2.844956	5.187645	C	-5.848444	-1.344743	-2.137878
C	4.720452	-0.879071	-2.130986	H	-6.602908	-0.951233	-1.450271
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C	2.338966	-0.997295	-2.593502	H	-6.432805	-3.405314	-1.730060
C	2.105179	0.284488	-2.007479	C	-4.761136	-2.817342	-0.465486
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C	0.516266	2.205436	-1.302517
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C	-1.318129	3.728736	-0.727086
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C	-3.205759	5.252802	-0.877270
C	-4.574684	5.088371	-1.523926
H	-4.473397	4.844918	-2.584817
H	-5.131252	4.284503	-1.033961
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H	-1.405999	6.444287	-1.142959
H	-2.203222	5.959190	-2.656955
C	-3.348428	5.604885	0.601015
H	-4.027889	4.915031	1.110331
H	-2.380139	5.597860	1.101619
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H	-0.934873	-0.430577	0.632236
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H	-1.496574	2.068304	-1.924743
O	-1.574148	0.410058	-2.463894
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H	-2.182432	-0.394255	-2.227189

IM8a-1

Free Energy = -3921.860980 Hartree

Energy = -3922.724432 Hartree

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H	1.824532	1.985772	4.045012
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H	5.905755	6.489749	1.626178
N	3.136537	3.396383	3.360788
N	0.738522	1.564899	-0.740178
N	-2.441252	1.467933	-0.602392
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C	-4.436739	0.199778	-0.303889
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F	-7.996809	3.588499	0.182372
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O	5.467150	5.871922	-0.991296
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H	7.229567	6.686112	-0.235661
C	1.844803	-5.555625	-4.226901
C	1.469878	-4.283688	-4.574147
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C	0.661514	-3.892224	-2.293419
C	1.042470	-5.220993	-1.965412
C	1.618560	-6.028667	-2.913400
H	0.619189	-1.773032	-5.005802
H	2.307536	-6.207479	-4.959918
H	1.630714	-3.916806	-5.583873
C	0.454855	-2.103037	-3.984267
C	0.091925	-2.985020	-1.366602
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H	1.900002	-7.044343	-2.655264
C	-0.289226	-1.732039	-1.764948
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C	-1.663850	-1.546130	1.404640

C	-2.052585	-0.429820	2.130277
C	-3.266735	-0.458369	2.812582
C	-4.068403	-1.597488	2.755610
C	-3.669147	-2.726481	2.041057
H	-1.414527	0.449383	2.151080
H	-3.592959	0.407333	3.378193
H	-5.021913	-1.610965	3.271928
H	-4.298186	-3.609555	2.011720
C	-1.597853	2.516140	-0.785327
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C	-1.664050	3.989926	-1.003925
C	-0.132792	3.963424	-1.095779
O	-2.522932	4.834280	-1.072832
O	0.762018	4.744970	-1.307880
S	-1.750773	-4.037314	0.452311
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C	5.263483	-0.258952	-1.264109
C	4.555625	-1.362141	-2.080715
H	3.176436	-2.550984	-0.855646
H	2.380724	-1.655599	-2.154915
H	5.150242	-2.279041	-1.994640
C	3.786747	-0.651175	0.702629
H	3.626364	0.195029	1.370037
H	3.510201	-1.558988	1.252036
C	5.250846	-0.702236	0.205037
H	5.877924	-0.040182	0.809181
H	5.663226	-1.713081	0.295312
H	6.286974	-0.126895	-1.624104
C	4.486771	1.066513	-1.351073
H	4.848743	1.740250	-0.566777
H	4.648612	1.575410	-2.306554
C	2.988478	0.758921	-1.165265
H	2.540718	0.563079	-2.147281
N	2.833008	-0.533249	-0.433501
C	4.419014	-1.047296	-3.544551
H	3.883104	-0.134345	-3.808011
C	4.883567	-1.820114	-4.520835
H	5.417020	-2.743180	-4.308124
H	4.751467	-1.559976	-5.566016
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N	0.978786	-3.660295	0.780188
C	1.133784	-3.522328	2.141361
O	0.228016	-3.262518	2.896813
O	2.422711	-3.726708	2.461045
C	2.847088	-3.609238	3.854473
C	4.345218	-3.870360	3.771312
H	4.540087	-4.860593	3.351202
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C	2.157854	-4.676204	4.697814
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H	1.085674	-4.492212	4.767407
H	2.323645	-5.665678	4.261800
C	2.572205	-2.198622	4.366931
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H	1.502485	-2.000361	4.430979
H	3.015088	-2.083854	5.360597
H	0.466242	0.665620	-0.361767
H	-2.000617	0.552925	-0.583339
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O	-0.811145	-0.978996	-0.750003
H	1.397373	-0.910581	0.401170
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O	0.618418	-0.958153	1.050291

7j

Free Energy = -1642.519464 Hartree

Energy = -1642.866072 Hartree

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C	-2.614999	-0.372161	-0.152119
C	-2.723489	0.930612	-0.704412
C	-3.955339	1.462053	-0.993226
H	-4.666873	-2.992753	0.738790
H	-6.104864	1.171286	-0.982700
H	-5.966426	-1.114321	-0.053852
C	-3.739631	-2.448124	0.585294
C	-1.381723	-0.992853	0.185119
H	-1.822793	1.493200	-0.920382
H	-4.019193	2.458090	-1.420002
C	-1.380214	-2.276130	0.670954
C	-2.540811	-3.039542	0.884113
H	-2.464735	-4.047416	1.274599
C	2.119866	-1.702409	-1.075797
C	2.061129	-2.071070	0.264116
C	3.095154	-2.775544	0.861753

C	4.201041	-3.129746	0.093134
C	4.254803	-2.772415	-1.253659
C	3.221970	-2.053026	-1.850396
H	3.026877	-3.035877	1.913036
H	5.021392	-3.679251	0.541504
H	5.120564	-3.046834	-1.848083
H	3.281245	-1.760976	-2.893520
S	0.726096	-0.773968	-1.646088
C	0.782314	-1.682915	0.938630
O	1.032452	-1.293327	2.254732
C	0.065429	-0.551770	0.081444
N	0.428563	0.715781	0.665682
C	0.542639	1.913601	0.021036
O	0.144278	2.155134	-1.100530
O	1.153586	2.785096	0.843668
C	1.357385	4.165398	0.425772
C	0.014815	4.841019	0.163987
H	-0.468218	4.432013	-0.723381
H	-0.646873	4.707249	1.024992
H	0.170690	5.913899	0.017686
C	2.276469	4.213774	-0.790409
H	2.534650	5.254006	-1.010020
H	3.202048	3.668929	-0.582711
H	1.796001	3.776670	-1.665722
C	2.039864	4.783220	1.640027
H	1.393840	4.713722	2.519257
H	2.976842	4.263631	1.857078
H	2.260765	5.837032	1.451693
H	0.896858	0.650116	1.561215
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H	0.207767	-1.389374	2.752244

3j'

Free Energy = -1642.508260 Hartree

Energy =-1642.851941 Hartree

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C	-0.748422	2.041891	-0.017845
C	-1.945407	1.988772	-0.786220
C	-2.456278	3.102597	-1.404912
H	1.355009	4.484144	1.187197
H	-2.215300	5.220162	-1.812344
H	-0.205469	5.418265	-0.376361
C	0.908695	3.500269	1.075337
C	-0.152471	0.909716	0.648284
H	-2.506196	1.068496	-0.848742
H	-3.382054	3.019062	-1.965253
C	0.747883	1.172877	1.676408
C	1.314355	2.460062	1.852859
H	2.069570	2.566038	2.623793
C	-2.564268	-1.524113	-0.738424
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C	-3.738538	-2.087377	1.326805
C	-4.842229	-2.467964	0.582086
C	-4.801687	-2.375756	-0.816095
C	-3.677585	-1.909719	-1.487439
H	-3.724620	-2.146532	2.410607
H	-5.735946	-2.835519	1.073215
H	-5.671600	-2.674783	-1.392609
H	-3.665645	-1.847952	-2.570405
S	-1.046825	-0.929203	-1.406694
C	-1.356226	-1.214755	1.286453
O	-1.056538	-1.349078	2.461606
C	-0.363849	-0.587338	0.282508
N	0.865158	-1.351303	0.379937
C	1.921297	-0.975649	-0.414701
O	1.799275	-0.272966	-1.396209
O	3.049716	-1.526945	0.046336
C	4.323815	-1.214472	-0.590219
C	5.320891	-1.993004	0.258347
H	5.280297	-1.658833	1.298344
H	5.095352	-3.062323	0.228809
H	6.335278	-1.839922	-0.119030
C	4.589389	0.284746	-0.496077
H	5.609154	0.496069	-0.830949
H	3.891095	0.850398	-1.113548
H	4.492971	0.615830	0.542440
C	4.330199	-1.718027	-2.029490
H	4.064240	-2.778792	-2.057038
H	3.626689	-1.158863	-2.646120
H	5.334939	-1.607268	-2.448044
H	1.117558	-1.702677	1.293590
O	1.194491	0.239360	2.559859
H	0.464715	-0.376498	2.758879

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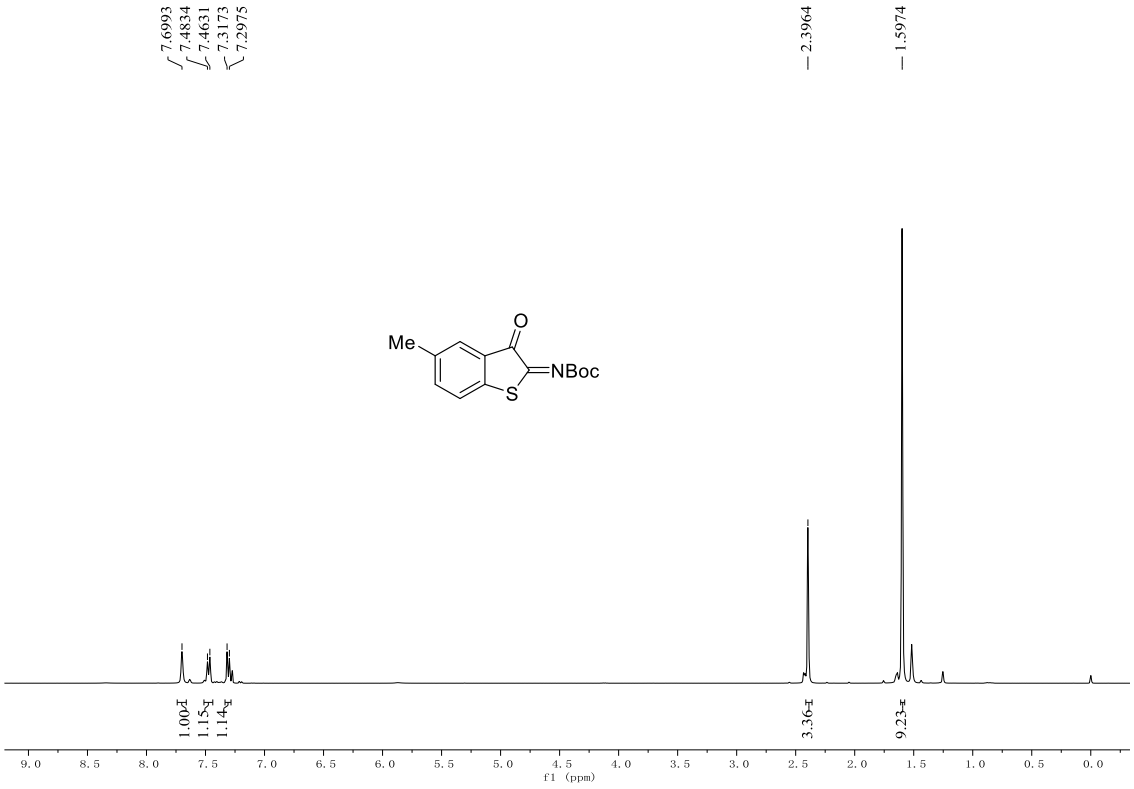
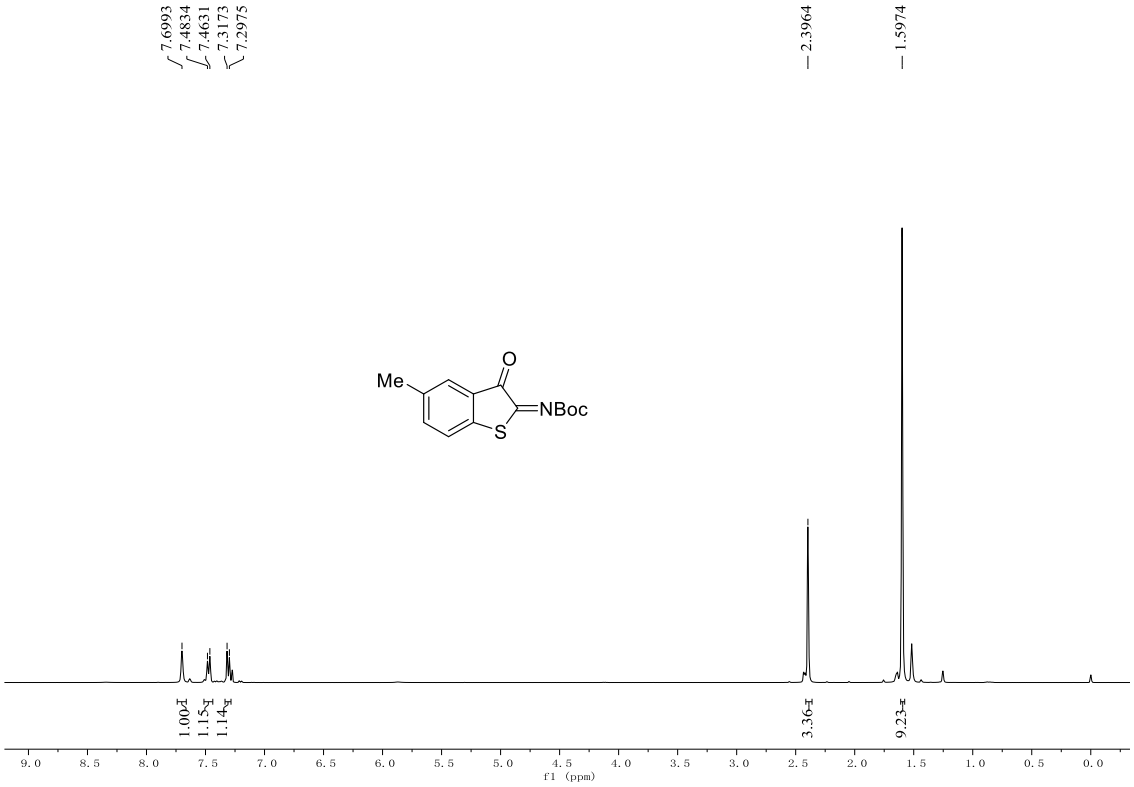
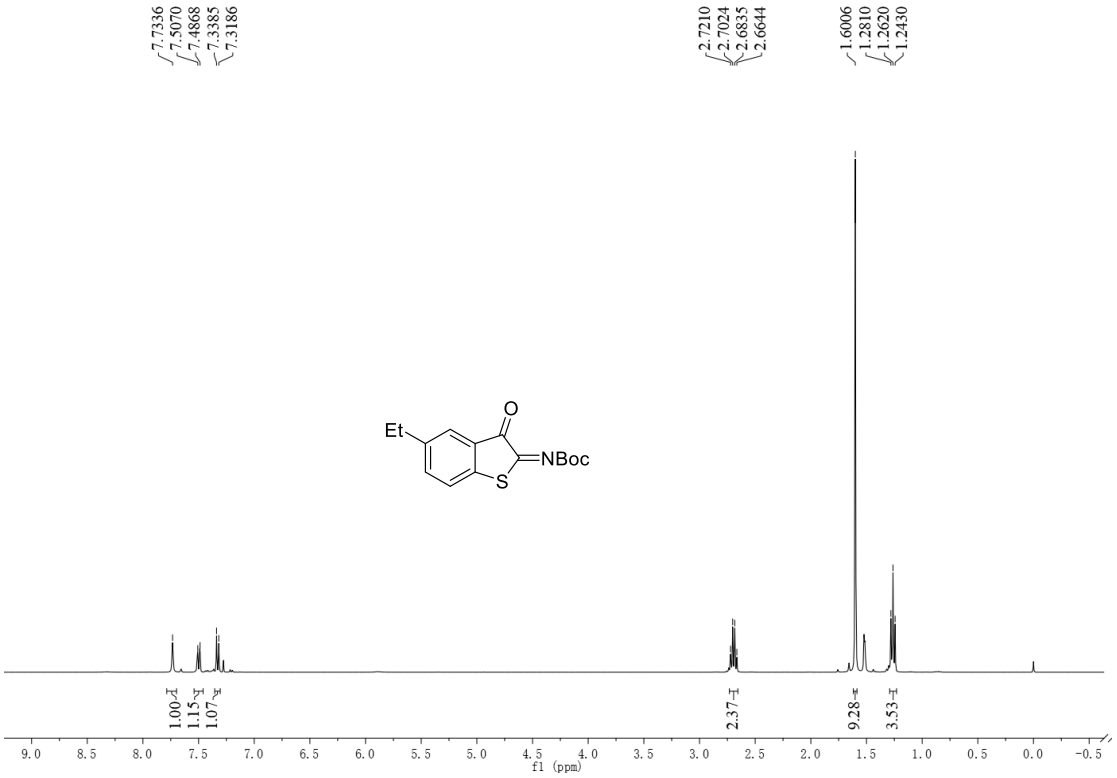
10. ^{1}H NMR, ^{13}C NMR and HPLC spectra for compounds

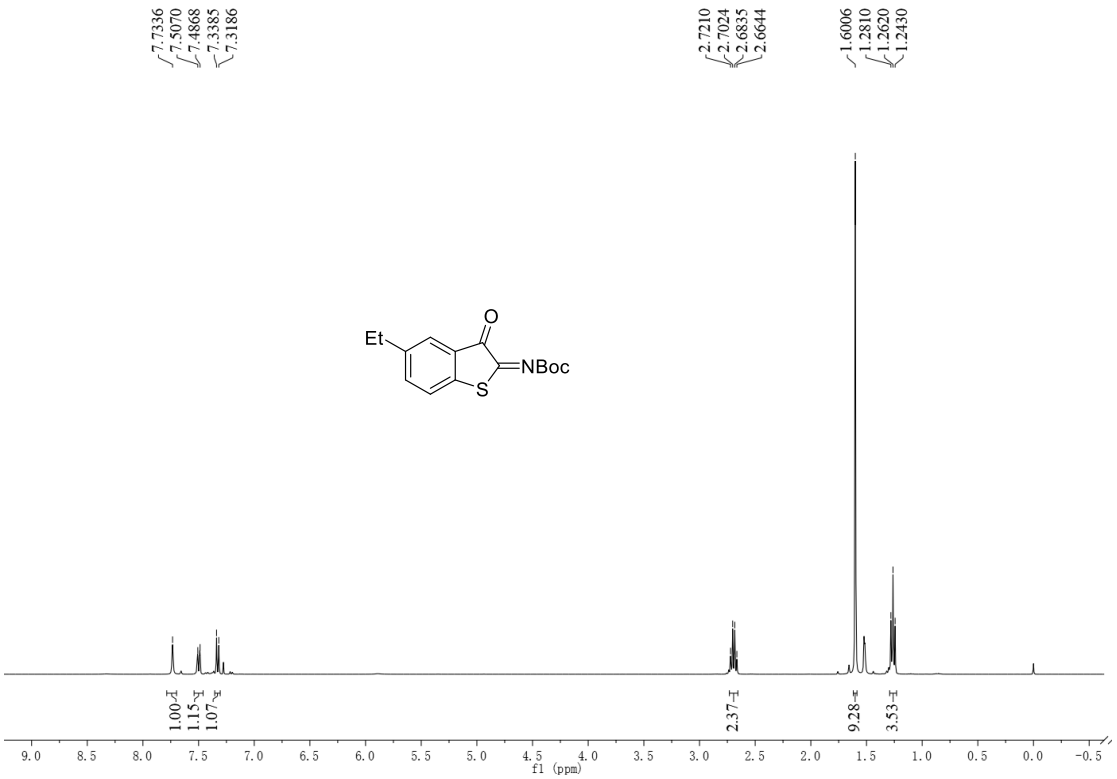
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1a



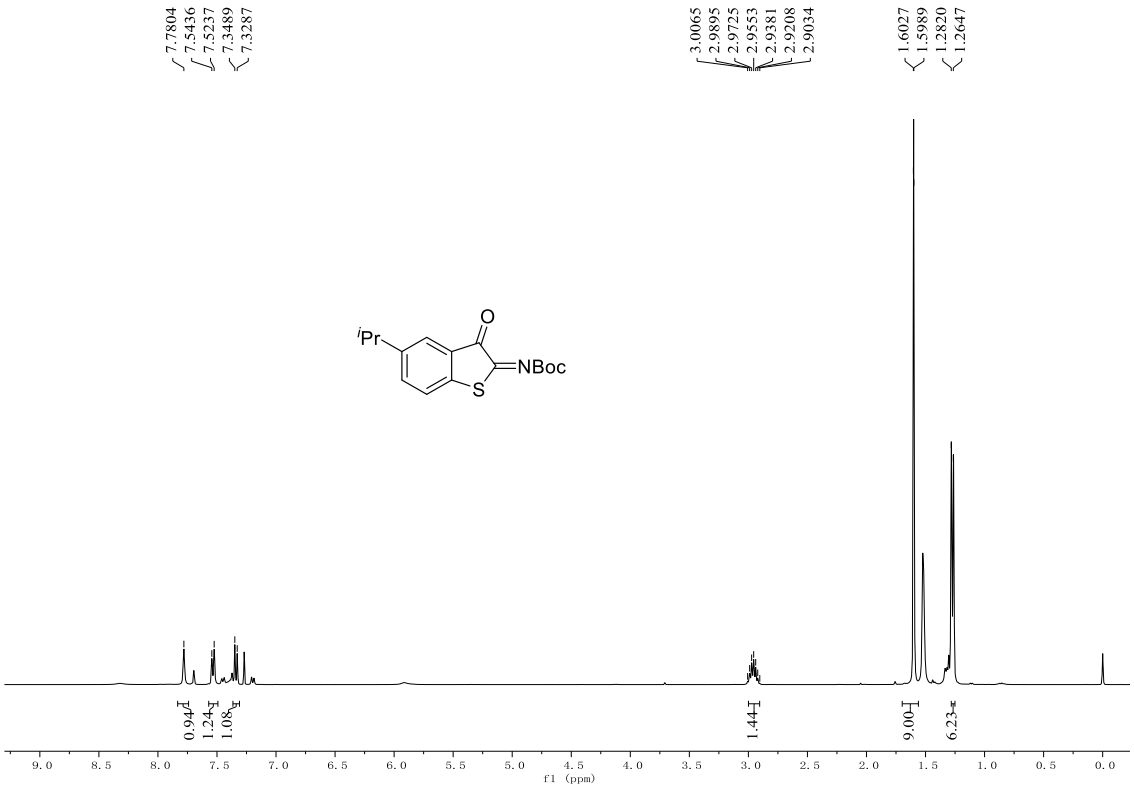


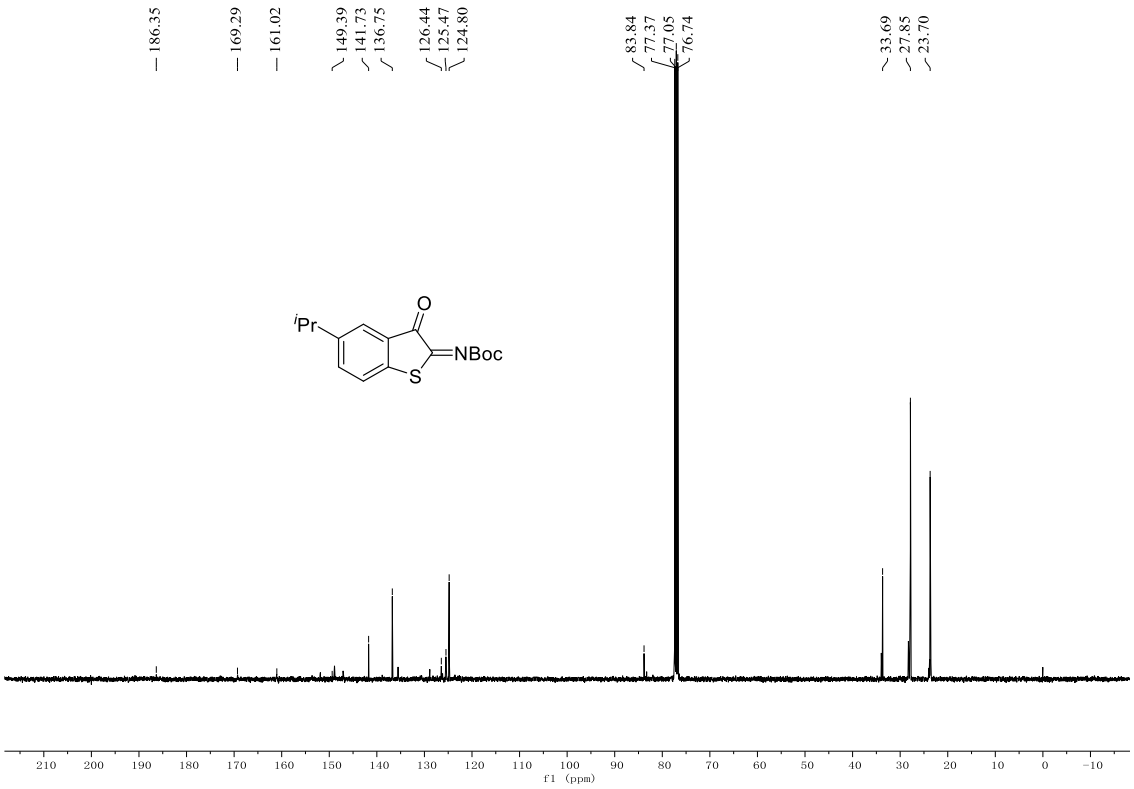
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1b



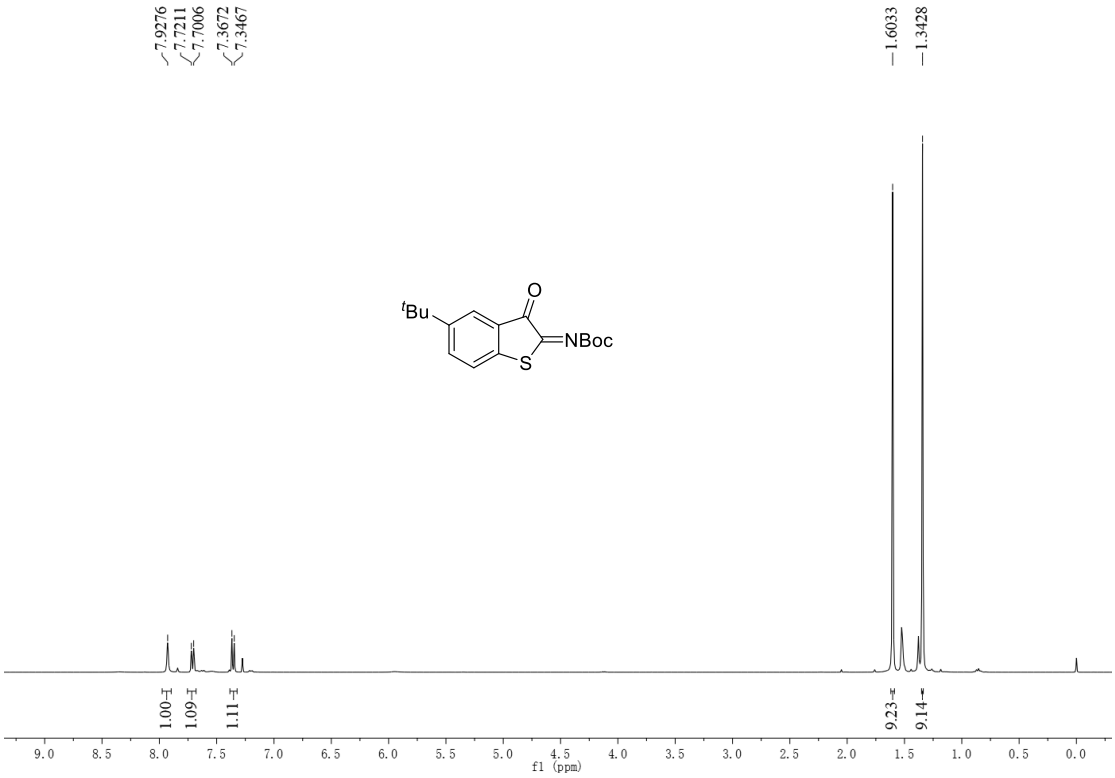


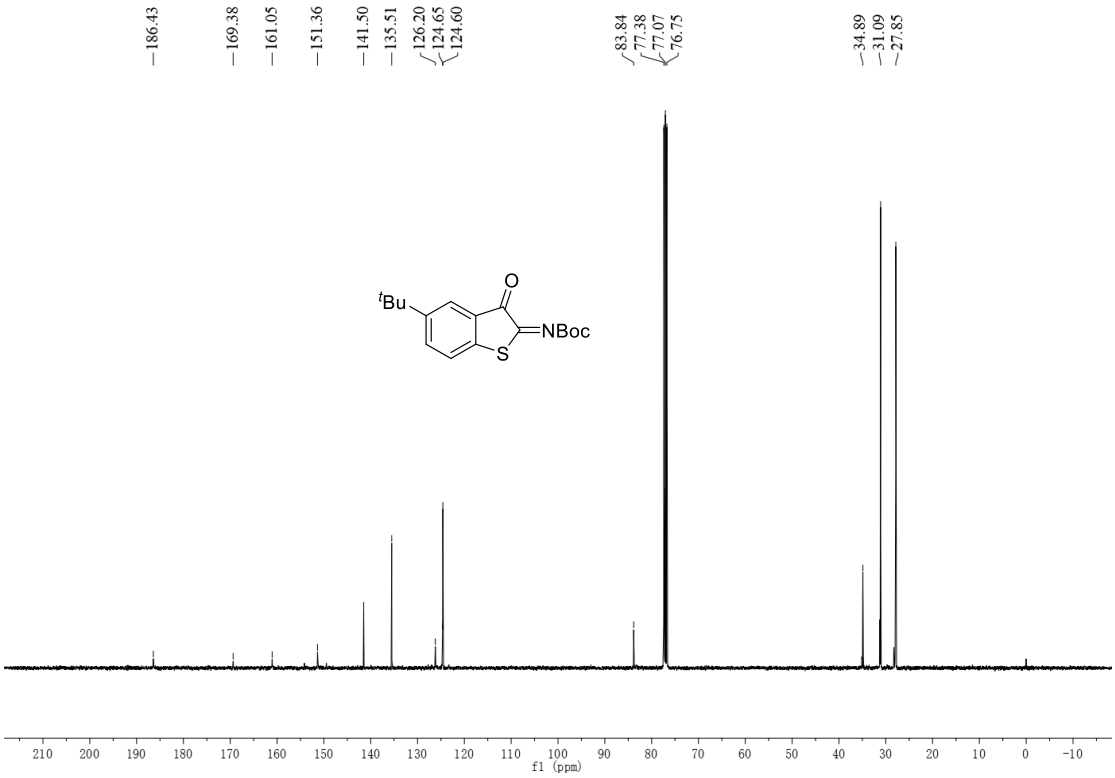
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1c



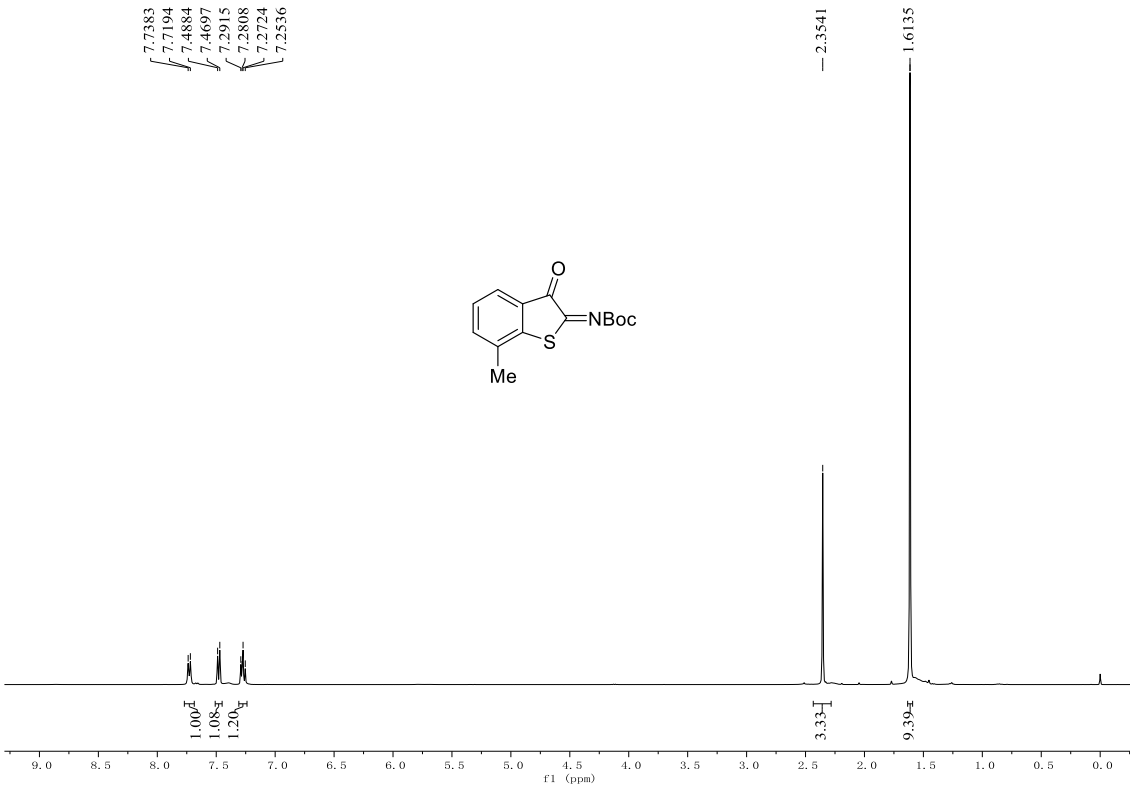


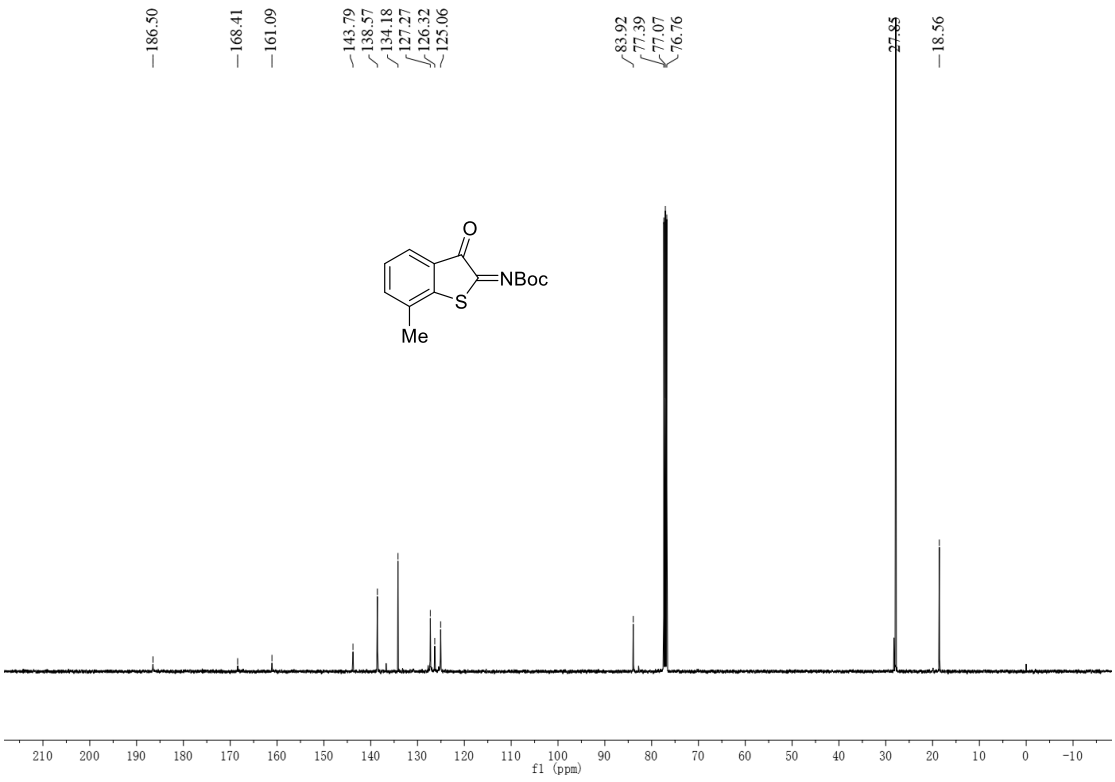
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1d



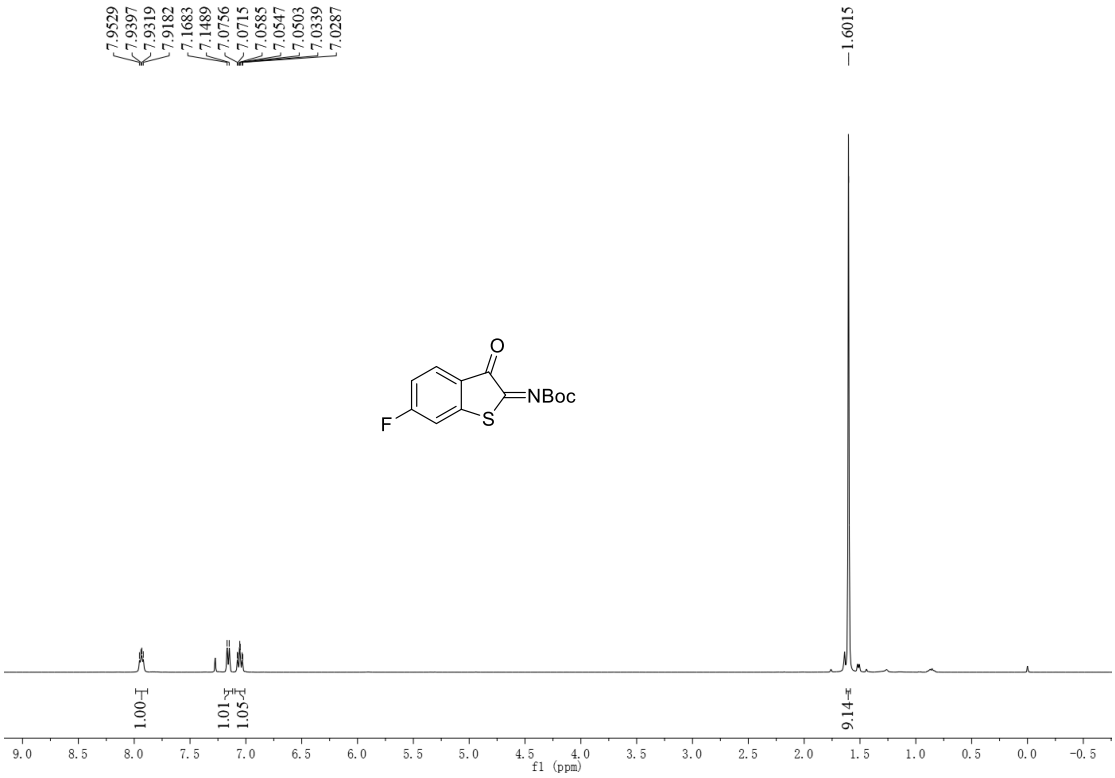


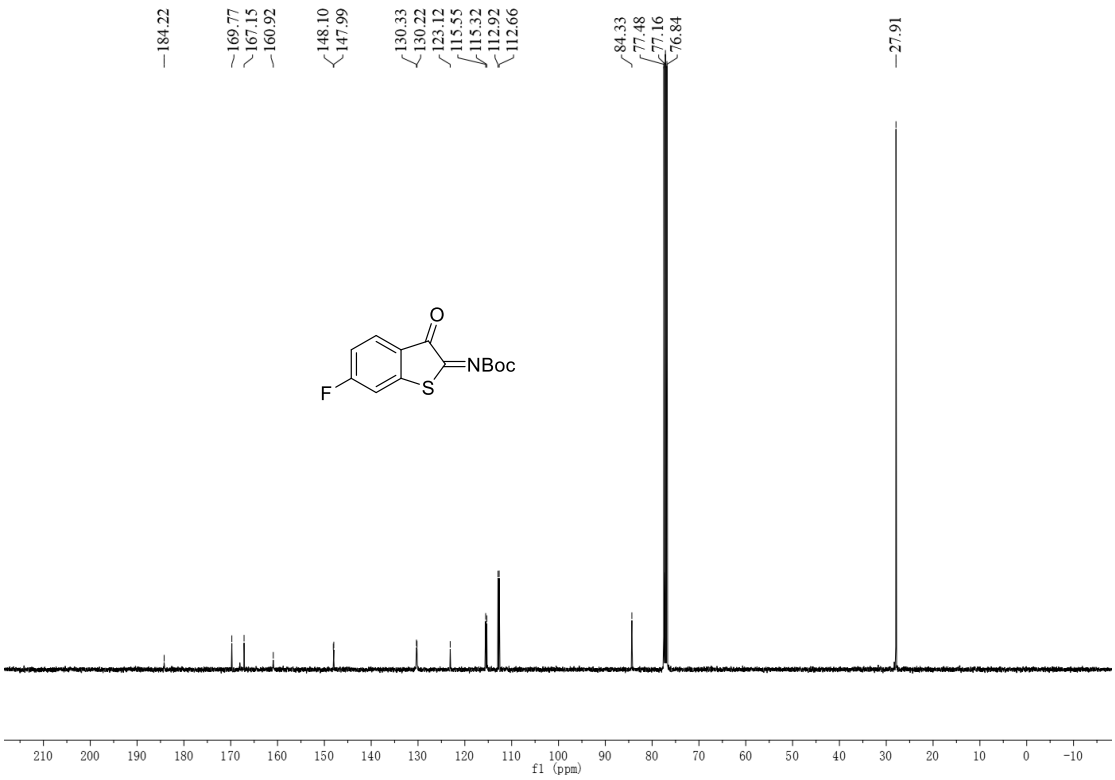
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1e



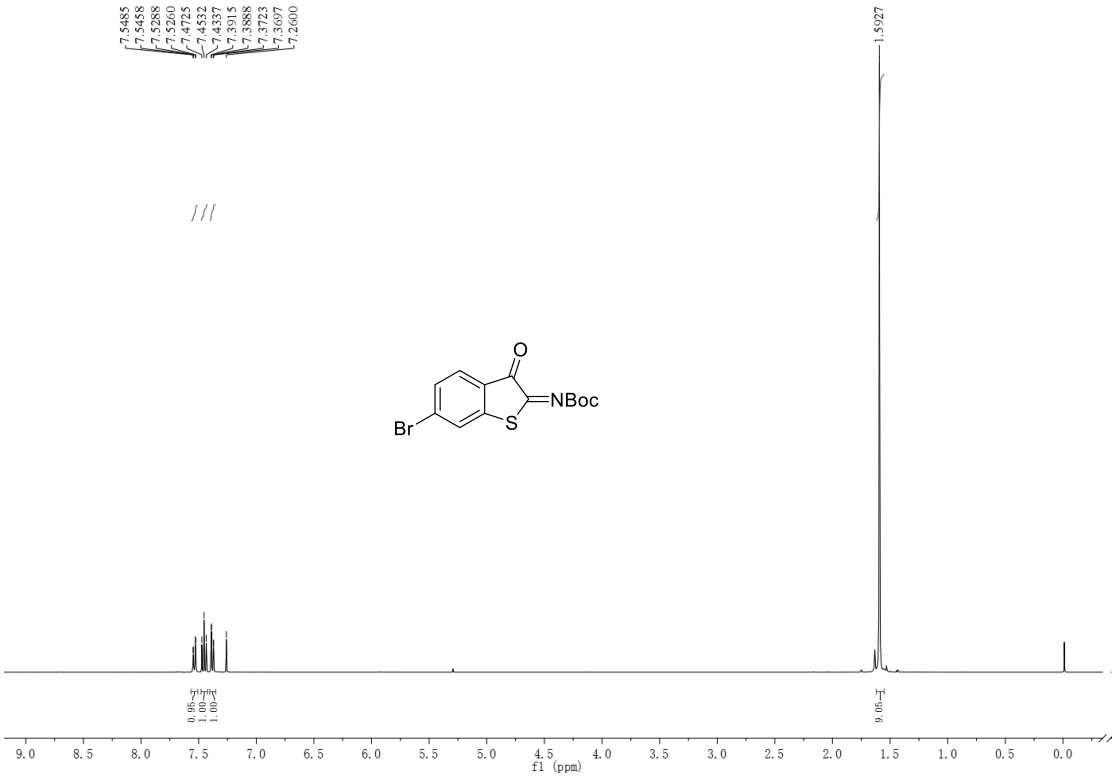


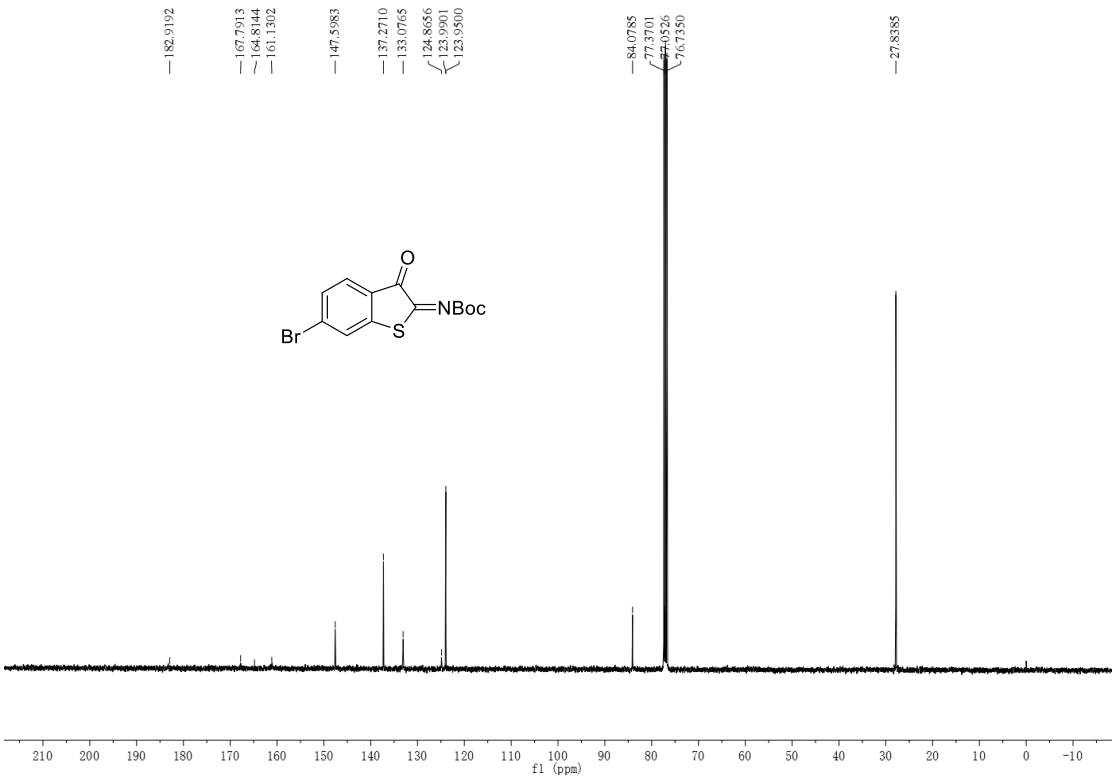
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1f



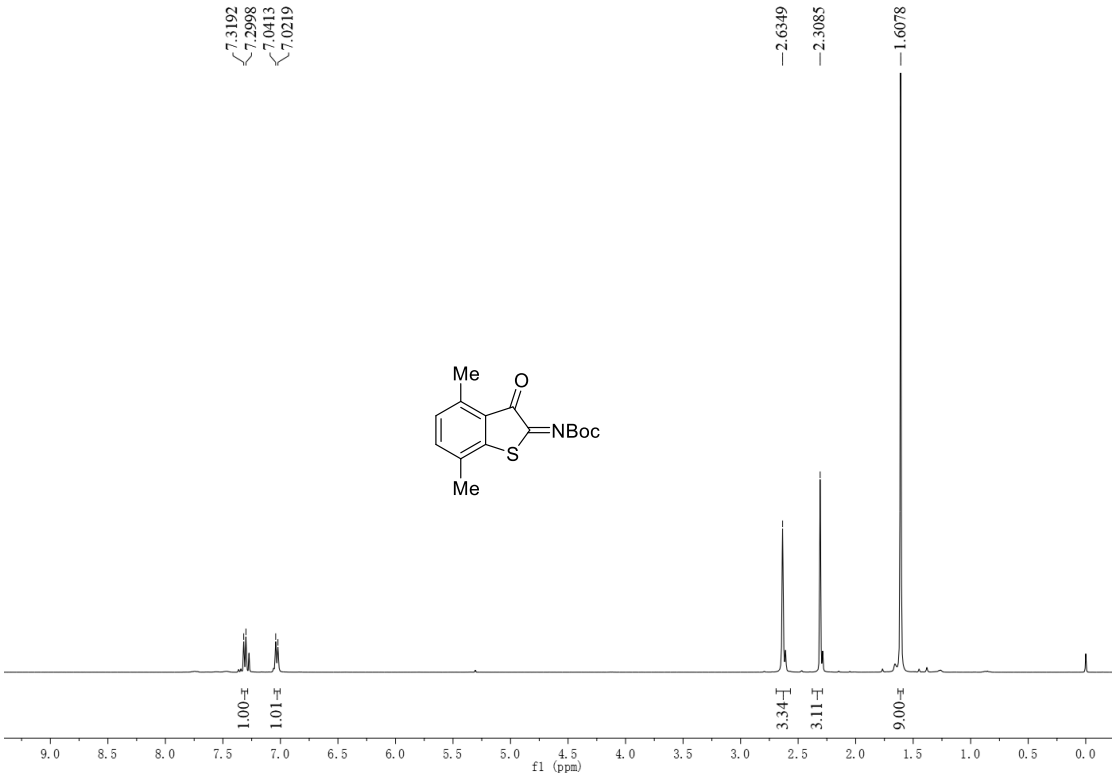


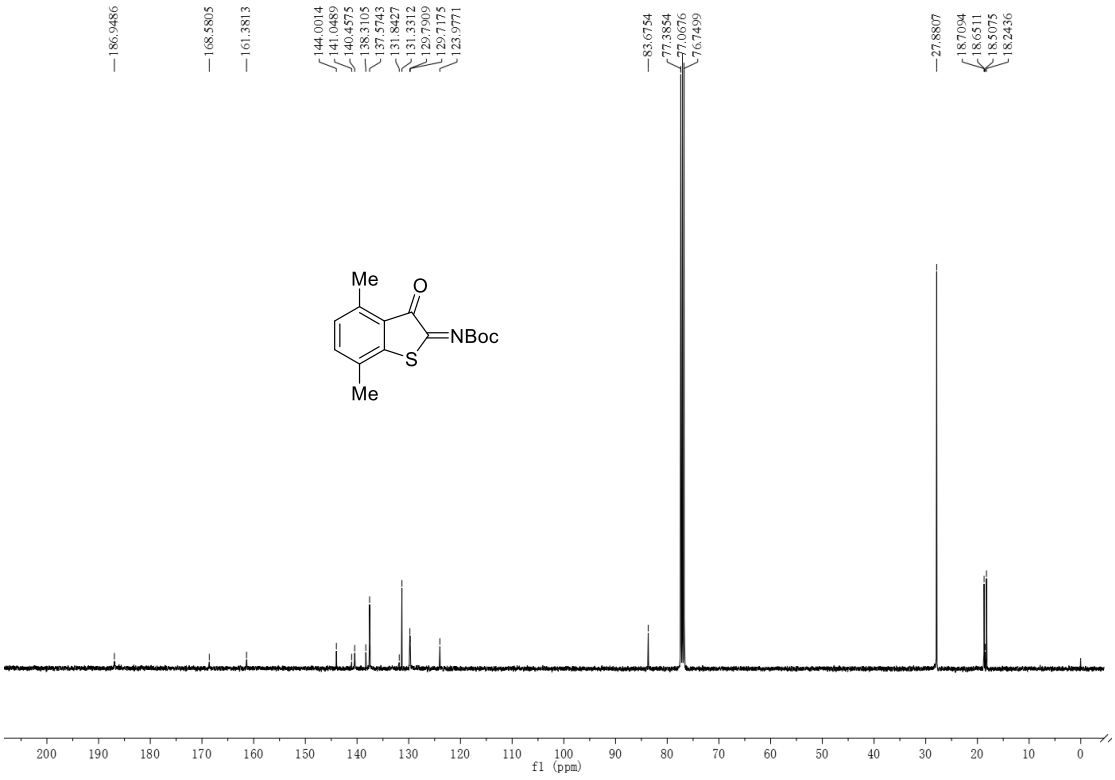
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1g



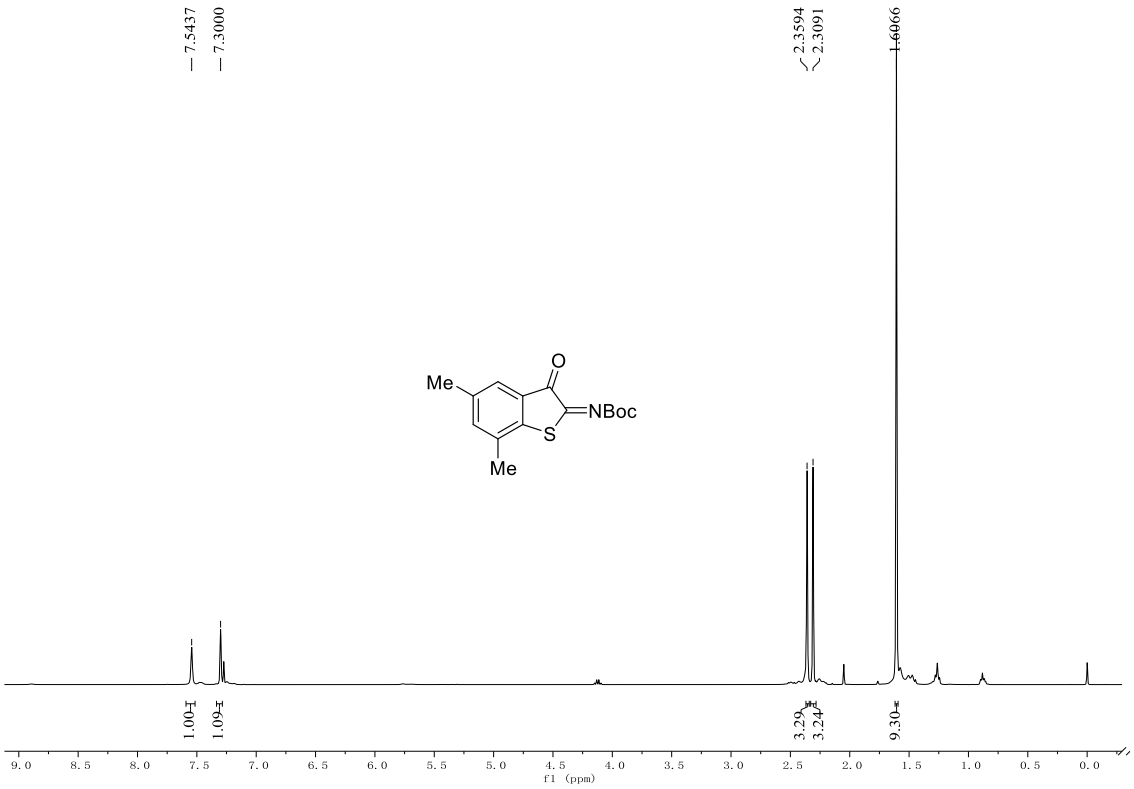


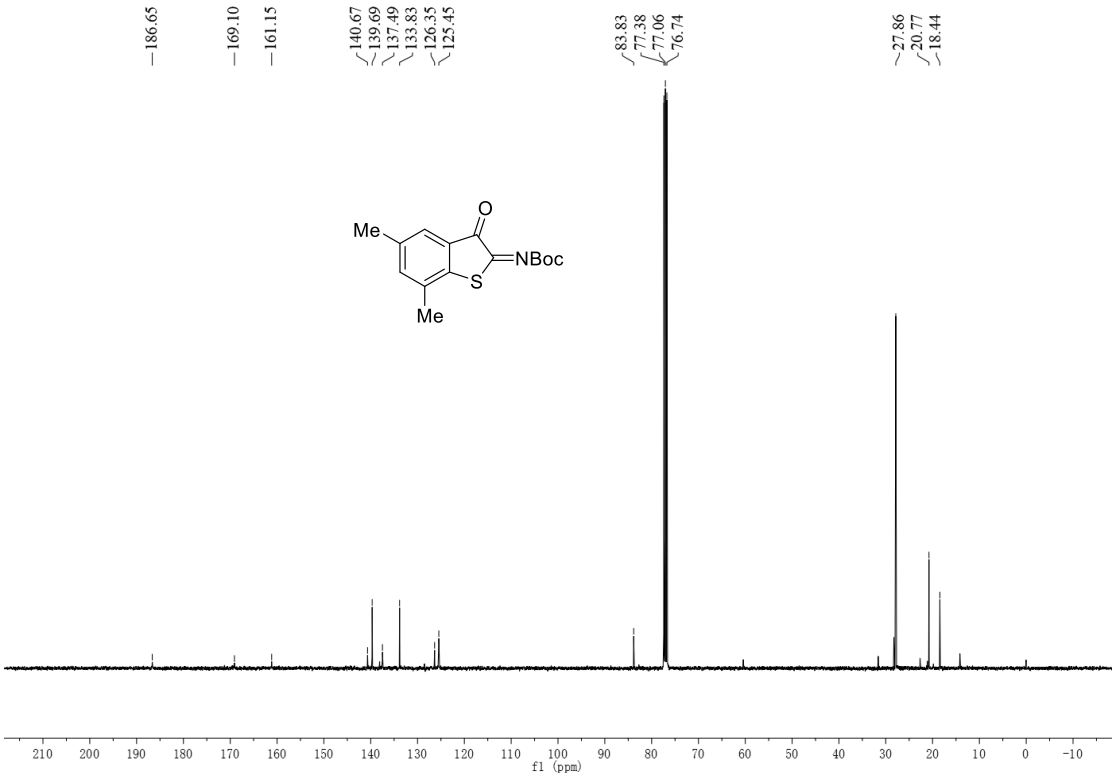
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1h



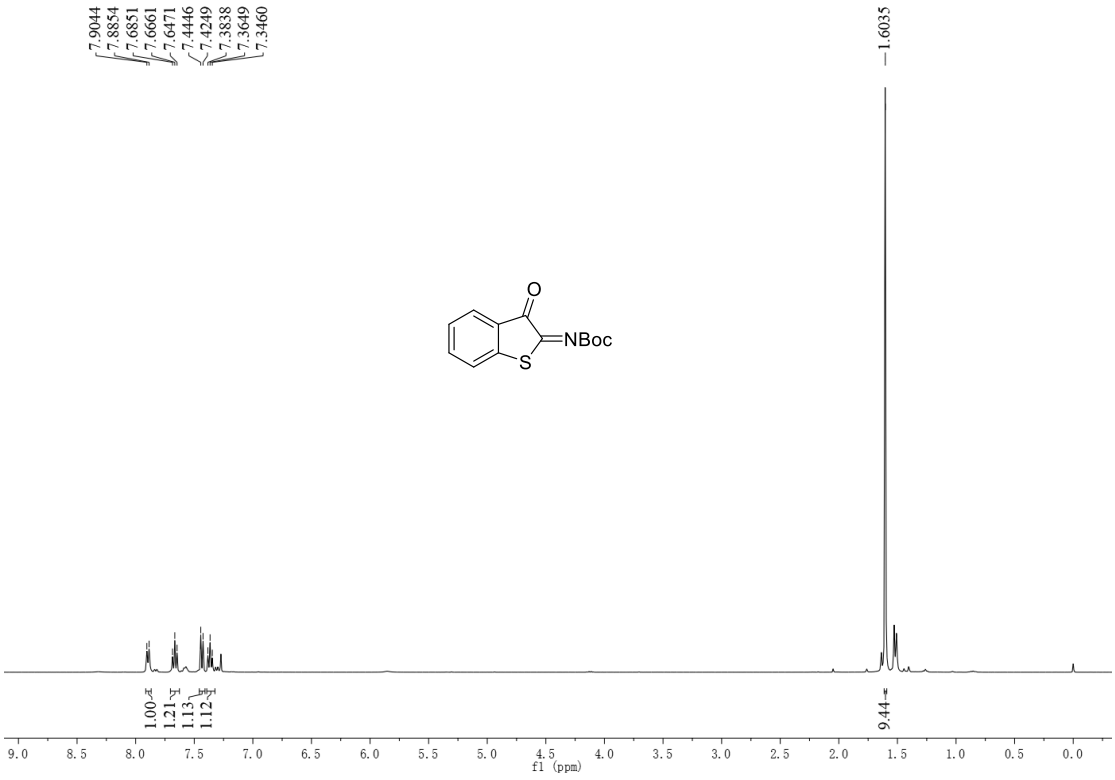


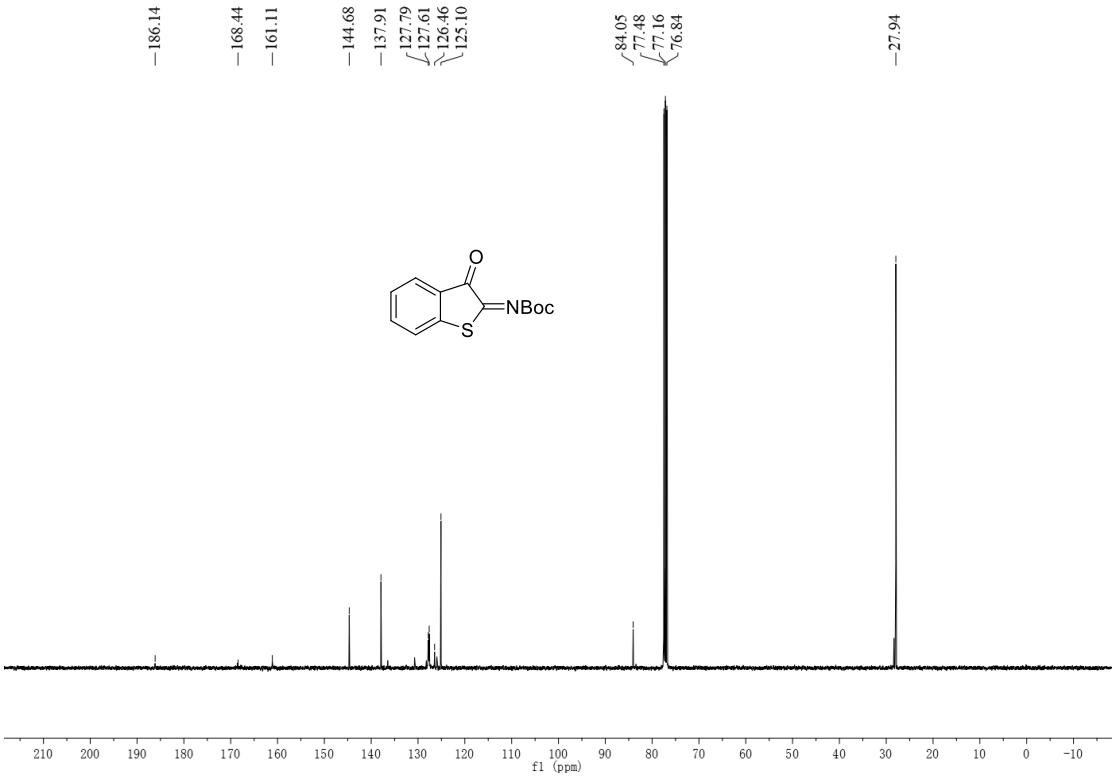
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1i



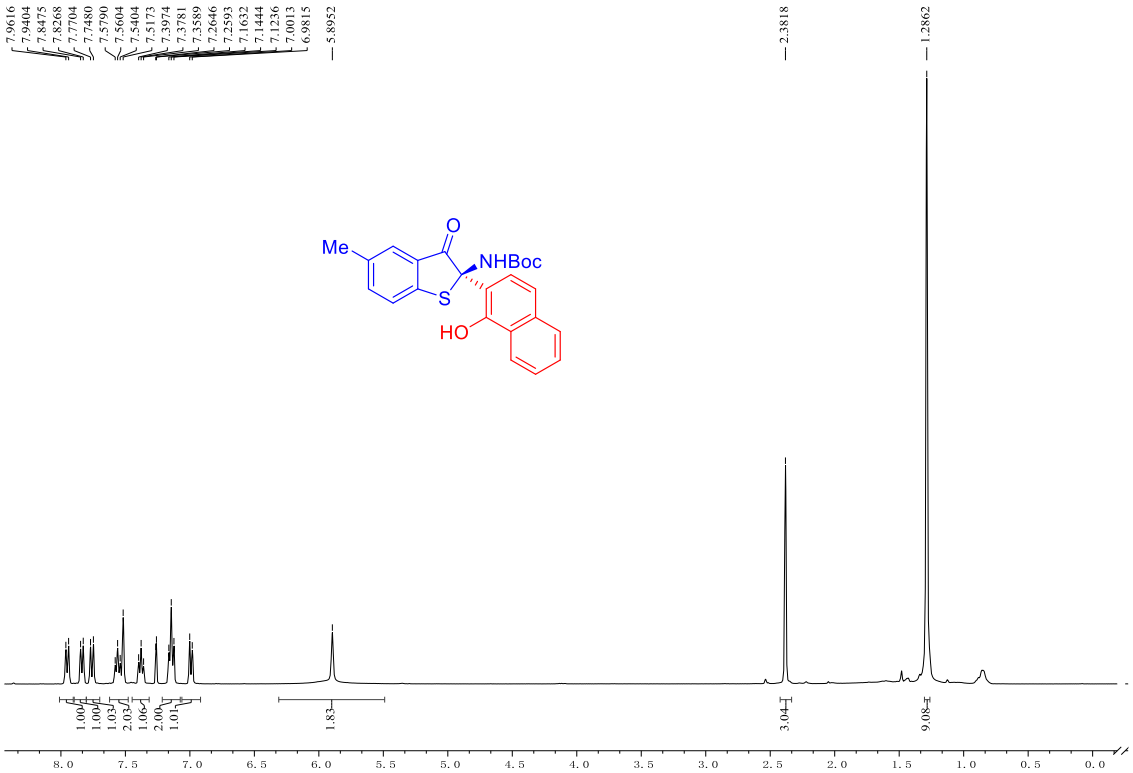


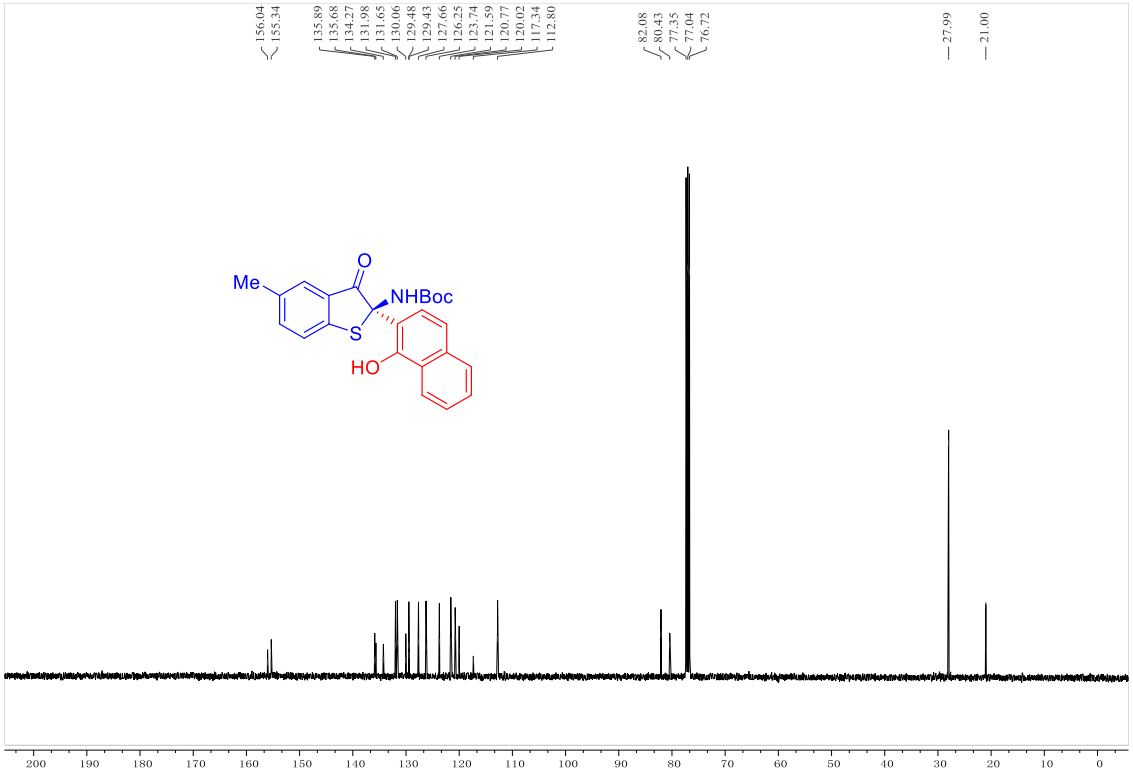
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 1j



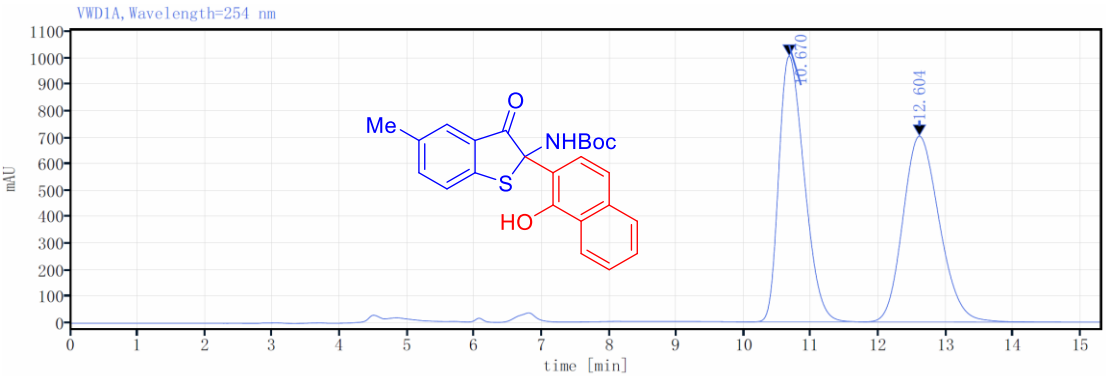


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3a



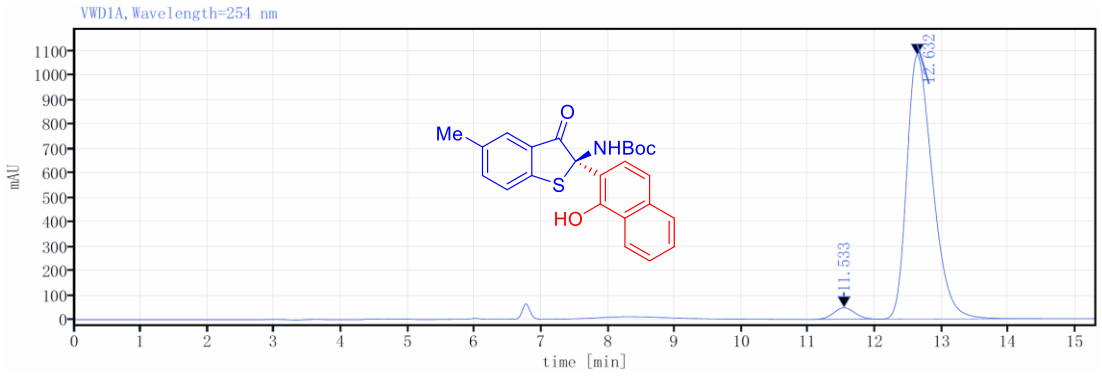


HPLC of 3a



Detector VWD1A, Wavelength=254 nm

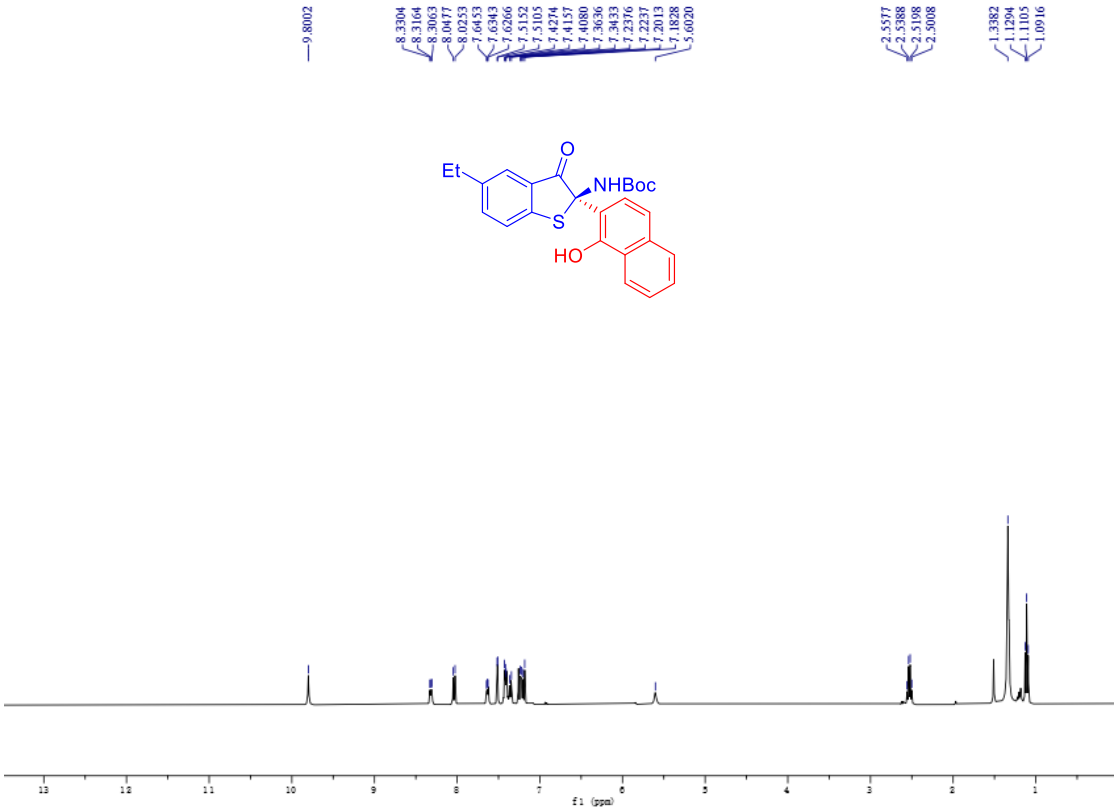
Peak	Ret.Time [min]	Area	Height	Area%
	10.670	26331.17	1004.37	50.03
	12.604	26300.75	701.90	49.97
		52631.92		100.00

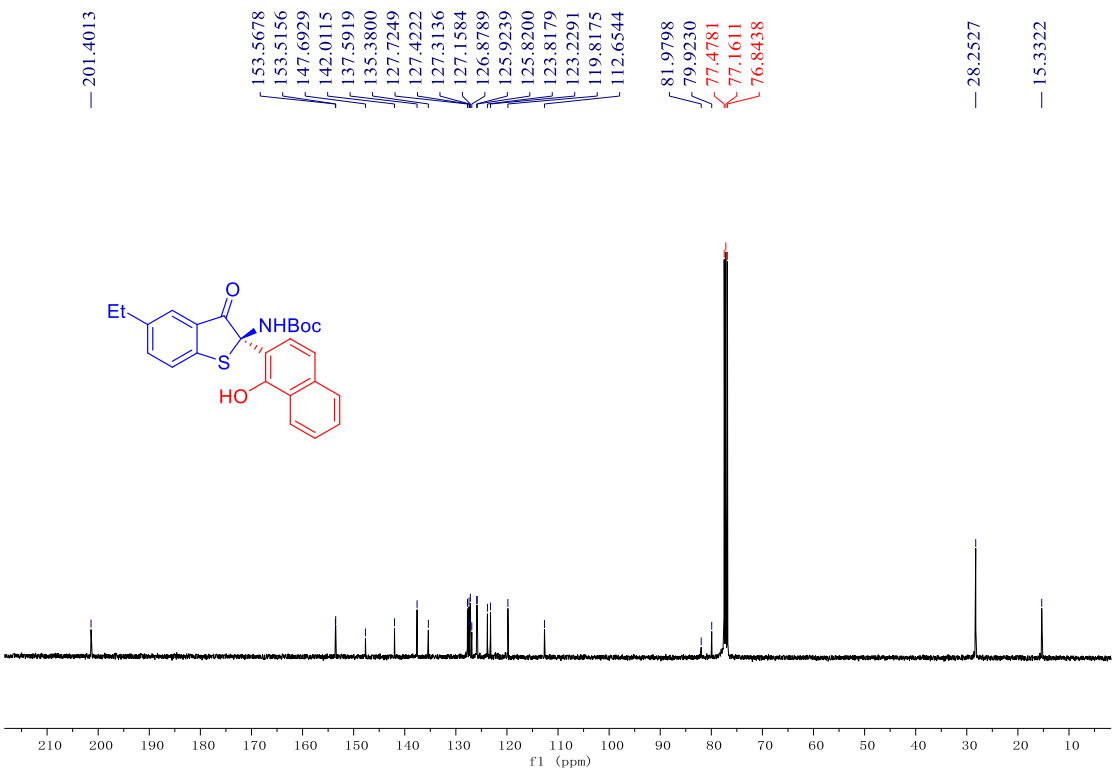


Detector VWD1A, Wavelength=254 nm

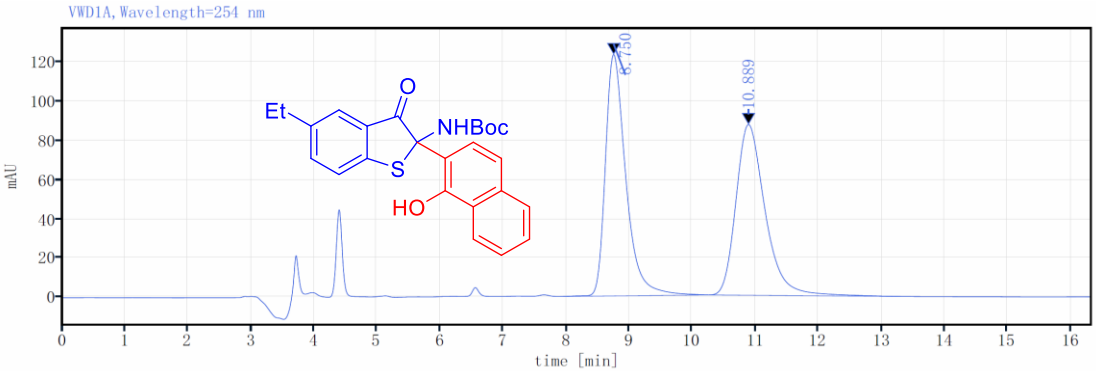
Peak	Ret.Time [min]	Area	Height	Area%
	11.533	1060.57	47.42	3.52
	12.632	29074.99	1082.63	96.48
		30135.56		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3b



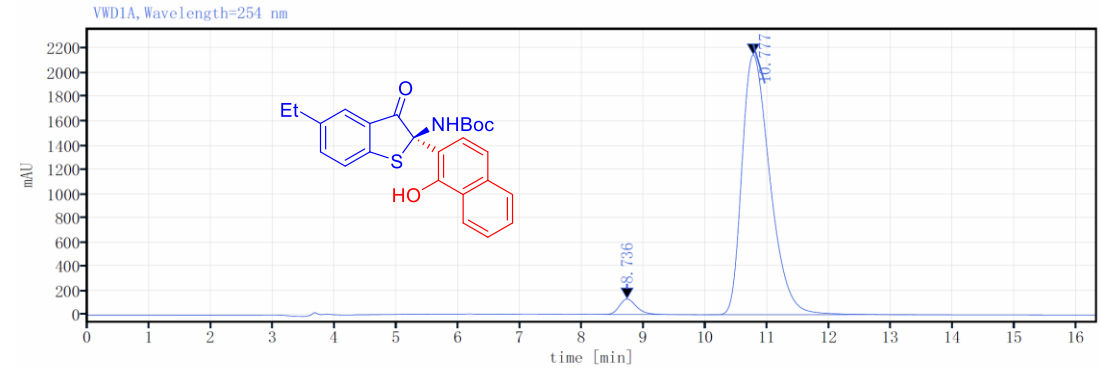


HPLC of 3b



Detector VWD1A, Wavelength=254 nm

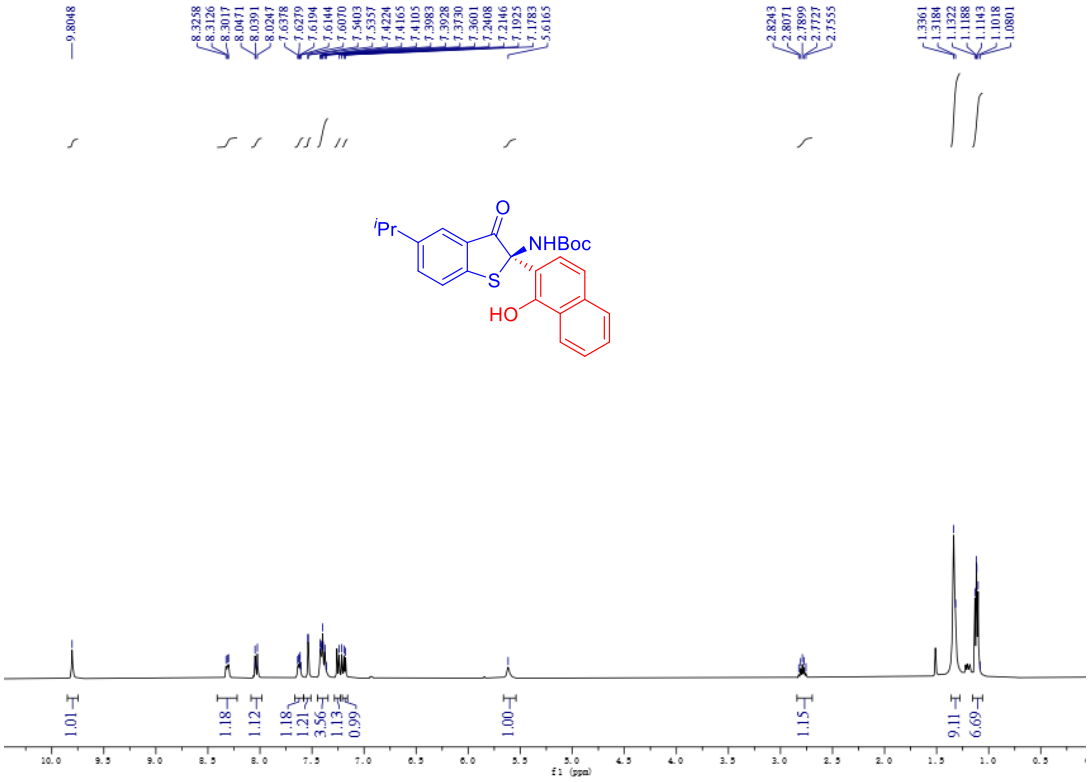
Peak	Ret.Time [min]	Area	Height	Area%
	8.750	2765.89	122.66	49.77
	10.889	2791.24	86.75	50.23
		5557.13		100.00

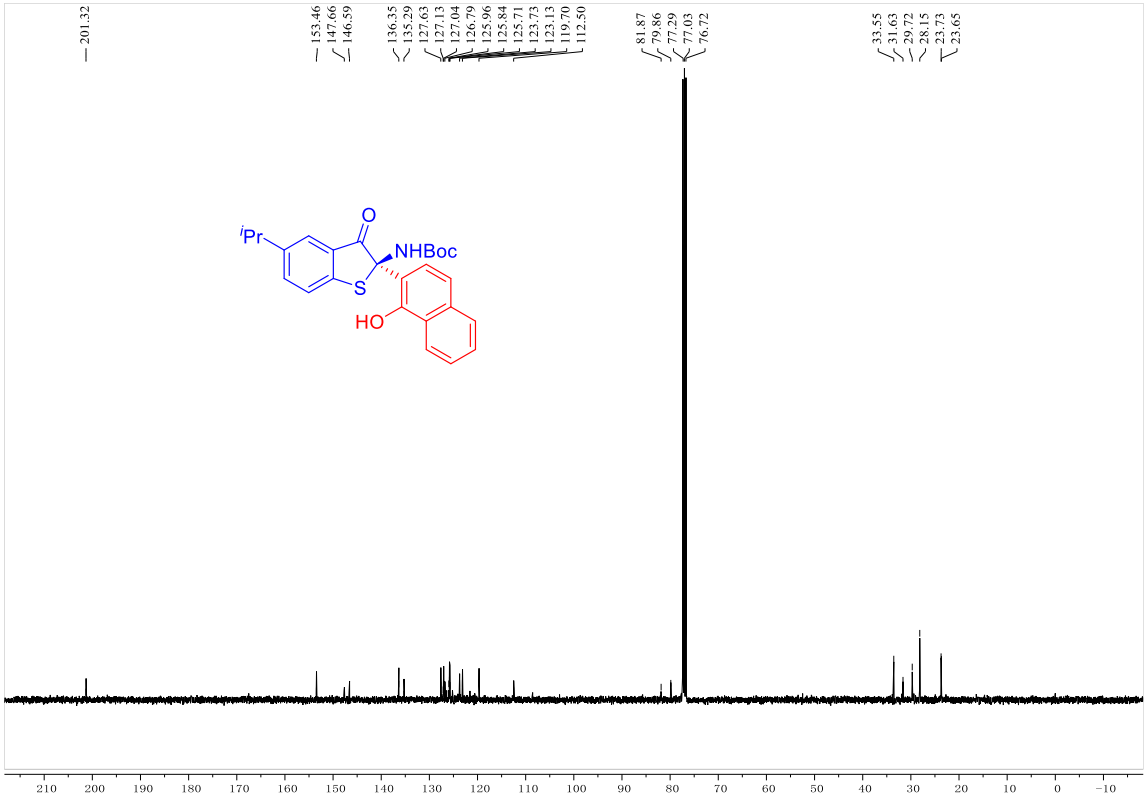


Detector VWD1A, Wavelength=254 nm

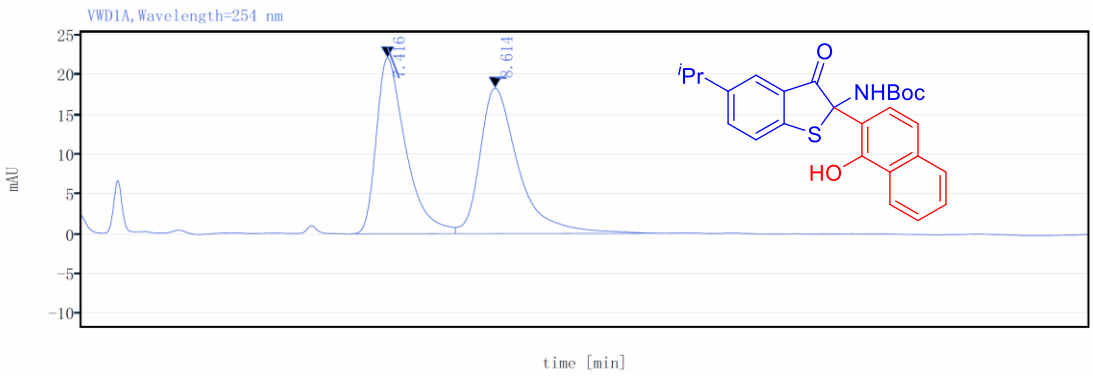
Peak	Ret.Time [min]	Area	Height	Area%
	8.736	2498.23	128.77	3.56
	10.777	67684.26	2147.34	96.44
		70182.49		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3c



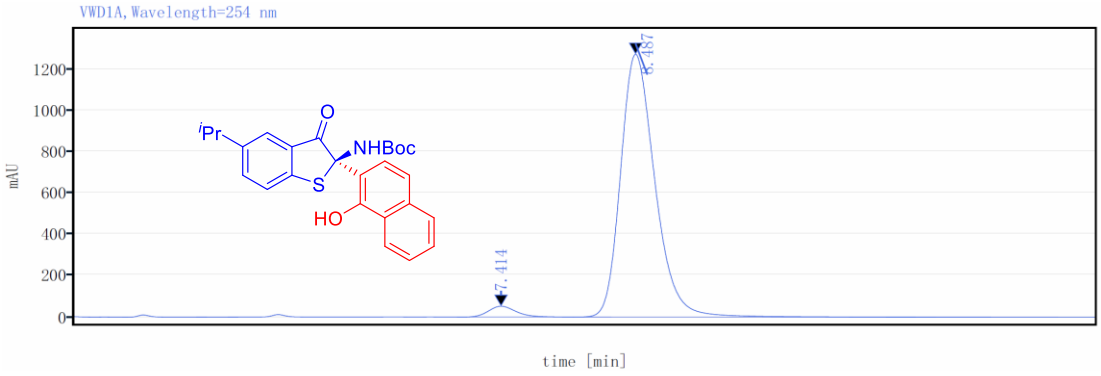


HPLC of 3c



Detector VWD1A, Wavelength=254 nm

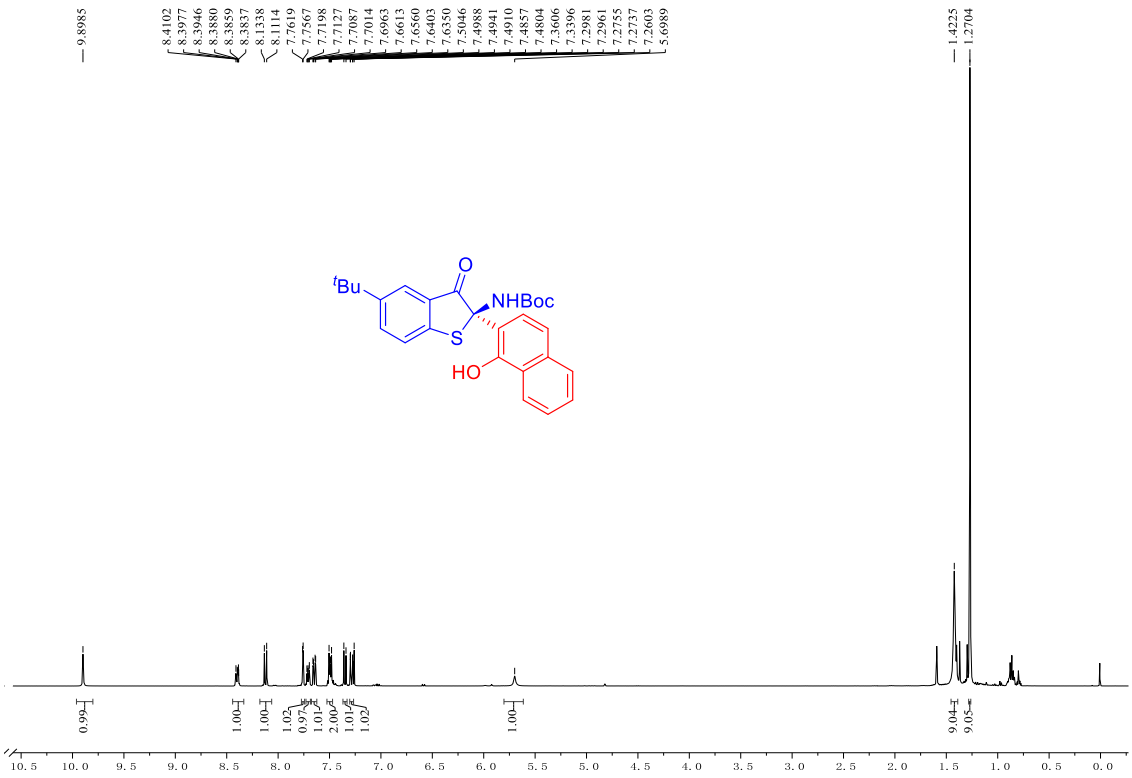
Peak	Ret.Time [min]	Area	Height	Area%
	7.416	503.06	22.10	48.08
	8.614	543.24	18.27	51.92
		1046.30		100.00

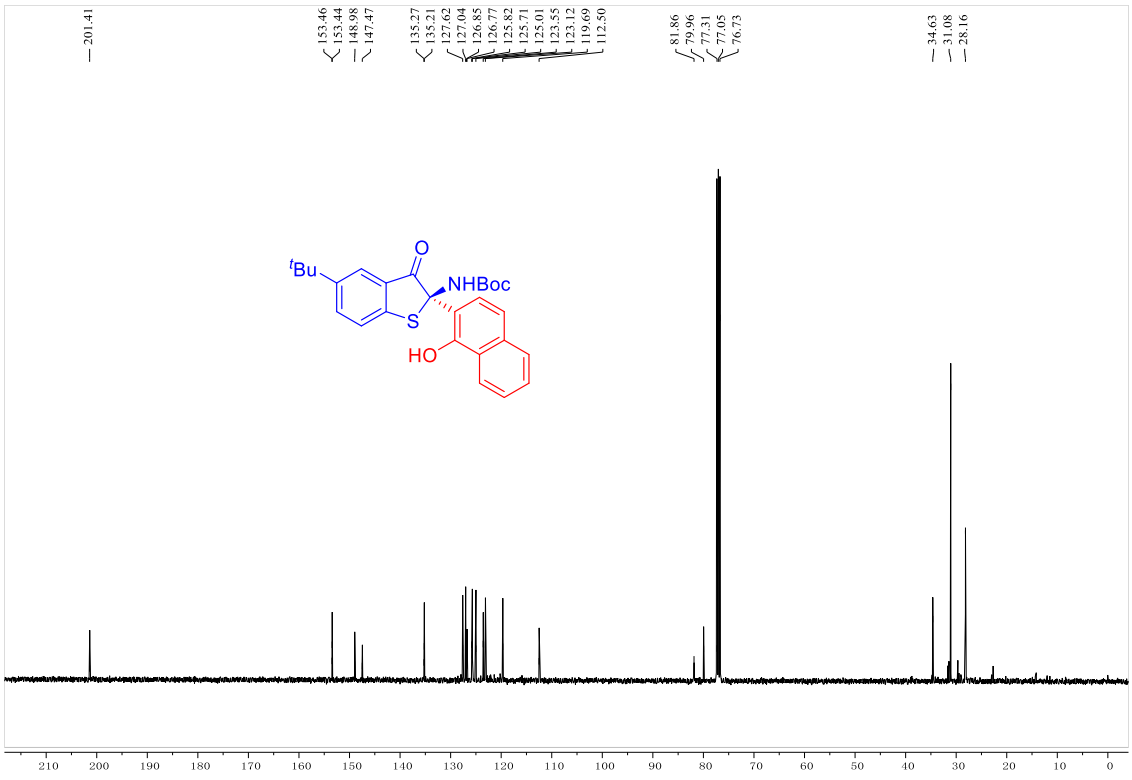


Detector VWD1A, Wavelength=254 nm

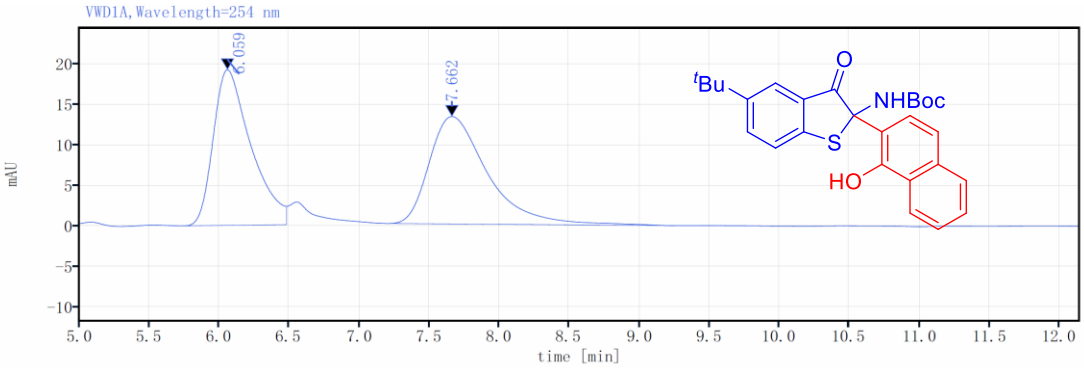
Peak	Ret.Time [min]	Area	Height	Area%
	7.414	810.52	52.34	3.23
	8.487	24318.60	1271.04	96.77
		25129.11		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3d



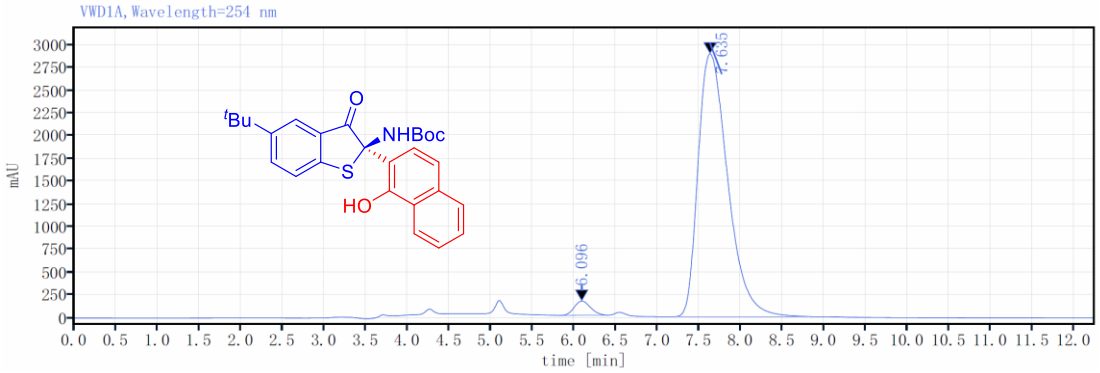


HPLC of 3d



Detector VWD1A, Wavelength=254 nm

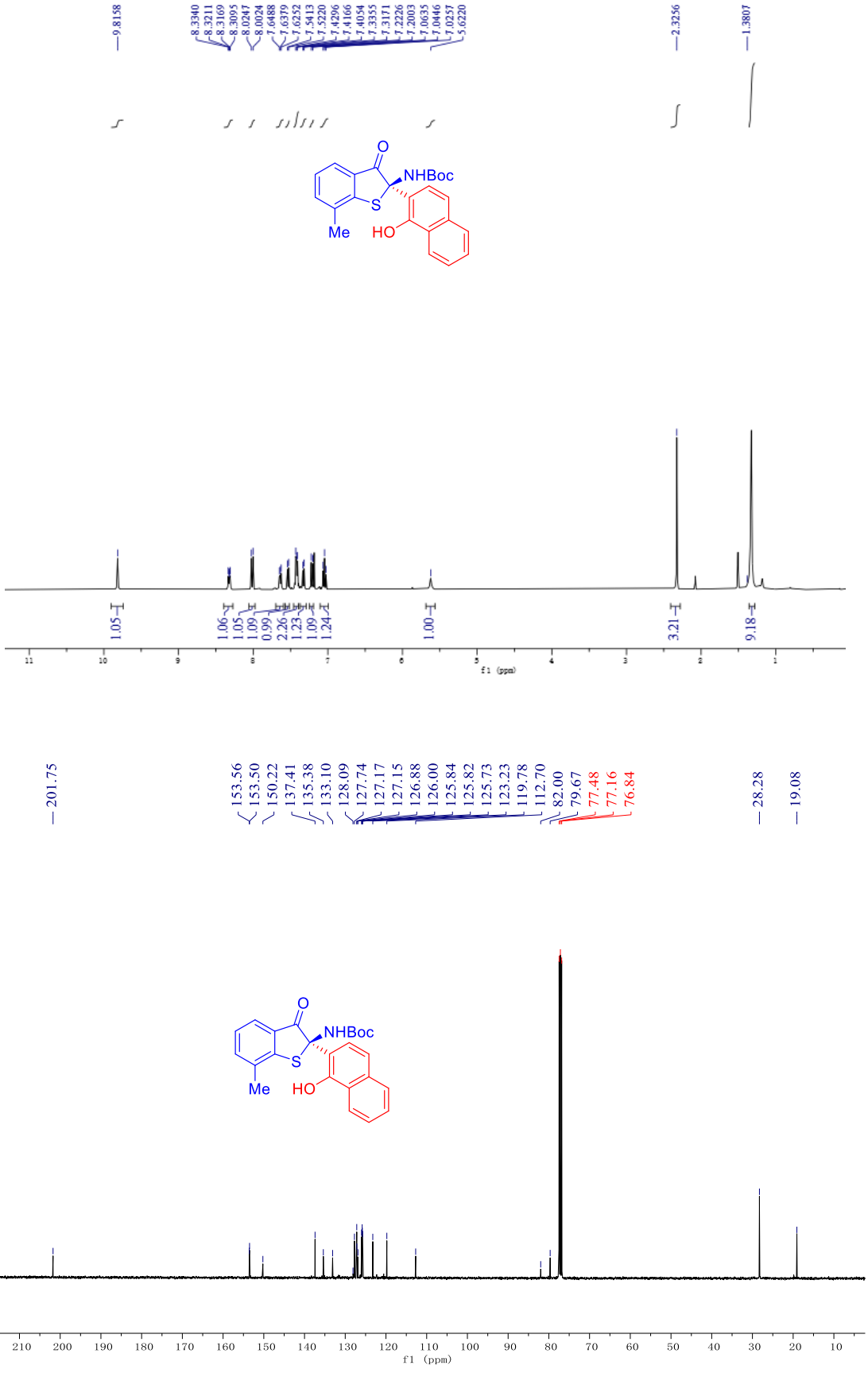
Peak	Ret.Time [min]	Area	Height	Area%
	6.059	359.86	19.21	48.39
	7.662	383.77	13.26	51.61
		743.63		100.00



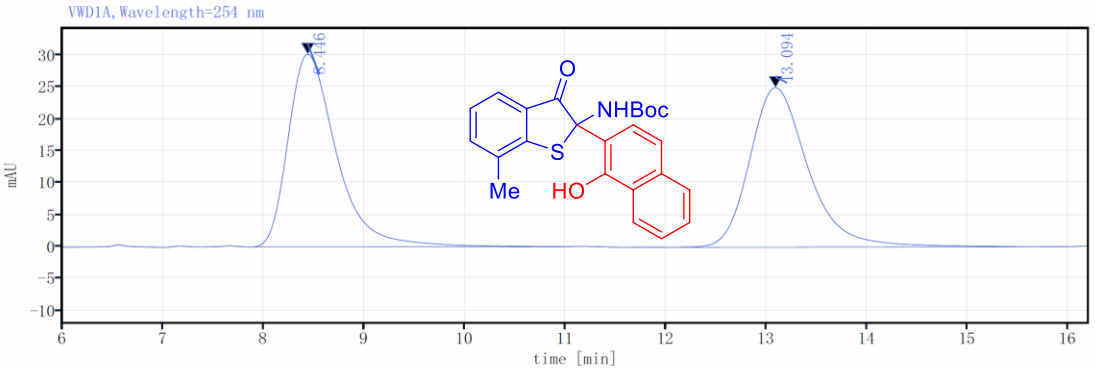
Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	6.096	2104.43	156.00	2.86
	7.635	71521.07	2888.73	97.14
		73625.50		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3e

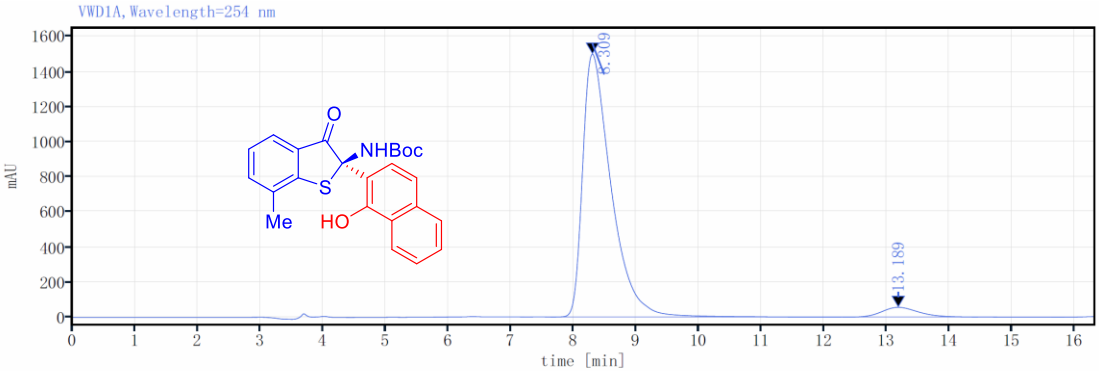


HPLC of 3e



Detector VWD1A, Wavelength=254 nm

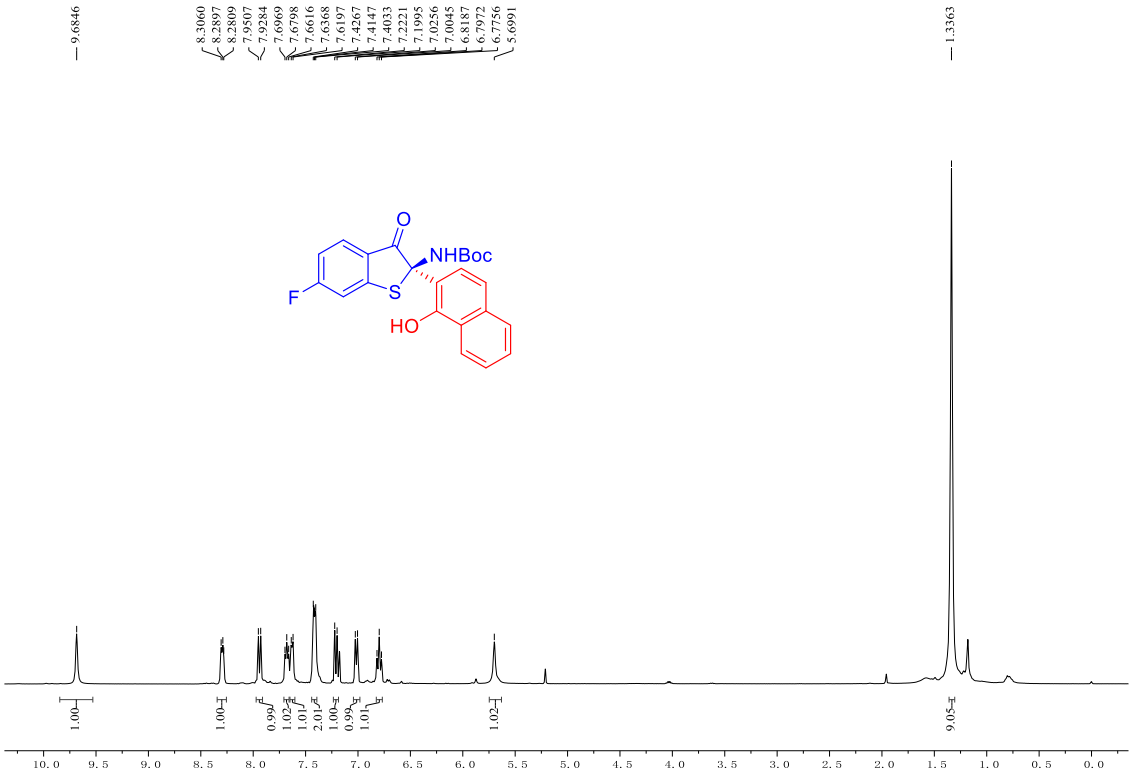
Peak	Ret.Time [min]	Area	Height	Area%
	8.446	1014.66	30.24	49.92
	13.094	1017.84	25.04	50.08
		2032.50		100.00

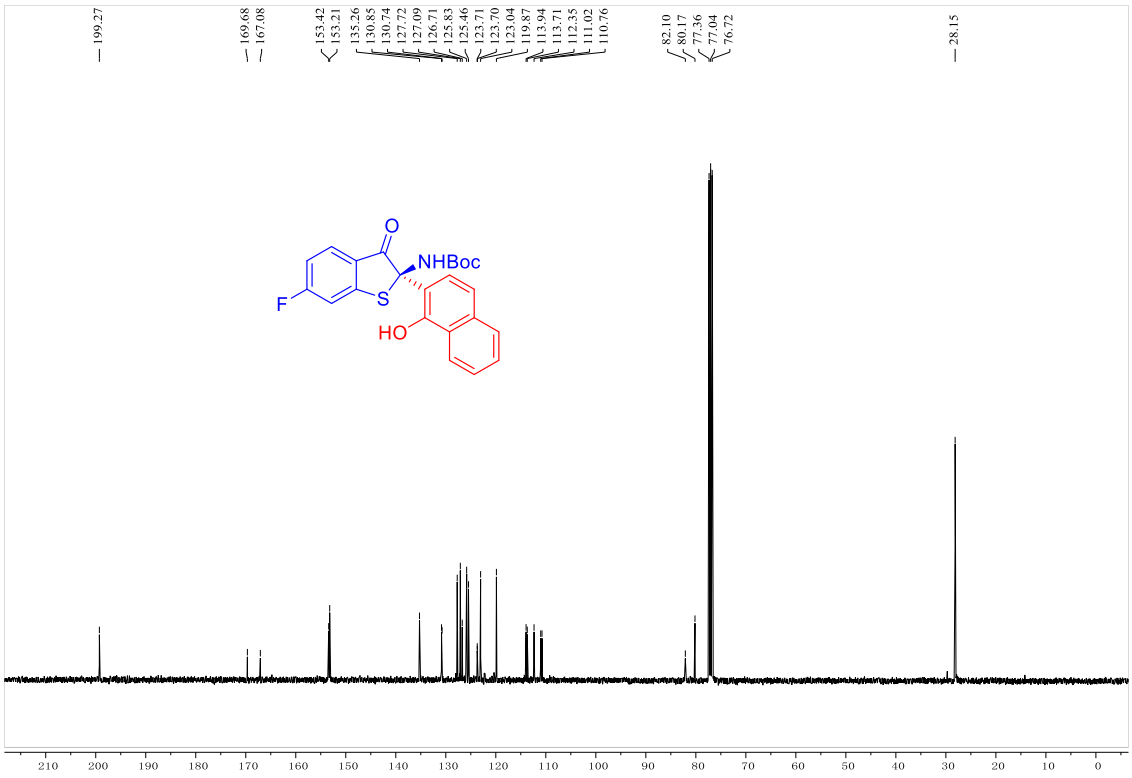


Detector VWD1A, Wavelength=254 nm

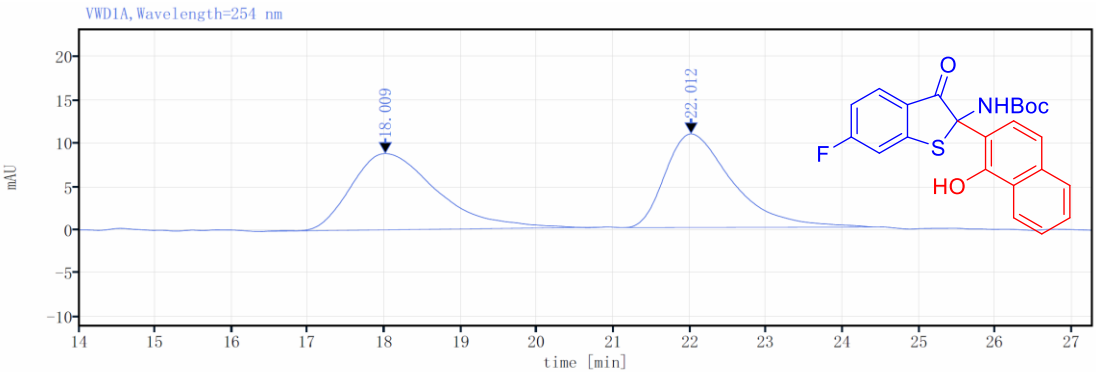
Peak	Ret.Time [min]	Area	Height	Area%
	8.309	47408.44	1499.34	95.52
	13.189	2223.95	55.09	4.48
		49632.39		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3f



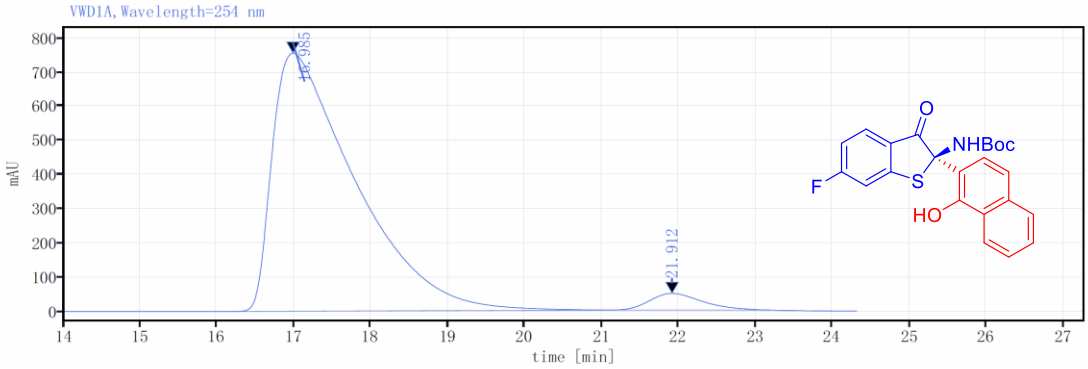


HPLC of **3f**



Detector VWD1A, Wavelength=254 nm

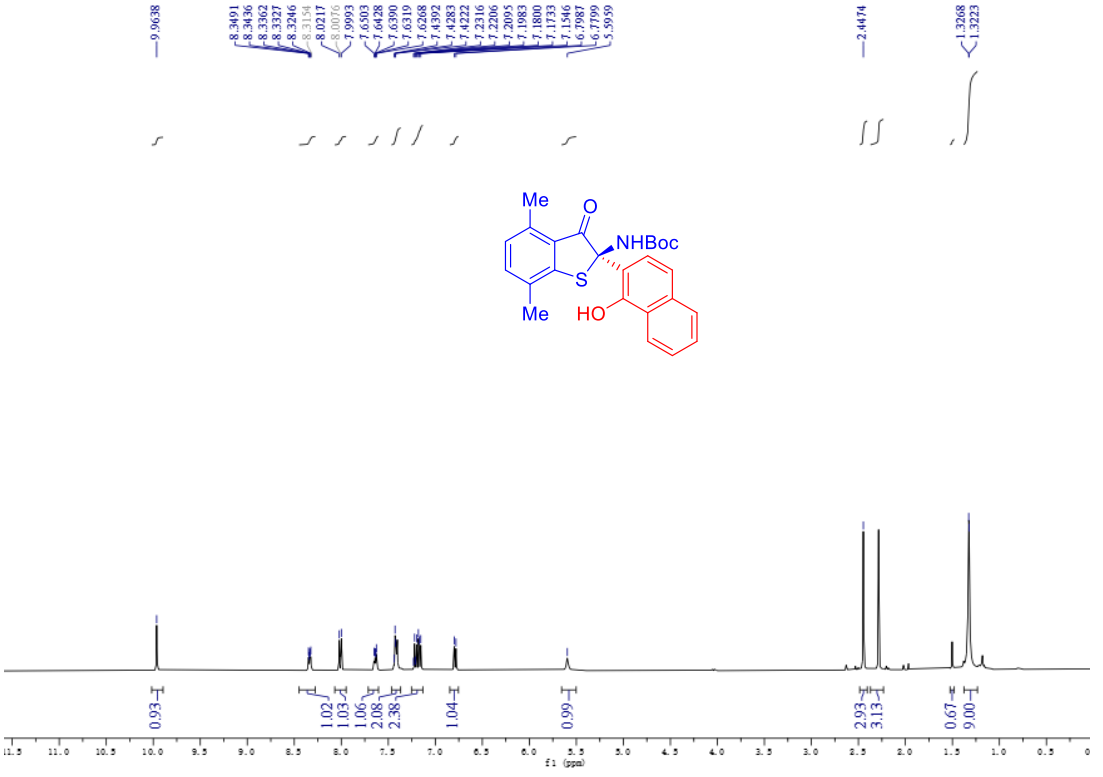
Peak	Ret.Time [min]	Area	Height	Area%
	18.009	688.79	8.82	50.97
	22.012	662.70	10.83	49.03
		1351.49		100.00

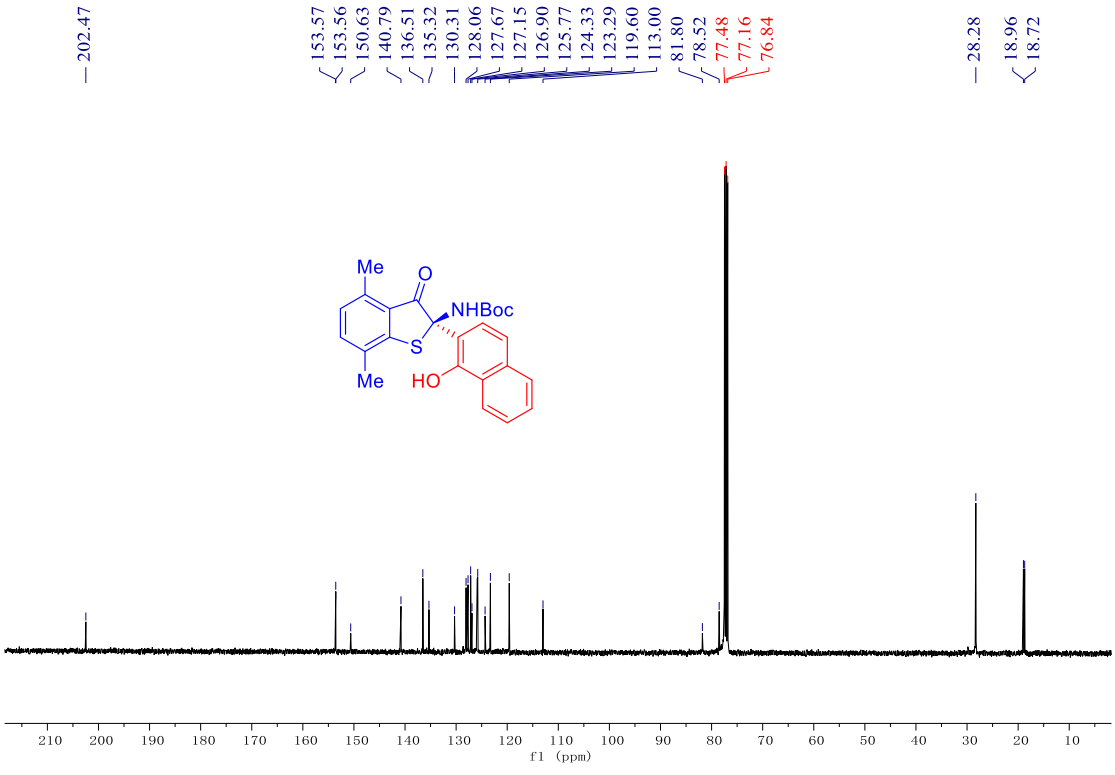


Detector VWD1A, Wavelength=254 nm

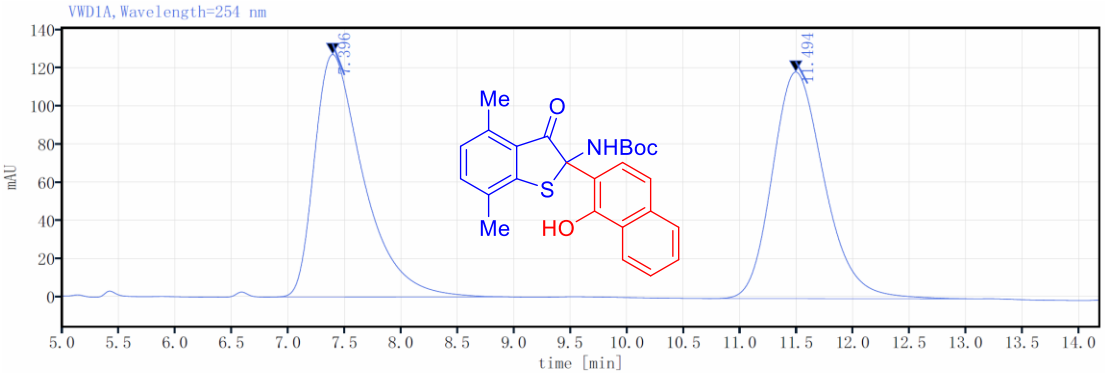
Peak	Ret.Time [min]	Area	Height	Area%
	16.985	56443.87	754.33	96.06
	21.912	2315.96	48.77	3.94
		58759.83		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3g



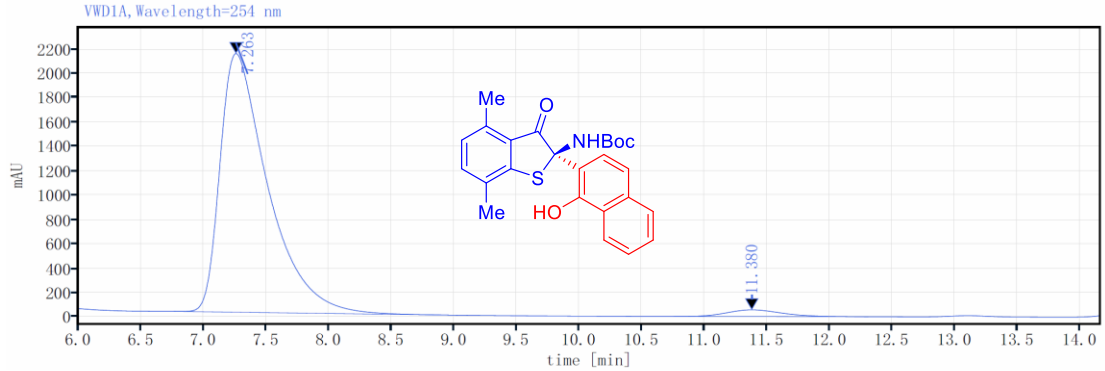


HPLC of 3g



Detector VWD1A, Wavelength=254 nm

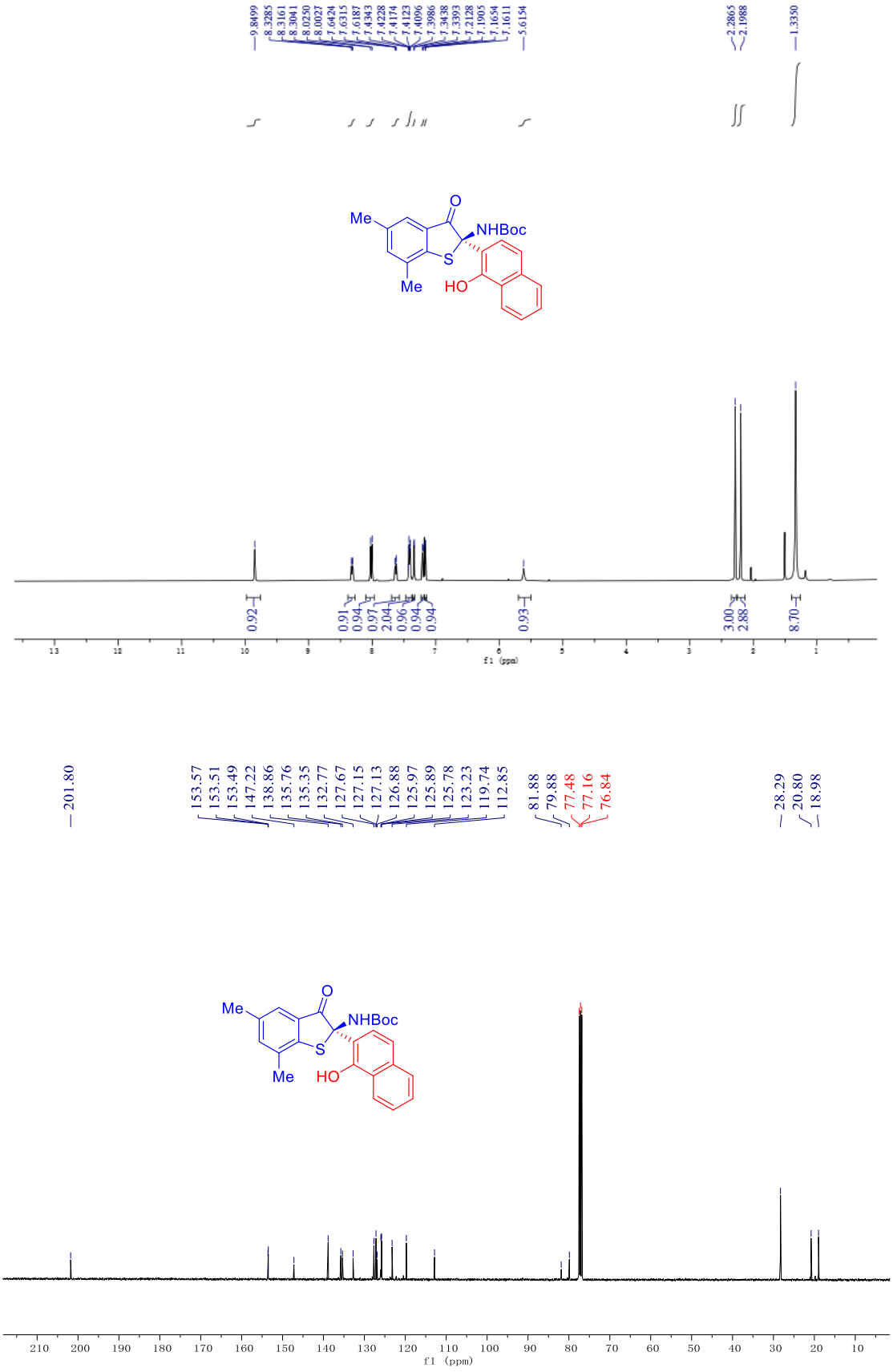
Peak	Ret.Time [min]	Area	Height	Area%
	7.396	3818.90	126.66	50.19
	11.494	3790.63	118.35	49.81
		7609.53		100.00



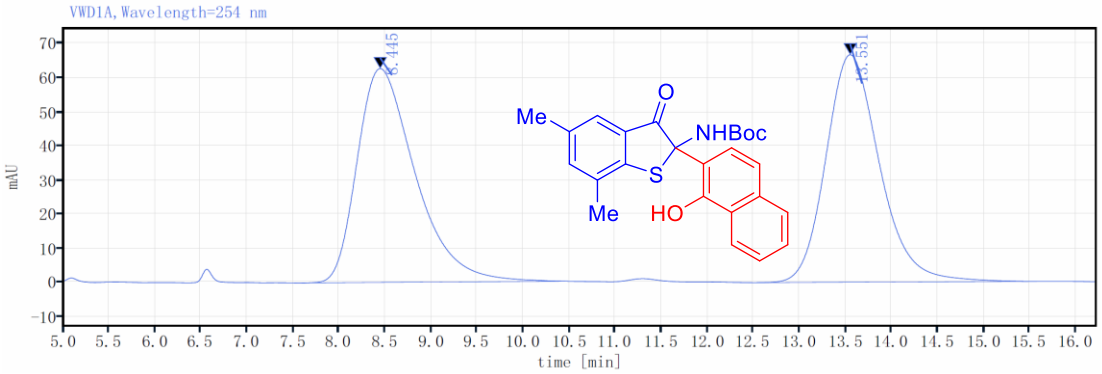
Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	7.263	56353.65	2121.61	97.14
	11.380	1660.93	54.49	2.86
		58014.58		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3h

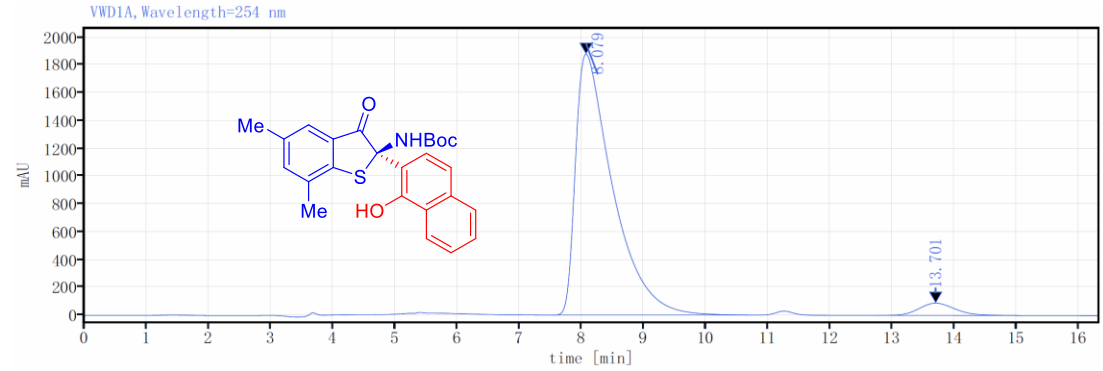


HPLC of 3h



Detector VWD1A, Wavelength=254 nm

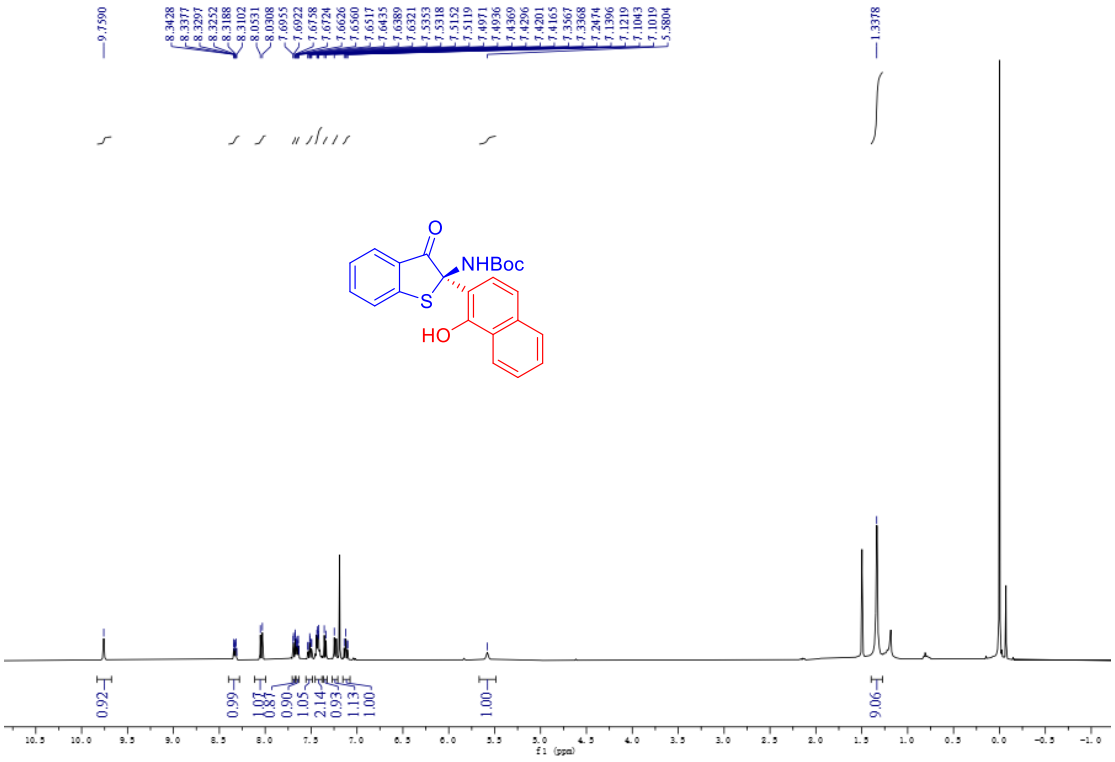
Peak	Ret.Time [min]	Area	Height	Area%
	8.445	2751.27	62.70	50.41
	13.551	2706.59	66.71	49.59
		5457.86		100.00

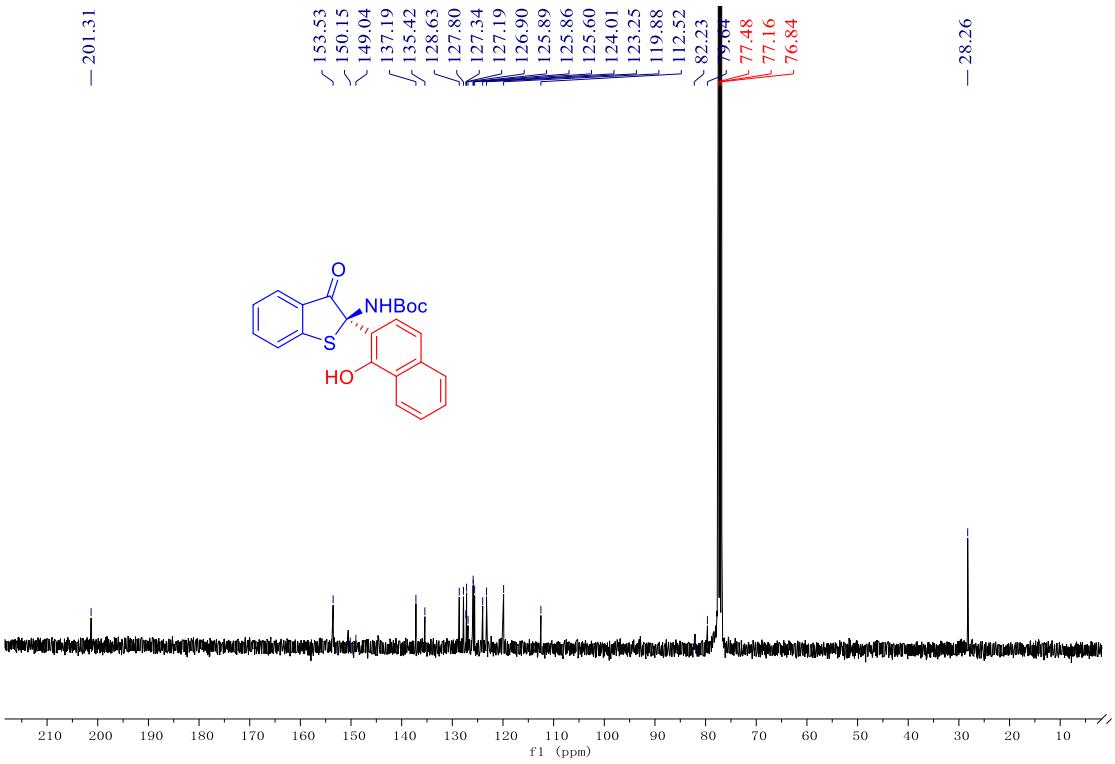


Detector VWD1A, Wavelength=254 nm

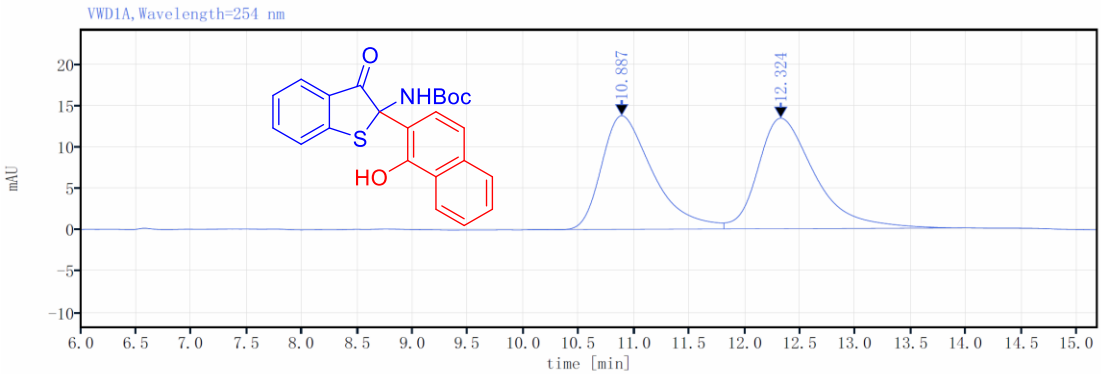
Peak	Ret.Time [min]	Area	Height	Area%
	8.079	78091.95	1876.52	95.59
	13.701	3603.09	88.95	4.41
		81695.04		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3i



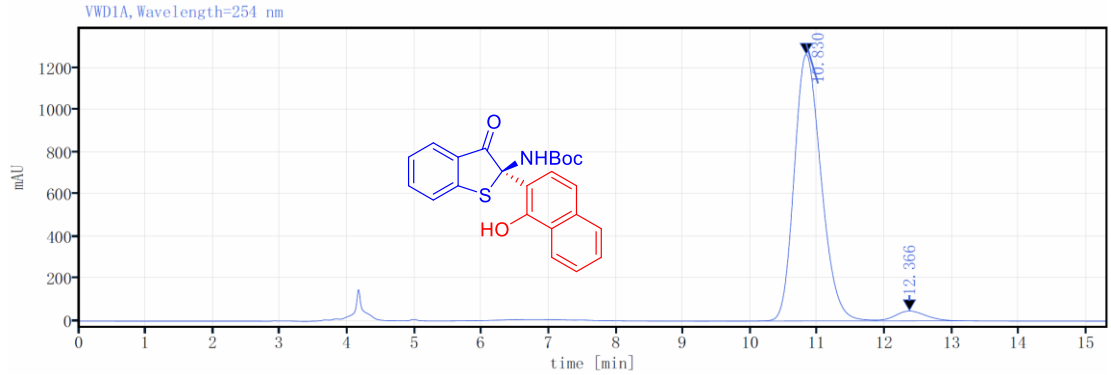


HPLC of 3i



Detector VWD1A, Wavelength=254 nm

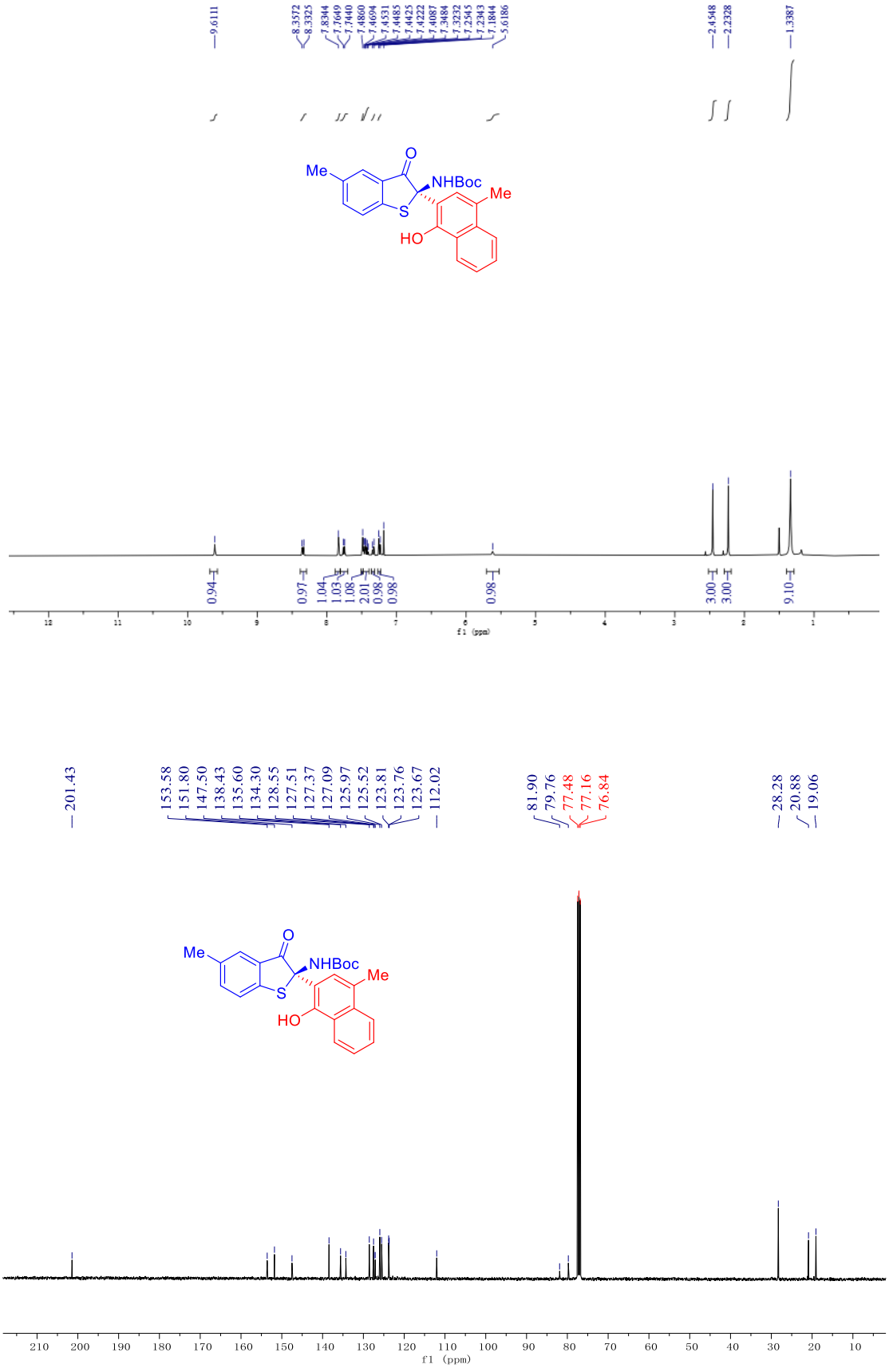
Peak	Ret.Time [min]	Area	Height	Area%
	10.887	444.35	13.74	48.21
	12.324	477.41	13.36	51.79
		921.76		100.00



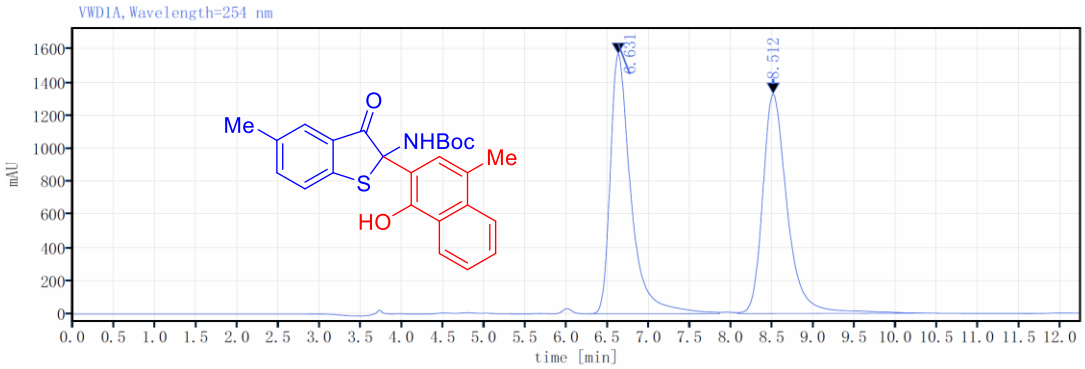
Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	10.830	35213.00	1264.67	95.90
	12.366	1506.02	46.97	4.10
		36719.02		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3j

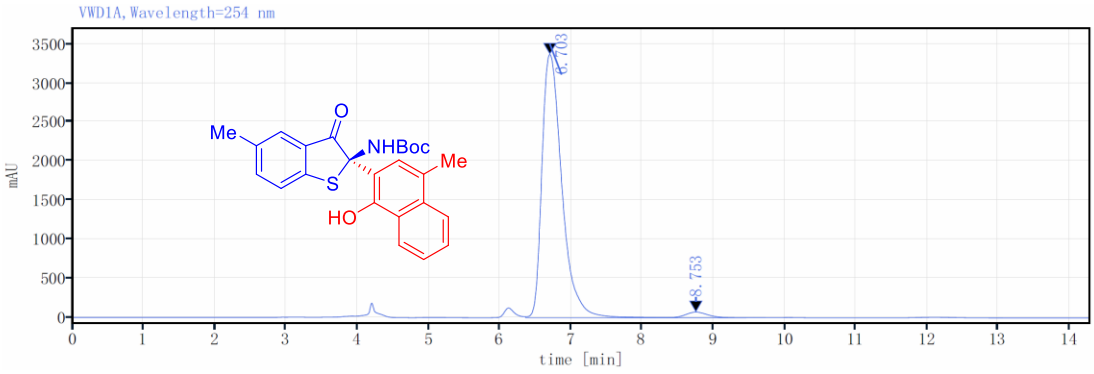


HPLC of 3j



Detector VWD1A, Wavelength=254 nm

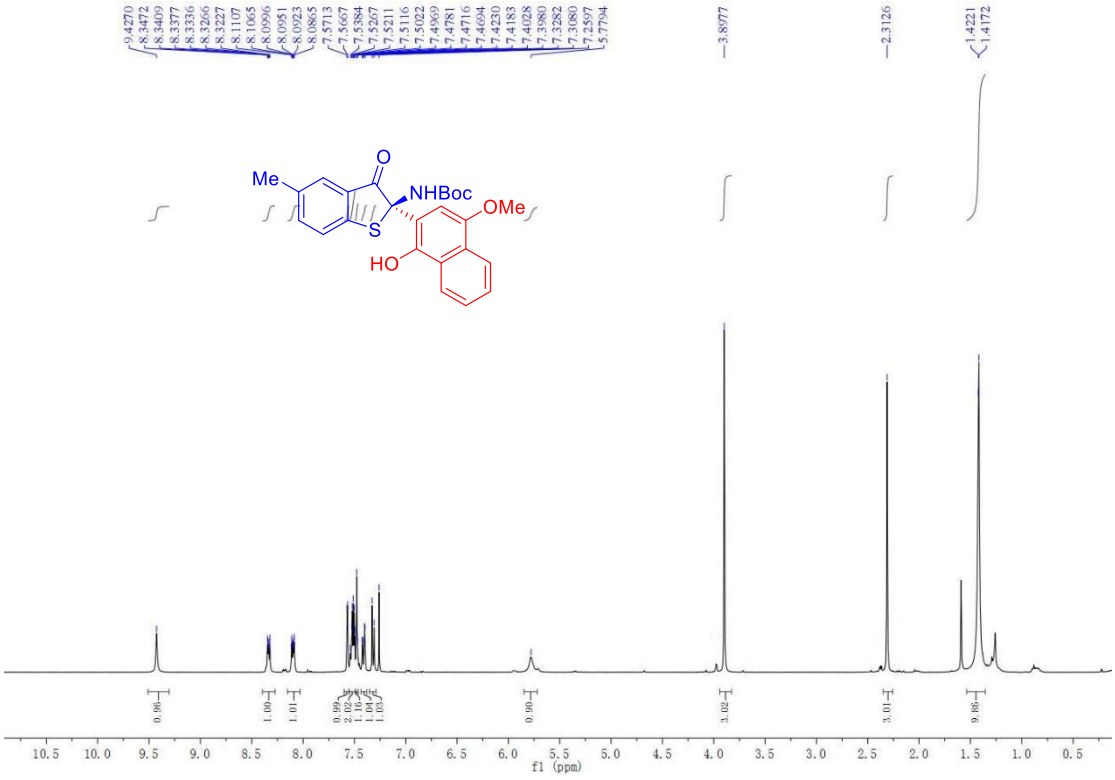
Peak	Ret.Time [min]	Area	Height	Area%
	6.631	27515.71	1570.32	49.91
	8.512	27618.73	1327.52	50.09
		55134.44		100.00

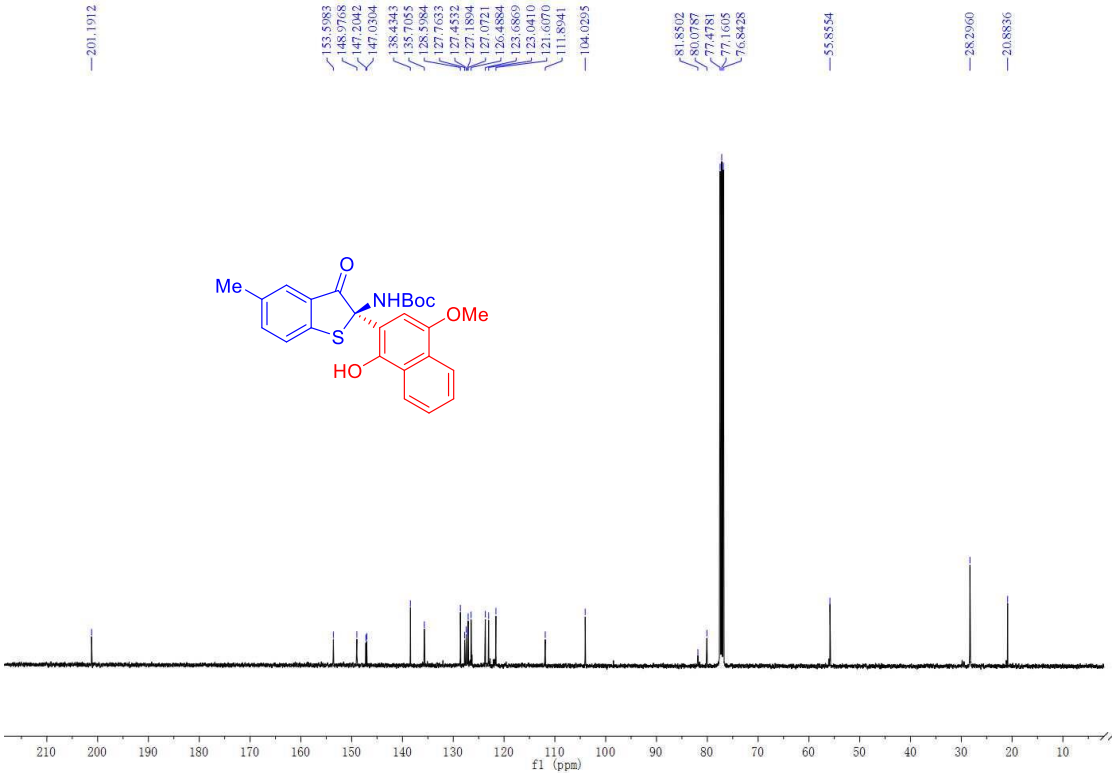


Detector VWD1A, Wavelength=254 nm

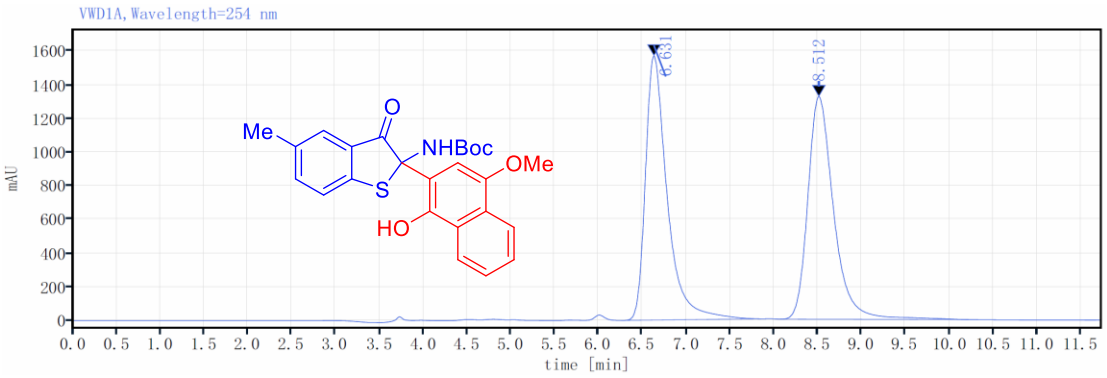
Peak	Ret.Time [min]	Area	Height	Area%
	6.703	65683.96	3372.06	97.61
	8.753	1610.68	72.72	2.39
		67294.63		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3k



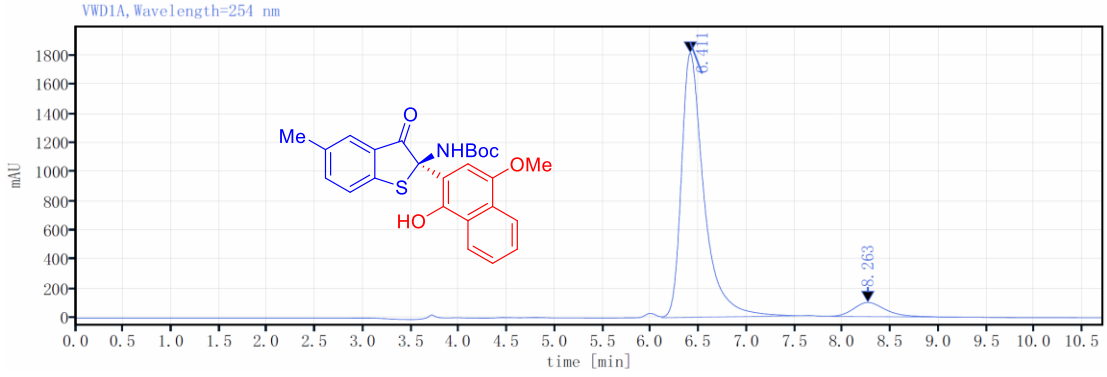


HPLC of 3k



Detector VWD1A, Wavelength=254 nm

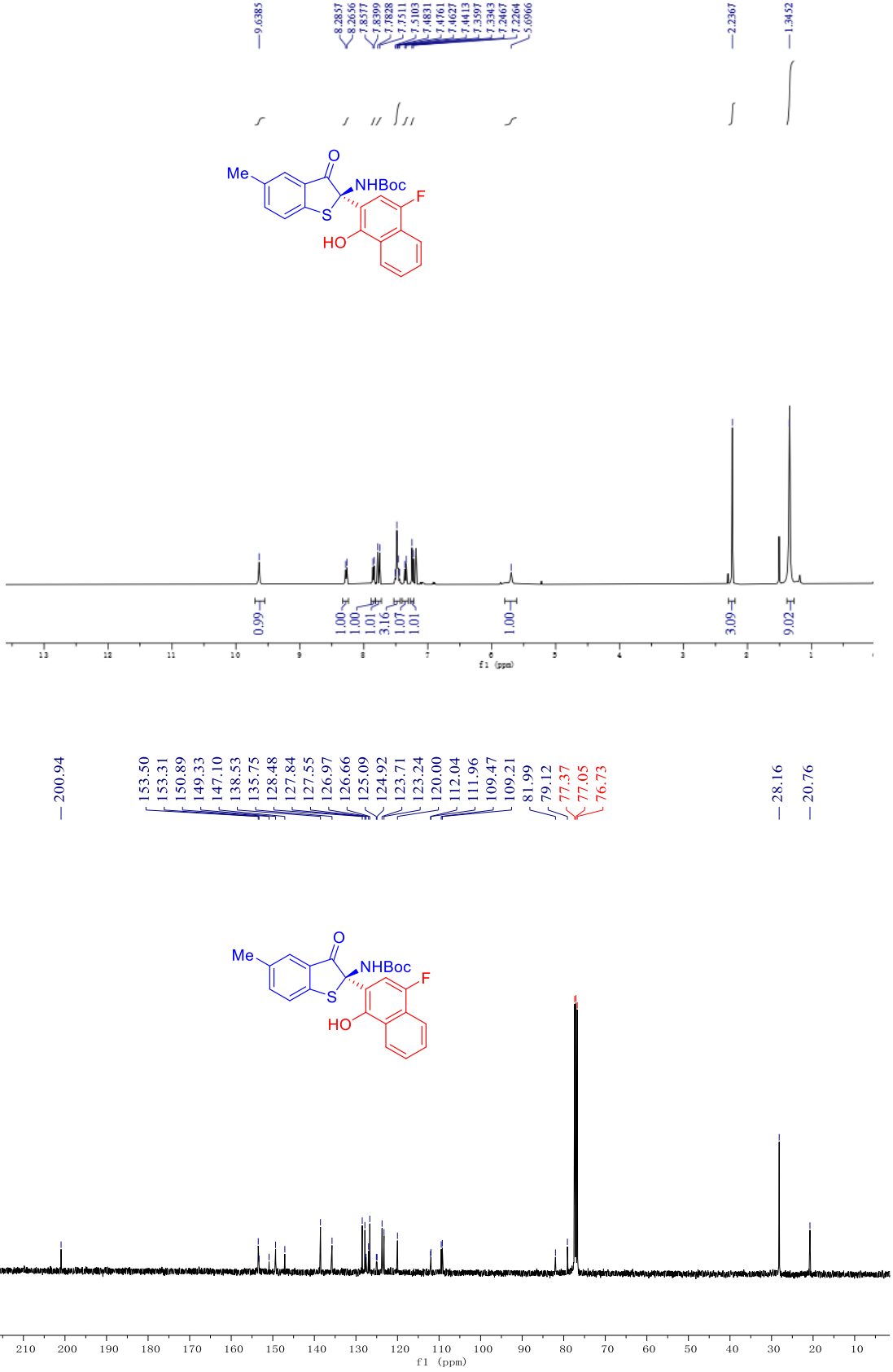
Peak	Ret.Time [min]	Area	Height	Area%
	6.631	27090.97	1568.27	50.01
	8.512	27076.82	1321.74	49.99
		54167.79		100.00



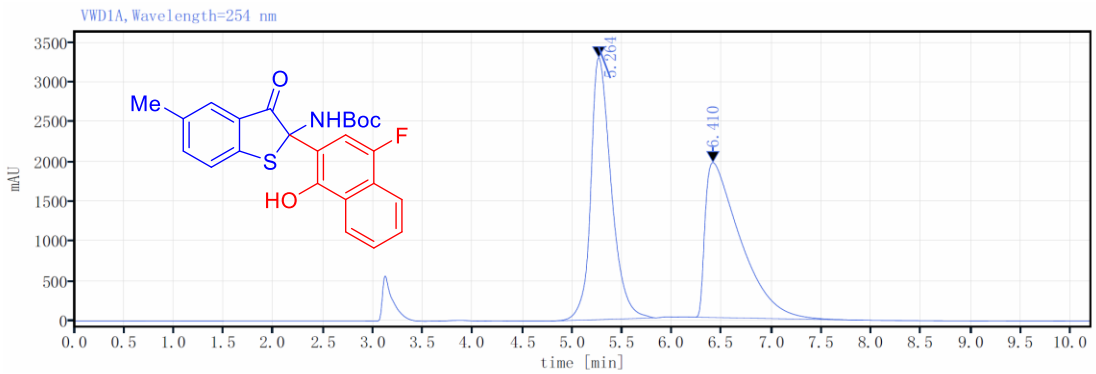
Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	6.411	29634.35	1809.84	92.97
	8.263	2241.92	96.51	7.03
		31876.26		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3l

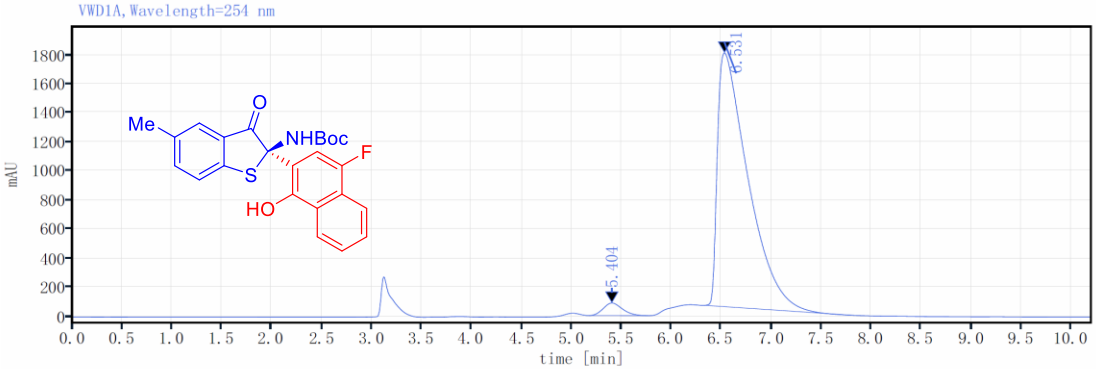


HPLC of 3l



Detector VWD1A, Wavelength=254 nm

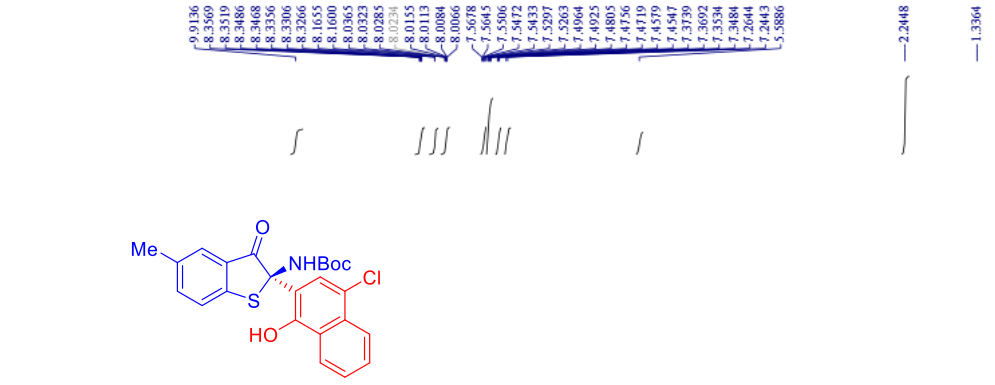
Peak	Ret.Time [min]	Area	Height	Area%
	5.264	47014.04	3291.04	49.53
	6.410	47901.35	1947.00	50.47
		94915.39		100.00

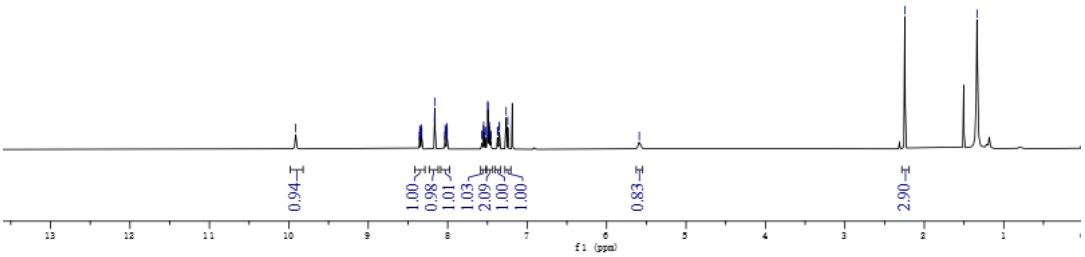


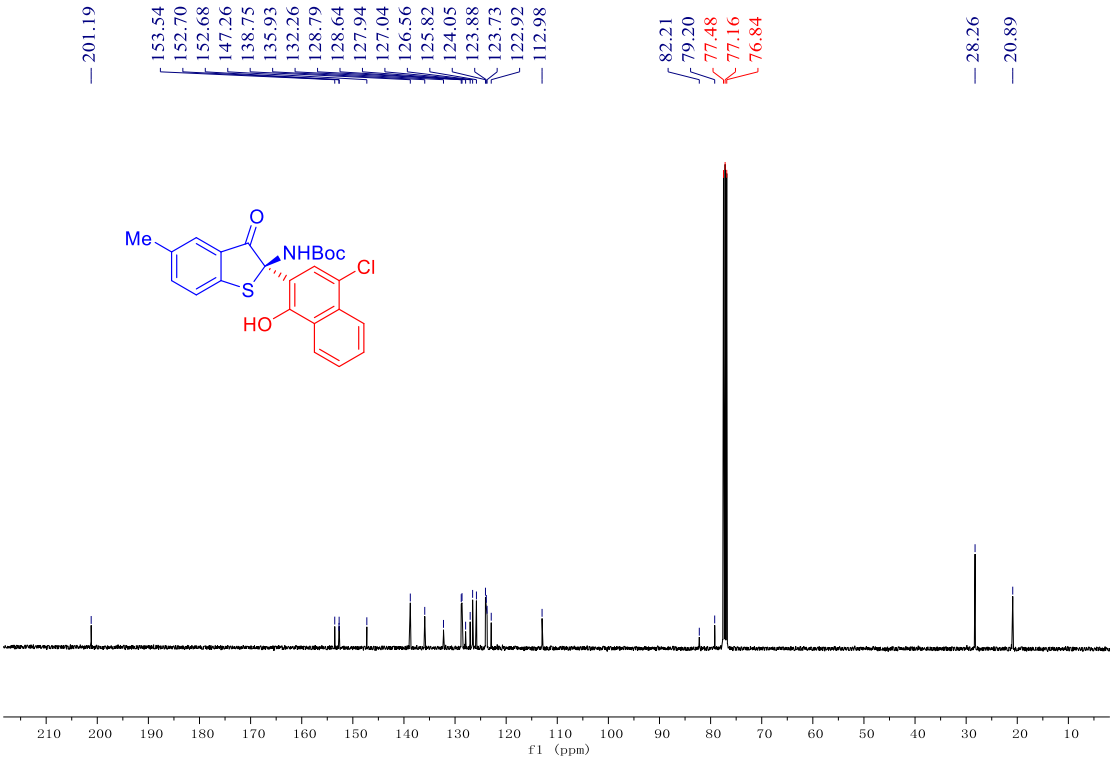
Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	5.404	1137.94	86.34	2.97
	6.531	37176.50	1746.85	97.03
		38314.45		100.00

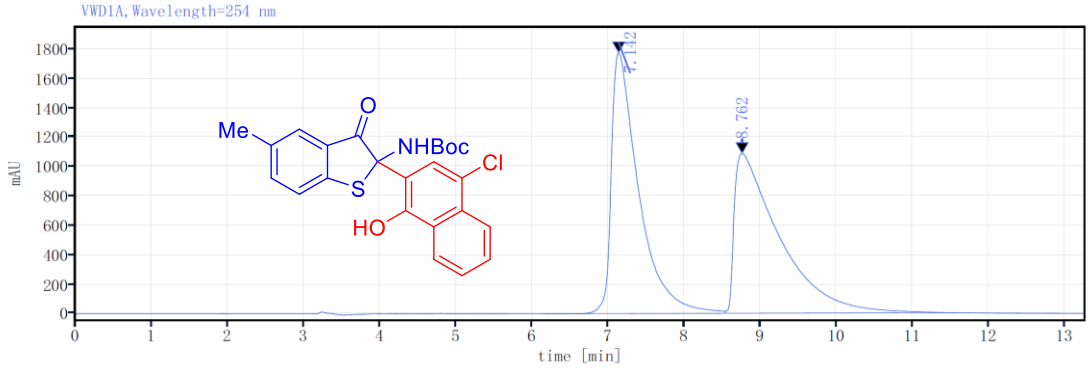
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3m





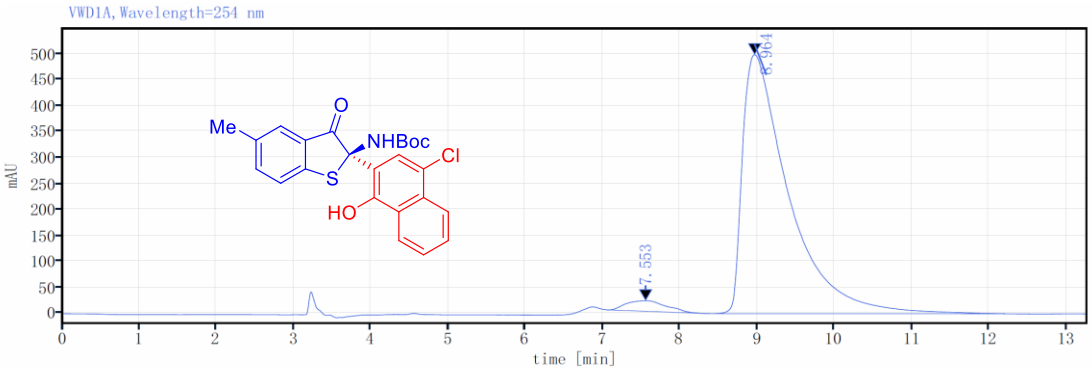


HPLC of 3m



Detector VWD1A, Wavelength=254 nm

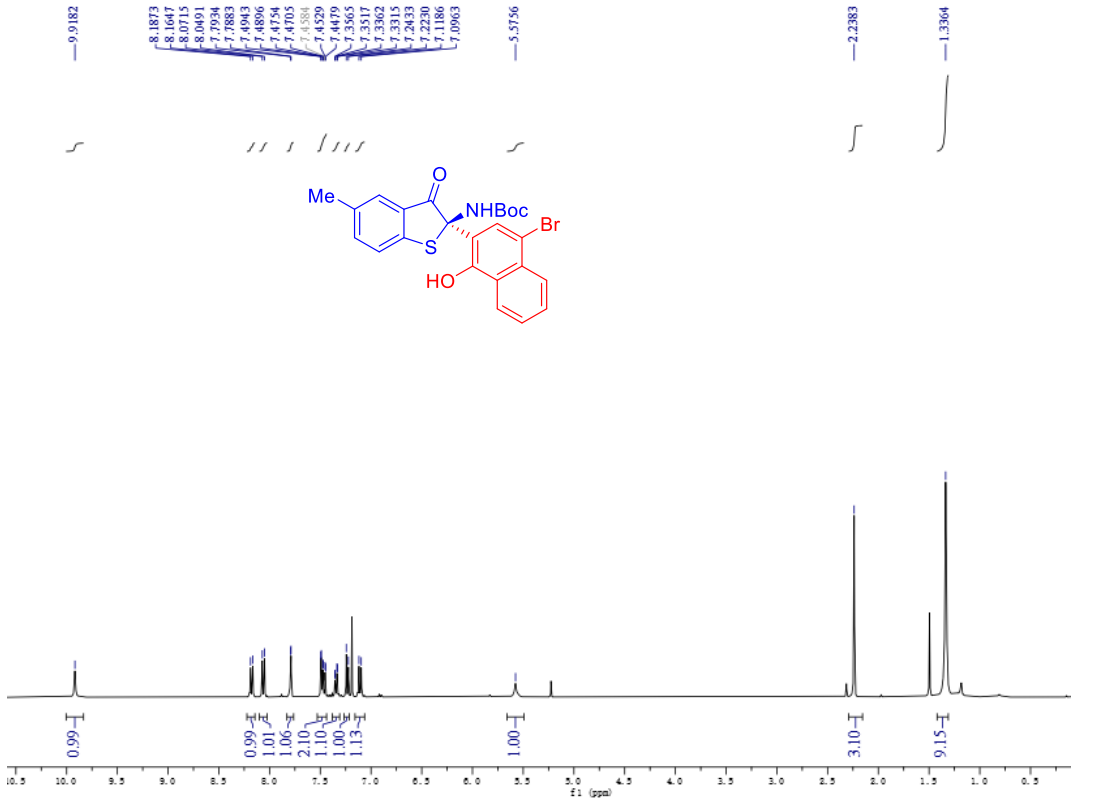
Peak	Ret.Time [min]	Area	Height	Area%
	7.142	44422.86	1774.28	49.77
	8.762	44840.73	1086.50	50.23
		89263.59		100.00

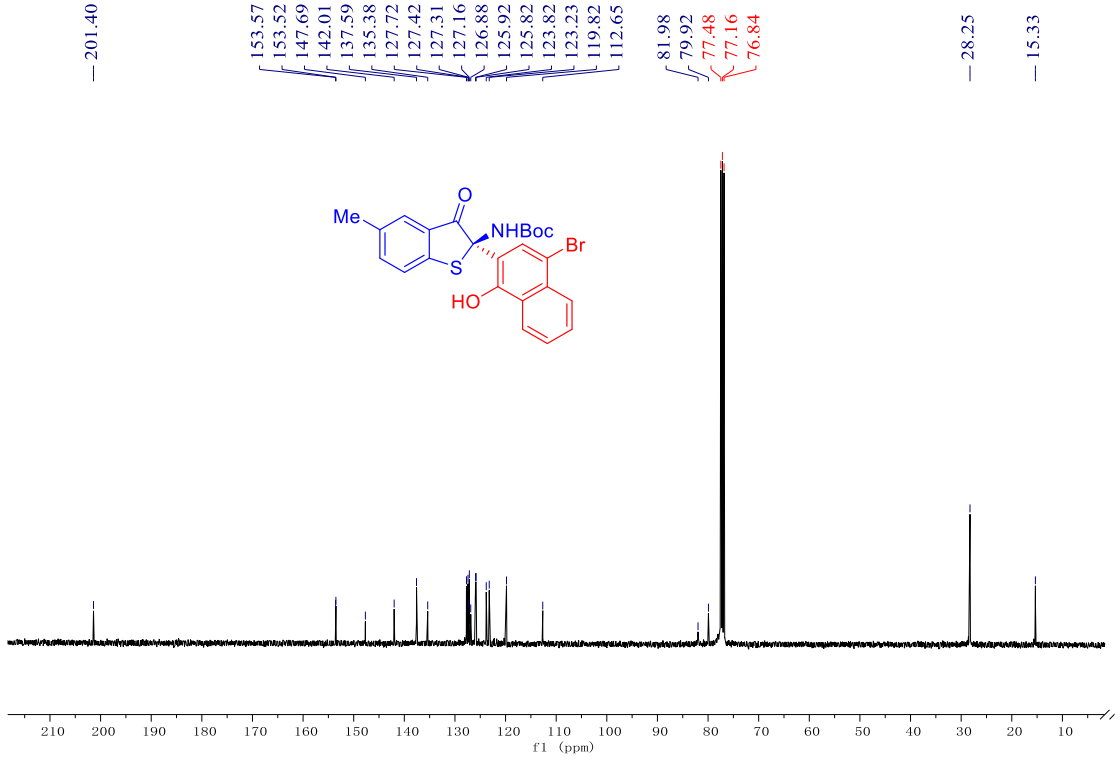


Detector VWD1A, Wavelength=254 nm

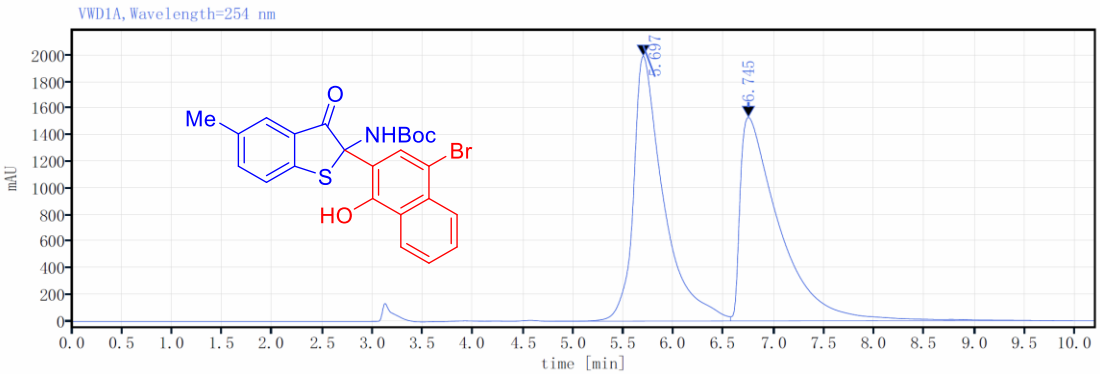
Peak	Ret.Time [min]	Area	Height	Area%
	7.553	734.28	20.42	3.42
	8.964	20748.05	498.47	96.58
		21482.33		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3n



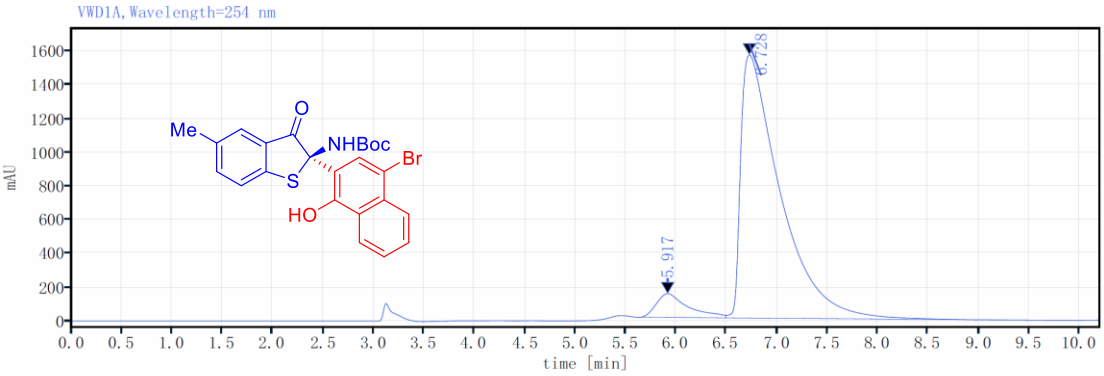


HPLC of 3n



Detector VWD1A, Wavelength=254 nm

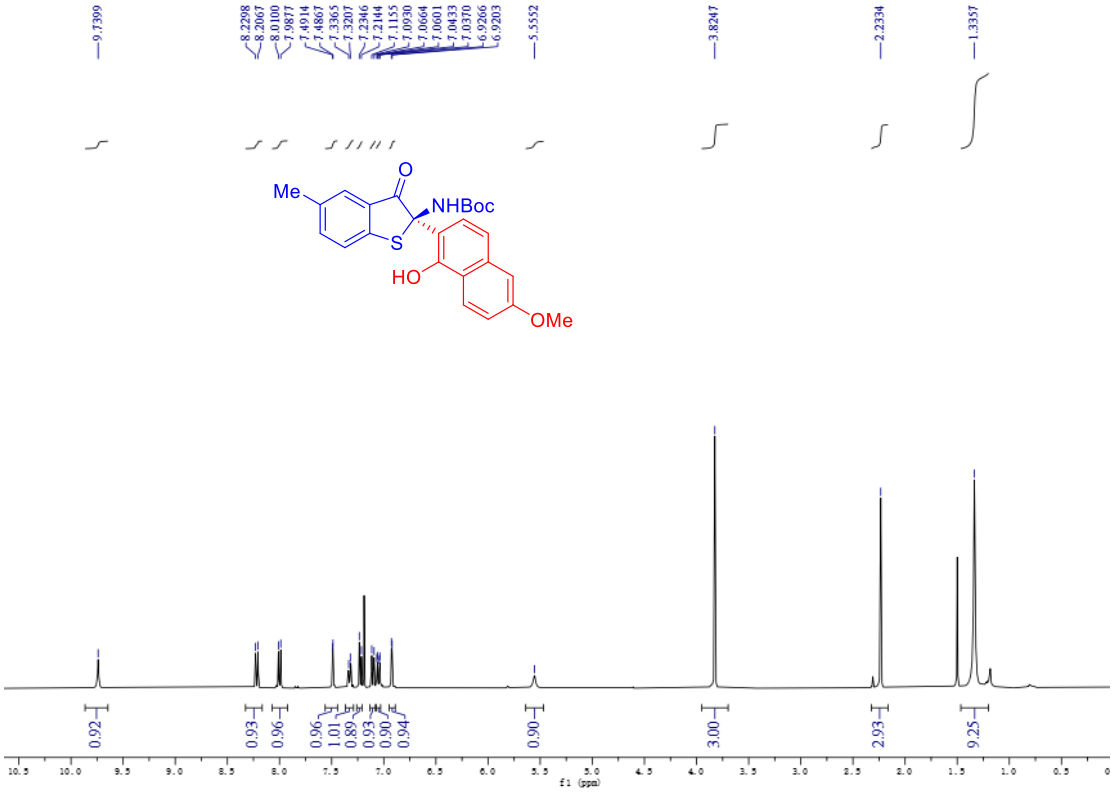
Peak	Ret.Time [min]	Area	Height	Area%
	5.697	41821.89	1992.41	50.11
	6.745	41640.05	1530.87	49.89
		83461.93		100.00

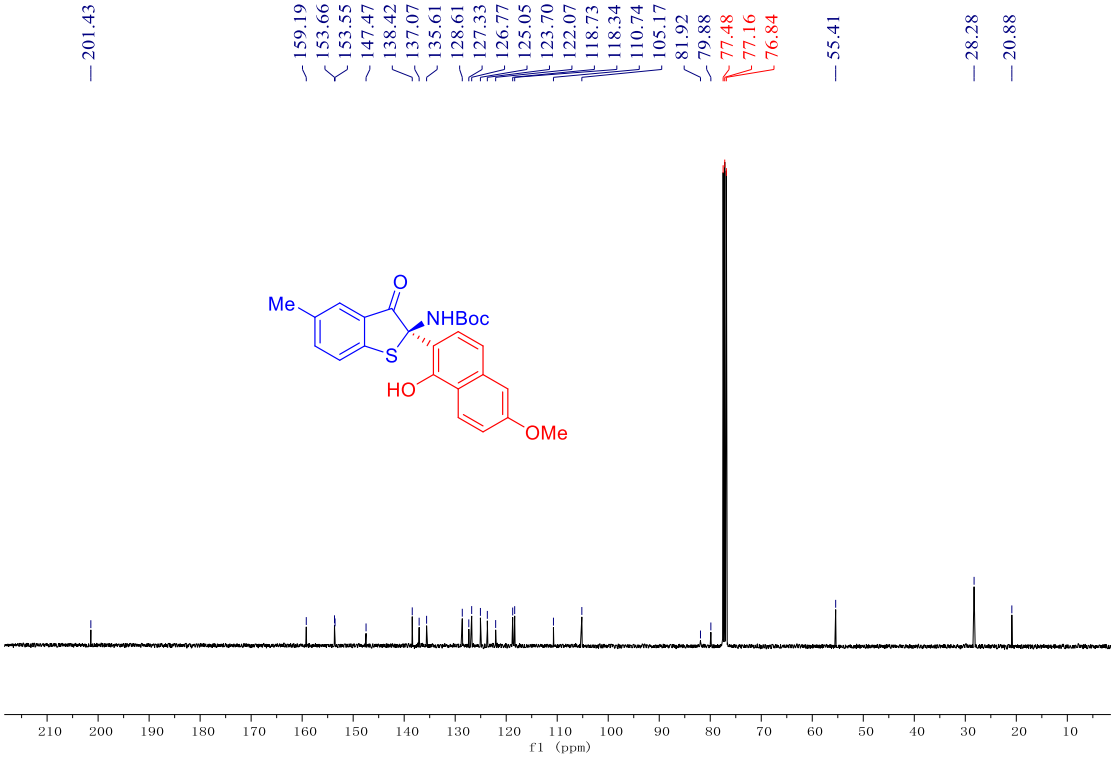


Detector VWD1A, Wavelength=254 nm

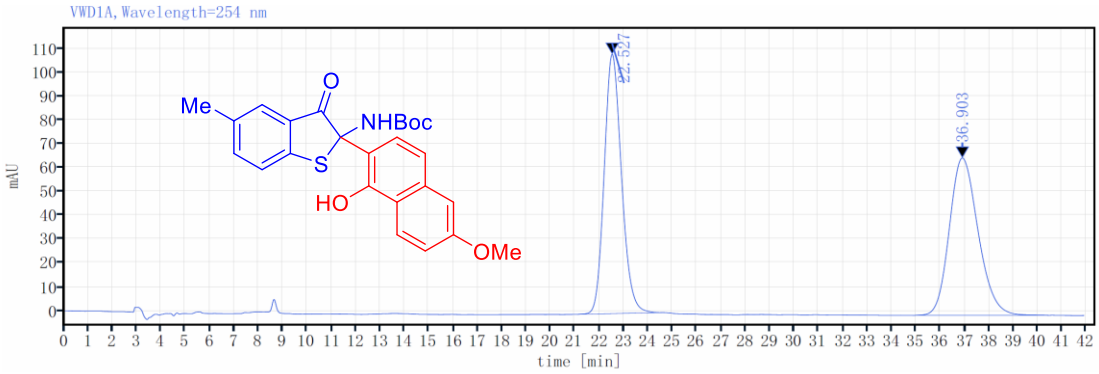
Peak	Ret.Time [min]	Area	Height	Area%
	5.917	3100.38	141.51	6.80
	6.728	42469.27	1562.98	93.20
		45569.65		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3o



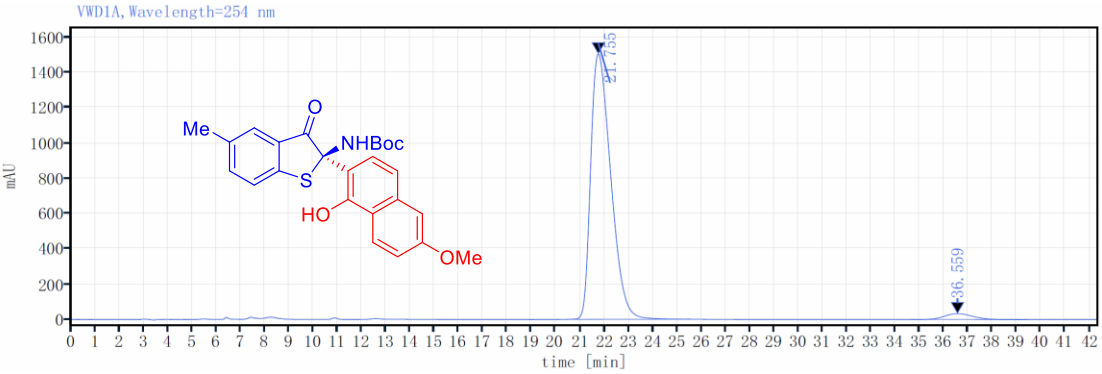


HPLC of 3o



Detector VWD1A, Wavelength=254 nm

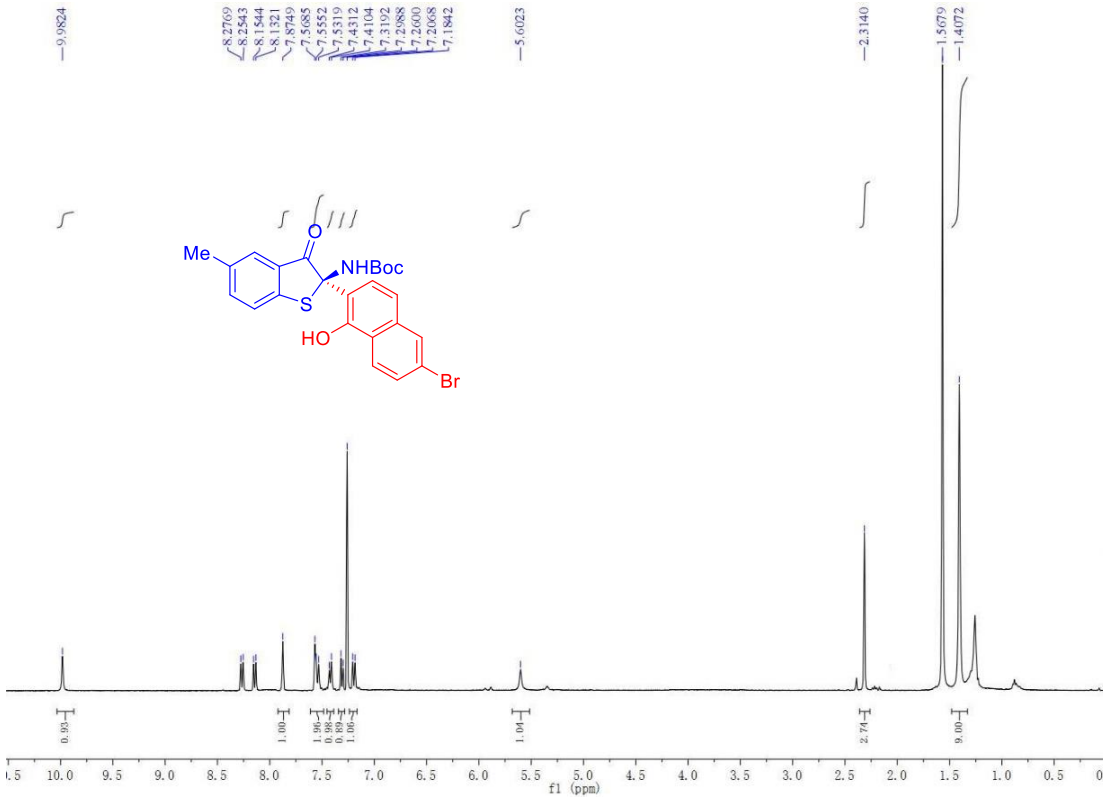
Peak	Ret.Time [min]	Area	Height	Area%
	22.527	5357.30	108.75	49.77
	36.903	5407.68	65.97	50.23
		10764.98		100.00

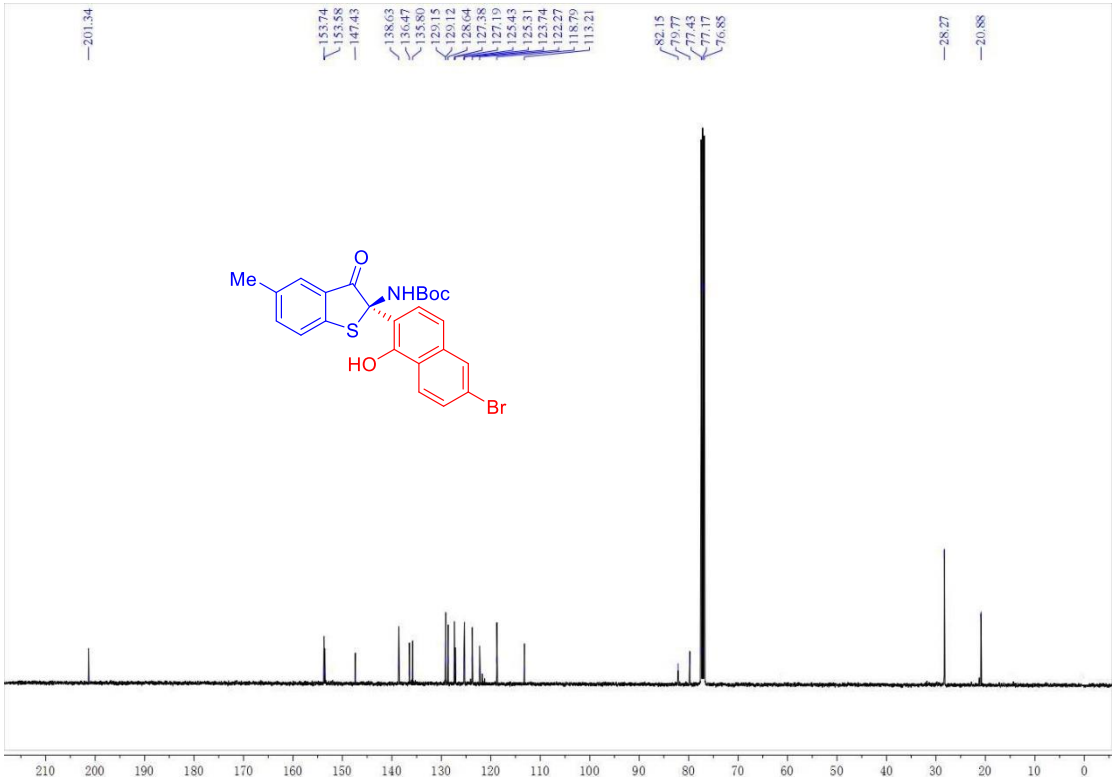


Detector VWD1A, Wavelength=254 nm

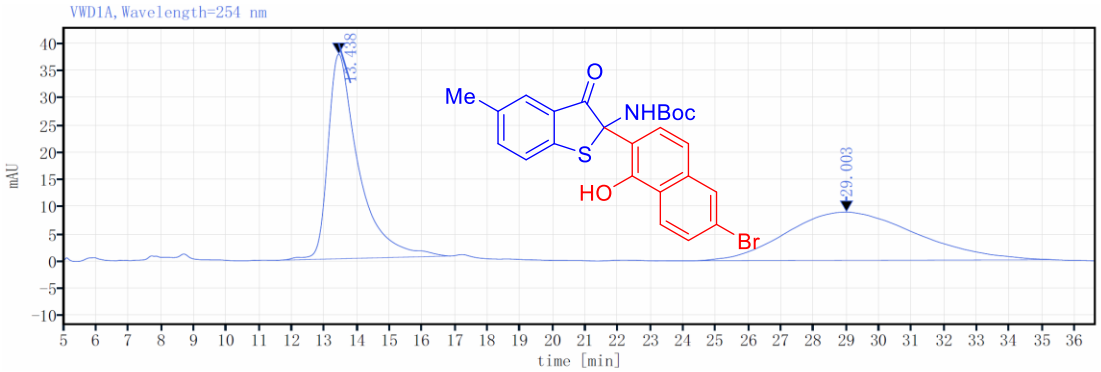
Peak	Ret.Time [min]	Area	Height	Area%
	21.755	86519.03	1503.35	96.88
	36.559	2783.06	33.92	3.12
		89302.09		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 3p



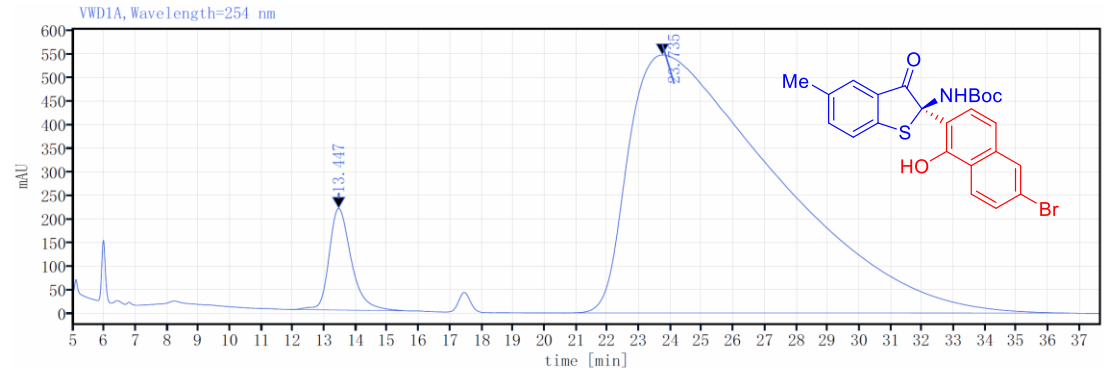


HPLC of 3p



Detector VWD1A, Wavelength=254 nm

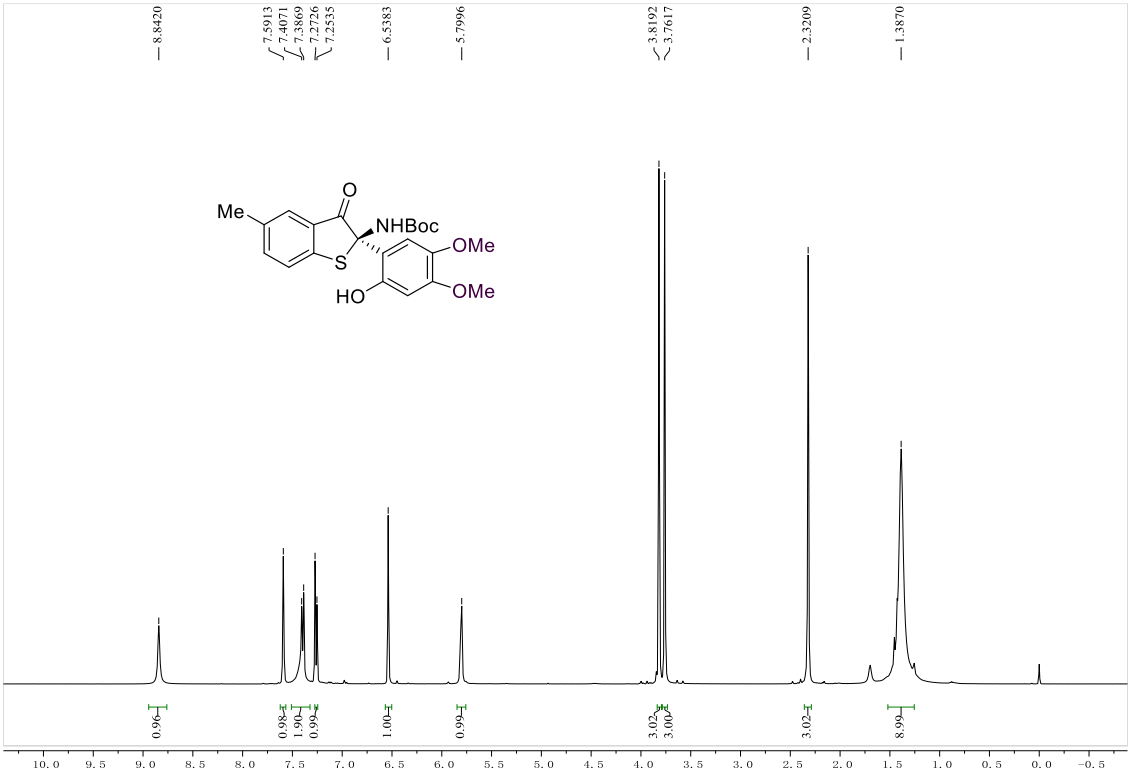
Peak	Ret.Time [min]	Area	Height	Area%
	13.438	2452.00	37.61	49.93
	29.003	2458.58	8.87	50.07
		4910.58		100.00

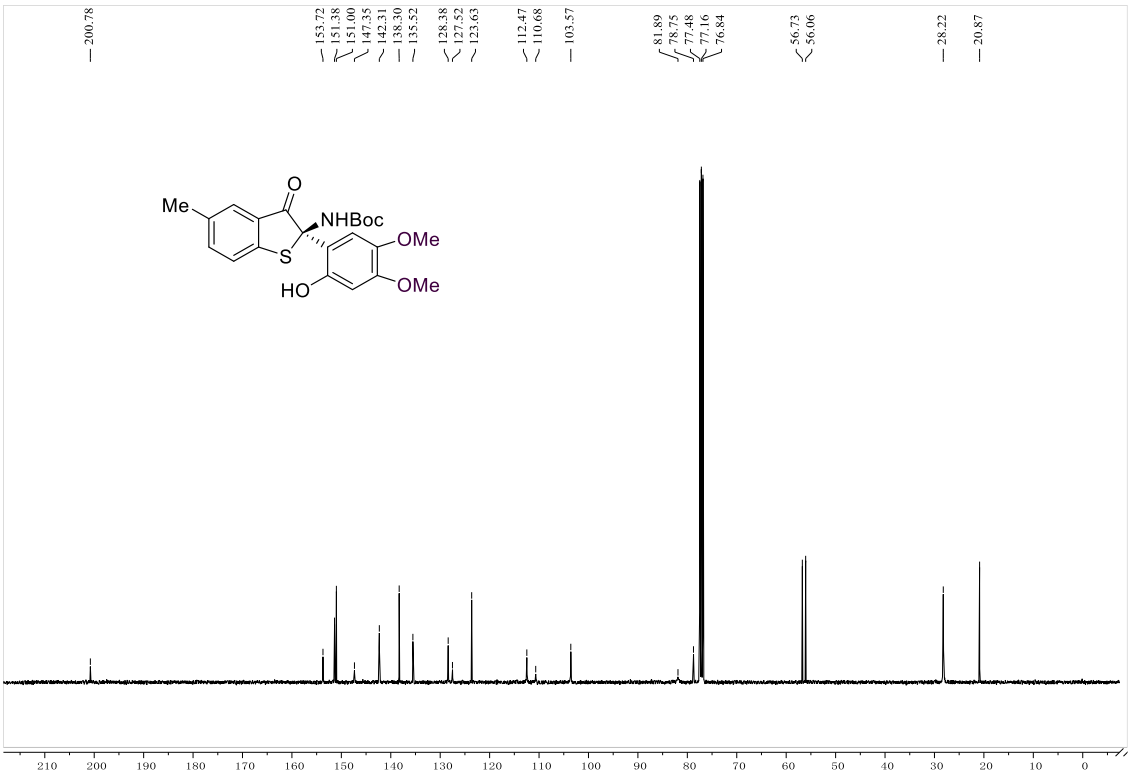


Detector VWD1A, Wavelength=254 nm

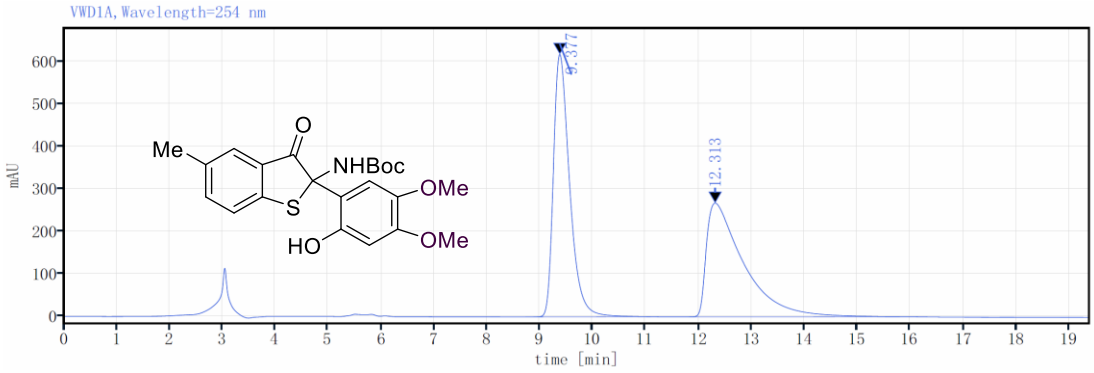
Peak	Ret.Time [min]	Area	Height	Area%
	13.447	10516.99	215.12	5.56
	23.735	178784.28	546.10	94.44
		189301.28		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5a



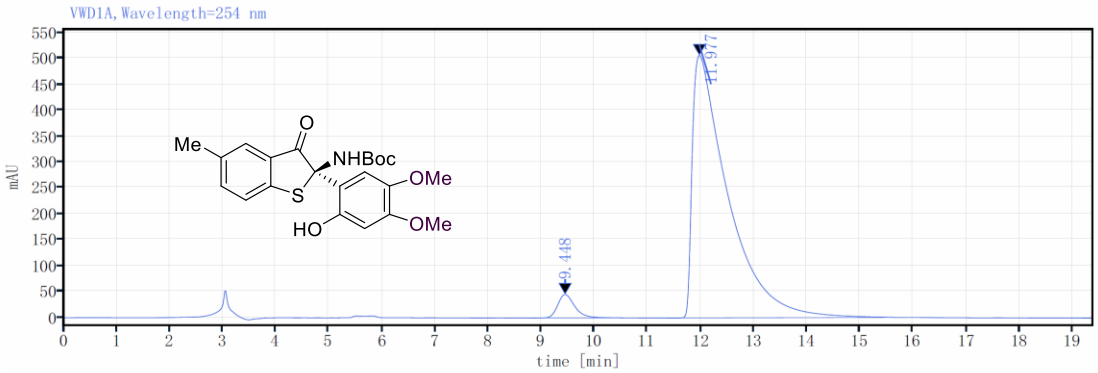


HPLC of 5a



Detector VWD1A, Wavelength=254 nm

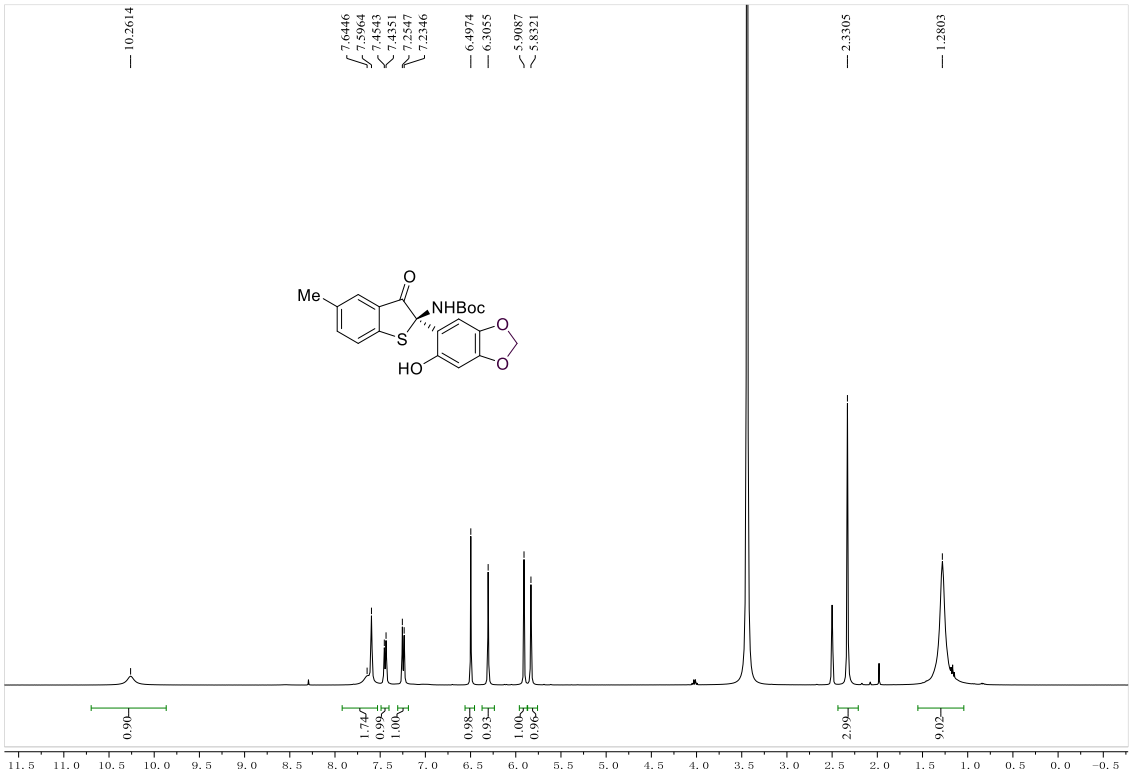
Peak	Ret.Time [min]	Area	Height	Area%
	9.377	13130.88	616.68	50.09
	12.313	13083.57	267.32	49.91
		26214.45		100.00

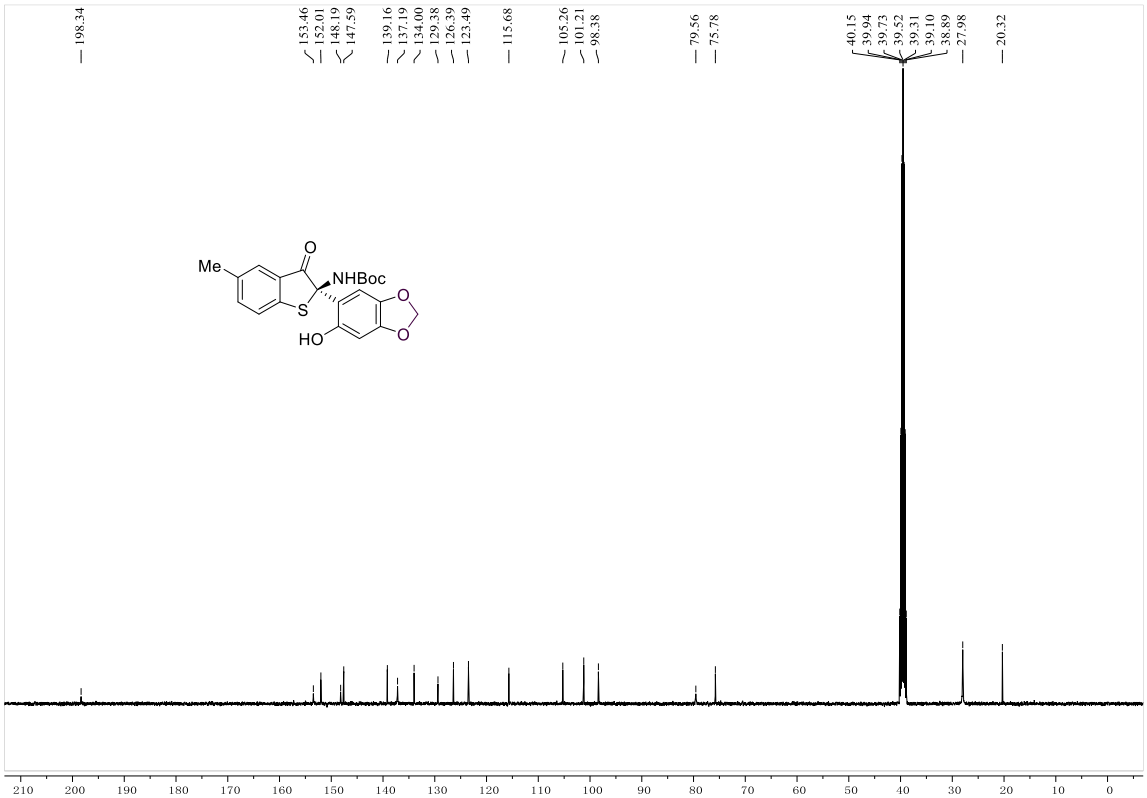


Detector VWD1A, Wavelength=254 nm

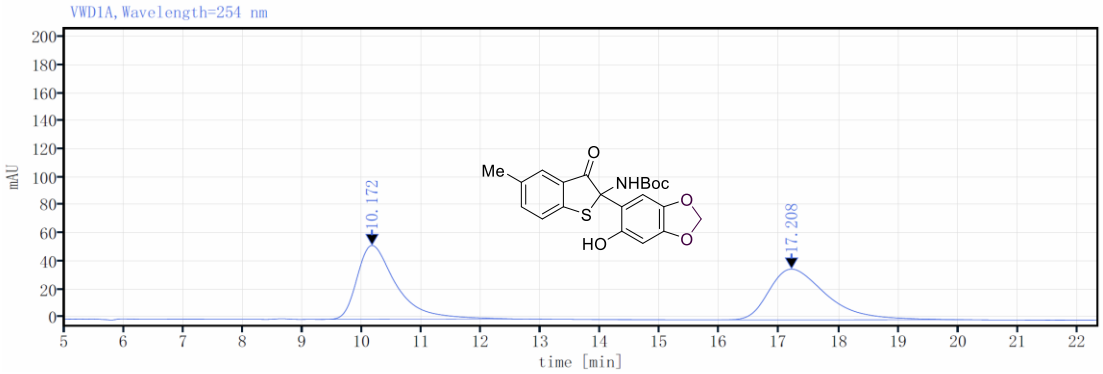
Peak	Ret.Time [min]	Area	Height	Area%
	9.448	1002.91	45.21	4.08
	11.977	23587.45	506.13	95.92
		24590.36		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 5b



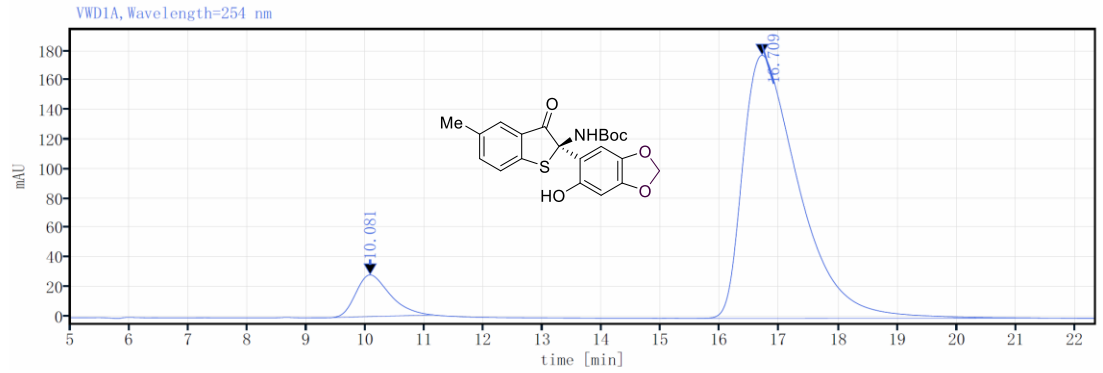


HPLC of 5b



Detector VWD1A, Wavelength=254 nm

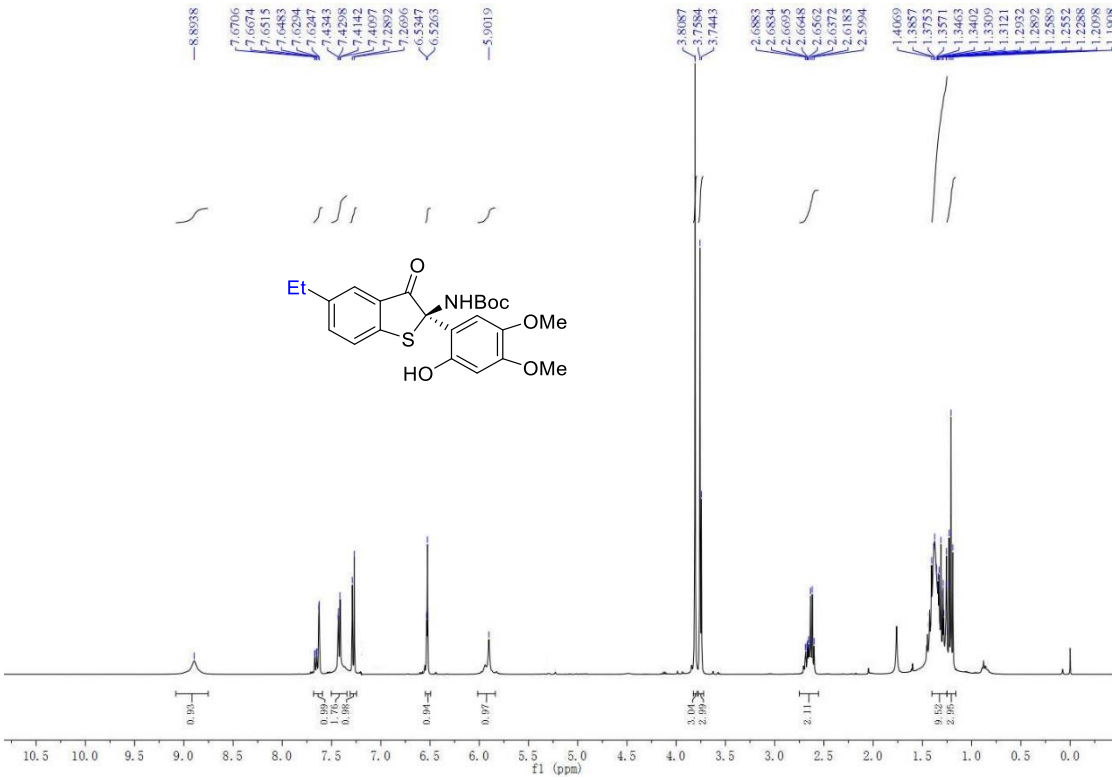
Peak	Ret.Time [min]	Area	Height	Area%
	10.172	2403.12	52.58	49.99
	17.208	2404.42	36.12	50.01
		4807.54		100.00

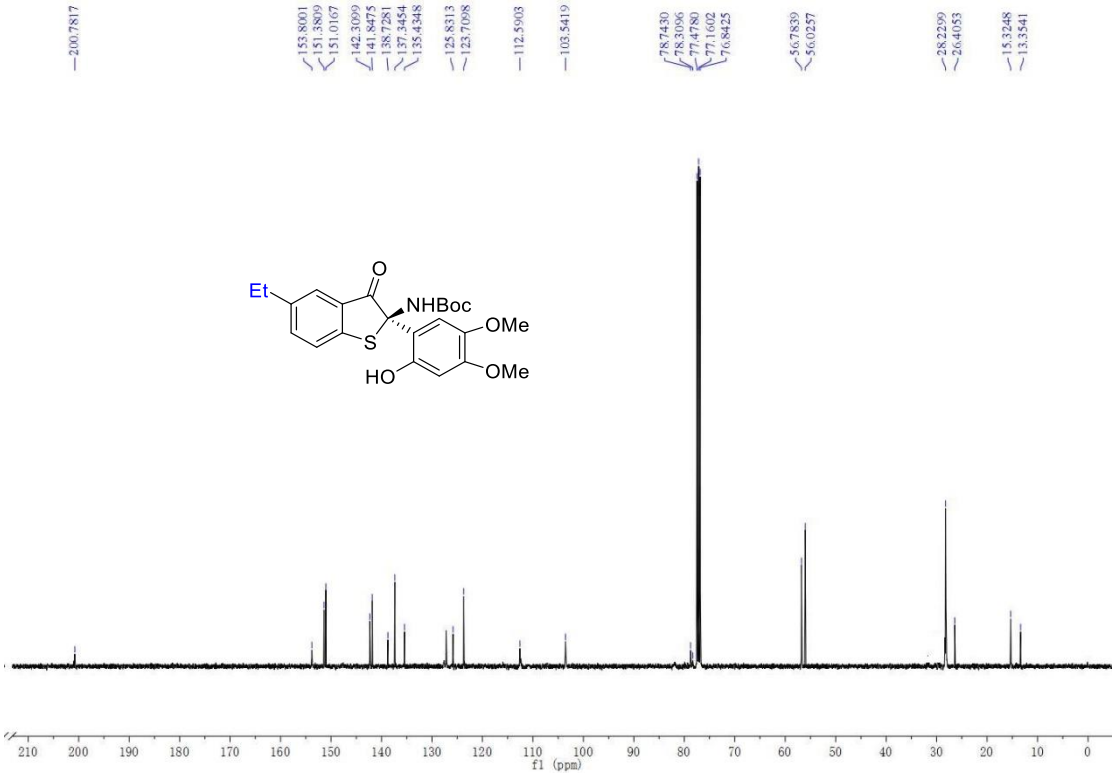


Detector VWD1A, Wavelength=254 nm

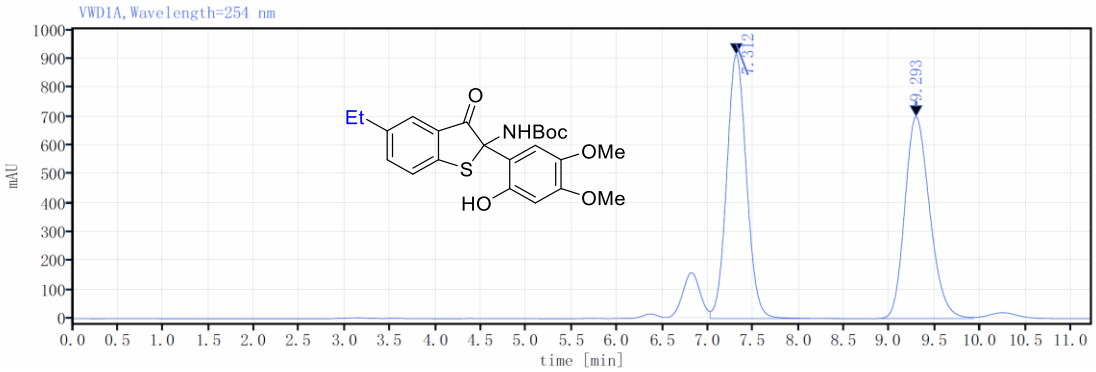
Peak	Ret.Time [min]	Area	Height	Area%
	10.081	1135.17	28.28	8.81
	16.709	11756.38	178.33	91.19
		12891.54		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5c



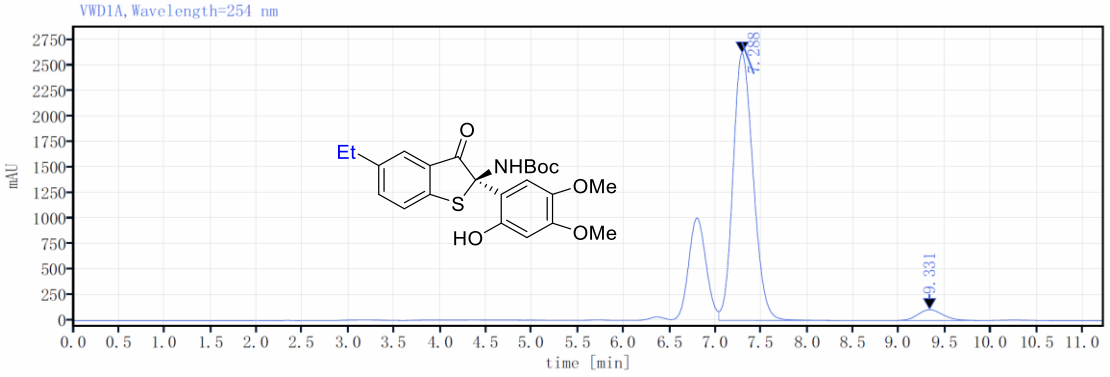


HPLC of 5c



Detector VWD1A, Wavelength=254 nm

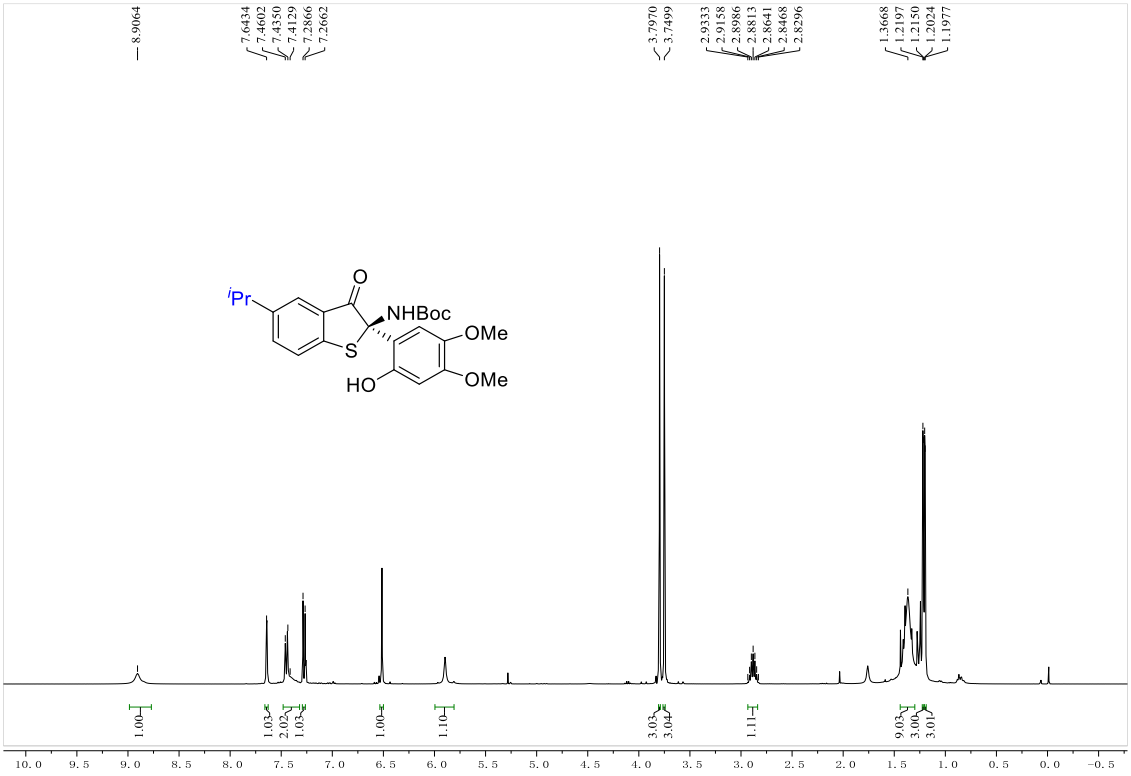
Peak	Ret.Time [min]	Area	Height	Area%
	7.312	13890.14	914.81	50.95
	9.293	13370.96	699.55	49.05
		27261.10		100.00

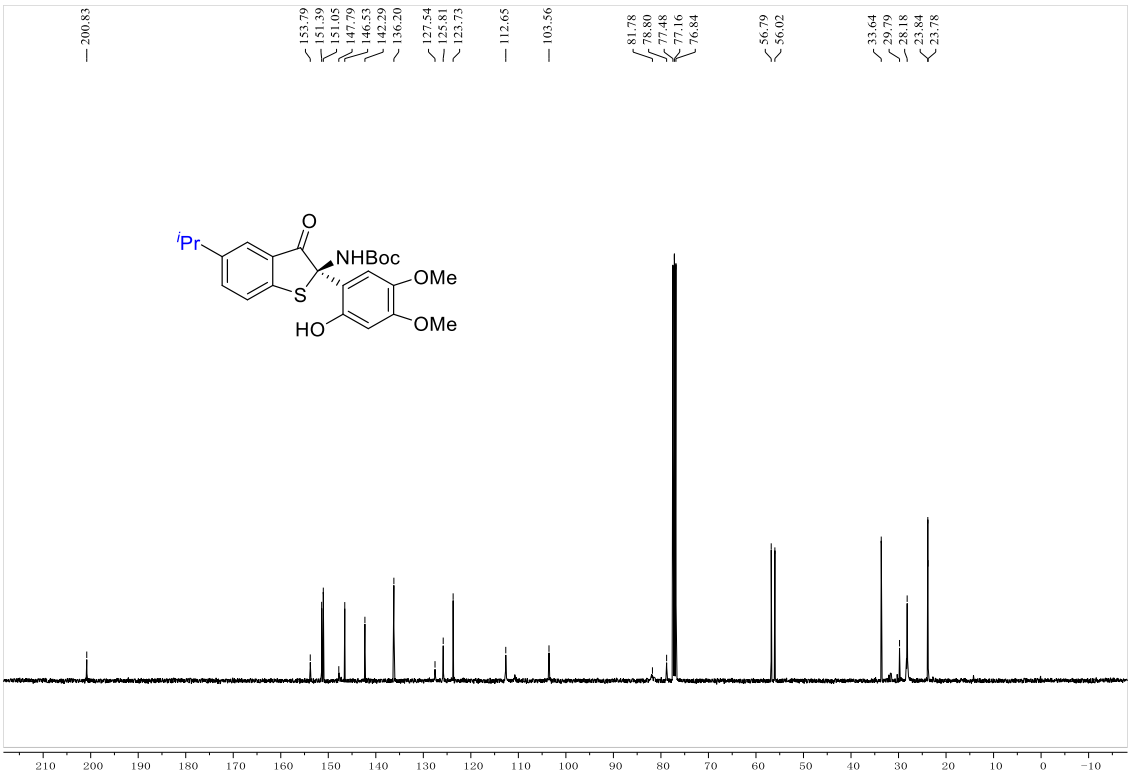


Detector VWD1A, Wavelength=254 nm

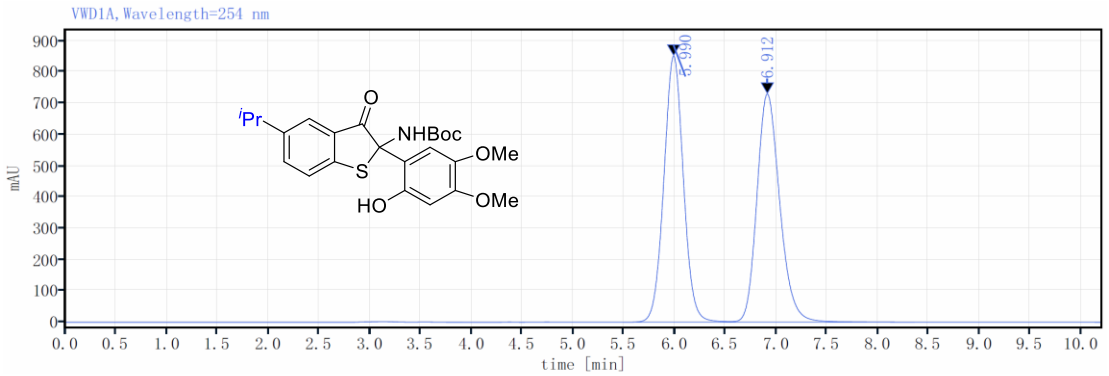
Peak	Ret.Time [min]	Area	Height	Area%
	7.288	40000.48	2619.88	95.26
	9.331	1992.28	105.64	4.74
		41992.76		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5d



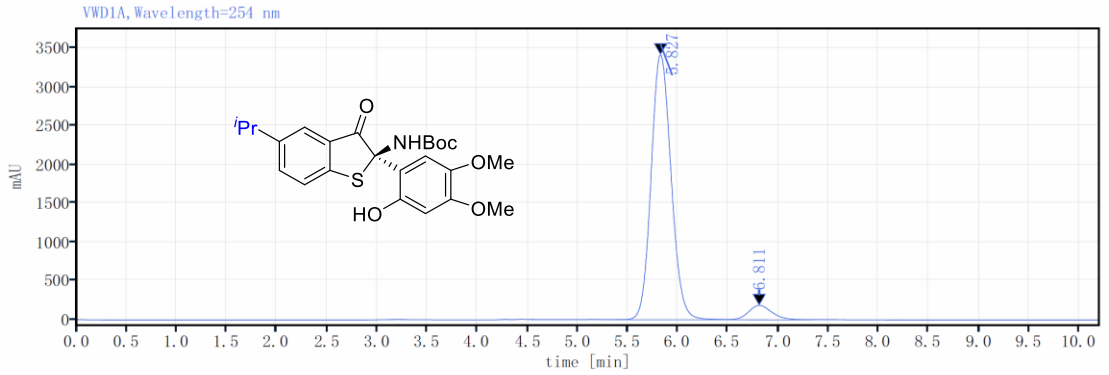


HPLC of 5d



Detector VWD1A, Wavelength=254 nm

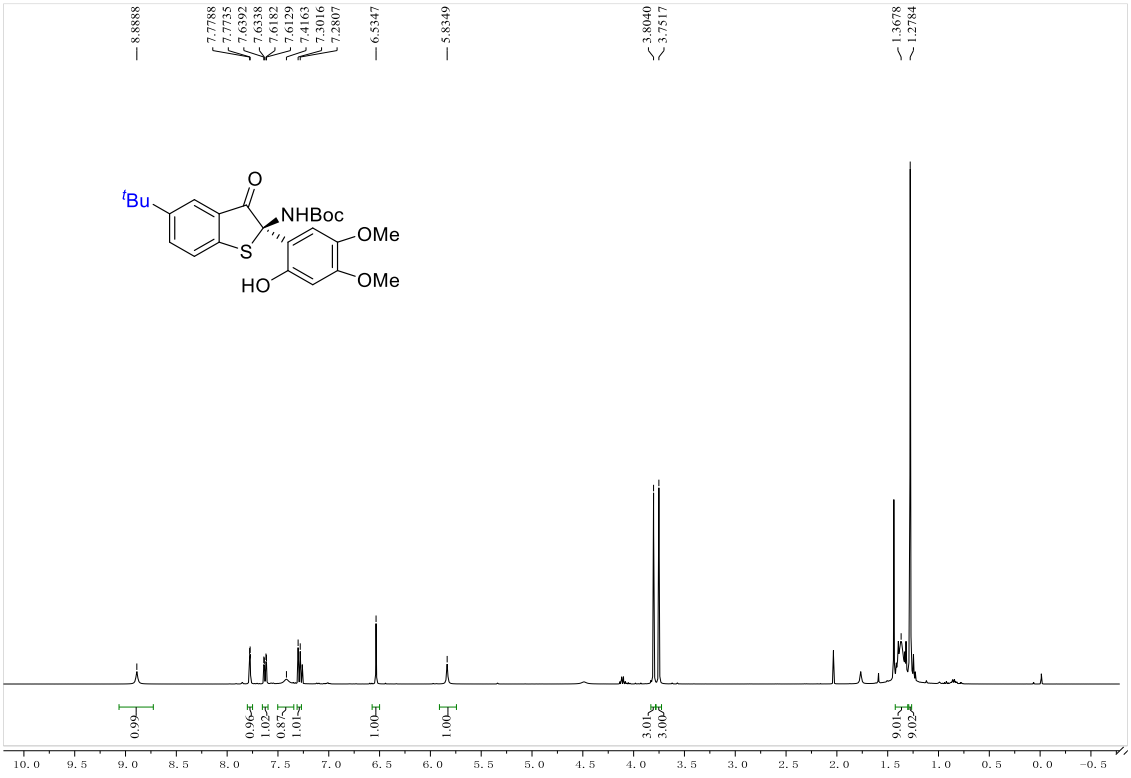
Peak	Ret.Time [min]	Area	Height	Area%
	5.990	11389.62	851.54	49.93
	6.912	11419.50	730.31	50.07
		22809.12		100.00

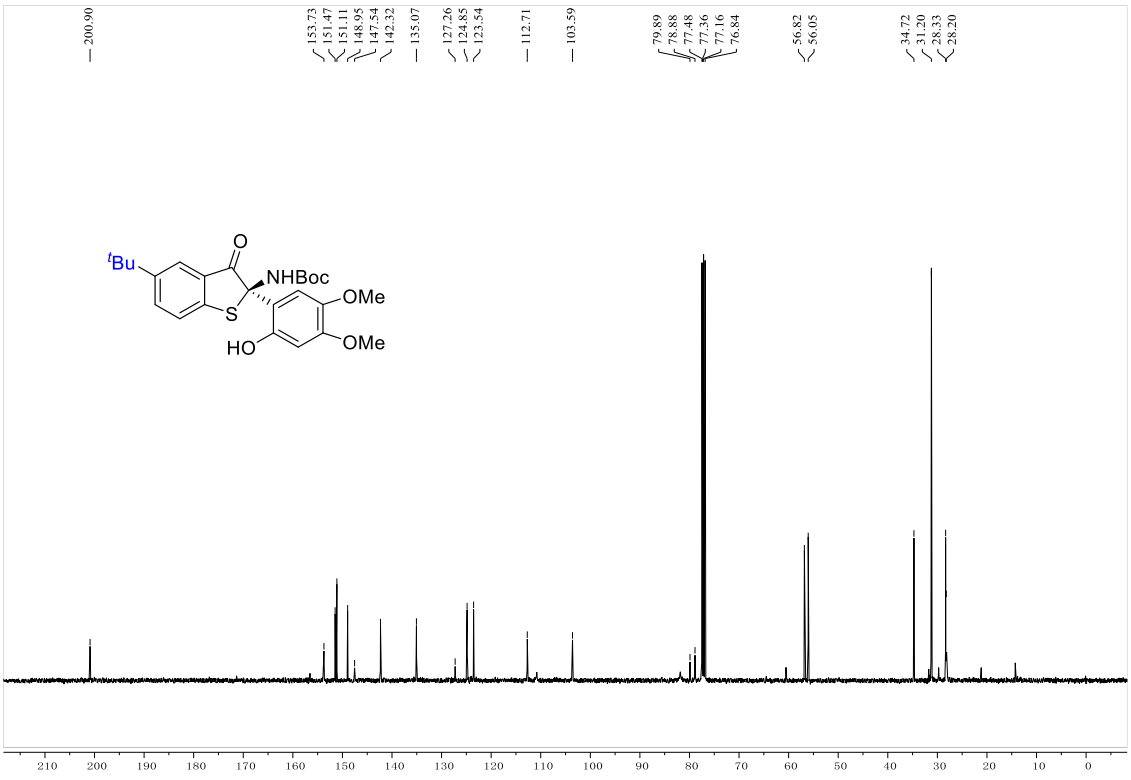


Detector VWD1A, Wavelength=254 nm

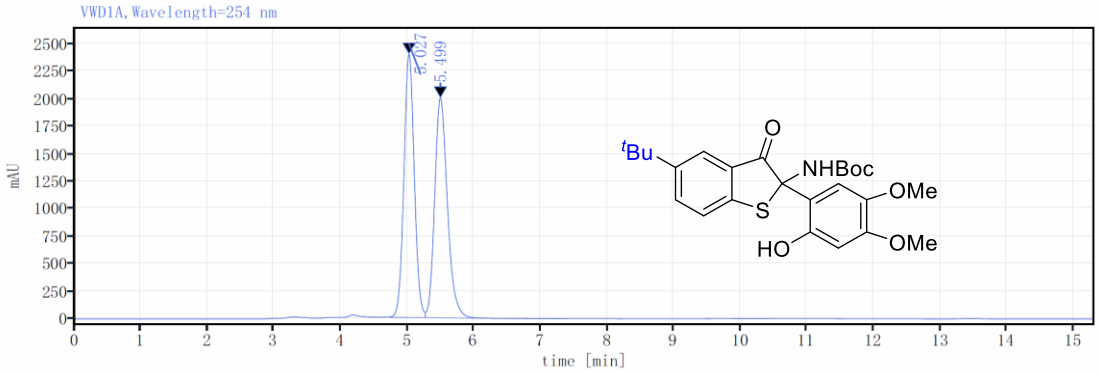
Peak	Ret.Time [min]	Area	Height	Area%
	5.827	47491.06	3427.44	93.91
	6.811	3081.89	187.47	6.09
		50572.95		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5e



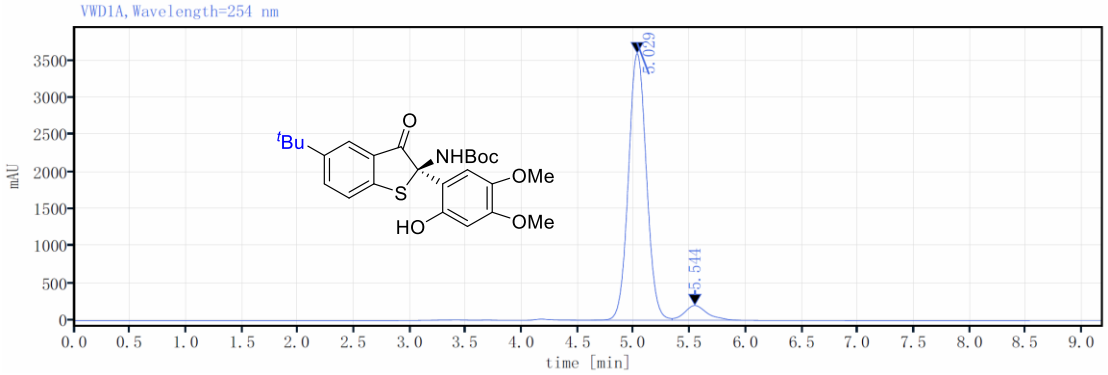


HPLC of 5e



Detector VWD1A, Wavelength=254 nm

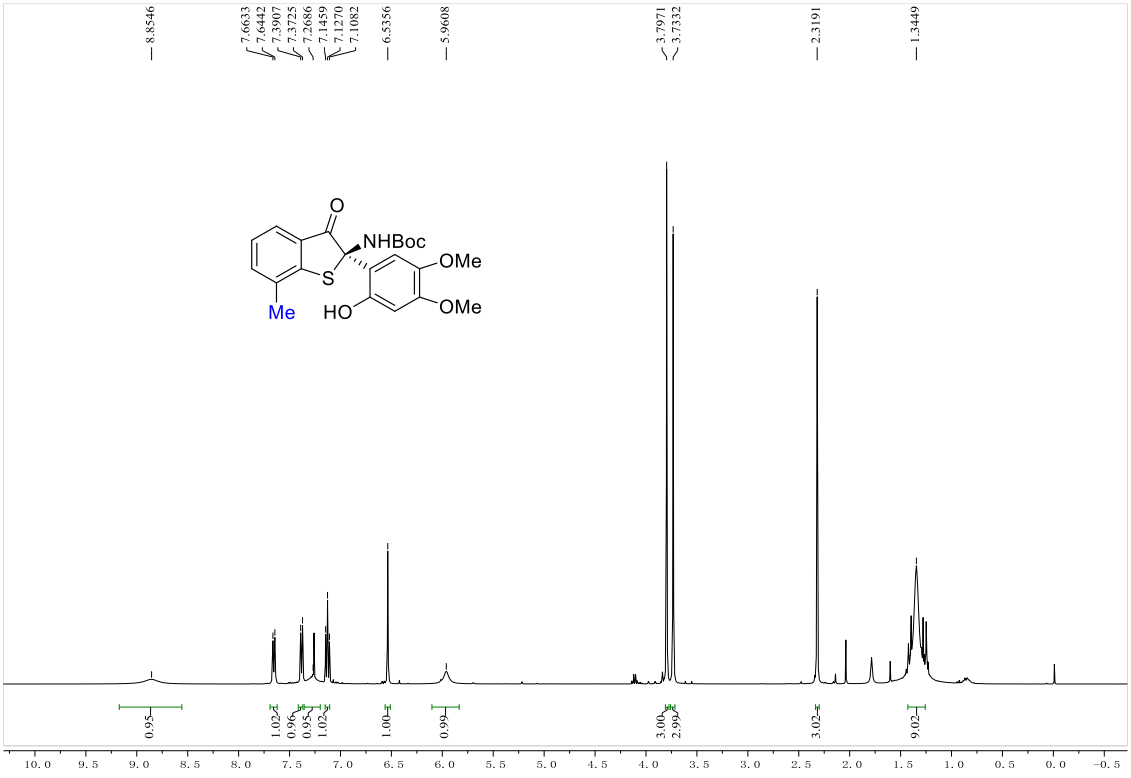
Peak	Ret.Time [min]	Area	Height	Area%
	5.027	25914.30	2396.64	49.36
	5.499	26582.65	2001.63	50.64
		52496.95		100.00

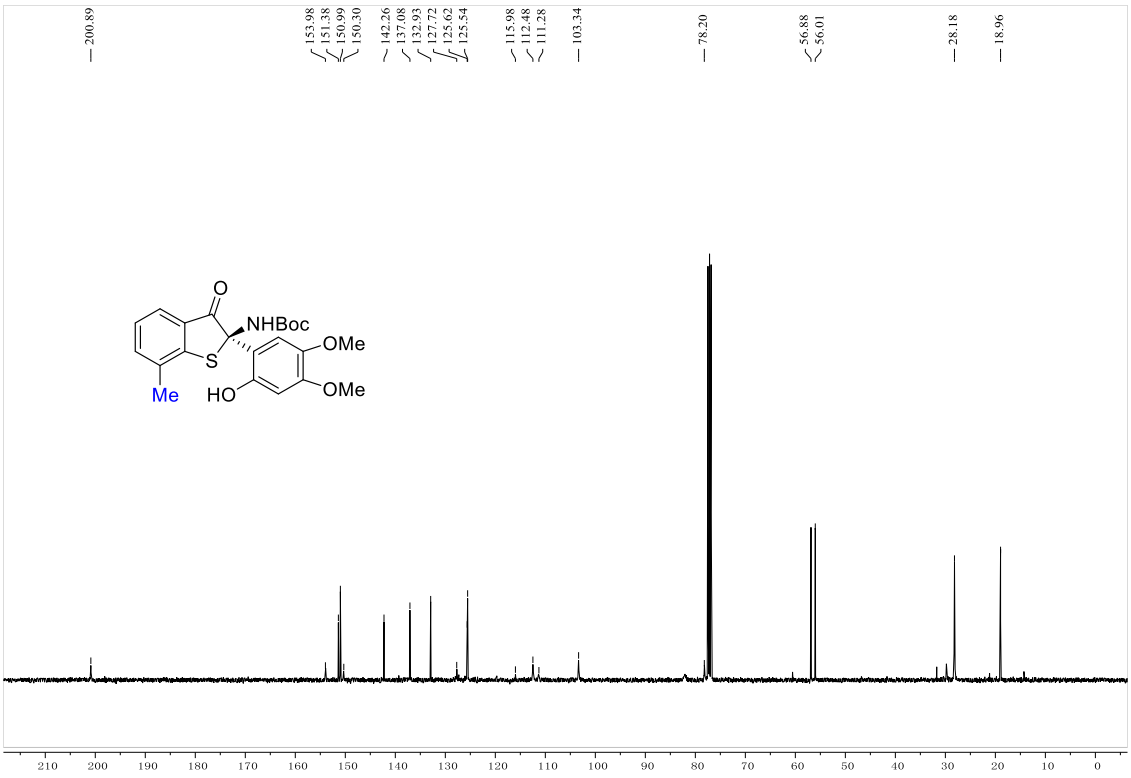


Detector VWD1A, Wavelength=254 nm

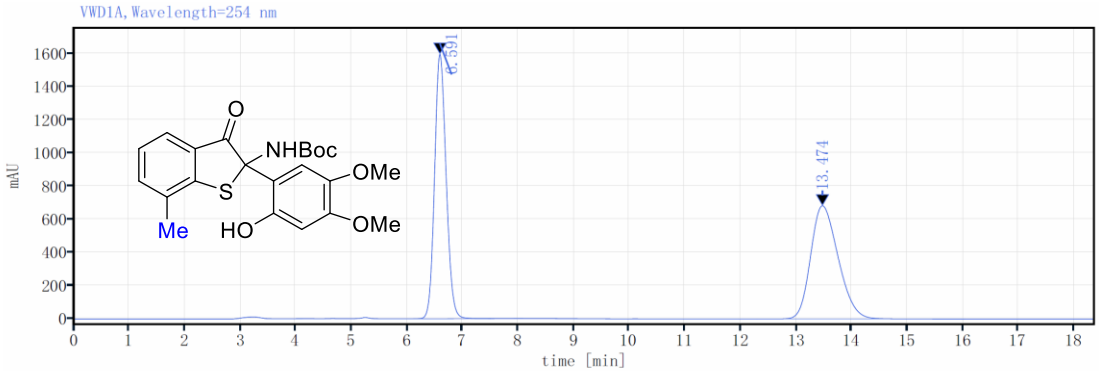
Peak	Ret.Time [min]	Area	Height	Area%
	5.029	40247.05	3592.30	93.52
	5.544	2788.59	197.75	6.48
		43035.63		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5f



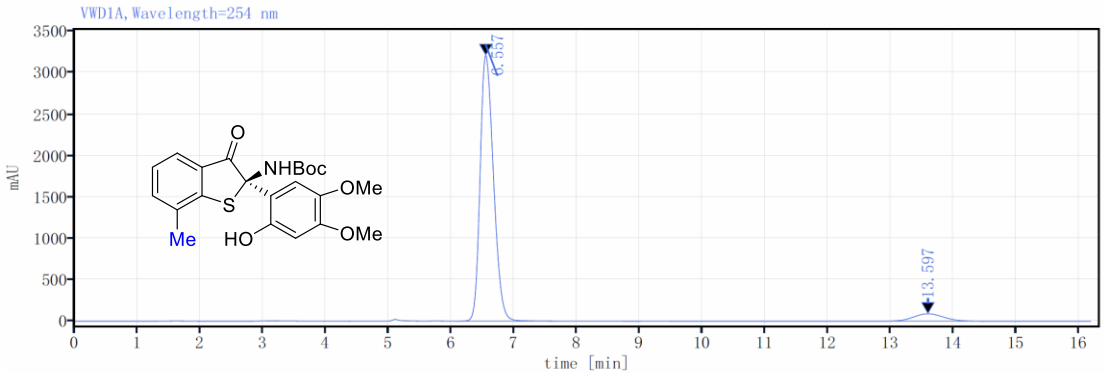


HPLC of 5f



Detector VWD1A, Wavelength=254 nm

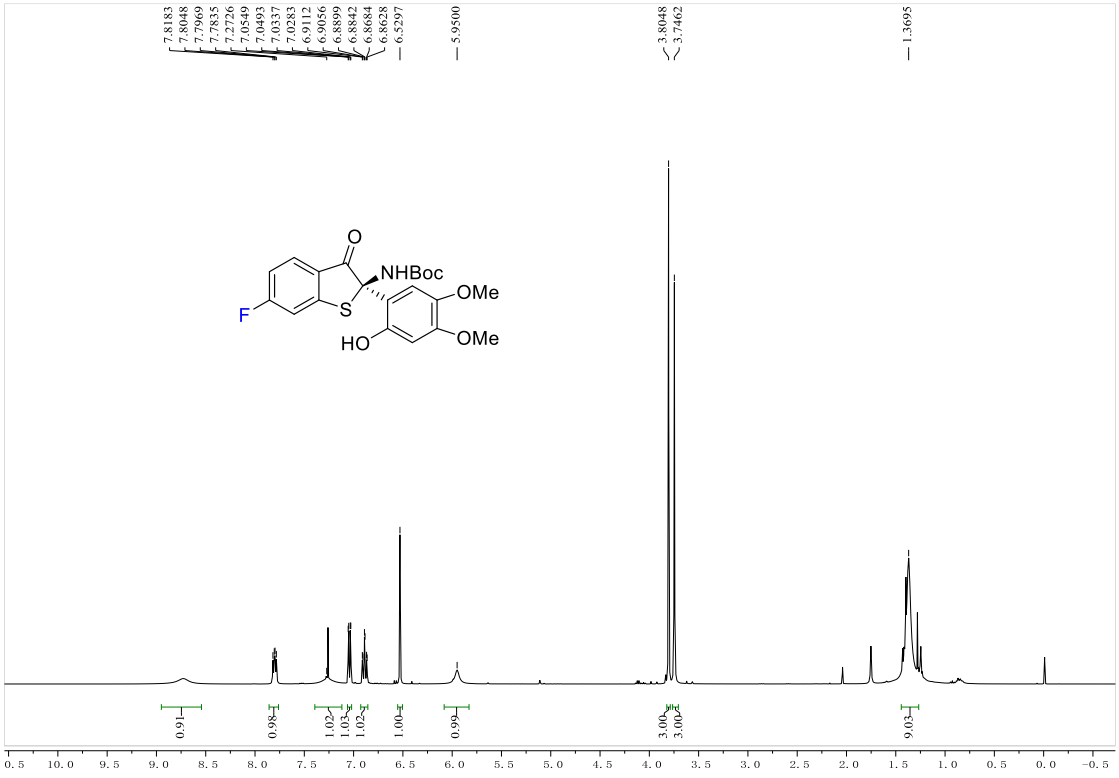
Peak	Ret.Time [min]	Area	Height	Area%
	6.591	23112.60	1600.23	49.60
	13.474	23484.93	684.32	50.40
		46597.53		100.00

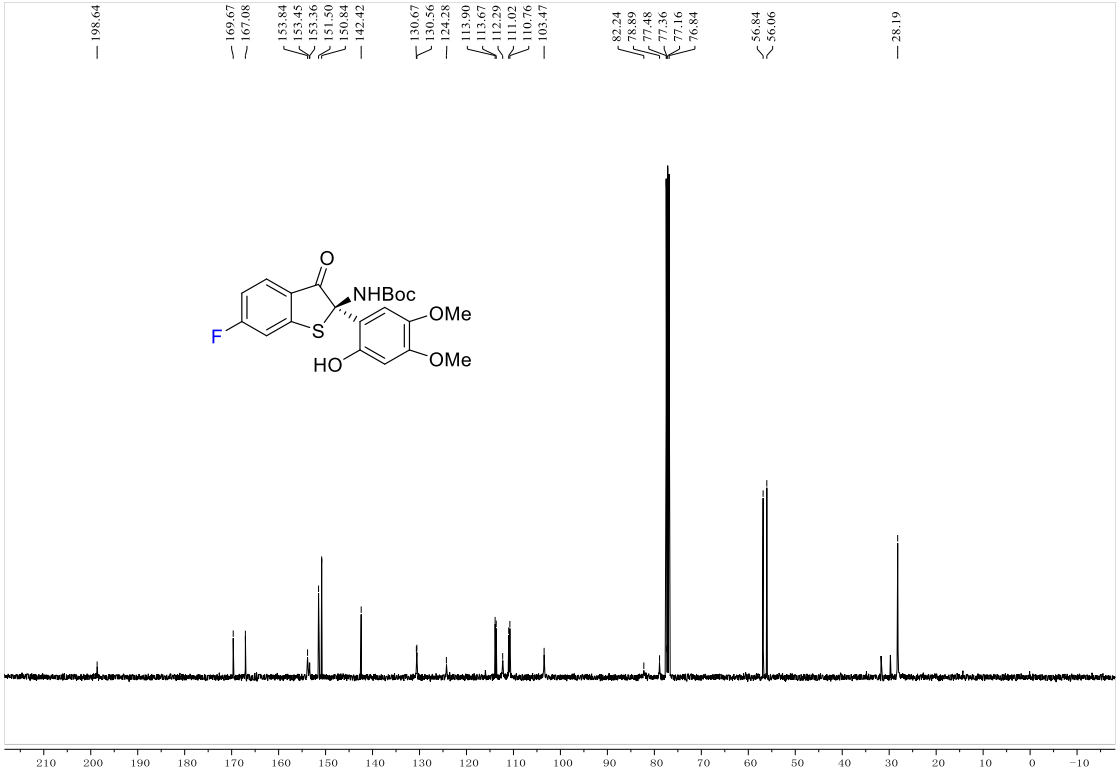


Detector VWD1A, Wavelength=254 nm

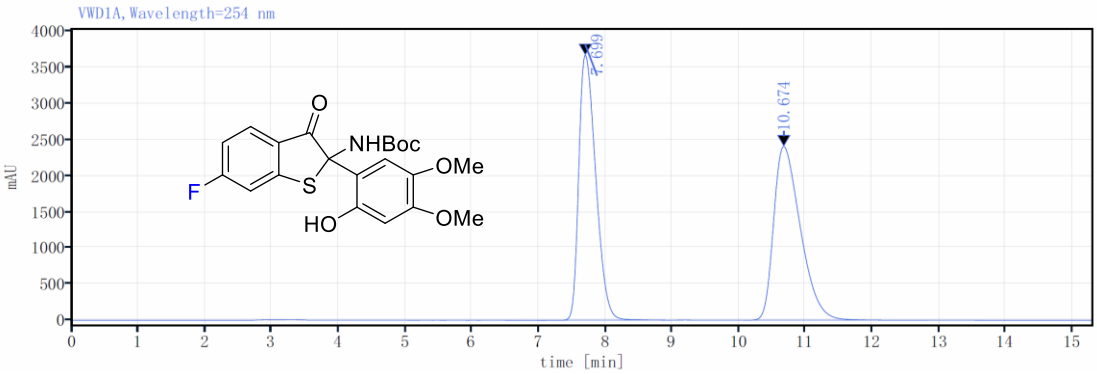
Peak	Ret.Time [min]	Area	Height	Area%
	6.557	47520.25	3211.32	94.11
	13.597	2972.14	89.68	5.89
		50492.38		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5g



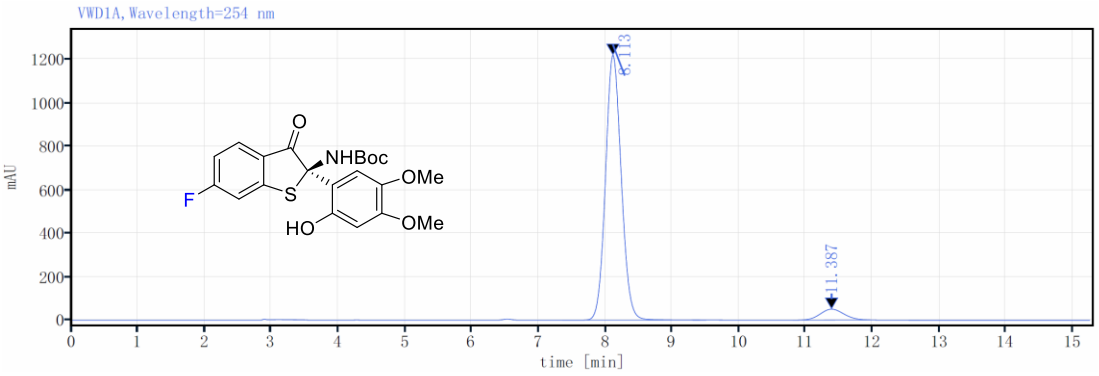


HPLC of 5g



Detector VWD1A, Wavelength=254 nm

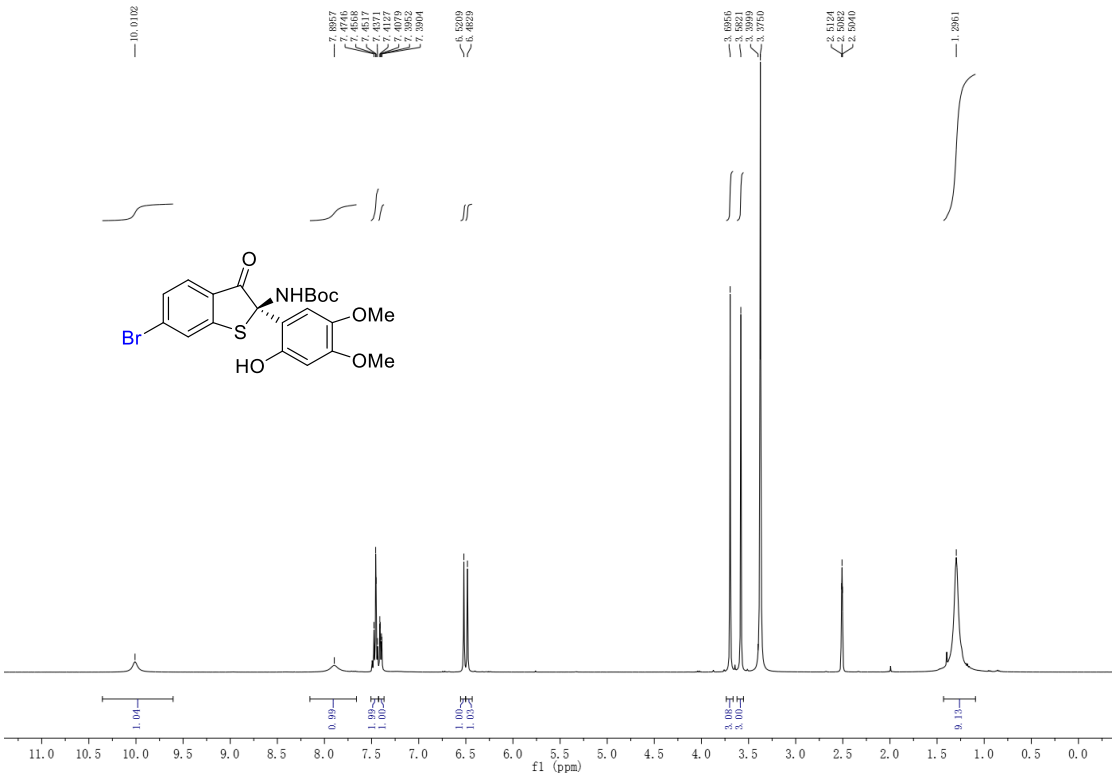
Peak	Ret.Time [min]	Area	Height	Area%
	7.699	64719.94	3667.80	49.17
	10.674	66903.09	2405.55	50.83
		131623.03		100.00

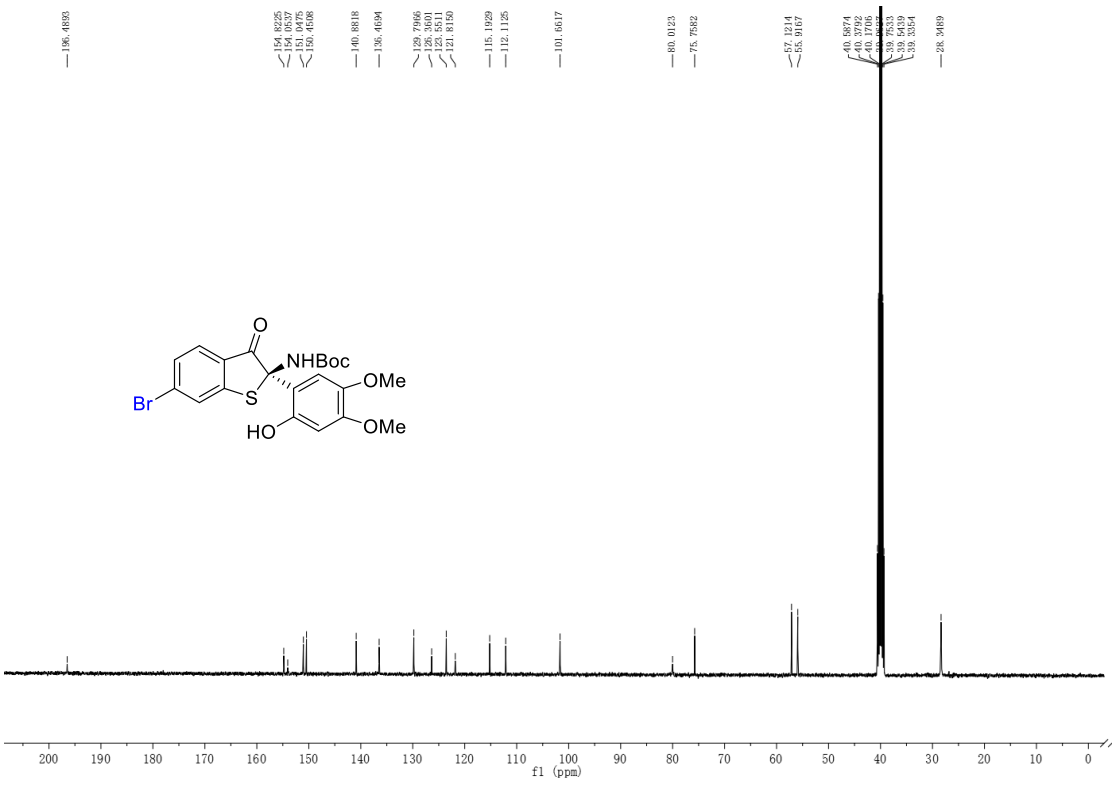


Detector VWD1A, Wavelength=254 nm

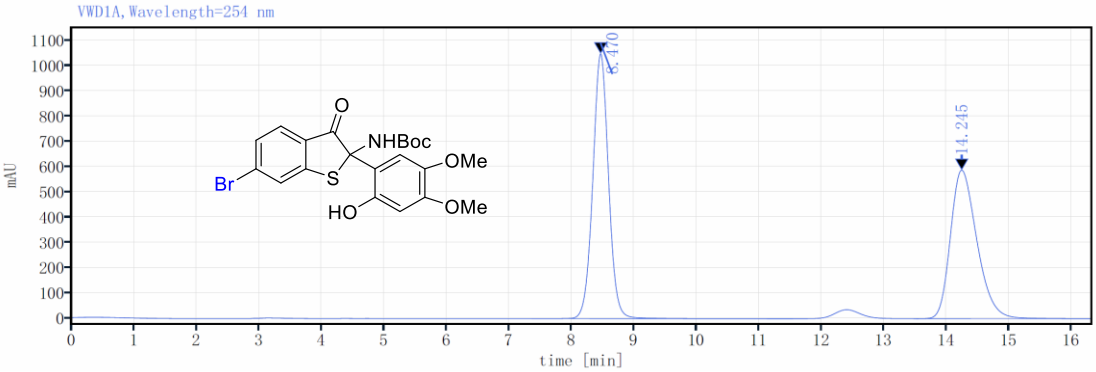
Peak	Ret.Time [min]	Area	Height	Area%
	8.113	19996.29	1220.38	94.09
	11.387	1256.38	50.44	5.91
		21252.67		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 5h



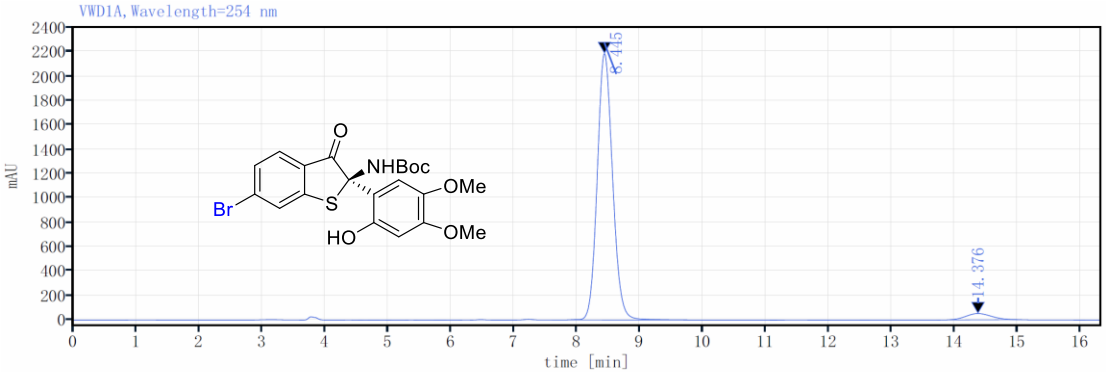


HPLC of 5h



Detector VWD1A, Wavelength=254 nm

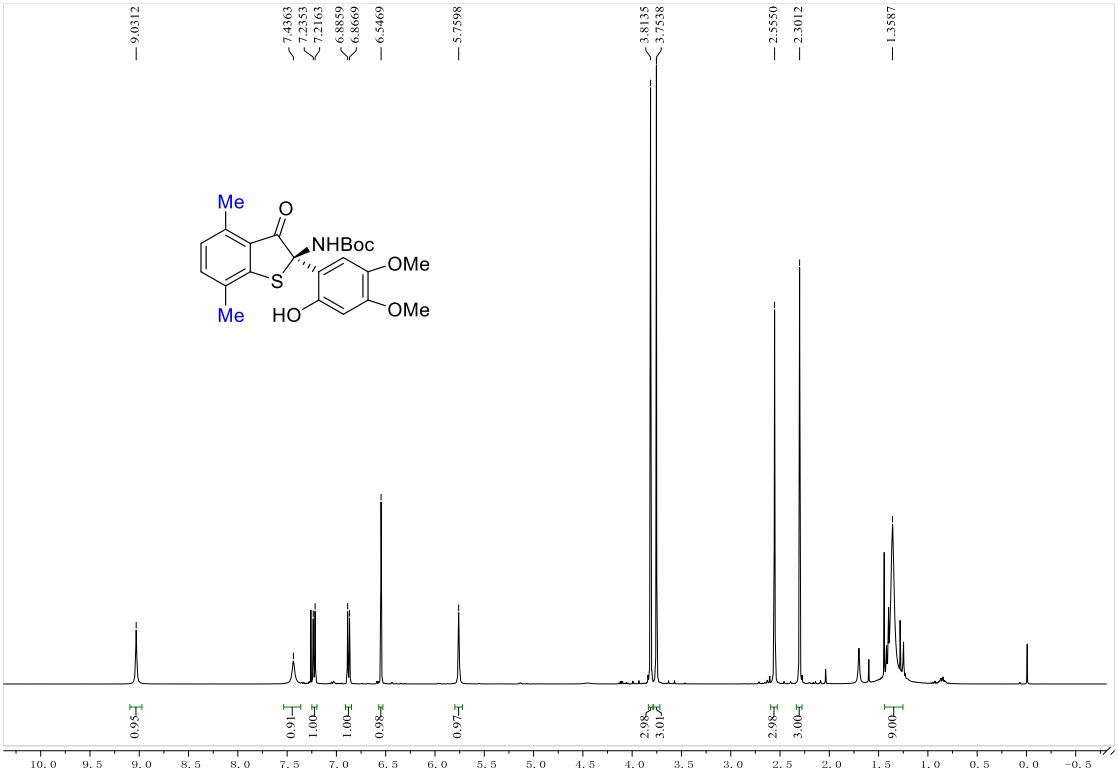
Peak	Ret.Time [min]	Area	Height	Area%
	8.470	18334.78	1047.47	51.47
	14.245	17284.59	587.40	48.53
		35619.37		100.00

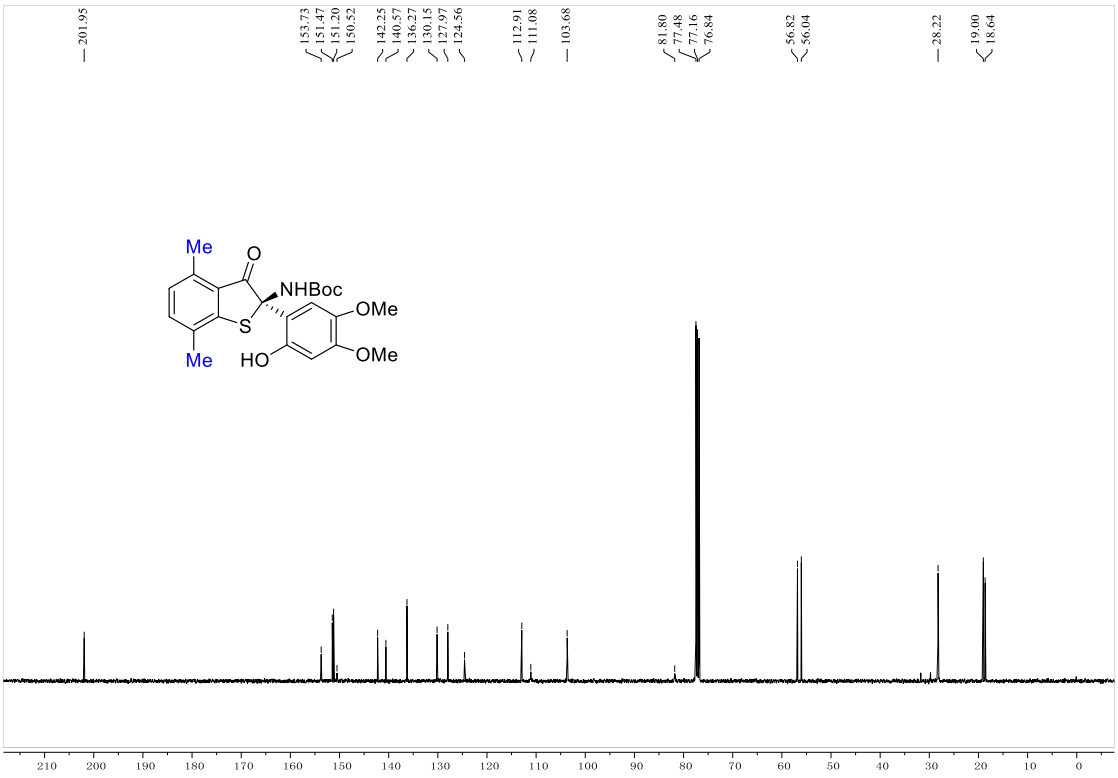


Detector VWD1A, Wavelength=254 nm

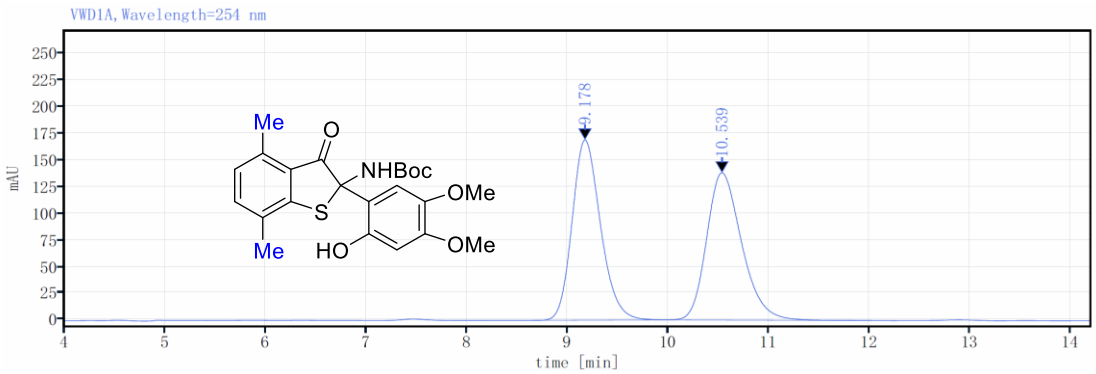
Peak	Ret.Time [min]	Area	Height	Area%
	8.445	37101.20	2189.15	96.20
	14.376	1464.54	51.61	3.80
		38565.73		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5i



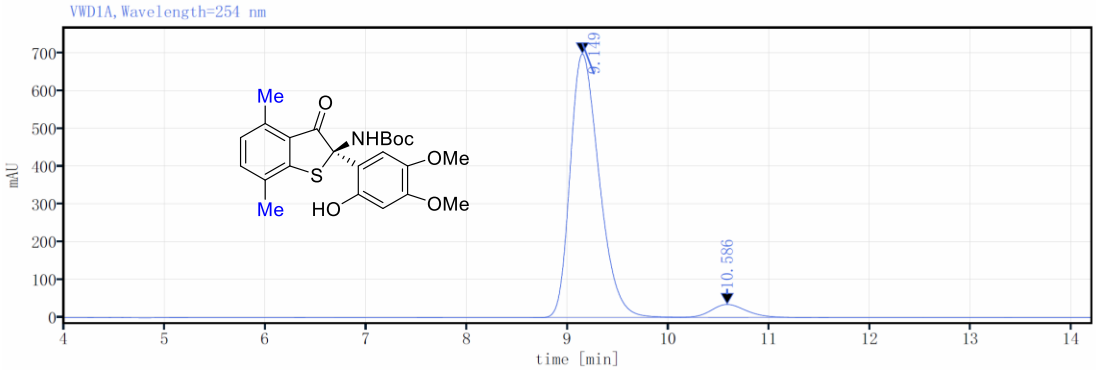


HPLC of 5i



Detector VWD1A, Wavelength=254 nm

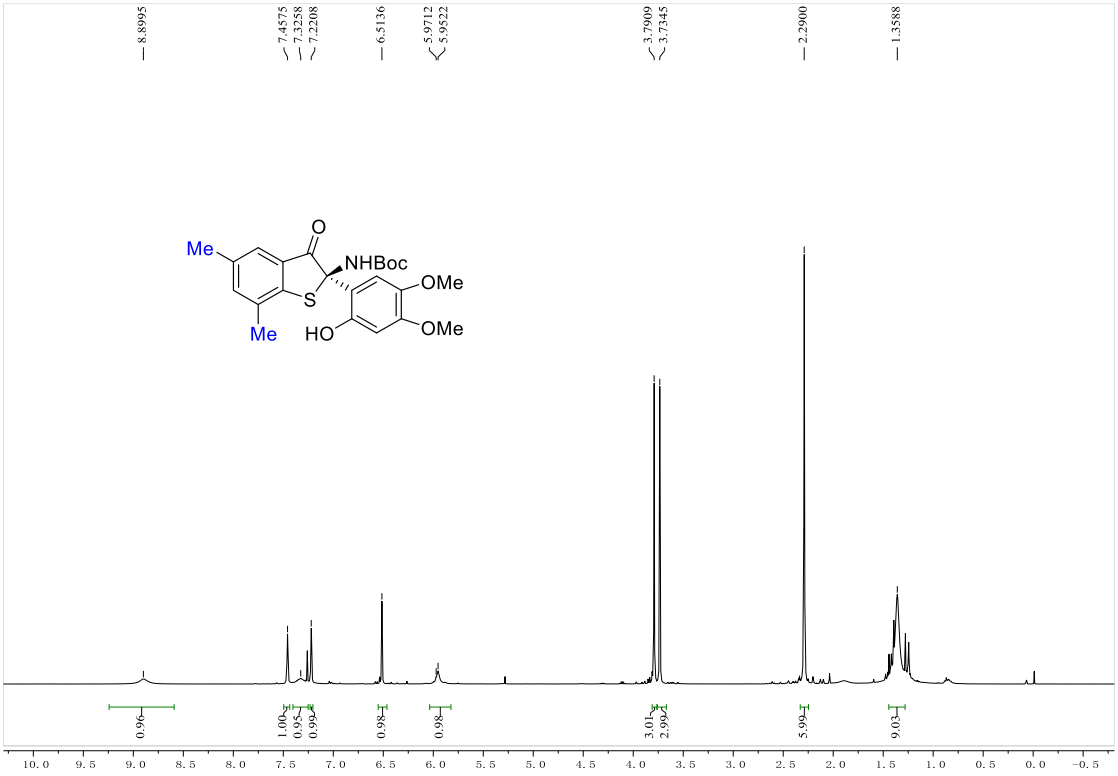
Peak	Ret.Time [min]	Area	Height	Area%
	9.178	3323.75	169.49	49.80
	10.539	3350.66	138.45	50.20
		6674.41		100.00

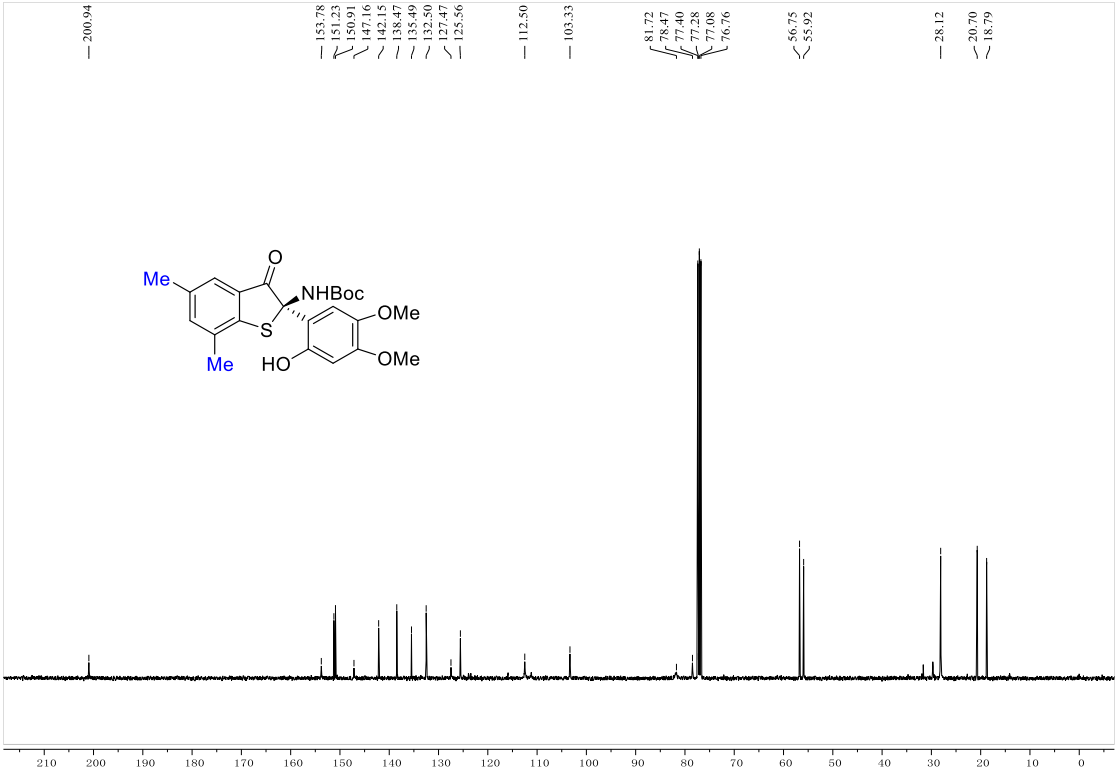


Detector VWD1A, Wavelength=254 nm

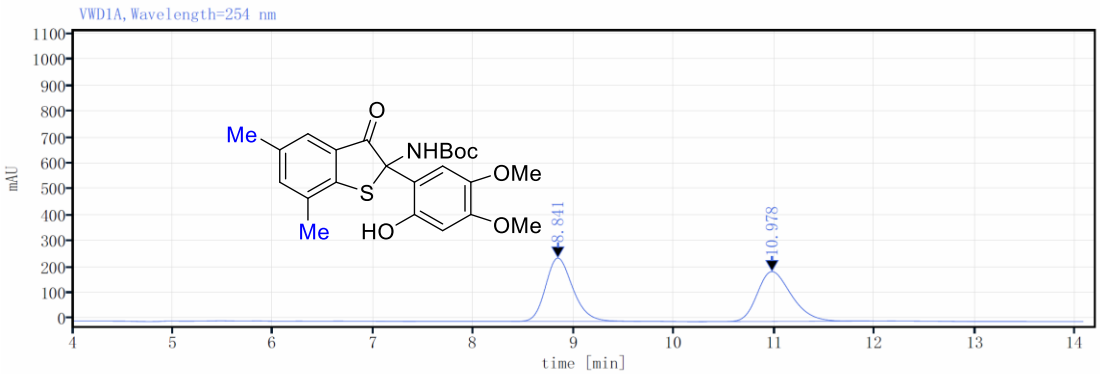
Peak	Ret.Time [min]	Area	Height	Area%
	9.149	14001.05	697.51	94.24
	10.586	856.04	34.73	5.76
		14857.09		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5j



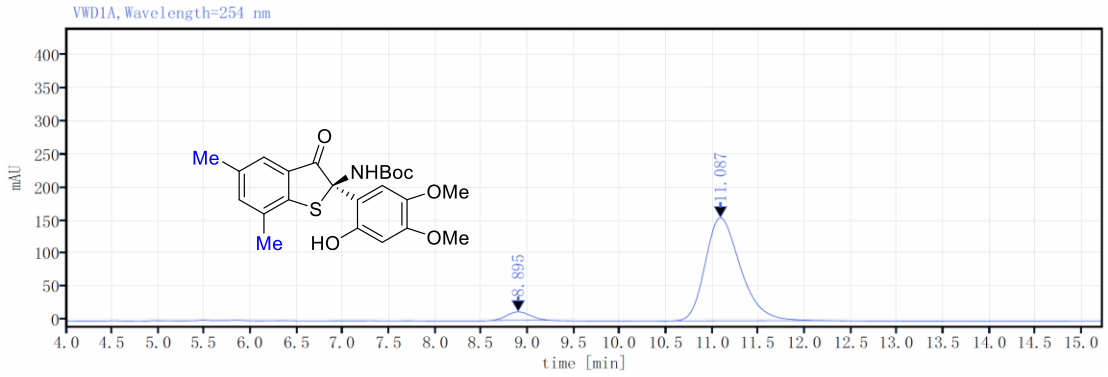


HPLC of 5j



Detector VWD1A, Wavelength=254 nm

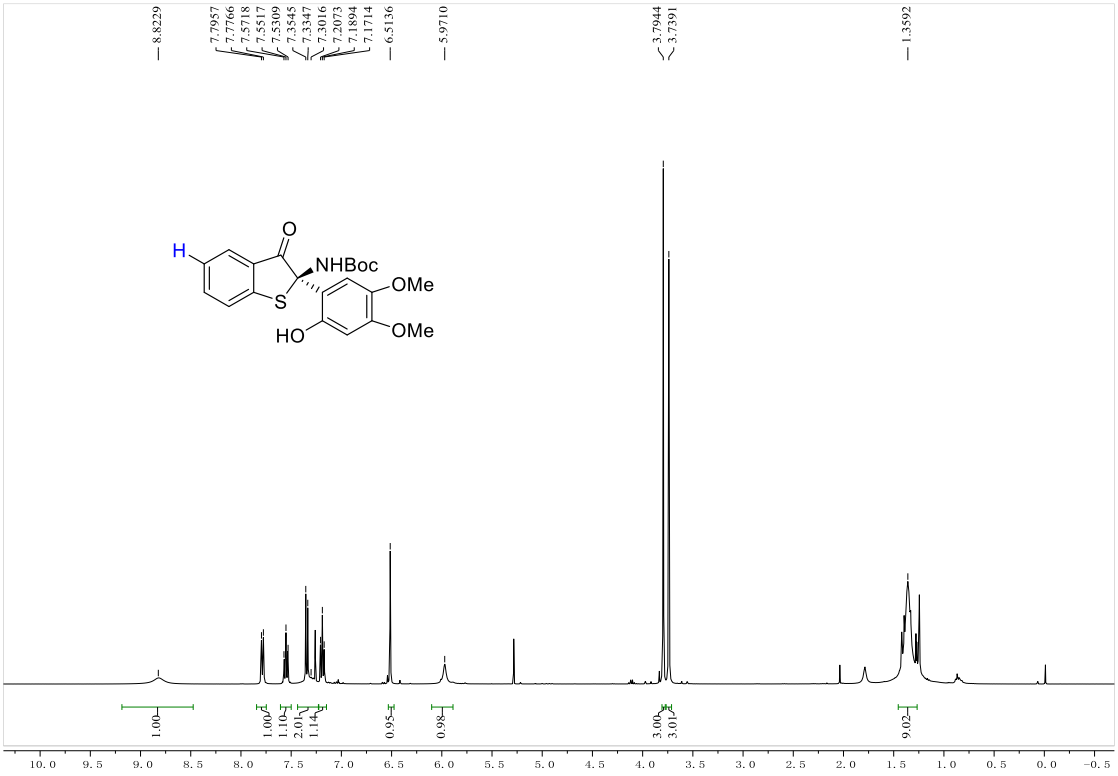
Peak	Ret.Time [min]	Area	Height	Area%
	8.841	4595.42	244.22	50.30
	10.978	4539.95	192.31	49.70
		9135.36		100.00

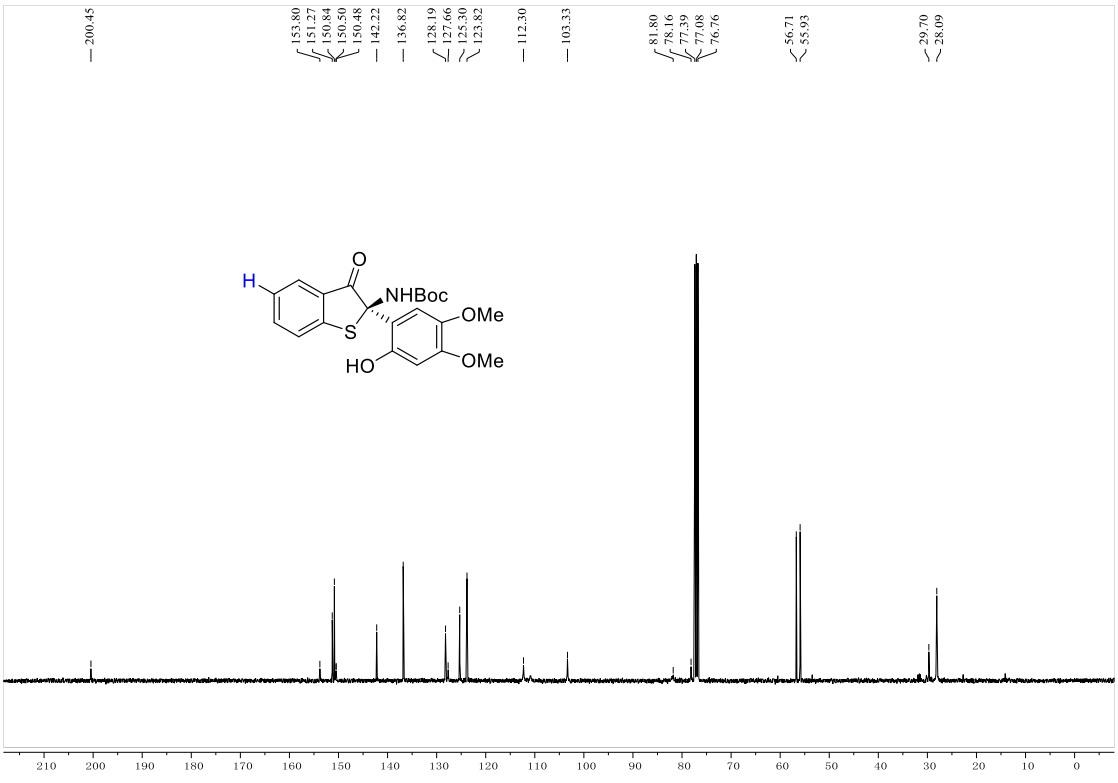


Detector VWD1A, Wavelength=254 nm

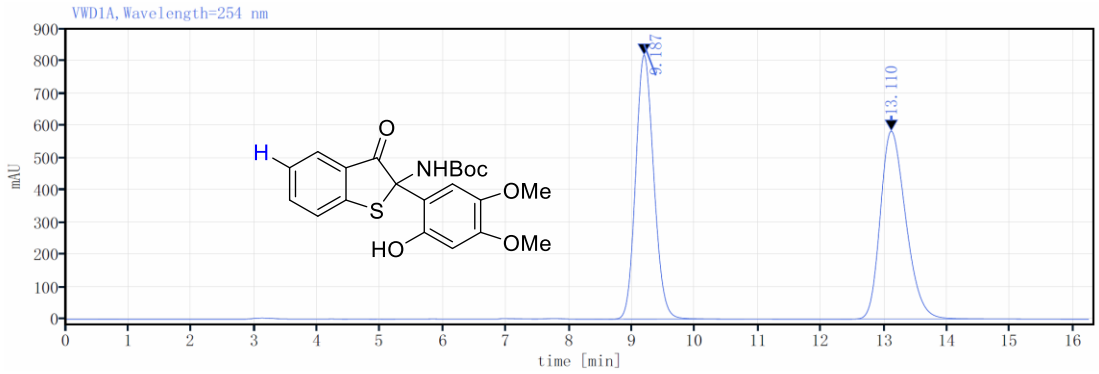
Peak	Ret.Time [min]	Area	Height	Area%
	8.895	232.70	13.04	5.33
	11.087	4136.84	155.57	94.67
		4369.54		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 5k



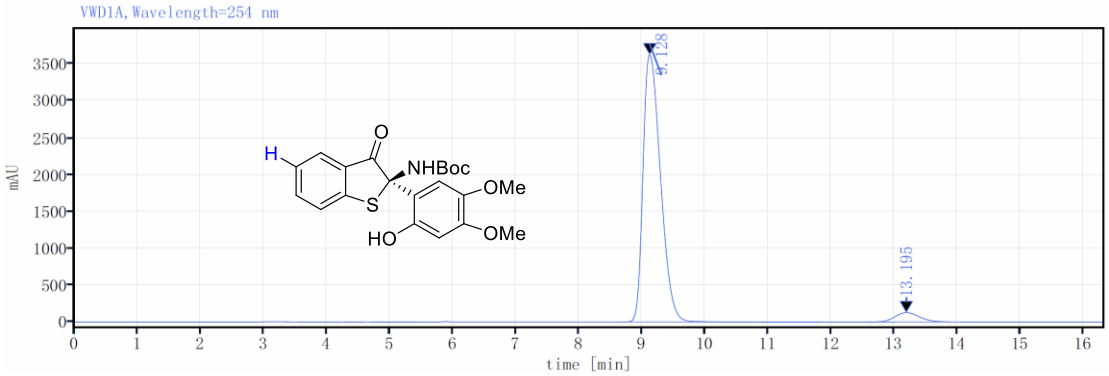


HPLC of 5k



Detector VWD1A, Wavelength=254 nm

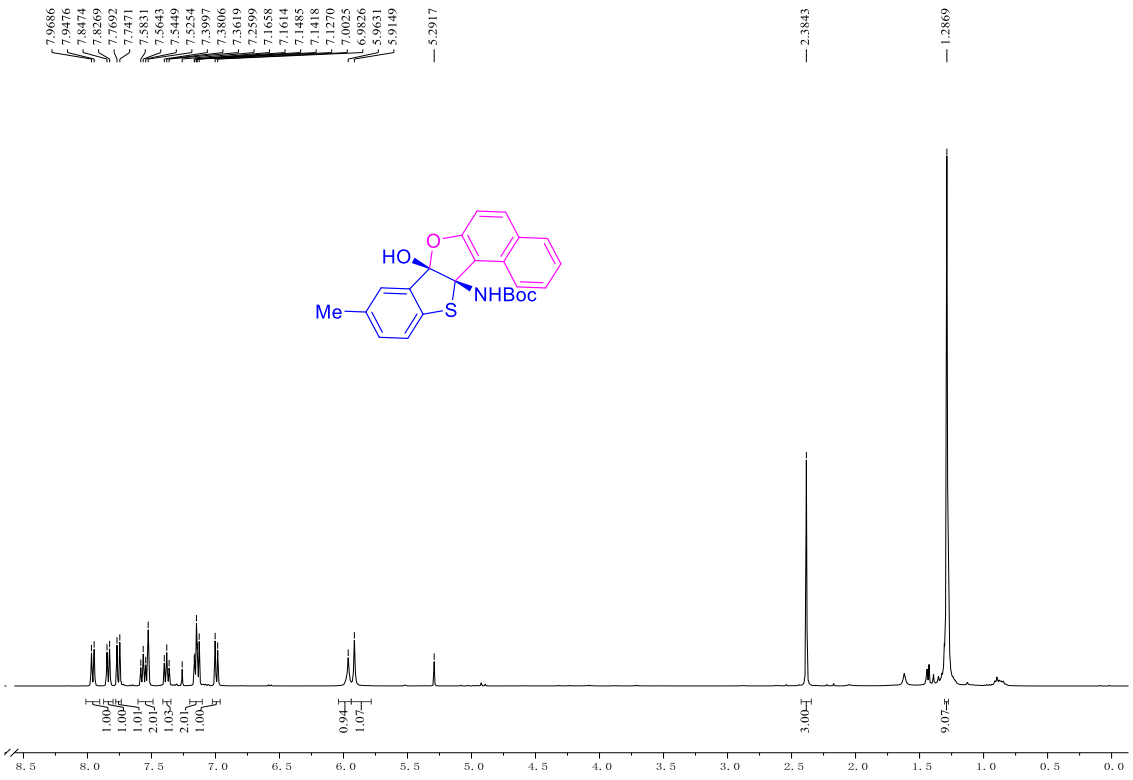
Peak	Ret.Time [min]	Area	Height	Area%
	9.187	16399.74	820.16	49.87
	13.110	16485.07	584.26	50.13
		32884.81		100.00

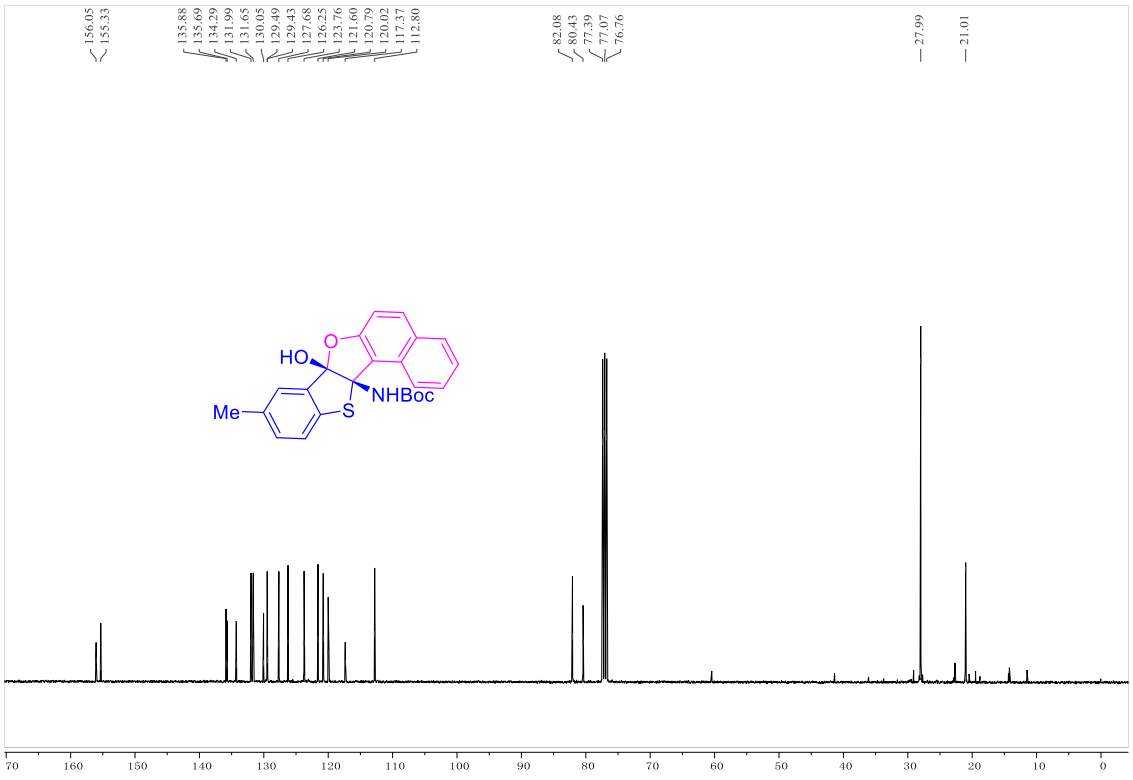


Detector VWD1A, Wavelength=254 nm

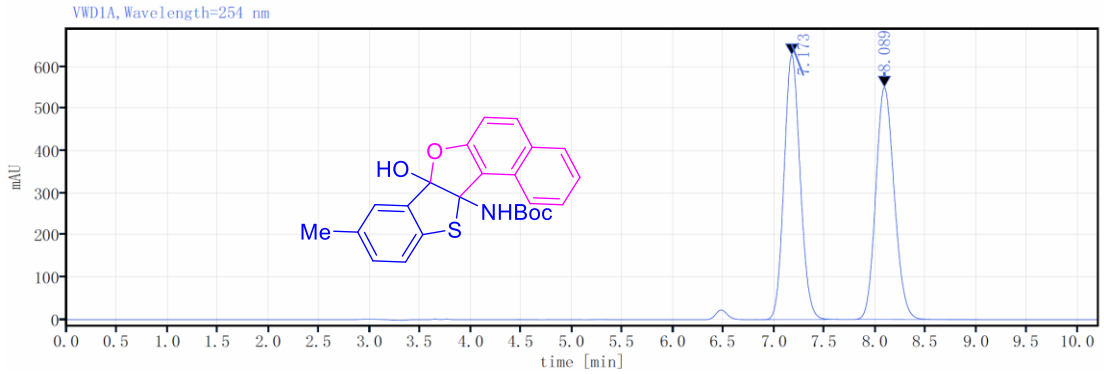
Peak	Ret.Time [min]	Area	Height	Area%
	9.128	69843.13	3631.14	95.27
	13.195	3467.60	127.78	4.73
		73310.73		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 7a



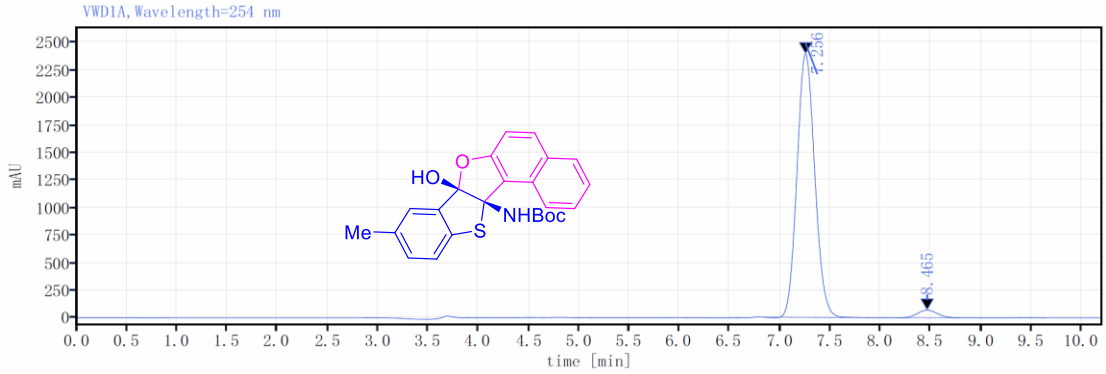


HPLC of 7a



Detector VWD1A, Wavelength=254 nm

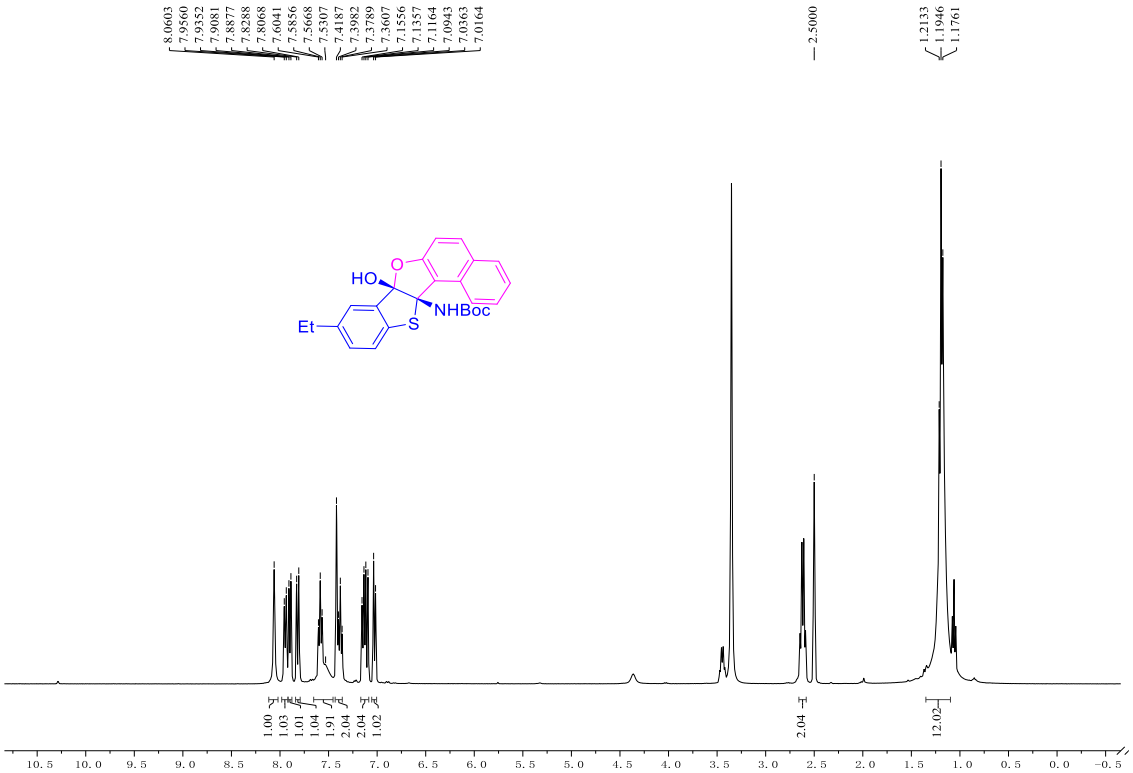
Peak	Ret.Time [min]	Area	Height	Area%
	7.173	6971.77	626.95	49.92
	8.089	6993.43	550.13	50.08
		13965.20		100.00

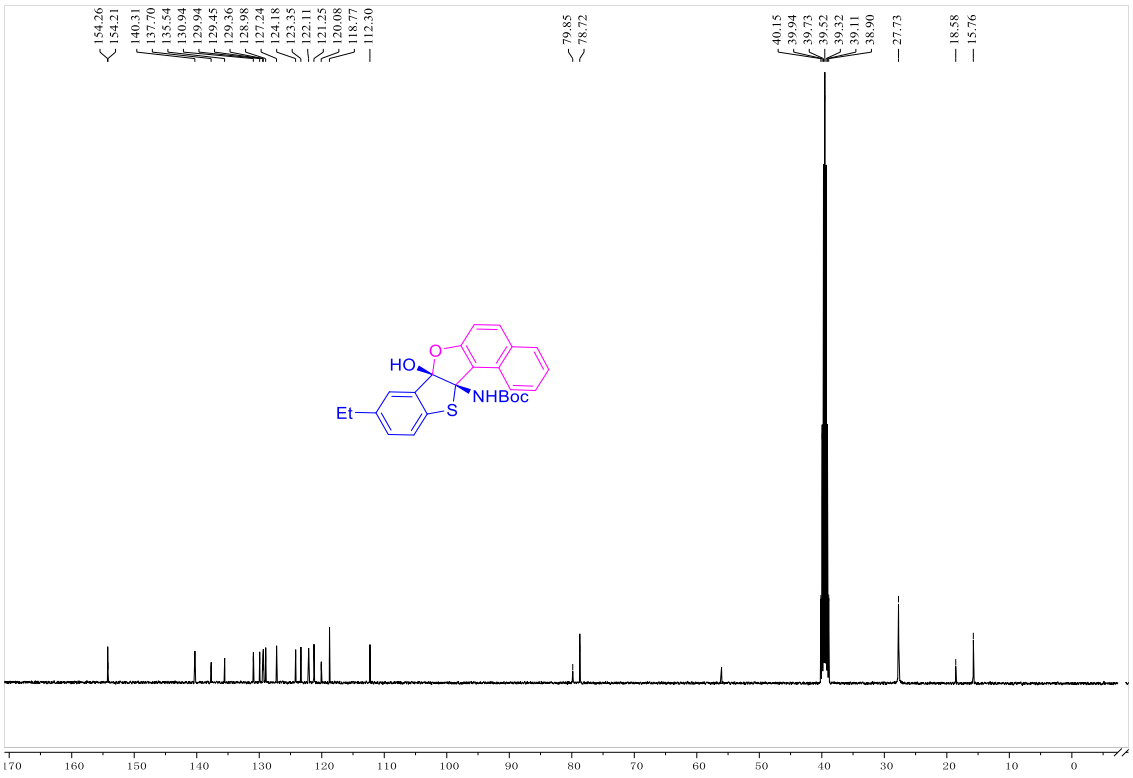


Detector VWD1A, Wavelength=254 nm

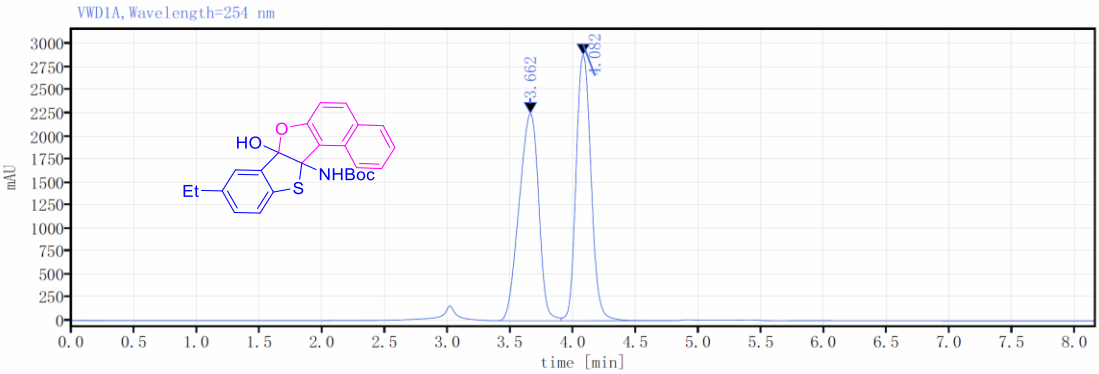
Peak	Ret.Time [min]	Area	Height	Area%
	7.256	29530.62	2396.96	96.80
	8.465	977.35	70.58	3.20
		30507.96		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7b



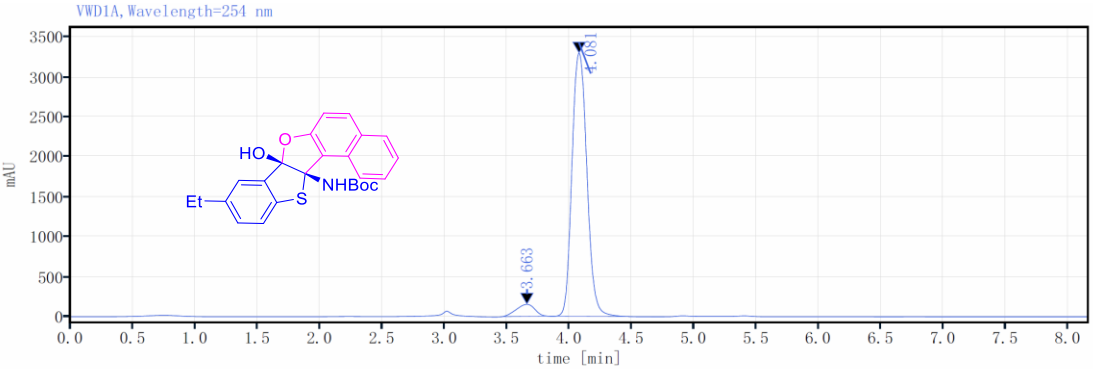


HPLC of 7b



Detector VWD1A, Wavelength=254 nm

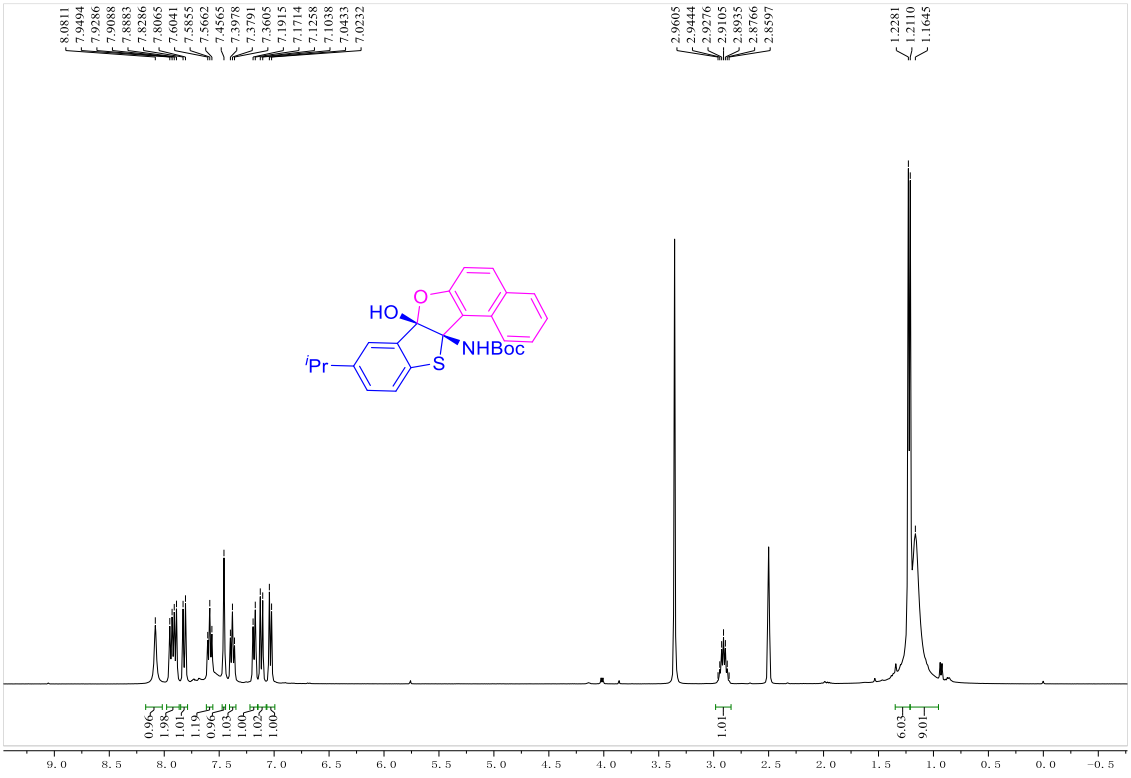
Peak	Ret.Time [min]	Area	Height	Area%
	3.662	24372.49	2248.72	50.44
	4.082	23945.58	2884.27	49.56
		48318.07		100.00

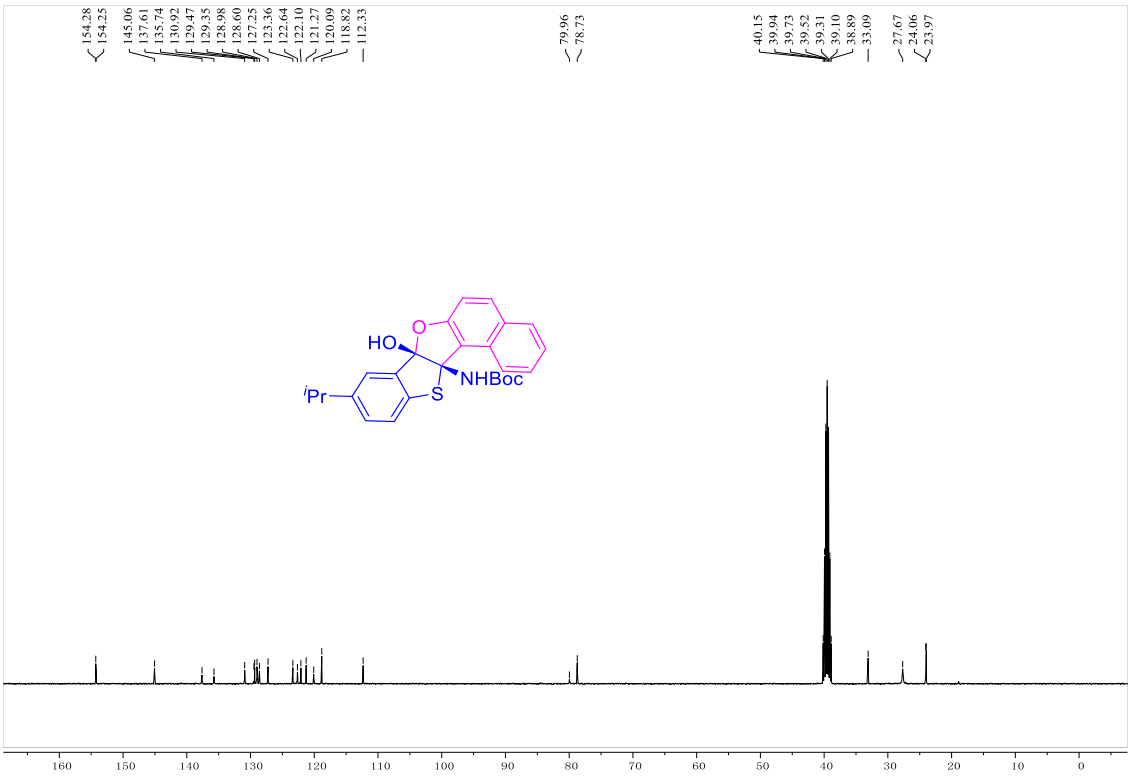


Detector VWD1A, Wavelength=254 nm

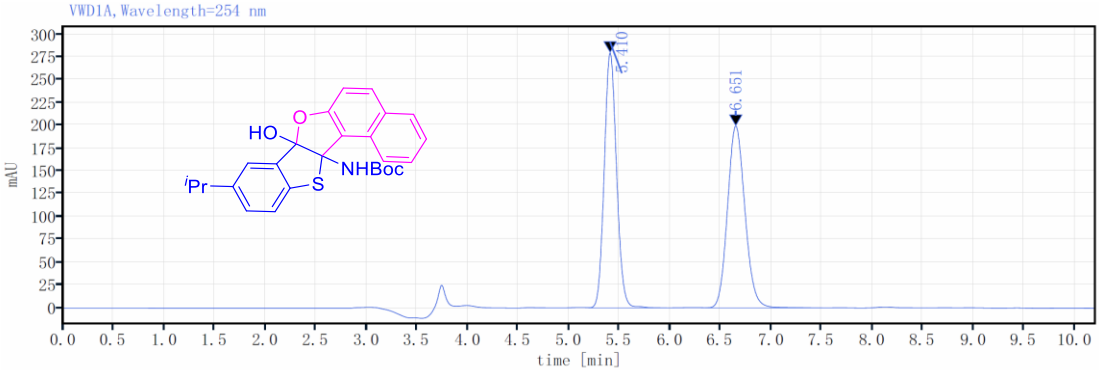
Peak	Ret.Time [min]	Area	Height	Area%
	3.663	1548.12	150.02	5.33
	4.081	27479.66	3296.84	94.67
		29027.79		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7c



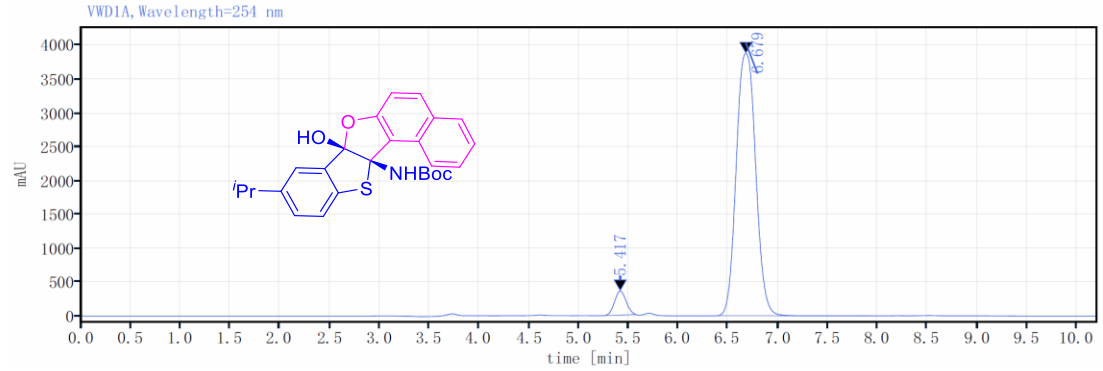


HPLC of 7c



Detector VWD1A, Wavelength=254 nm

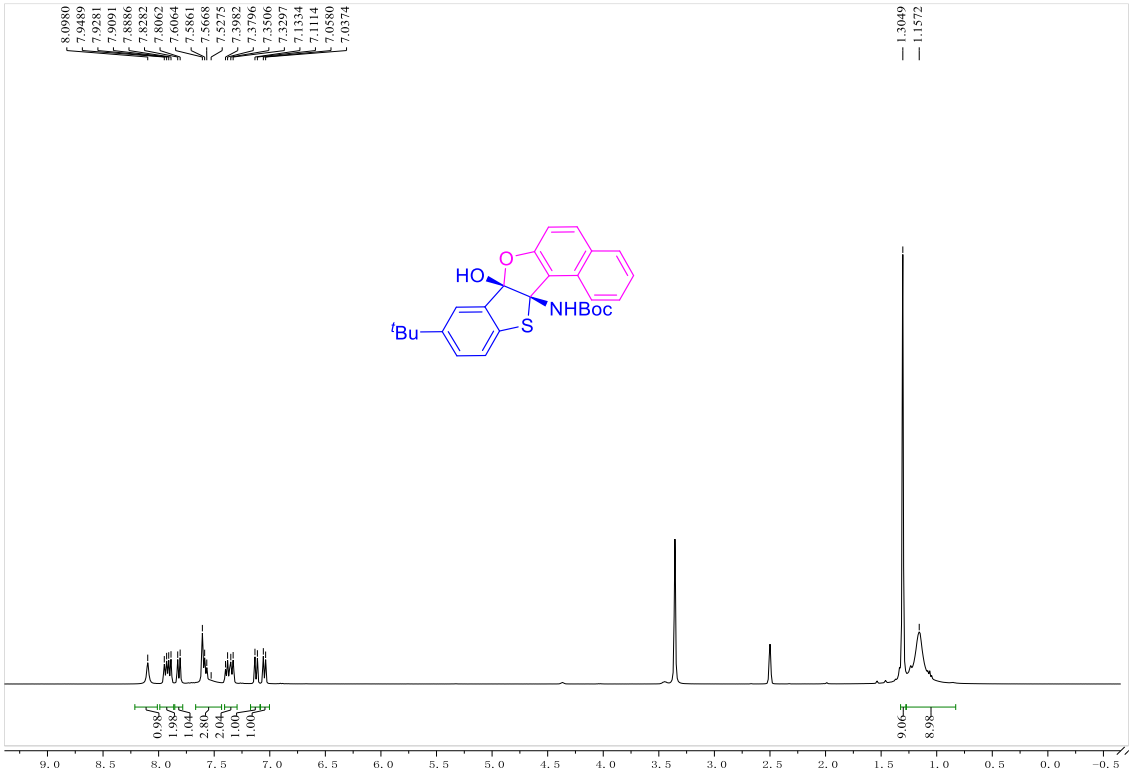
Peak	Ret.Time [min]	Area	Height	Area%
	5.410	2365.26	279.71	49.74
	6.651	2390.23	199.39	50.26
		4755.48		100.00

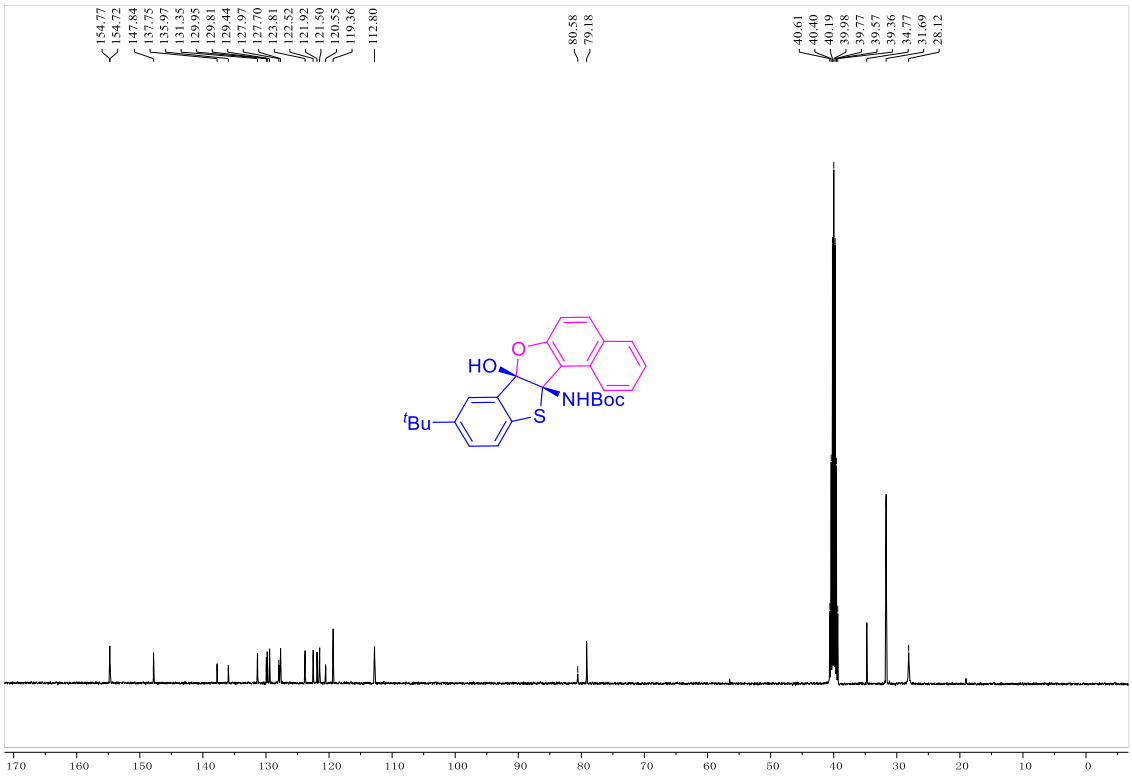


Detector VWD1A, Wavelength=254 nm

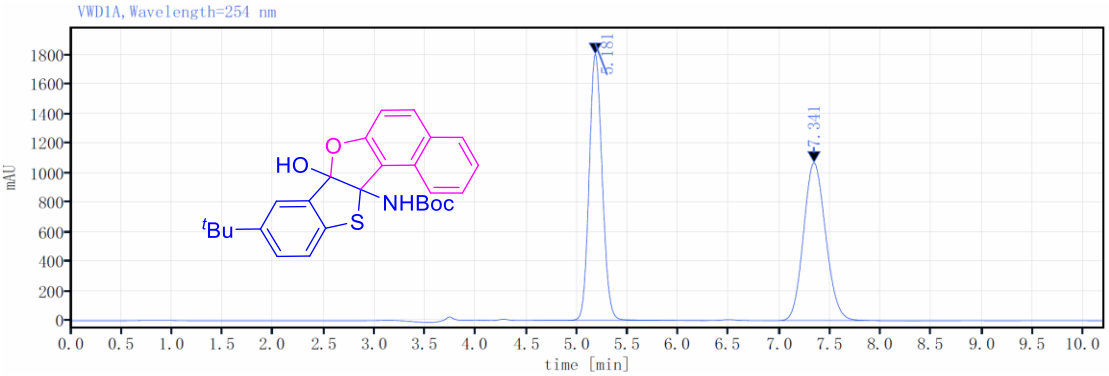
Peak	Ret.Time [min]	Area	Height	Area%
	5.417	2883.71	356.77	5.19
	6.679	52723.77	3882.70	94.81
		55607.49		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7d



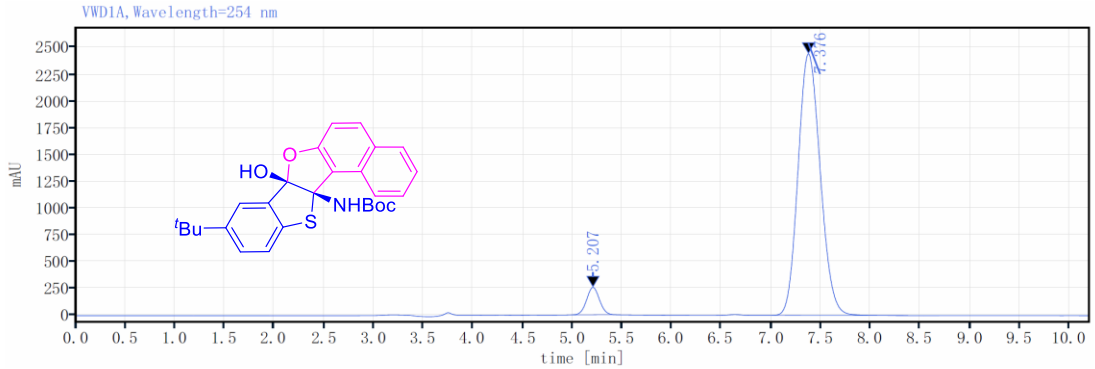


HPLC of 7d



Detector VWD1A, Wavelength=254 nm

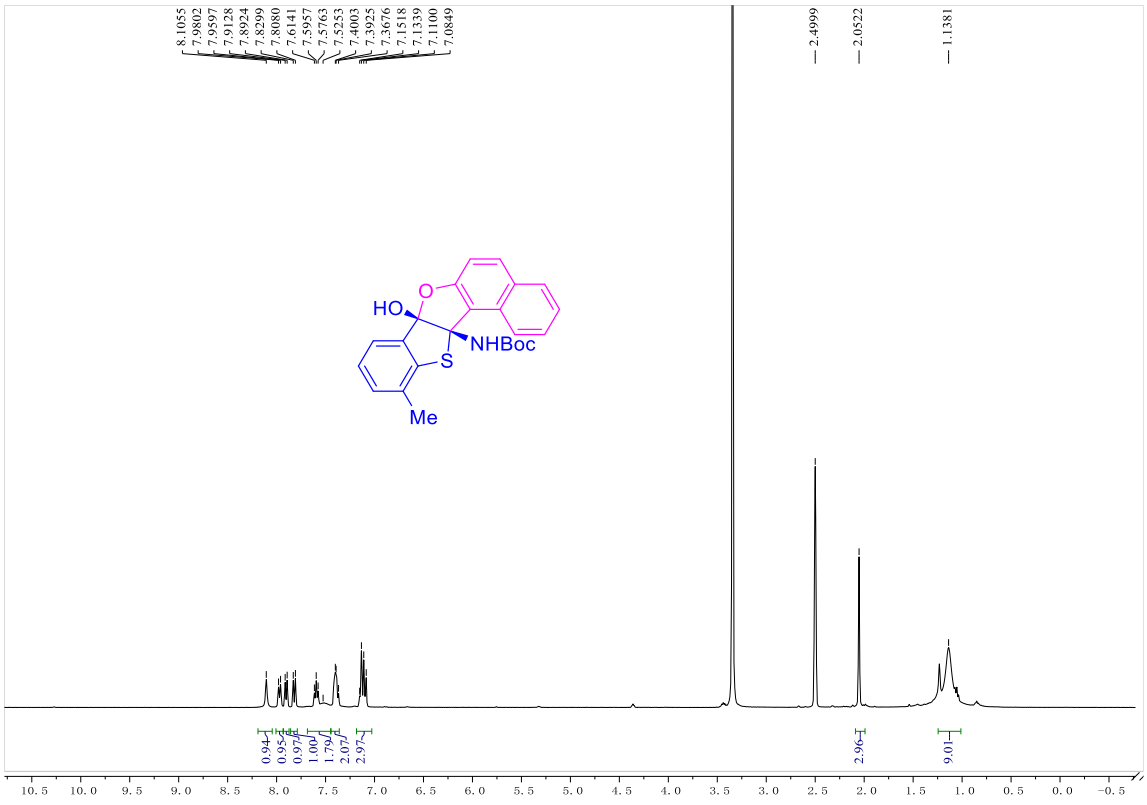
Peak	Ret.Time [min]	Area	Height	Area%
	5.181	16257.54	1805.69	49.91
	7.341	16314.68	1070.20	50.09
		32572.21		100.00

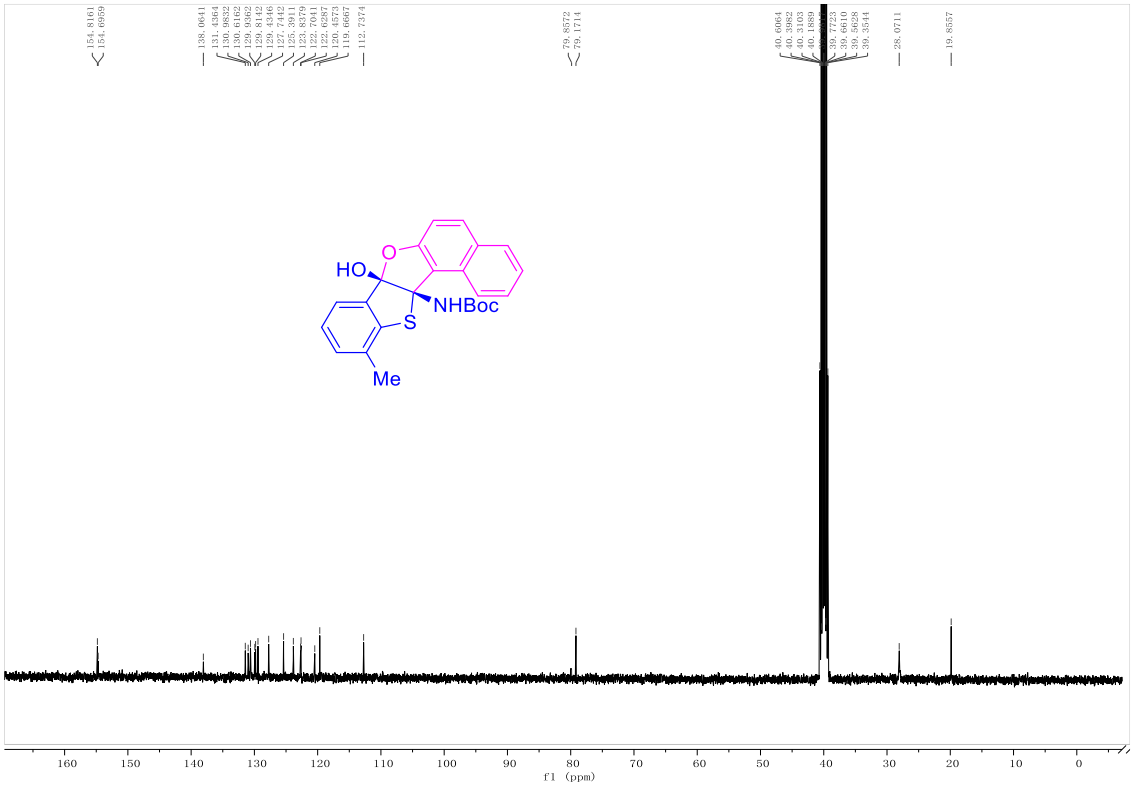


Detector VWD1A, Wavelength=254 nm

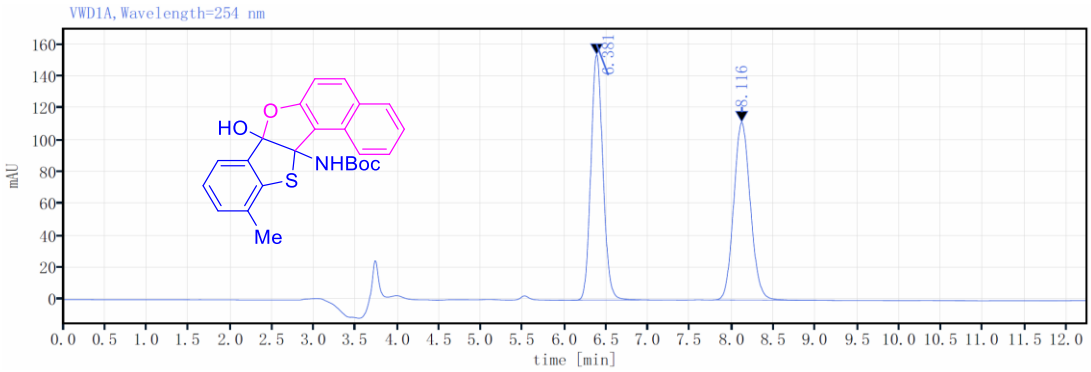
Peak	Ret.Time [min]	Area	Height	Area%
	5.207	2304.43	256.21	5.73
	7.376	37945.16	2442.01	94.27
		40249.59		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7e



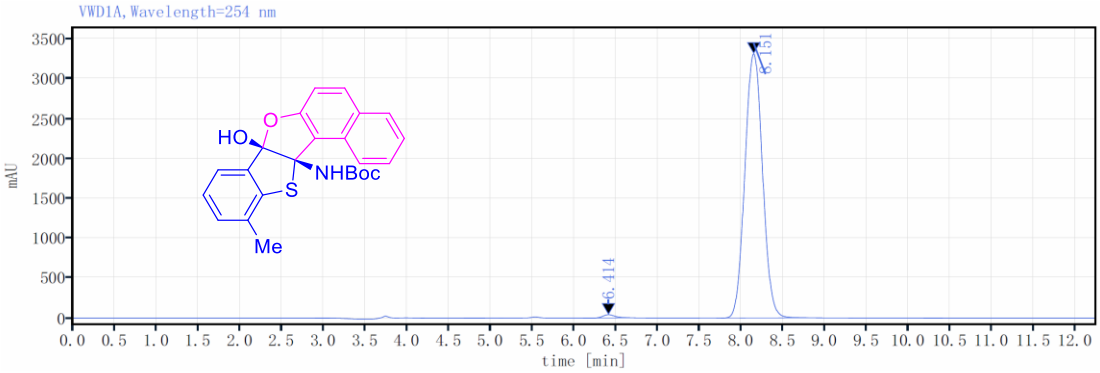


HPLC of 7e



Detector VWD1A, Wavelength=254 nm

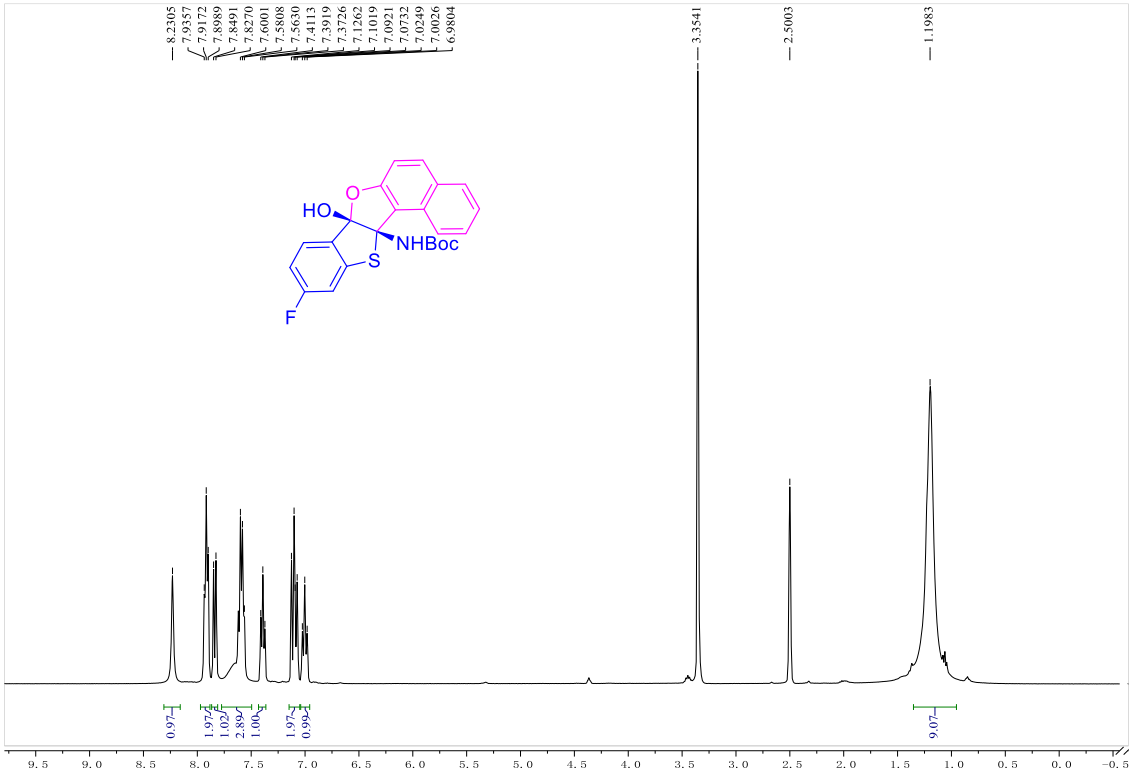
Peak	Ret.Time [min]	Area	Height	Area%
	6.381	1547.62	154.09	49.96
	8.116	1550.27	111.67	50.04
		3097.90		100.00

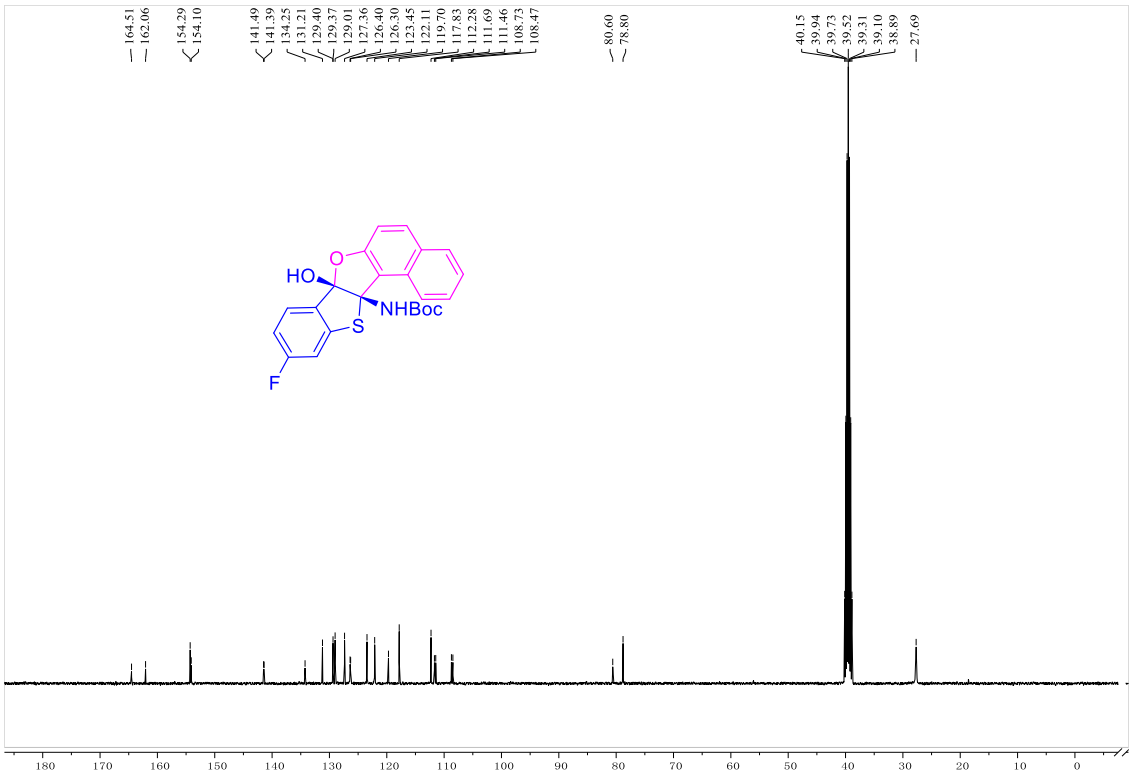


Detector VWD1A, Wavelength=254 nm

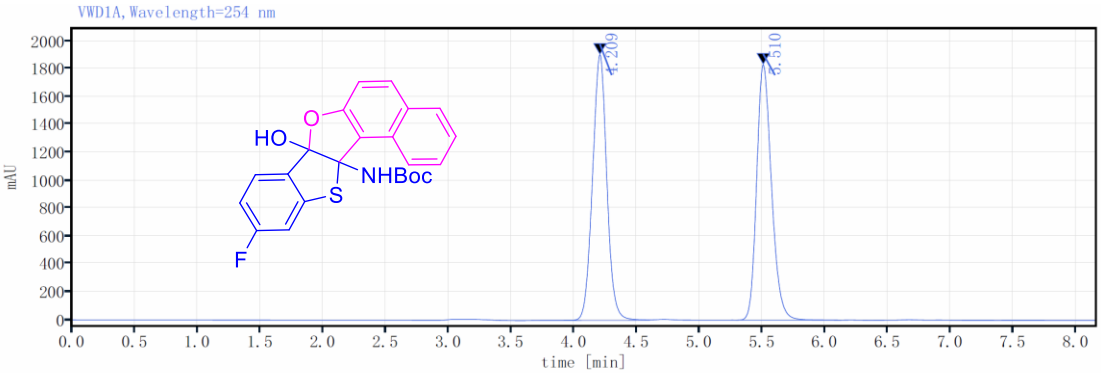
Peak	Ret.Time [min]	Area	Height	Area%
	6.414	399.08	40.00	0.81
	8.151	48861.68	3318.52	99.19
		49260.76		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7f



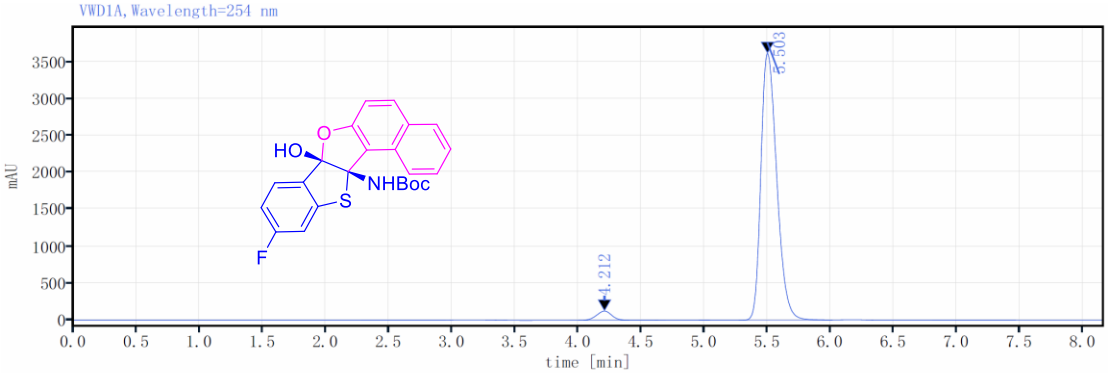


HPLC of 7f



Detector VWD1A, Wavelength=254 nm

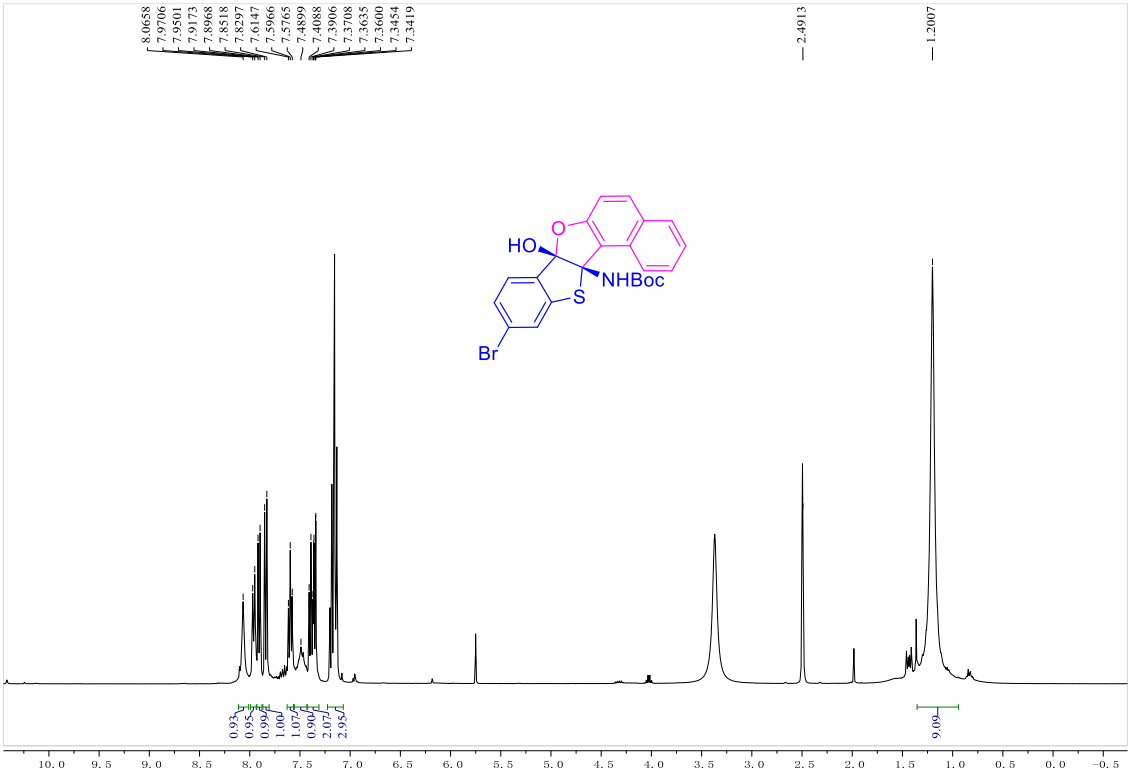
Peak	Ret.Time [min]	Area	Height	Area%
	4.209	15126.46	1905.51	50.07
	5.510	15087.07	1832.71	49.93
		30213.53		100.00

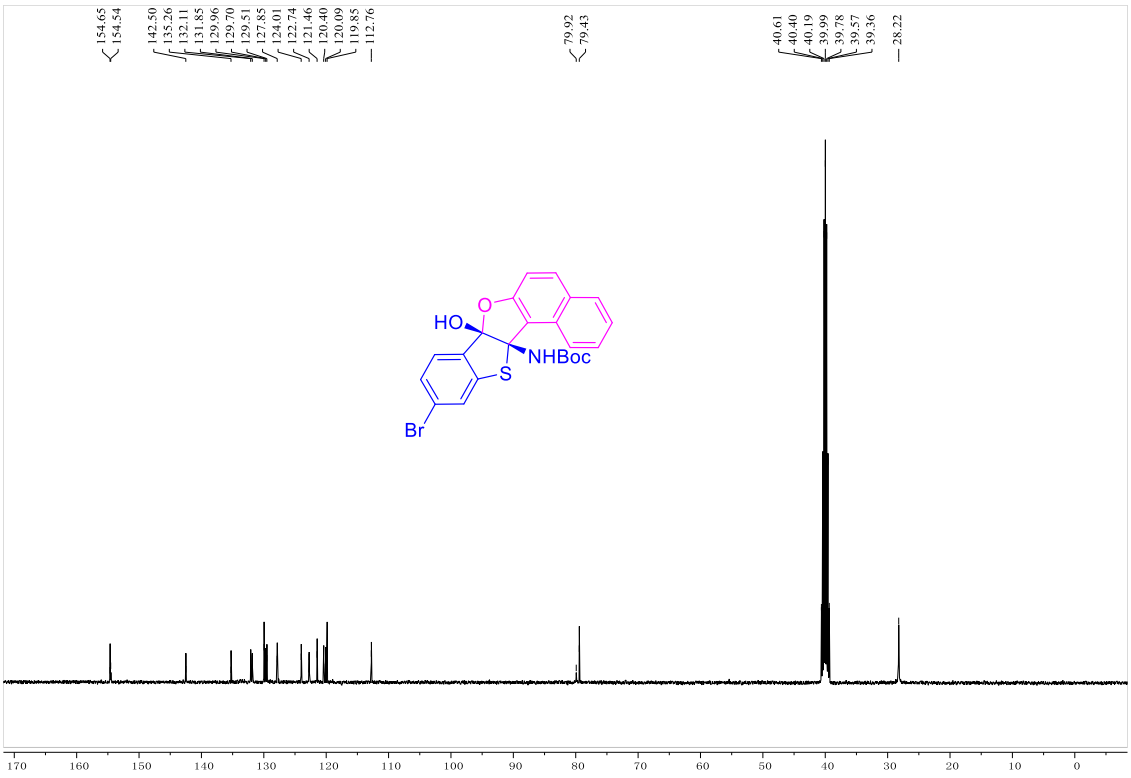


Detector VWD1A, Wavelength=254 nm

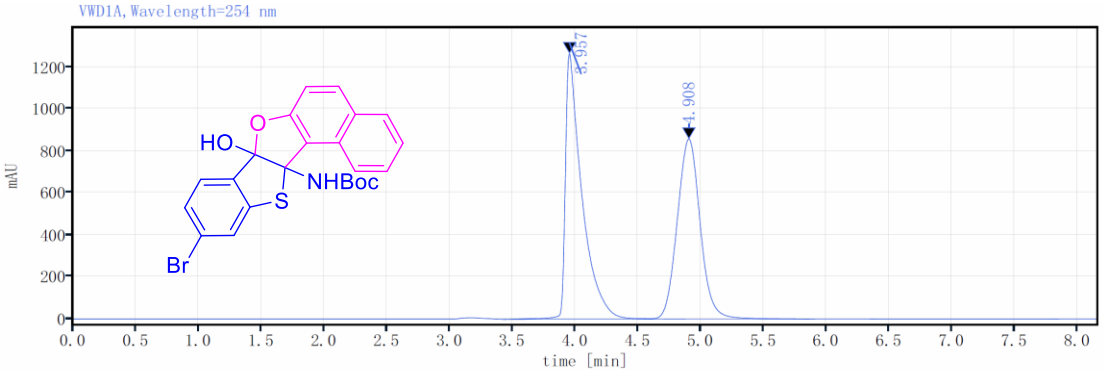
Peak	Ret.Time [min]	Area	Height	Area%
	4.212	1071.21	125.36	3.28
	5.503	31634.39	3616.18	96.72
		32705.60		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7g



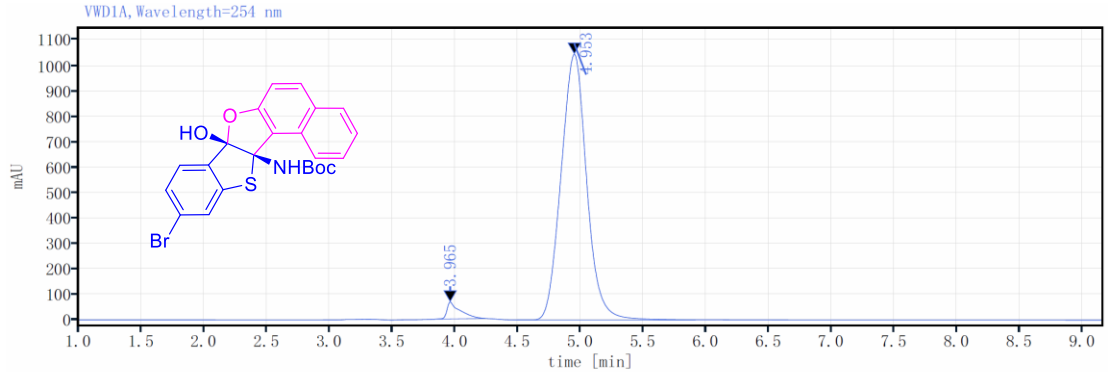


HPLC of 7g



Detector VWD1A, Wavelength=254 nm

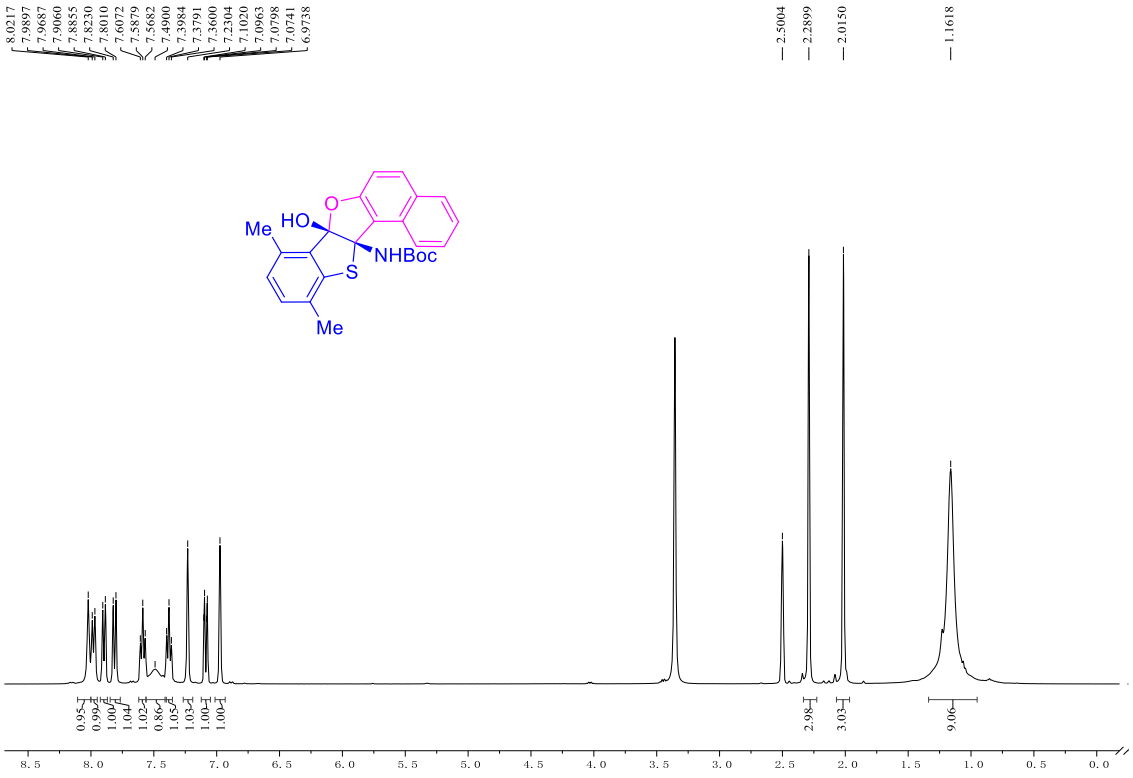
Peak	Ret.Time [min]	Area	Height	Area%
	3.957	11577.13	1268.15	51.36
	4.908	10964.28	859.90	48.64
		22541.40		100.00

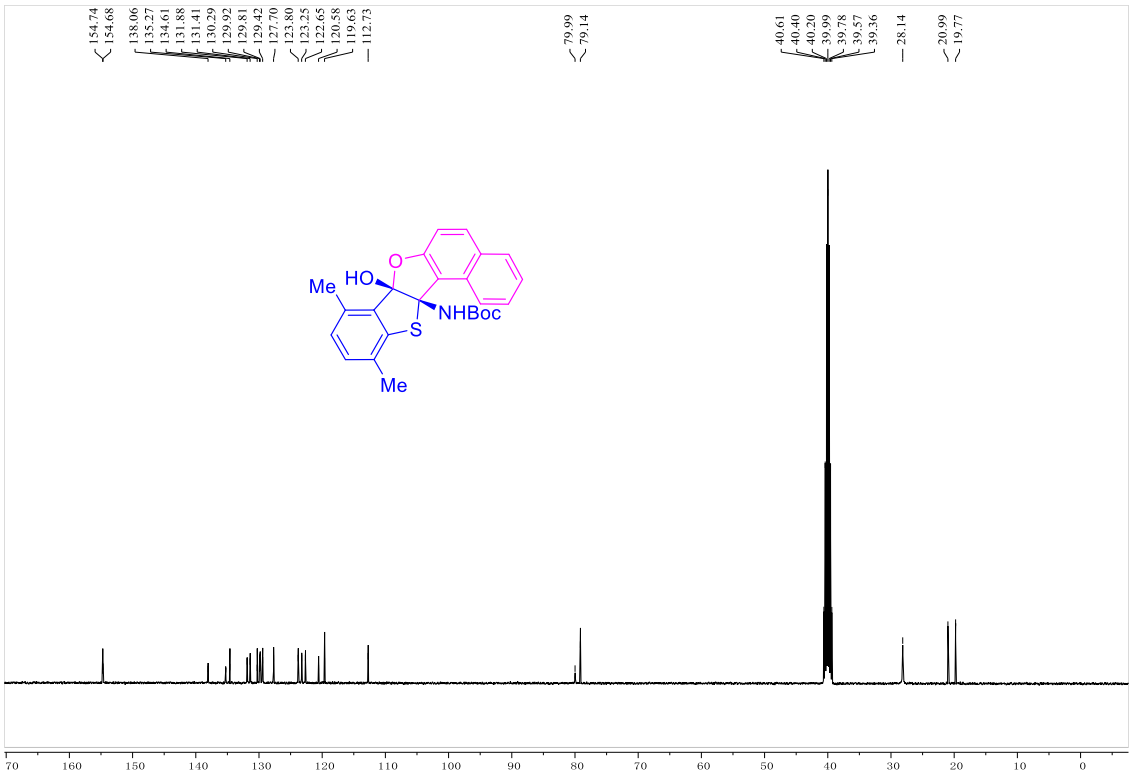


Detector VWD1A, Wavelength=254 nm

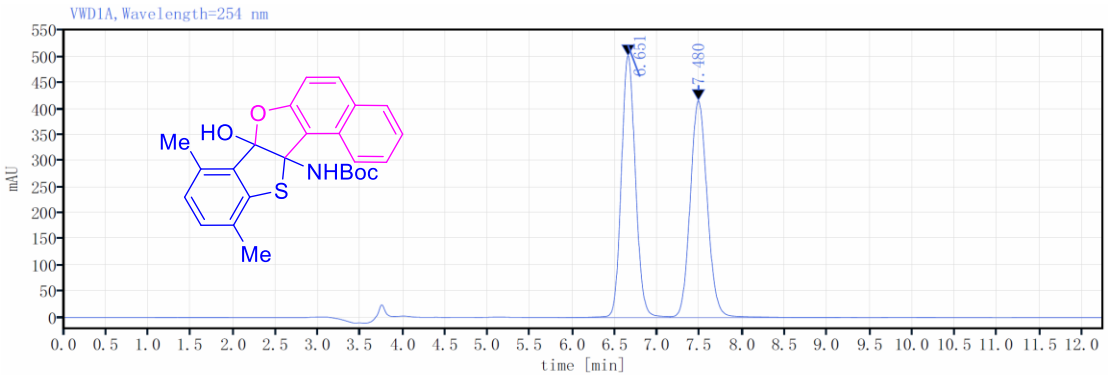
Peak	Ret.Time [min]	Area	Height	Area%
	3.965	484.24	67.05	3.15
	4.953	14868.95	1045.60	96.85
		15353.19		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7h



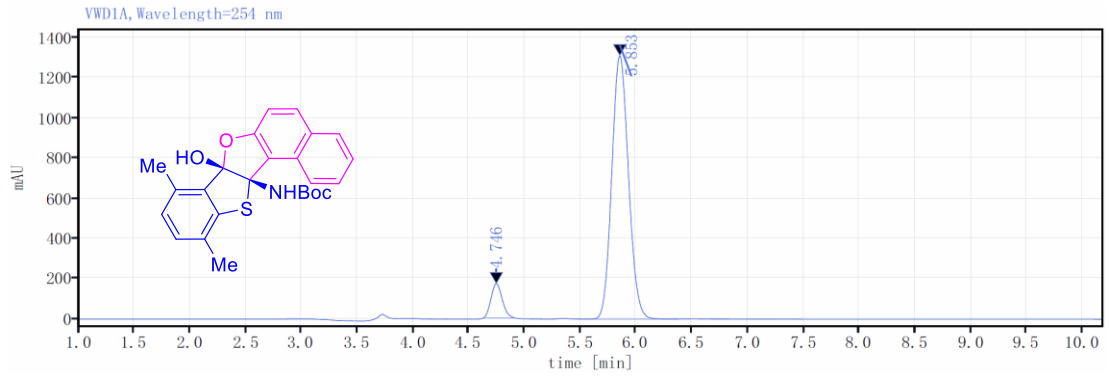


HPLC of 7h



Detector VWD1A, Wavelength=254 nm

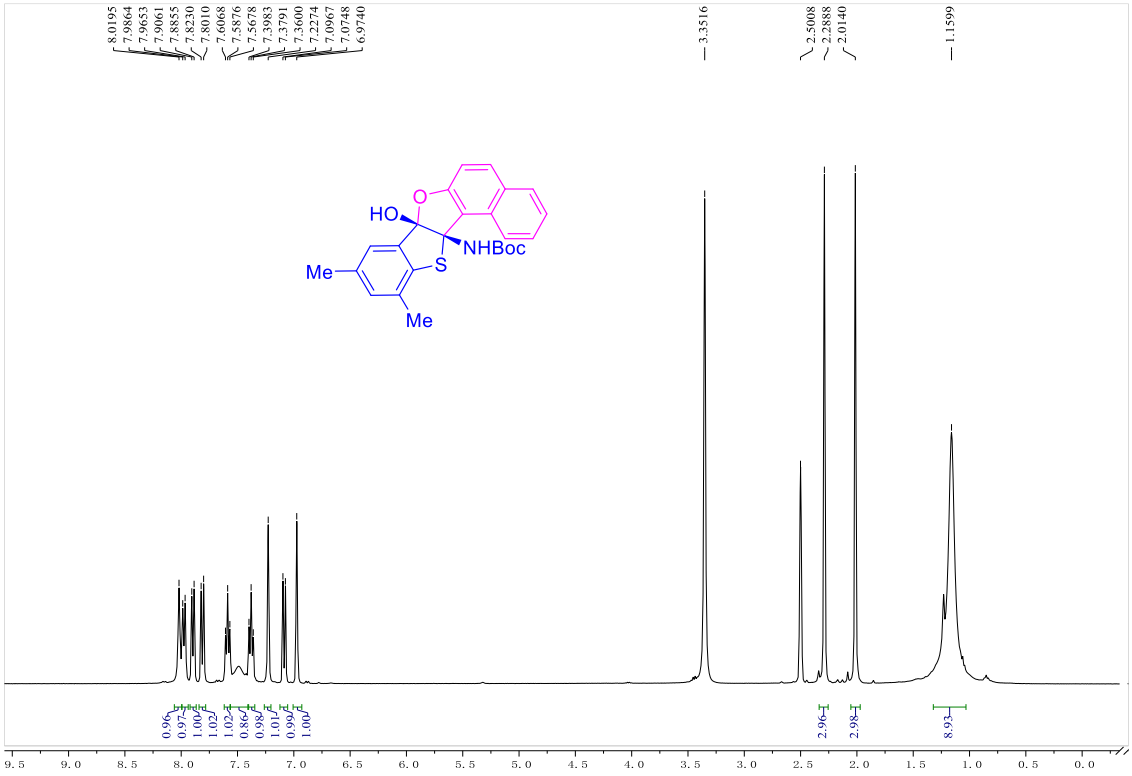
Peak	Ret.Time [min]	Area	Height	Area%
	6.651	5797.31	501.61	49.87
	7.480	5826.42	415.87	50.13
		11623.72		100.00

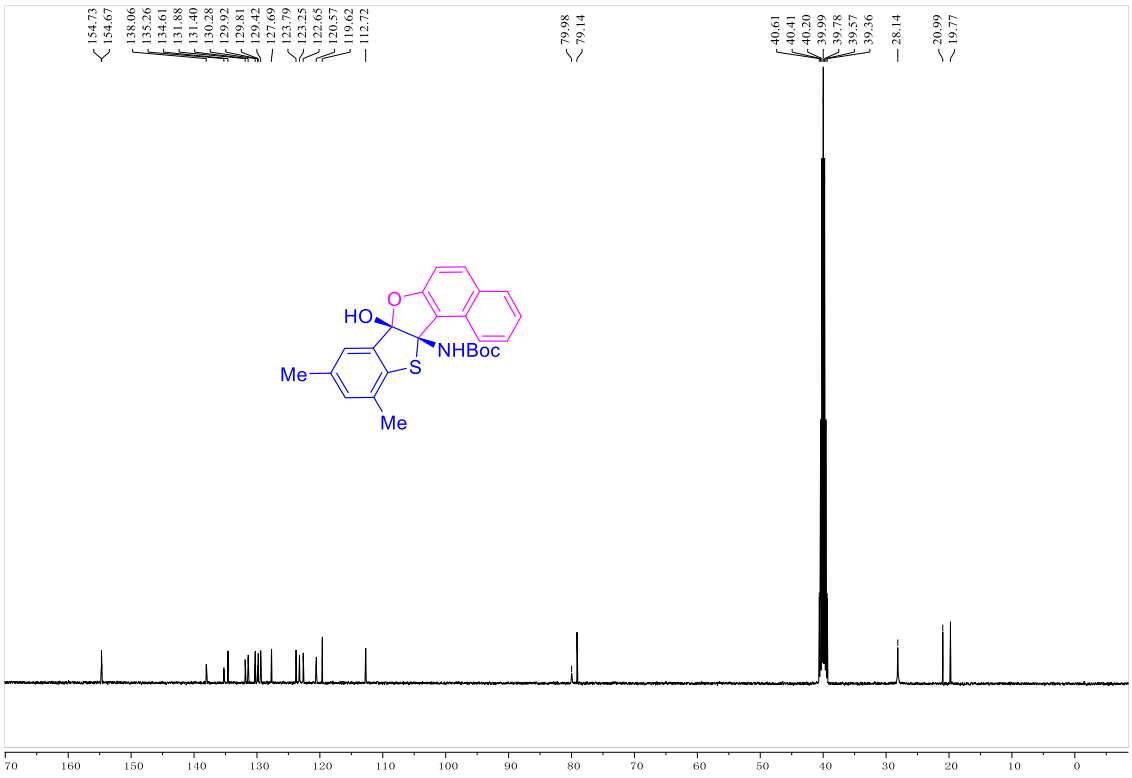


Detector VWD1A, Wavelength=254 nm

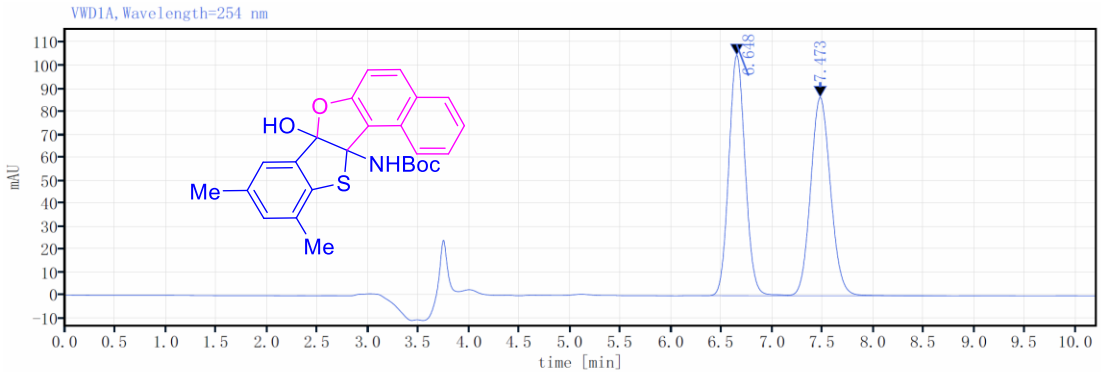
Peak	Ret.Time [min]	Area	Height	Area%
	4.746	1193.21	170.57	8.04
	5.853	13639.02	1310.42	91.96
		14832.24		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7i



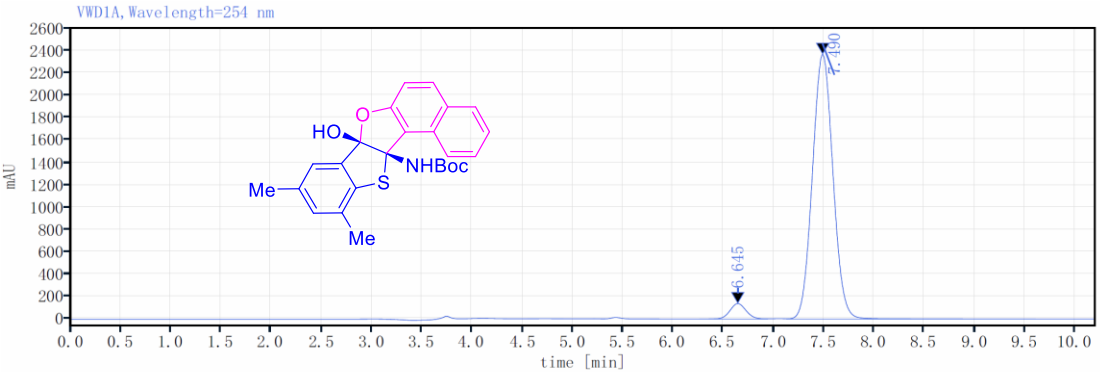


HPLC of 7i



Detector VWD1A, Wavelength=254 nm

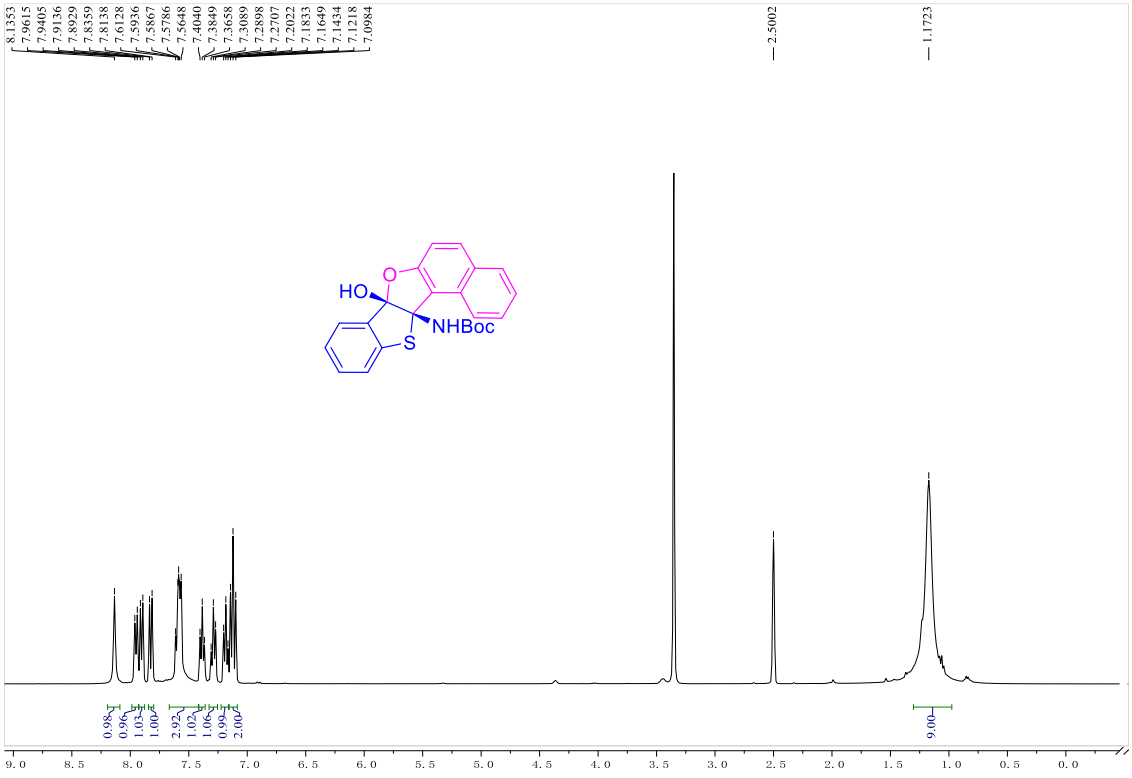
Peak	Ret.Time [min]	Area	Height	Area%
	6.648	1181.28	104.79	49.86
	7.473	1187.94	86.45	50.14
		2369.22		100.00

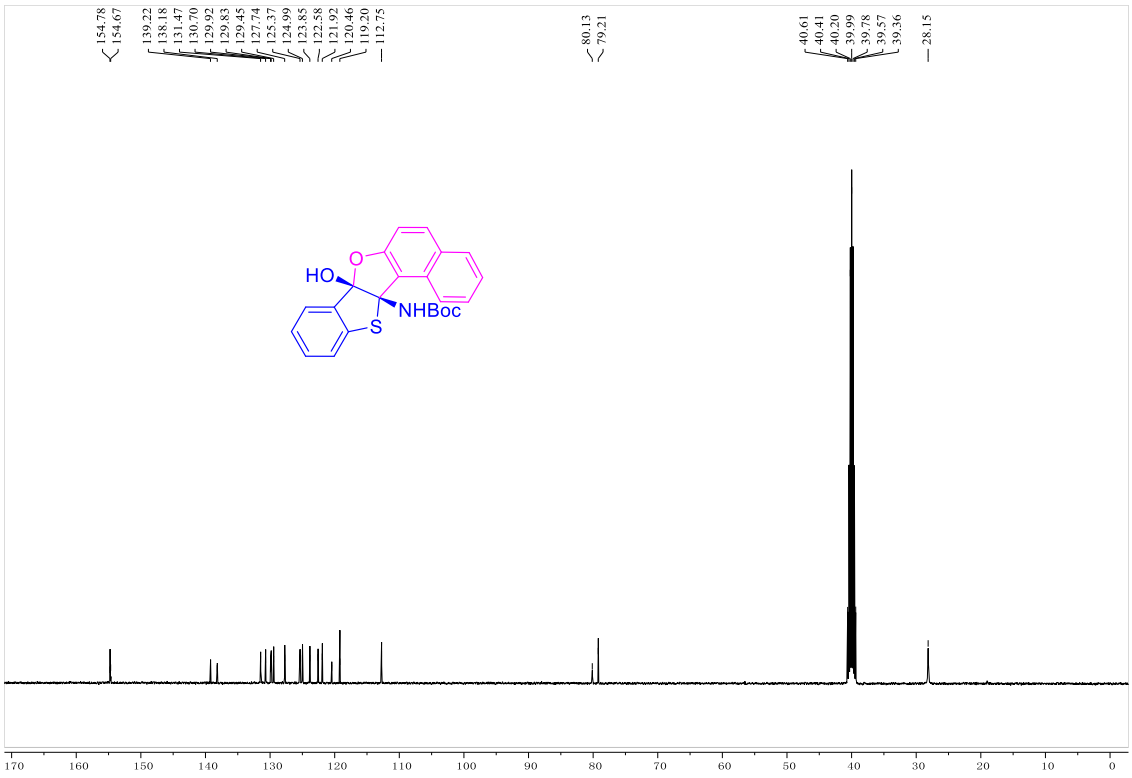


Detector VWD1A, Wavelength=254 nm

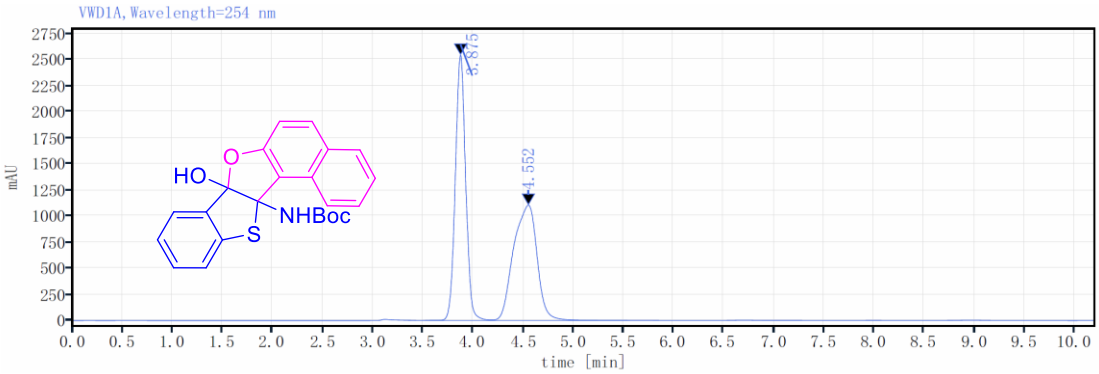
Peak	Ret.Time [min]	Area	Height	Area%
	6.645	1556.29	138.04	4.41
	7.490	33734.23	2365.11	95.59
		35290.52		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7j



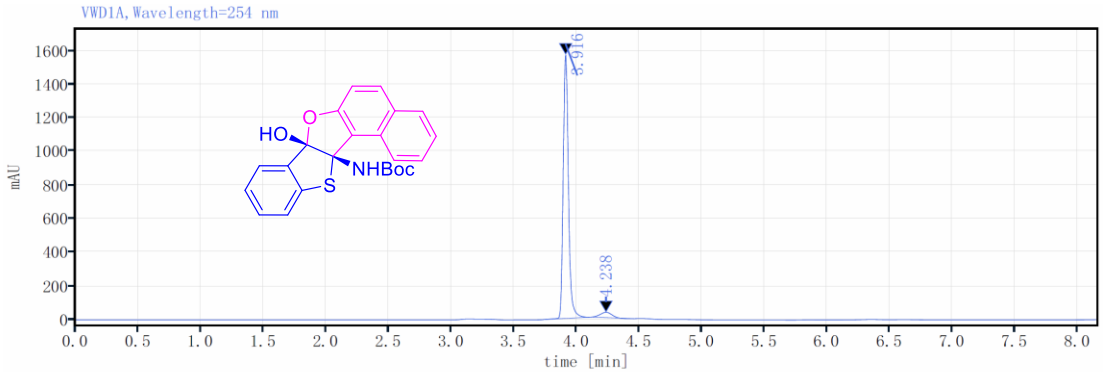


HPLC of 7j



Detector VWD1A, Wavelength=254 nm

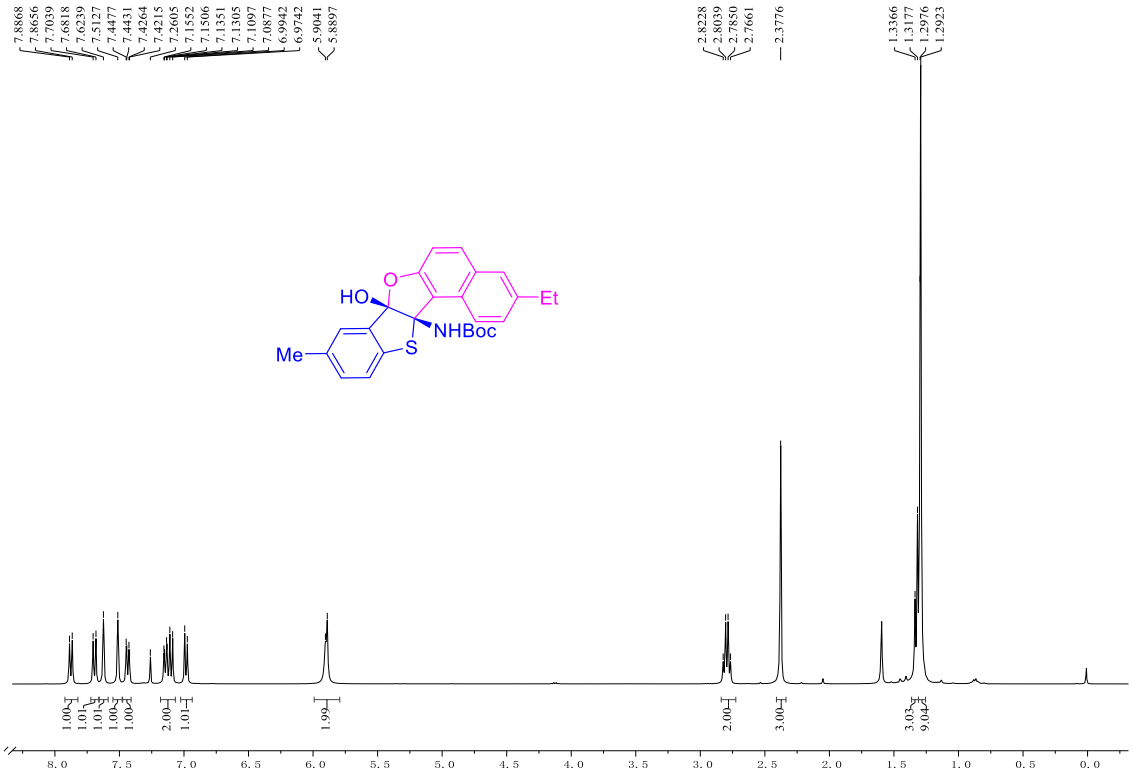
Peak	Ret.Time [min]	Area	Height	Area%
	3.875	18262.25	2547.15	50.28
	4.552	18060.17	1106.91	49.72
		36322.42		100.00

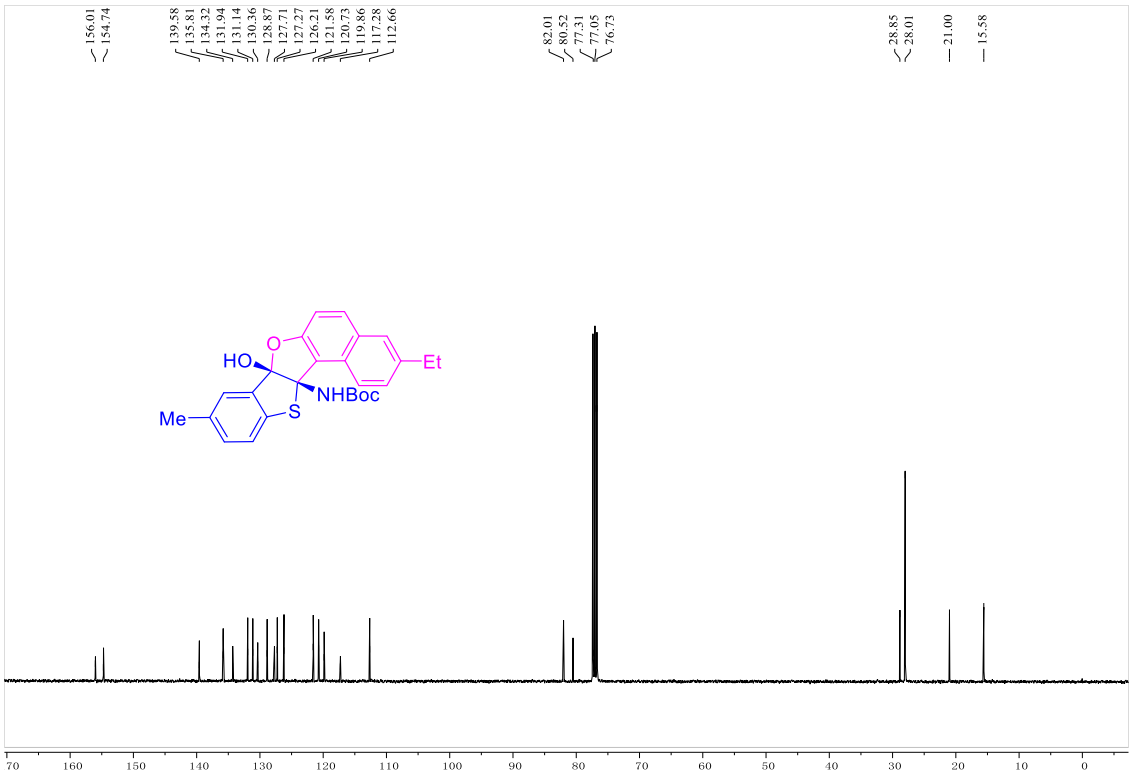


Detector VWD1A, Wavelength=254 nm

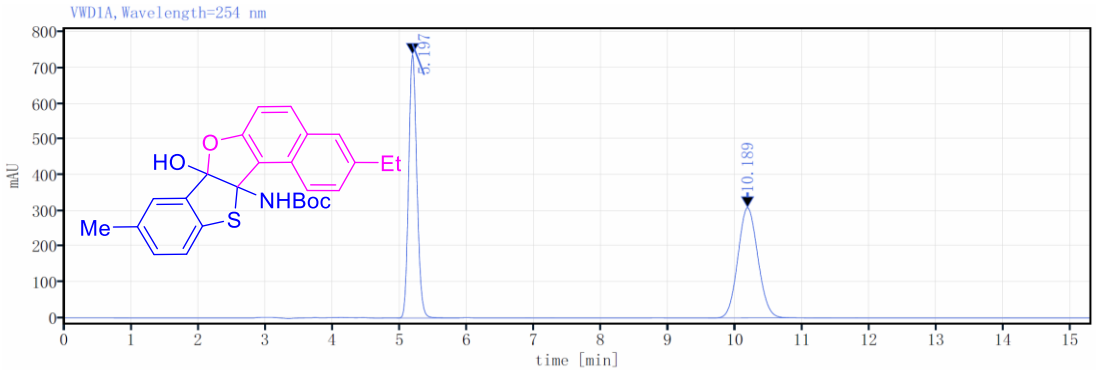
Peak	Ret.Time [min]	Area	Height	Area%
	3.916	4526.27	1568.45	95.82
	4.238	197.38	31.99	4.18
		4723.65		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 7k



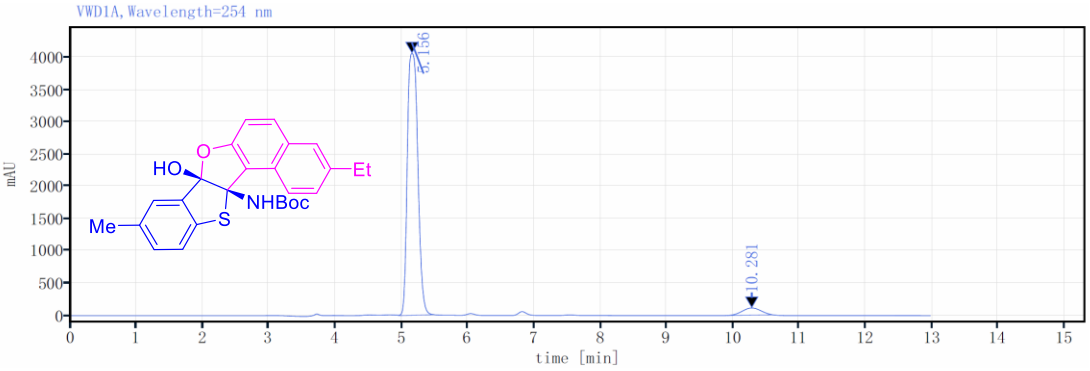


HPLC of 7k



Detector VWD1A, Wavelength=254 nm

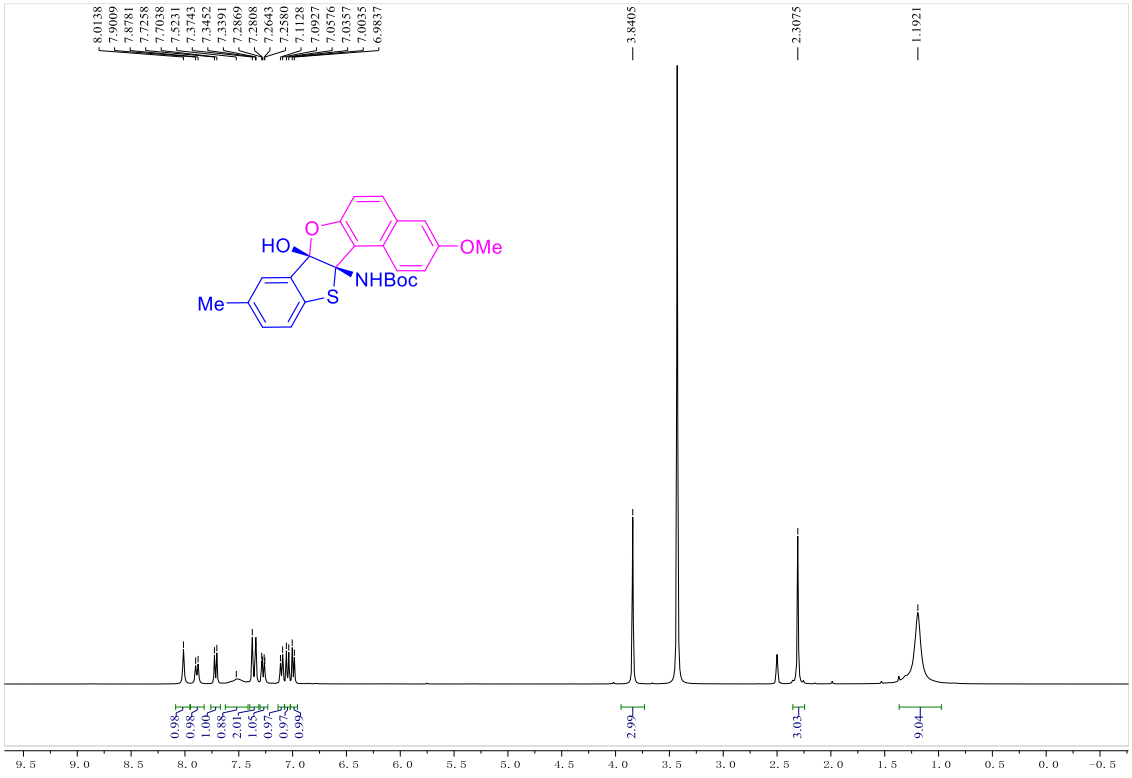
Peak	Ret.Time [min]	Area	Height	Area%
	5.197	6298.96	739.88	49.62
	10.189	6395.30	309.14	50.38
		12694.26		100.00

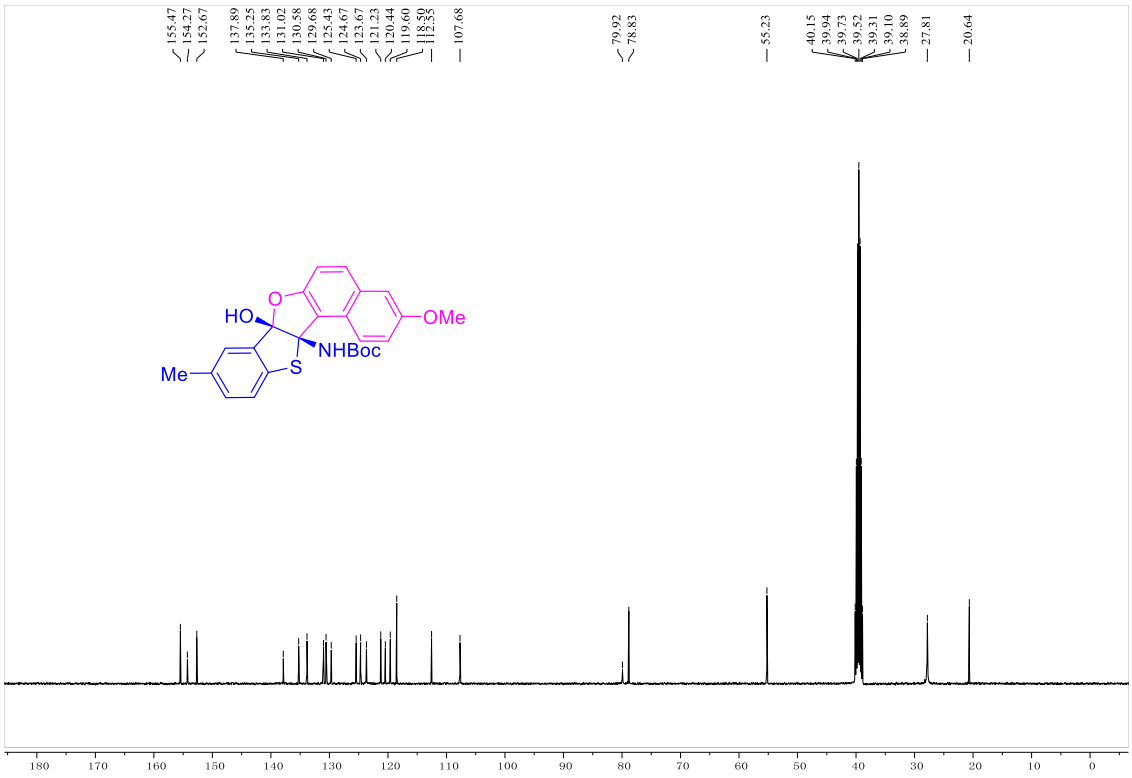


Detector VWD1A, Wavelength=254 nm

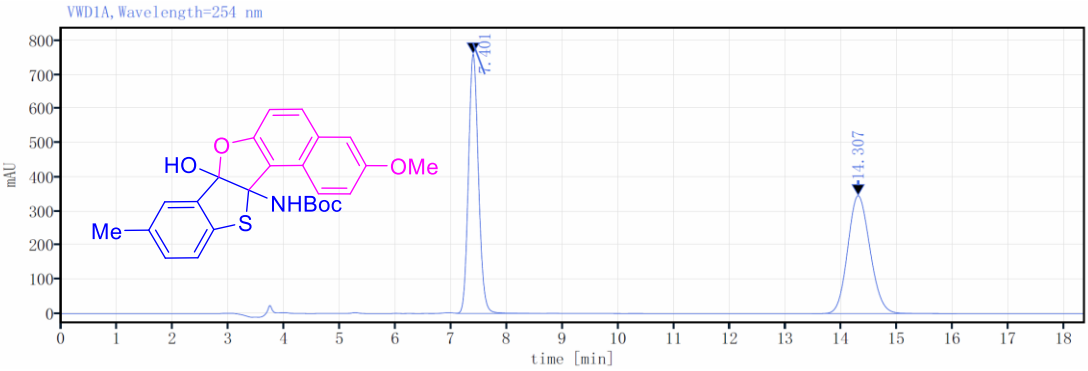
Peak	Ret.Time [min]	Area	Height	Area%
	5.156	44803.95	4064.23	95.38
	10.281	2168.60	110.85	4.62
		46972.55		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7l



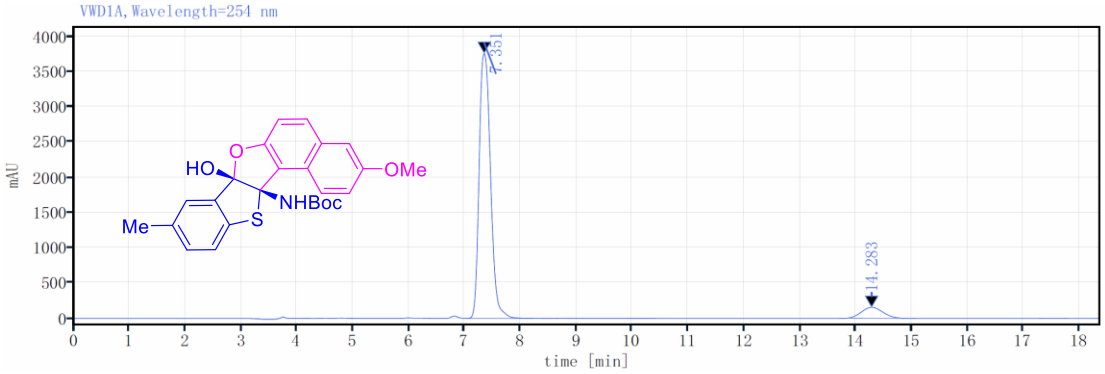


HPLC of 7l



Detector VWD1A, Wavelength=254 nm

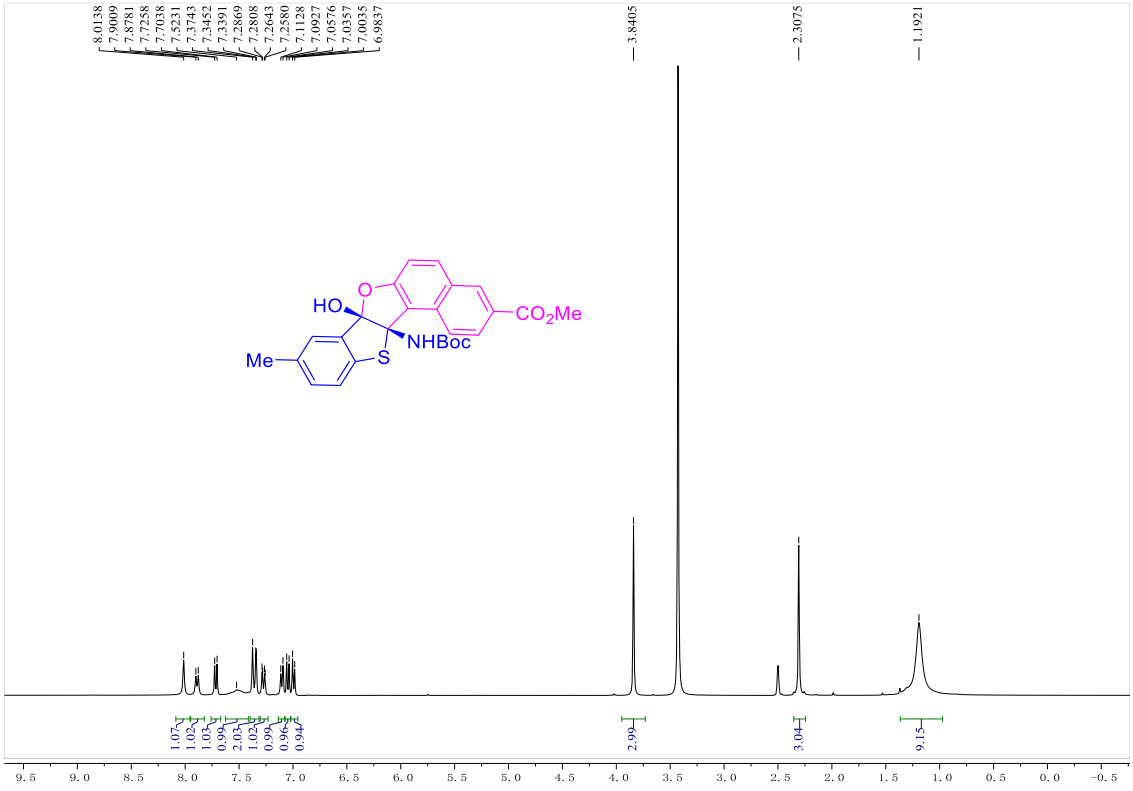
Peak	Ret.Time [min]	Area	Height	Area%
	7.401	9462.28	760.62	49.67
	14.307	9586.74	345.42	50.33
		19049.02		100.00

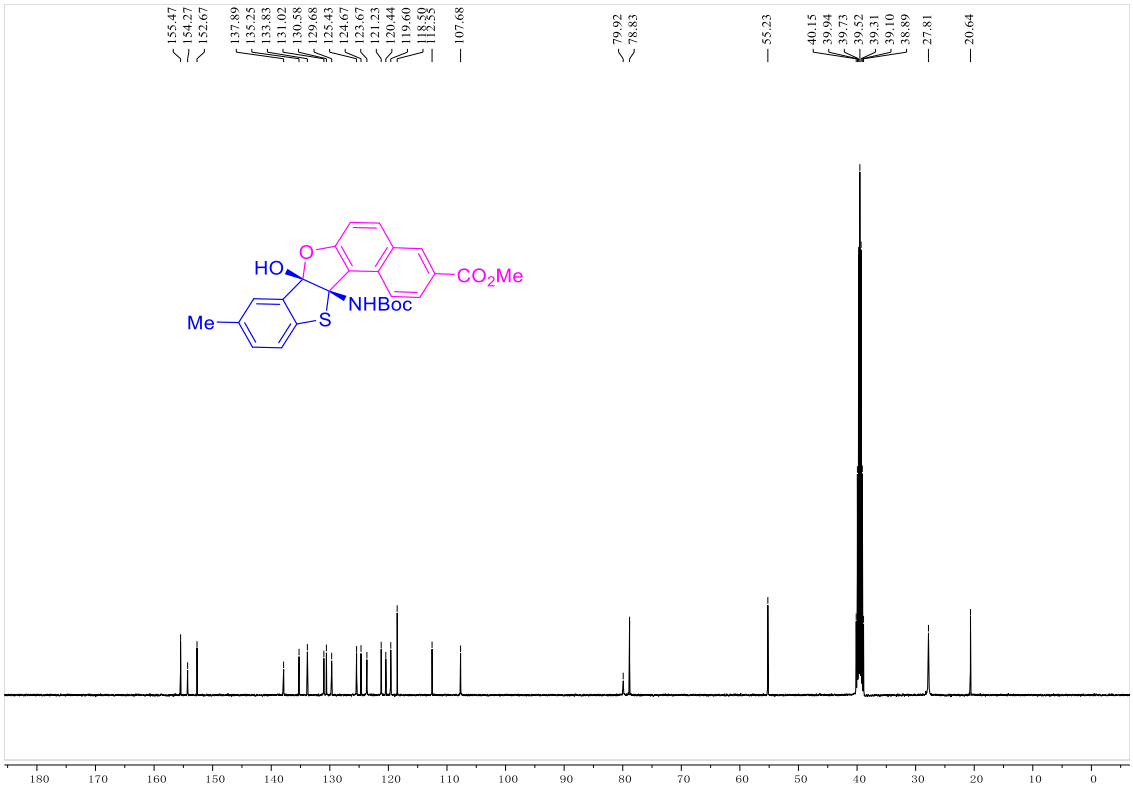


Detector VWD1A, Wavelength=254 nm

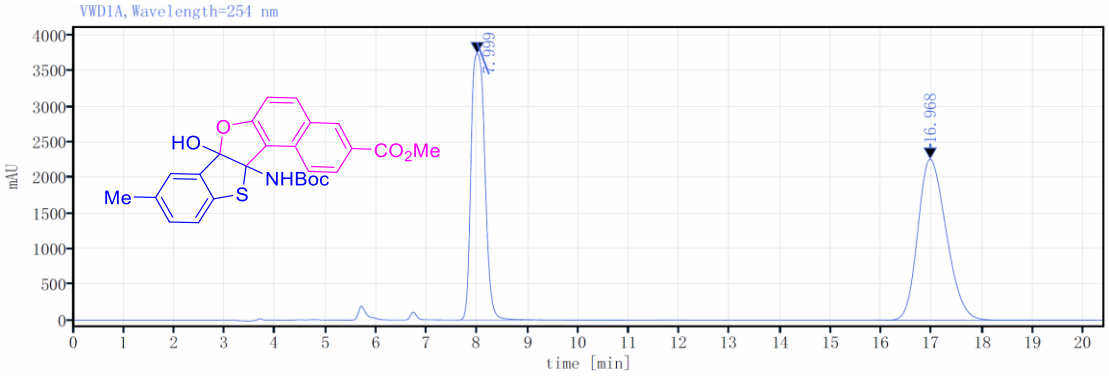
Peak	Ret.Time [min]	Area	Height	Area%
	7.351	53133.98	3758.95	92.79
	14.283	4126.59	155.44	7.21
		57260.56		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7m



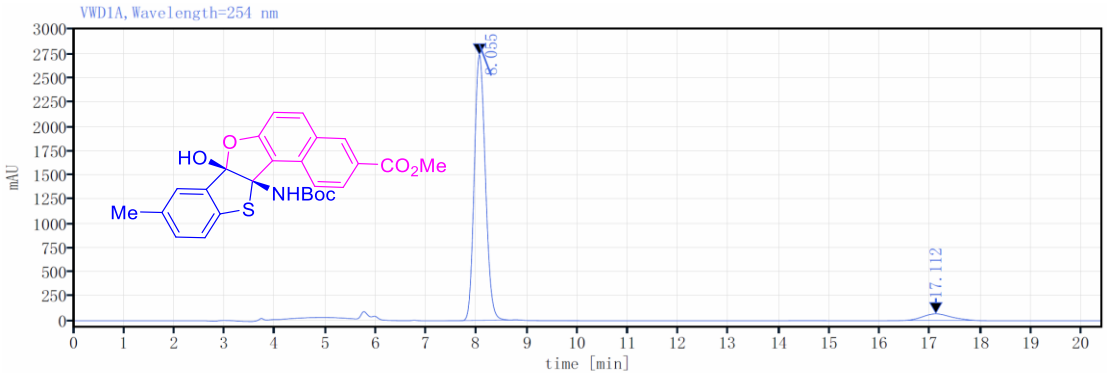


HPLC of 7m



Detector VWD1A, Wavelength=254 nm

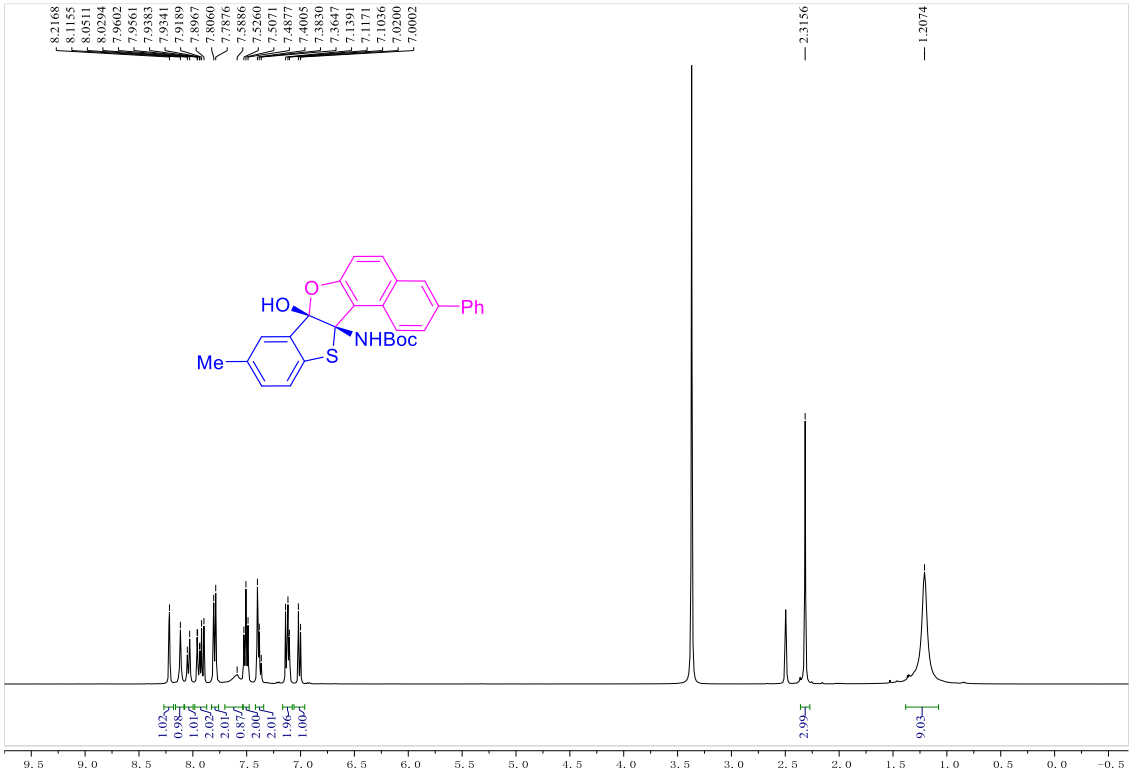
Peak	Ret.Time [min]	Area	Height	Area%
	7.999	71449.68	3741.25	44.63
	16.968	88641.79	2262.26	55.37
		160091.47		100.00

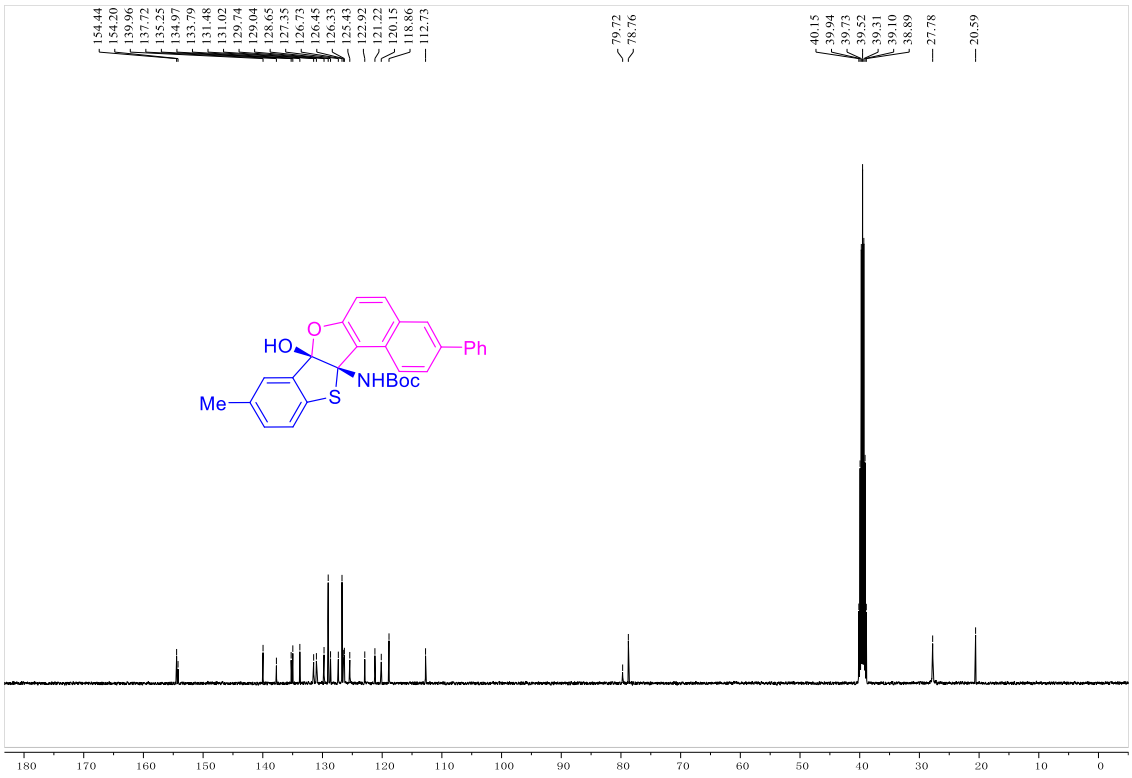


Detector VWD1A, Wavelength=254 nm

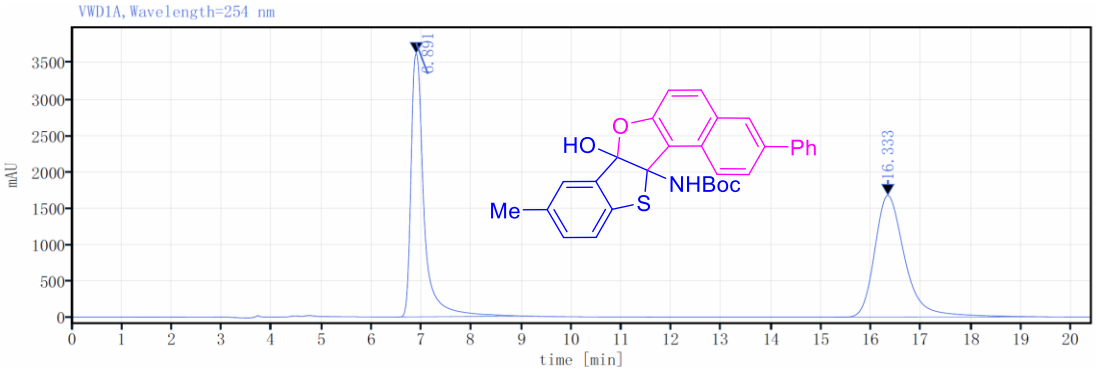
Peak	Ret.Time [min]	Area	Height	Area%
	8.055	41870.19	2735.77	94.09
	17.112	2629.40	68.34	5.91
		44499.59		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7n



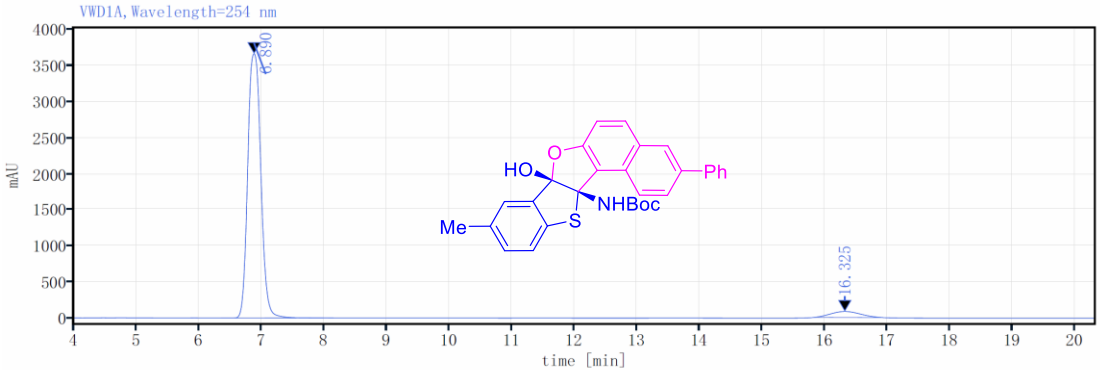


HPLC of 7n



Detector VWD1A, Wavelength=254 nm

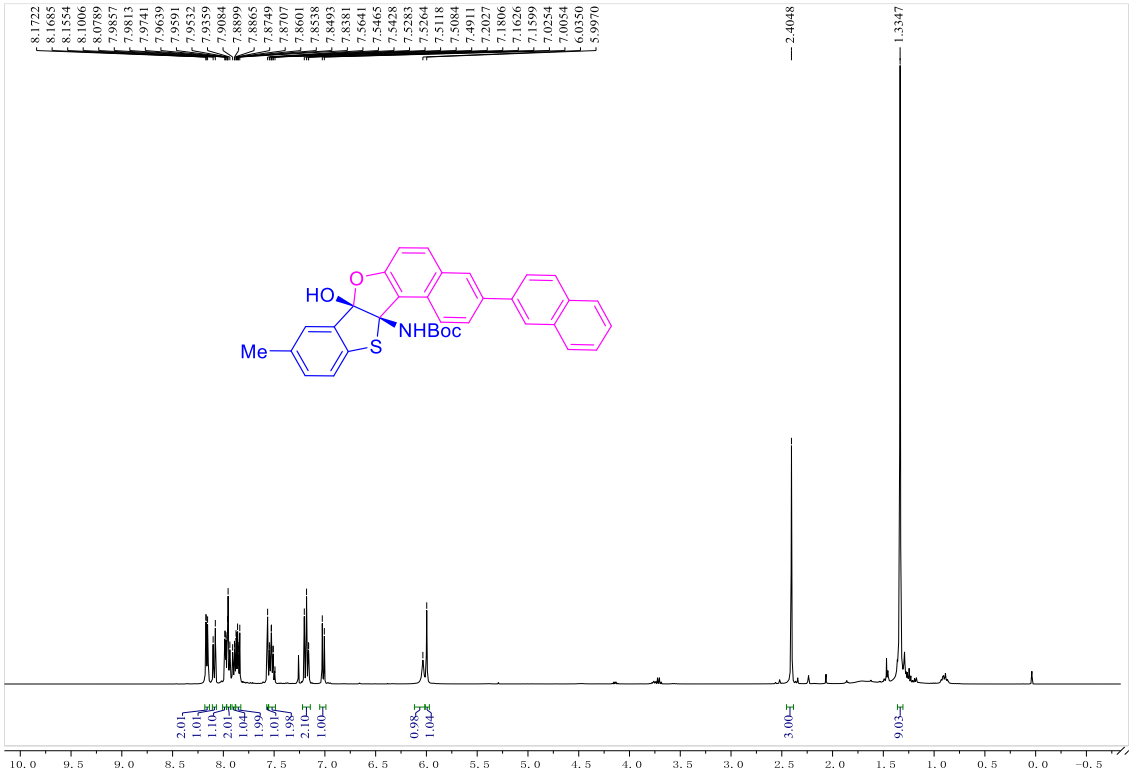
Peak	Ret.Time [min]	Area	Height	Area%
	6.891	65530.68	3630.84	48.12
	16.333	70662.52	1677.35	51.88
		136193.20		100.00

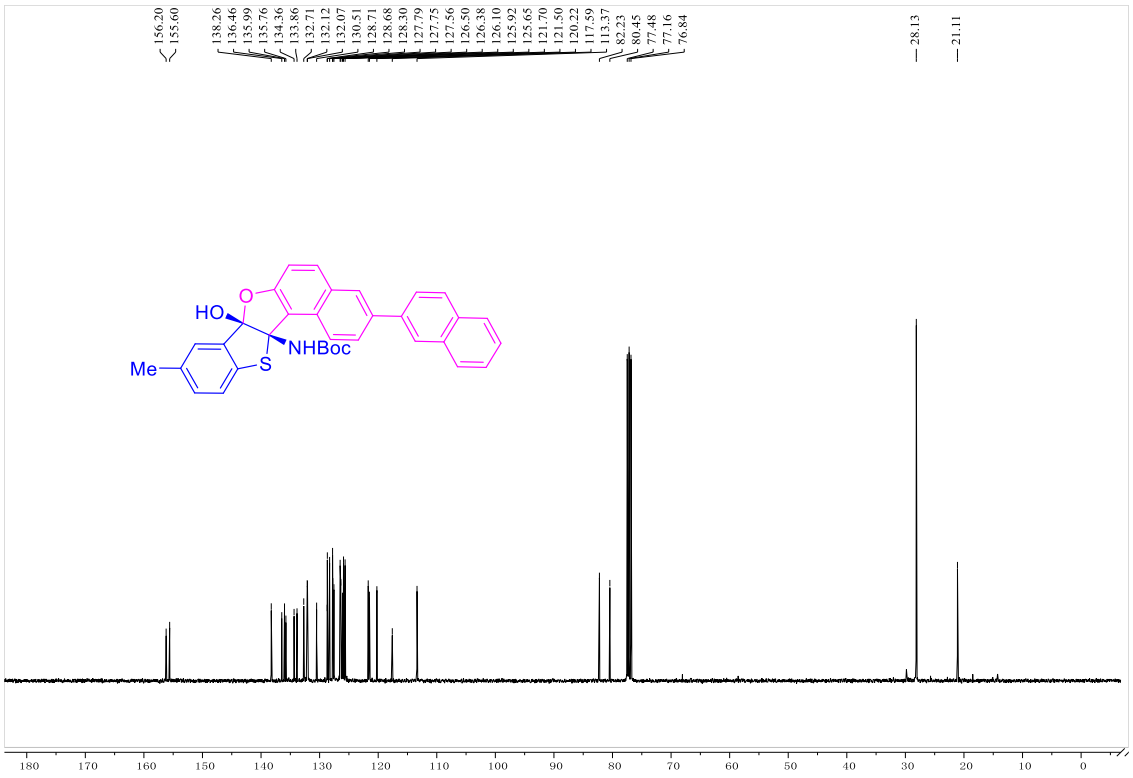


Detector VWD1A, Wavelength=254 nm

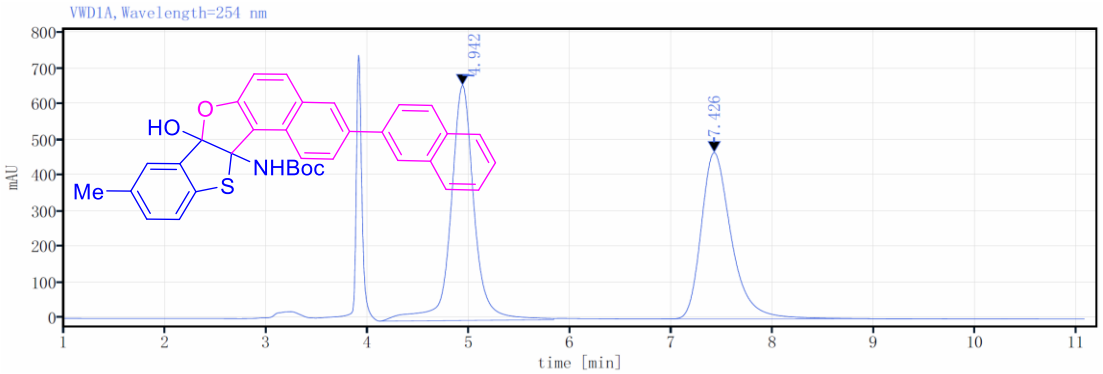
Peak	Ret.Time [min]	Area	Height	Area%
	6.890	53309.98	3675.38	95.19
	16.325	2694.25	82.44	4.81
		56004.23		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 7o



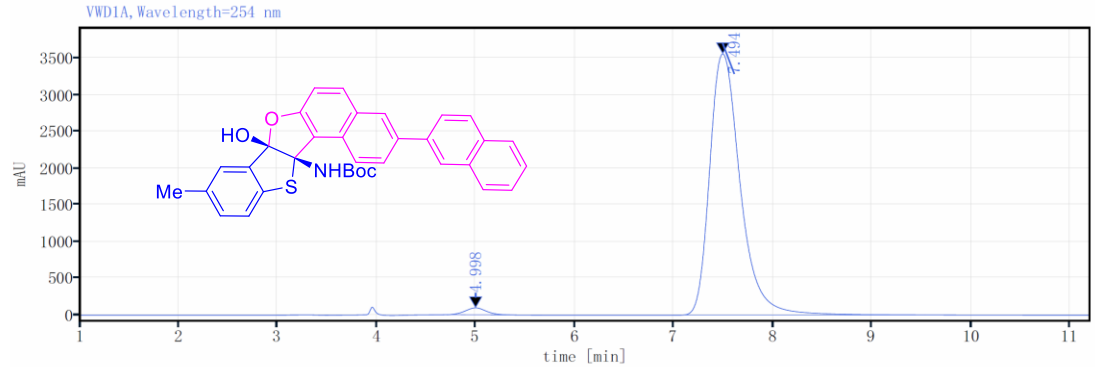


HPLC of 7o



Detector VWD1A, Wavelength=254 nm

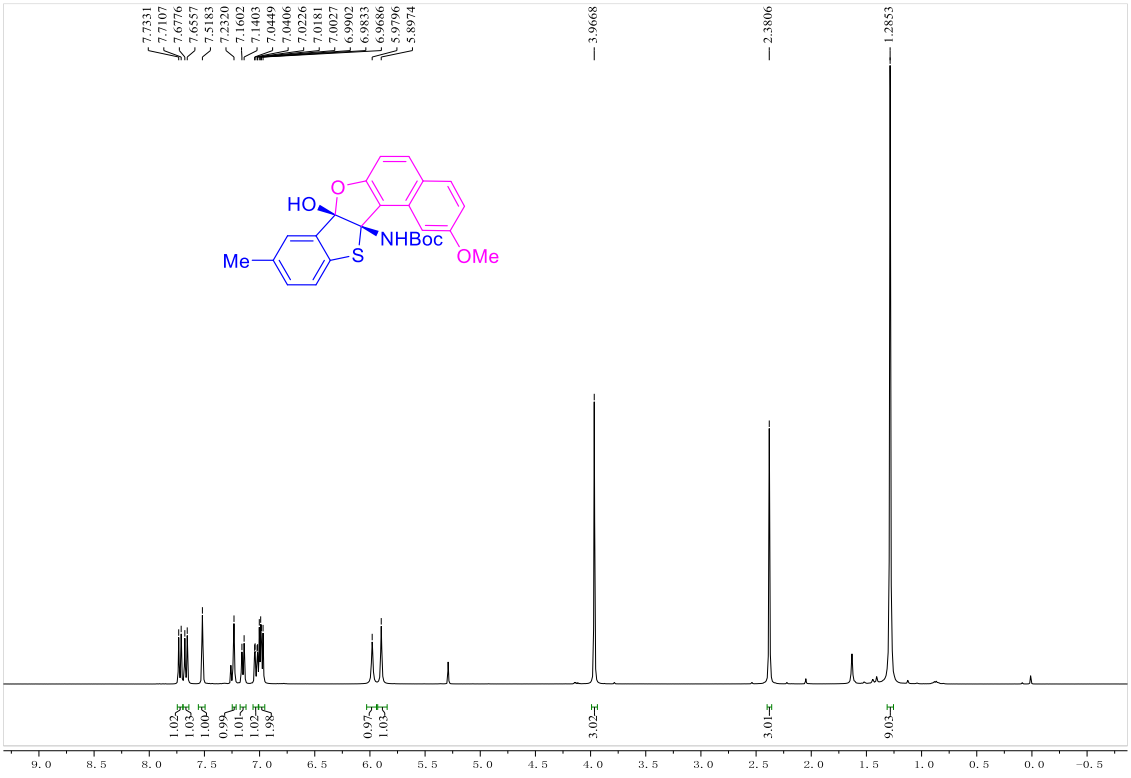
Peak	Ret.Time [min]	Area	Height	Area%
	4.942	10598.57	658.32	52.32
	7.426	9657.77	465.81	47.68
		20256.34		100.00

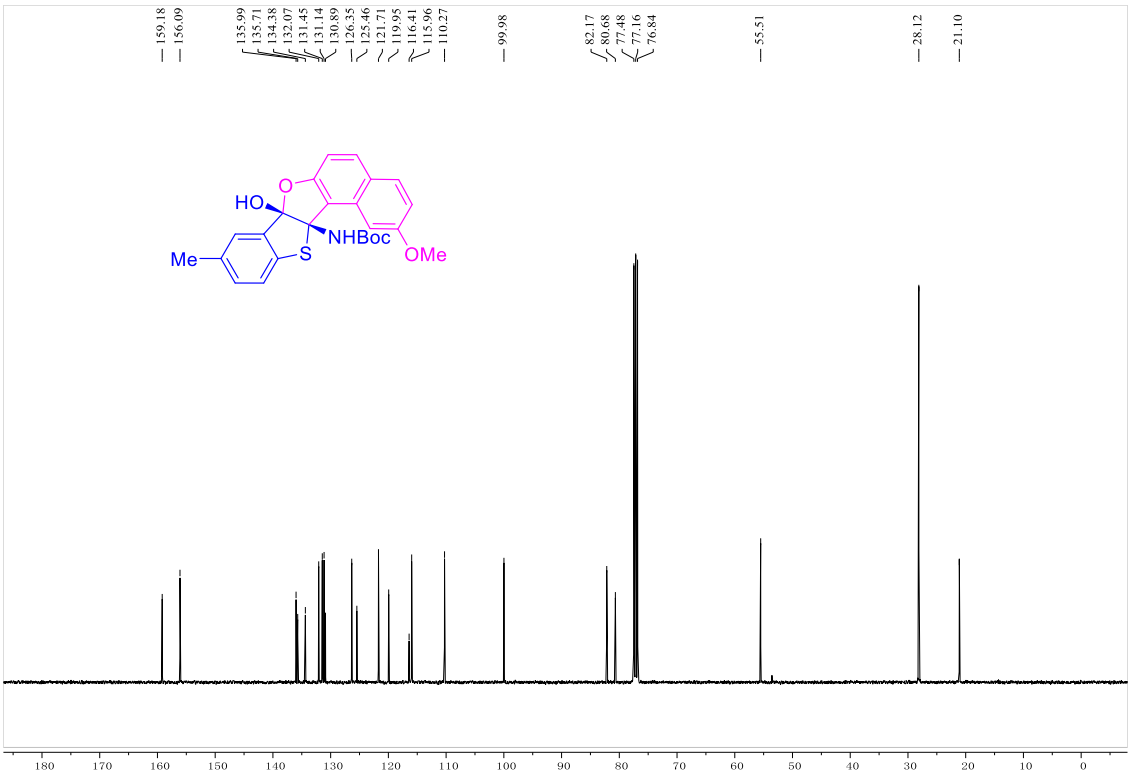


Detector VWD1A, Wavelength=254 nm

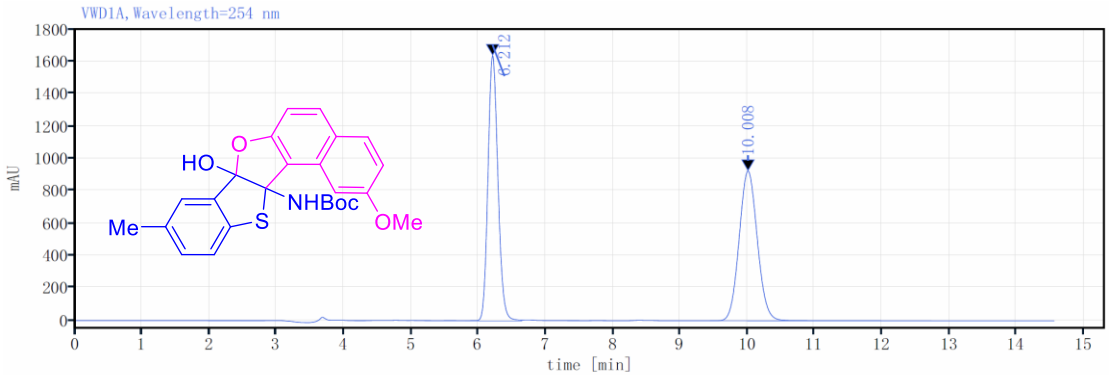
Peak	Ret.Time [min]	Area	Height	Area%
	4.998	1398.31	94.68	1.78
	7.494	77102.65	3565.48	98.22
		78500.97		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 7p



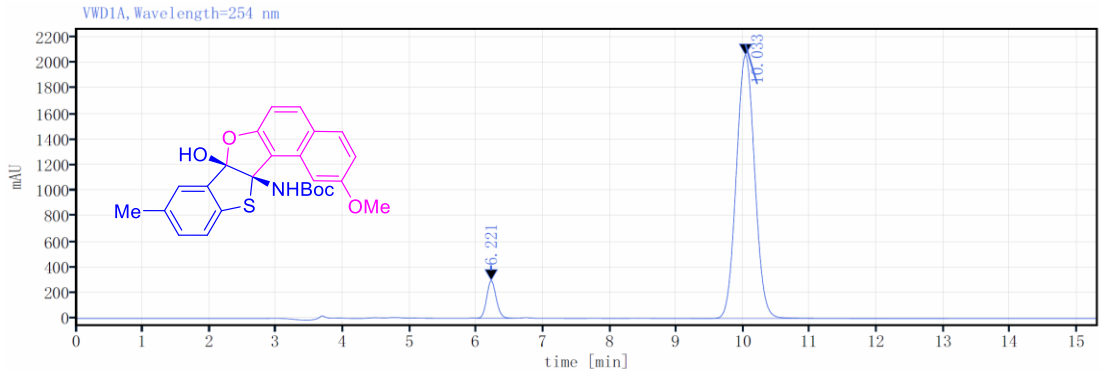


HPLC of 7p



Detector VWD1A, Wavelength=254 nm

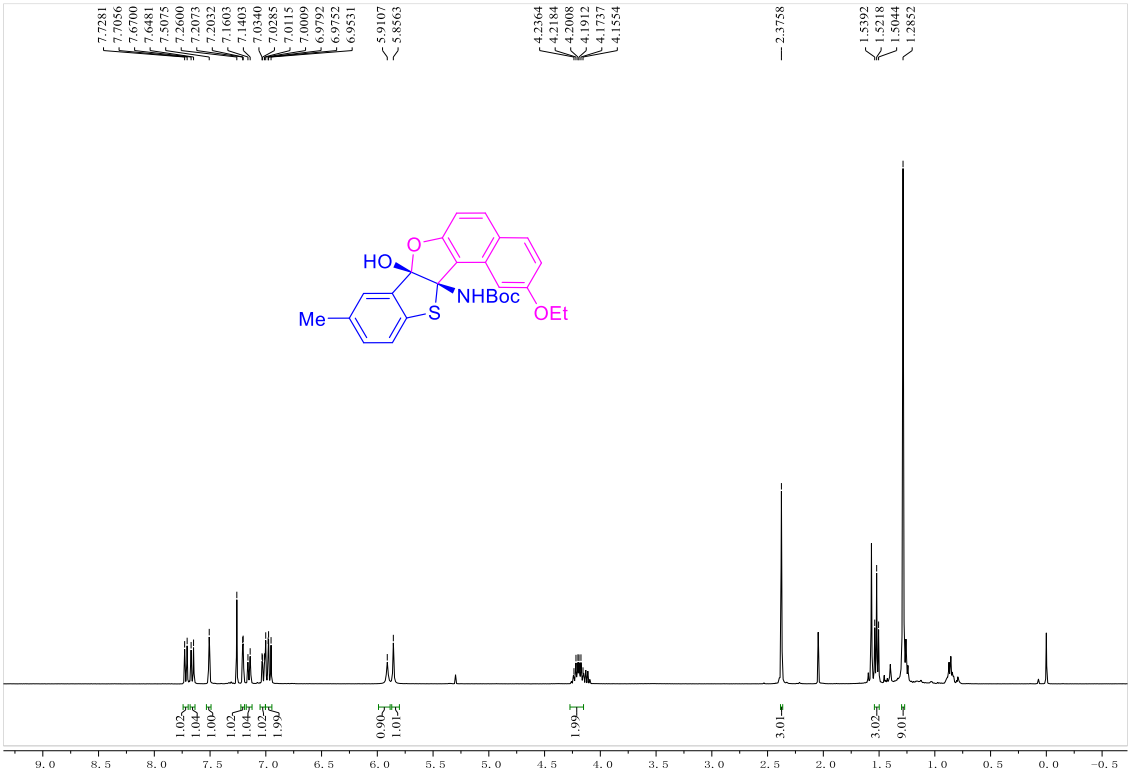
Peak	Ret.Time [min]	Area	Height	Area%
	6.212	16780.85	1636.63	49.14
	10.008	17368.07	924.50	50.86
		34148.92		100.00

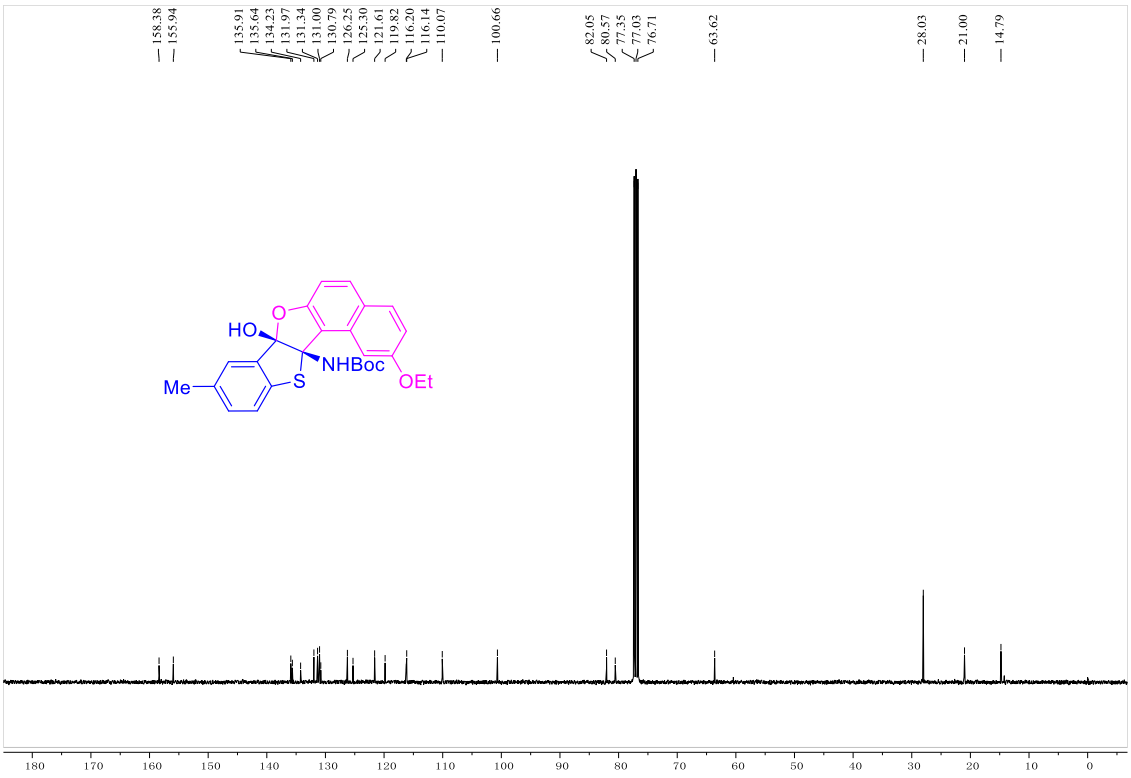


Detector VWD1A, Wavelength=254 nm

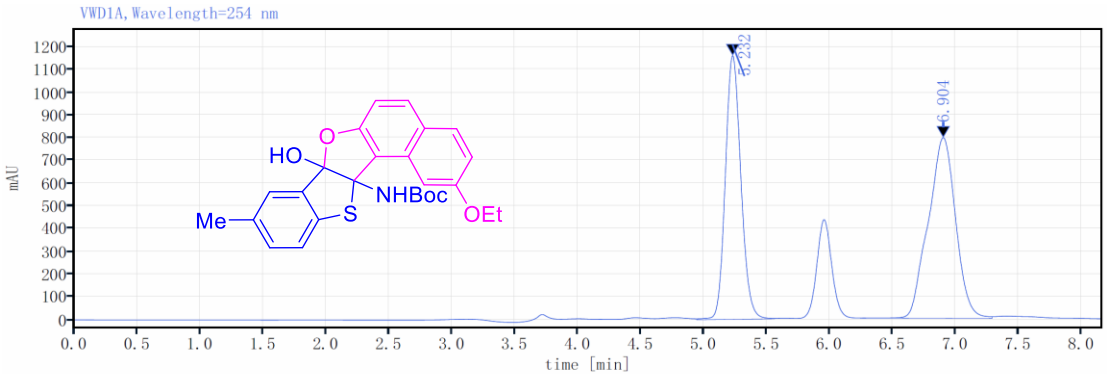
Peak	Ret.Time [min]	Area	Height	Area%
	6.221	2949.44	295.08	6.93
	10.033	39616.03	2061.94	93.07
		42565.47		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 7q



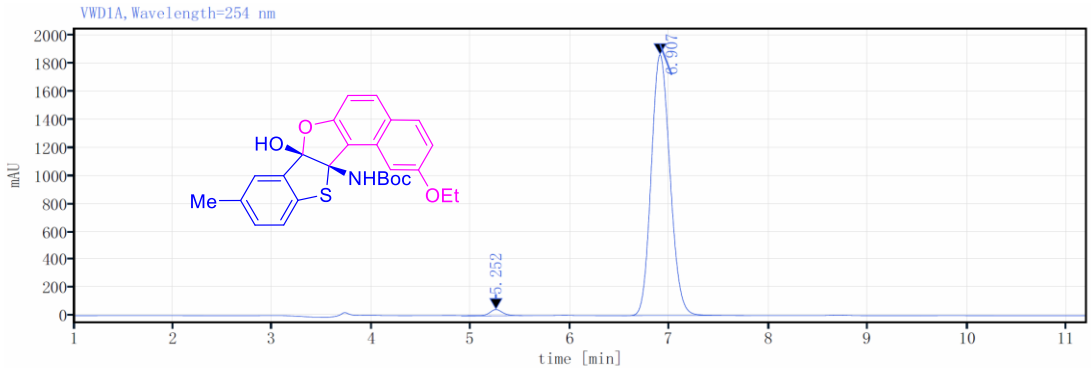


HPLC of 7q



Detector VWD1A, Wavelength=254 nm

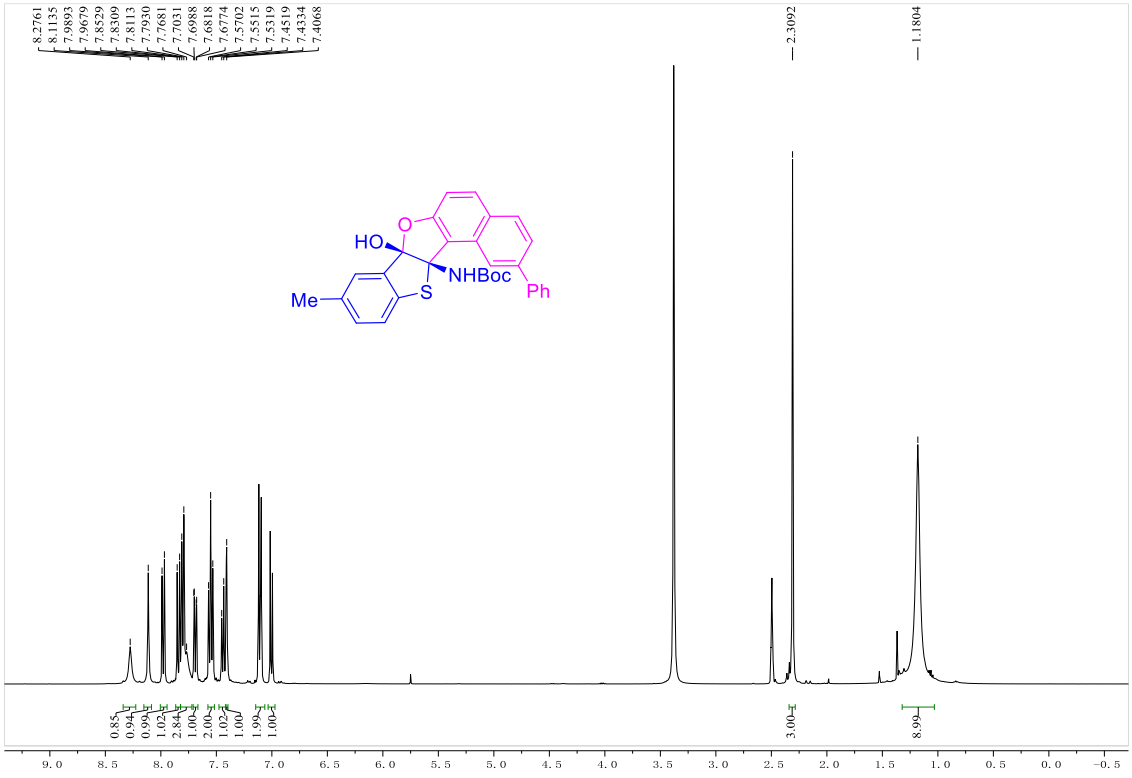
Peak	Ret.Time [min]	Area	Height	Area%
	5.232	9955.16	1159.89	45.31
	6.904	12015.27	794.34	54.69
		21970.43		100.00

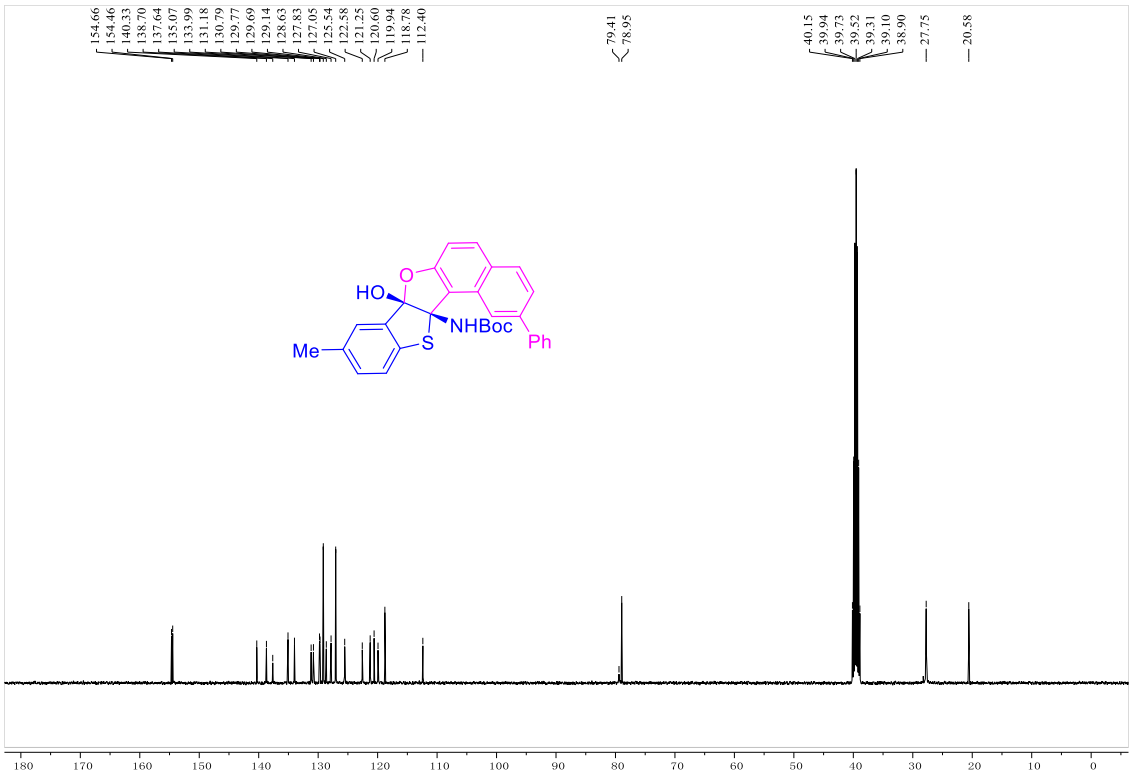


Detector VWD1A, Wavelength=254 nm

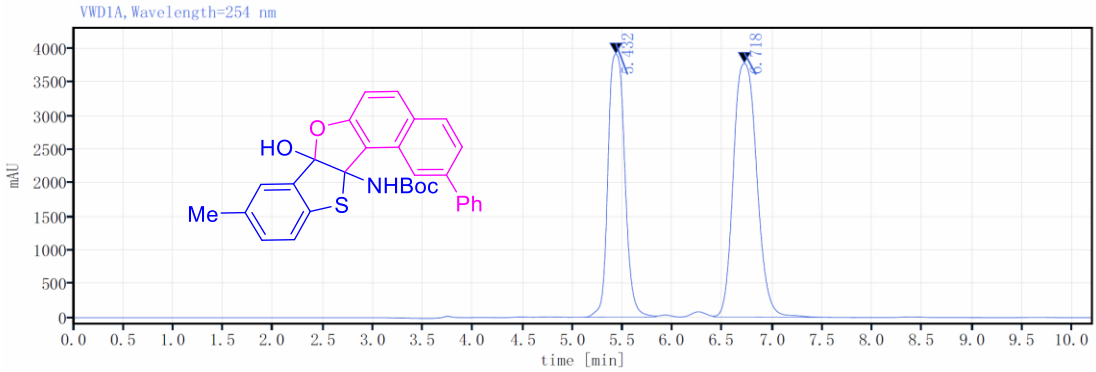
Peak	Ret.Time [min]	Area	Height	Area%
	5.252	458.04	45.11	1.83
	6.907	24507.53	1865.97	98.17
		24965.57		100.00

^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 7r



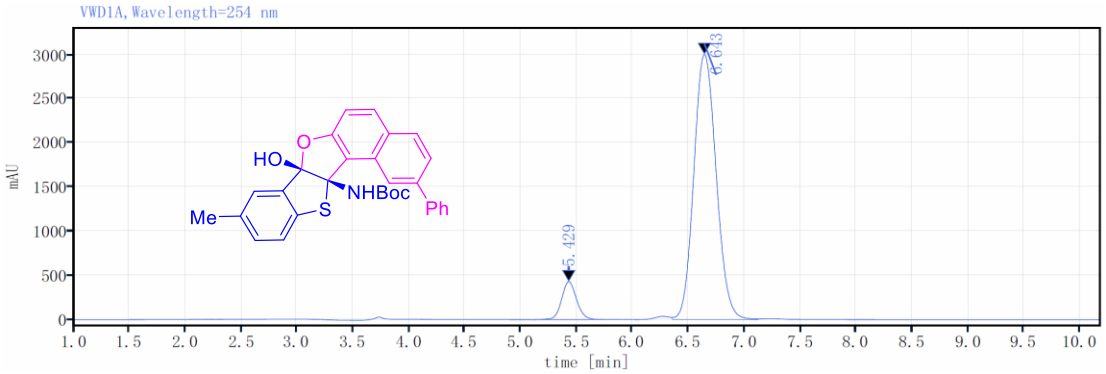


HPLC of 7r



Detector VWD1A, Wavelength=254 nm

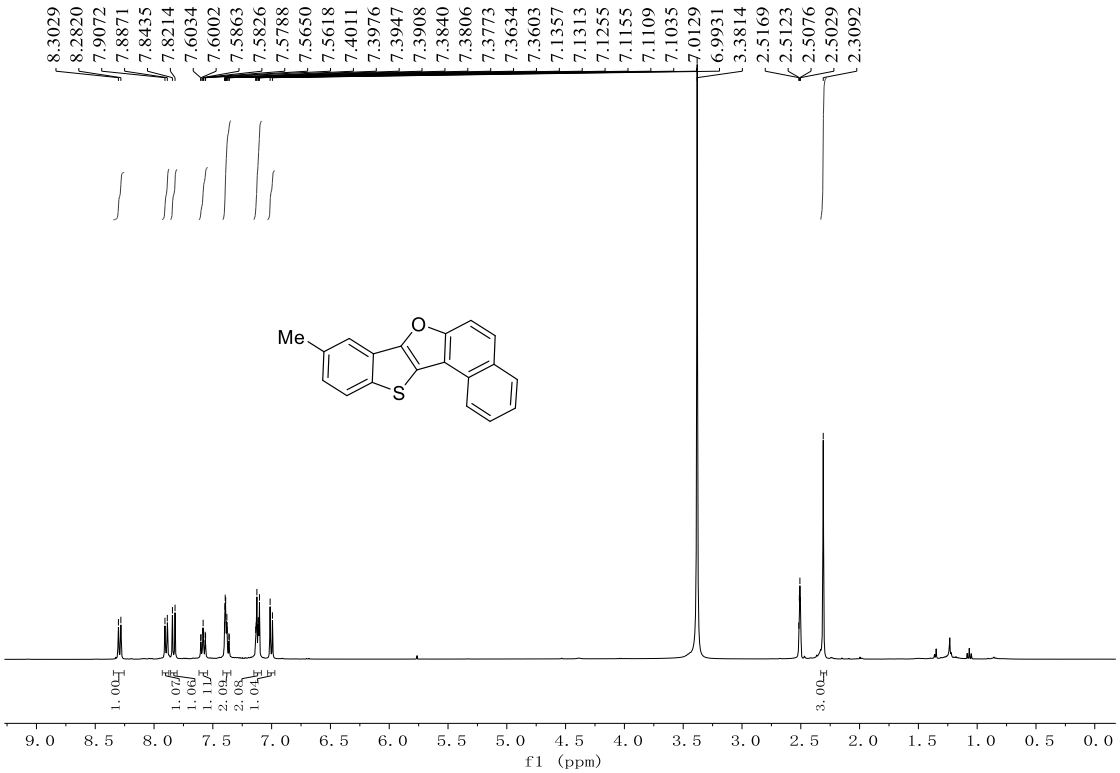
Peak	Ret.Time [min]	Area	Height	Area%
	5.432	45737.73	3910.08	42.59
	6.718	61649.22	3771.18	57.41
		107386.95		100.00

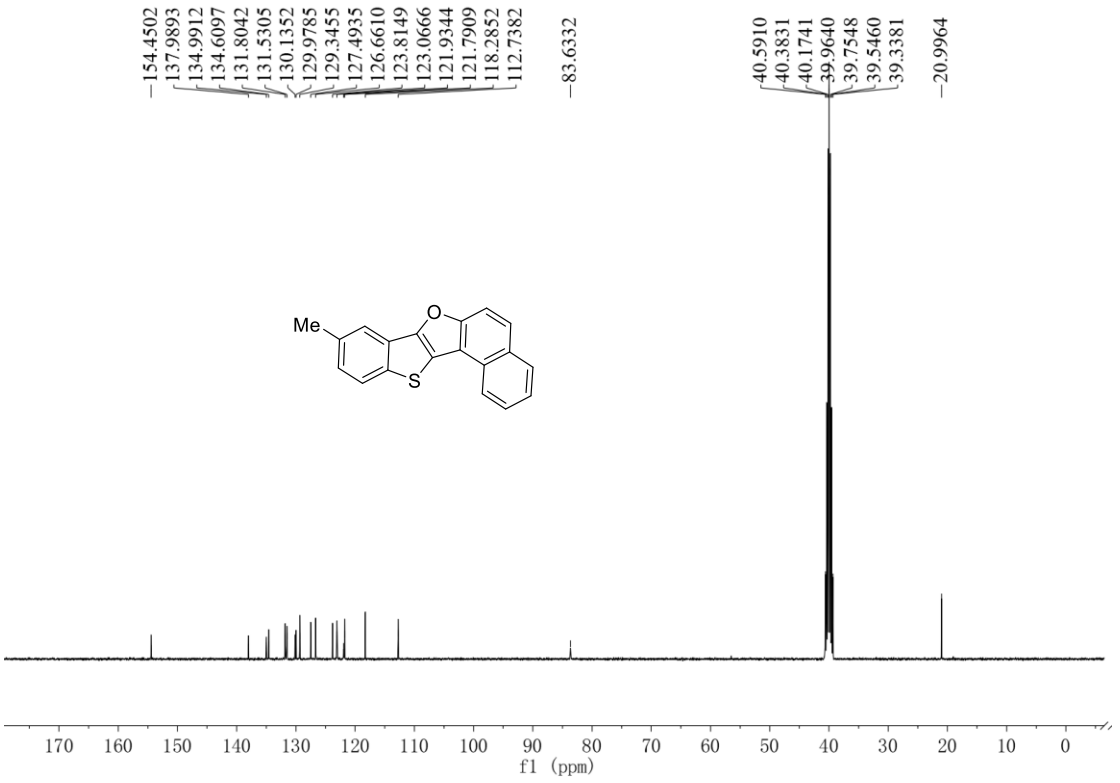


Detector VWD1A, Wavelength=254 nm

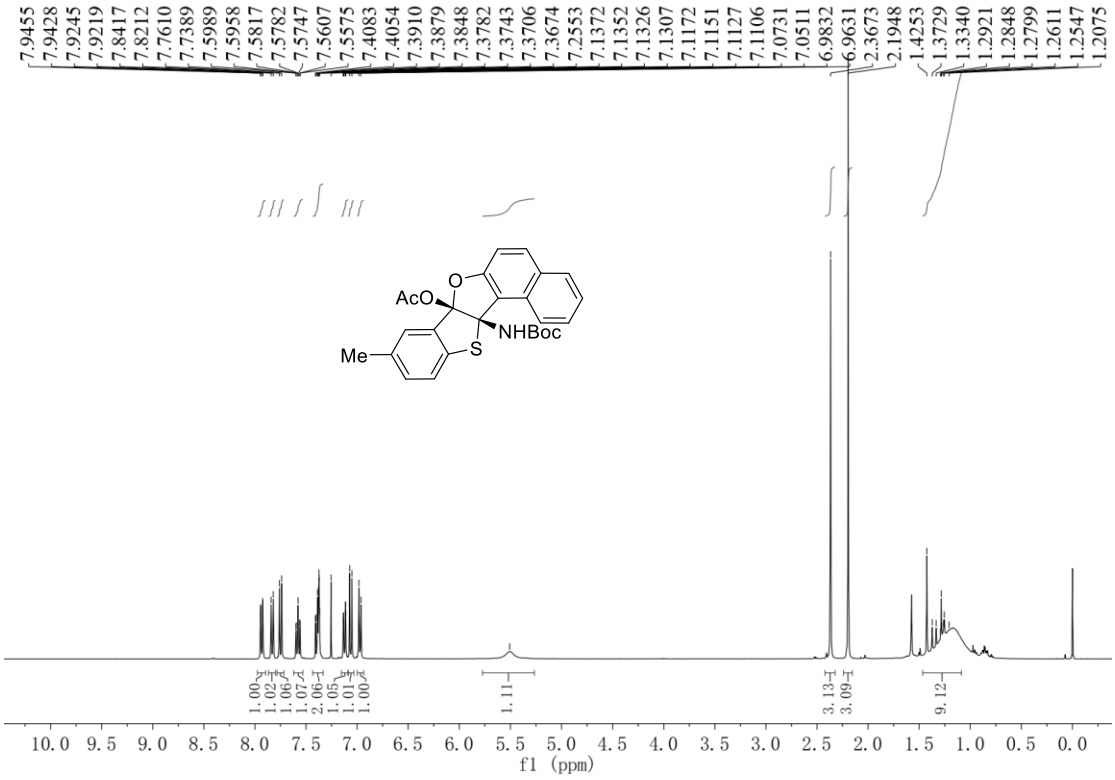
Peak	Ret.Time [min]	Area	Height	Area%
	5.429	4006.54	431.46	8.74
	6.643	41836.80	3007.94	91.26
		45843.33		100.00

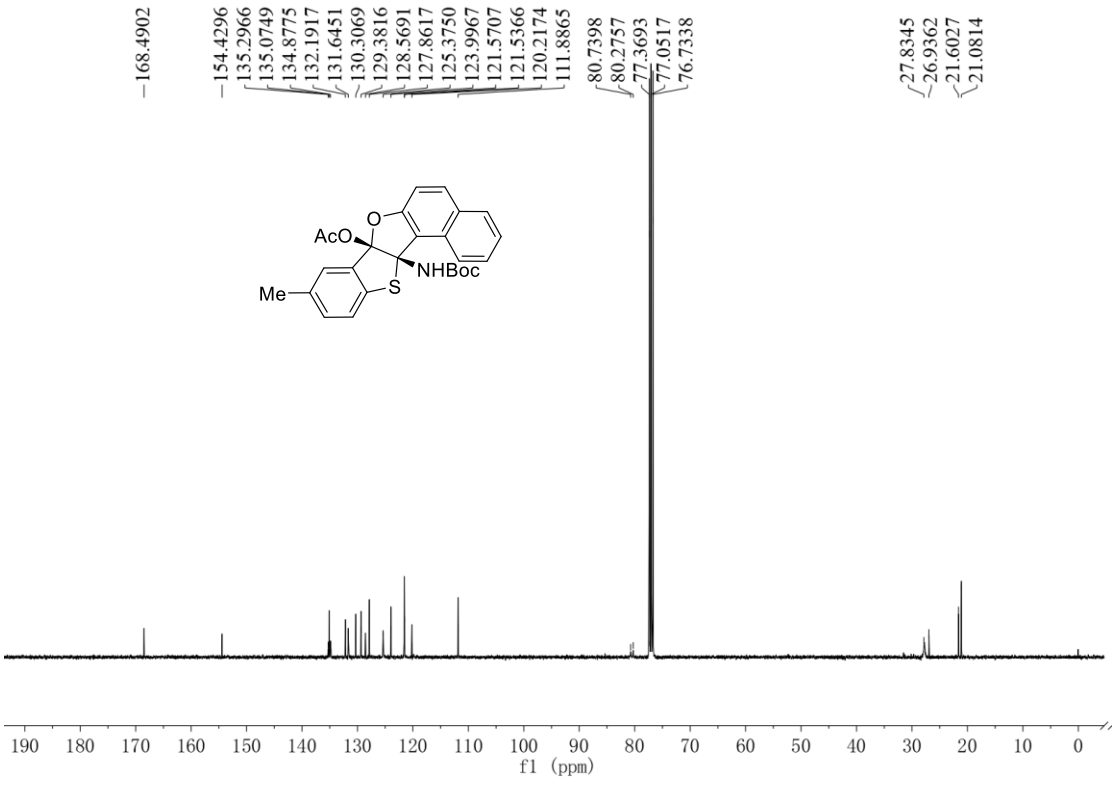
^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (101 MHz, DMSO-d_6) of 8



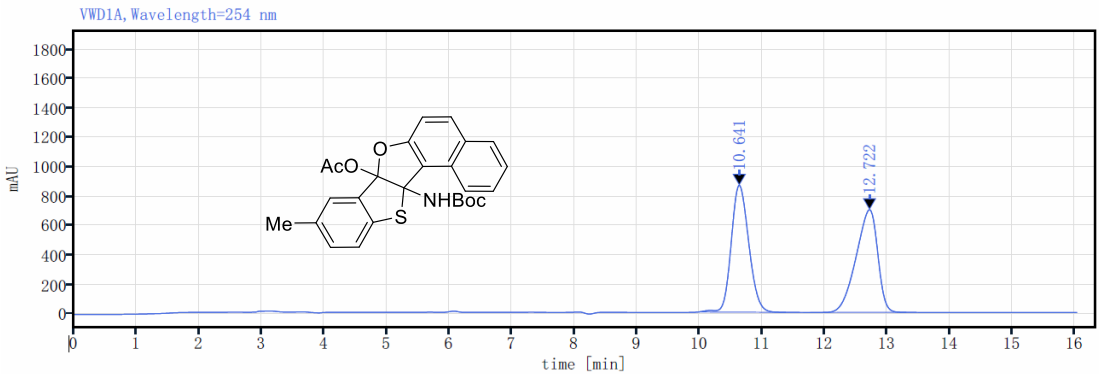


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 9



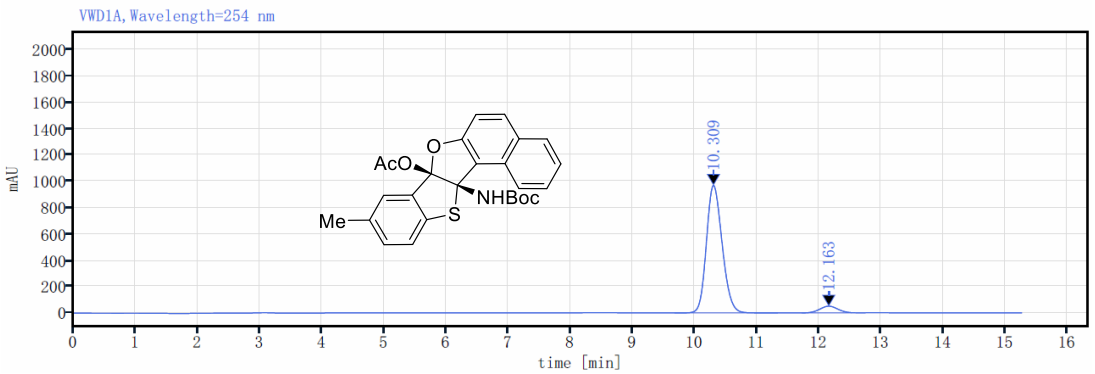


HPLC of 9



Detector VWD1A, Wavelength=254 nm

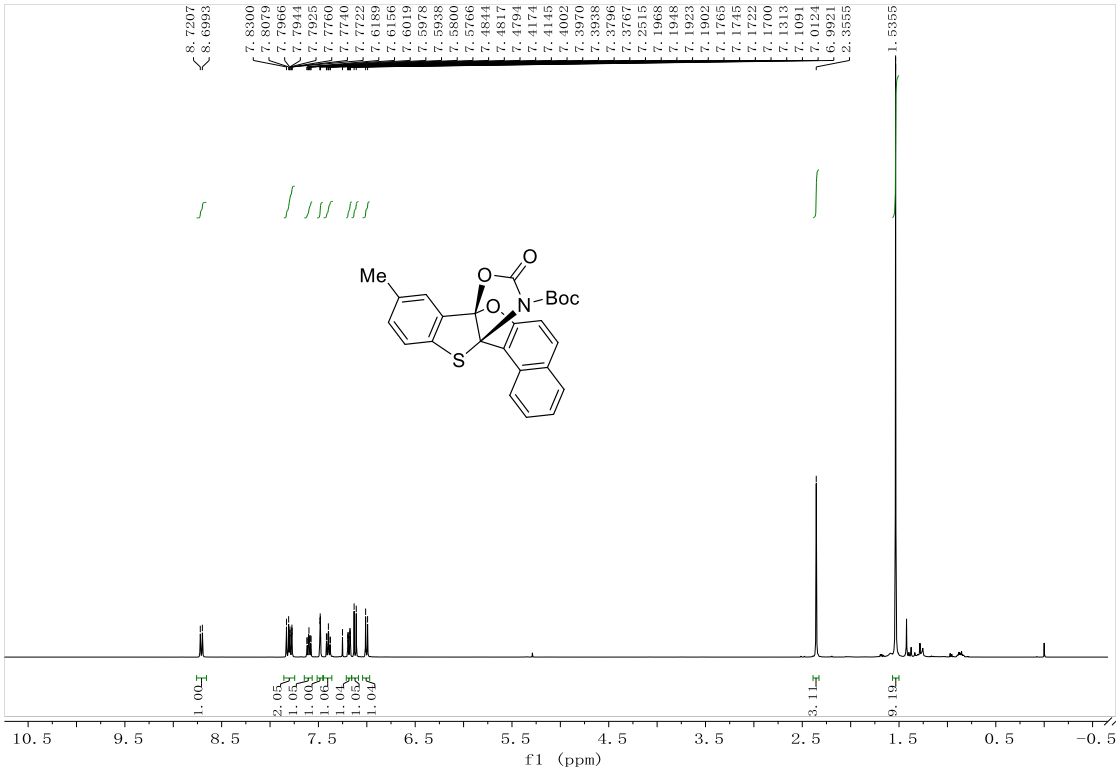
Peak	Ret.Time [min]	Area	Height	Area%
	10.641	16789.98	861.55	50.06
	12.722	16749.08	697.79	49.94
		33539.06		100.00

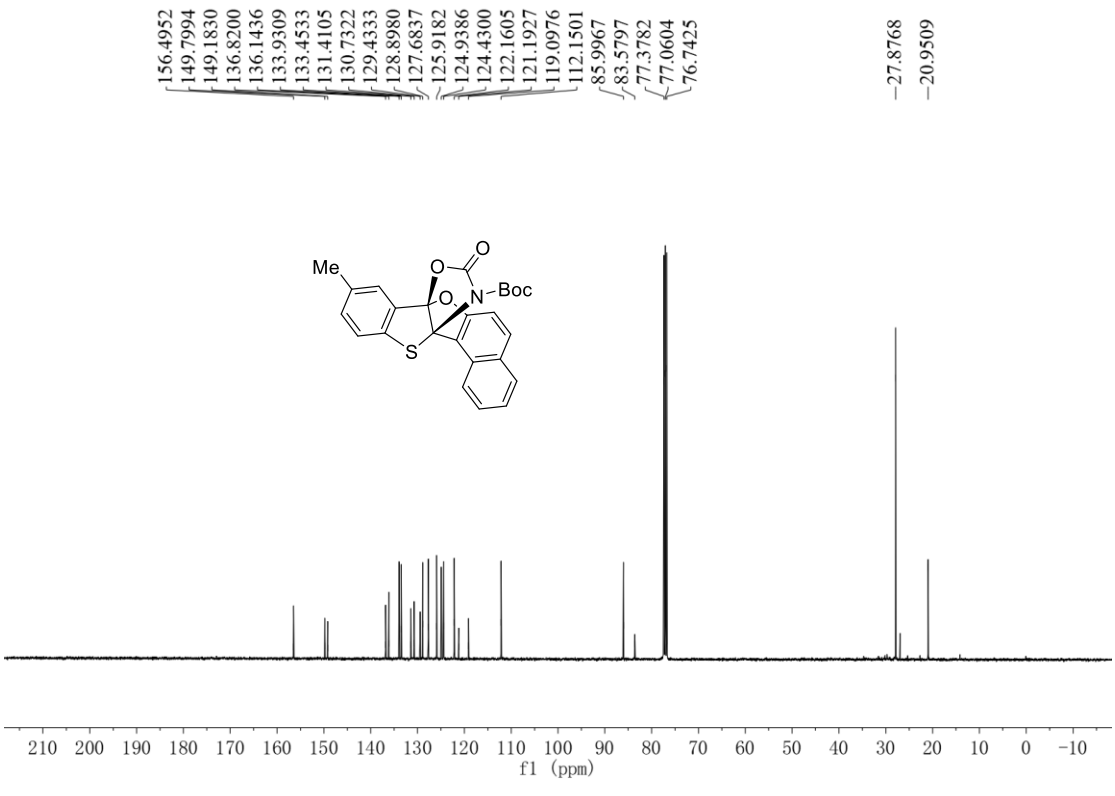


Detector VWD1A, Wavelength=254 nm

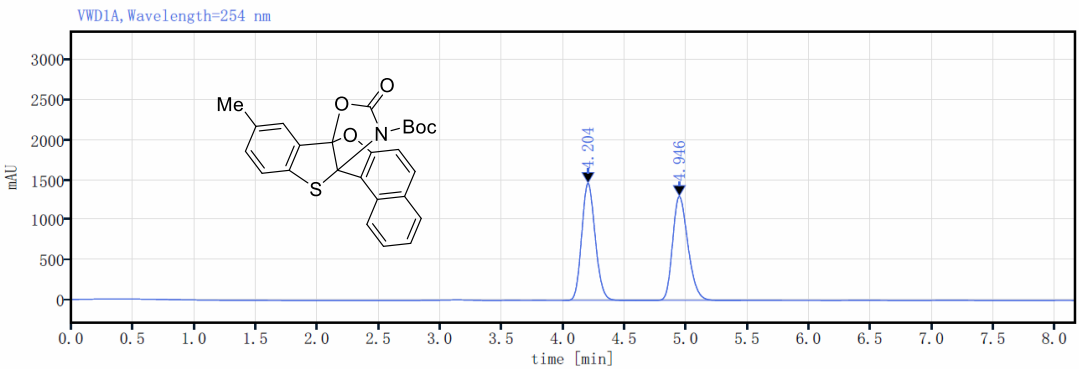
Peak	Ret.Time [min]	Area	Height	Area%
	10.309	17029.72	970.35	94.39
	12.163	1011.37	50.44	5.61
		18041.08		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10a



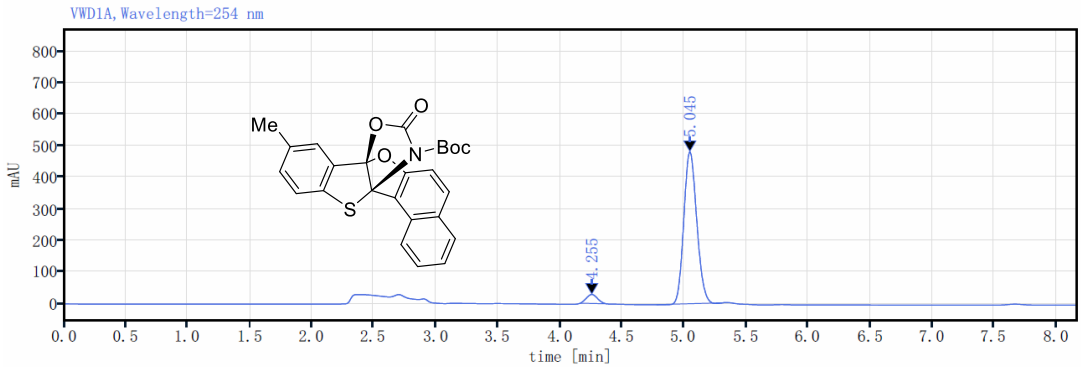


HPLC of 10a



Detector VWD1A, Wavelength=254 nm

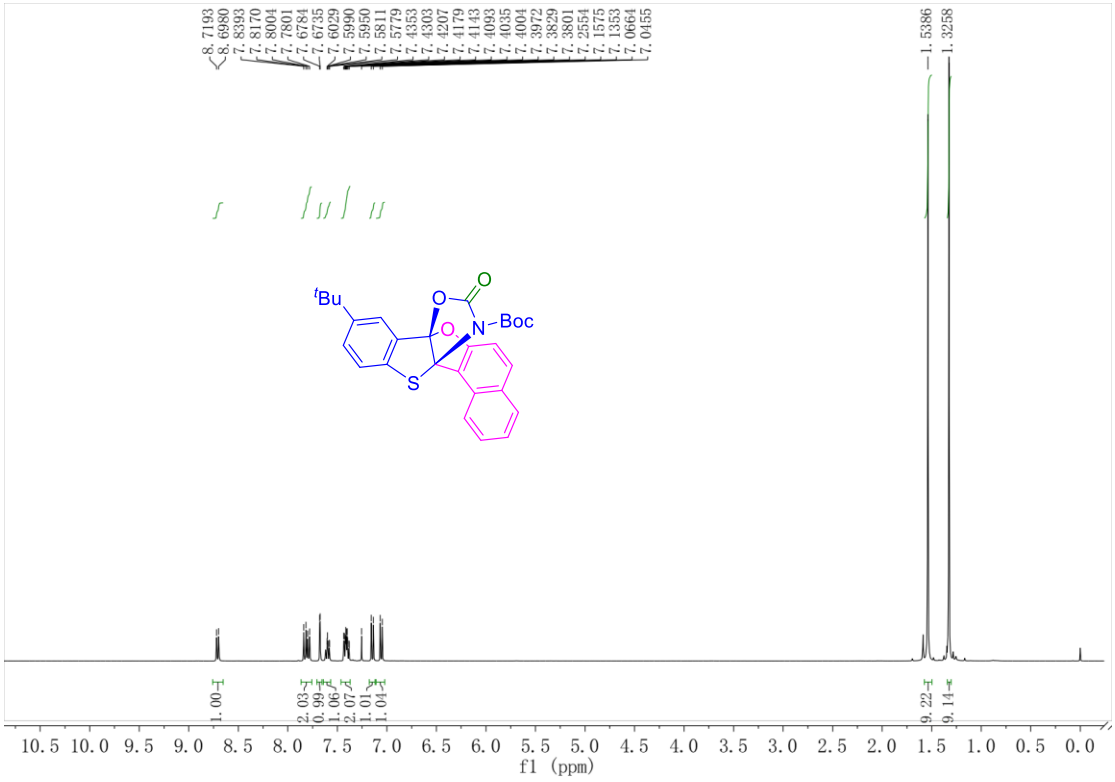
Peak	Ret.Time [min]	Area	Height	Area%
	4.204	11176.92	1461.26	49.84
	4.946	11247.06	1297.89	50.16
		22423.98		100.00

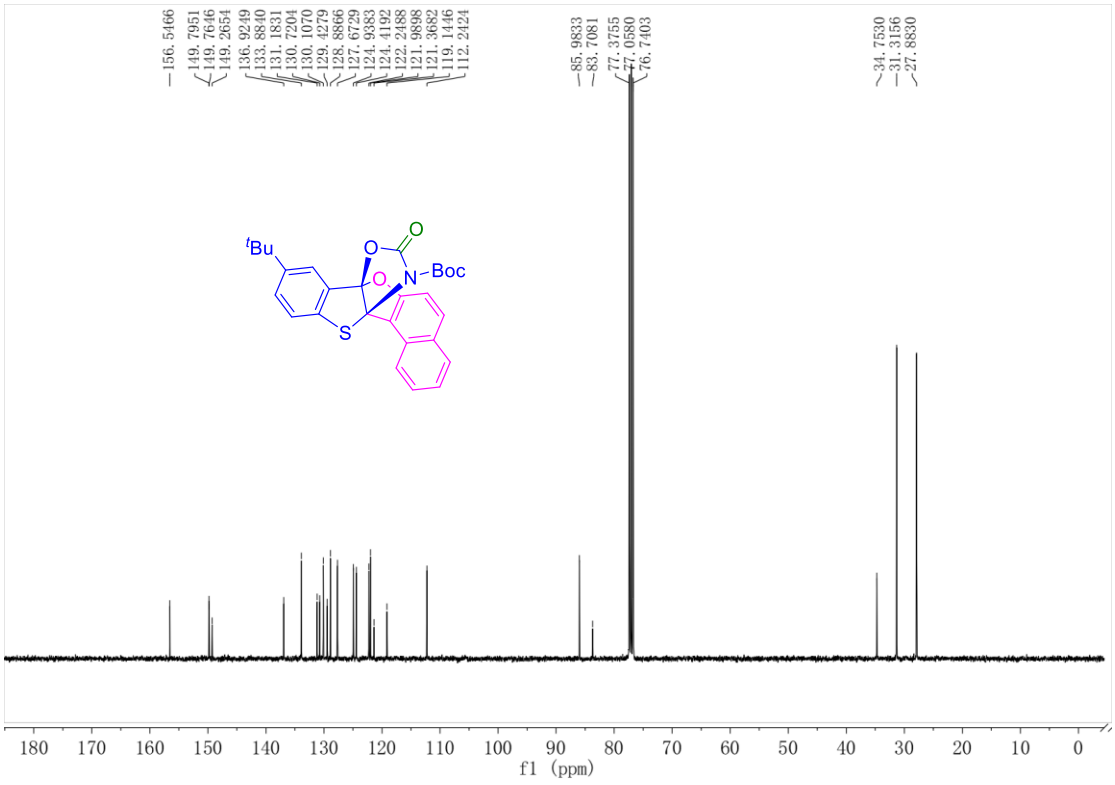


Detector VWD1A, Wavelength=254 nm

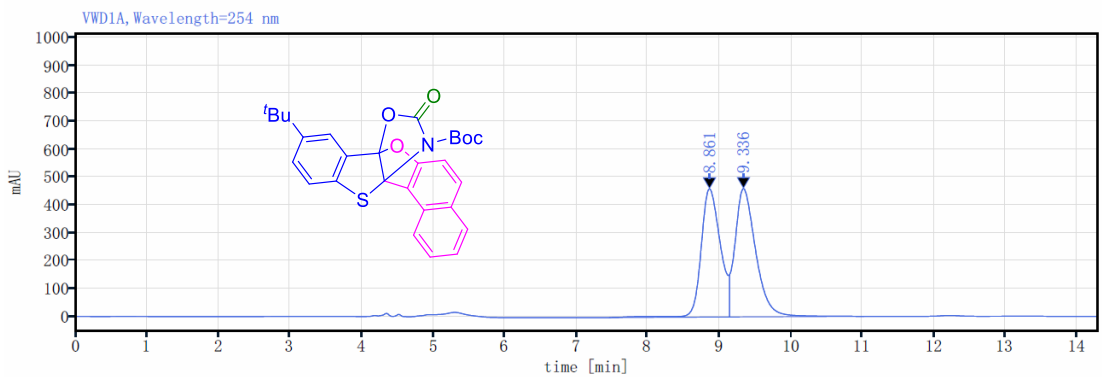
Peak	Ret.Time [min]	Area	Height	Area%
	4.255	175.55	28.30	4.81
	5.045	3470.99	480.70	95.19
		3646.55		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10b



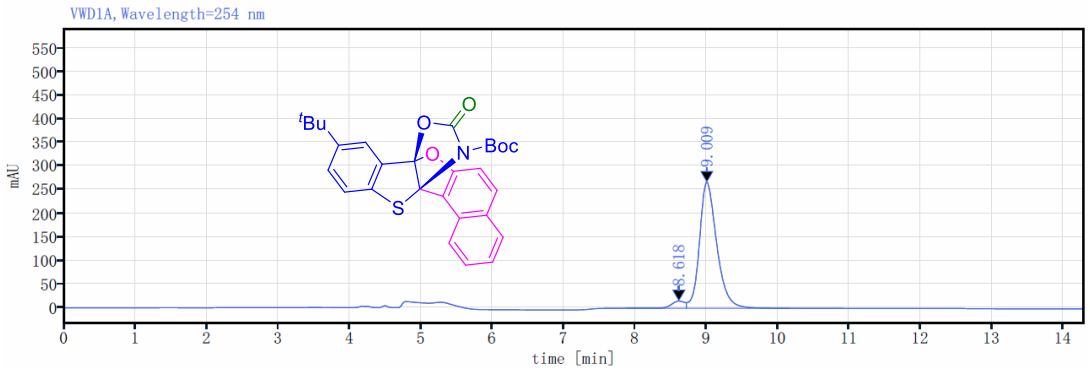


HPLC of 10b



Detector VWD1A, Wavelength=254 nm

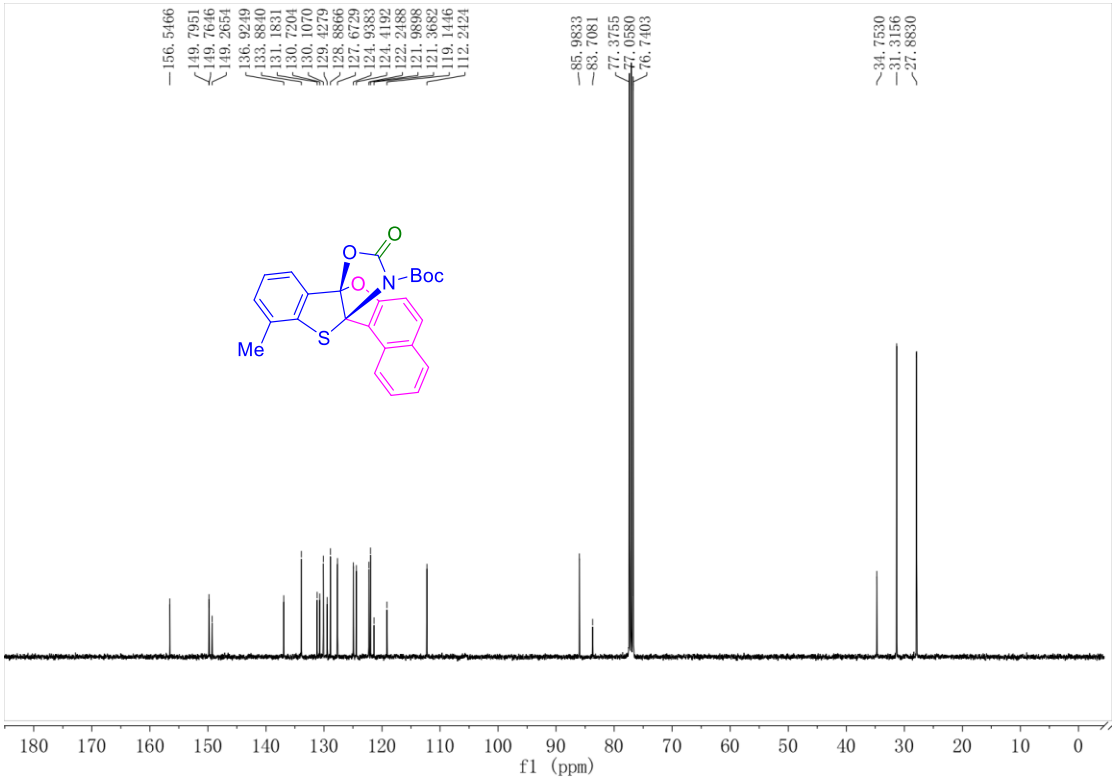
Peak	Ret.Time [min]	Area	Height	Area%
	8.861	8643.52	460.03	48.27
	9.336	9264.73	460.40	51.73
		17908.26		100.00

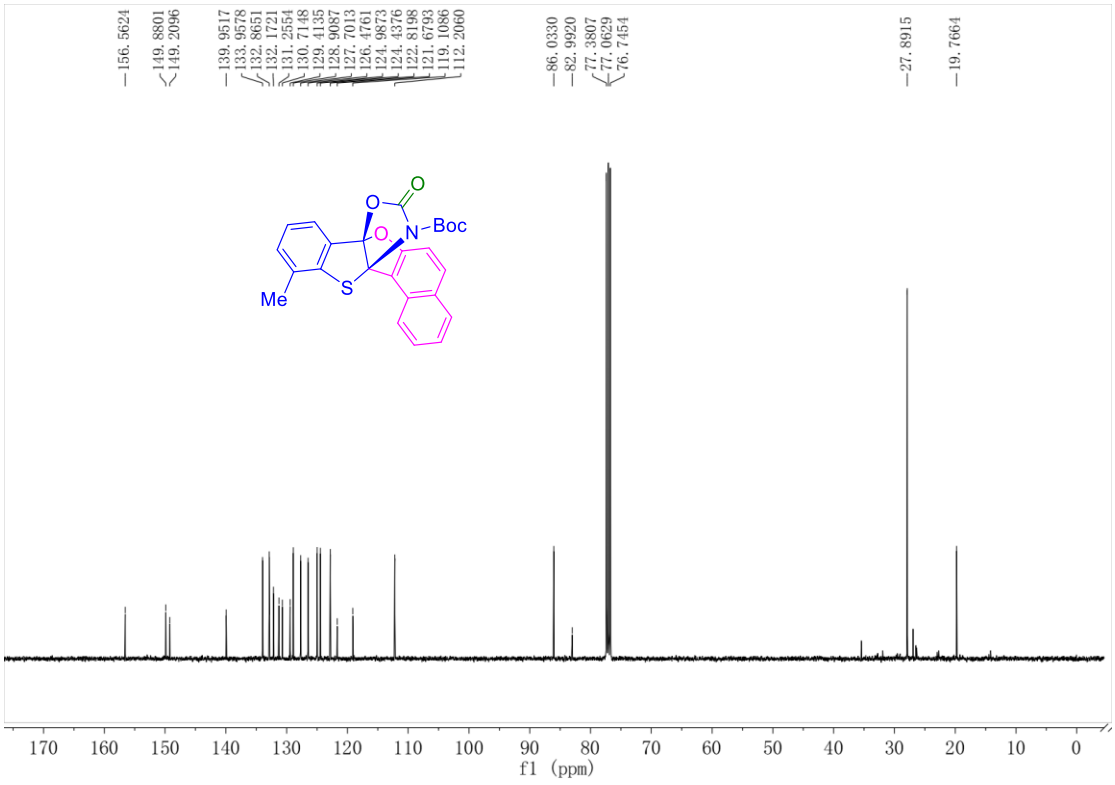


Detector VWD1A, Wavelength=254 nm

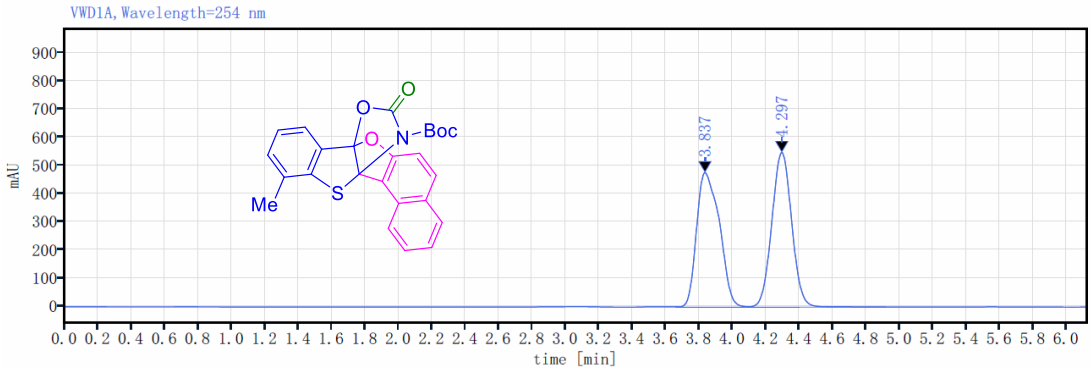
Peak	Ret.Time [min]	Area	Height	Area%
	8.618	192.71	15.03	4.12
	9.009	4489.32	266.86	95.88
		4682.04		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10c



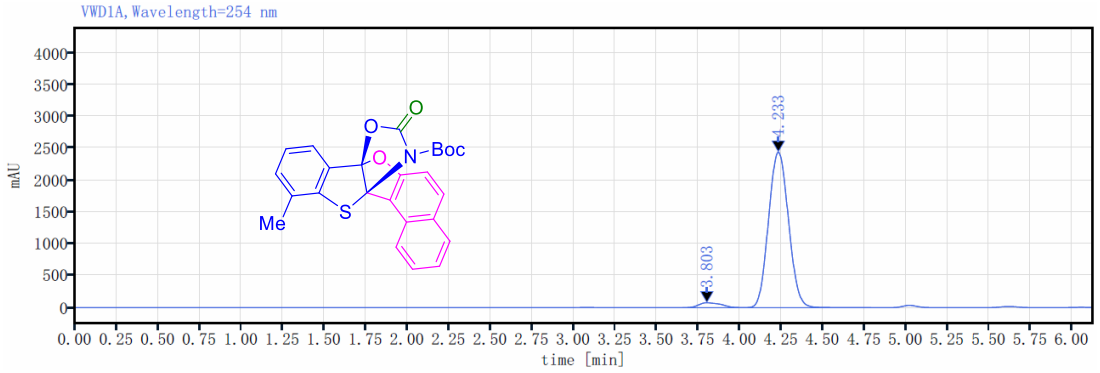


HPLC of 10c



Detector VWD1A, Wavelength=254 nm

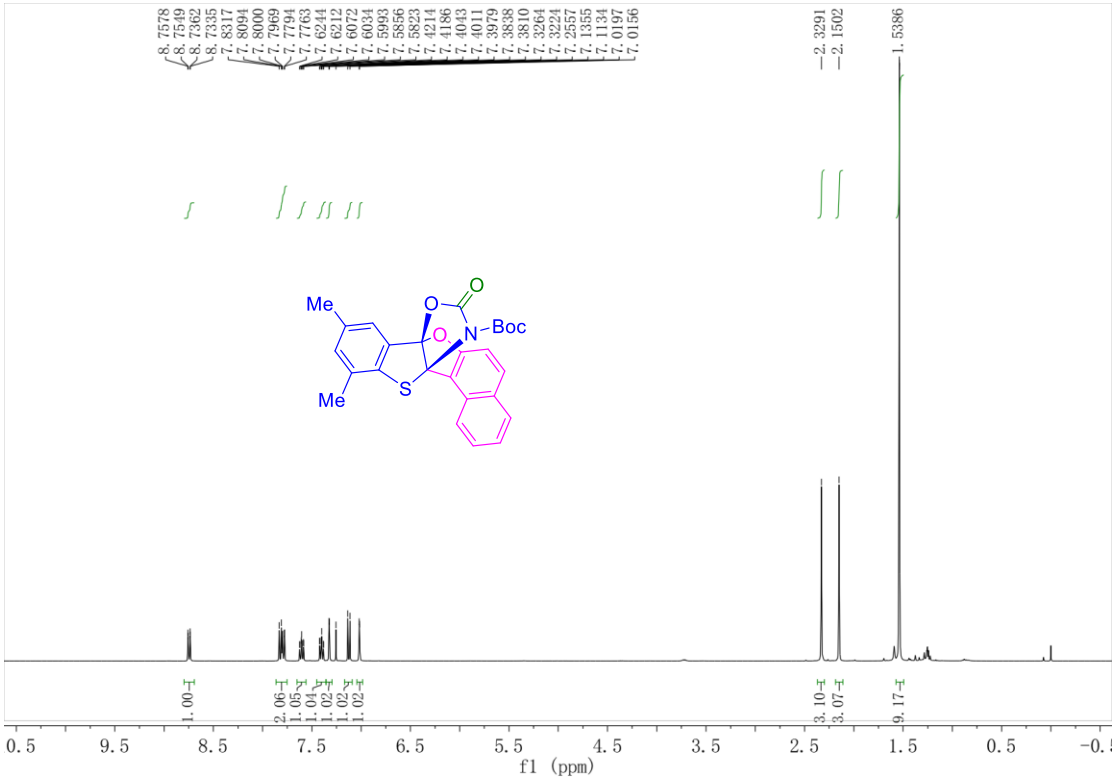
Peak	Ret.Time [min]	Area	Height	Area%
	3.837	4532.43	477.50	49.98
	4.297	4536.64	548.78	50.02
		9069.07		100.00

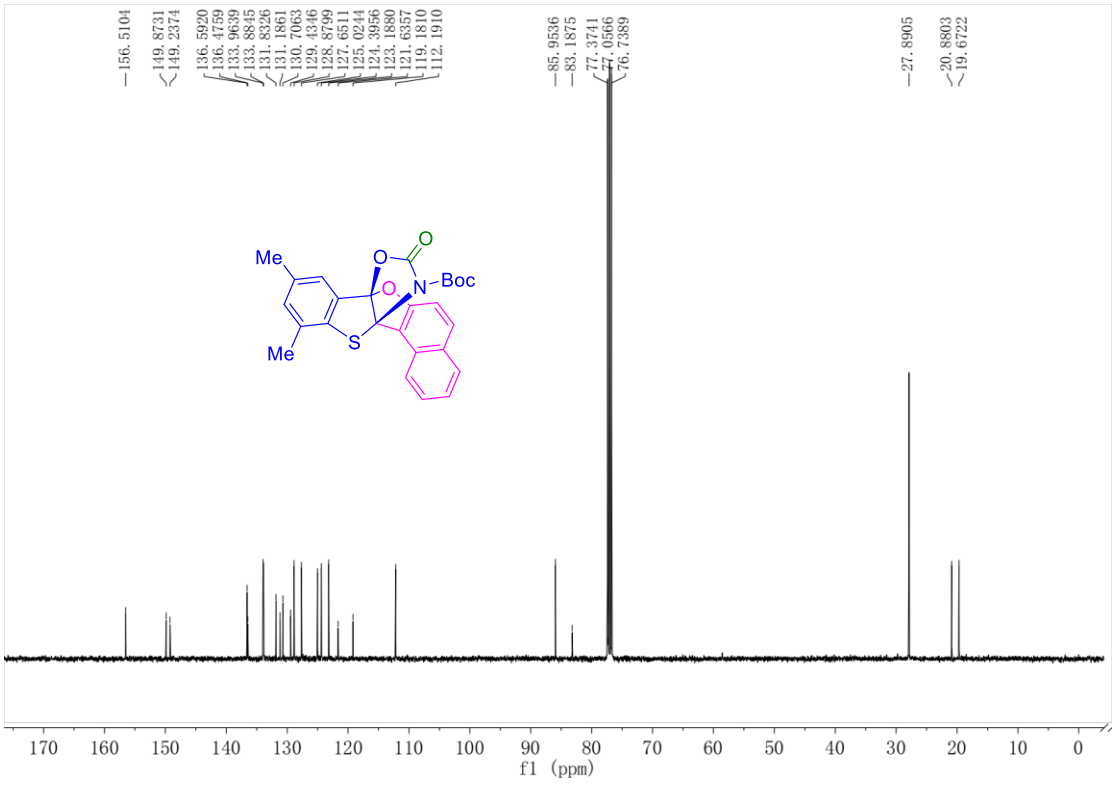


Detector VWD1A, Wavelength=254 nm

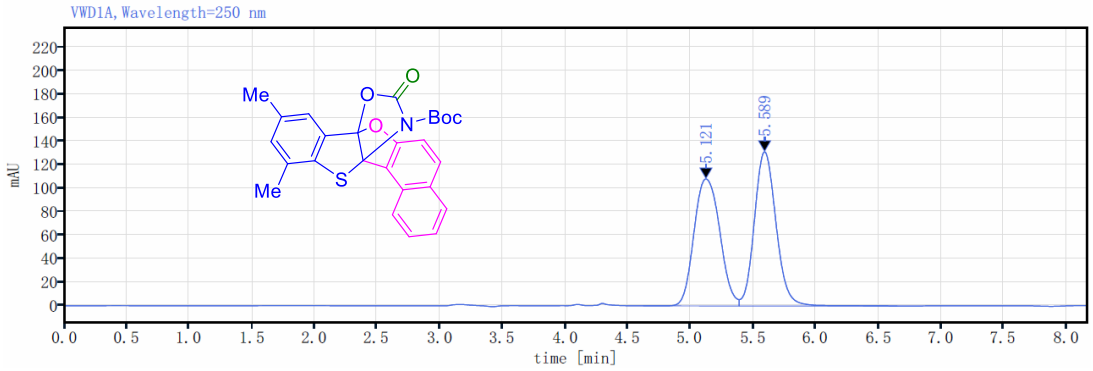
Peak	Ret.Time [min]	Area	Height	Area%
	3.803	729.56	77.81	3.45
	4.233	20409.69	2445.44	96.55
		21139.25		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10d



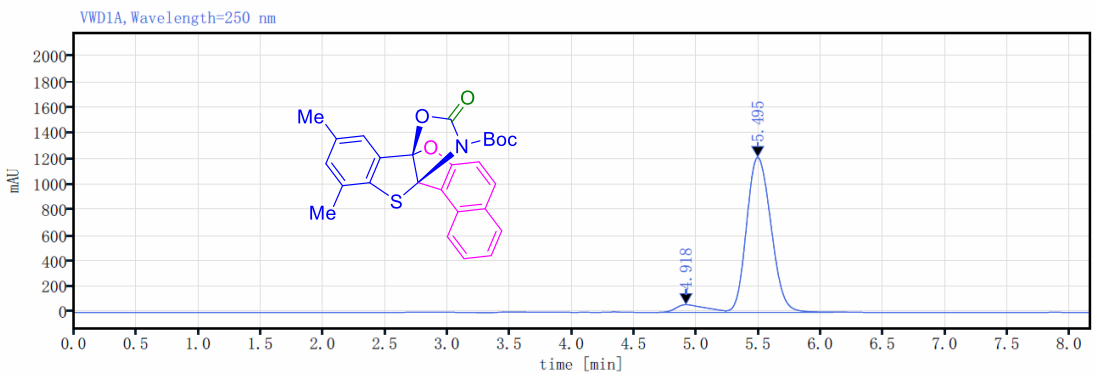


HPLC of 10d



Detector VWD1A, Wavelength=250 nm

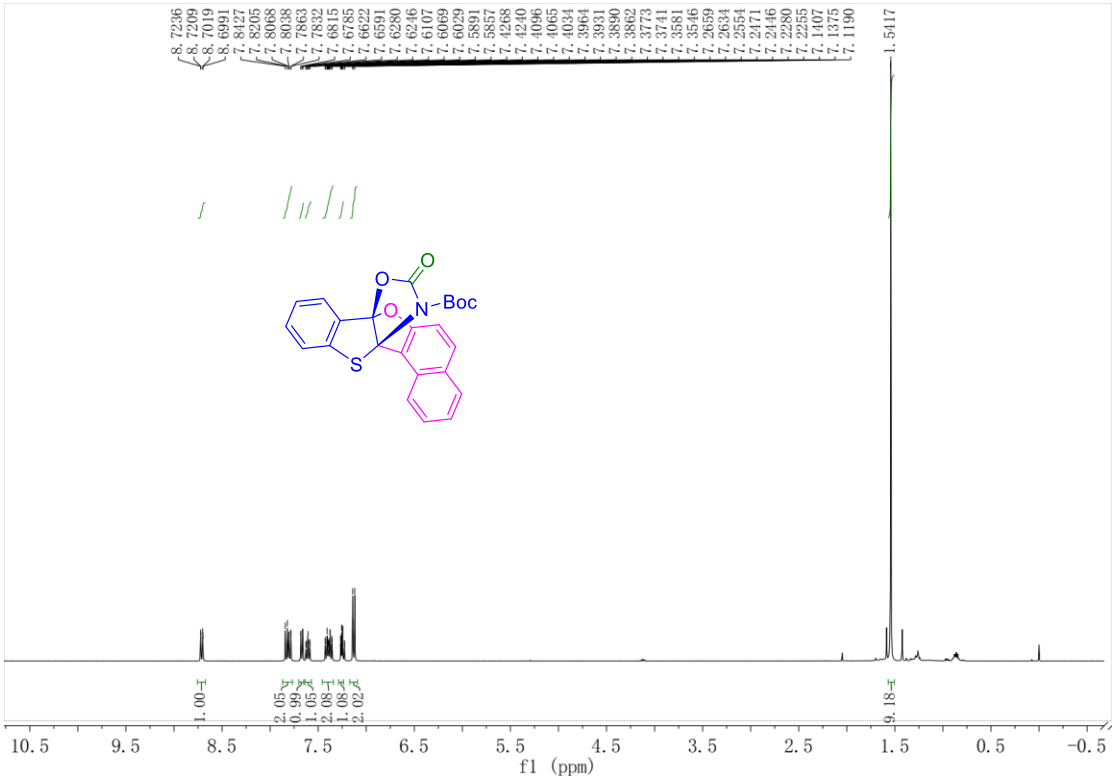
Peak	Ret.Time [min]	Area	Height	Area%
	5.121	1547.84	108.20	49.38
	5.589	1586.58	131.35	50.62
		3134.42		100.00

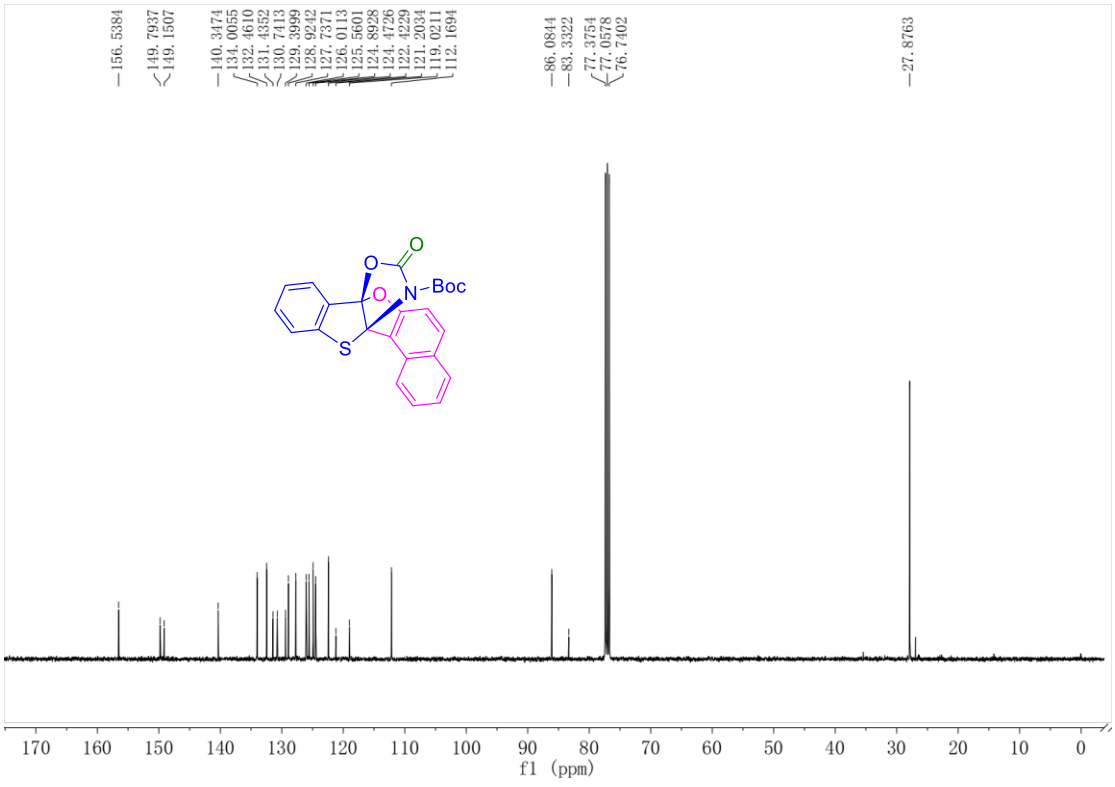


Detector VWD1A, Wavelength=250 nm

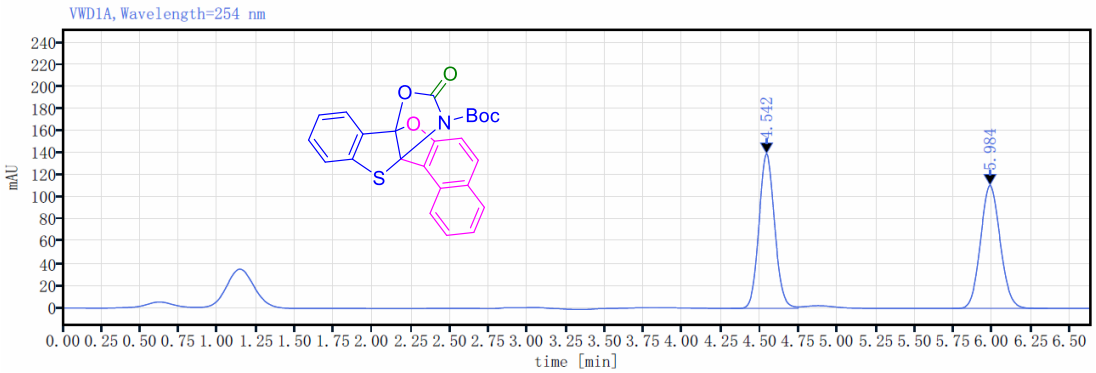
Peak	Ret.Time [min]	Area	Height	Area%
	4.918	1020.79	60.39	5.80
	5.495	16576.33	1212.10	94.20
		17597.12		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10e



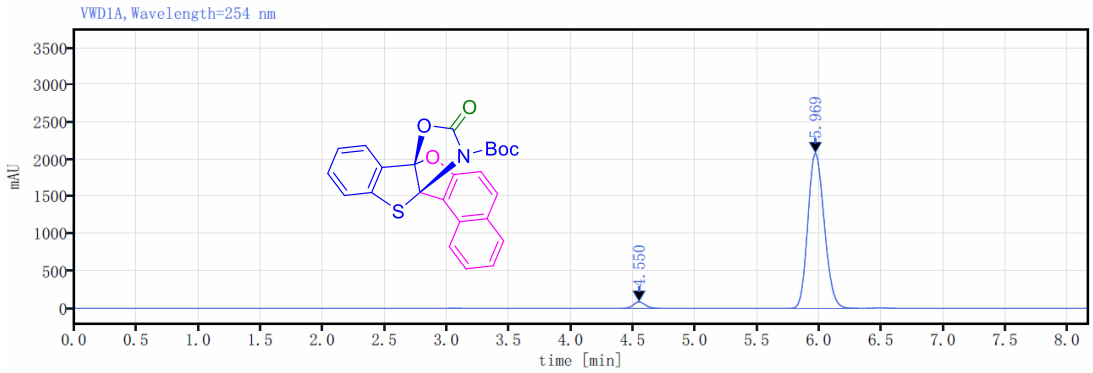


HPLC of 10e



Detector VWD1A, Wavelength=254 nm

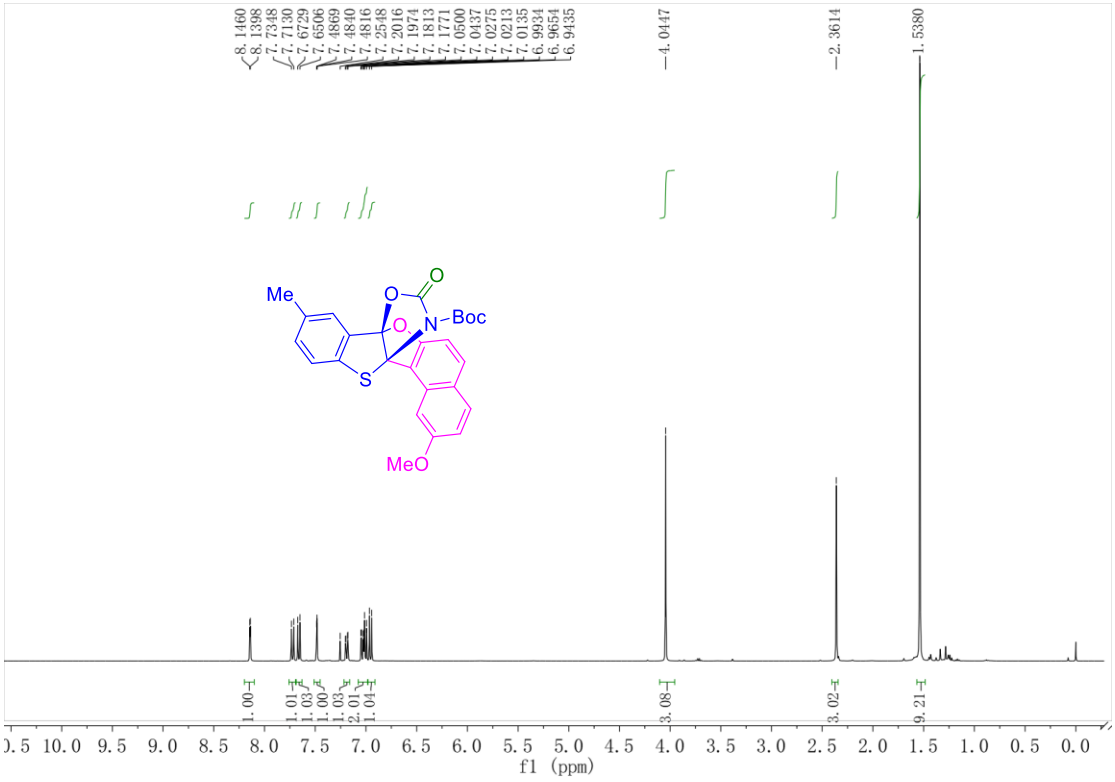
Peak	Ret.Time [min]	Area	Height	Area%
	4.542	982.99	139.53	50.03
	5.984	981.70	111.07	49.97
		1964.69		100.00

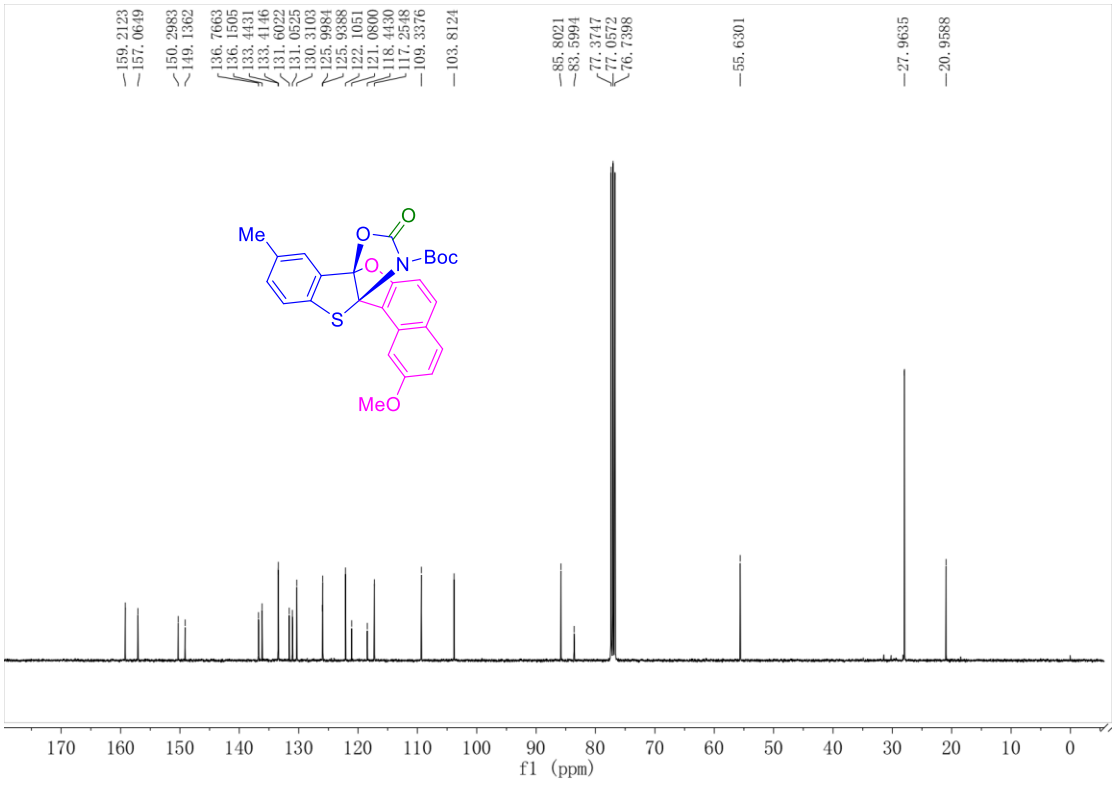


Detector VWD1A, Wavelength=254 nm

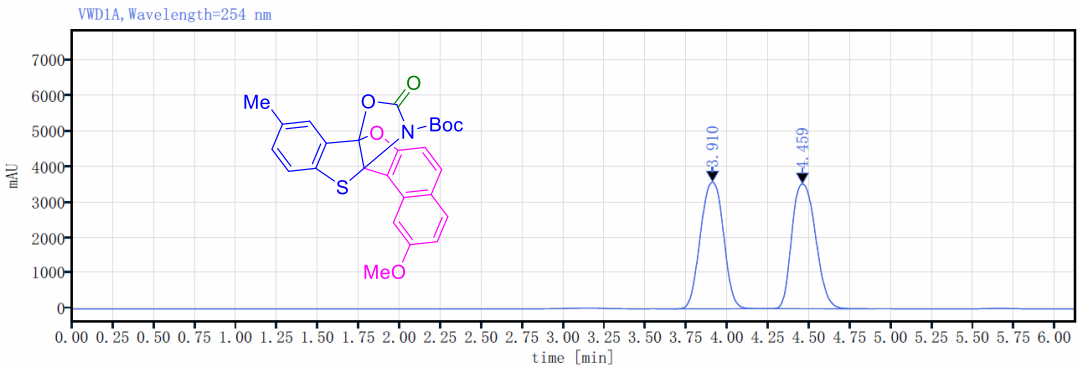
Peak	Ret.Time [min]	Area	Height	Area%
	4.550	576.26	86.15	2.92
	5.969	19179.39	2085.87	97.08
		19755.65		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10f



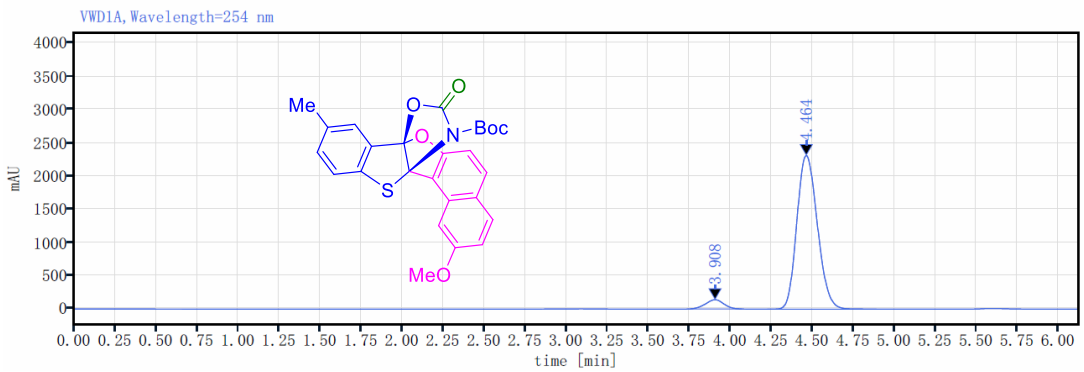


HPLC of 10f



Detector VWD1A, Wavelength=254 nm

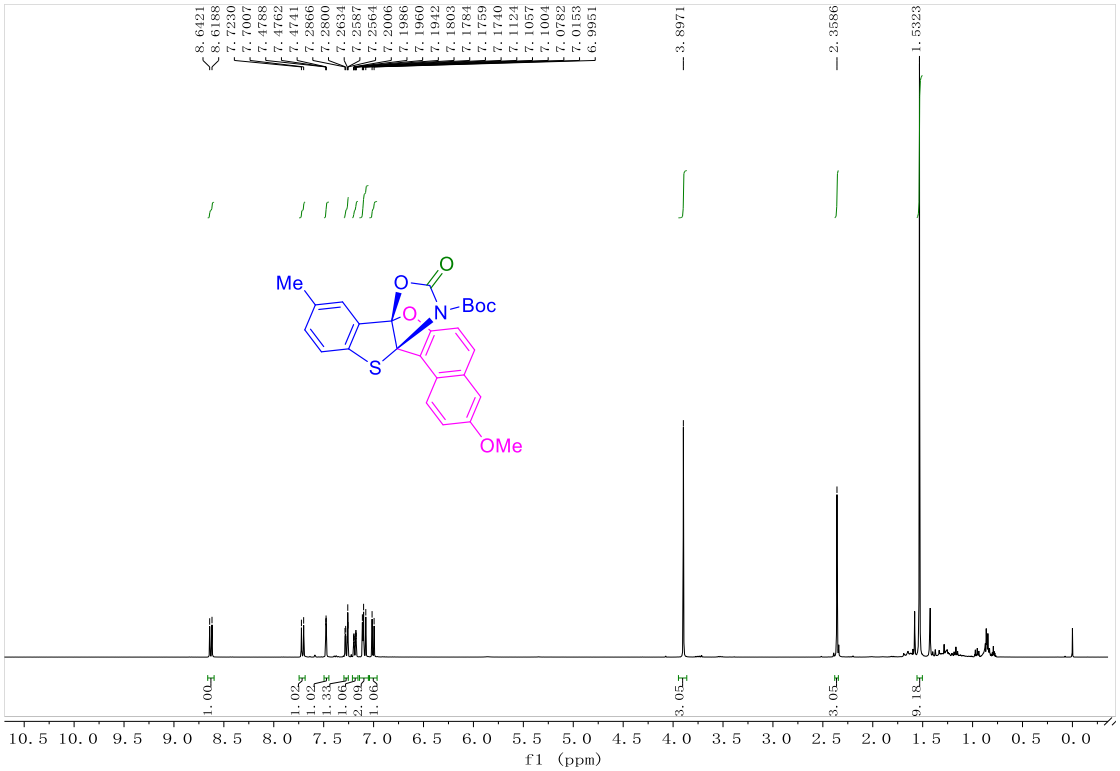
Peak	Ret.Time [min]	Area	Height	Area%
	3.910	35013.35	3575.97	49.59
	4.459	35590.30	3523.14	50.41
		70603.65		100.00

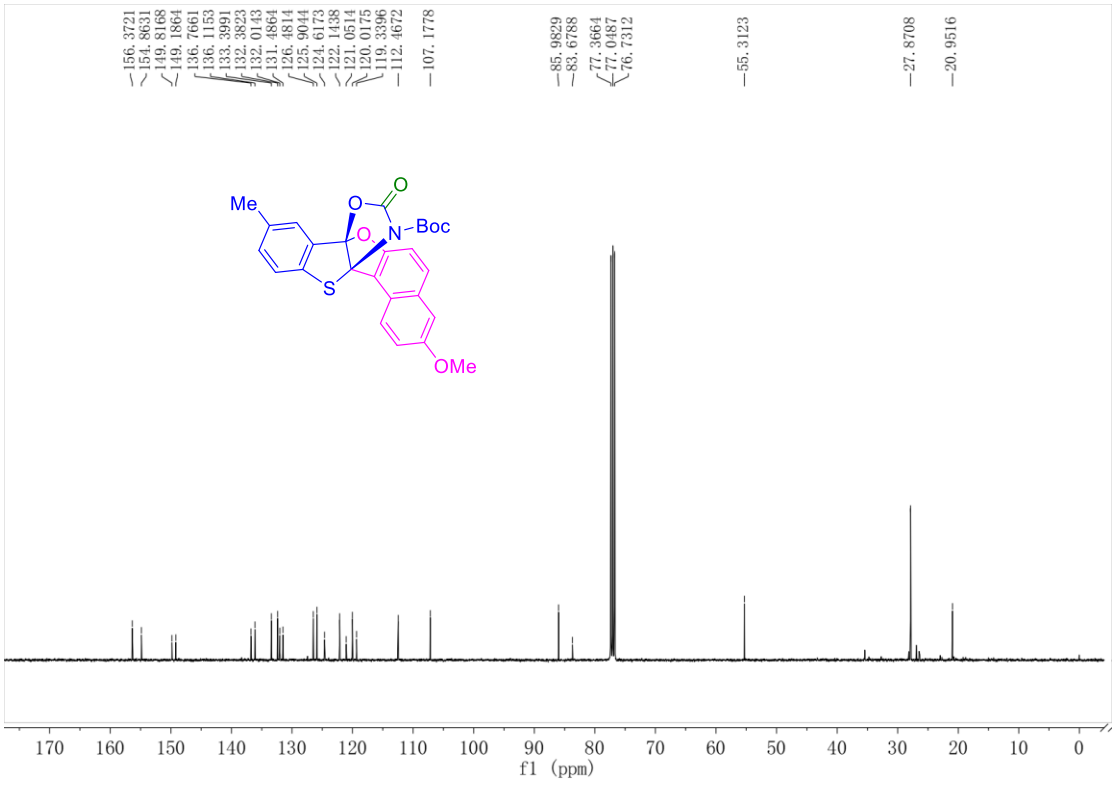


Detector VWD1A, Wavelength=254 nm

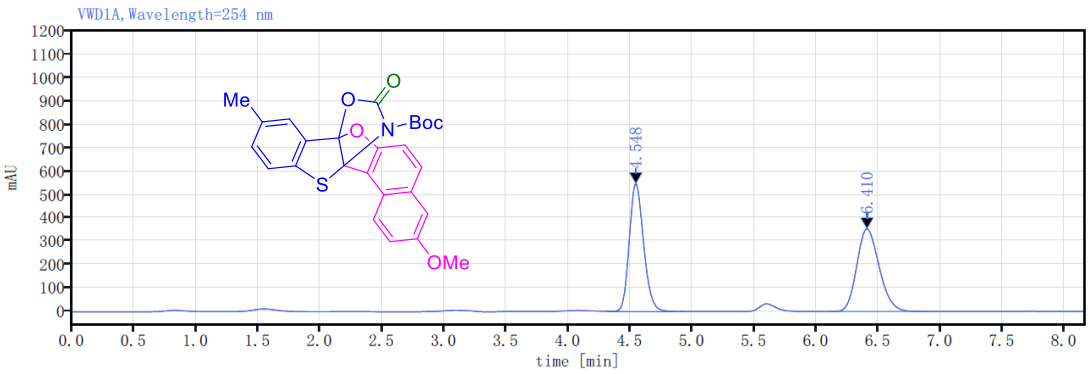
Peak	Ret.Time [min]	Area	Height	Area%
	3.908	1070.45	139.50	5.06
	4.464	20077.76	2311.30	94.94
		21148.22		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10g



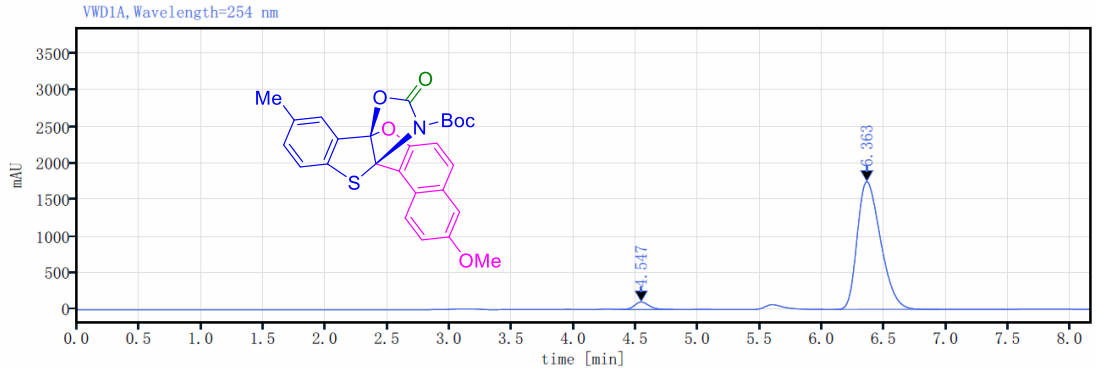


HPLC of 10g



Detector VWD1A, Wavelength=254 nm

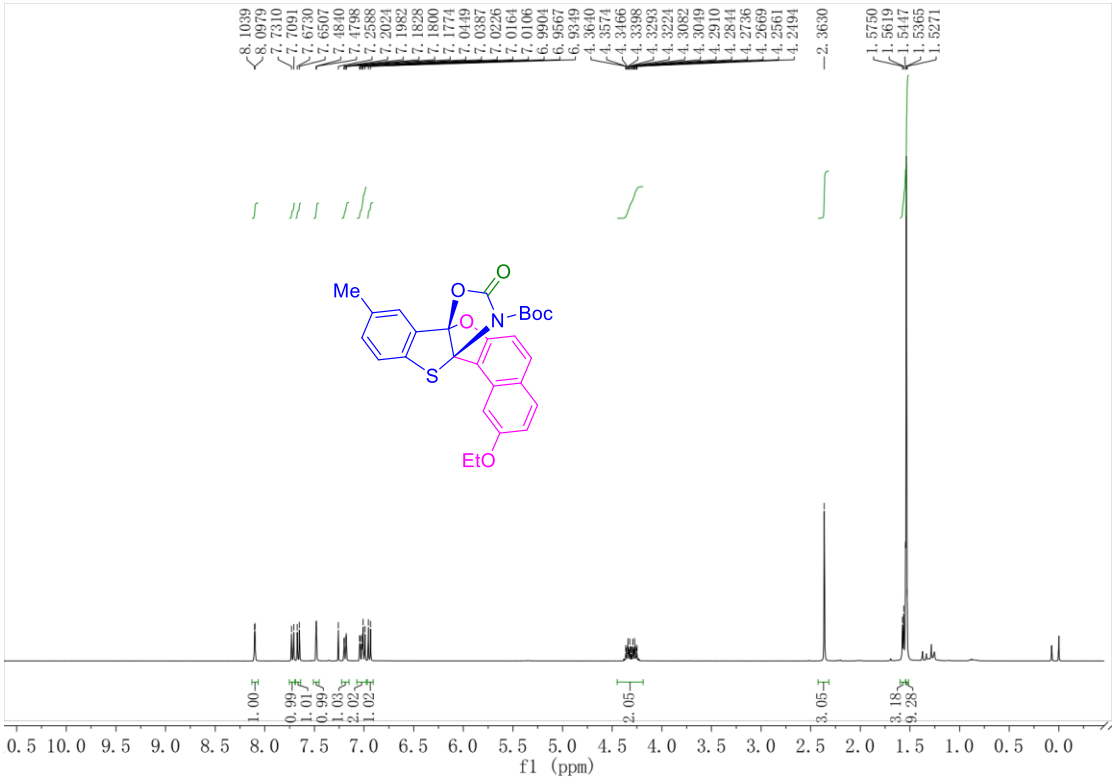
Peak	Ret.Time [min]	Area	Height	Area%
	4.548	4409.87	545.88	49.93
	6.410	4422.74	352.65	50.07
		8832.60		100.00

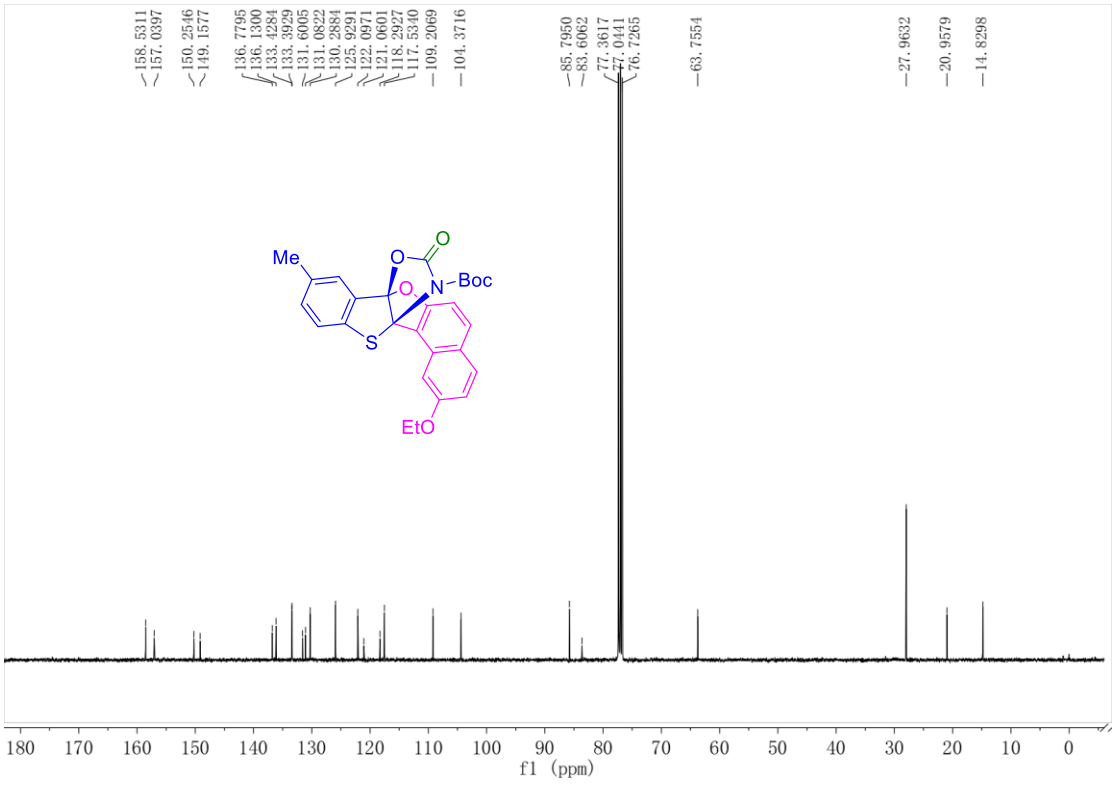


Detector VWD1A, Wavelength=254 nm

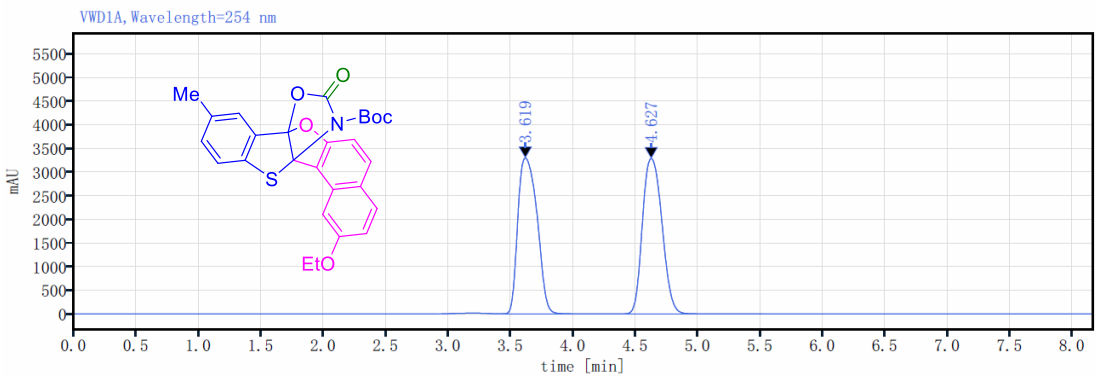
Peak	Ret.Time [min]	Area	Height	Area%
	4.547	851.49	103.36	3.59
	6.363	22860.60	1746.77	96.41
		23712.09		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10h



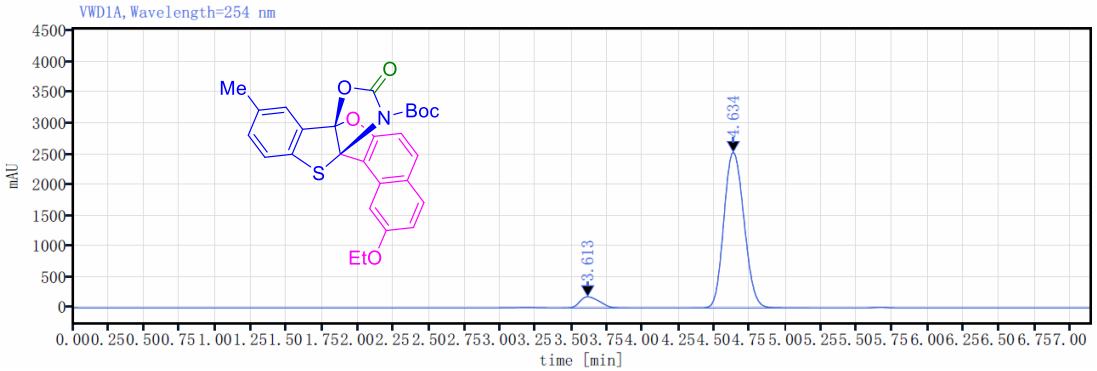


HPLC of 10h



Detector VWD1A, Wavelength=254 nm

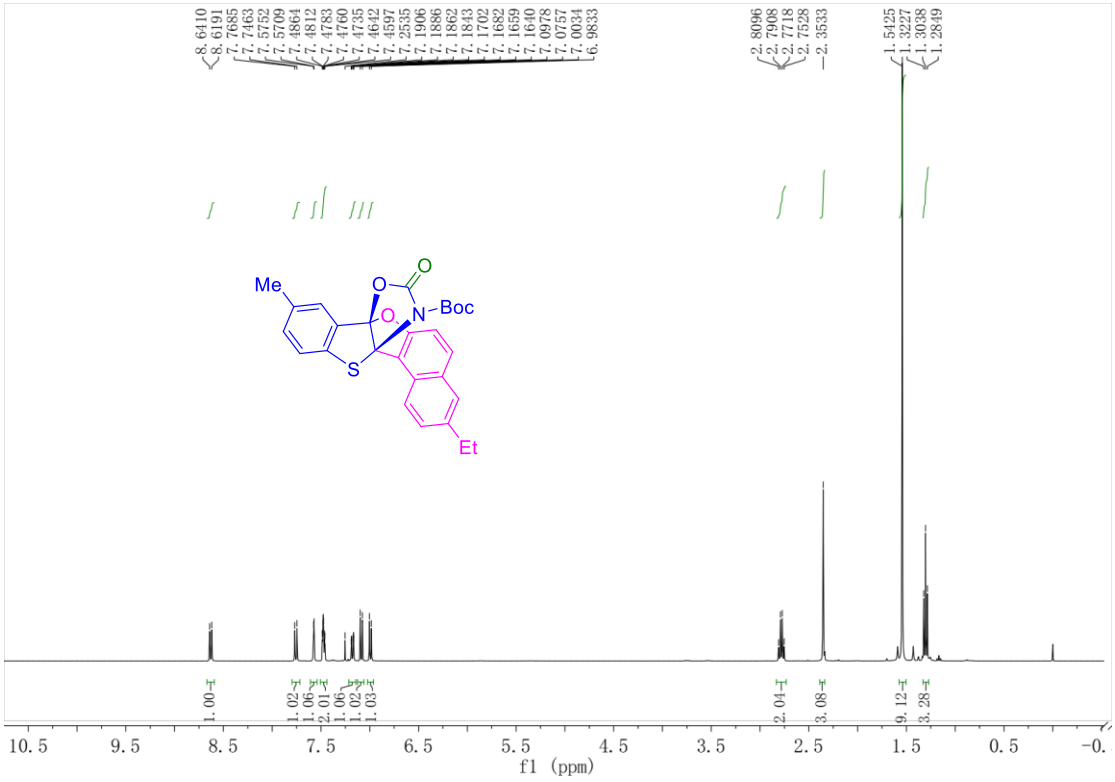
Peak	Ret.Time [min]	Area	Height	Area%
	3.619	35393.11	3297.64	49.72
	4.627	35793.94	3285.79	50.28
		71187.05		100.00

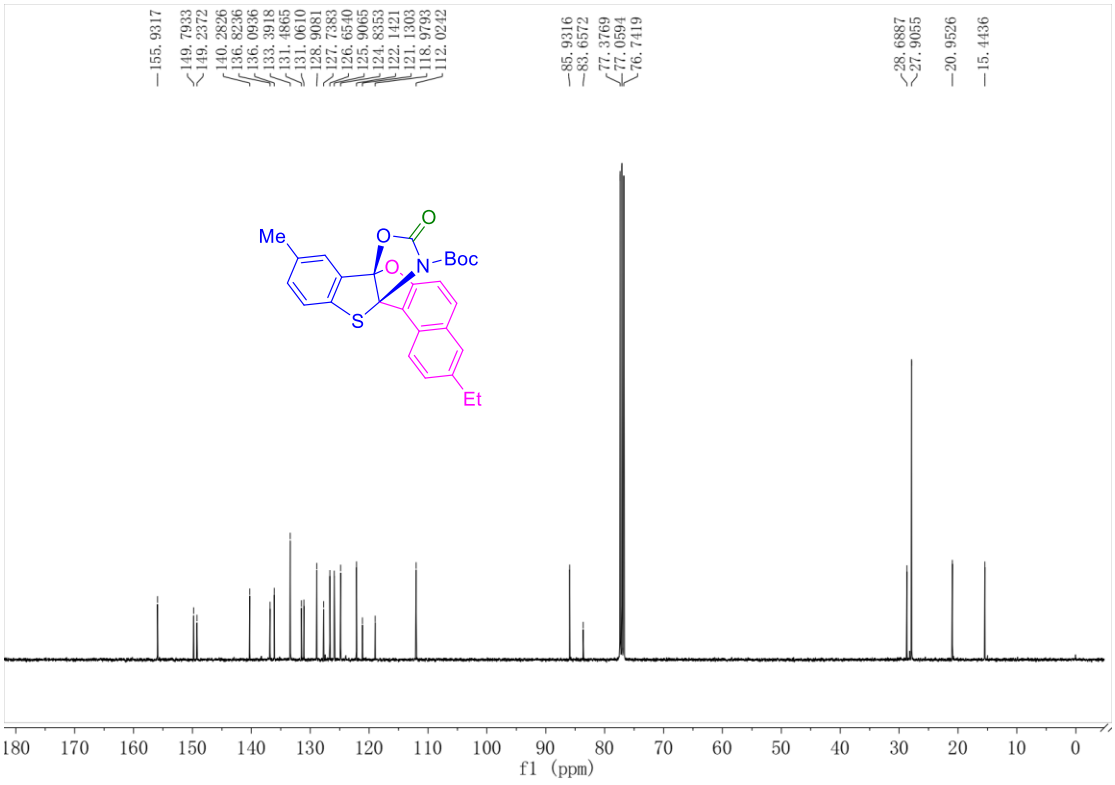


Detector VWD1A, Wavelength=254 nm

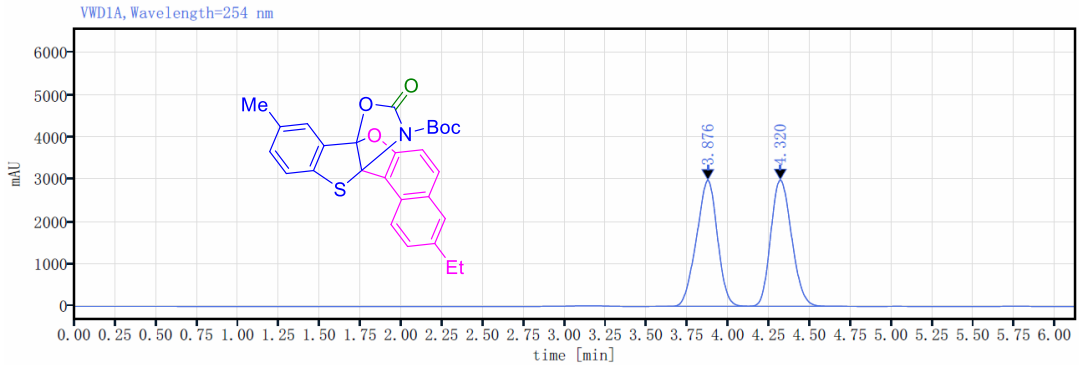
Peak	Ret.Time [min]	Area	Height	Area%
	3.613	1736.02	183.15	6.52
	4.634	24880.61	2528.14	93.48
		26616.64		100.00

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) of 10i



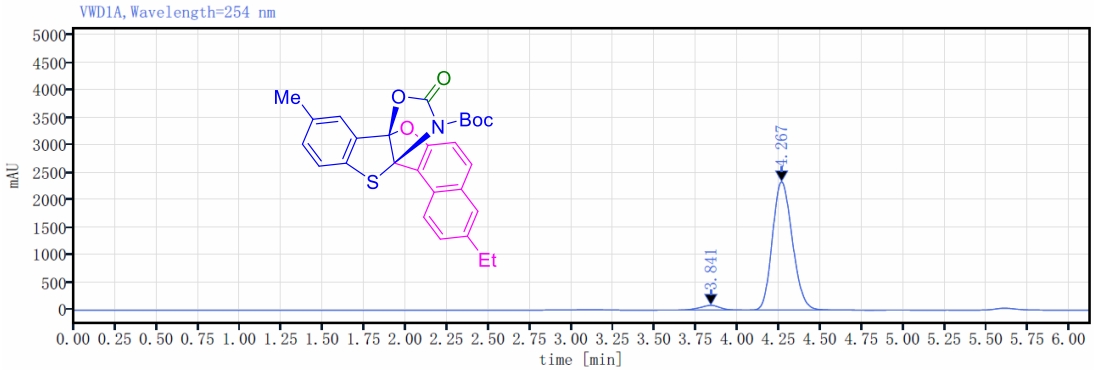


HPLC of 10i



Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	3.876	26556.79	2981.33	50.02
	4.320	26536.17	2986.33	49.98
		53092.97		100.00



Detector VWD1A, Wavelength=254 nm

Peak	Ret.Time [min]	Area	Height	Area%
	3.841	716.33	87.43	3.53
	4.267	19558.53	2335.67	96.47
		20274.86		100.00