

Enantioselective Organocatalyzed Sulfenylation of 3-Substituted Oxindoles

Xin Li,^{*} Cong Liu, Xiao-Song Xue, Jin-Pei Cheng^{*}

Contribution from the State Key Laboratory of Elemento-Organic Chemistry,

Department of Chemistry, Nankai University, Tianjin 300071, China.

E-mail: xin_li@nankai.edu.cn; chengjp@most.cn

Supporting Information

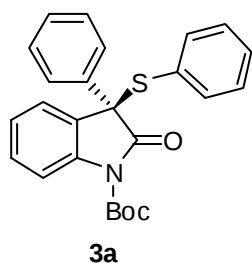
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General Information: Commercial reagents were used as received, unless otherwise stated. ^1H and ^{13}C NMR were recorded on a 400 MHz spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s= singlet, d= doublet, t= triplet, q= quartet, h= heptet, m= multiplet, br= broad. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). Mass spectra were obtained using electron ionization (EI) mass spectrometer.

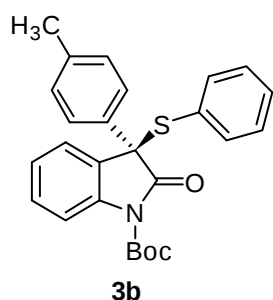
General experimental Michael reaction procedure

To a stirred solution of 3-Boc-N-phenyl oxindole **1a** 31 mg (0.1 mmol) and electrophilic sulfur reagents **2a** 25 mg (1.2 equiv.) in dry CH₂Cl₂ (2 mL) was added quinidine 3.2 mg (0.1 equiv) at -80°C. After the reaction completed, the reaction solution was concentrated *in vacuo* and the crude was purified by flash chromatography to afford the product.



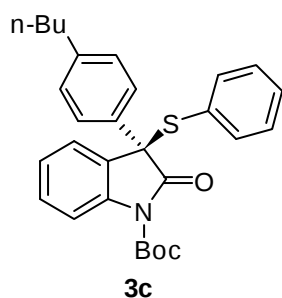
The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. $[\alpha]_D^{22}$ -64.4° (c = 2.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.69 (2H, d, *J* = 7.22 Hz), 7.56 (1H, d, *J* = 8.44 Hz), 7.44 (1H, d, *J* = 7.22 Hz),

7.40-7.34 (3H, m), 7.27-7.23 (3H, m), 7.14 (2H, d, *J* = 7.37 Hz), 7.08 (2H, t, *J* = 7.37 Hz), 1.54 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.4, 148.6, 139.3, 136.6, 135.7, 129.8, 129.3, 129.1, 128.7, 128.5, 128.4, 126.3, 124.5, 114.7, 84.1, 62.8, 28.0 ppm; HRMS (ESI⁺): calcd. for [C₂₅H₂₃NO₃S+Na]⁺ 440.1291, found 440.1290. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=3:97), 1.0 mL/min; *t_R* = 5.2 min (minor), 7.1 min (major).

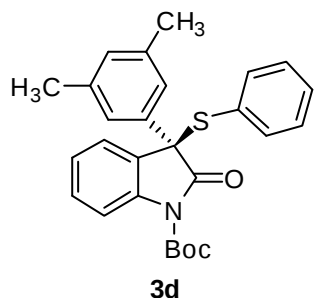


The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. $[\alpha]_D^{22}$ -173.7°

(c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.56 (3H, t, *J* = 8.29 Hz), 7.45-7.42 (1H, m), 7.25-7.22 (3H, m), 7.18 (2H, d, *J* = 8.29 Hz), 7.14 (2H, d, *J* = 7.06 Hz), 7.08 (2H, t, *J* = 7.37 Hz), 2.34 (3H, s), 1.53 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.5, 148.7, 139.3, 138.4, 136.5, 132.7, 129.7, 129.5, 129.4, 129.0, 128.8, 128.4, 128.3, 126.2, 124.4, 114.7, 84.0, 62.6, 28.0, 21.1 ppm; HRMS (ESI⁺): calcd. for [C₂₆H₂₅NO₃S+Na]⁺ 454.1447, found 454.1451. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R* = 5.1 min (minor), 7.5 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. [α]_D²² -93.8° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.61 (2H, d, *J* = 8.38 Hz), 7.57 (1H, t, *J* = 4.59 Hz), 7.48 (1H, t, *J* = 4.39 Hz), 7.28-7.25 (3H, m), 7.21 (2H, d, *J* = 7.98 Hz), 7.16 (2H, d, *J* = 7.58 Hz), 7.10 (2H, t, *J* = 7.59 Hz), 2.62 (2H, t, *J* = 7.58 Hz), 1.64-1.59 (2H, m), 1.56 (9H, s), 1.42-1.32 (2H, m), 0.94 (3H, t, *J* = 7.25 Hz); ¹³C NMR (100.6MHz, CDCl₃): δ 173.6, 148.7, 143.4, 139.3, 136.5, 132.8, 129.7, 129.5, 129.0, 128.9, 128.7, 128.4, 128.3, 126.3, 124.4, 114.7, 84.1, 62.6, 35.3, 34.5, 28.0, 22.4, 14.0 ppm; HRMS (ESI⁺): calcd. for [C₂₉H₃₁NO₃S+Na]⁺ 496.1917, found 496.1922. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R* = 4.5 min (minor), 6.3 min (major).

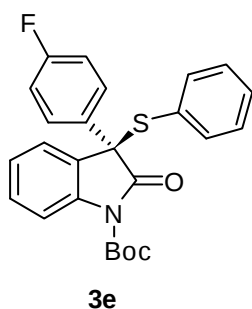


The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield.

$[\alpha]_D^{15}$ -80.3° (c = 1.5, CHCl₃); ¹H NMR (400MHz, CDCl₃):

δ 7.57 (1H, t, *J* = 4.55 Hz), 7.47 (1H, t, *J* = 4.40 Hz), 7.30

-7.25 (5H, m), 7.17 (2H, d, *J* = 7.28 Hz), 7.11 (2H, d, *J* = 7.28 Hz), 7.00 (1H, s), 2.34 (6H, s), 1.57 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.6, 148.7, 139.3, 138.3, 136.6, 135.5, 130.3, 129.7, 129.4, 129.1, 128.9, 128.4, 126.3, 126.0, 124.5, 114.6, 84.0, 62.9, 28.0, 21.5 ppm; HRMS (ESI⁺): calcd. for [C₂₇H₂₇NO₃S+Na]⁺ 468.1604, found 468.1602. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R*= 4.4 min (minor), 4.9 min (major).



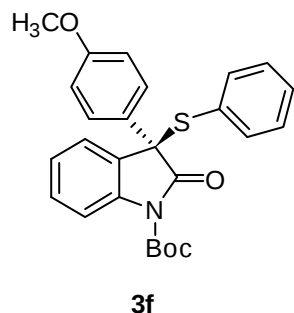
The sulfenyl product was synthesized according to the general procedure as colorless oil in 85% overall yield. $[\alpha]_D^{22}$ -107.1° (c

= 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.72 (2H, t, *J* =

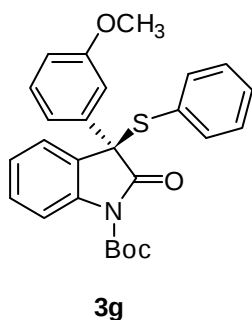
6.98 Hz), 7.59 (1H, d, *J* = 8.80 Hz), 7.45-7.43 (1H, m),

7.31-7.27 (3H, m), 7.16-7.07 (6H, m), 1.56 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.3, 164.0, 161.5, 148.5, 139.3, 136.6, 131.4, 130.5, 130.4, 129.9, 129.3, 129.2, 128.5, 128.3, 126.2, 124.6, 115.6, 115.4, 114.9, 84.3, 62.1, 28.0 ppm; HRMS (ESI⁺): calcd. for [C₂₅H₂₂FO₃S+Na]⁺ 458.1197, found 458.1201. The enantiomeric excess

was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 5.0 min (minor), 6.1 min (major).

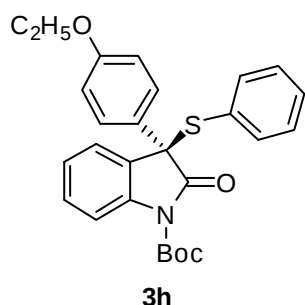


The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. $[\alpha]_D^{22}$ -104.1° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.64 (2H, d, J = 8.80 Hz), 7.58 (1H, d, J = 6.68 Hz), 7.46 (1H, d, J = 4.58 Hz), 7.28-7.25 (3H, m), 7.17-7.09 (4H, m), 6.93 (2H, d, J = 8.80 Hz), 3.83 (3H, s), 1.56 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.6, 159.7, 148.7, 139.3, 136.5, 129.8, 129.5, 129.0, 128.8, 128.4, 127.5, 126.3, 124.4, 114.7, 114.0, 84.1, 62.3, 55.3, 28.0 ppm; HRMS (ESI⁺): calcd. for [C₂₆H₂₅NO₄S+Na]⁺ 470.1396, found 470.1401. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 10.1 min (minor), 14.8 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. $[\alpha]_D^{22}$ -107.4° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.58 (1H, d, J = 7.59 Hz), 7.47 (1H, d, J = 6.68 Hz), 7.33 -7.25 (6H, m), 7.18 (2H, d, J = 7.28 Hz), 7.11 (2H, t, J = 7.59 Hz), 6.91 (1H, d, J = 7.83 Hz), 3.85 (3H, s), 1.58 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.3, 159.7, 148.6, 139.3, 137.2,

136.6, 129.8, 129.6, 129.4, 129.1, 128.7, 128.4, 126.3, 124.5, 120.7, 114.7, 114.5, 114.1, 84.1, 62.7, 55.4, 28.0 ppm; HRMS (ESI⁺): calcd. for [C₂₆H₂₅NO₄S+Na]⁺ 470.1396, found 470.1394. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R*= 7.6 min (minor), 10.7 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 83% overall yield.

[α]_D²² -53.7° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃):

δ 7.61 (2H, d, *J* = 8.80 Hz), 7.57 -7.55 (1H, m), 7.44 (1H, t,

J = 4.55 Hz), 7.26 -7.23 (3H, m), 7.13 (2H, d, *J* = 7.28 Hz), 7.08 (2H, t, *J* = 7.59 Hz),

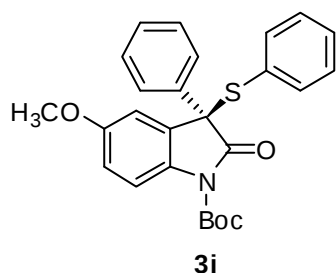
6.89 (2H, d, *J* = 8.80 Hz), 4.03 (2H, q, *J* = 6.98, 13.96 Hz), 1.53 (9H, s), 1.41 (3H, t, *J*

= 6.98 Hz); ¹³C NMR (100.6MHz, CDCl₃): δ 173.6, 159.1, 148.7, 139.3, 136.5, 129.7,

129.6, 129.0, 128.8, 128.4, 127.3, 126.3, 124.4, 114.7, 114.5, 84.1, 63.5, 62.3, 28.0,

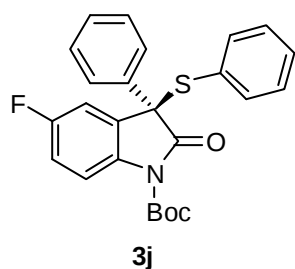
14.8 ppm; HRMS (ESI⁺): calcd. for [C₂₇H₂₇NO₄S+Na]⁺ 484.1553, found 484.1550.

The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R*= 7.4 min (minor), 11.5 min (major).



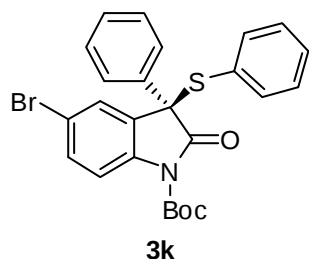
The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield.

$[\alpha]_D^{22}$ -95.5° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.69 (2H, d, *J* = 7.28 Hz), 7.50 (1H, d, *J* = 8.95 Hz), 7.41-7.34 (3H, m), 7.26 (1H, t, *J* = 7.28 Hz), 7.18 (2H, d, *J* = 6.98 Hz), 7.11 (2H, t, *J* = 7.59 Hz), 6.94 (1H, d, *J* = 2.73 Hz), 6.81-6.78 (1H, m), 3.81 (3H, s), 1.53 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.4, 156.8, 148.7, 136.5, 135.7, 132.8, 129.9, 129.8, 129.3, 128.7, 128.5, 115.8, 114.8, 111.4, 84.0, 63.2, 55.8, 28.0 ppm; HRMS (ESI⁺): calcd. for [C₂₆H₂₅NO₄S+Na]⁺ 470.1396, found 470.1393. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R* = 8.6 min (minor), 10.6 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 91% overall yield.

$[\alpha]_D^{22}$ -89.7° (c = 0.67, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.67 (2H, d, *J* = 7.20 Hz), 7.58-7.54 (1H, m), 7.44-7.40 (2H, m), 7.38-7.34 (1H, m), 7.30-7.26 (2H, m), 7.15-7.10 (4H, m), 6.95 (1H, t, *J* = 8.76 Hz), 1.54 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.1, 1641.1, 158.6, 148.6, 136.6, 136.4, 135.1, 130.1, 129.0, 128.9, 128.8, 128.6, 128.3, 128.2, 116.2, 116.0, 115.7, 113.4, 113.1, 84.4, 62.8, 28.0, 26.3 ppm; HRMS (ESI⁺): calcd. for [C₂₅H₂₂FNO₃S+Na]⁺ 458.1197, found 458.1199. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R* = 5.5 min (minor), 6.9 min (major).



The sulfenyl product was synthesized according to the general procedure as white solid in 93% overall yield.

$[\alpha]_D^{22}$ -18.7° (c = 1.0, CHCl₃); ¹H NMR (300MHz, CDCl₃):

δ 7.57 (2H, d, *J* = 6.50 Hz), 7.41-7.38 (2H, m), 7.33-7.22

(4H, m), 7.18 (1H, t, *J* = 6.91 Hz), 7.09-7.00 (4H, m), 1.44 (9H, s); ¹³C NMR (75MHz,

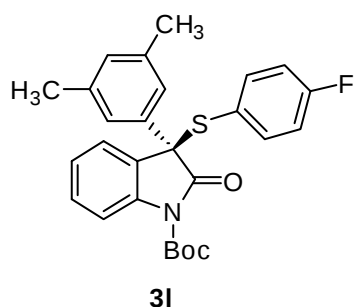
CDCl₃): δ 172.6, 148.5, 138.3, 136.7, 135.1, 132.0, 131.1, 130.1, 129.1, 129.0, 128.9,

128.8, 128.6, 128.4, 117.4, 116.5, 84.6, 62.6, 28.0 ppm; HRMS (ESI⁺): calcd. for

[C₂₅H₂₂BrNO₃S+Na]⁺ 518.0396, found 518.0399. The enantiomeric excess was

determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98),

1.0 mL/min; *t_R* = 5.6 min (minor), 7.1 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield.

$[\alpha]_D^{22}$ -149.5° (c = 1.0, CHCl₃); ¹H NMR (400MHz,

CDCl₃): δ 7.59-7.56 (1H, m), 7.49-7.46 (1H, m),

7.31-7.25 (4H, m), 7.16-7.12 (2H, m), 7.00 (1H, s), 6.80 (2H, t, *J* = 8.51 Hz), 2.33

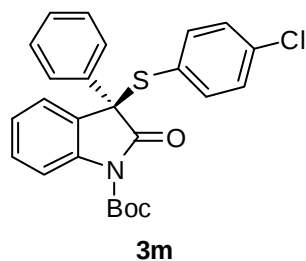
(6H, s), 1.57 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.5, 165.1, 162.7, 148.5,

139.2, 138.7, 138.6, 138.3, 135.2, 130.3, 129.1, 129.0, 126.2, 126.0, 124.8, 124.6,

115.6, 115.4, 114.7, 84.3, 62.9, 28.0, 21.4 ppm; HRMS (ESI⁺): calcd. for

[C₂₇H₂₆FNO₃S+Na]⁺ 486.1510, found 486.1514. The enantiomeric excess was

determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 4.2 min (minor), 4.6 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 98% overall yield.

$[\alpha]_D^{22}$ -98.6° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃):

δ 7.70 (2H, d, J = 6.62 Hz), 7.61 (1H, d, J = 7.57 Hz), 7.48

(1H, d, J = 7.25 Hz), 7.43-7.37 (3H, m), 7.32-7.27 (2H, m), 7.09 (4H, s), 1.58 (9H, s);

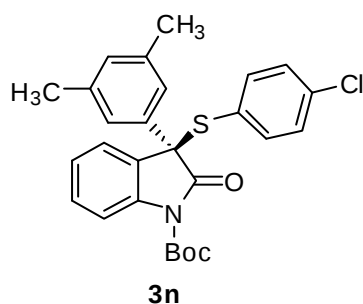
¹³C NMR (100.6MHz, CDCl₃): δ 173.2, 148.4, 139.3, 137.8, 136.5, 135.3, 129.3,

128.7, 128.5, 128.4, 127.9, 126.2, 124.6, 114.9, 84.3, 62.8, 28.0 ppm; HRMS (ESI⁺):

calcd. for [C₂₅H₂₂ClNO₃S+Na]⁺ 474.0901, found 474.0902. The enantiomeric excess

was determined by HPLC with an OD-H column at 210 nm (2-propanol:

hexane=2:98), 1.0 mL/min; t_R = 5.8 min (minor), 9.9 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 98% overall yield.

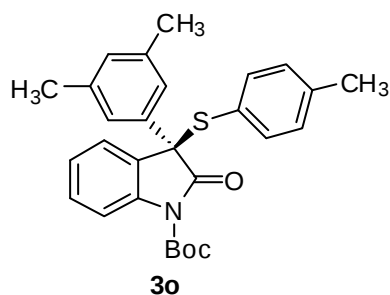
$[\alpha]_D^{22}$ -26.0° (c = 1.0, CHCl₃); ¹H NMR (300MHz,

CDCl₃): δ 7.49 (1H, d, J = 7.50 Hz), 7.36 (1H, d, J =

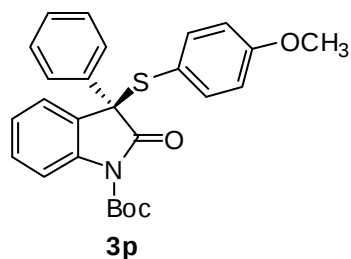
7.15 Hz), 7.21-7.12 (4H, m), 6.97 (4H, s), 6.88 (1H, s), 2.22 (6H, s), 1.46 (9H, s); ¹³C

NMR (75MHz, CDCl₃): δ 173.3, 148.6, 139.3, 138.4, 137.8, 136.5, 135.3, 130.4,

129.3, 129.0, 128.7, 128.1, 126.3, 126.1, 124.7, 114.8, 84.4, 63.0, 28.1, 21.5ppm;
 HRMS (EI⁺): calcd. for [C₂₇H₂₆ClNO₃S] 479.1322, found 479.1327. The
 enantiomeric excess was determined by HPLC with an OD-H column at 210 nm
 (2-propanol: hexane=2:98), 1.0 mL/min; *t_R*= 4.2 min (minor), 4.6 min (major).

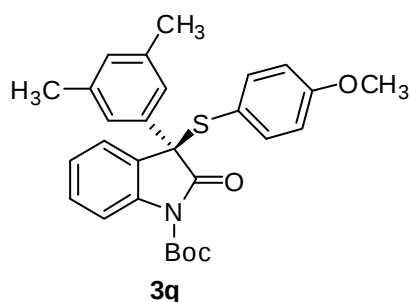


The sulfenyl product was synthesized according to
 the general procedure as colorless oil in 99% overall
 yield. $[\alpha]_D^{22}$ -83.1° (c = 1.0, CHCl₃); ¹H NMR
 (400MHz, CDCl₃): δ 7.59 (1H, d, *J* = 9.08 Hz), 7.46
 (1H, d, *J* = 9.08 Hz), 7.30-7.25 (4H, m), 7.04 (2H, d, *J* = 8.05 Hz), 6.99 (1H, s), 6.91
 (2H, d, *J* = 7.99 Hz), 2.34 (6H, s), 2.27(3H, s), 1.57(9H, s); ¹³C NMR (100.6MHz,
 CDCl₃): δ 173.6, 148.7, 139.9, 139.3, 138.2, 136.5, 135.6, 130.2, 129.4, 129.2, 128.9,
 126.4, 126.2, 126.1, 125.9, 124.5, 114.6, 83.9, 62.9, 28.0, 21.4, 21.2 ppm; HRMS
 (EI⁺): calcd. for [C₂₈H₂₉NO₃S] 459.1868, found 459.1873. The enantiomeric excess
 was determined by HPLC with an AD-H column at 210 nm (2-propanol:
 hexane=2:98), 1.0 mL/min; *t_R*= 5.4 min (minor), 7.0 min (major).

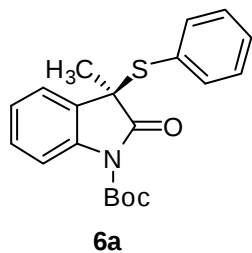


The sulfenyl product was synthesized according to the
 general procedure as colorless oil in 99% overall yield.
 $[\alpha]_D^{22}$ -108.8° (c = 0.67, CHCl₃); ¹H NMR (400MHz,

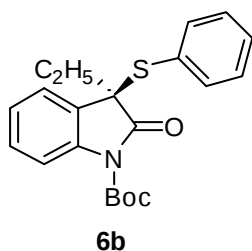
CDCl₃): δ 7.71 (2H, d, J = 7.25 Hz), 7.60 (1H, d, J = 7.25 Hz), 7.45 (1H, d, J = 6.94 Hz), 7.42-7.35 (3H, m), 7.30-7.24 (2H, m), 7.08 (2H, d, J = 8.83 Hz), 6.63 (2H, d, J = 8.83 Hz), 3.74 (3H, s), 1.57 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.5, 161.0, 148.7, 139.3, 138.2, 135.7, 129.0, 128.9, 128.6, 128.5, 128.4, 126.2, 124.4, 120.1, 114.8, 113.9, 84.1, 62.9, 55.2, 28.0 ppm; HRMS (ESI⁺): calcd. for [C₂₆H₂₅NO₄S+Na]⁺ 470.1396, found 470.1392. The enantiomeric excess was determined by HPLC with an AD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 12.1 min (minor), 21.9 min (major).



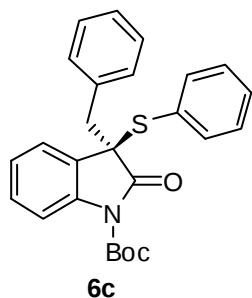
The sulfenyl product was synthesized according to the general procedure as colorless oil in 95% overall yield. $[\alpha]_D^{22}$ -84.5° (c = 1.0, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.56 (1H, d, J = 8.52 Hz), 7.43 (1H, d, J = 8.52 Hz), 7.26-7.23 (4H, m), 7.04 (2H, d, J = 8.52 Hz), 6.96 (1H, s), 6.60 (2H, d, J = 8.52 Hz), 3.71 (3H, s), 2.31 (6H, s), 1.54 (9H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 173.8, 161.0, 148.7, 139.3, 138.2, 138.1, 135.5, 130.2, 129.3, 128.9, 126.2, 126.1, 124.5, 120.2, 114.7, 113.9, 84.0, 63.0, 55.2, 28.0, 21.5 ppm; HRMS (ESI⁺): calcd. for [C₂₈H₂₉NO₄S+Na]⁺ 498.1709, found 498.1701. The enantiomeric excess was determined by HPLC with an AD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 8.4 min (minor), 10.9 min (major).



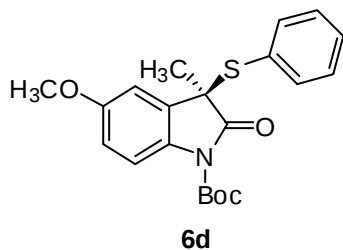
The sulfenyl product was synthesized according to the general procedure as little yellow oil in 83% overall yield. $[\alpha]_D^{22}$ -3.8° ($c = 0.6$, CHCl_3); ^1H NMR (400MHz, CDCl_3): δ 7.56 (1H, d, $J = 7.44$ Hz), 7.44 (1H, d, $J = 7.44$ Hz), 7.32-7.20 (5H, m), 7.15 (2H, t, $J = 7.59$ Hz), 1.77 (3H, s), 1.60 (9H, s); ^{13}C NMR (100.6MHz, CDCl_3): δ 175.3, 138.7, 136.6, 130.1, 129.7, 129.4, 129.0, 128.4, 124.5, 123.8, 114.6, 84.0, 54.6, 28.1, 21.2 ppm; HRMS (EI^+): calcd. for $[\text{C}_{20}\text{H}_{21}\text{NO}_3\text{S}]$ 355.1242, found 355.1248. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=3:97), 1.0 mL/min; t_R = 4.9 min (minor), 8.7 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. $[\alpha]_D^{22}$ -30.2° ($c = 1.0$, CHCl_3); ^1H NMR (400MHz, CDCl_3): δ 7.54 (1H, d, $J = 8.80$ Hz), 7.40-7.37 (1H, m), 7.28-7.18 (5H, m), 7.13 (2H, t, $J = 7.59$ Hz), 2.37-2.28 (1H, m), 2.21-2.12 (1H, m), 1.59 (9H, s), 0.76 (3H, t, $J = 7.28$ Hz); ^{13}C NMR (100.6MHz, CDCl_3): δ 174.7, 148.7, 139.6, 136.7, 129.6, 129.0, 128.9, 128.3, 128.1, 124.5, 124.0, 114.6, 84.0, 59.8, 28.2, 28.1, 9.5 ppm; HRMS (ESI^+): calcd. for $[\text{C}_{21}\text{H}_{23}\text{NO}_3\text{S} + \text{Na}]^+$ 392.1291, found 392.1297. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 4.7 min (minor), 5.1 min (major).

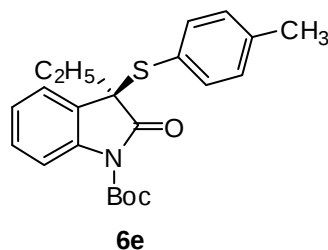


The sulfenyl product was synthesized according to the general procedure as little yellow oil in 93% overall yield. $[\alpha]_D^{22}$ -15.8° ($c = 1.0$, CHCl_3); ^1H NMR (400MHz, CDCl_3): δ 7.61-7.55 (1H, m), 7.46 (1H, d, $J = 7.25$ Hz), 7.42-7.37 (2H, m), 7.25 (2H, d, $J = 7.57$ Hz), 7.16 (4H, q, $J = 7.57$, 15.14 Hz), 7.11 (2H, s), 7.02 (2H, s), 3.58 (1H, d, $J = 13.25$ Hz), 3.43 (1H, d, $J = 13.25$ Hz), 1.55 (9H, s); ^{13}C NMR (100.6MHz, CDCl_3): δ 174.2, 148.4, 139.4, 136.7, 136.6, 135.4, 134.7, 131.6, 130.3, 129.7, 129.4, 129.3, 129.0, 128.9, 128.5, 128.0, 127.6, 126.9, 124.9, 124.3, 124.1, 114.6, 83.9, 60.1, 41.1, 28.0 ppm; HRMS (ESI^+): calcd. for $[\text{C}_{26}\text{H}_{25}\text{NO}_3\text{S}+\text{Na}]^+$ 454.1474, found 454.1469. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=3:97), 1.0 mL/min; t_R = 5.8 min (minor), 7.4 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. $[\alpha]_D^{22}$ 17.9° ($c = 1.0$, CHCl_3); ^1H NMR (400MHz, CDCl_3): δ 7.47 (1H, d, $J = 8.83$ Hz), 7.31 (1H, d, $J = 7.25$ Hz), 7.23 (2H, d, $J = 7.57$ Hz), 7.16 (2H, t, $J = 7.57$ Hz), 6.97 (1H, s), 6.77 (1H, d, $J = 8.83$ Hz), 3.86 (3H, s), 1.75 (3H, s), 1.58 (9H, s); ^{13}C NMR (100.6MHz, CDCl_3): δ 175.3, 157.0, 148.7, 136.5, 132.0, 131.4, 129.8, 129.3, 128.4, 115.7, 114.3, 109.3, 83.9, 55.7, 54.9, 28.1, 21.4 ppm; HRMS (ESI^+): calcd. for $[\text{C}_{21}\text{H}_{23}\text{NO}_4\text{S}+\text{Na}]^+$ 408.1240, found 408.1242. The enantiomeric excess was determined by HPLC with

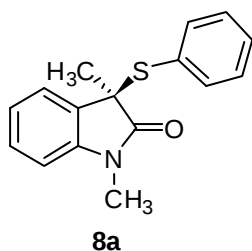
an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 6.6 min (minor), 20.5 min (major).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 96% overall yield.

$[\alpha]_D^{22}$ -42.7° (c = 0.75, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.55 (1H, d, *J* = 7.51 Hz), 7.36 (1H, d, *J* = 7.83

Hz), 7.25-7.18 (2H, m), 7.06 (2H, d, *J* = 7.99 Hz), 6.93 (2H, d, *J* = 7.51 Hz), 2.30-2.26 (1H, m), 2.25 (3H, s), 2.17-2.08 (1H, m), 1.57 (9H, s), 0.72 (3H, t, *J* = 7.51 Hz); ¹³C NMR (100.6MHz, CDCl₃): δ 174.6, 148.7, 139.9, 139.6, 136.6, 130.9, 129.2, 128.8, 125.5, 124.5, 124.0, 114.7, 83.9, 59.6, 28.1, 28.0, 21.3, 9.6 ppm; HRMS (ESI⁺): calcd. for [C₂₂H₂₅NO₃S+Na]⁺ 406.1447, found 406.1448. The enantiomeric excess was determined by HPLC with an AD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 6.2 min (minor), 6.8 min (major).

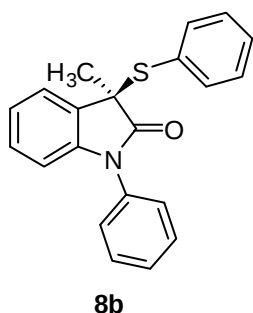


The sulfenyl product was synthesized according to the general procedure as colorless oil in 74% overall yield. $[\alpha]_D^{22}$ 11.6° (c =

0.5, CHCl₃); ¹H NMR (400MHz, CDCl₃): δ 7.40 (1H, d, *J* = 7.25 Hz), 7.26-7.16 (4H, m), 7.11 (3H, t, *J* = 7.57 Hz), 6.53 (1H,

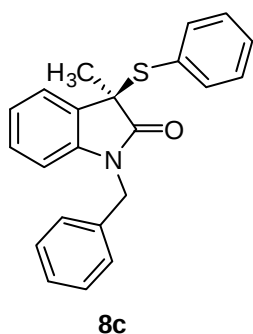
d, *J* = 7.88 Hz), 2.90 (3H, s), 1.74 (3H, s); ¹³C NMR (100.6MHz, CDCl₃): δ 176.8,

142.6, 136.3, 131.7, 130.0, 129.3, 128.6, 128.1, 123.8, 122.6, 107.7, 54.9, 26.0, 21.0 ppm; HRMS (ESI⁺): calcd. for [C₁₆H₁₅NOS+Na]⁺ 292.0767, found 292.0768. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R*= 12.1 min (major), 15.0 min (minor).



The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. [α]_D²² -21.5° (c = 0.8, CHCl₃); ¹H NMR (300MHz, CDCl₃): δ 7.42 (1H, d, *J* = 6.47 Hz), 7.34-7.16 (4H, m), 7.11-6.98 (6H, m), 6.80 (2H, d, *J* = 7.15

Hz), 6.38 (1H, d, *J* = 6.91 Hz), 1.74 (3H, s); ¹³C NMR (75MHz, CDCl₃): δ 176.1, 142.8, 136.6, 134.1, 131.7, 130.1, 129.6, 129.5, 129.2, 128.8, 128.6, 128.5, 128.2, 128.1, 126.4, 124.2, 123.2, 109.2, 55.2, 21.5 ppm; HRMS (ESI⁺): calcd. for [C₂₁H₁₇NOS+Na]⁺ 354.0923, found 354.0921. The enantiomeric excess was determined by HPLC with an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; *t_R*= 12.7 min (minor), 26.4 min (major).



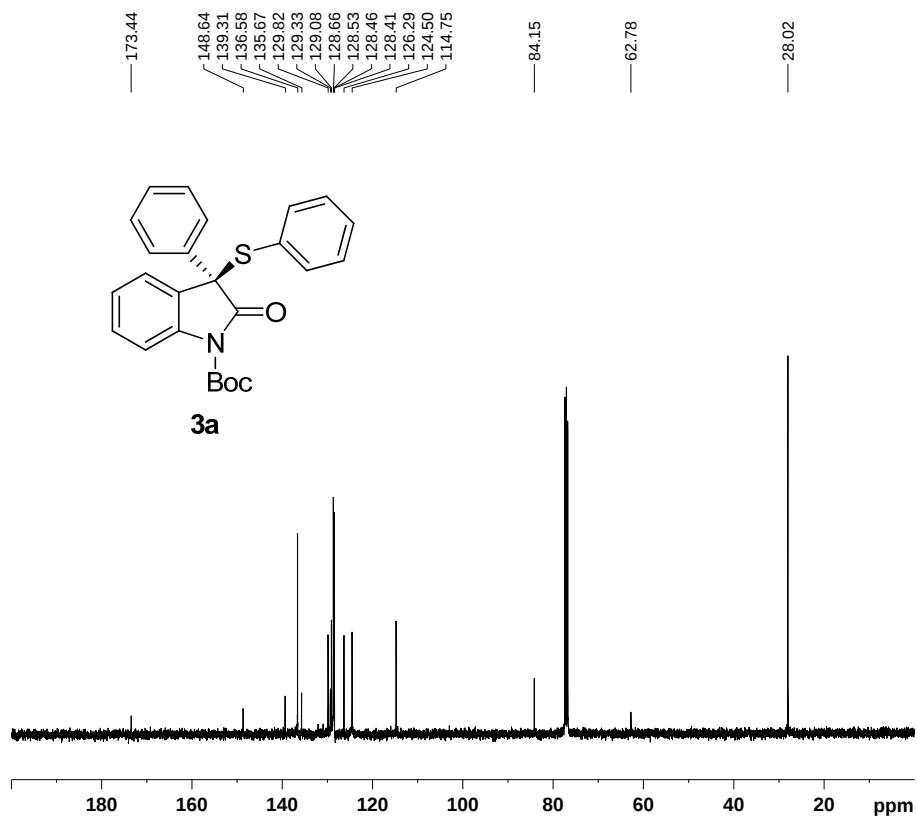
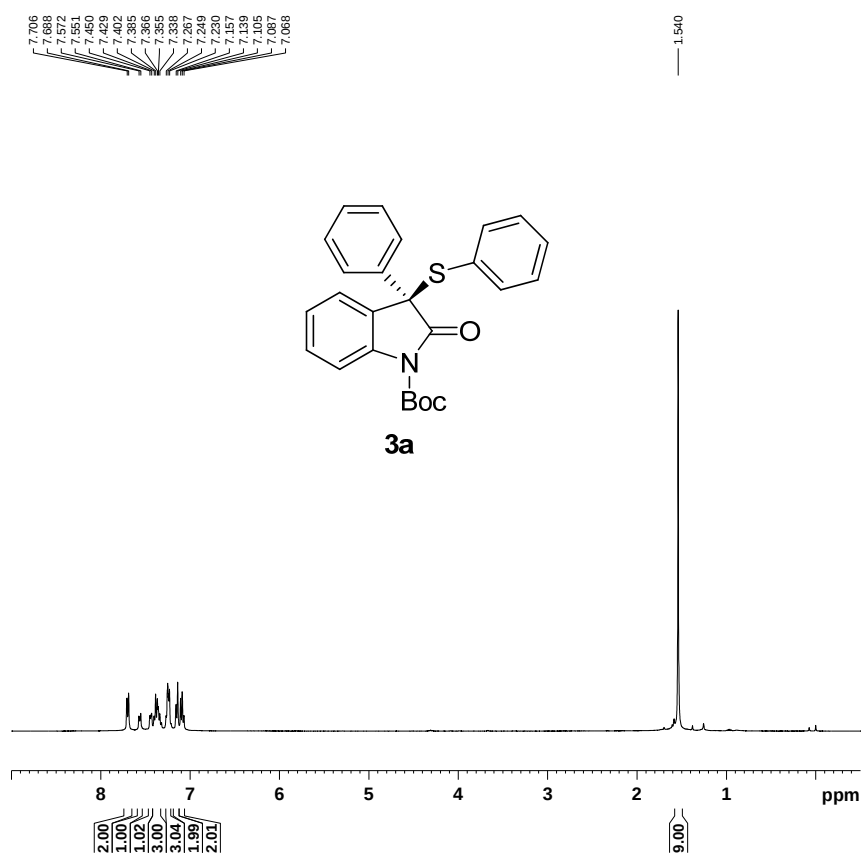
The sulfenyl product was synthesized according to the general procedure as colorless oil in 99% overall yield. [α]_D²² 1.9° (c = 1.0, CHCl₃); ¹H NMR (300MHz, CDCl₃): δ 7.42 (1H, t, *J* = 4.37 Hz), 7.29-7.18 (6H, m), 7.12-7.03 (4H, m), 6.91-6.88 (2H, m),

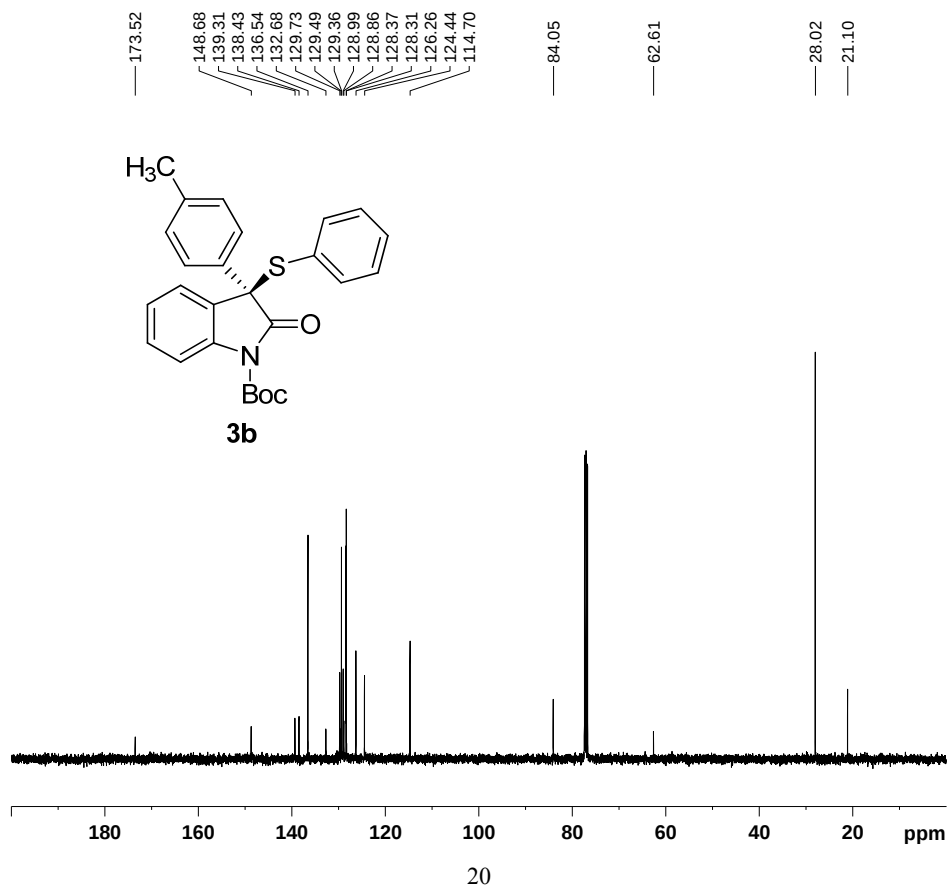
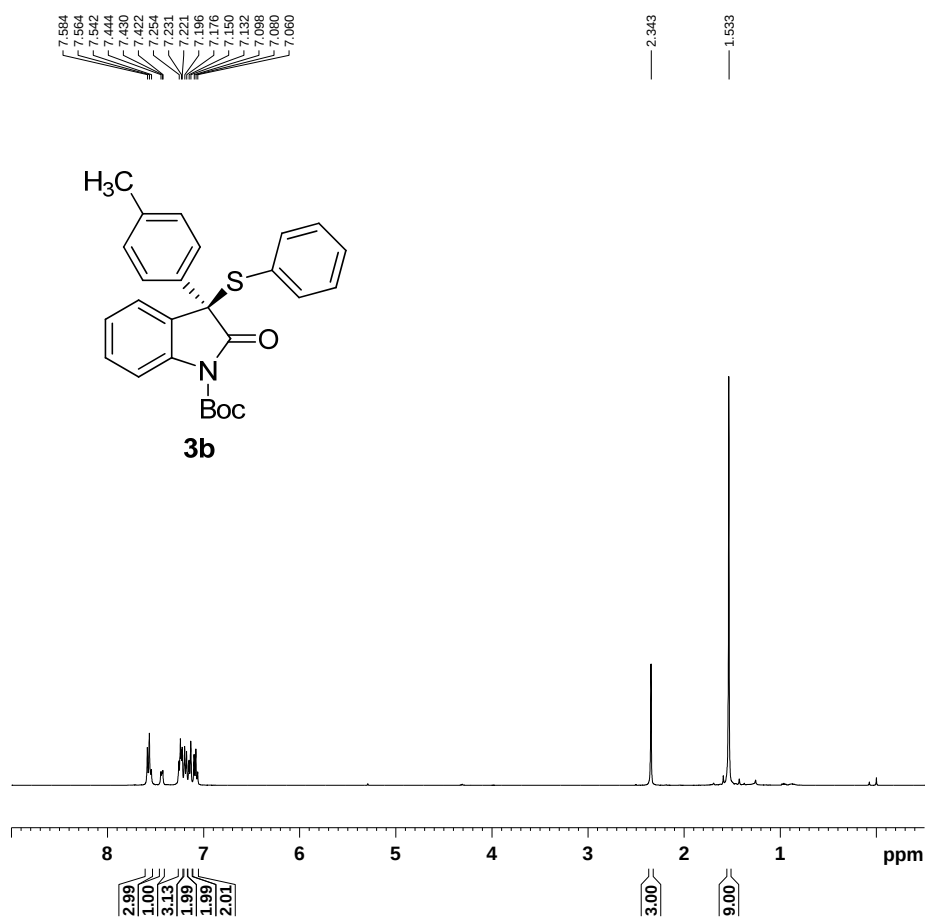
6.42 (1H, t, $J = 5.24$ Hz), 4.73-4.58 (2H, m), 1.75 (3H, s); ^{13}C NMR (75MHz, CDCl_3):
 δ 177.0, 141.9, 136.5, 135.5, 131.8, 130.1, 129.5, 128.7, 128.5, 127.4, 127.0, 124.1,
122.8, 109.2, 54.9, 44.0, 22.3 ppm; HRMS (ESI^+): calcd. for $[\text{C}_{22}\text{H}_{19}\text{NOS}+\text{Na}]^+$
368.1080, found 368.1085. The enantiomeric excess was determined by HPLC with
an OD-H column at 210 nm (2-propanol: hexane=2:98), 1.0 mL/min; t_R = 16.3 min
(major), 18.2 min (minor).

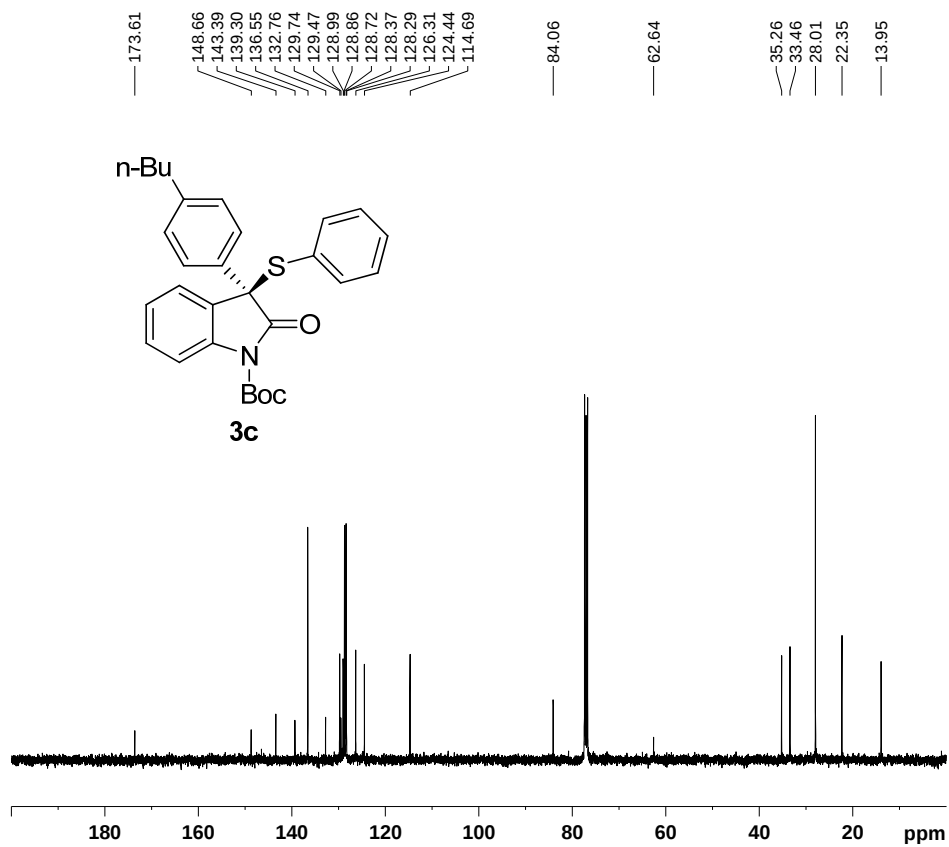
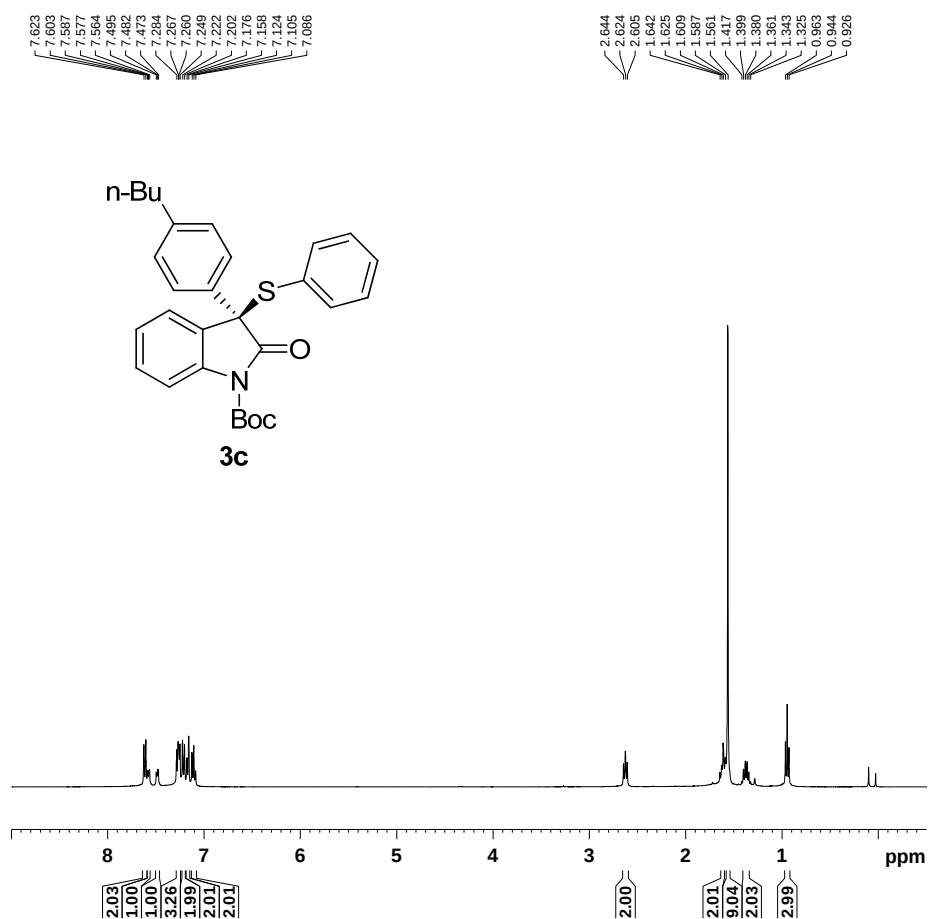
Table S1. Crystal data and structure refinement for shelxl.

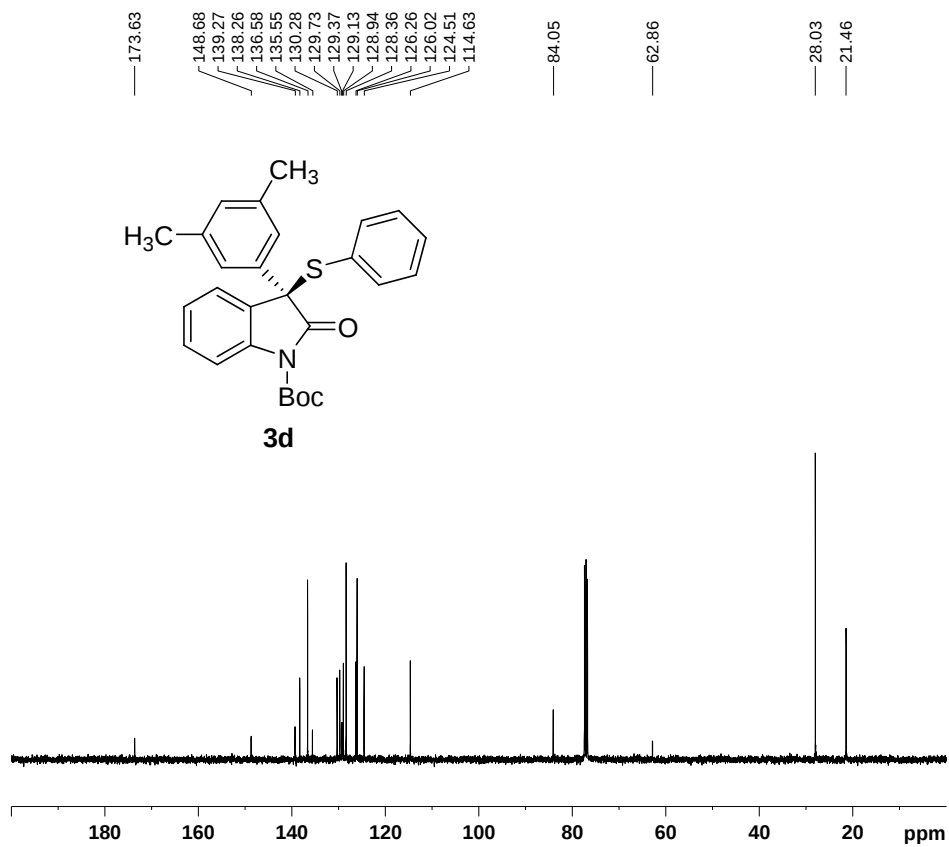
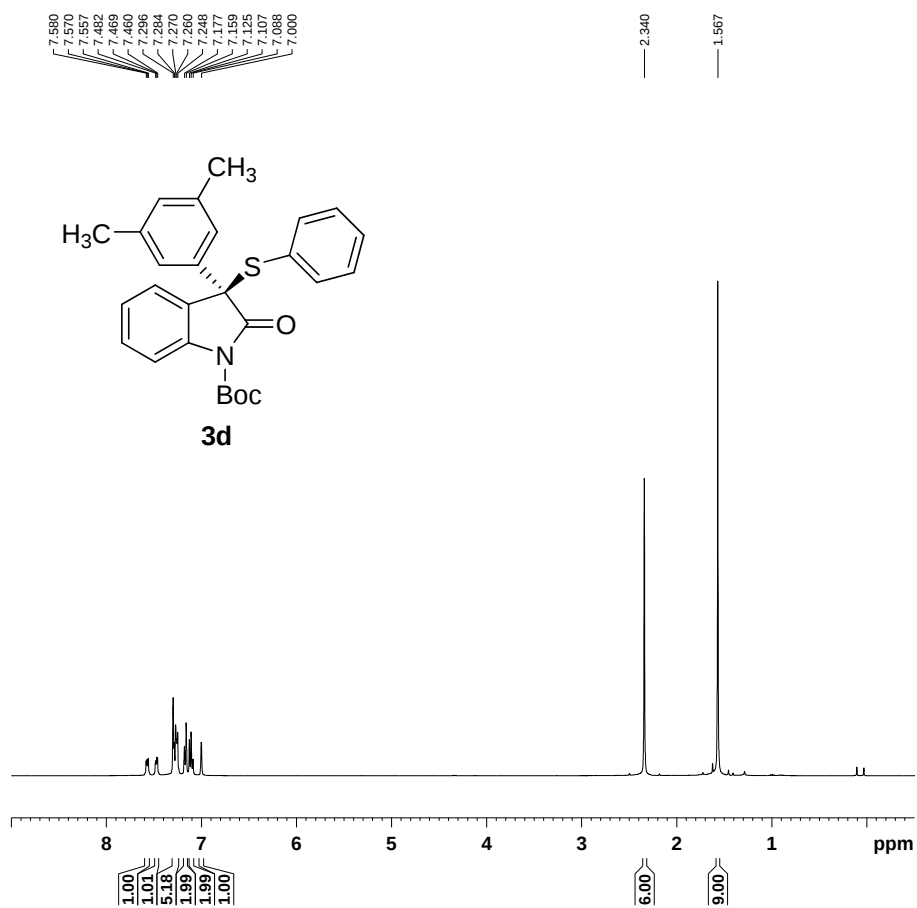
Identification code	shelxl
Empirical formula	C ₂₅ H ₂₂ Br ₁ N ₁ O ₃ S ₁
Formula weight	496.41
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.6278(17) Å α = 90 deg. b = 14.856(3) Å β = 90 deg. c = 17.839(4) Å γ = 90 deg.
Volume	2286.5(8) Å ³
Z, Calculated density	4, 1.442 Mg/m ³
Absorption coefficient	1.916 mm ⁻¹
F(000)	1016
Crystal size	0.24 x 0.20 x 0.18 mm
Theta range for data collection	2.96 to 27.48 deg.
Limiting indices	-11 ≤ h ≤ 11, -19 ≤ k ≤ 19, -22 ≤ l ≤ 23
Reflections collected / unique	14403 / 5223 [R(int) = 0.0474]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.5288
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5223 / 0 / 283
Goodness-of-fit on F ²	1.138
Final R indices [I > 2σ(I)]	R1 = 0.0446, wR2 = 0.0794
R indices (all data)	R1 = 0.0494, wR2 = 0.0821
Absolute structure parameter	0.024(7)
Largest diff. peak and hole	0.305 and -0.390 e.Å ⁻³

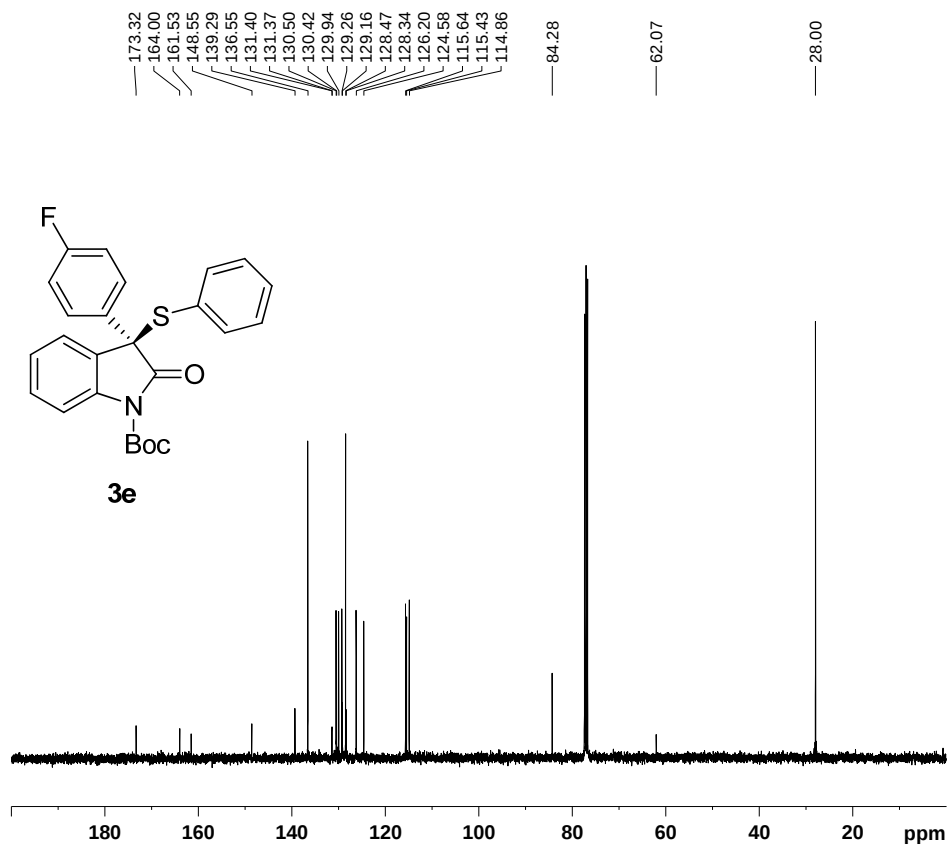
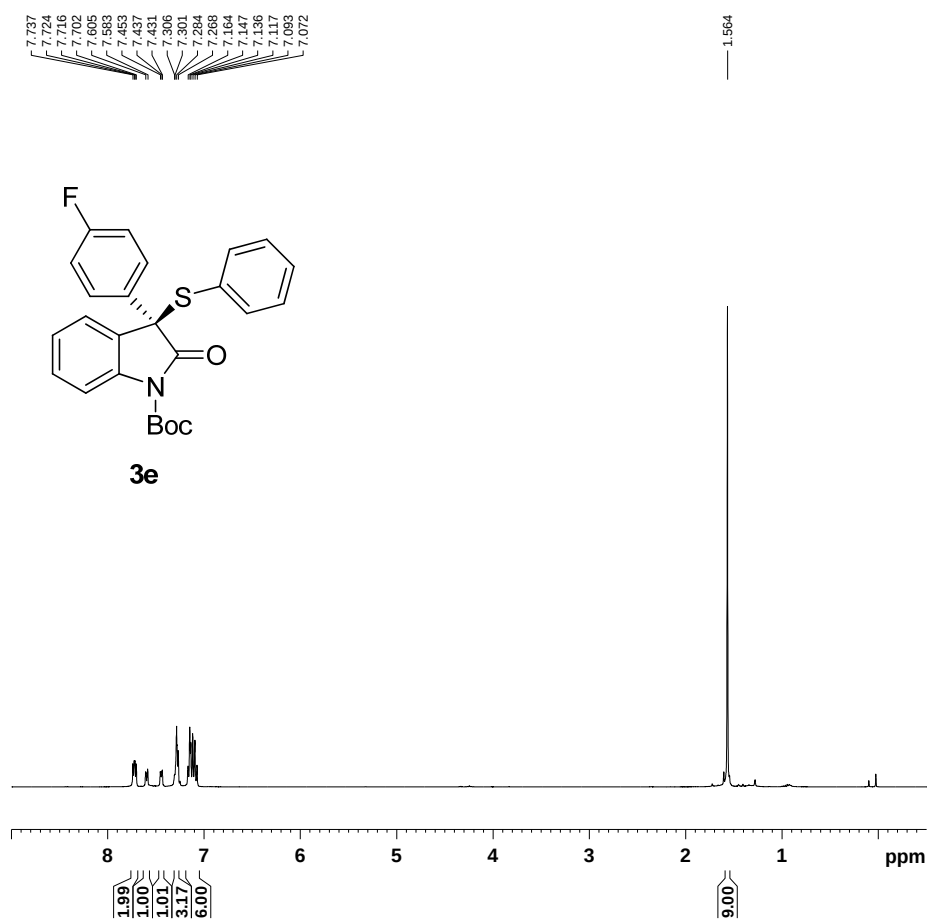
NMR spectrum for the sulfonylation products:

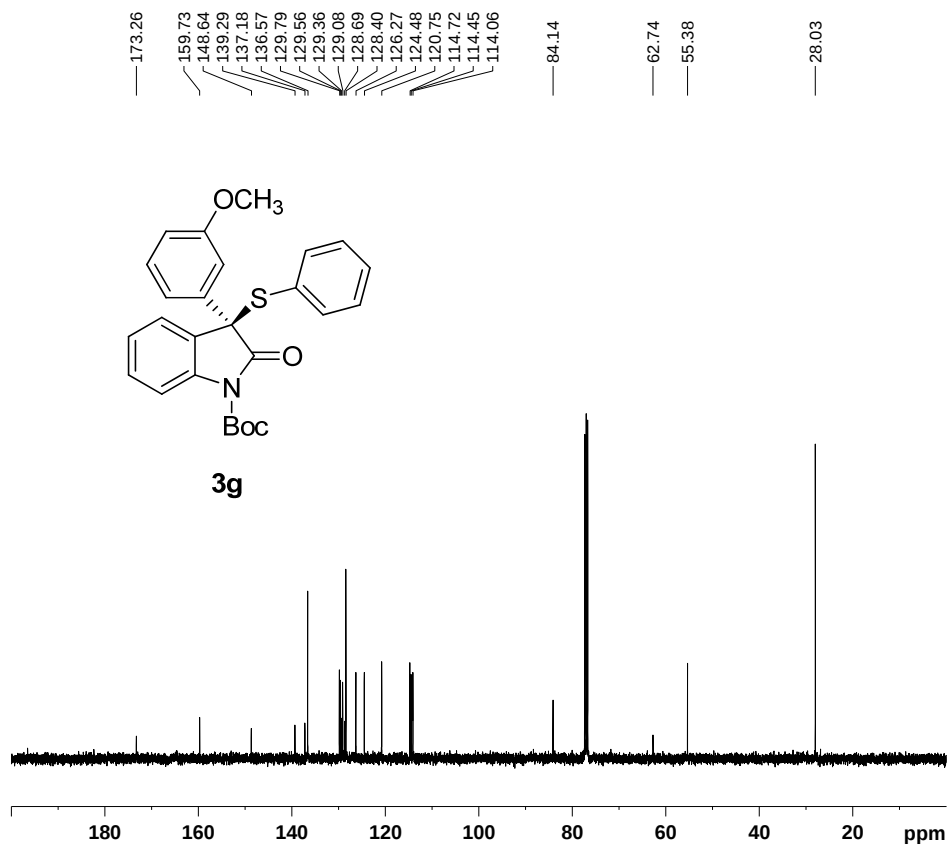
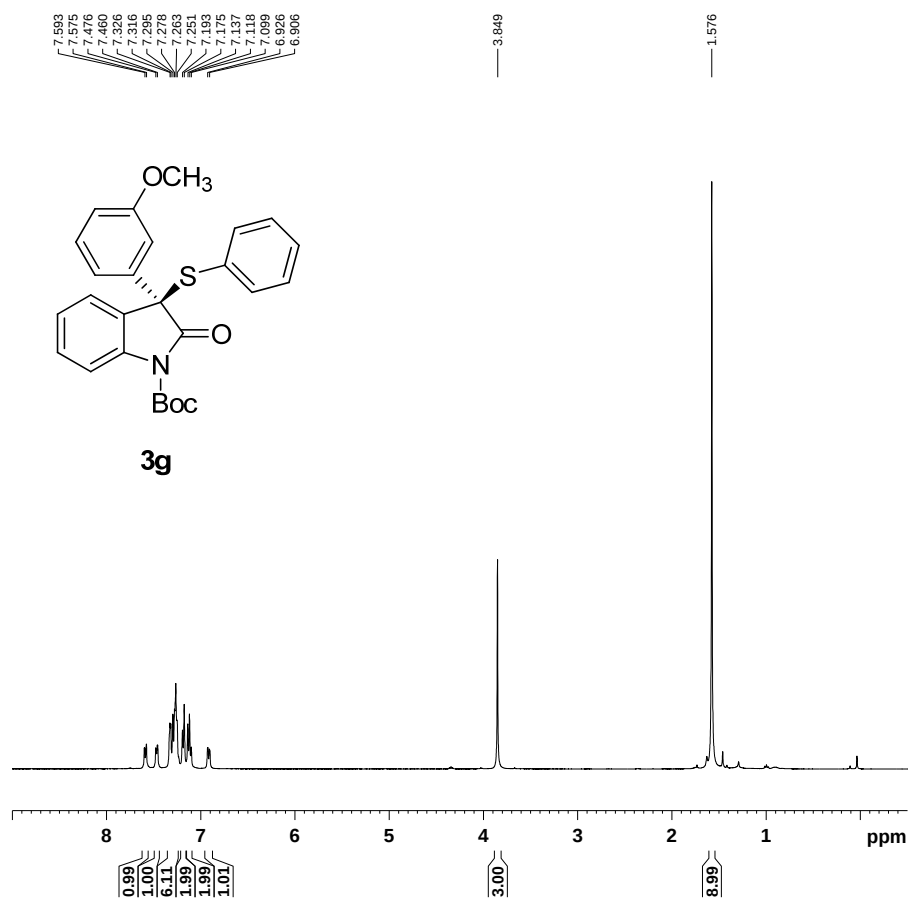


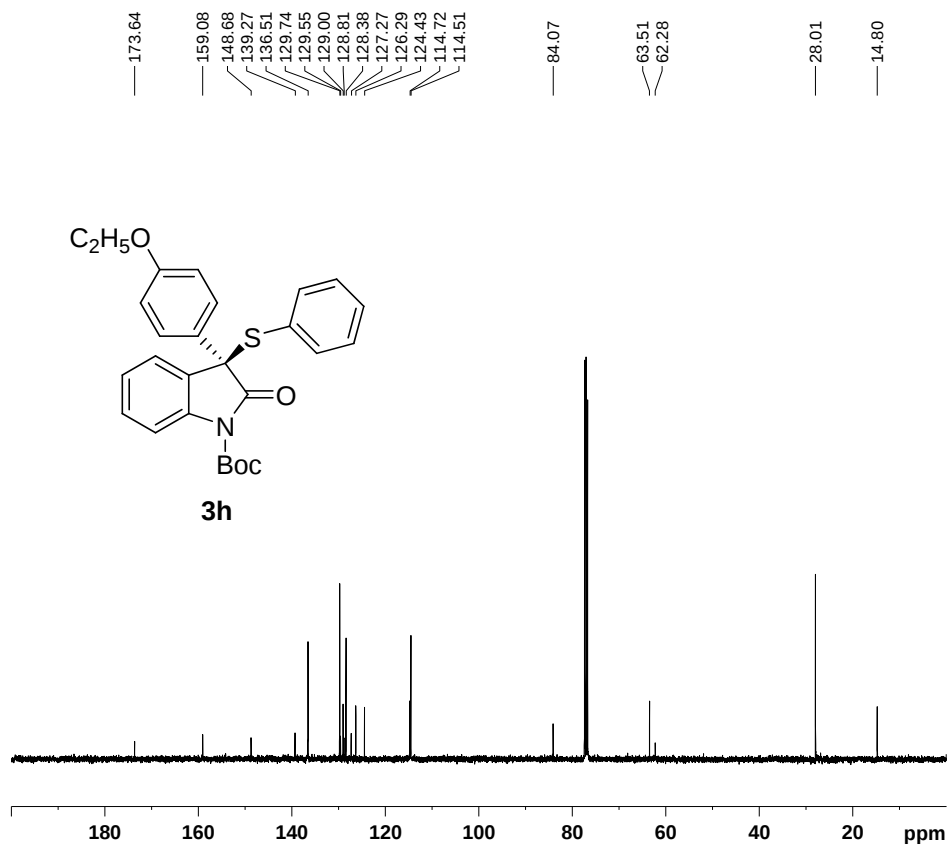
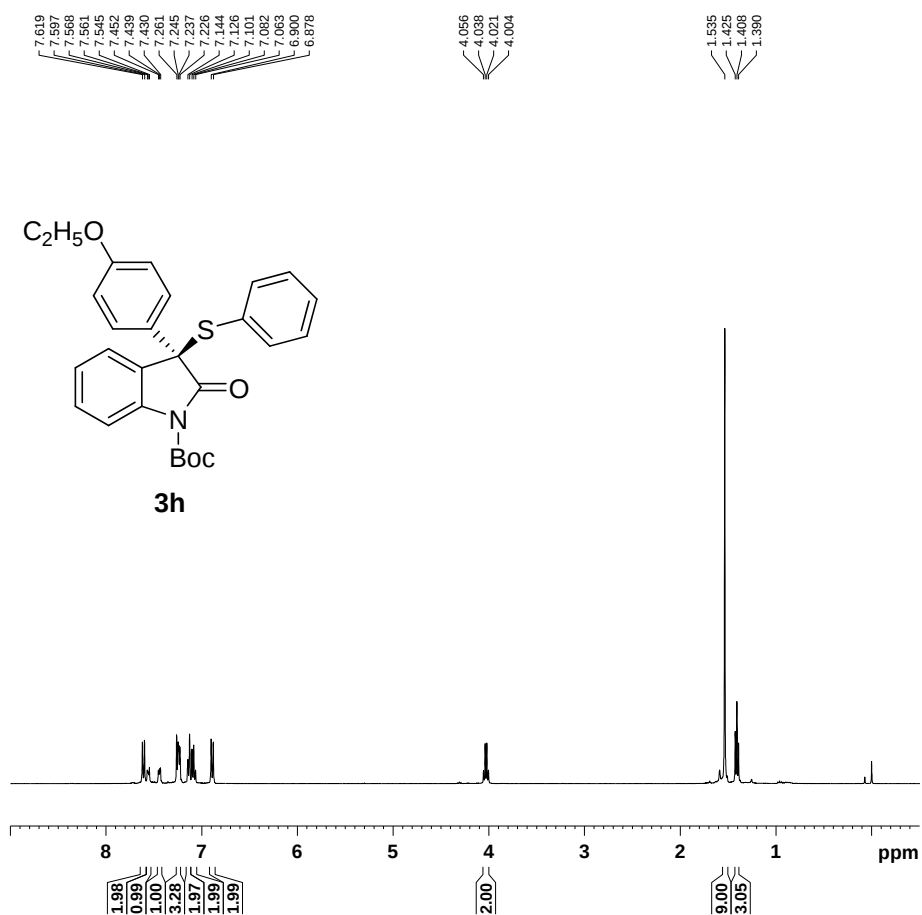


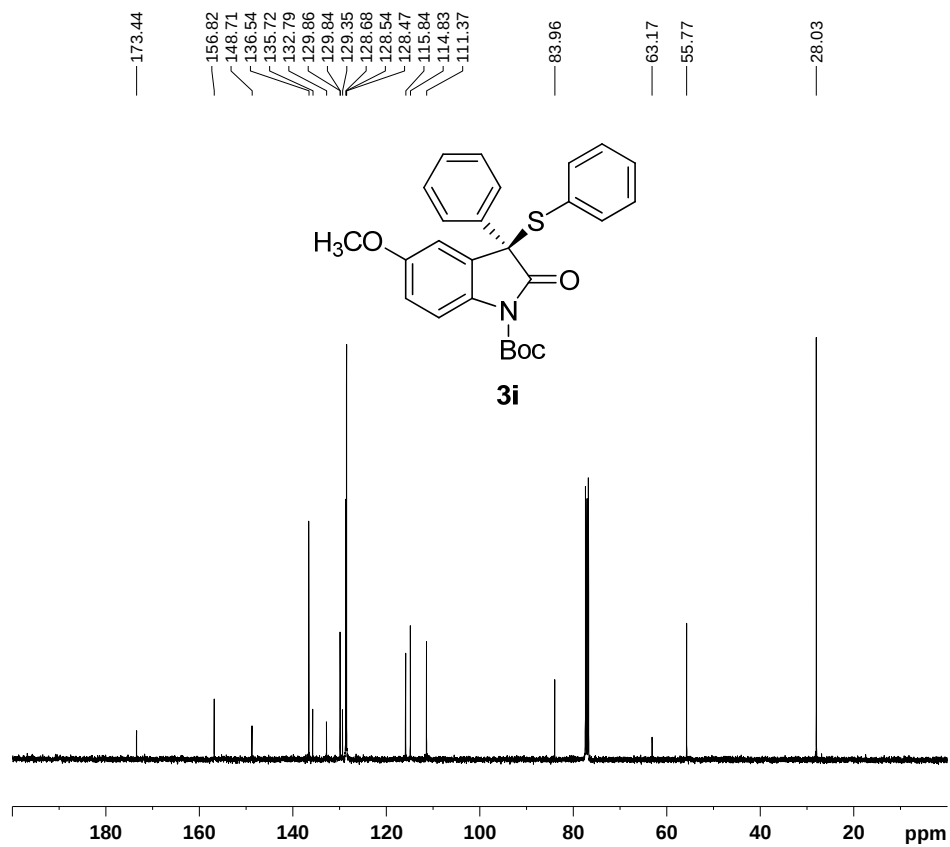
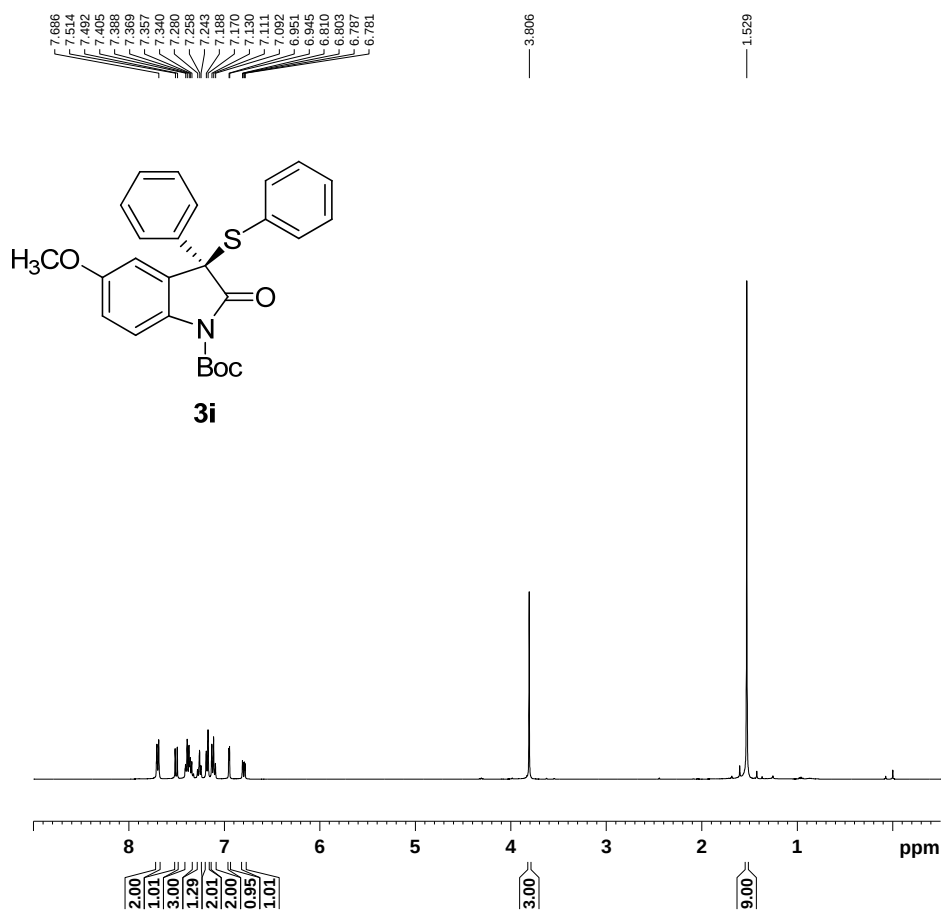


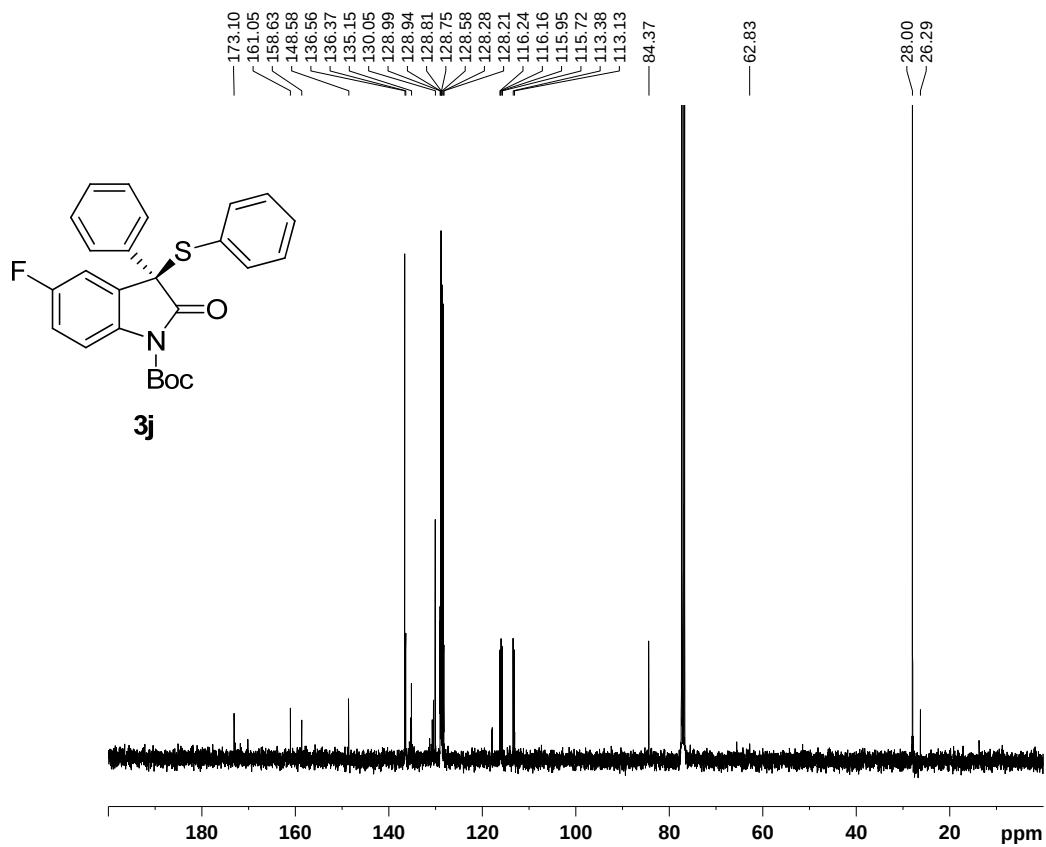
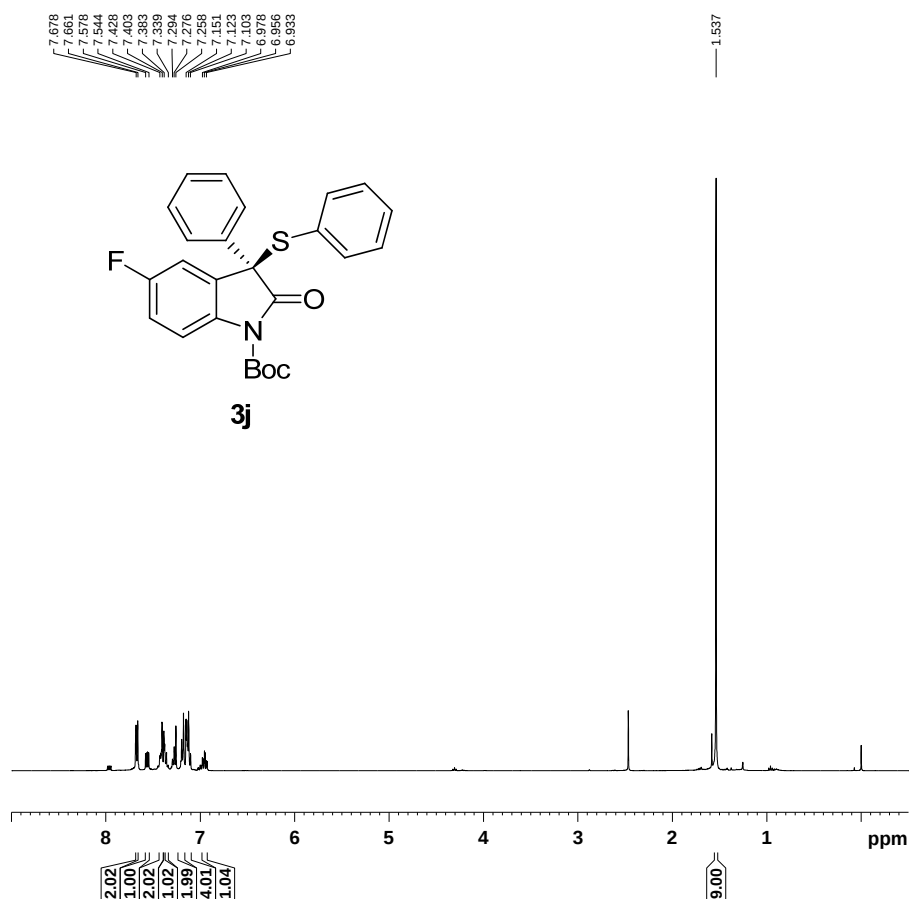


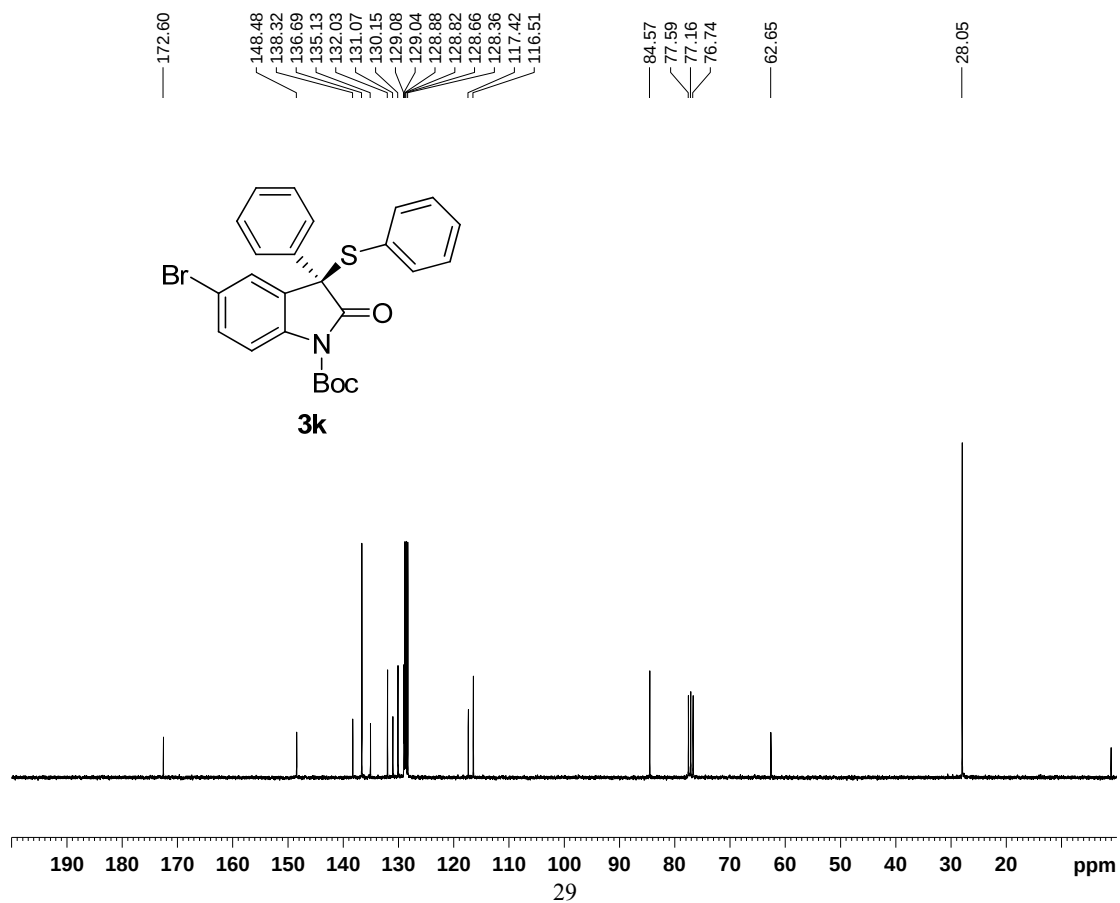
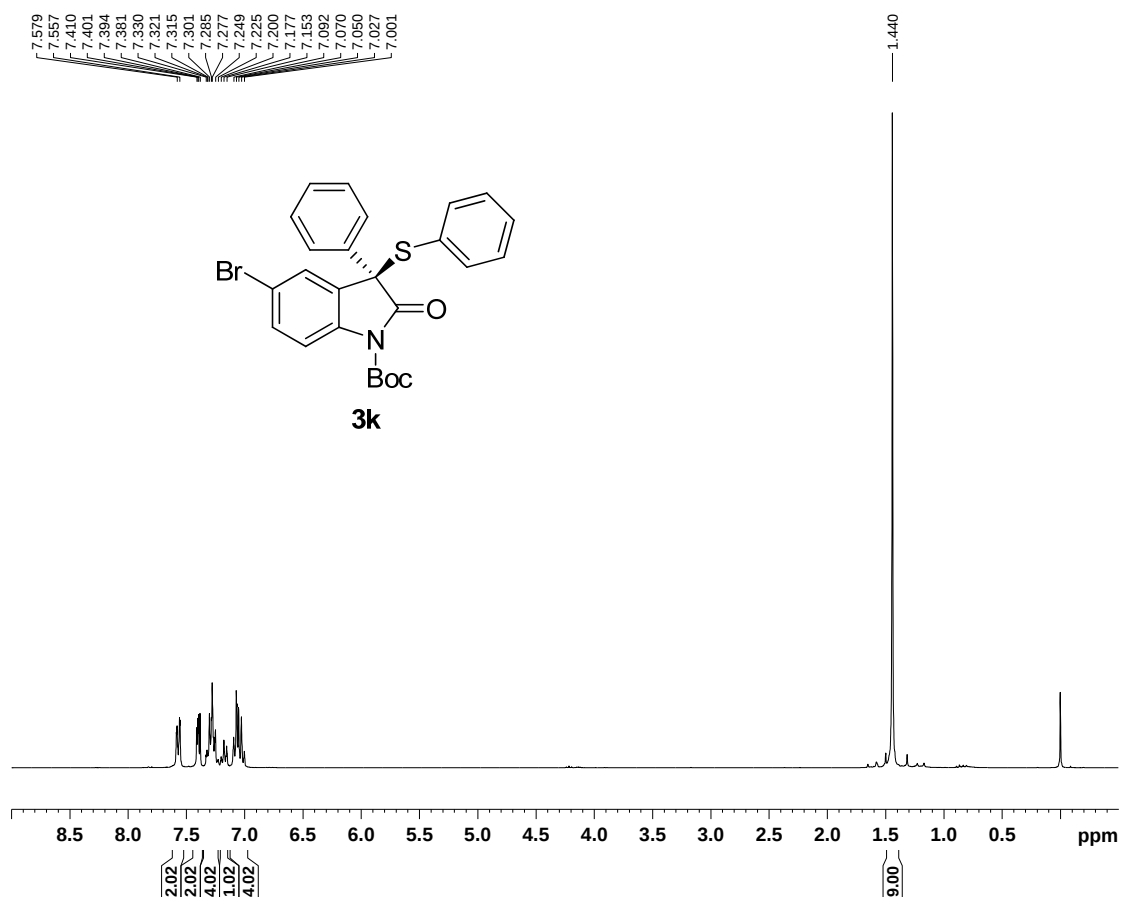


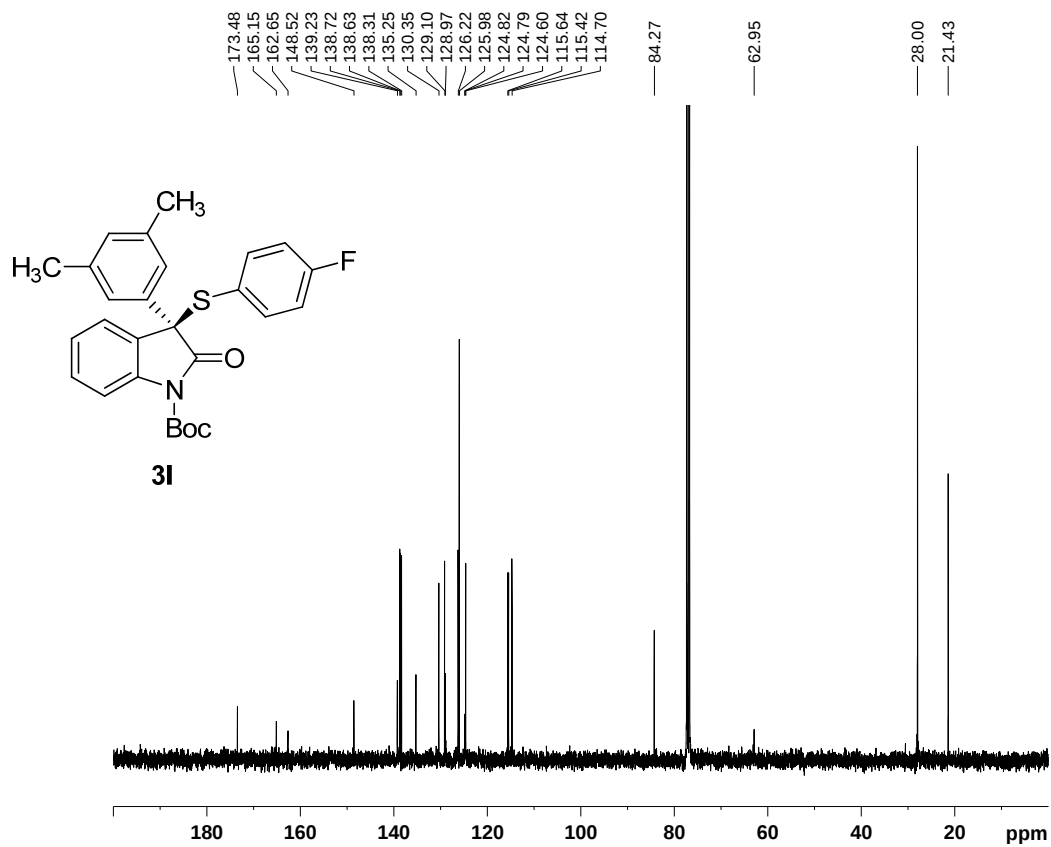
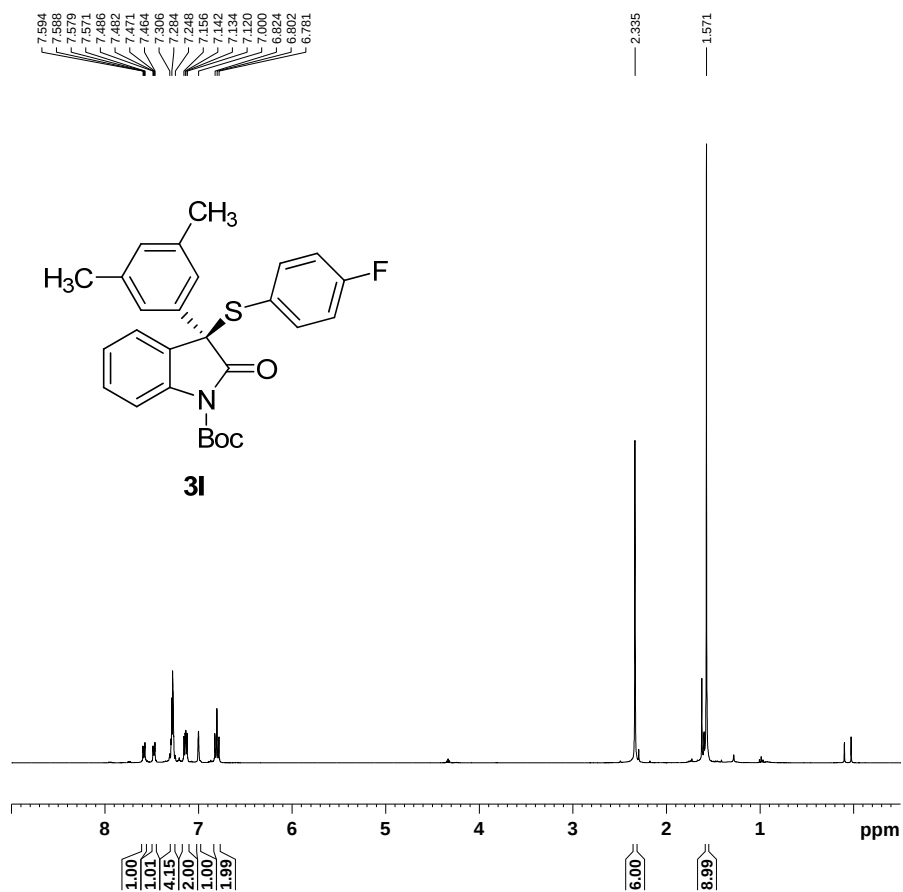


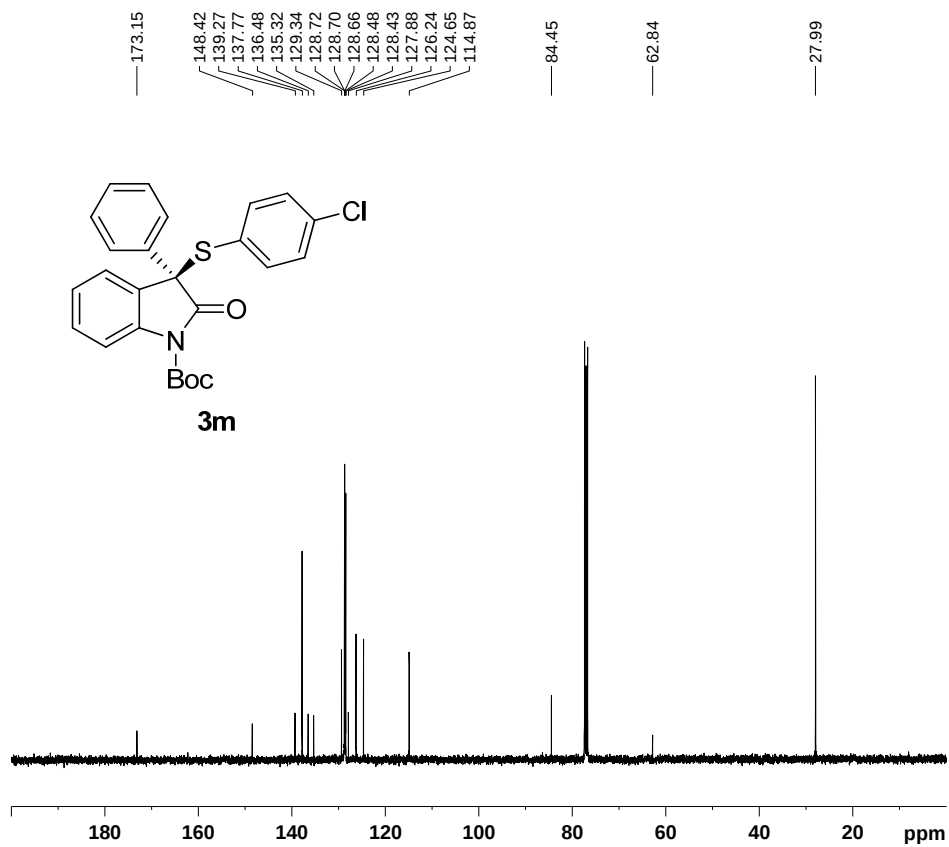
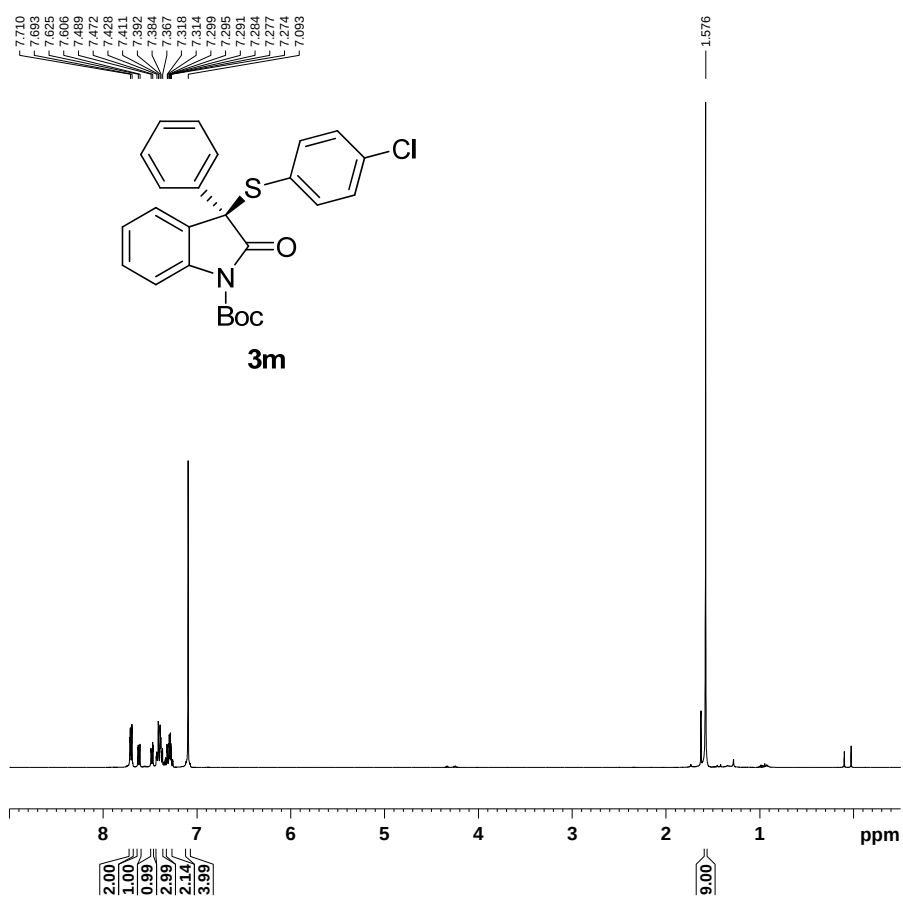


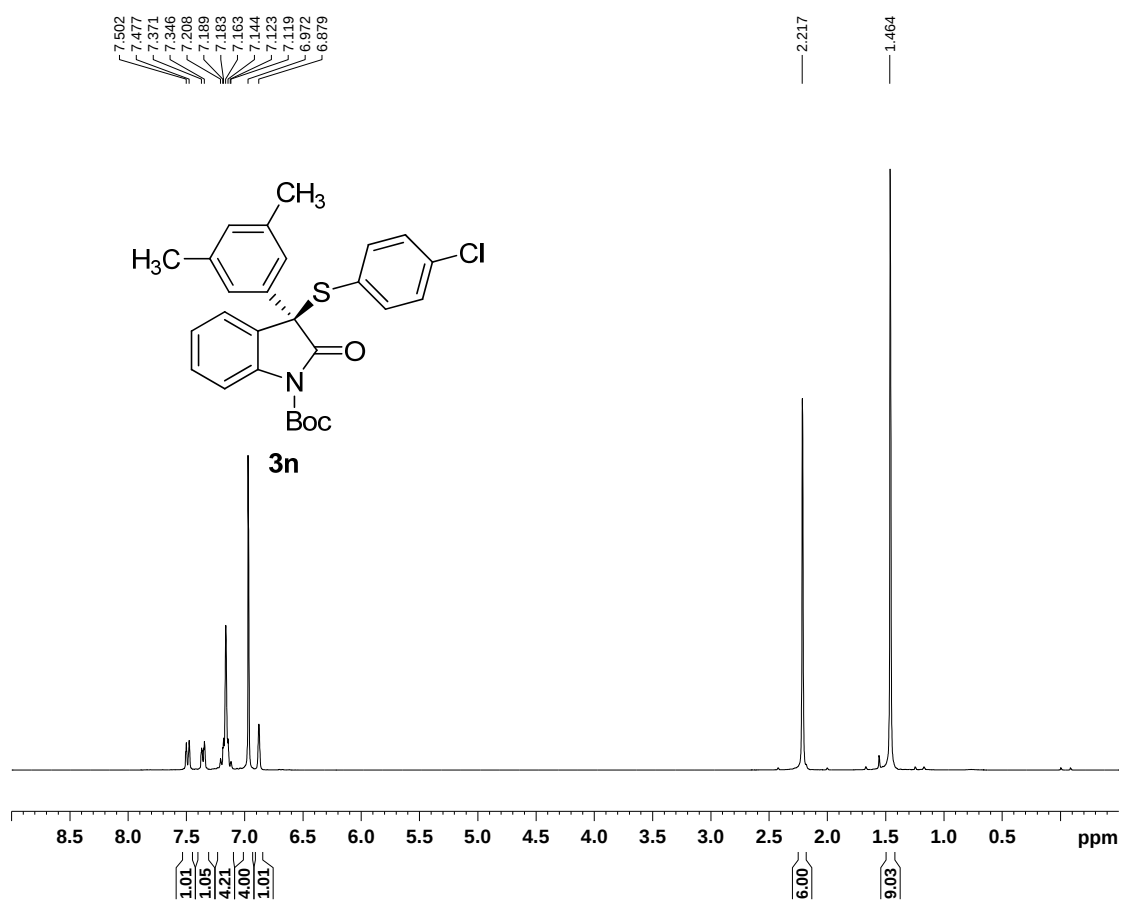


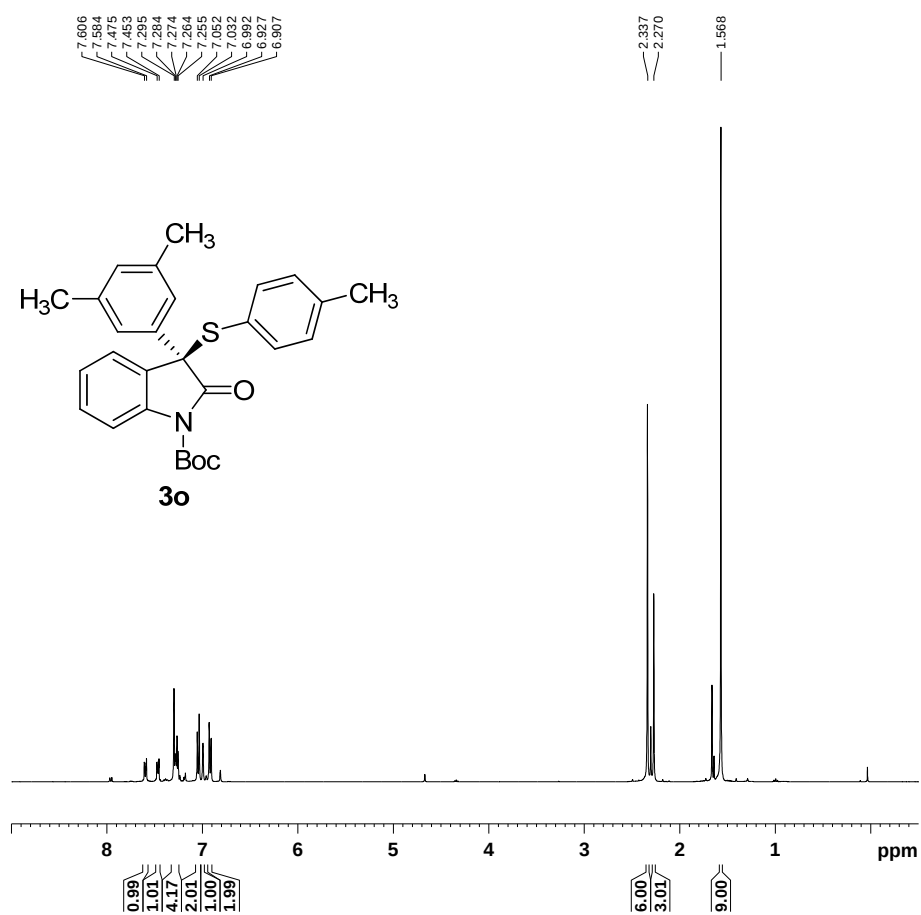
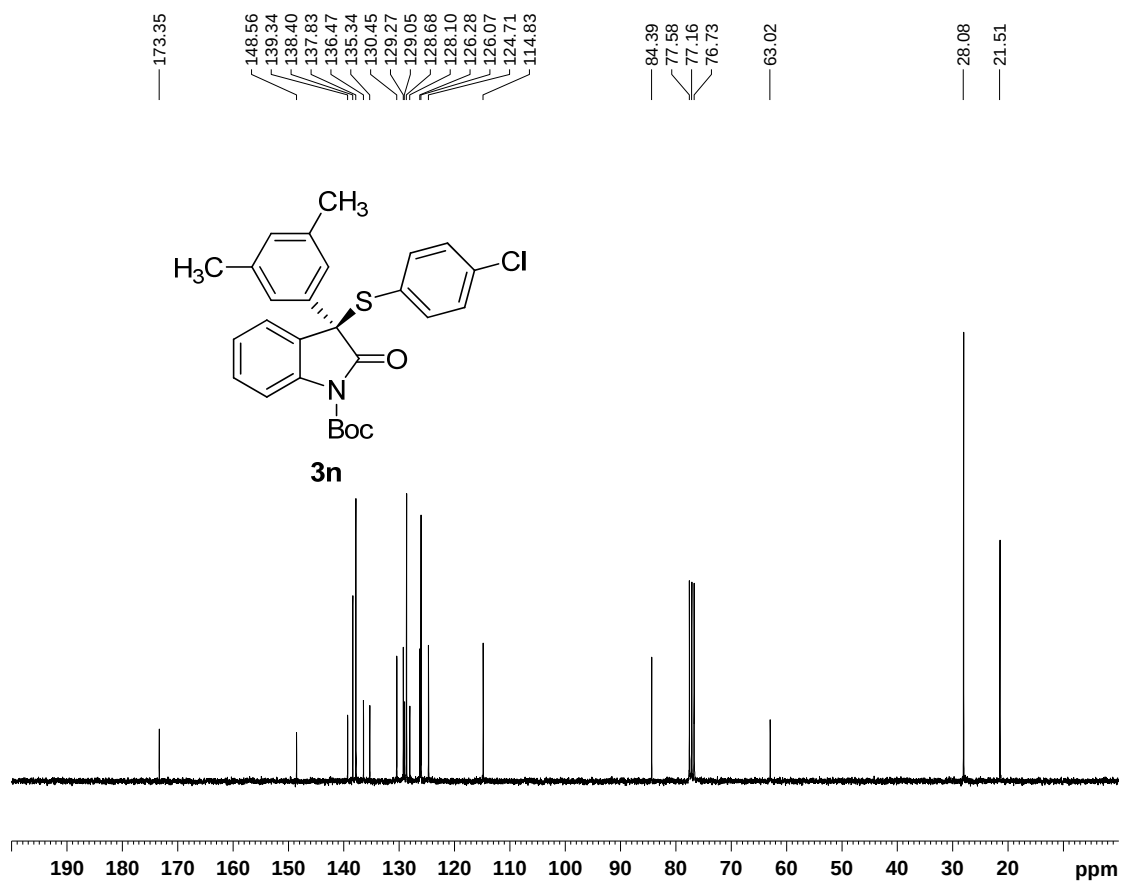


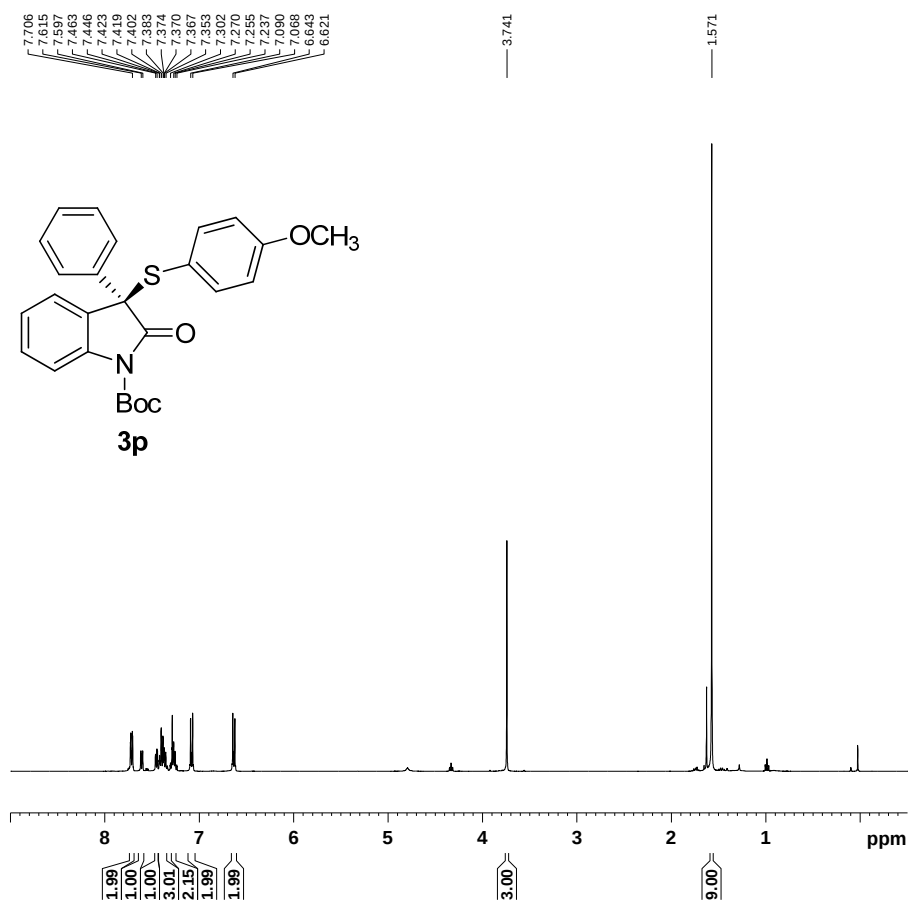
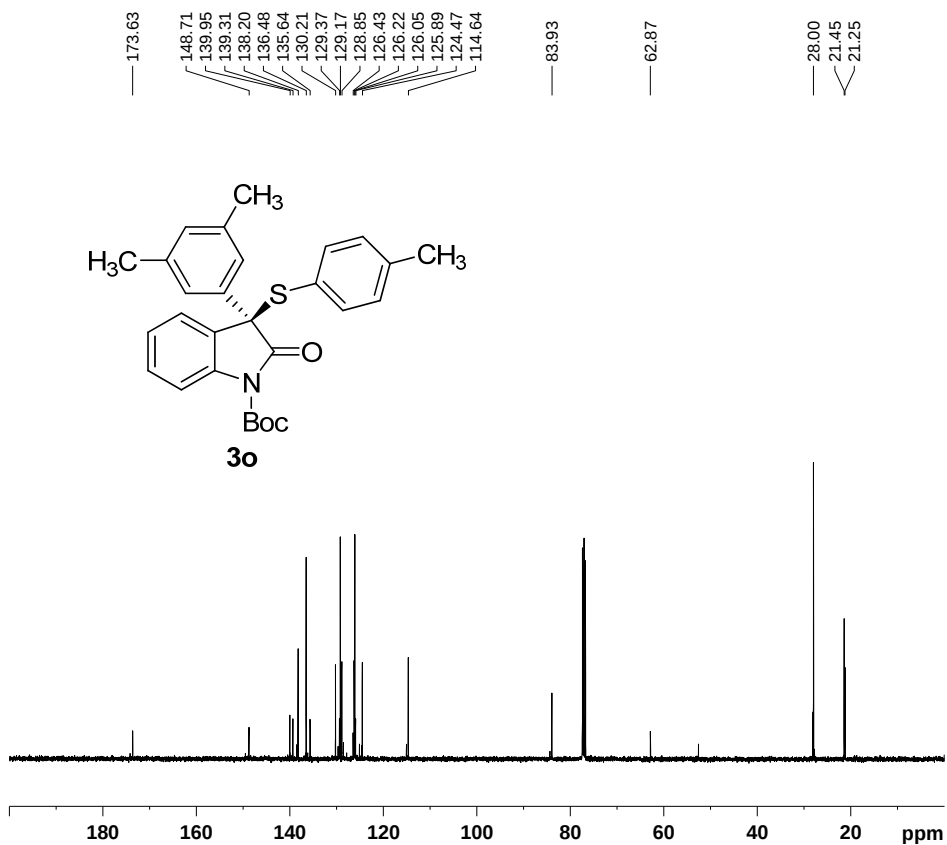


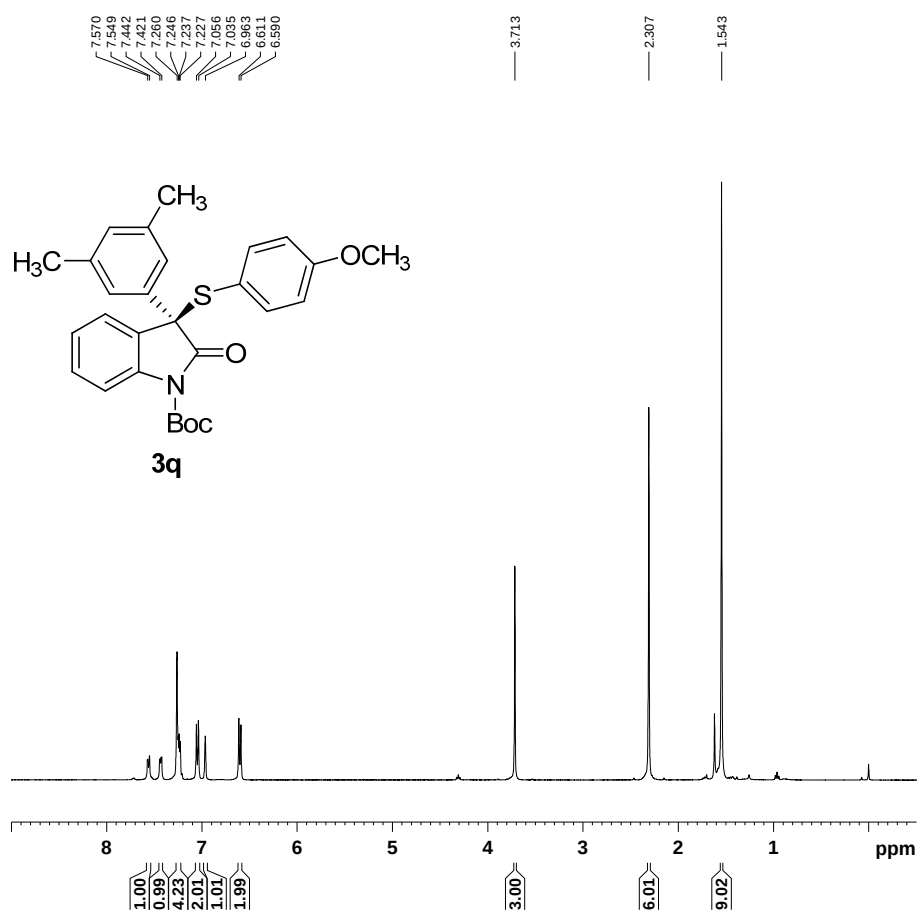
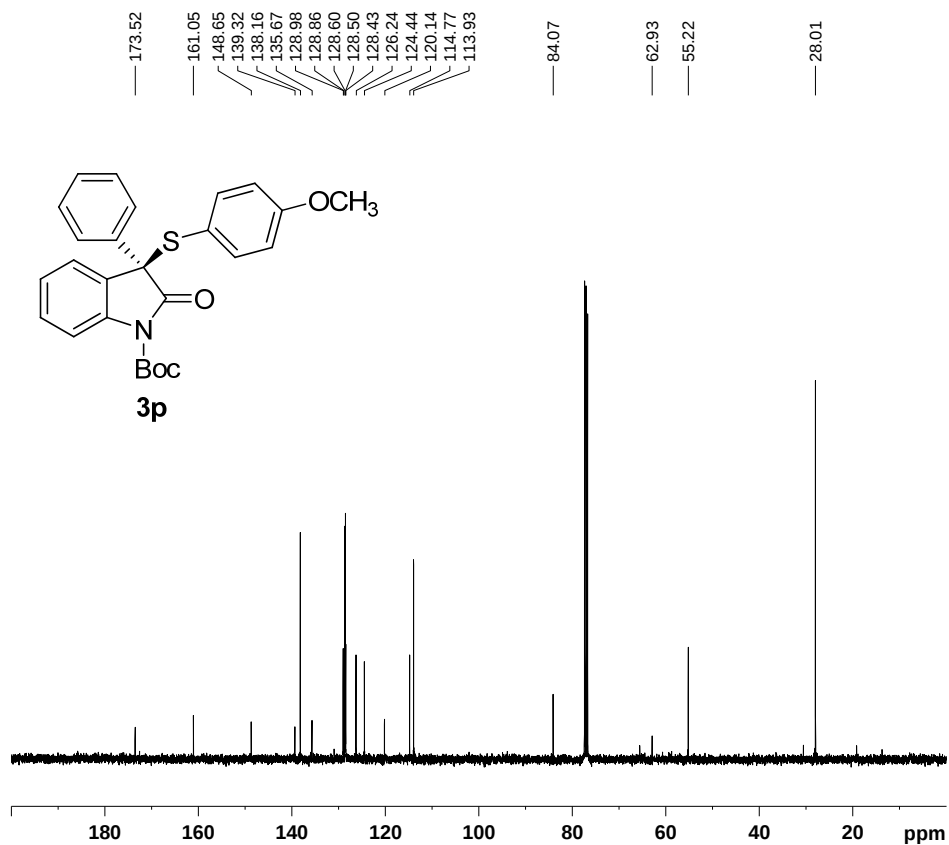


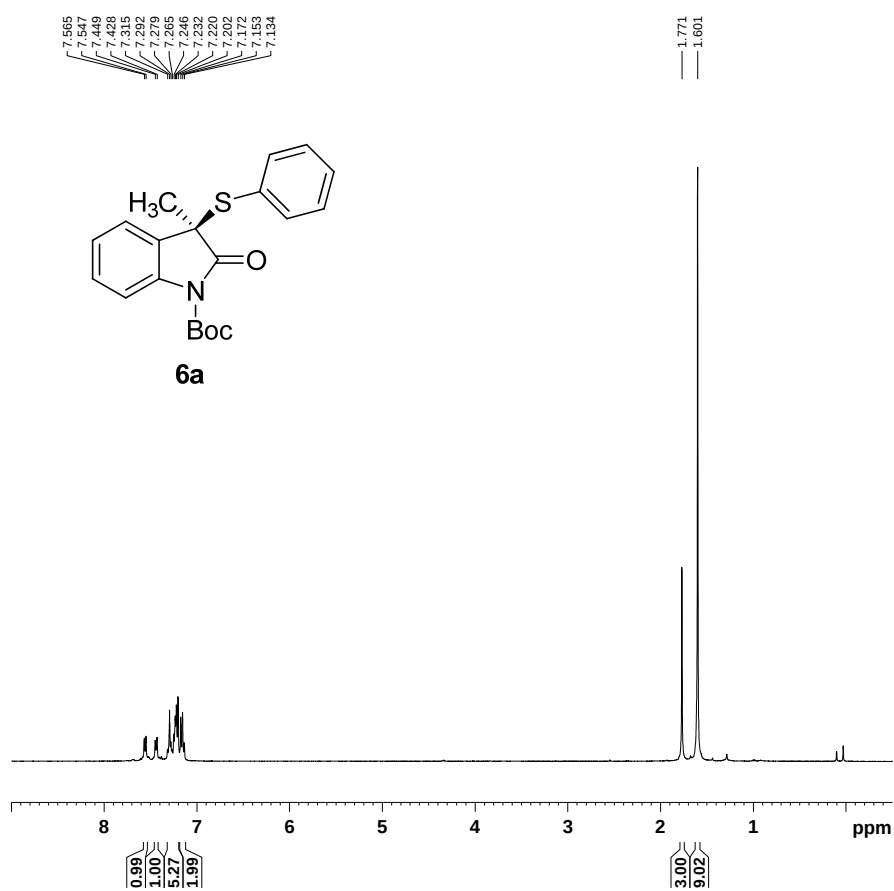
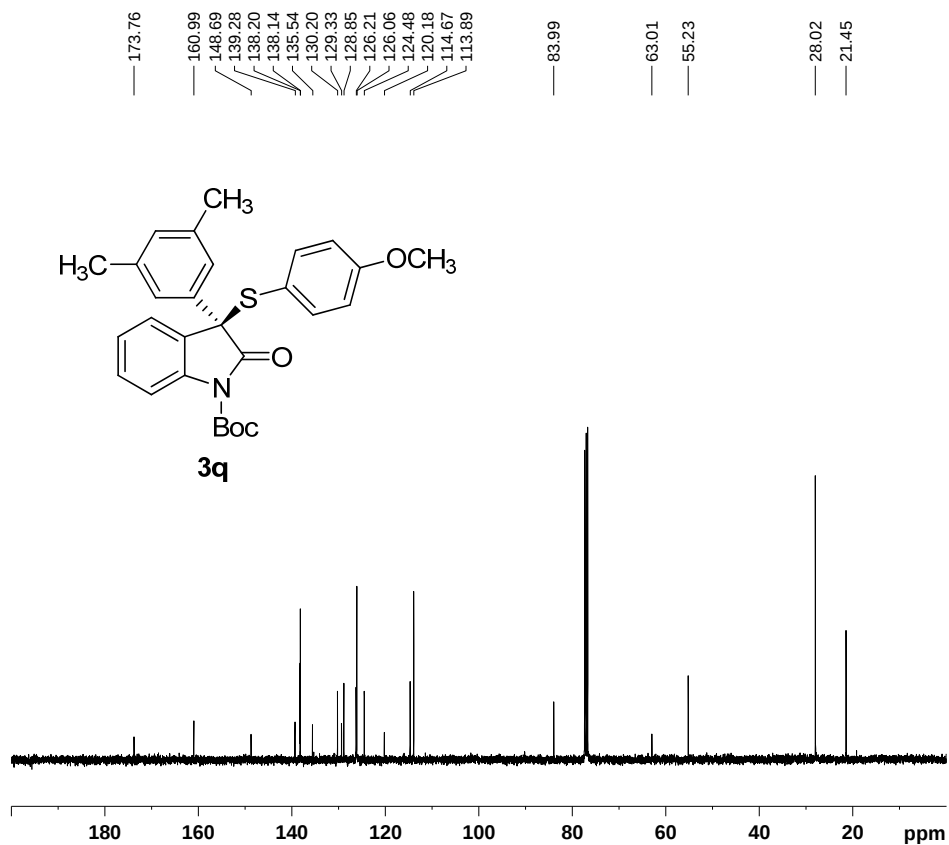


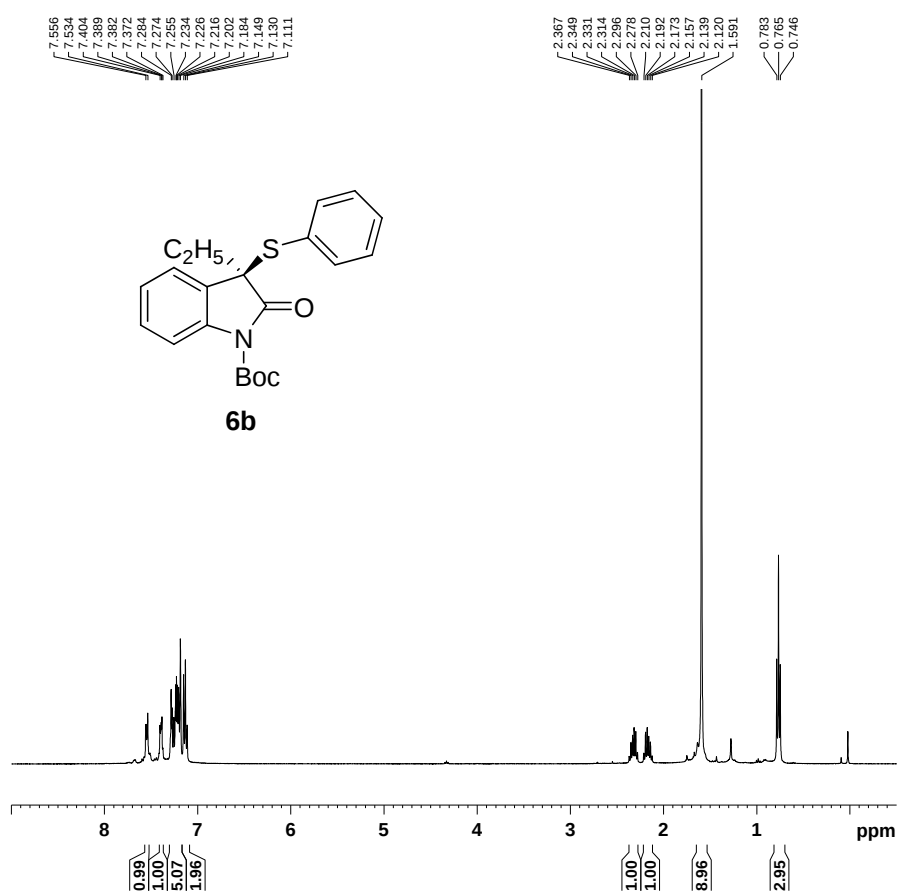
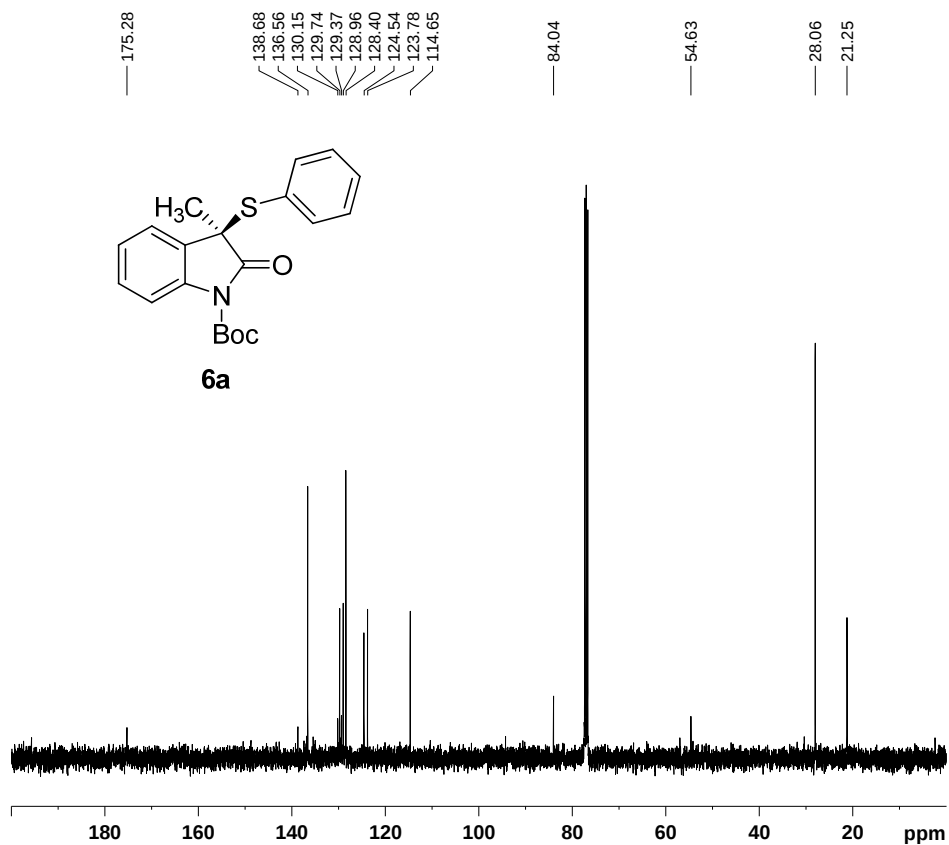


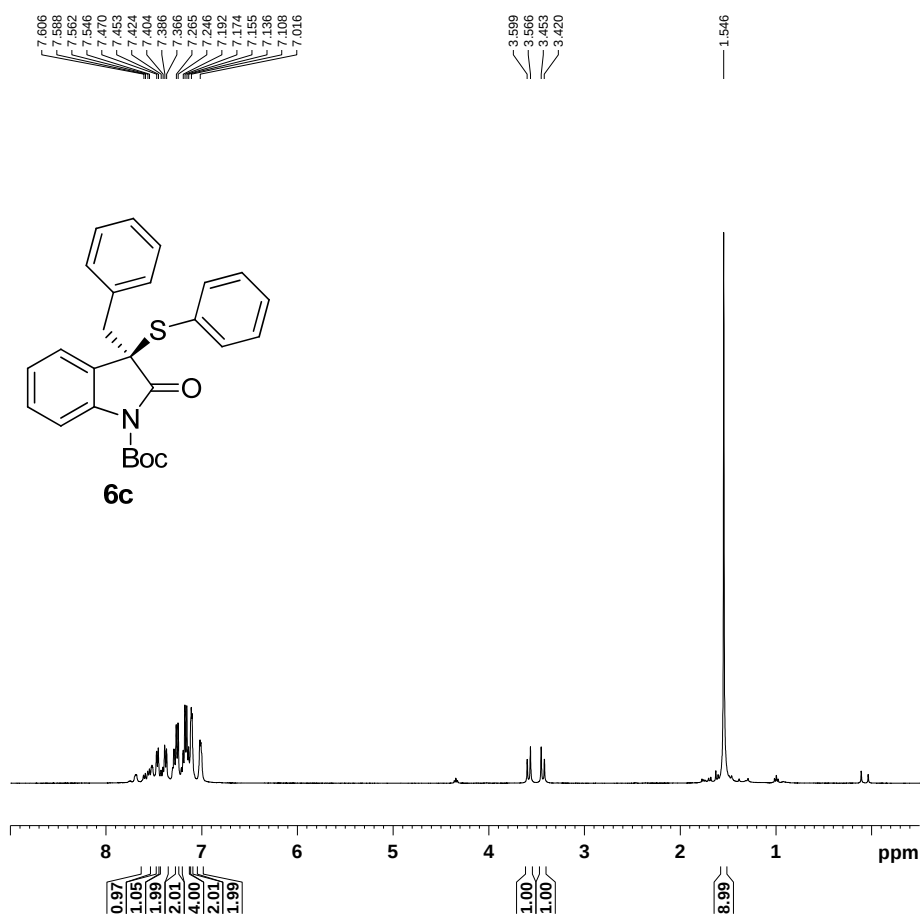
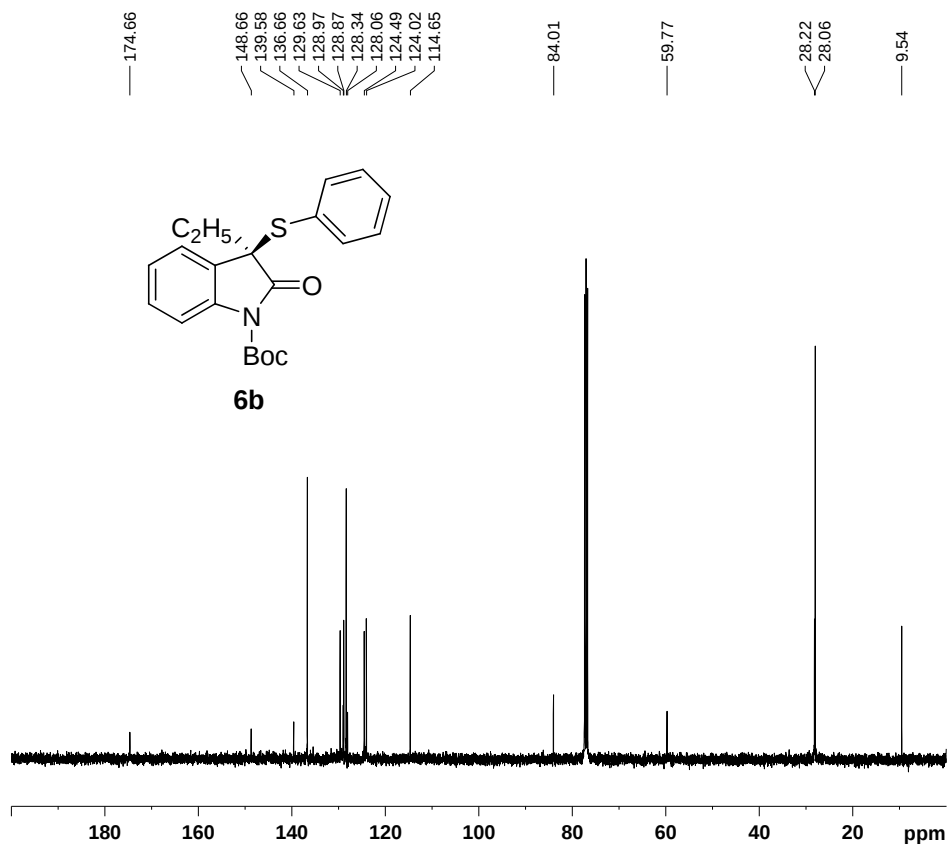


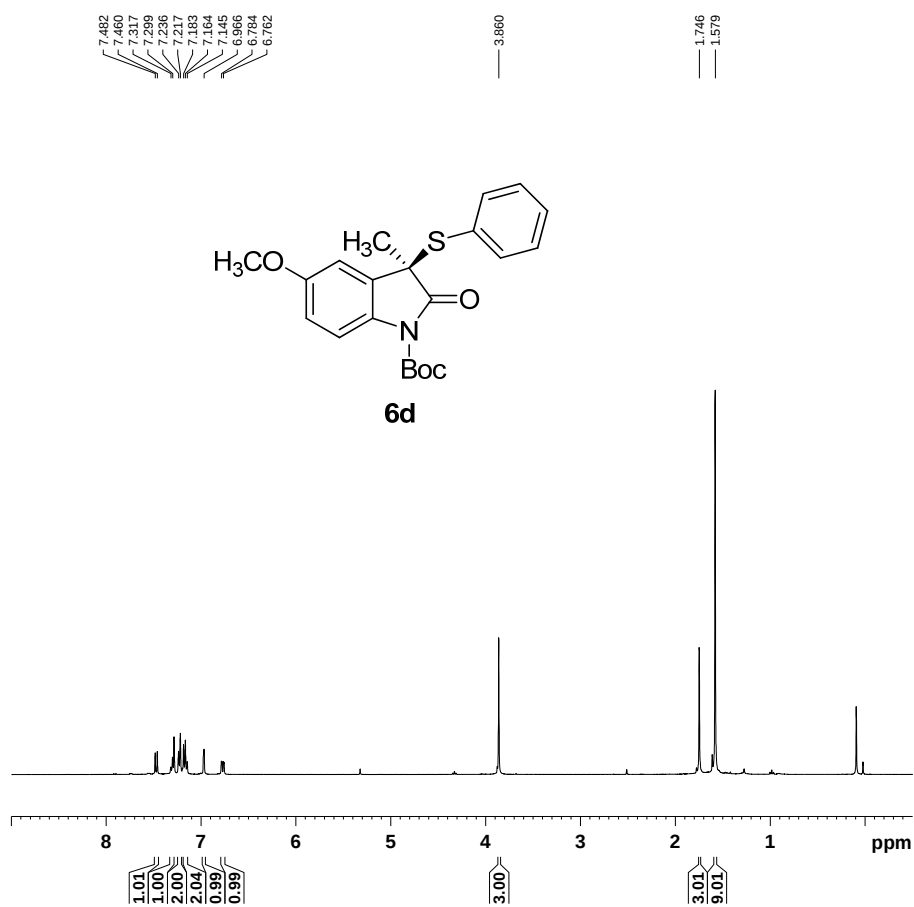
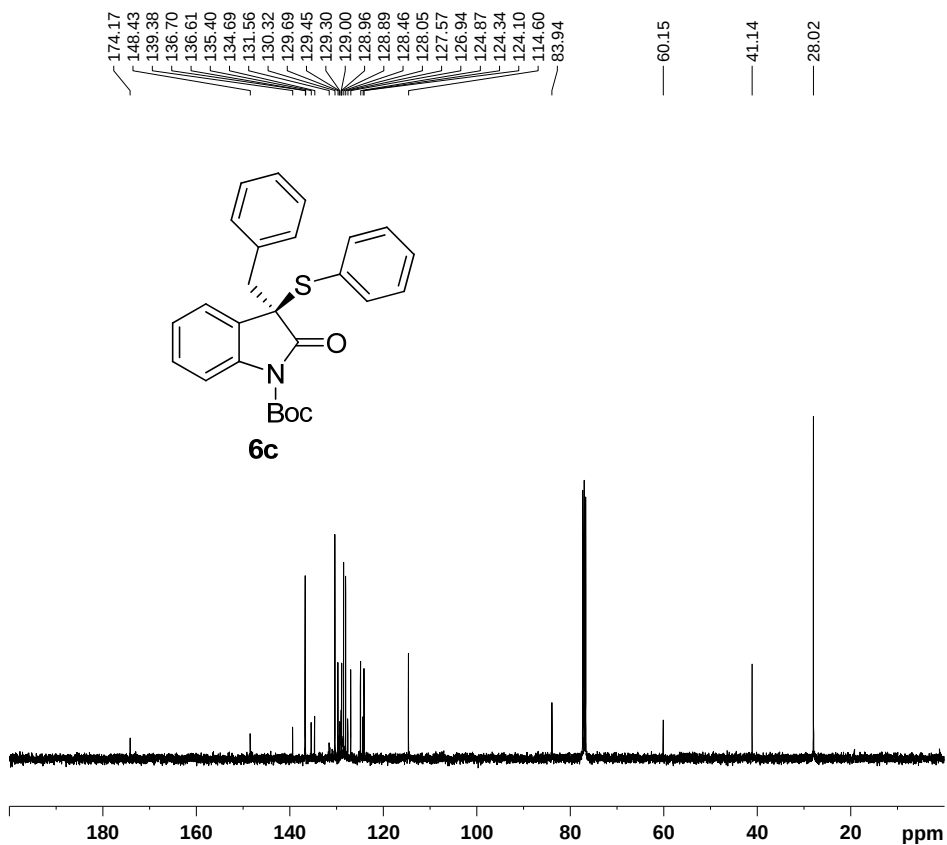


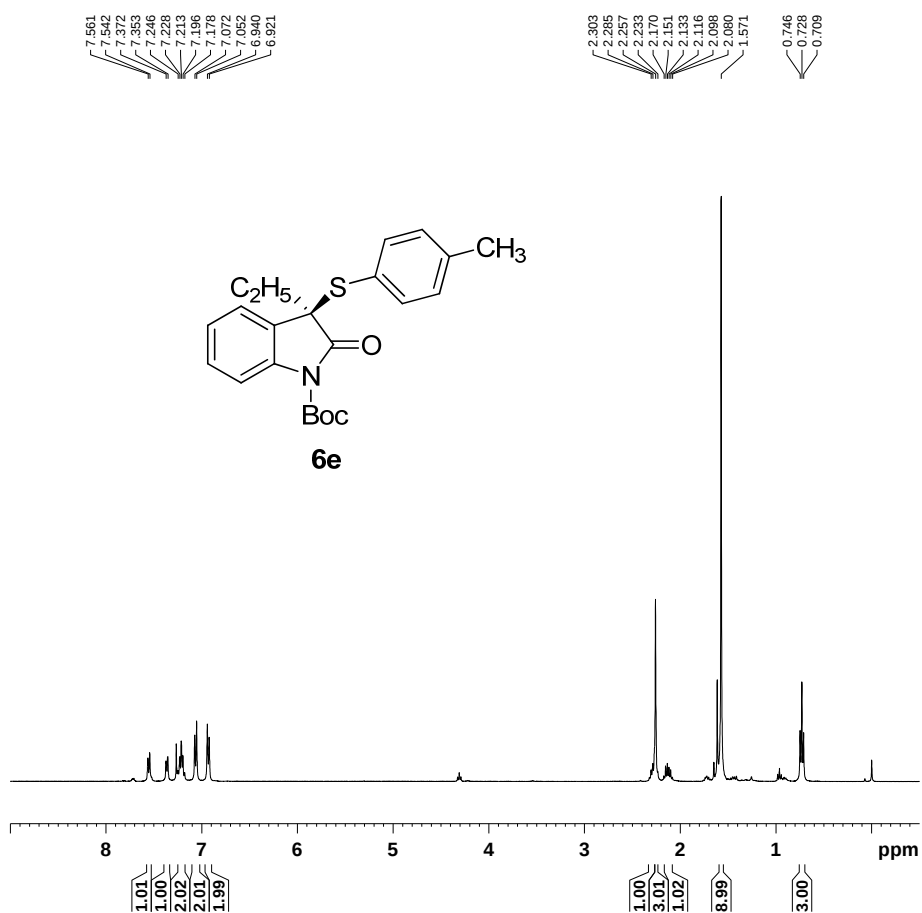
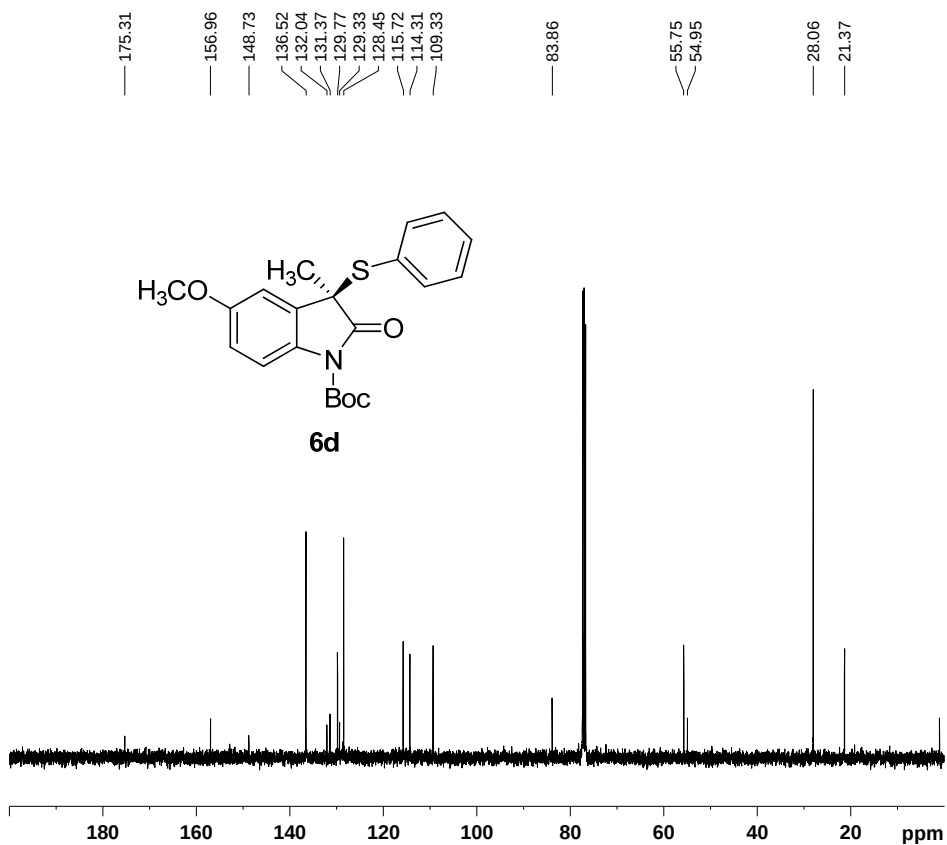


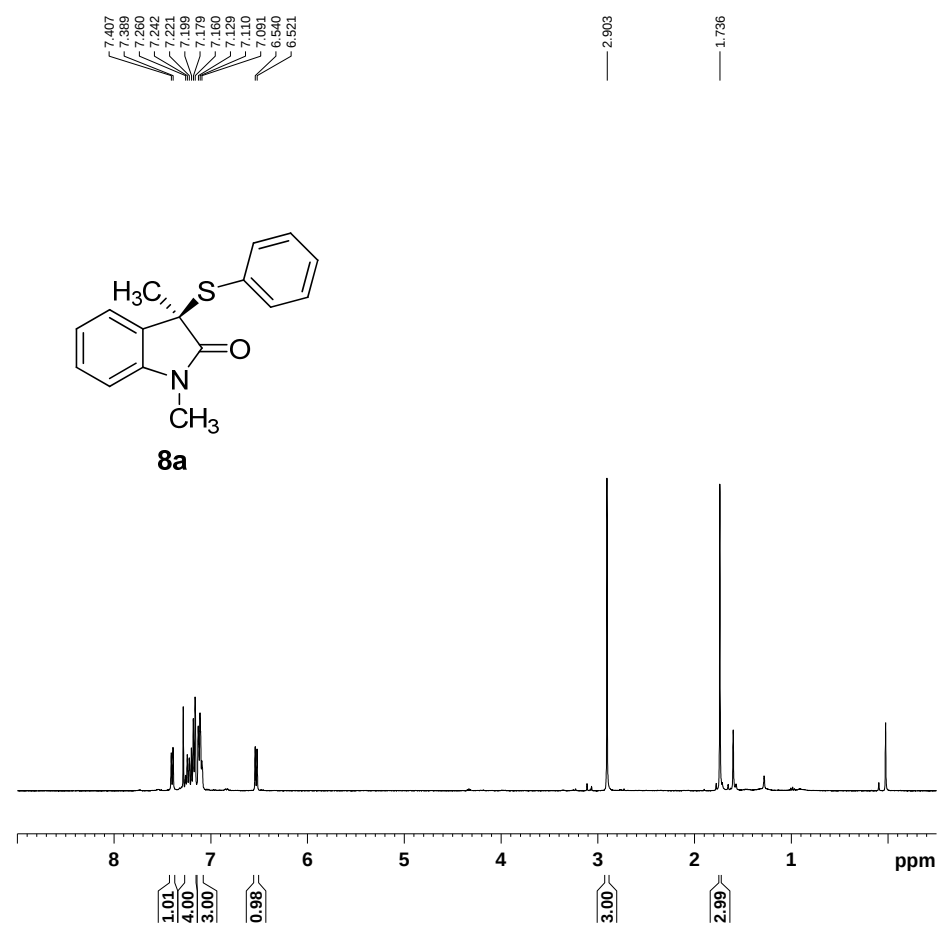
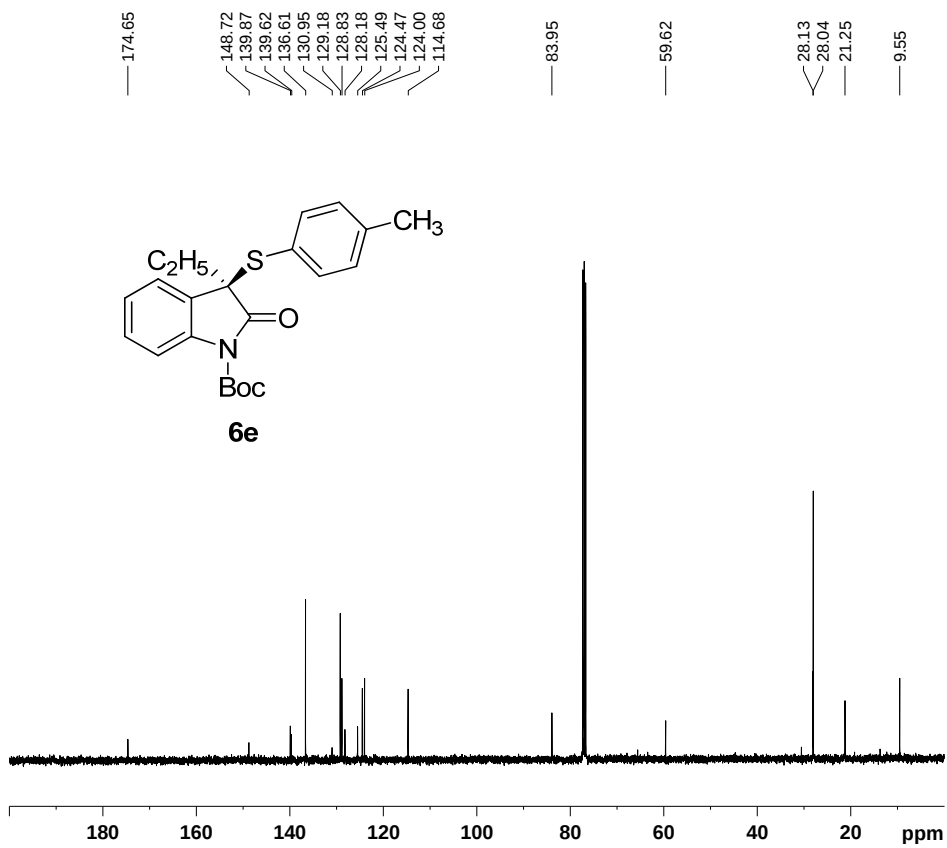


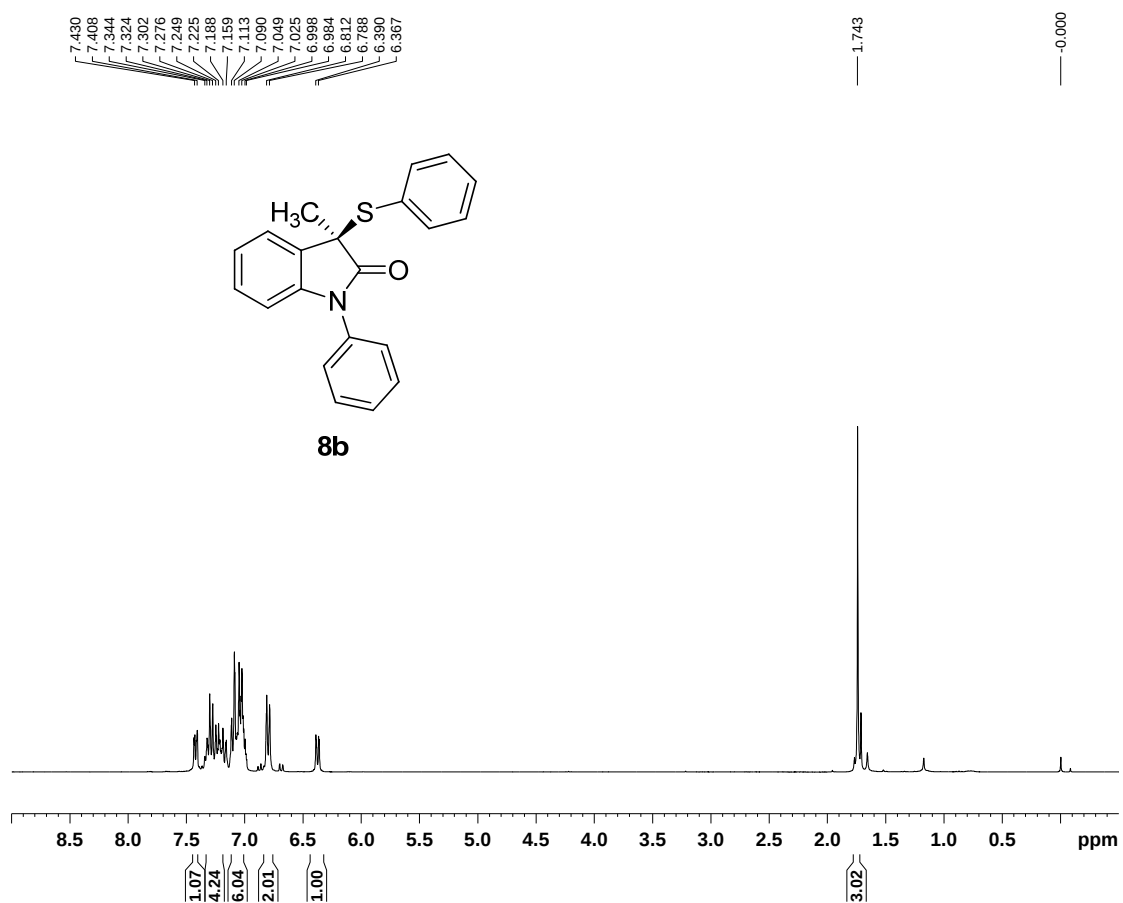
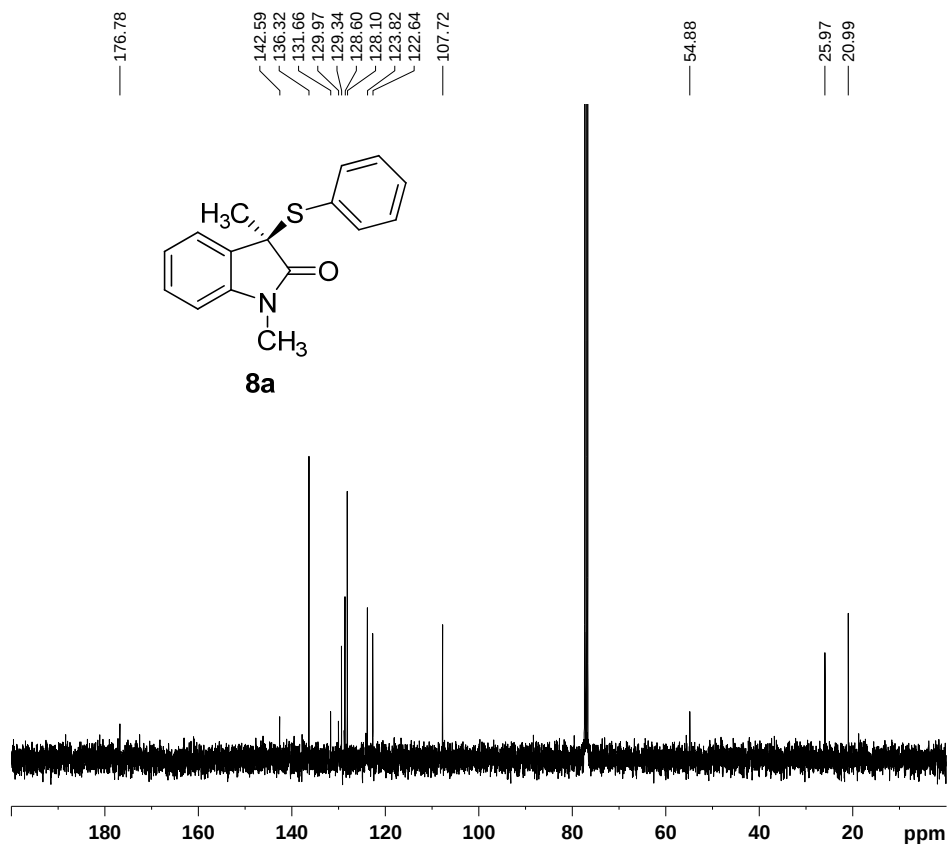


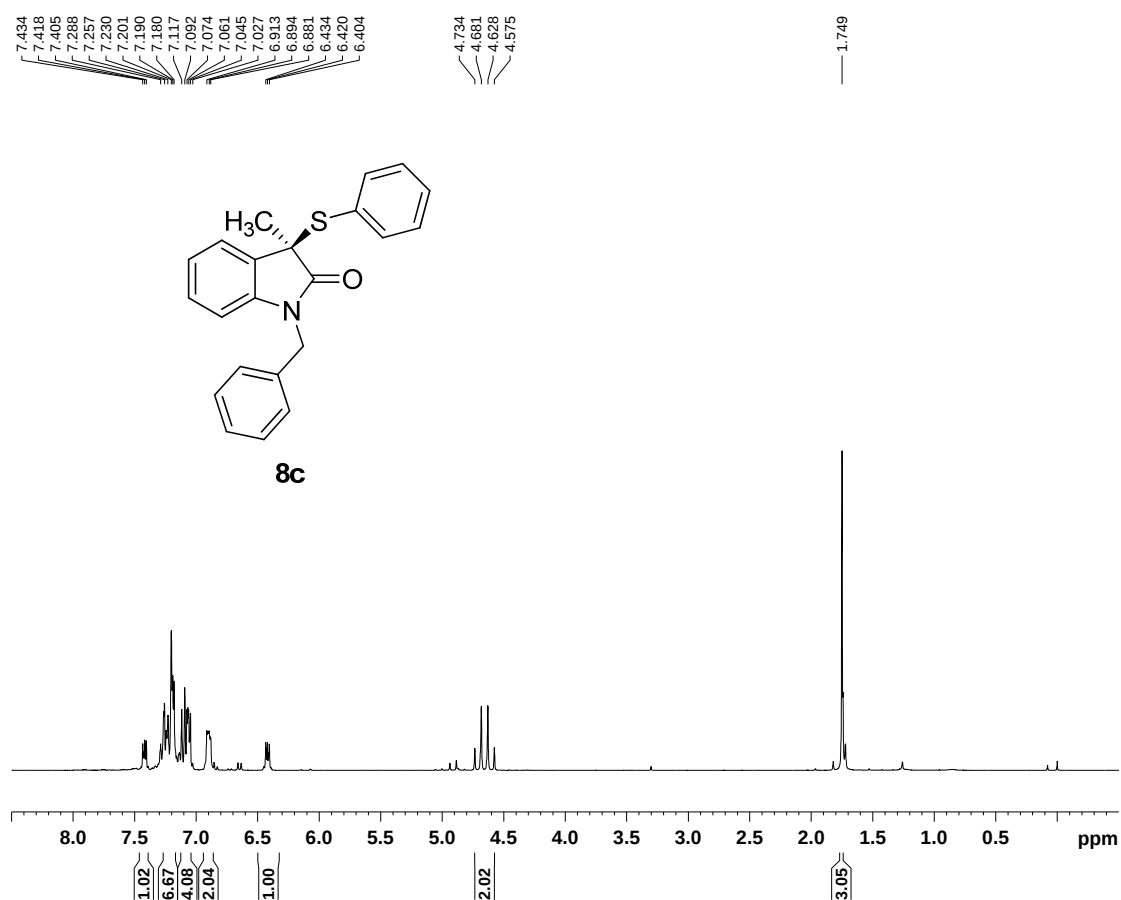
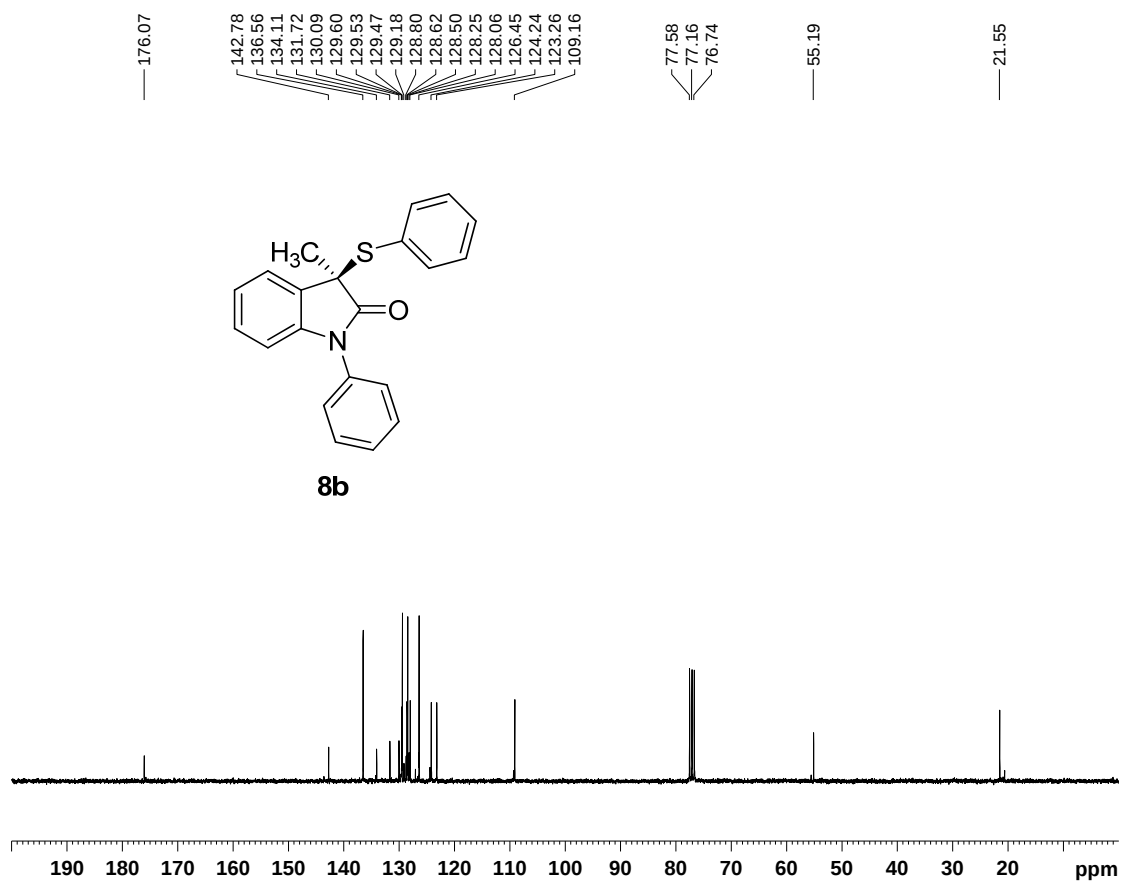


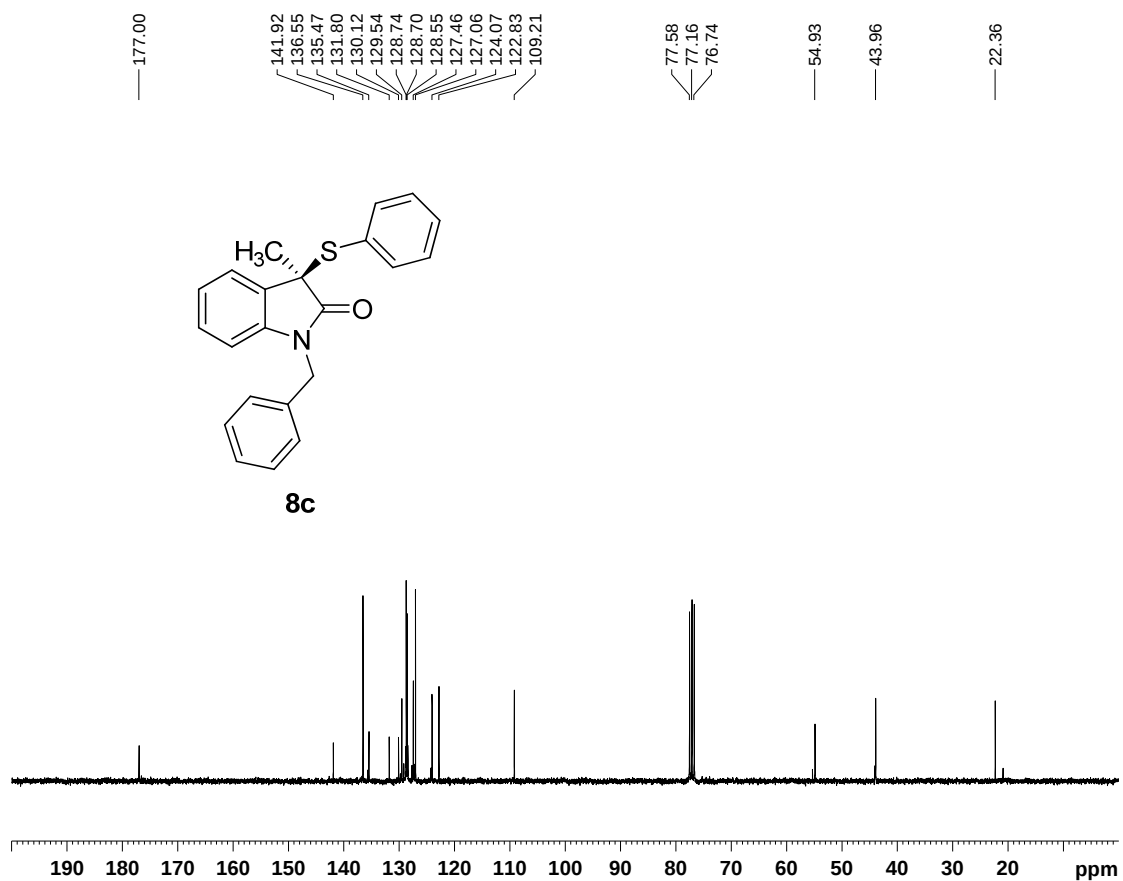




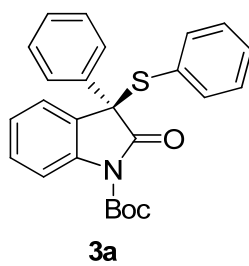


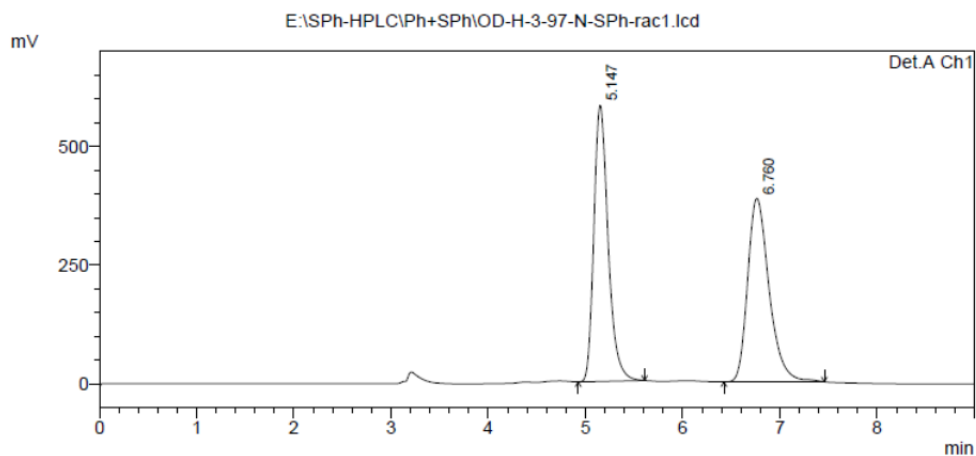






HPLC spectrum for the sulfenylation products:



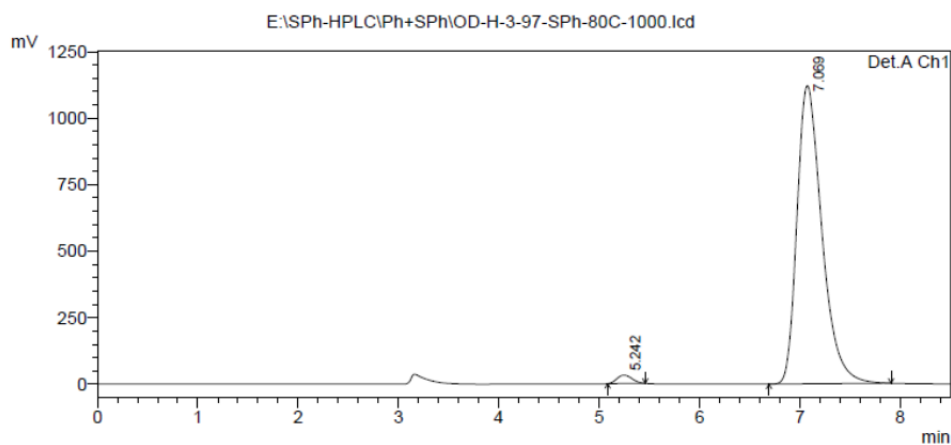


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.147	5934706	582462	49.949	60.092
2	6.760	5946898	386824	50.051	39.908
Total		11881604	969286	100.000	100.000

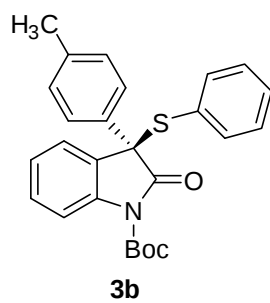


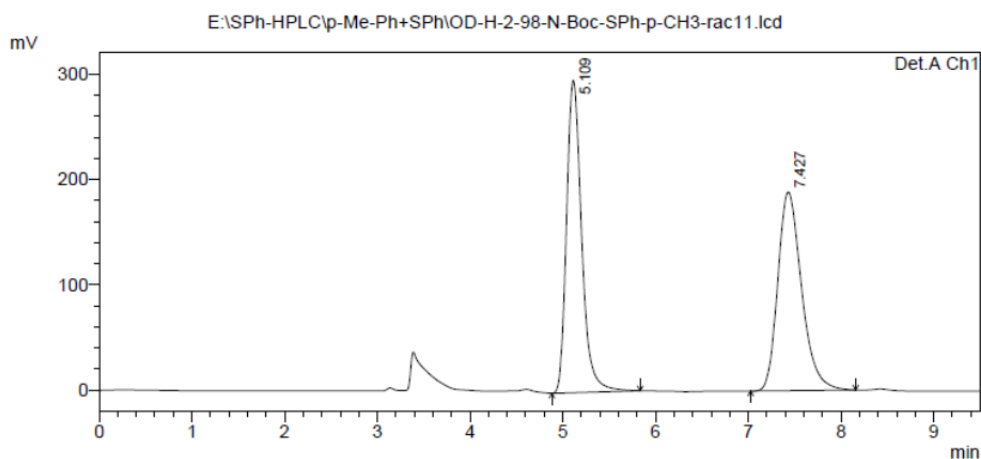
1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.242	325284	31704	1.652	2.750
2	7.069	19360282	1121274	98.348	97.250
Total		19685566	1152978	100.000	100.000

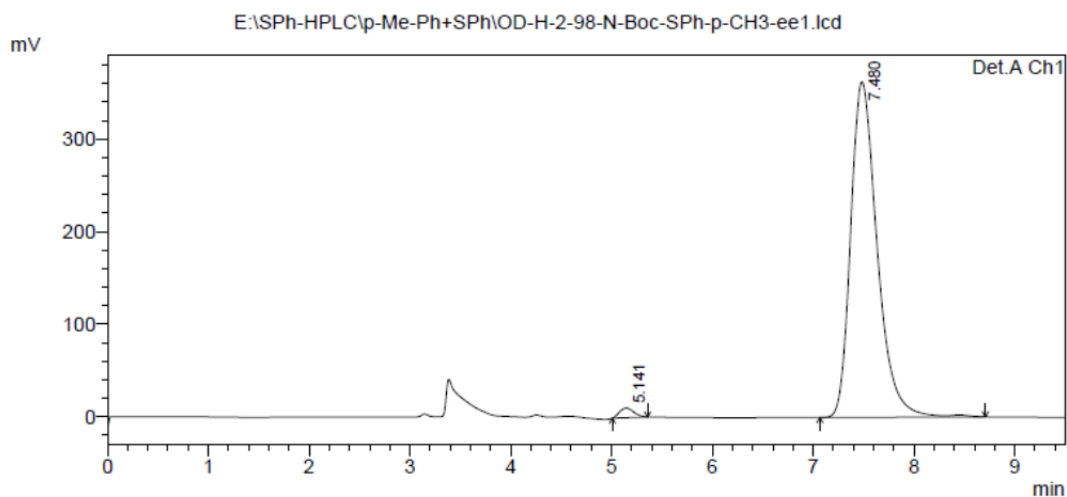




PeakTable

Detector A Ch1 210nm

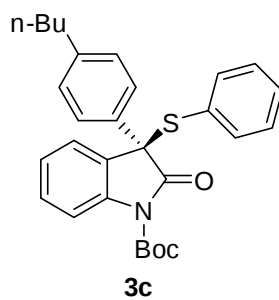
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.109	3355961	296395	49.905	61.107
2	7.427	3368677	188648	50.095	38.893
Total		6724638	485043	100.000	100.000

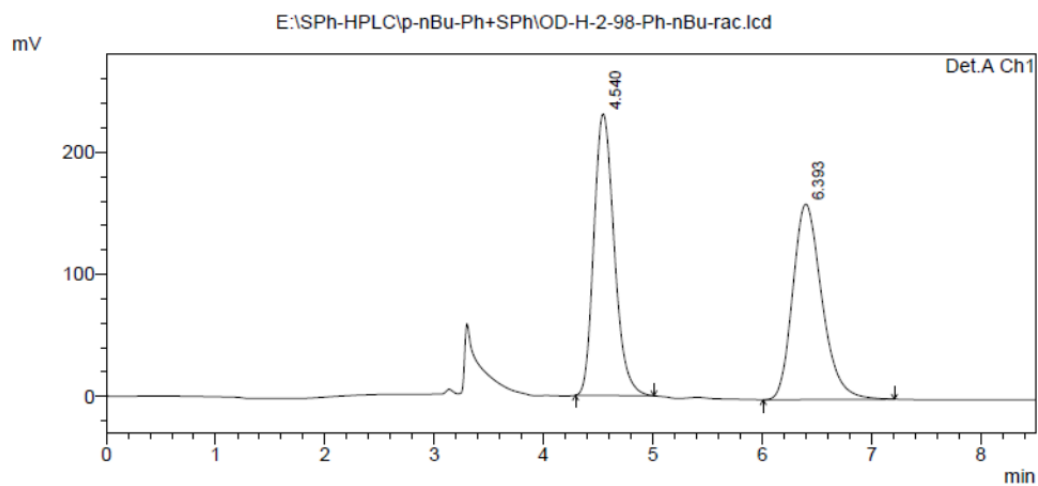


PeakTable

Detector A Ch1 210nm

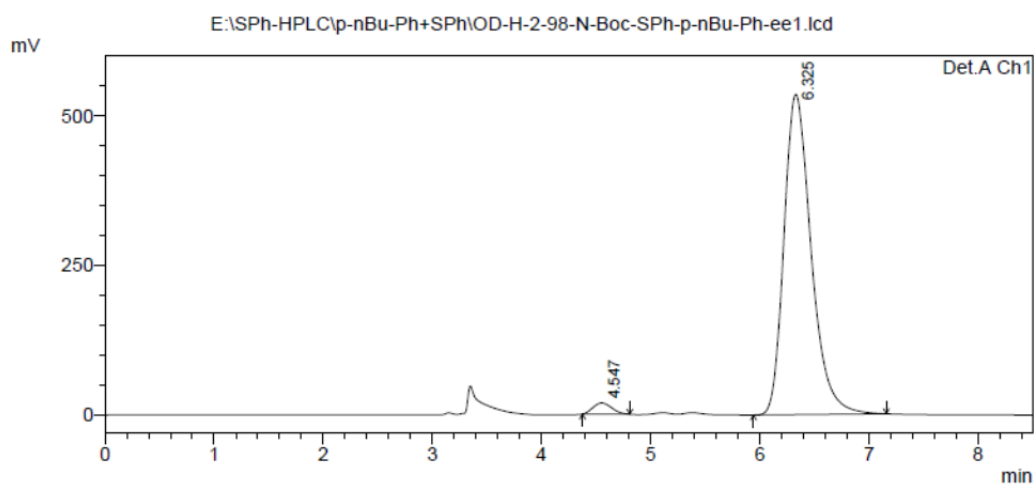
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.141	103751	10369	1.544	2.780
2	7.480	6615613	362583	98.456	97.220
Total		6719364	372952	100.000	100.000





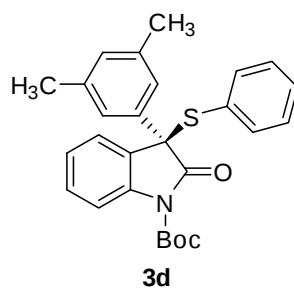
PeakTable

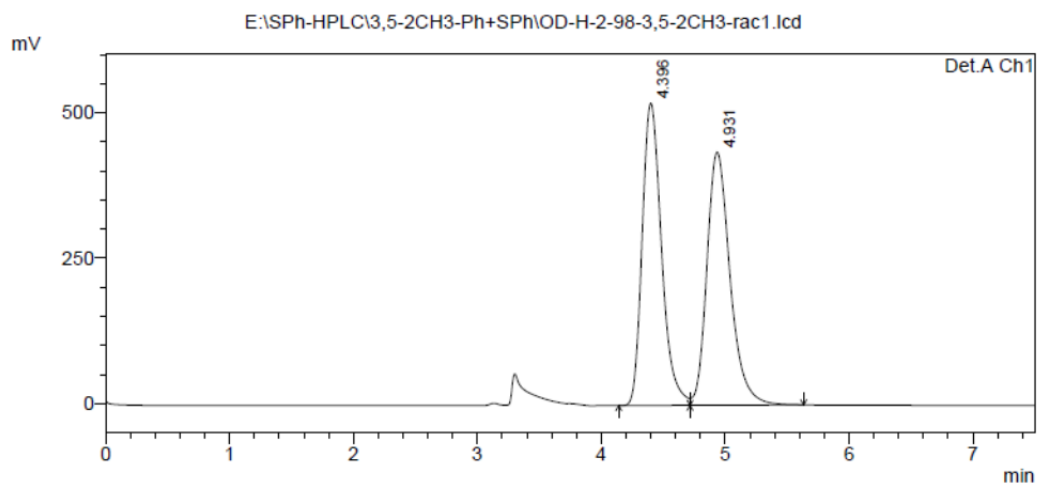
Detector A Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.540	2983504	230744	50.101	59.019
2	6.393	2971465	160220	49.899	40.981
Total		5954969	390964	100.000	100.000



PeakTable

Detector A Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.547	223669	18695	2.356	3.371
2	6.325	9269413	535880	97.644	96.629
Total		9493082	554576	100.000	100.000

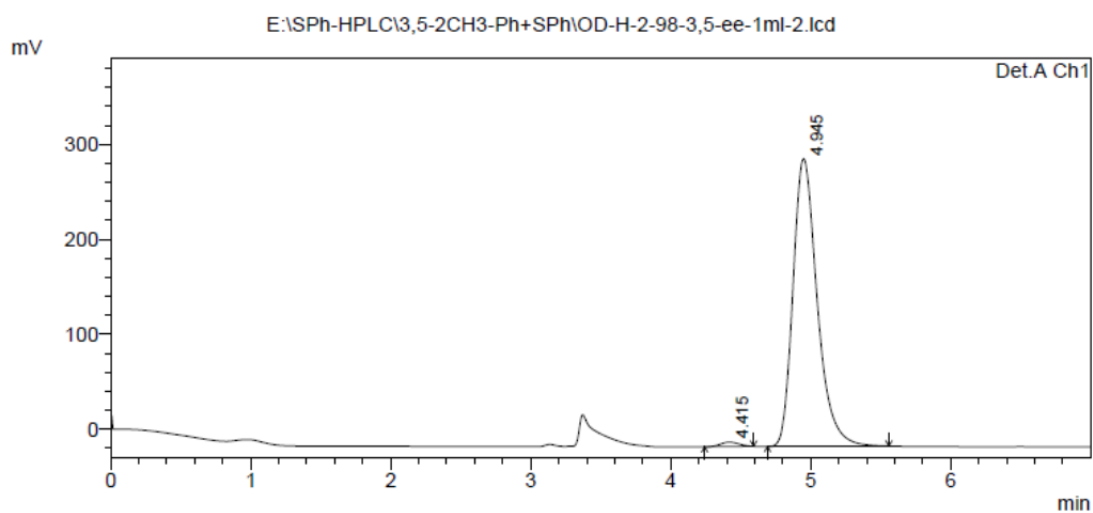




PeakTable

Detector A Ch1 210nm

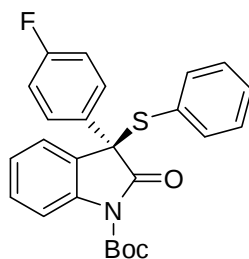
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.396	5646921	520245	49.908	54.427
2	4.931	5667734	435607	50.092	45.573
Total		11314655	955852	100.000	100.000



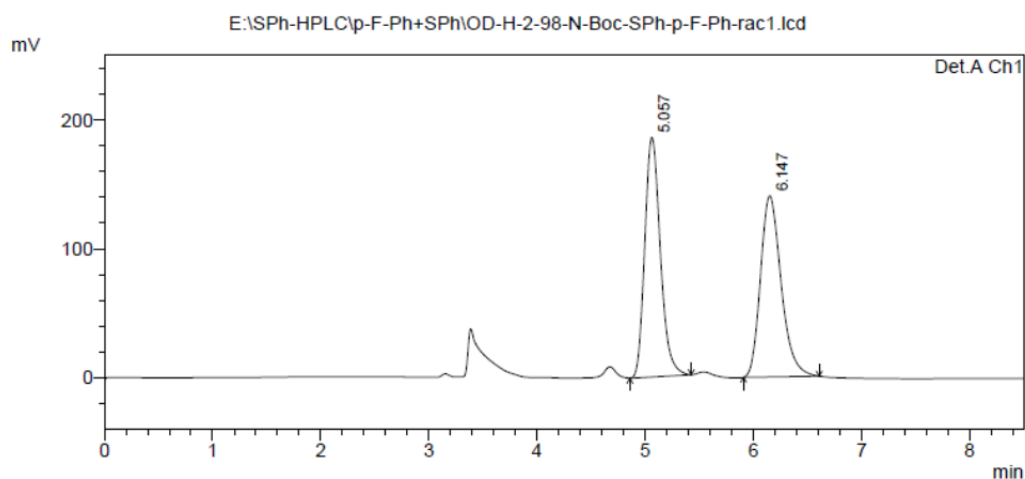
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.415	42433	4619	1.153	1.501
2	4.945	3637959	303132	98.847	98.499
Total		3680392	307752	100.000	100.000



3e

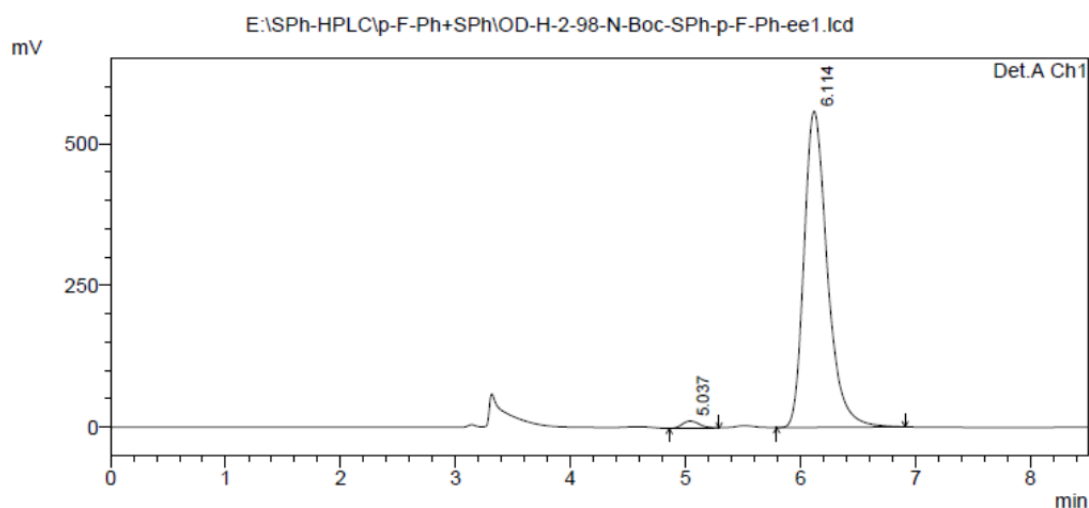


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.057	1864349	185969	49.957	56.919
2	6.147	1867533	140758	50.043	43.081
Total		3731883	326727	100.000	100.000

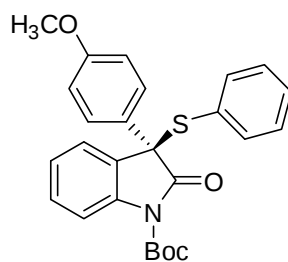


1 Det.A Ch1/210nm

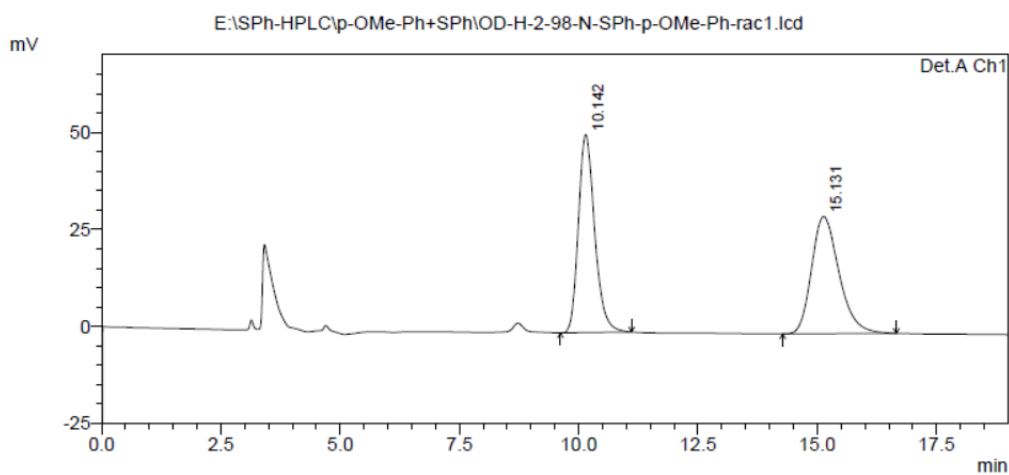
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.037	134704	12733	1.682	2.229
2	6.114	7873012	558453	98.318	97.771
Total		8007716	571186	100.000	100.000

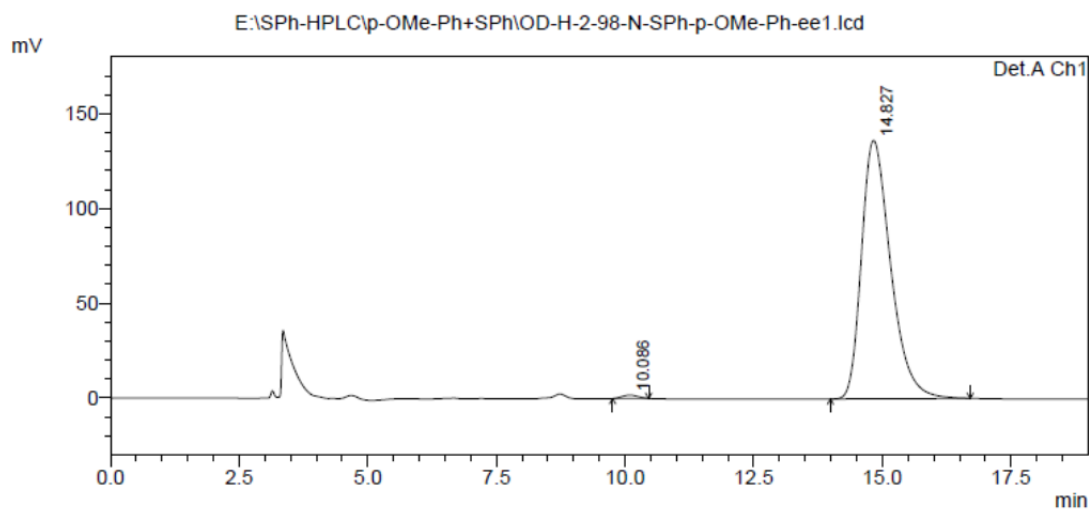


3f



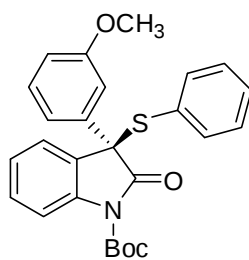
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.142	1213380	51033	50.026	62.787
2	15.131	1212104	30247	49.974	37.213
Total		2425484	81280	100.000	100.000

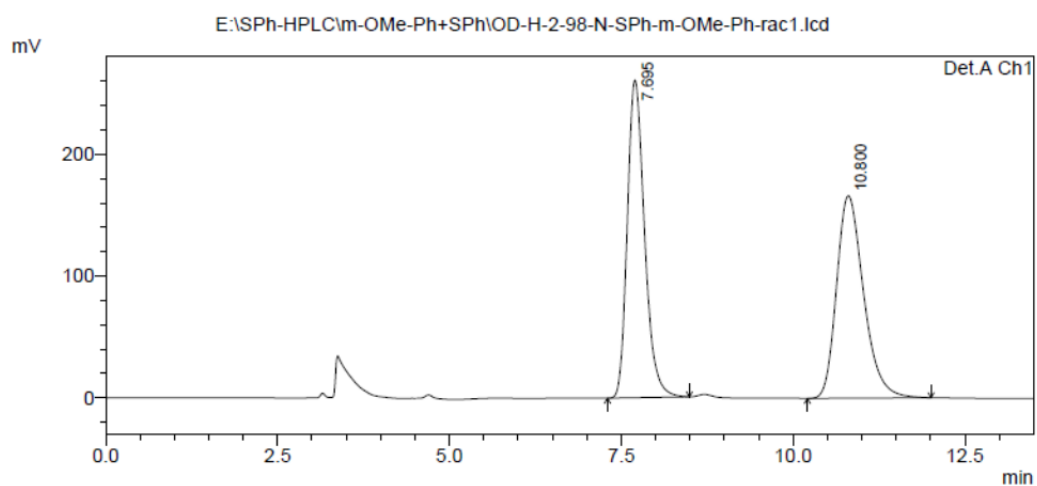


PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.086	38472	1832	0.709	1.325
2	14.827	5384571	136422	99.291	98.675
Total		5423043	138254	100.000	100.000



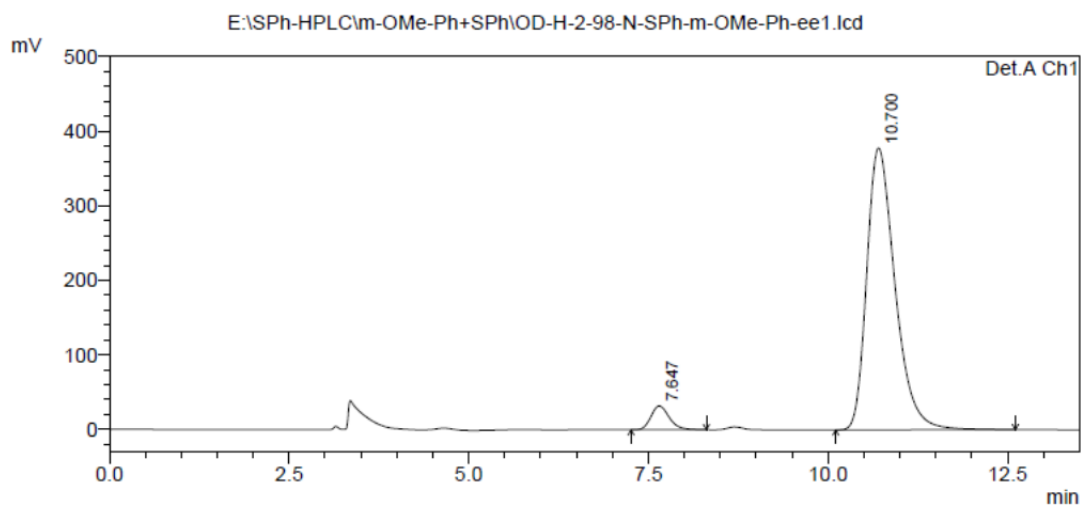
3g



Detector A Ch1 210nm

PeakTable

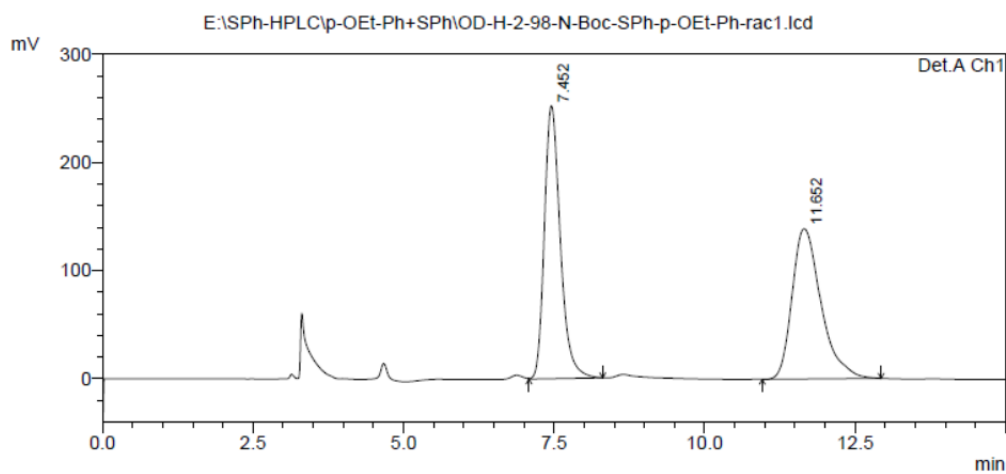
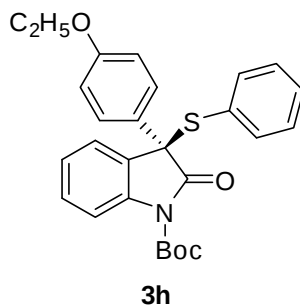
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.695	4555263	260979	50.010	61.073
2	10.800	4553479	166343	49.990	38.927
Total		9108742	427323	100.000	100.000



PeakTable

Detector A Ch1 210nm

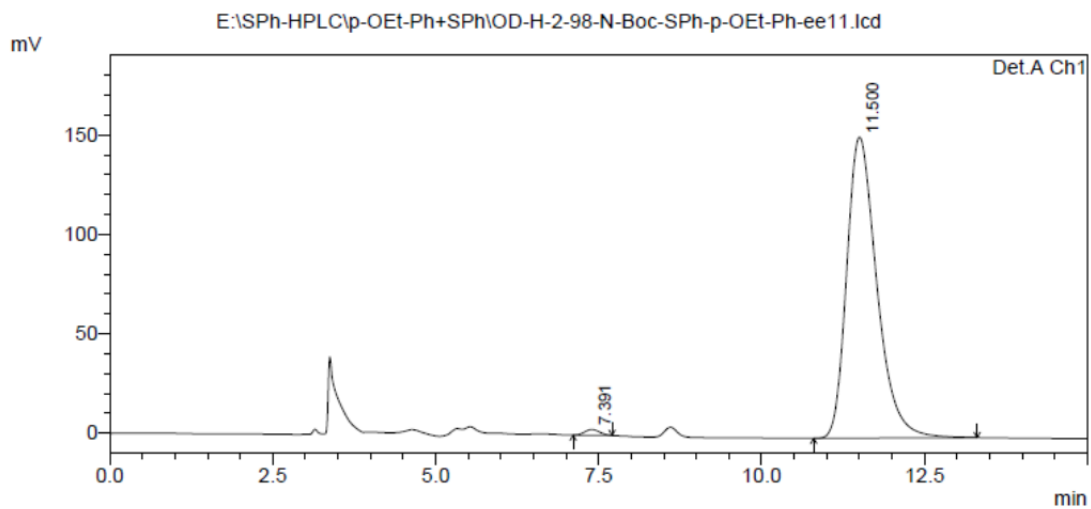
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.647	562535	31938	5.148	7.787
2	10.700	10365476	378225	94.852	92.213
Total		10928011	410164	100.000	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.452	4646170	252509	49.976	64.458
2	11.652	4650706	139235	50.024	35.542
Total		9296876	391745	100.000	100.000

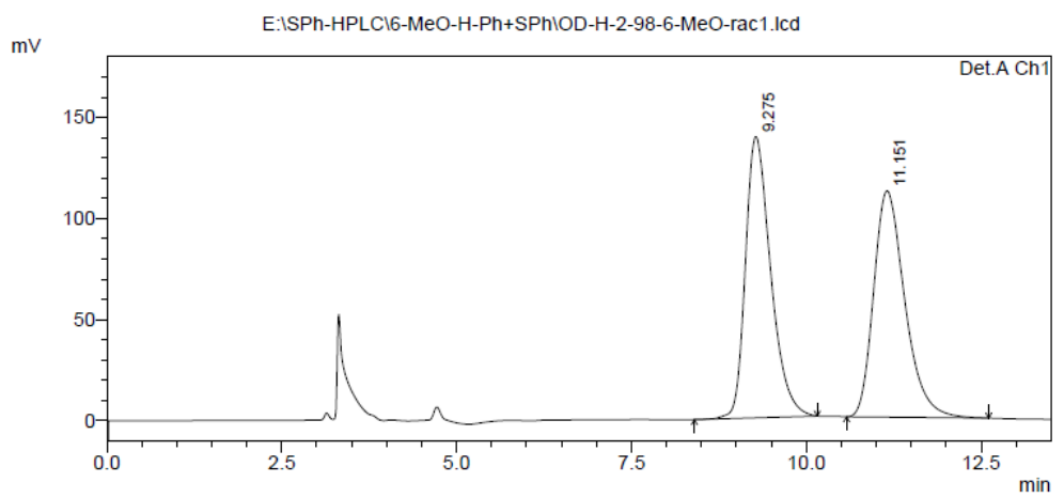
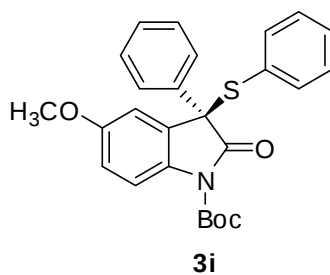


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.391	46098	2929	0.936	1.897
2	11.500	4880333	151489	99.064	98.103
Total		4926431	154418	100.000	100.000

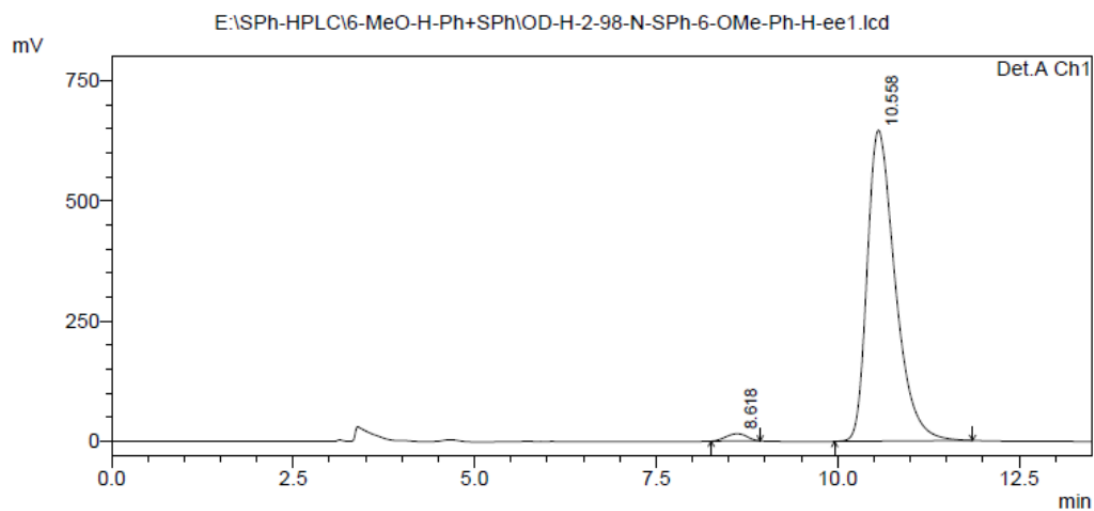


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

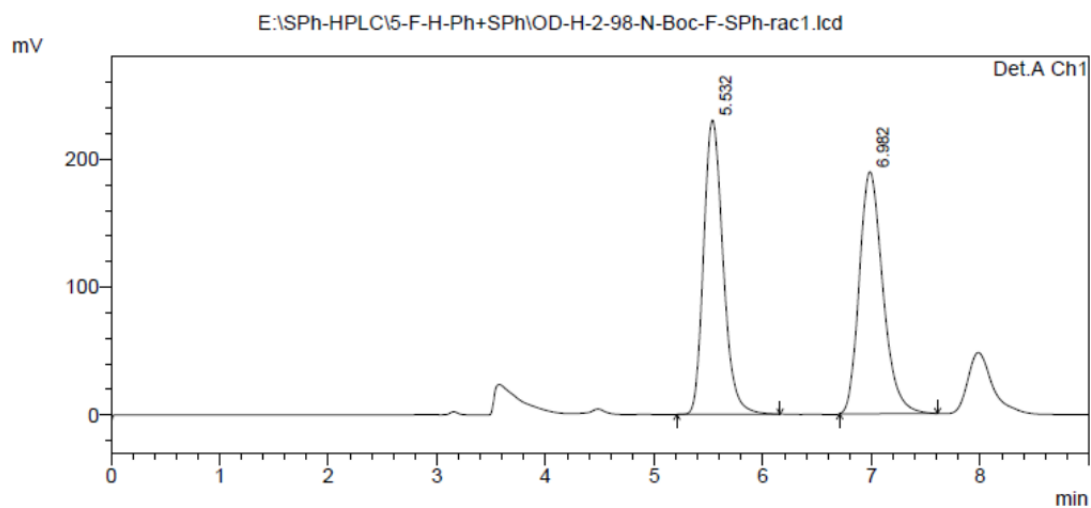
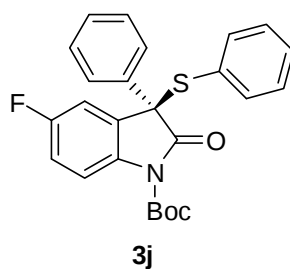
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.275	3499907	139132	50.197	55.412
2	11.151	3472446	111955	49.803	44.588
Total		6972353	251086	100.000	100.000



PeakTable

Detector A Ch1 210nm

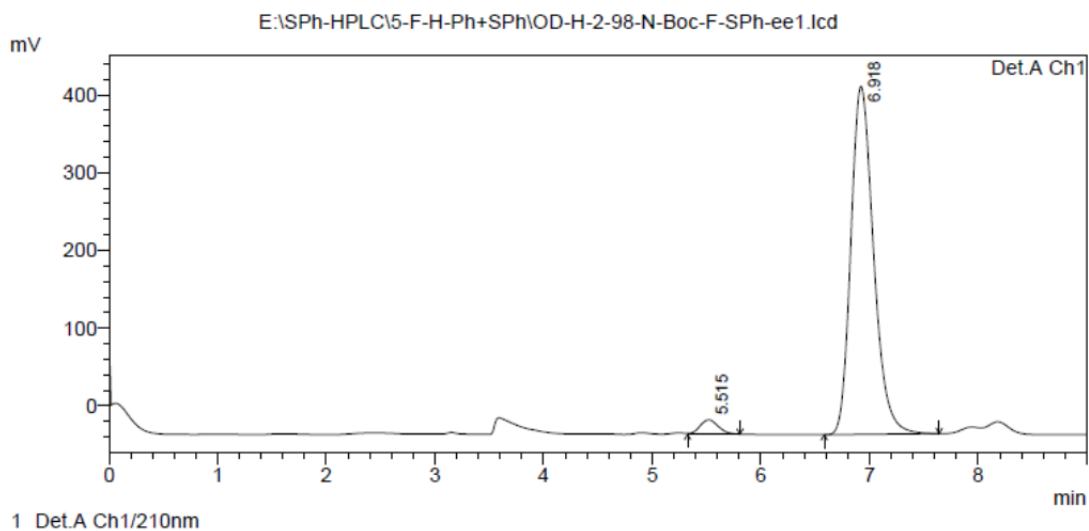
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.618	305423	15241	1.728	2.301
2	10.558	17369505	647232	98.272	97.699
Total		17674928	662473	100.000	100.000



PeakTable

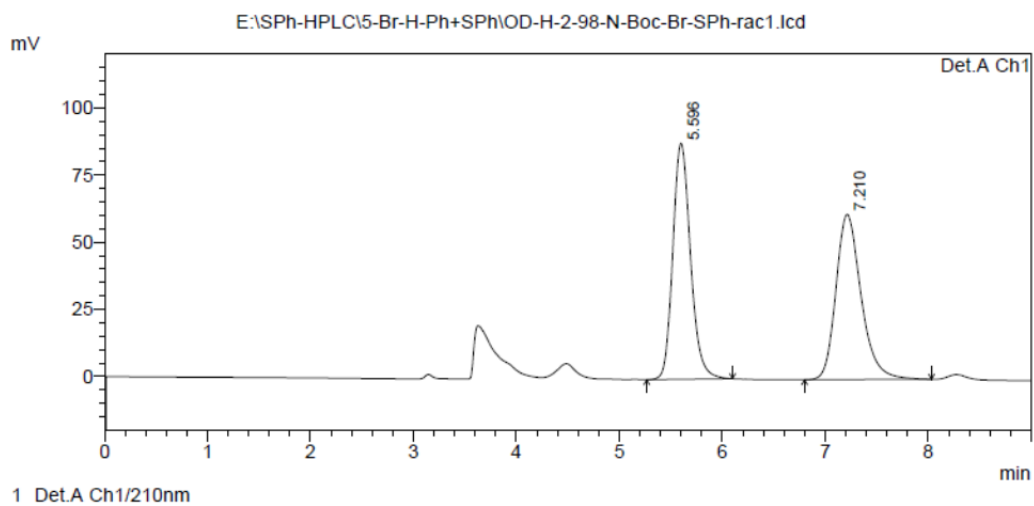
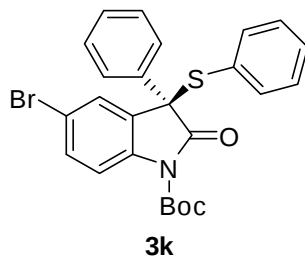
Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.532	2867690	230073	50.023	54.856
2	6.982	2865097	189337	49.977	45.144
Total		5732787	419410	100.000	100.000



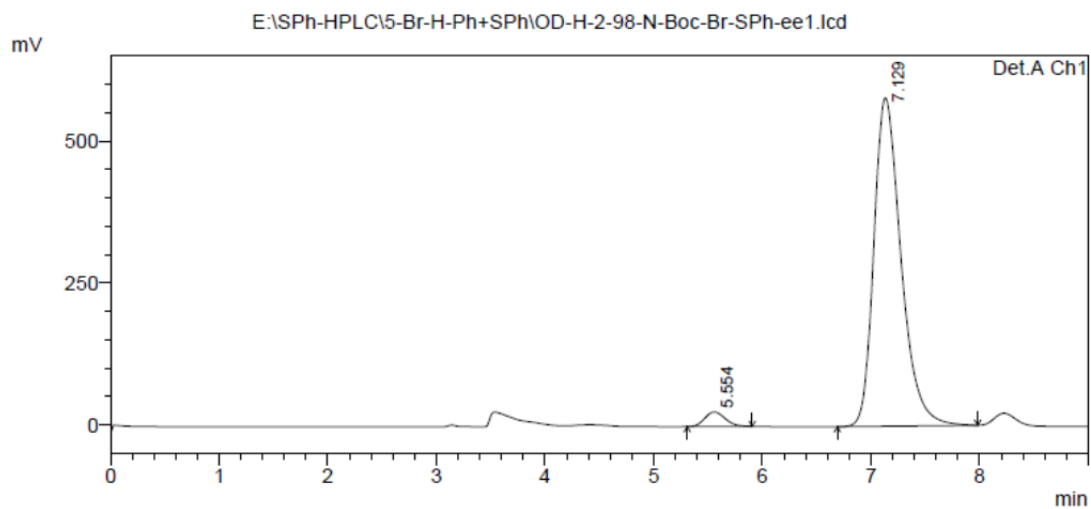
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.515	217094	18444	3.227	3.956
2	6.918	6510759	447821	96.773	96.044
Total		6727853	466266	100.000	100.000



PeakTable

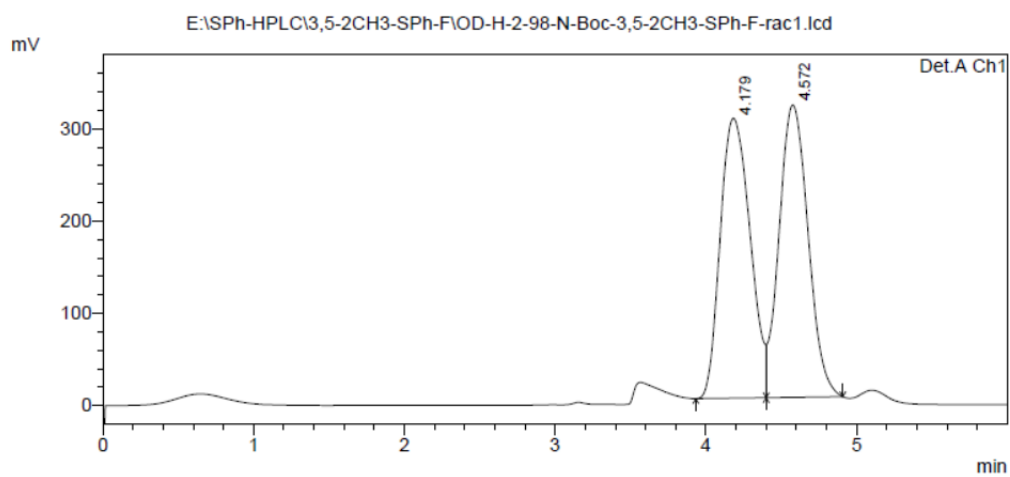
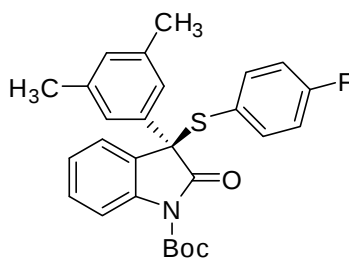
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.596	1050415	86250	50.083	58.528
2	7.210	1046948	61116	49.917	41.472
Total		2097363	147366	100.000	100.000



PeakTable

Detector A Ch1 210nm

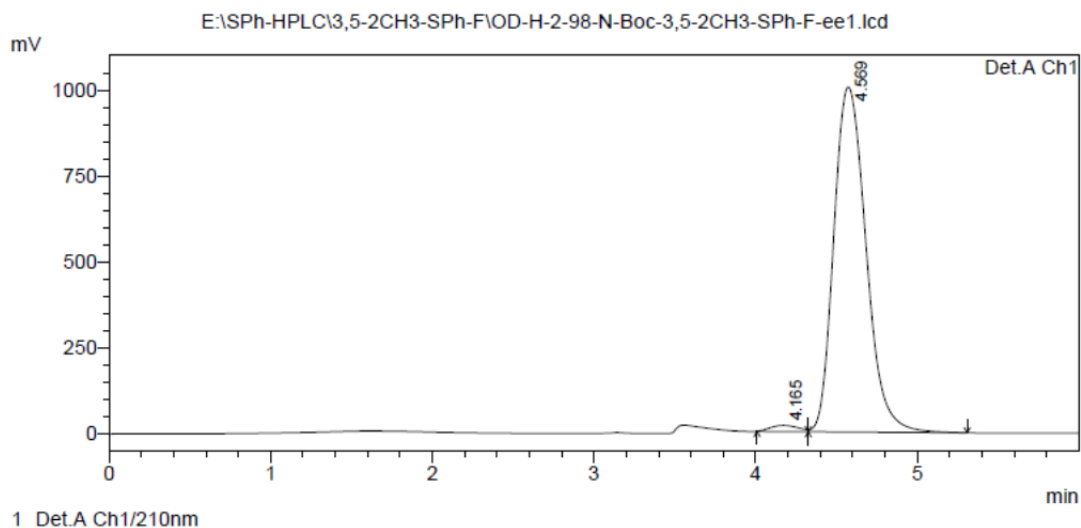
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.554	334675	25516	3.219	4.222
2	7.129	10062680	578873	96.781	95.778
Total		10397355	604389	100.000	100.000



PeakTable

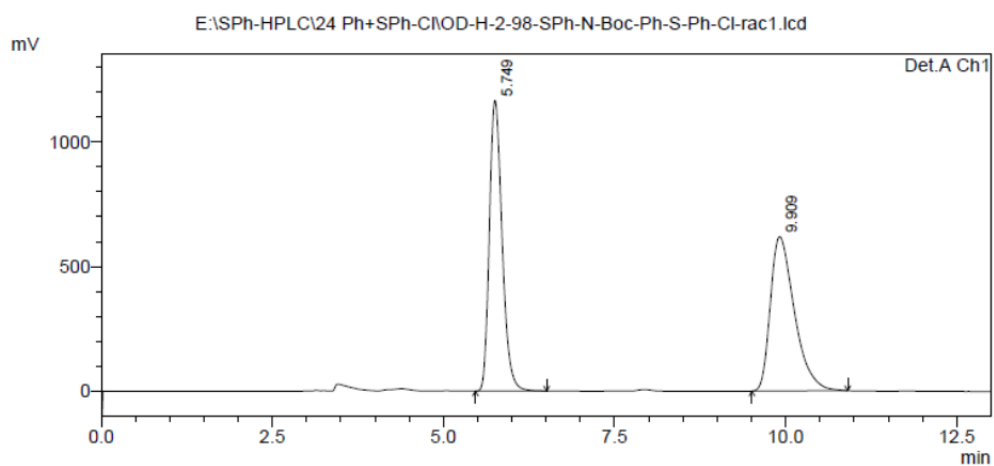
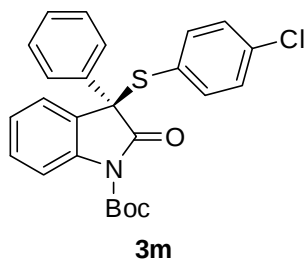
Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.179	4193452	303592	49.747	48.913
2	4.572	4236081	317089	50.253	51.087
Total		8429533	620682	100.000	100.000



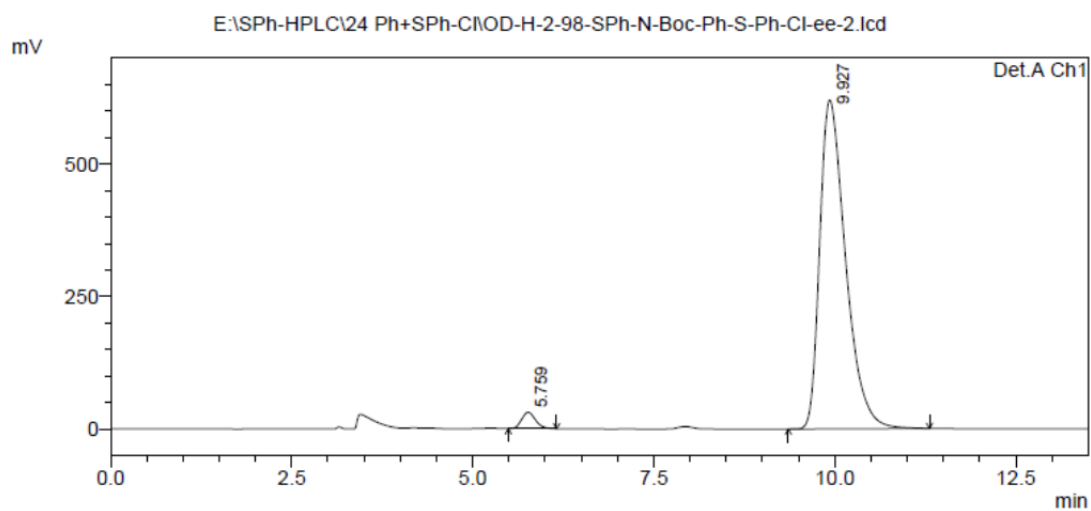
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.165	213855	17816	1.515	1.744
2	4.569	13900334	1003815	98.485	98.256
Total		14114189	1021631	100.000	100.000



PeakTable

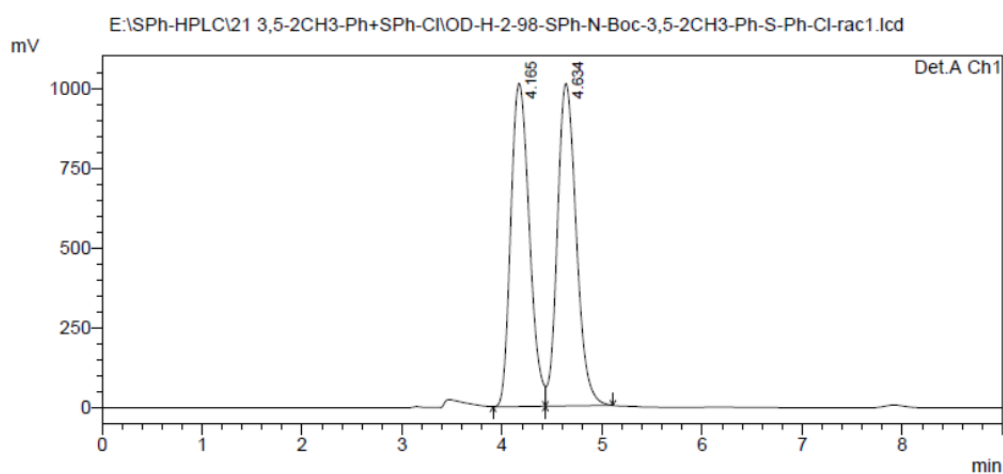
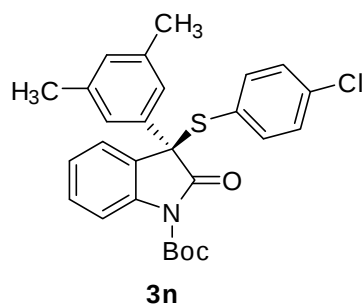
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.749	15117814	1166060	49.967	65.310
2	9.909	15137961	619369	50.033	34.690
Total		30255775	1785429	100.000	100.000



PeakTable

Detector A Ch1 210nm

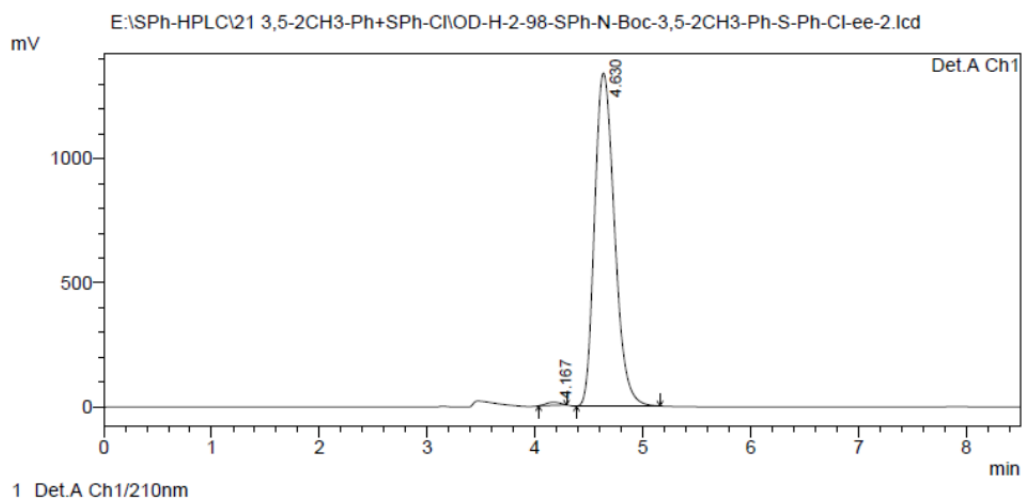
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.759	413930	30966	2.615	4.750
2	9.927	15416099	620898	97.385	95.250
Total		15830028	651864	100.000	100.000



PeakTable

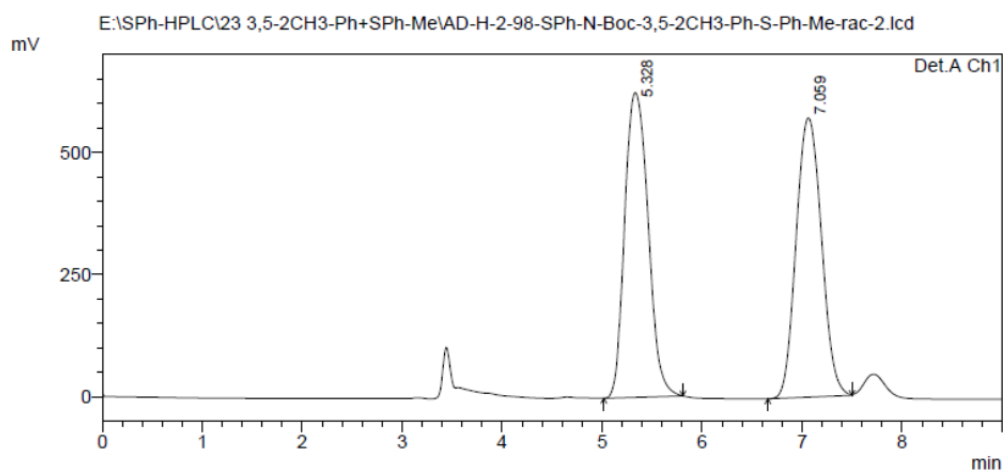
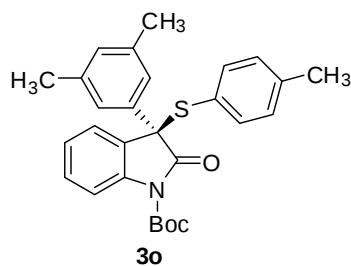
Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.165	13041949	1011773	49.612	50.066
2	4.634	13245738	1009090	50.388	49.934
Total		26287687	2020863	100.000	100.000



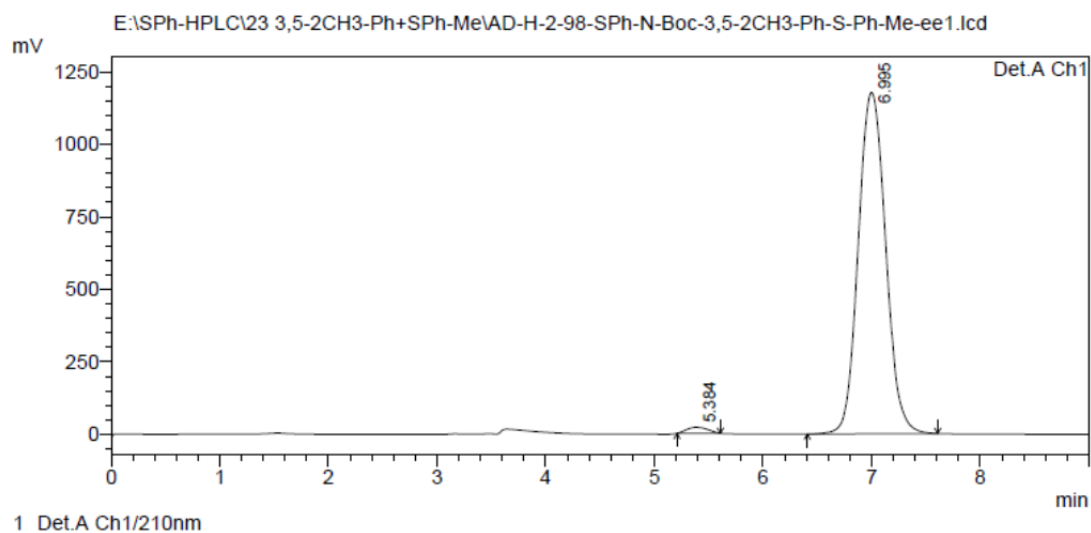
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.167	112846	12724	0.650	0.940
2	4.630	17244496	1341510	99.350	99.060
Total		17357342	1354234	100.000	100.000



PeakTable

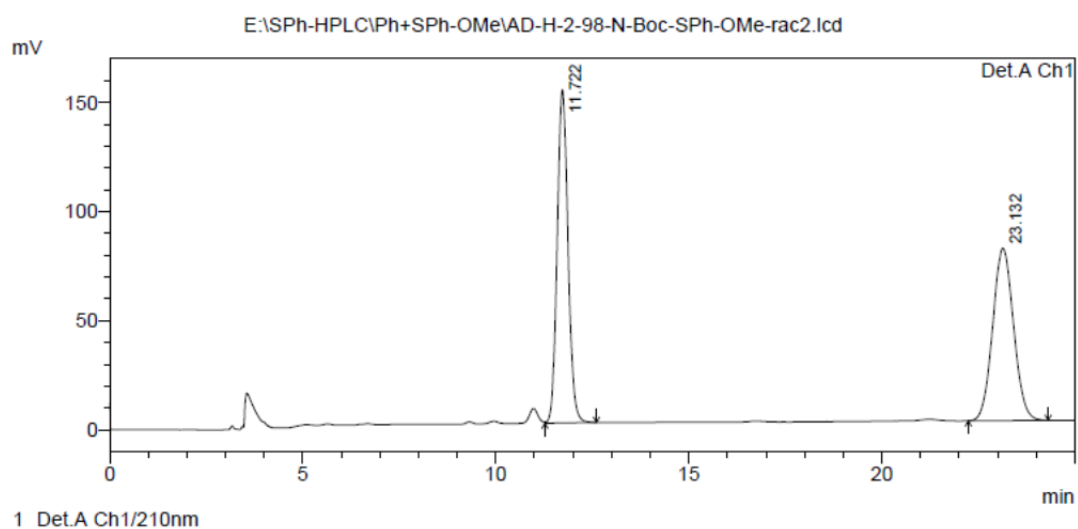
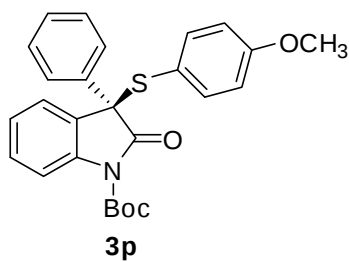
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.328	10184973	624220	50.219	52.178
2	7.059	10096013	572120	49.781	47.822
Total		20280986	1196340	100.000	100.000



PeakTable

Detector A Ch1 210nm

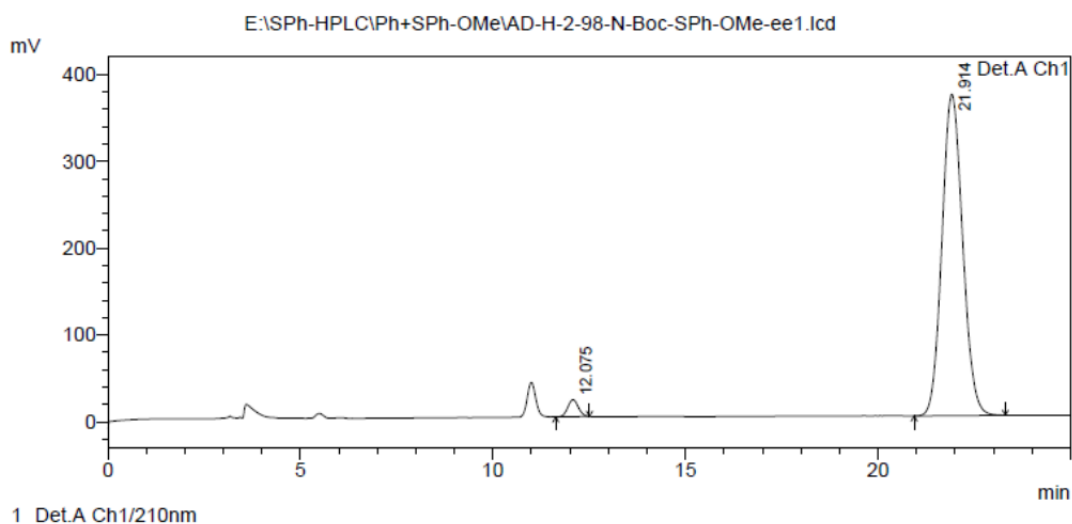
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.384	282346	20652	1.350	1.723
2	6.995	20624791	1178259	98.650	98.277
Total		20907137	1198912	100.000	100.000



PeakTable

Detector A Ch1 210nm

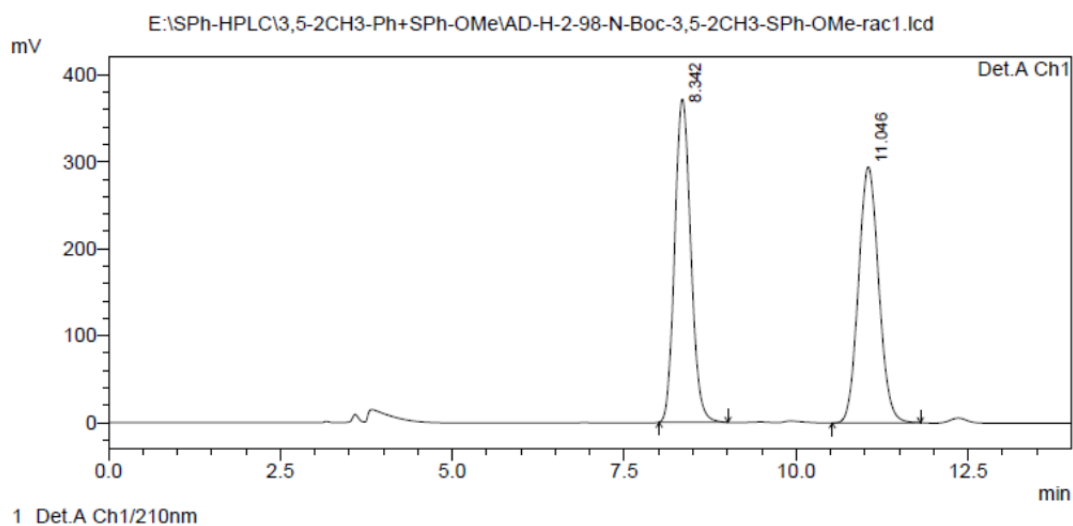
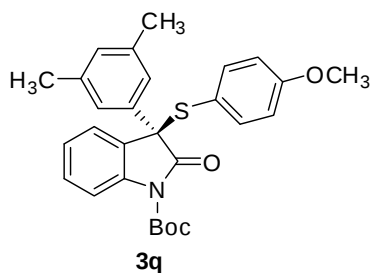
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.722	2976756	152683	50.000	65.899
2	23.132	2976757	79008	50.000	34.101
Total		5953513	231691	100.000	100.000



PeakTable

Detector A Ch1 210nm

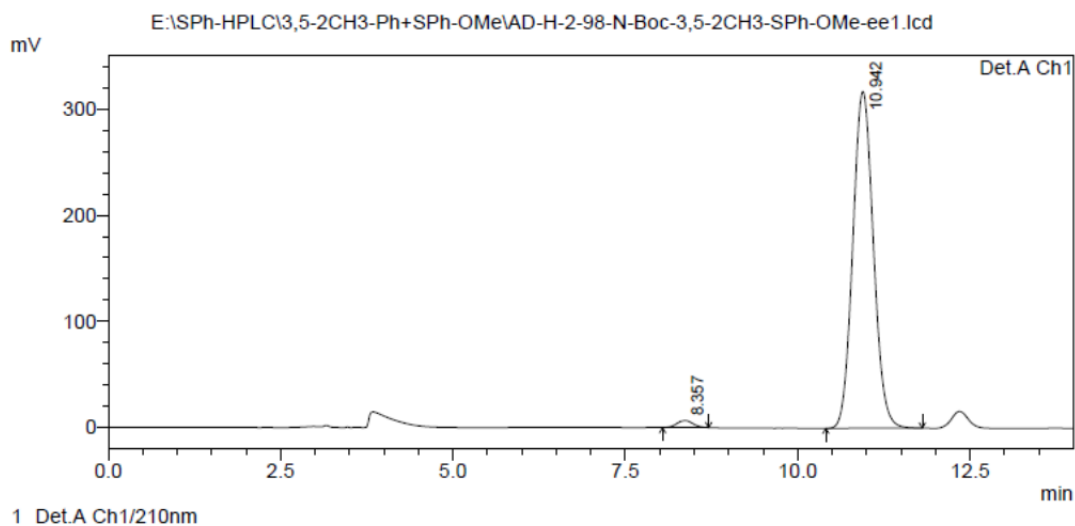
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.075	377075	19585	2.653	5.024
2	21.914	13834674	370261	97.347	94.976
Total		14211749	389846	100.000	100.000



PeakTable

Detector A Ch1 210nm

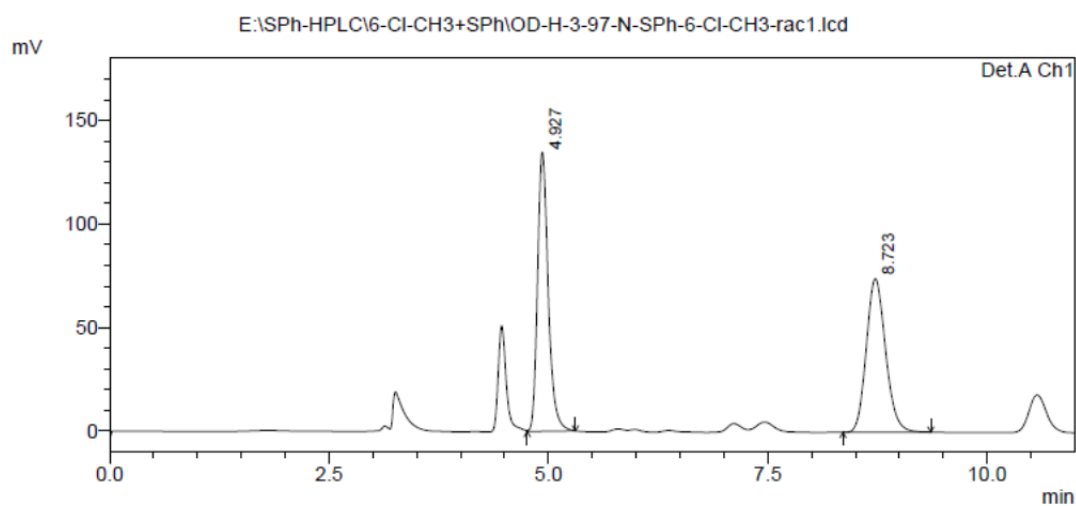
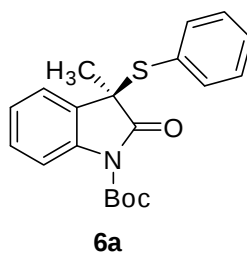
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.342	6045265	371524	50.028	55.789
2	11.046	6038514	294418	49.972	44.211
Total		12083779	665943	100.000	100.000



PeakTable

Detector A Ch1 210nm

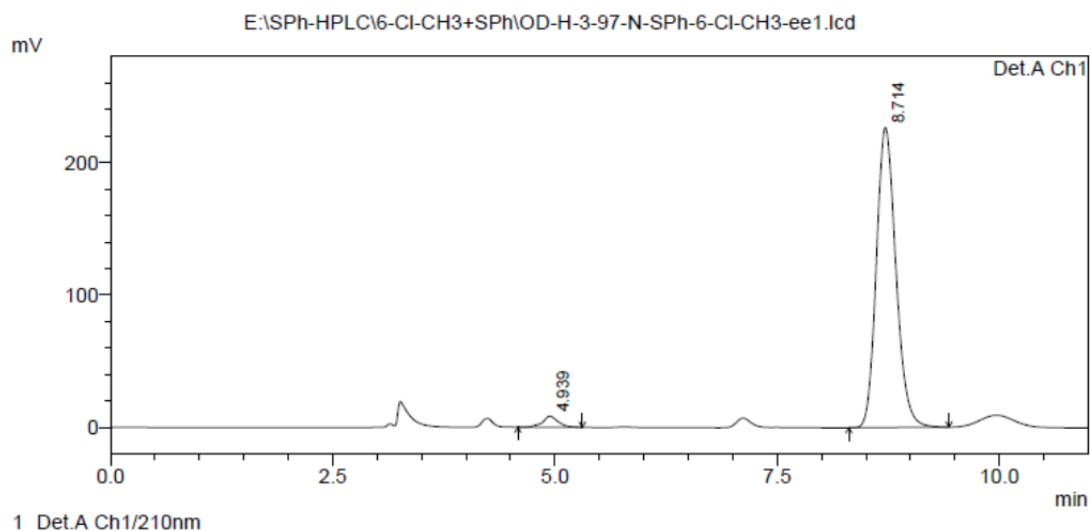
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.357	109749	6711	1.637	2.071
2	10.942	6593446	317363	98.363	97.929
Total		6703194	324074	100.000	100.000



PeakTable

Detector A Ch1 210nm

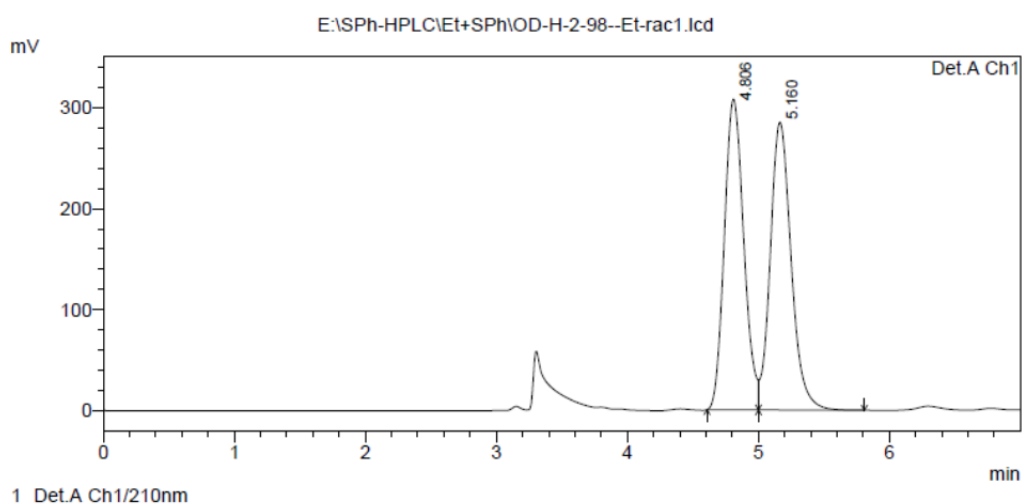
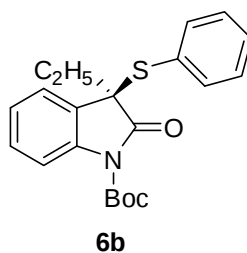
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.927	1140517	134919	50.072	64.512
2	8.723	1137229	74219	49.928	35.488
Total		2277746	209138	100.000	100.000



PeakTable

Detector A Ch1 210nm

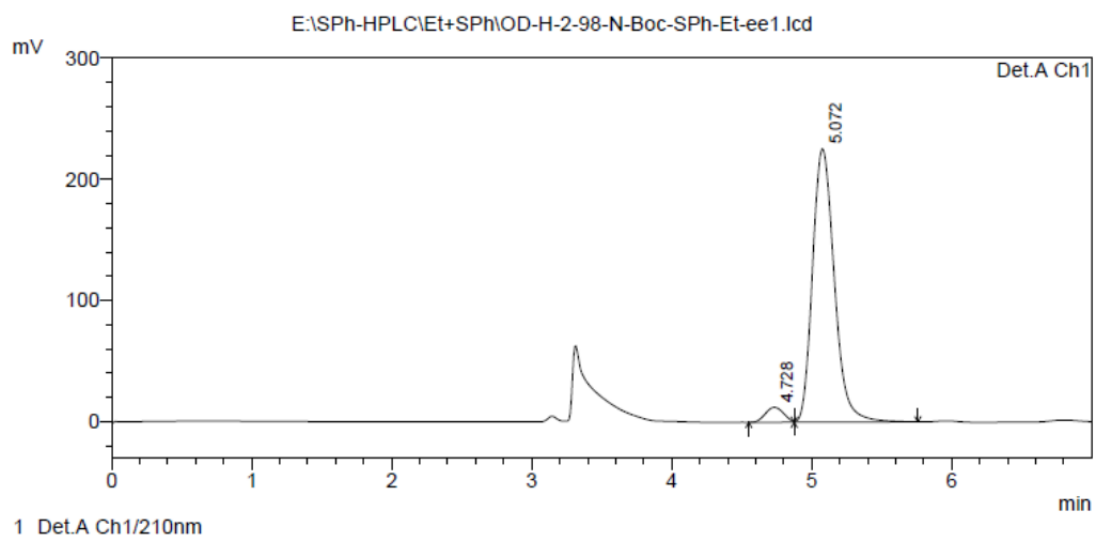
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.939	100338	8345	2.811	3.552
2	8.714	3469238	226591	97.189	96.448
Total		3569576	234936	100.000	100.000



PeakTable

Detector A Ch1 210nm

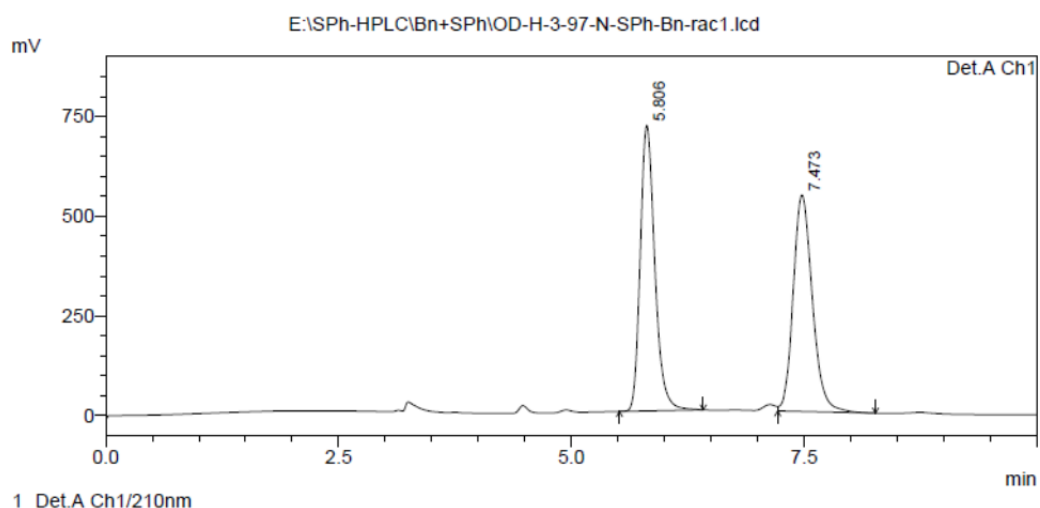
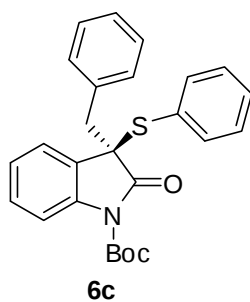
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.806	3170106	307537	50.158	51.929
2	5.160	3150146	284692	49.842	48.071
Total		6320252	592229	100.000	100.000



PeakTable

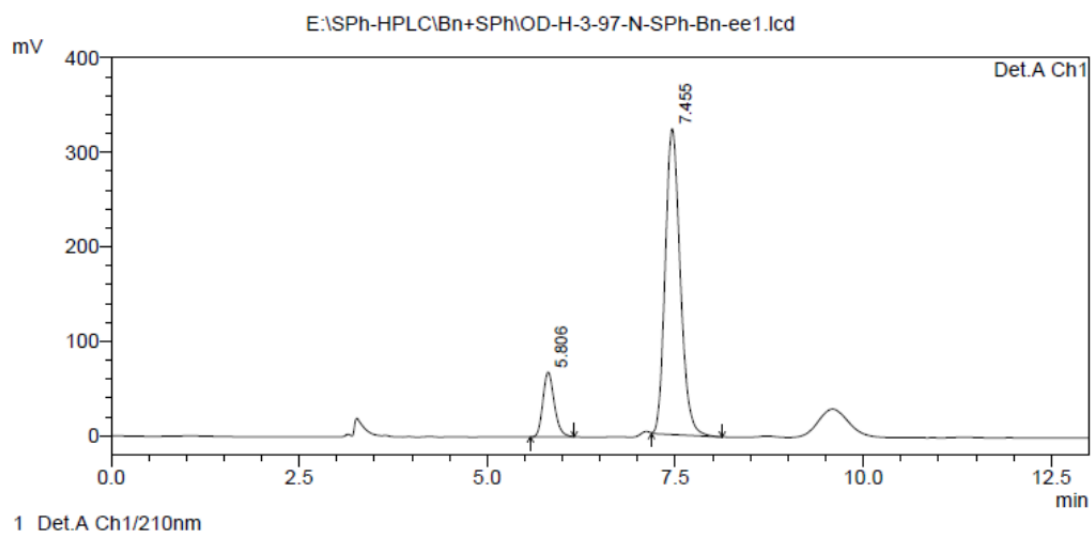
Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.728	112422	12330	4.389	5.177
2	5.072	2449179	225820	95.611	94.823
Total		2561601	238150	100.000	100.000



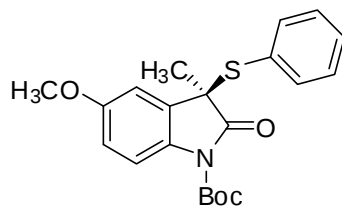
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.806	7804075	715037	50.070	56.862
2	7.473	7782244	542461	49.930	43.138
Total		15586318	1257498	100.000	100.000

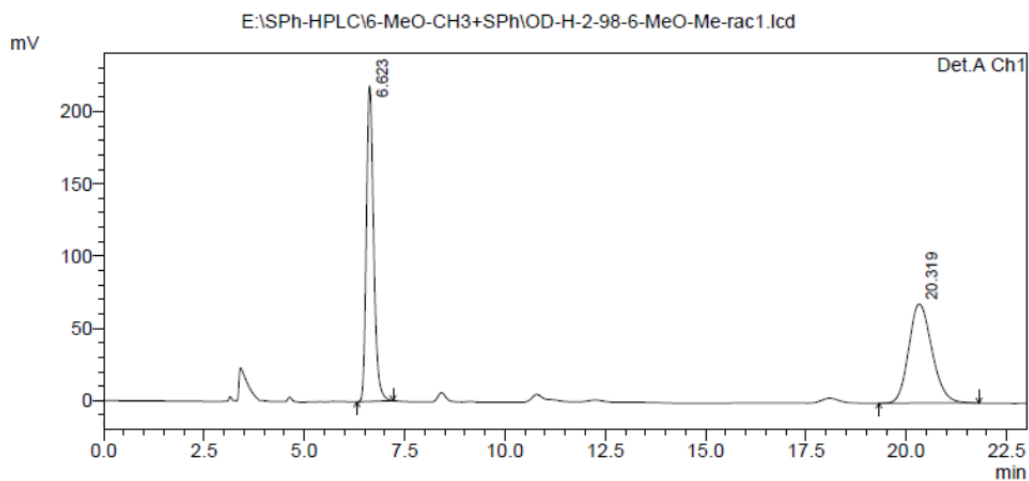


PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.806	723763	68514	13.864	17.466
2	7.455	4496646	323754	86.136	82.534
Total		5220410	392268	100.000	100.000



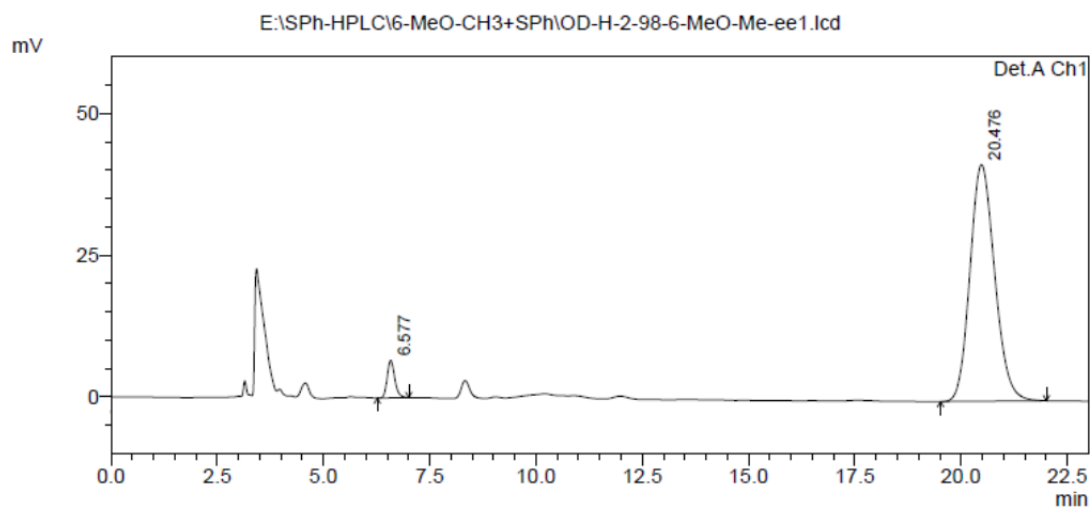
6d



PeakTable

Detector A Ch1 210nm

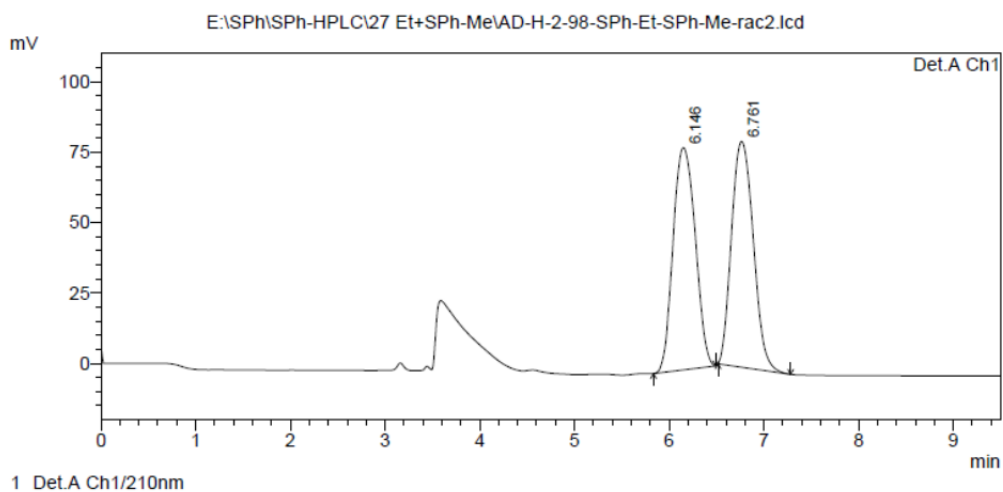
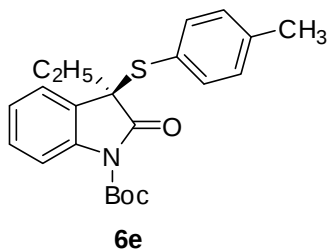
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.623	2756090	218628	50.005	76.116
2	20.319	2755486	68604	49.995	23.884
Total		5511575	287232	100.000	100.000



PeakTable

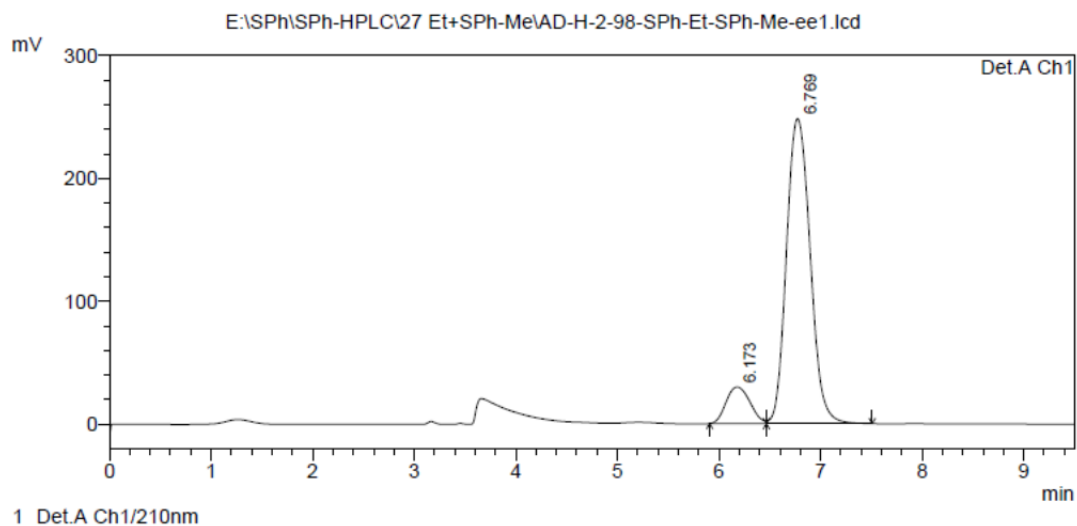
Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.577	82537	6618	4.654	13.673
2	20.476	1690786	41785	95.346	86.327
Total		1773322	48403	100.000	100.000



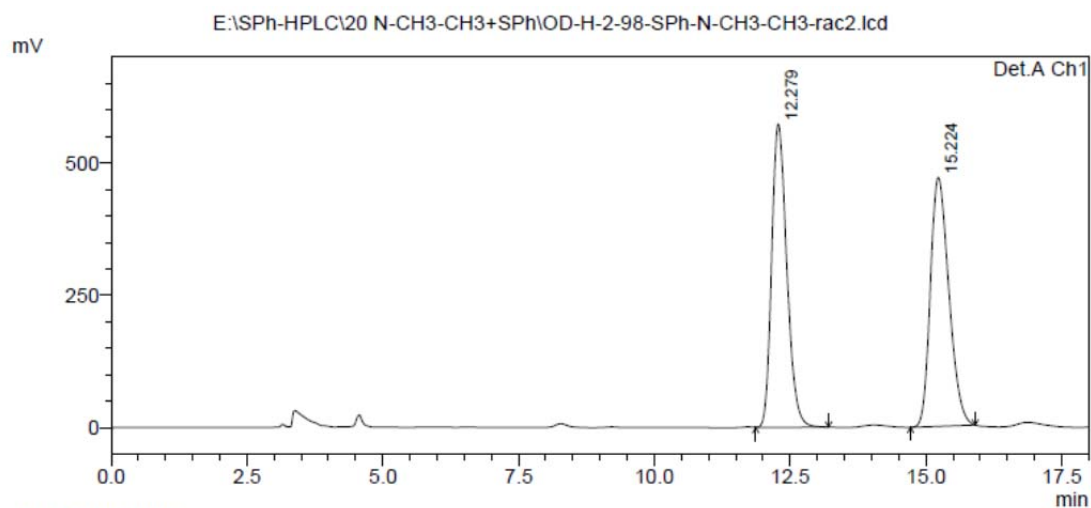
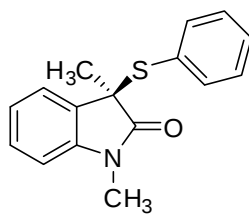
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.146	1285011	78990	49.998	49.603
2	6.761	1285098	80254	50.002	50.397
Total		2570109	159244	100.000	100.000



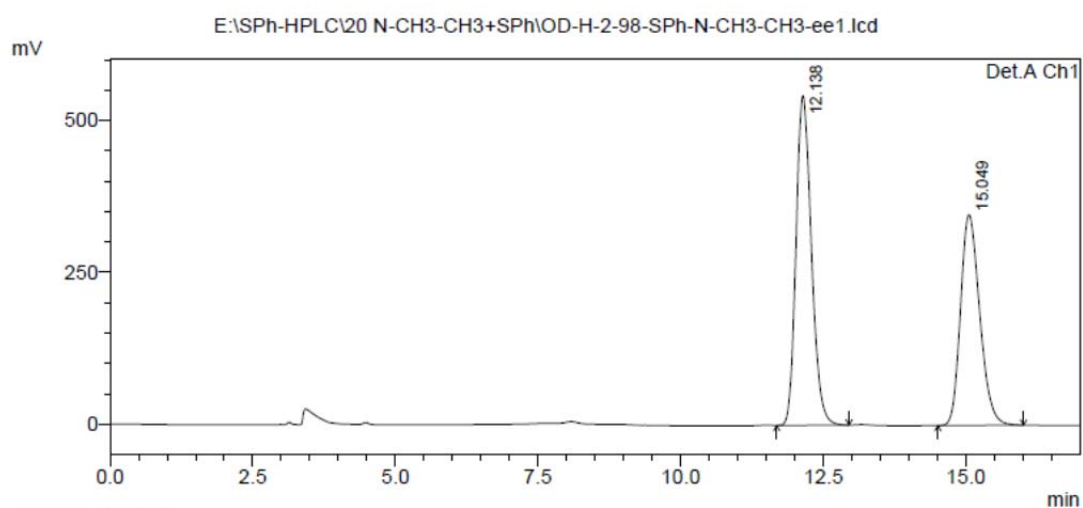
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.173	485663	29694	10.766	10.677
2	6.769	4025283	248405	89.234	89.323
Total		4510946	278099	100.000	100.000



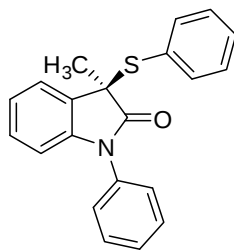
PeakTable

Detector A Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.279	11139716	573616	49.919	54.925
2	15.224	11175884	470740	50.081	45.075
Total		22315600	1044356	100.000	100.000

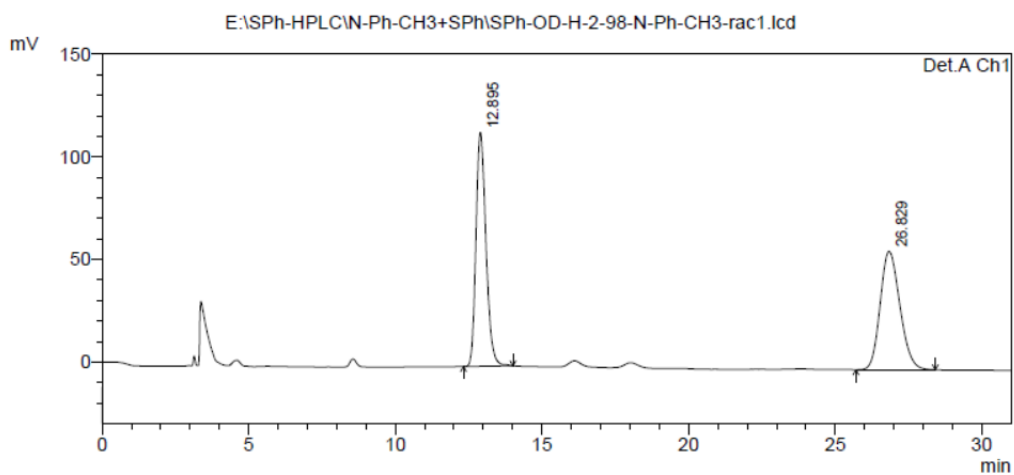


PeakTable

Detector A Ch1 210nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.138	10210550	543181	55.728	61.041
2	15.049	8111626	346684	44.272	38.959
Total		18322176	889865	100.000	100.000



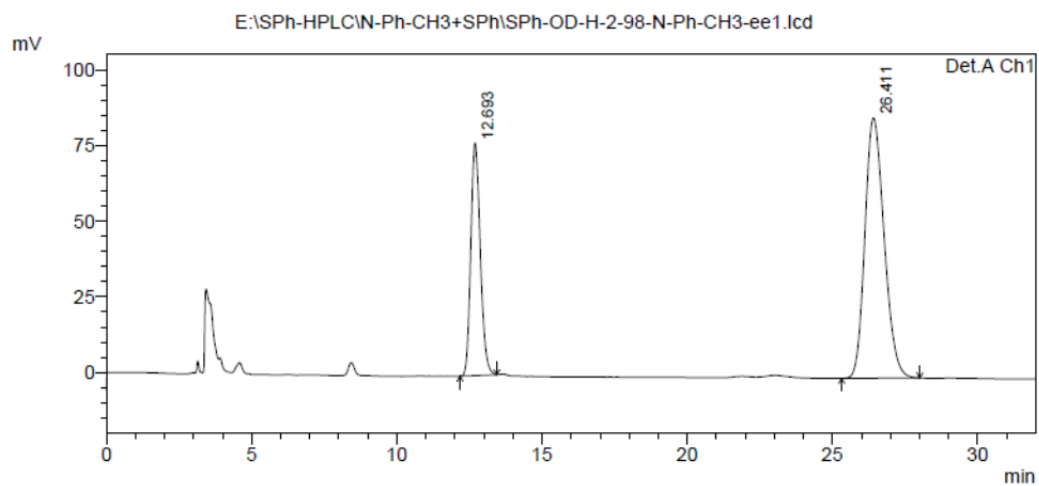
8b



Detector A Ch1 210nm

PeakTable

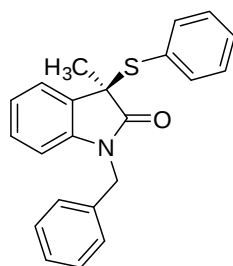
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.895	2702269	114078	50.002	66.384
2	26.829	2702093	57767	49.998	33.616
Total		5404362	171845	100.000	100.000



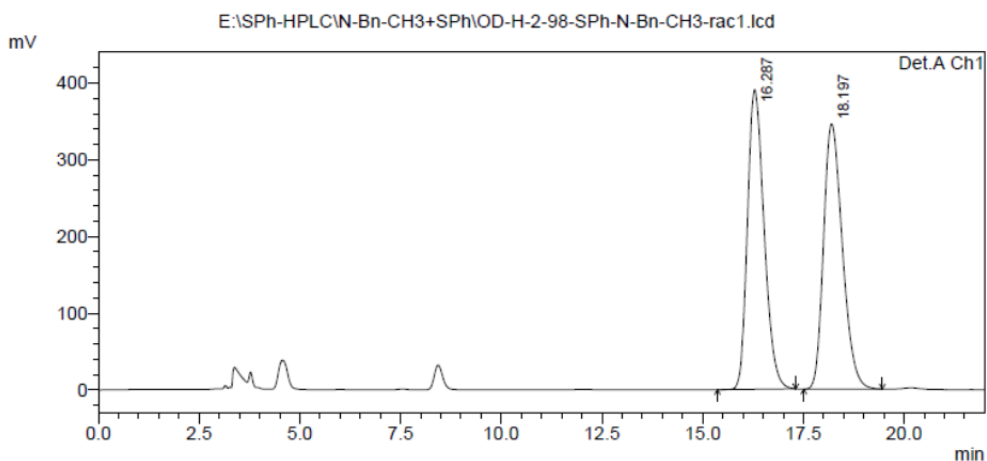
Detector A Ch1 210nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.693	1750697	76812	30.677	47.188
2	26.411	3956093	85966	69.323	52.812
Total		5706790	162778	100.000	100.000



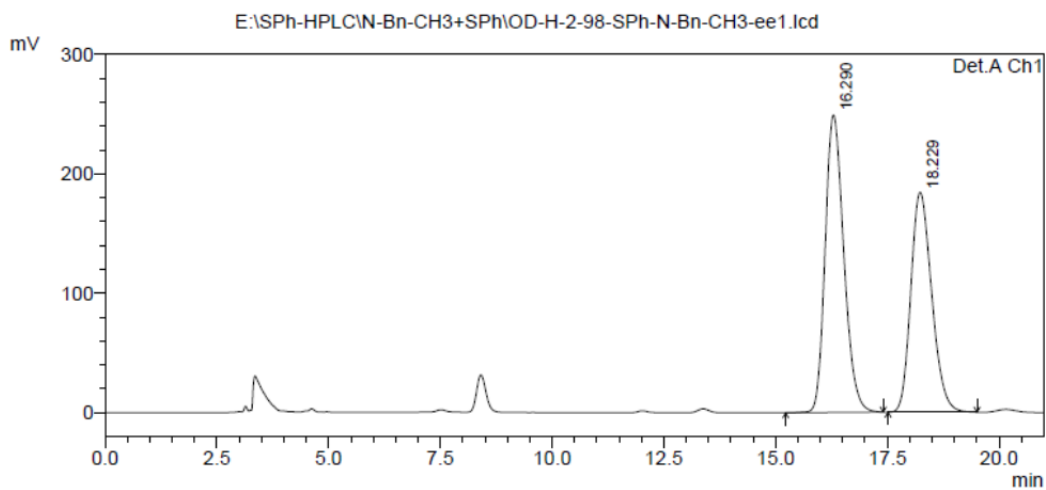
8c



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.287	11254431	390667	50.003	53.028
2	18.197	11253035	346056	49.997	46.972
Total		22507467	736722	100.000	100.000

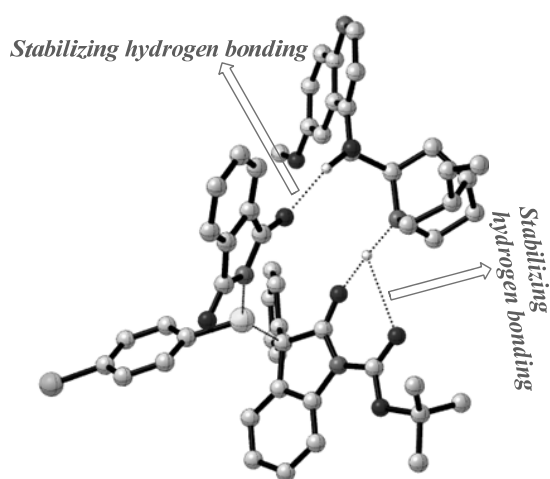


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.290	7238477	249368	54.717	57.494
2	18.229	5990398	184364	45.283	42.506
Total		13228875	433732	100.000	100.000

Scheme S1. Proposed transition state.



The favored TS model

Scheme S2. Reactions carried out on a large scale

