Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Enantioselective Conjugate Addition Reaction of 3-Substituted Benzothiophen-2-ones and 2-Phthalimidoacrylates

Shoulei Li, ‡ Enge Zhang, ‡ Junjun Feng and Xin Li*

State Key Laboratory of Elemento-organic Chemistry, College of Chemistry, Collaborative Innovation Center of Chemical Science and Engineering, Nankai University, Tianjin 300071, China

xin_li@nankai.edu.cn (X. Li)

Contents

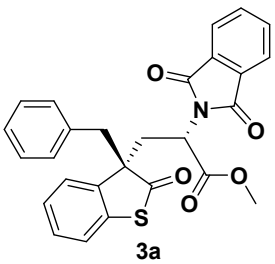
General Information.

Commercial reagents were used as received, unless otherwise stated. ^{1}H and ^{13}C NMR were recorded in $CDCl_3$ on 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 mutiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. 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). Mass spectra were obtained using electrospray ionization (ESI). Substrates **1** and **2** were synthesized according to the reported literatures.[1,2,3]

General procedure for synthesis of products 3.

To a reaction tube, benzothiophenones **1** (0.1 mmol), acrylates **2** (0.15 mmol), catalyst **C2** (0.01 mmol), 3Å MS (40 mg) were added. The tube was cooled to -20 °C and then cooled toluene (1 mL, -20 °C) was added. The resulting mixture was stirred at -20 °C. After monitored by TLC, the reaction solution was concentrated in vacuum and the products **3** were obtained by silica gel column chromatography (EA:PE=1:8).

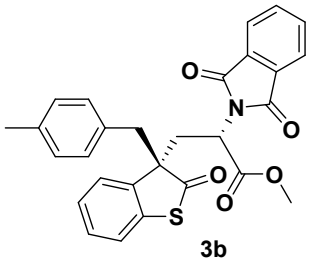
Methyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3a).



3a

White solid, 45 mg, 96 % yield, 4 days; $[\alpha]_D^{25}$ -40.4 (*c* = 1.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.72 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.41 – 7.32 (m, 2H), 7.30 – 7.26 (m, 1H), 7.21 – 7.18 (m, 1H), 7.13 – 7.07 (m, 1H), 7.05 – 6.99 (m, 2H), 6.73 – 6.65 (m, 2H), 4.47 (dd, *J* = 11.9, 2.6 Hz, 1H), 3.67 (s, 3H), 3.46 (dd, *J* = 14.9, 12.0 Hz, 1H), 3.18 (d, *J* = 12.9 Hz, 1H), 3.05 (d, *J* = 12.9 Hz, 1H), 2.99 (dd, *J* = 14.9, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 169.3, 167.2, 137.1, 136.6, 134.3, 133.9, 131.9, 130.3, 129.4, 127.9, 127.1, 126.7, 124.9, 123.7, 123.6, 63.4, 53.2, 48.5, 48.1, 37.2; HRMS (ESI): m/z calcd for $[C_{27}H_{21}NNaO_5S]^+$ 492.1038, found 492.1036; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4 , Flow rate = 1 mL/min, UV = 210 nm, t_R = 16.1 min (minor) and t_R = 23.0 min (major).

Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-(4-methylbenzyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3b).

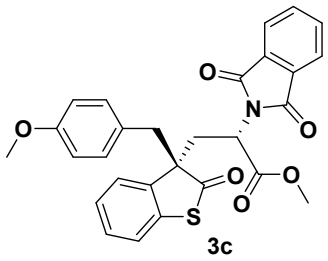


3b

White solid, 48 mg, 99 % yield, 4 days; $[\alpha]_D^{25}$ -35.6 (*c* = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.71 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.40-7.32 (m, 2H), 7.29 – 7.17 (m,2H), 6.83 (d, *J* = 7.9 Hz, 2H), 6.57 (d, *J* = 8.0 Hz, 2H), 4.46 (dd, *J* = 11.9, 2.5 Hz, 1H), 3.66 (s, 3H), 3.44 (dd, *J* = 14.9, 12.0 Hz, 1H), 3.13 (d, *J* = 13.0 Hz, 1H), 3.06 – 2.93 (m, 2H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 169.3, 167.1, 137.2, 136.6, 136.6, 134.3, 131.9, 130.8, 130.1, 129.2, 128.6, 126.6, 124.9, 123.7, 123.5, 63.4, 53.2, 48.5, 47.6, 37.1, 21.1; HRMS (ESI): m/z calcd for $[C_{28}H_{23}NNaO_5S]^+$ 508.1189, found 508.1192; HPLC: Daicel ChiralpakIC-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 20.7 min (minor) and t_R = 68.1

min (major).

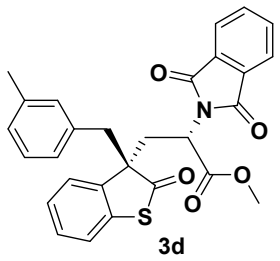
Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-(4-methoxybenzyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3c).



3c

White solid, 49 mg, 99 % yield, 4 days; $[\alpha]_D^{25}$ -29.3 (c = 0.8, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.42 – 7.32 (m,2H), 7.29 – 7.18 (m, 2H), 6.63 – 6.52 (m, 4H), 4.47 (dd, *J* = 11.9, 2.5 Hz, 1H), 3.68 (s, 3H), 3.66 (s, 3H), 3.43 (dd, *J* = 14.9, 12.0 Hz, 1H), 3.12 (d, *J* = 13.1 Hz, 1H), 3.04 – 2.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.5, 169.3, 167.2, 158.6, 137.2, 136.6, 134.3, 131.9, 131.3, 129.2, 126.7, 126.0, 124.9, 123.7, 123.6, 113.2, 63.5, 55.2, 53.12, 48.56, 47.3, 37.0; HRMS (ESI): m/z calcd for $[C_{28}H_{23}NNaO_6S]^+$ 524.1144, found 524.1143; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 21.7 min (minor) and t_R = 32.8 min (major).

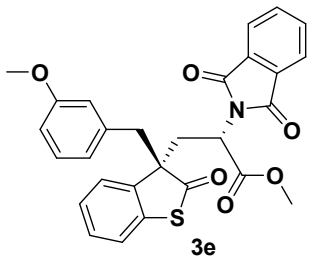
Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-(3-methylbenzyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3d).



3d

White solid, 47 mg, 97 % yield, 4 days; $[\alpha]_D^{25}$ -29.7 (*c* = 1.5, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.41-7.32 (m, 2H), 7.30 – 7.24 (m, 1H), 7.22 – 7.17 (m, 1H), 6.92 – 6.86 (m, 2H), 6.53 – 6.43 (m, 2H), 4.48 (dd, *J* = 11.9, 2.6 Hz, 1H), 3.66 (s, 3H), 3.45 (dd, *J* = 14.9, 12.0 Hz, 1H), 3.13 (d, *J* = 12.8 Hz, 1H), 3.06 – 2.94 (m, 2H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 169.3, 167.1, 137.3, 137.2, 136.6, 134.3, 133.7, 131.9, 131.1, 129.2, 127.8, 127.6, 127.2, 126.6, 124.9, 123.6, 123.5, 63.4, 53.2, 48.5, 48.0, 37.1, 21.3; HRMS (ESI): m/z calcd for $[C_{28}H_{23}NNaO_5S]^+$ 508.1195, found 508.1193; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 12.2 min (minor) and t_R = 19.0 min (major).

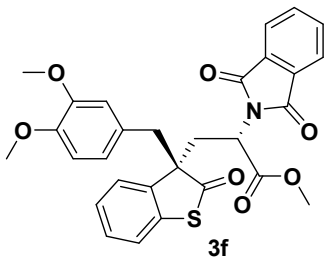
Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-(3-methoxybenzyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3e).



3e

White solid, 49 mg, 99 % yield, 4 days; $[\alpha]_D^{25}$ -47.8 (*c* = 0.8, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.72 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.35 – 7.20 (m, 3H), 7.16 – 7.03 (m, 2H), 6.86 – 6.78 (m, 1H), 6.74-6.69 (m, 1H), 6.64 (d, *J* = 8.2 Hz, 1H), 4.43 (dd, *J* = 11.8, 2.6 Hz, 1H), 3.65 (s, 3H), 3.46 (s, 3H), 3.42 (dd, *J* = 15.0, 11.9 Hz, 1H), 3.17 (dd, *J* = 28.9, 13.0 Hz, 2H), 3.00 (dd, *J* = 15.0, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.1, 169.4, 167.1, 157.7, 137.4, 135.8, 134.2, 132.2, 131.9, 128.8, 128.6, 125.9, 125.6, 123.6, 123.1, 122.8, 119.9, 110.1, 63.1, 54.8, 53.1, 48.6, 40.8, 36.2; HRMS (ESI): m/z calcd for $[C_{28}H_{23}NNaO_6S]^+$ 524.1144, found 524.1143; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 14.6 min (minor) and t_R = 16.1 min (major).

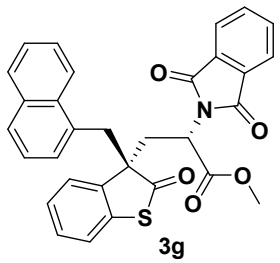
Methyl (S)-3-((S)-3-(3,4-dimethoxybenzyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3f).



3f

White solid, 49 mg, 92 % yield, 4 days; $[\alpha]_D^{25}$ -48.9 (*c* = 0.7, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.45 – 7.31 (m, 3H), 7.21 (d, *J* = 7.4 Hz, 1H), 6.54 (d, *J* = 8.2 Hz, 1H), 6.31 (dd, *J* = 8.2, 1.7 Hz, 1H), 6.04 (d, *J* = 1.7 Hz, 1H), 4.49 (dd, *J* = 12.0, 2.4 Hz, 1H), 3.75 (s, 3H), 3.67 (s, 3H), 3.50 (s, 3H), 3.45 (dd, *J* = 11.4, 8.5 Hz, 1H), 3.14 (d, *J* = 13.1 Hz, 1H), 3.04 – 2.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 169.3, 167.1, 148.0, 147.9, 137.4, 137.0, 134.3, 131.8, 129.2, 126.6, 126.3, 124.8, 123.7, 122.5, 112.9, 110.4, 63.6, 55.7, 55.5, 53.2, 48.5, 47.8, 37.1; HRMS (ESI): m/z calcd for $[C_{29}H_{25}NNaO_7S]^+$ 554.1250, found 554.1248; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 32.4 min (minor) and t_R = 37.2 min (major).

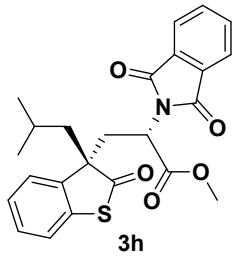
Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-(naphthalen-1-ylmethyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3g).



3g

White solid, 51 mg, 99 % yield, 4 days; $[\alpha]_D^{25}$ +7.2 (*c* = 1.5, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.51 (m, 7H), 7.38 – 7.12 (m, 6H), 6.93 (dd, *J* = 20.8, 7.4 Hz, 2H), 4.47 (dd, *J* = 11.8, 2.3 Hz, 1H), 3.78 (d, *J* = 13.6 Hz, 1H), 3.69 (s, 3H), 3.56 (dd, *J* = 14.9, 11.9 Hz, 1H), 3.40 (d, *J* = 13.6 Hz, 1H), 3.12 (dd, *J* = 14.9, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.0, 169.3, 167.1, 136.9, 136.3, 134.3, 133.6, 132.6, 131.8, 130.5, 129.2, 129.1, 128.4, 128.1, 126.5, 125.6, 125.4, 124.7, 124.0, 123.7, 123.5, 123.1, 63.3, 53.2, 48.6, 43.0, 36.3; HRMS (ESI): m/z calcd for $[C_{31}H_{23}NNaO_5S]^+$ 544.1195, found 544.1193; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 15.4 min (minor) and t_R = 26.3 min (major).

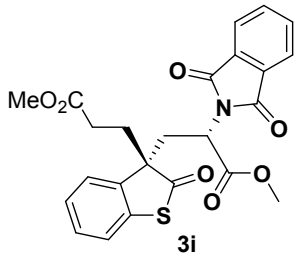
Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-isobutyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3h).



3h

Colorless oil, 38 mg, 87 % yield, 1 day; $[\alpha]_D^{25}$ -39.2 (*c* = 0.5, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.28 (m, 2H), 7.76 – 7.72 (m, 2H), 7.40 – 7.34 (m, 3H), 7.28 – 7.26 (m, 1H), 4.40 (d, *J* = 9.5 Hz, 1H), 3.64 (s, 3H), 3.32 (dd, *J* = 14.9, 11.9 Hz, 1H), 2.78 (d, *J* = 12.5 Hz, 1H), 2.02 (dd, *J* = 13.8, 5.9 Hz, 1H), 1.76 (dd, *J* = 13.8, 6.2 Hz, 1H), 1.46 – 1.38 (m, 1H), 0.76 (d, *J* = 6.6 Hz, 3H), 0.51 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.5, 169.2, 167.1, 138.5, 136.2, 134.2, 131.8, 129.0, 126.8, 124.4, 123.6, 61.8, 53.0, 51.2, 48.2, 39.7, 24.7, 24.4, 24.0; HRMS (ESI): m/z calcd for $[C_{24}H_{27}N_2O_5S]^+$ 455.1635, found 455.1621; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/9, Flow rate = 1 mL/min, UV = 210 nm, t_R = 16.7 min (minor) and t_R = 23.5 min (major).

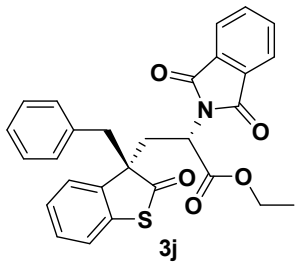
Methyl (S)-2-(1,3-dioxoisoindolin-2-yl)-3-((S)-3-(3-methoxy-3-oxopropyl)-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)propanoate (3i).



3i

White solid, 34 mg, 72 % yield, 2 days; $[\alpha]_D^{25}$ -34.8 (*c* = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.61 (m, 4H), 7.43 – 7.27 (m, 4H), 4.44 (d, *J* = 9.5 Hz, 1H), 3.65 (s, 3H), 3.54 (s, 3H), 3.41 – 3.29 (m, 1H), 2.87 (d, *J* = 12.7 Hz, 1H), 2.31 – 2.12 (m, 3H), 1.97 – 1.89 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.4, 172.5, 169.0, 167.0, 137.0, 136.0, 134.2, 131.8, 129.4, 127.2124.2, 123.8, 123.6, 61.1, 53.1, 51.7, 48.4, 37.8, 36.8, 28.1; HRMS (ESI): m/z calcd for $[C_{24}H_{25}N_2O_7S]^+$ 485.1377, found 485.1360; HPLC: Daicel Chiralpak AS-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 22.8 min (minor) and t_R = 25.8 min (major).

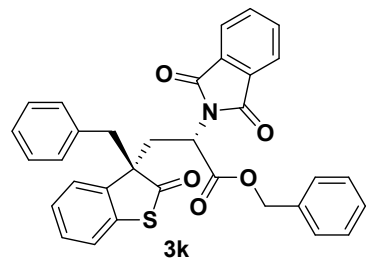
Ethyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3j).



3j

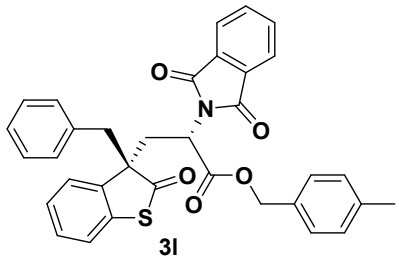
White solid, 41 mg, 86 % yield, 4 days; $[\alpha]_D^{25}$ -27.1 (*c* = 1.1, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.43 – 7.32 (m, 2H), 7.30 – 7.26 (m, 1H), 7.22 – 7.17 (m, 1H), 7.12-7.06 (m, 1H), 7.06 – 6.99 (m, 2H), 6.72 – 6.63 (m, 2H), 4.45 (dd, *J* = 11.9, 2.6 Hz, 1H), 4.20 – 4.05 (m, 2H), 3.45 (dd, *J* = 14.9, 11.9 Hz, 1H), 3.18 (d, *J* = 12.9 Hz, 1H), 3.05 (d, *J* = 12.9 Hz, 1H), 2.99 (dd, *J* = 14.9, 2.6 Hz, 1H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 168.8, 167.2, 137.1, 136.6, 134.3, 134.0, 131.9, 130.3, 129.2, 127.8, 127.1, 126.7, 124.9, 123.6, 123.6, 63.4, 62. 4, 48.7, 48.1, 37.2, 14.1; HRMS (ESI): m/z calcd for $[C_{28}H_{23}NNaO_5S]^+$ 508.1195, found 508.1192; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 15.2 min (minor) and t_R = 24.0 min (major).

Benzyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3k).



3k

White solid, 43 mg, 78 % yield, 4 days; $[\alpha]_D^{25}$ -20.2 (*c* = 1.1, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.70 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.37 – 7.33 (m, 2H), 7.31 – 7.26 (m, 3H), 7.24 – 7.17 (m, 4H), 7.12-7.06 (m, 1H), 7.04 – 6.97 (m, 2H), 6.72 – 6.64 (m, 2H), 5.11 (q, *J* = 12.4 Hz, 2H), 4.52 (dd, *J* = 11.9, 2.6 Hz, 1H), 3.49 (dd, *J* = 14.9, 11.9 Hz, 1H), 3.17 (d, *J* = 12.9 Hz, 1H), 3.06 – 2.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 168.7, 167.2, 137.0, 136.6, 135.1, 134.3, 133.9, 131.8, 130.3, 129.3, 128.6, 128.4, 128.0, 127.8, 127.1, 126.7, 124.9, 123.7, 123.5, 67.9, 63.4, 48.8, 48.0, 37.2; HRMS (ESI): m/z calcd for $[C_{33}H_{25}NNaO_5S]^+$ 570.1351, found 570.1349; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4 , Flow rate = 1 mL/min, UV = 210 nm, t_R = 26.6 min (minor) and t_R = 36.8 min (major).



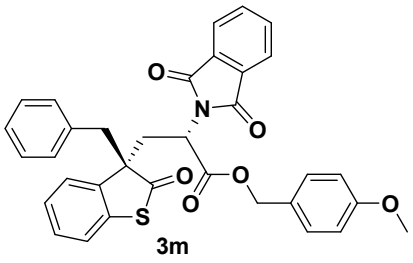
3l

4-methylbenzyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-

yl)propanoate (3l).

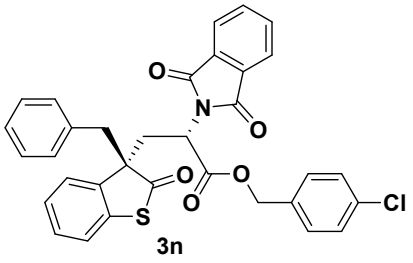
White solid, 45 mg, 80 % yield, 4 days; $[\alpha]_D^{25}$ -16.9 (c = 0.9, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, J = 5.5, 3.0 Hz, 2H), 7.70 (dd, J = 5.5, 3.1 Hz, 2H), 7.40 – 7.30 (m, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.16 (m, 1H), 7.13 – 7.06 (m, 5H), 7.04-6.98 (m, 2H), 6.72 – 6.61 (m, 2H), 5.07 (dd, J = 27.1, 12.2 Hz, 2H), 4.50 (dd, J = 11.9, 2.6 Hz, 1H), 3.48 (dd, J = 14.9, 12.0 Hz, 1H), 3.16 (d, J = 12.9 Hz, 1H), 3.06 – 2.94 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 168.7, 167.2, 138.3, 137.0, 136.5, 134.3, 133.9, 132.1, 131.8, 130.3, 129.3, 129.2, 128.2, 127.8, 127.1, 126.7, 124.9, 123.6, 123.5, 67.9, 63.4, 48.8, 48.1, 37.2, 21.3; HRMS (ESI): m/z calcd for $[C_{34}H_{27}NNaO_5S]^+$ 584.1508, found 584.1508; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4 , Flow rate = 1 mL/min, UV = 210 nm, t_R = 23.3 min (minor) and t_R = 30.0 min (major).

4-methoxybenzyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3m).



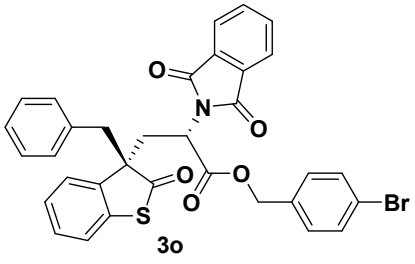
White solid, 29 mg, 50 % yield, 4 days; $[\alpha]_D^{25}$ -7.0 (c = 0.2, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, J = 5.5, 3.0 Hz, 2H), 7.70 (dd, J = 5.5, 3.1 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.24 – 7.20 (m, 1H), 7.20 – 7.16 (m, 2H), 7.15 – 7.13 (m, 1H), 712-7.06 (m,1H), 7.04-6.98 (m, 2H), 6.86 – 6.79 (m, 2H), 6.70-6.66 (m, 2H), 5.05 (dd, J = 23.2, 12.0 Hz, 2H), 4.48 (dd, J = 11.9, 2.6 Hz, 1H), 3.78 (s, 3H), 3.46 (dd, J = 14.9, 11.9 Hz, 1H), 3.25 – 3.10 (m, 1H), 3.02 (d, J = 12.9 Hz, 1H), 2.97 (dd, J = 14.9, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 168.8, 167.2, 159.8, 137.1, 136.6, 134.3, 134.0, 131.9, 130.3, 130.0, 129.3, 127.7, 127.3, 127.1, 126.7, 125.0, 123.7, 123.6, 114.0, 67.9, 63.4, 55.4, 48.8, 48.1, 37.2; HRMS (ESI): m/z calcd for $[C_{34}H_{27}NNaO_6S]^+$ 600.1457, found 600.1455; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV =210 nm, t_R = 20.3 min (minor) and t_R = 24.0 min (major).

4-chlorobenzyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3n).



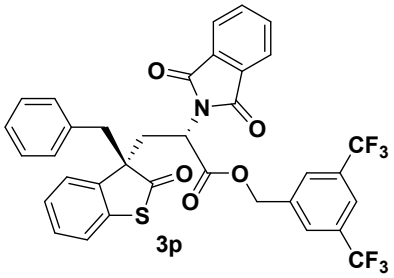
White solid, 44 mg, 76 % yield, 4 days; $[\alpha]_D^{25}$ -21.6 (c = 0.8, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, J = 5.5, 3.0 Hz, 2H), 7.71 (dd, J = 5.5, 3.1 Hz, 2H), 7.39 – 7.31 (m, 2H), 7.28 – 7.18 (m, 4H), 7.16 – 7.06 (m, 3H), 7.05 – 6.99 (m, 2H), 6.71 – 6.65 (m, 2H), 5.06 (s, 2H), 4.51 (dd, J = 11.9, 2.6 Hz, 1H), 3.47 (dd, J = 14.9, 11.9 Hz, 1H), 3.16 (d, J = 12.9 Hz, 1H), 3.03 (d, J = 12.9 Hz, 1H), 2.97 (dd, J = 15.0, 2.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 168.7, 167.1, 137.0, 136.6, 134.4, 133.9, 133.6, 131.8, 130.3, 129.5, 129.3, 128.9, 127.9, 127.1, 126.7, 124.9, 123.7, 123.6, 67.1, 63.4, 48.7, 48.0, 37.1; HRMS (ESI): m/z calcd for $[C_{33}H_{24}ClNNaO_5S]^+$ 604.0962, found 604.0960; HPLC: Daicel Chiralpak OD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 18.6 min (minor) and t_R = 21.2 min (major).

4-bromobenzyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3o).



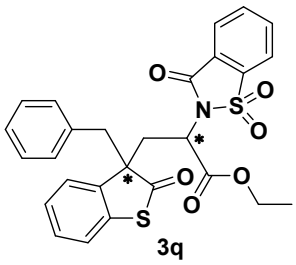
White solid, 43 mg, 68 % yield, 4 days; $[\alpha]_D^{25}$ -19.4 (*c* = 0.4, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.47 – 7.30 (m, 4H), 7.24 – 7.16 (m, 2H), 7.15 – 6.98 (m, 5H), 6.68 (d, *J* = 7.3 Hz, 2H),5.05 (s, 2H), 4.50 (dd, *J* = 11.9, 2.5 Hz, 1H), 3.47 (dd, *J* = 14.9, 12.0 Hz, 1H), 3.16 (d, *J* = 12.9 Hz, 1H), 3.03 (d, *J* = 12.9 Hz, 1H), 2.97 (dd, *J* = 15.0, 2.5 Hz, 1H); ^{13}C NMR (10 MHz, $CDCl_3$) δ 208.2, 168.7, 167.1, 137.0, 136.6, 134.4, 134.1, 133.9, 131.8, 130.3, 129.8, 129.3, 127.9, 127.2, 126.7, 124.9, 123.7, 123.6, 122.6, 67.1, 63.4, 48.7, 48.1, 37.2; HRMS (ESI): m/z calcd for $[C_{33}H_{24}BrNNaO_5S]^+$ 648.0457, found 648.0455; HPLC: Daicel Chiralpak OD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210m, t_R = 17.9 min (minor) and t_R = 20.7 min (major).

3,5-bis(trifluoromethyl)benzyl (S)-3-((S)-3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,3-dioxoisoindolin-2-yl)propanoate (3p).



White solid, 33 mg, 49 % yield, 4 days; $[\alpha]_D^{25}$ -28.0 (*c* = 0.7, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.77 (s, 1H), 7.73 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.61 (s, 2H), 7.41 – 7.32 (m, 2H), 7.27-7.18 (m, 2H), 7.13-7.07 (m, 1H), 7.05-7.00 (m,2H), 6.71 – 6.66 (m, 2H), 5.31 (d, *J* = 13.2 Hz, 1H), 5.07 (d, *J* = 13.2 Hz, 1H), 4.56 (dd, *J* = 11.8, 2.6 Hz, 1H), 3.48 (dd, *J* = 14.9, 11.8 Hz, 1H), 3.18 (d, *J* = 12.9 Hz, 1H), 3.05 (d, *J* = 12.9 Hz, 1H), 3.00 (dd, *J* = 14.9, 2.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 168.6, 167.1, 137.6, 137.0, 136.6, 134.5, 133.8, 131.9, 131.7, 130.3, 129.4, 127.9, 127.2, 126.8, 124.9, 123.8, 123.7, 122.4, 66.0, 63.3, 48.5, 48.0, 37.2; HRMS (ESI): m/z calcd for $[C_{35}H_{23}F_6NNaO_5S]^+$ 706.1092, found 706.1100; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 12.2 min (minor) and t_R = 16.6 min (major).

Ethyl 3-(3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-(1,1-dioxido-3-oxobenzo[*d*]isothiazol-2(*3H*)-yl)propanoate (3q).

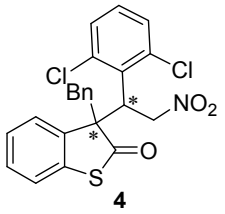


White solid, 51 mg, 98 % yield, 4 days; $[\alpha]_D^{25}$ +34.0 (*c* = 1.3, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.09-7.78 (m, 4H), 7.33-6.95 (m, 7H), 6.73 (d, *J* = 7.4 Hz, 2H), 4.65-4.49 (m, 1H), 4.22-4.10 (m, 2H), 3.45-3.05 (m, 4H), 1.24-1.14 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 207.7, 167.7, 167.3, 159.5, 158.8, 137.6, 137.5, 136.9, 136.6, 136.5, 136.3, 135.0, 134.9, 134.4, 134.2, 133.9, 130.2, 129.0, 128.5, 127.7, 127.0, 126.7, 126.2, 125.5, 125.4, 125.2, 125.1, 123.3, 123.1, 121.0, 120.8, 63.7, 63.2, 62.6, 51.1, 50.8, 48.0, 47.4, 36.0, 35.8, 13.9; HRMS (ESI): m/z calcd for$[C_{27}H_{23}NNaO_6S_2]^+$ 544.0865, found 544.0862; HPLC: Daicel ChiralpakIC-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 33.7 min (major) and t_R = 38.0 min (minor).

General procedure for synthesis of product 4.

To a reaction tube, benzothiophenone 1a (24 mg, 0.1 mmol), nitroolefin A (32.5 mg, 0.15 mmol), catalyst C7 (5.11 mg, 0.01 mmol), 3Å MS (40 mg) were added. The tube was cooled to -20 °C and then cooled toluene (0.4 mL, -20 °C) was added. The resulting mixture was stirred at -20 °C. After monitored by TLC, the reaction solution was concentrated in vacuum and the product 4 was obtained by silica gel column chromatography (EA:PE=1:8).

3-benzyl-3-(1-(2,6-dichlorophenyl)-2-nitroethyl)benzo[*b*]thiophen-2(*3H*)-one (4).



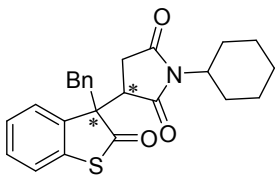
4

Yellow solid, 32 mg, 70 % yield, 7 days; $[\alpha]_D^{25}$ -58.9 (*c* = 0.2, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.24-7.16 (m, 2H), 7.15-6.92 (m, 8H), 6.85-6.76 (m, 2H), 5.66 (d, *J* = 9.5 Hz, 1H), 5.39 (d, *J* = 10.0 Hz, 2H), 3.50 (d, *J* = 12.8 Hz, 1H), 3.35 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 138.0, 136.5, 135.6, 135.5, 133.1, 132.6, 131.0, 129.9, 129.7, 128.9, 128.7, 128.0, 127.6, 126.4, 125.5, 122.7, 77.5, 77.2, 76.8, 74.9, 65.1, 48.8, 46.8; HRMS (ESI): m/z calcd for $[C_{23}H_{17}Cl_2NNaO_3S]^+$ 480.0204, found 480.0202; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 9.1 min (major) and t_R = 9.8 min (minor).

General procedure for synthesis of product 5.

To a reaction tube, benzothiophenone 1a (24 mg, 0.1 mmol), maleimide B (26.8 mg, 0.15 mmol), catalyst C1 (4.13 mg, 0.01 mmol), 3Å MS (40 mg) were added. The tube was cooled to -20 °C and then cooled DCM (0.4 mL, -20 °C) was added. The resulting mixture was stirred at -20 °C. After monitored by TLC, the reaction solution was concentrated in vacuum and the product 5 was obtained by silica gel column chromatography (EA:PE=1:8).

3-(3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-1-cyclohexylpyrrolidine-2,5-dione (5).



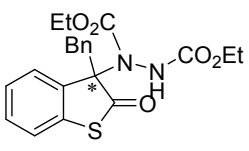
5

White solid, 41.5 mg, 99 % yield, 4 days; $[\alpha]_D^{25}$ -112.3 (*c* = 0.5, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.34 (m, 1H), 7.27 (dt, *J* = 6.2, 2.0 Hz, 2H), 7.20 – 7.15 (m, 1H), 7.11 – 6.99 (m, 3H), 6.78 (d, *J* = 7.0 Hz, 2H), 4.21 – 3.78 (m, 2H), 3.43 (dd, *J* = 8.8, 4.7 Hz, 2H), 2.68 (dd, *J* = 18.4, 9.3 Hz, 1H), 2.35 – 1.96 (m, 3H), 1.84 (s, 2H), 1.68 (d, *J* = 11.9 Hz, 1H), 1.57 (t, *J* = 11.8 Hz, 2H), 1.40 – 1.22 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.2, 177.0, 175.2, 136.6, 135.1, 134.5, 130.2, 129.7, 127.9, 126.9, 126.7, 125.5, 123.5, 65.9, 52.1, 45.5, 43.4, 31.0, 28.0, 26.0, 25.1; HRMS (ESI): m/z calcd for$[C_{25}H_{25}NNaO_3S]^+$ 442.1453, found 442.1450; HPLC: Daicel Chiralpak IA-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 7.5 min (major) and t_R = 10.1 min (minor).

General procedure for synthesis of product 6.

To a reaction tube, benzothiophenone 1a (24 mg, 0.1 mmol), azodicarboxylate C (26.1 mg, 0.15 mmol), $(DHQD)_2PYR$ (8.81 mg, 0.01 mmol), 3Å MS (40 mg) were added. The tube was cooled to -20 °C and then cooled DCM (0.5 mL, -20 °C) was added. The resulting mixture was stirred at -20 °C. After monitored by TLC, the reaction solution was concentrated in vacuum and the product 6 was obtained by silica gel column chromatography (EA:PE=1:10).

Diethyl 1-(3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)hydrazine-1,2-dicarboxylate (6).



6

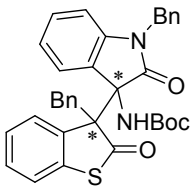
White solid, 40.6 mg, 98 % yield, 2 days; $[\alpha]_D^{25}$ +87.8 (*c* = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.29-7.20 (m, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 7.08-6.96 (m, 4H), 6.64 (d, *J* = 7.3 Hz, 2H), 4.38-4.26 (m, 2H), 4.00 (d, *J* = 6.9 Hz, 2H), 3.43 (d, *J* = 12.1 Hz, 1H), 3.16 (d, *J* = 12.2 Hz, 1H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.2, 157.4, 154.4, 137.3, 134.7, 131.7, 130.7, 129.1, 127.7,

127.3, 126.9, 125.6, 122.6, 78.2, 63.4, 62.7, 44.5, 14.6, 13.9; HRMS (ESI): m/z calcd for $[C_{21}H_{22}N_2NaO_5S]^+$ 437.1147, found 437.1145; HPLC: Daicel Chiralpak IA-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 6.8 min (major) and t_R = 11.7 min (minor).

General procedure for synthesis of product 7.

To a reaction tube, benzothiophenone 1a (36 mg, 0.15 mmol), ketimine D (33.5 mg, 0.1 mmol), $(DHQD)_2AQN$ (8.57 mg, 0.01 mmol) were added. The tube was cooled to -20 °C and then cooled MTBE (0.4 mL, -20 °C) was added. The resulting mixture was stirred at -20 °C. After monitored by TLC, the reaction solution was concentrated in vacuum and the product 7 was obtained by silica gel column chromatography (EA:PE=1:8).

tert-butyl (1-benzyl-3-(3-benzyl-2-oxo-2,3-dihydrobenzo[*b*]thiophen-3-yl)-2-oxoindolin-3-yl)carbamate (7).



7

White solid, 53.5 mg, 93 % yield, 4 days; $[\alpha]_D^{25}$ +151.0 (*c* = 1.5, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.3 Hz, 1H), 7.45 (s, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.22 – 7.02 (m, 7H), 6.98 (t, *J* = 7.4 Hz, 2H), 6.79 (t, *J* = 7.6 Hz, 1H), 6.71 – 6.62 (m, 4H), 6.56 (d, *J* = 7.8 Hz, 1H), 5.90 (d, *J* = 7.8 Hz, 1H), 4.75 (d, *J* = 15.8 Hz, 1H), 4.31 (d, *J* = 15.7 Hz, 1H), 3.86 (d, *J* = 12.8 Hz, 1H), 3.42 (d, *J* = 12.8 Hz, 1H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.0, 174.9, 154.6, 144.8, 137.0, 135.4, 133.9, 133.3, 130.6, 130.1, 129.6, 128.6, 127.9, 127.2, 127.1, 127.1, 126.9, 126.4, 125.5, 124.8, 123.0, 122.6, 109.73, 80.6, 67.9, 64.6, 44.4, 40.1, 28.2; HRMS (ESI): m/z calcd for $[C_{35}H_{32}N_2O_4SH]^+$ 577.2162, found 577.2146; HPLC: Daicel Chiralpak AD-H, *i*-PrOH /*n*-hexane =1/4, Flow rate = 1 mL/min, UV = 210 nm, t_R = 7.0 min (minor) and t_R = 29.4 min (major).

References

1. K. Ohmatsu, Y. Hara and T. Ooi, *Chem. Sci.*, 2014, **5**, 3645.

2. W.-L. Chen, Y.-L. Shi, H. Feng, M. Du, J.-Z. Zhang, J.-H. Hu and D. Yang, *J. Phys. Chem. B*, 2012, **116**, 9231.

3. (a) Y.-C. Fan and O. Kwon, *Org. Lett.*, 2012, **14**, 3264; (b) B. M. Trost and G. R. Dake, *J. Am. Chem. Soc*., 1997, **119**, 7595.

X-ray crystallography data of 3f

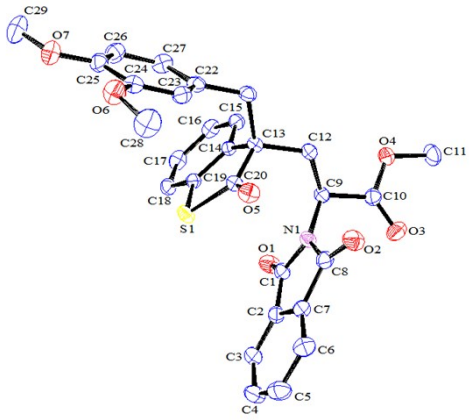
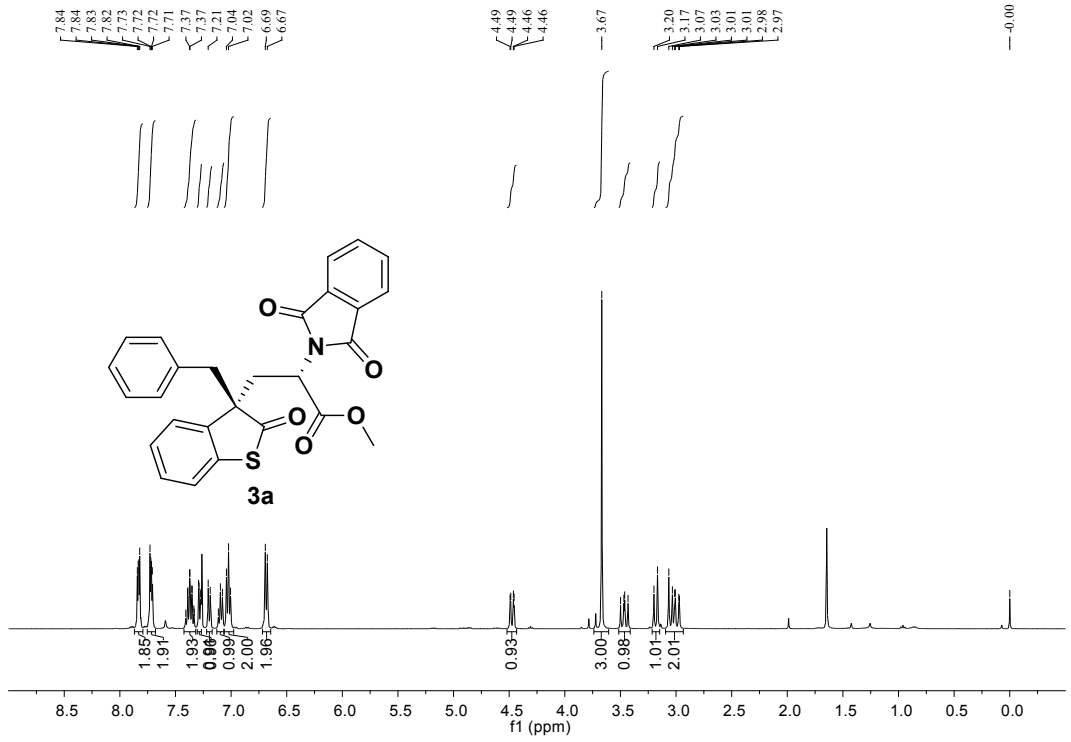


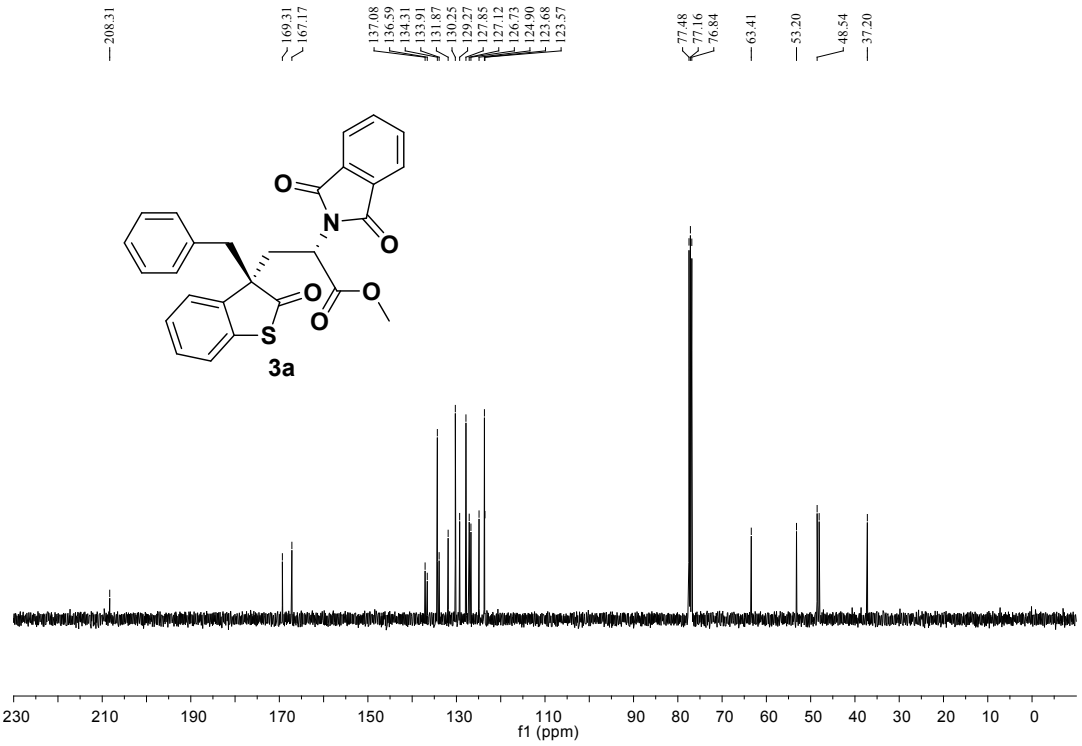
Fig. S1 ORTEP diagram showing of compound **3f**.

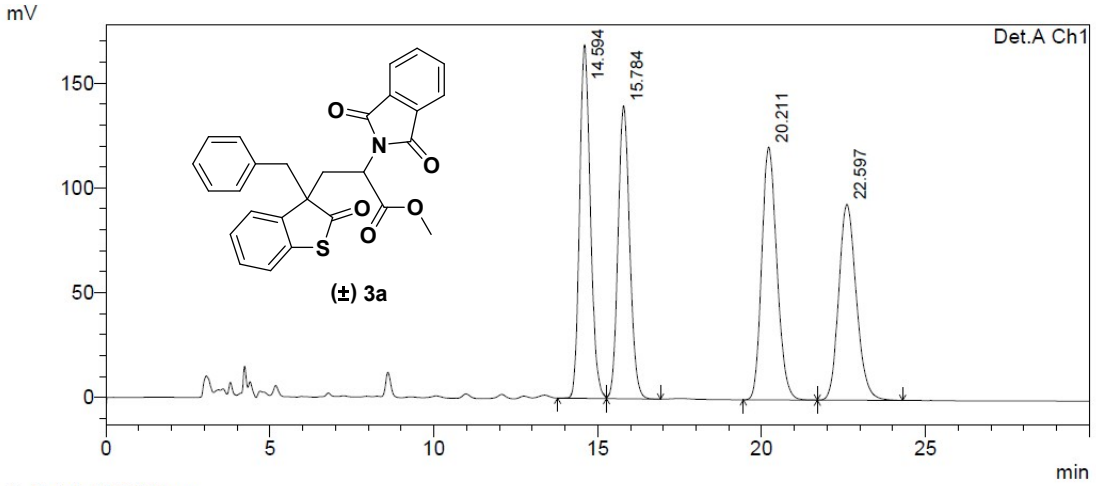
Table 1 Crystal data and structure refinement for shelx.

Identification code	shelx
Empirical formula	C29H25NO7S
Formula weight	531.56
Temperature	133(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.0159(11) A alpha = 90 deg.
	b = 15.545(3) A beta = 90 deg.
	c = 21.174(3) A gamma = 90 deg.
Volume	2638.4(7) A^3
Z, Calculated density	4, 1.338 Mg/m^3
Absorption coefficient	0.171 mm^-1
F(000)	1112
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	3.02 to 27.64 deg.
Limiting indices	-10<=h<=10, -19<=k<=20, -27<=l<=27
Reflections collected / unique	29028 / 6099 [R(int) = 0.0340]
Completeness to theta = 27.64	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9798 and 0.9666
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6099 / 0 / 346
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0276, wR2 = 0.0700
R indices (all data)	R1 = 0.0315, wR2 = 0.0720
Absolute structure parameter	0.00(5)
Largest diff. peak and hole	0.210 and -0.165 e.A^-3

NMR Spectra and HPLC Spectra


7.84
7.84
7.83
7.82
7.73
7.72
7.72
7.71
7.37
7.37
7.21
7.04
7.02
6.69
6.67
4.49
4.49
4.46
4.46
3.67
3.20
3.17
3.07
3.03
3.01
3.01
2.98
2.97
0.00
O
N
O
O
O
O
S
3a
1.85
1.91
1.93
0.99
2.00
1.96
0.93
3.00
0.98
1.01
2.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


208.31
169.31
167.17
137.08
136.59
134.31
133.91
131.87
130.25
129.27
127.85
127.12
126.73
124.90
123.68
123.57
77.48
77.16
76.84
63.41
53.20
48.54
37.20
O
N
O
O
O
O
S
3a
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

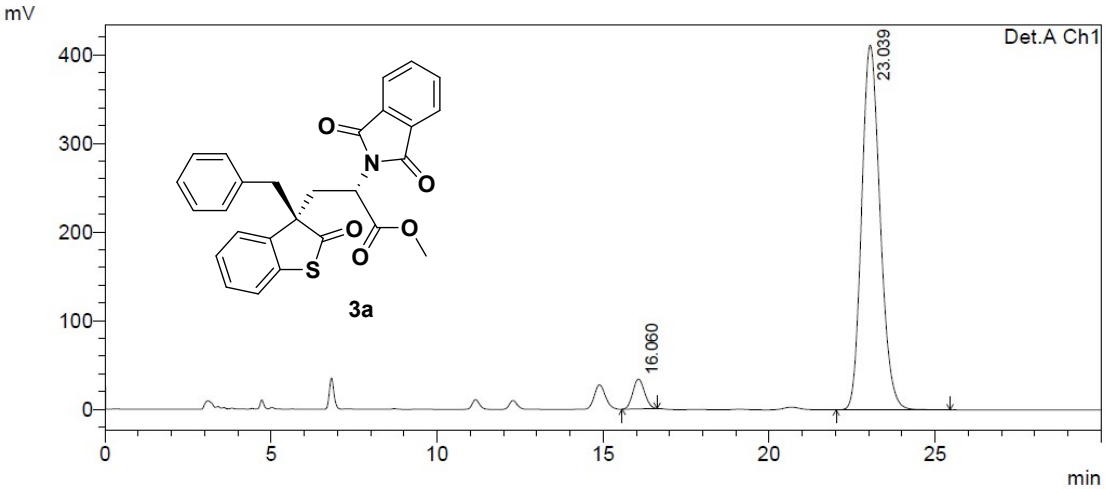


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.594	3867141	168793	26.313	32.291
2	15.784	3452738	139765	23.493	26.737
3	20.211	3889779	120681	26.467	23.086
4	22.597	3487031	93494	23.727	17.886
Total		14696689	522733	100.000	100.000

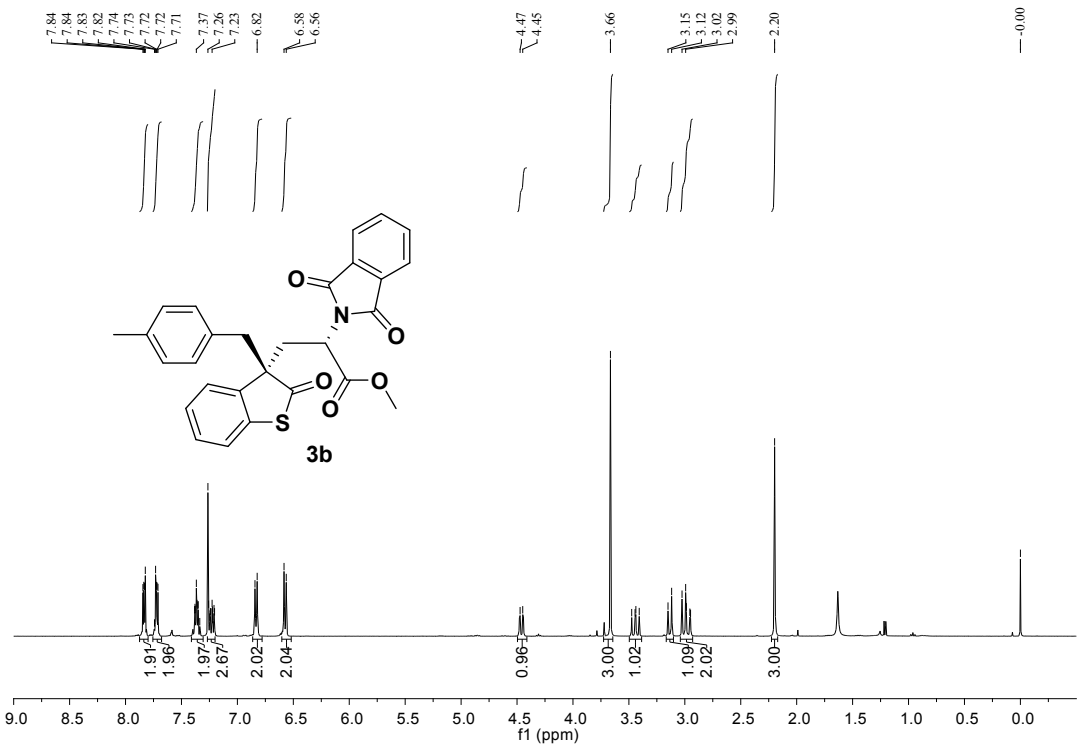


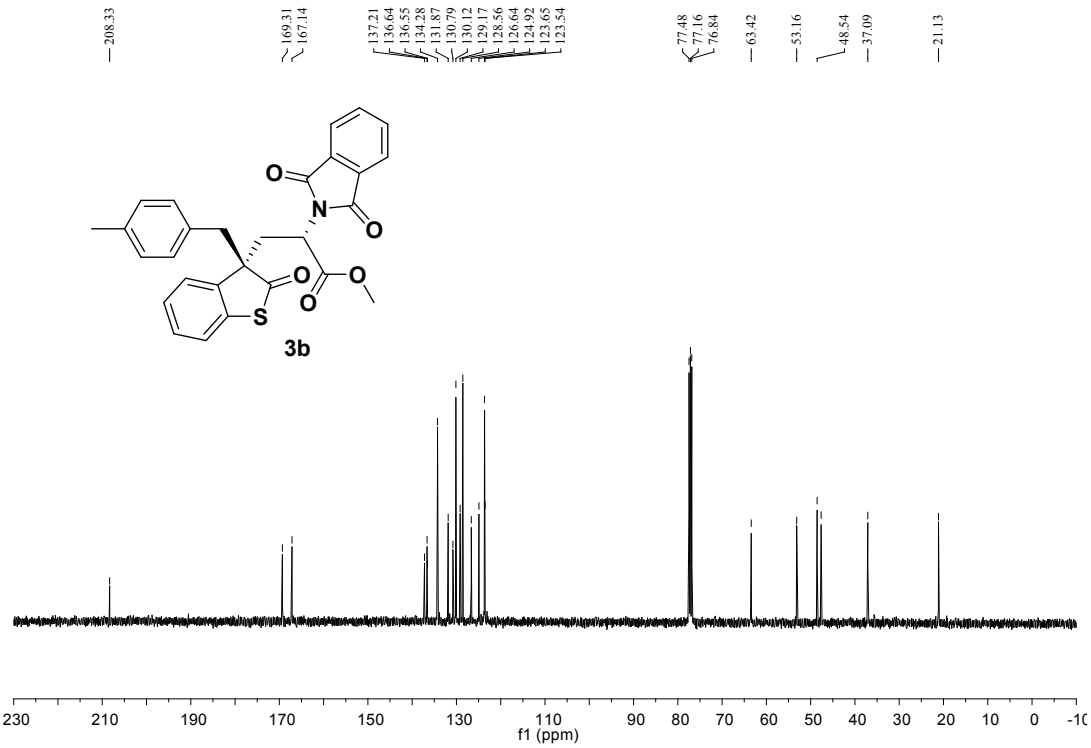
1 Det.A Ch1/210nm

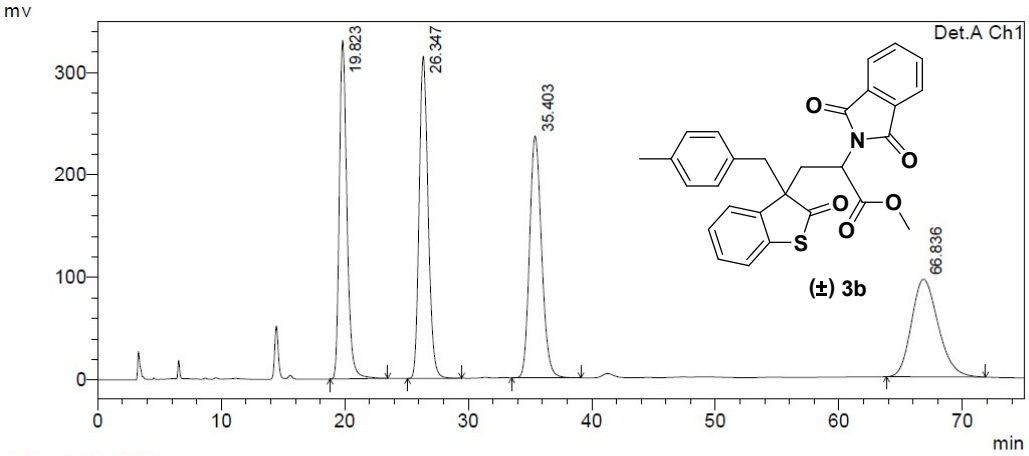
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.060	827080	33619	4.946	7.549
2	23.039	15896098	411747	95.054	92.451
Total		16723178	445367	100.000	100.000


7.84
7.84
7.83
7.82
7.74
7.73
7.72
7.72
7.72
7.71
7.37
7.26
7.23
6.82
6.58
6.56
4.47
4.45
3.66
3.15
3.12
3.02
2.99
2.20
-0.00
3b
1.91
1.96
1.97
2.67
2.02
2.04
0.96
3.00
1.02
1.09
2.02
3.00
f1 (ppm)

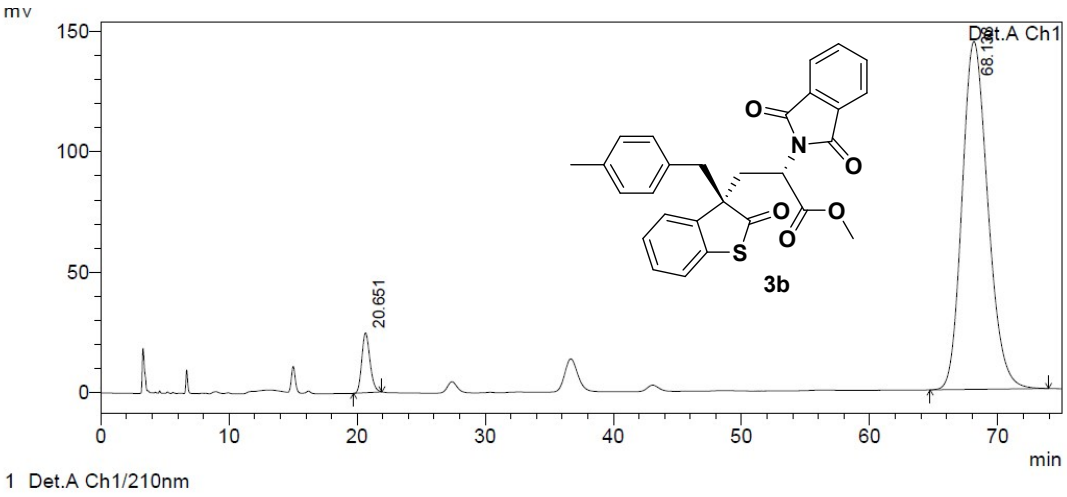

208.33
169.31
167.14
137.21
136.64
136.55
134.28
131.87
130.79
130.12
129.17
128.56
126.64
124.92
123.65
123.54
77.48
77.16
76.84
63.42
53.16
48.54
37.09
21.13
3b
f1 (ppm)



PeakTable

Detector A Ch1 210nm

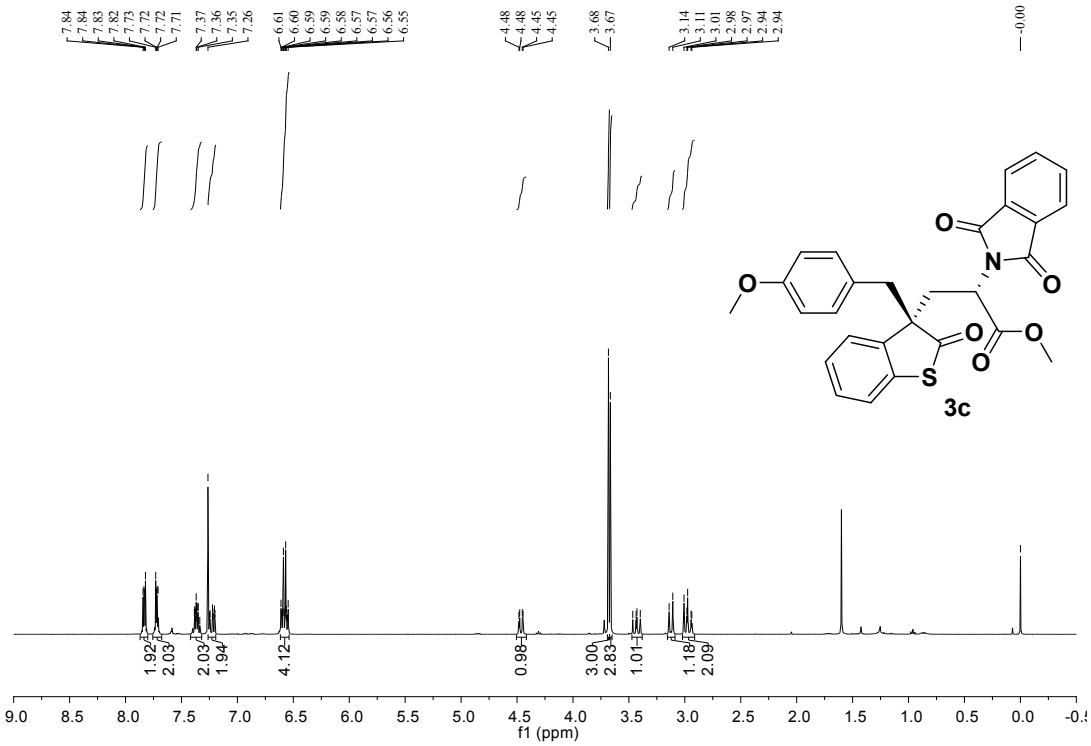
Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.823	14230183	330336	23.565	33.856
2	26.347	15888400	314187	26.311	32.201
3	35.403	15955399	235940	26.422	24.182
4	66.836	14313927	95239	23.703	9.761
Total		60387910	975702	100.000	100.000

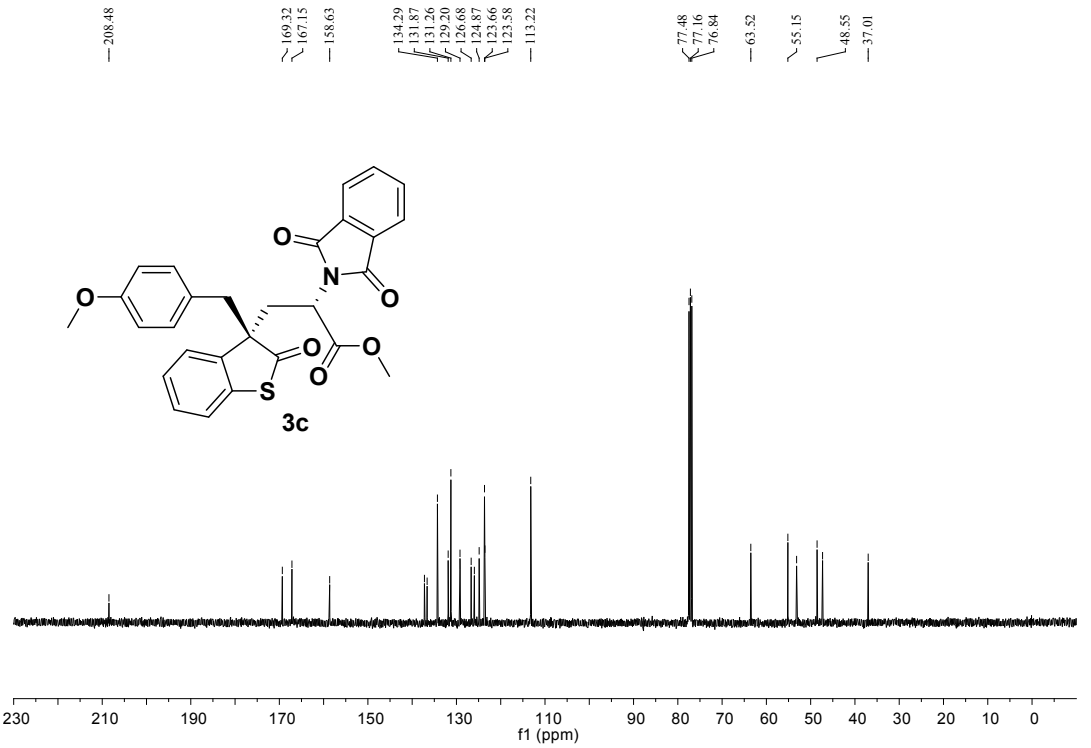


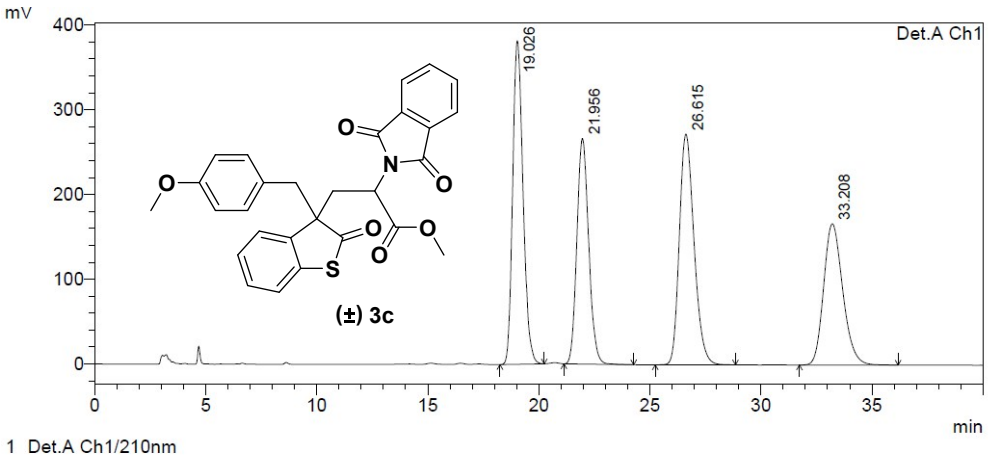
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.651	1106512	24823	5.188	14.673
2	68.133	20222466	144356	94.812	85.327
Total		21328978	169180	100.000	100.000


7.84
7.84
7.83
7.82
7.73
7.72
7.72
7.71
7.37
7.36
7.35
7.26
6.61
6.60
6.59
6.59
6.58
6.57
6.57
6.56
6.55
4.48
4.48
4.45
4.45
3.68
3.67
3.14
3.11
3.01
2.98
2.97
2.94
2.94
-0.00
1.92
2.03
2.03
1.94
4.12
0.98
3.00
2.83
1.01
1.18
2.09
f1 (ppm)
3c


208.48
169.32
167.15
158.63
134.29
131.87
131.26
129.20
126.68
124.87
123.66
123.58
113.22
77.48
77.16
76.84
63.52
55.15
48.55
37.01
f1 (ppm)
3c

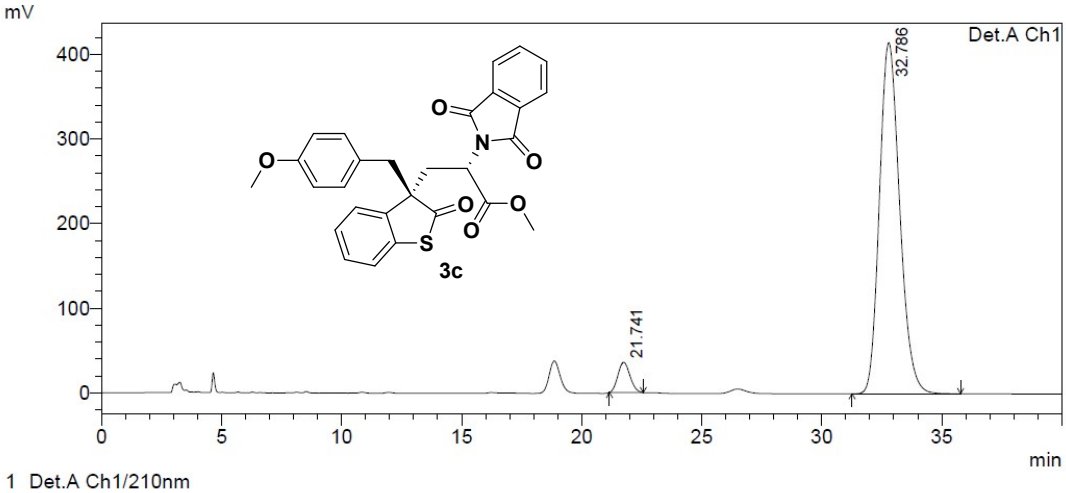


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.026	12378372	381973	27.659	35.121
2	21.956	9874048	266444	22.063	24.499
3	26.615	12534992	272455	28.009	25.051
4	33.208	9965749	166717	22.268	15.329
Total		44753161	1087589	100.000	100.000

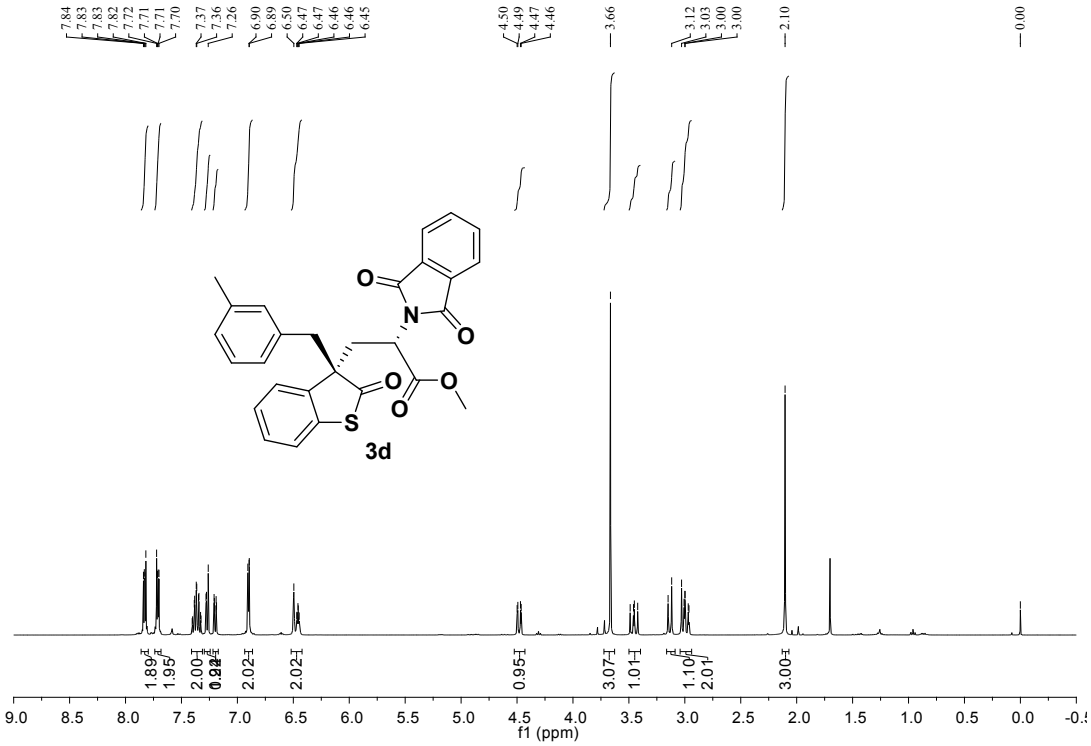


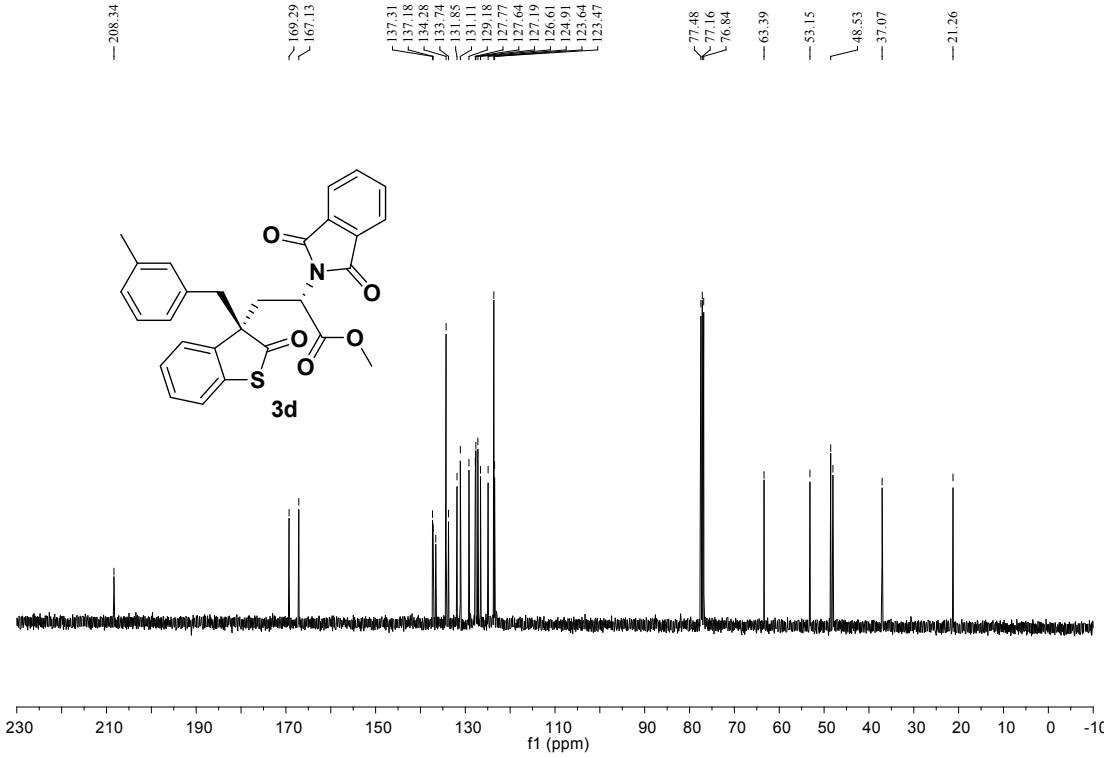
1 Det.A Ch1/210nm

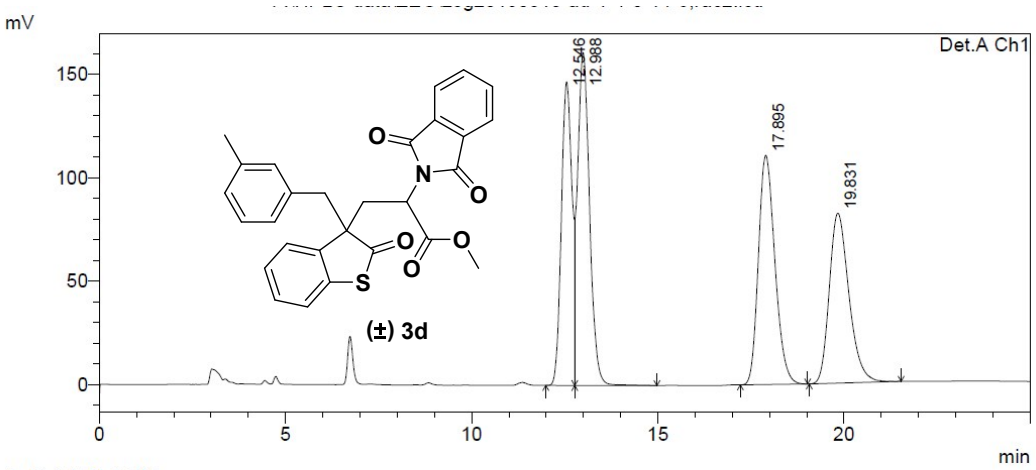
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.741	1254294	35930	4.898	7.968
2	32.786	24354554	414994	95.102	92.032
Total		25608848	450924	100.000	100.000


7.84
7.83
7.83
7.82
7.72
7.71
7.71
7.70
7.37
7.36
7.26
6.90
6.89
6.50
6.47
6.47
6.46
6.46
6.45
4.50
4.49
4.47
4.46
3.66
3.12
3.03
3.00
3.00
2.10
0.00
O
N
O
O
O
O
S
3d
1.89
1.95
2.00
2.02
2.02
0.95
3.07
1.01
1.10
2.01
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


208.34
169.29
167.13
137.31
137.18
134.28
133.74
131.85
131.11
129.18
127.77
127.64
127.19
126.61
124.91
123.64
123.47
77.48
77.16
76.84
63.39
53.15
48.53
37.07
21.26
O
N
O
O
O
O
S
3d
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

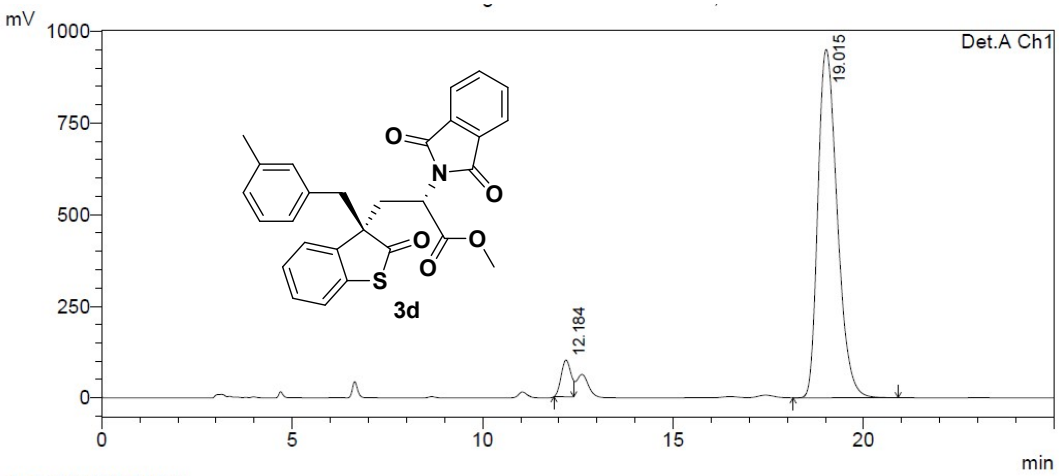


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.546	2911703	146841	22.463	29.310
2	12.988	3609222	161068	27.844	32.149
3	17.895	3420284	110894	26.387	22.134
4	19.831	3021004	82197	23.306	16.407
Total		12962213	501000	100.000	100.000

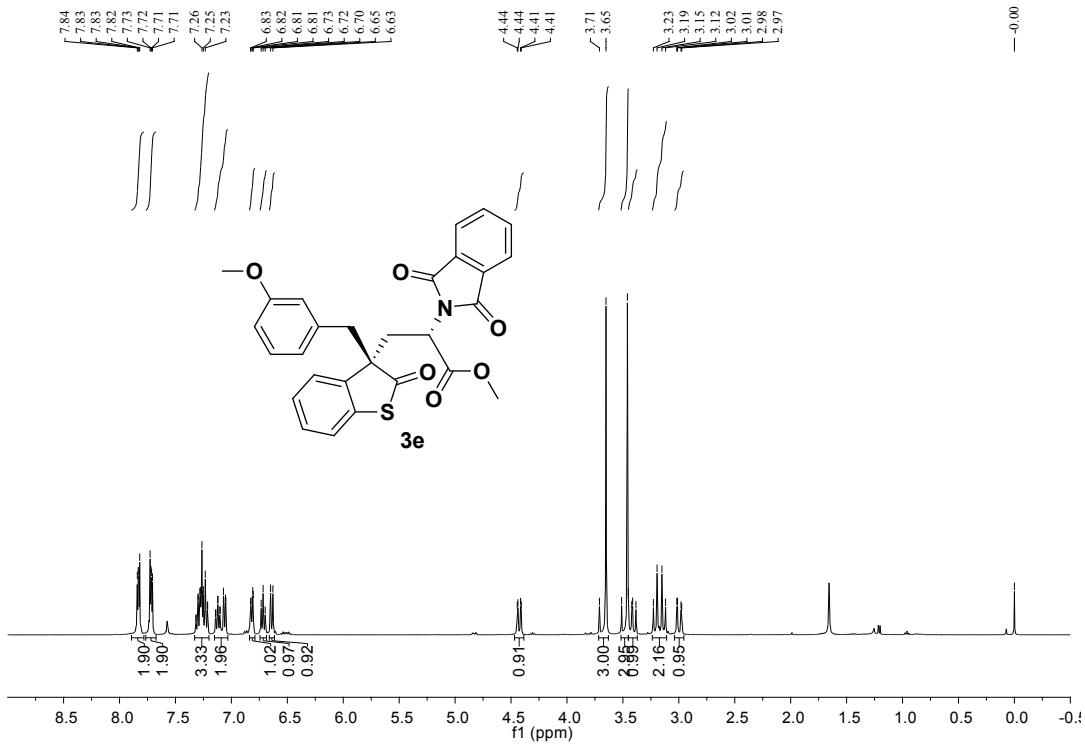


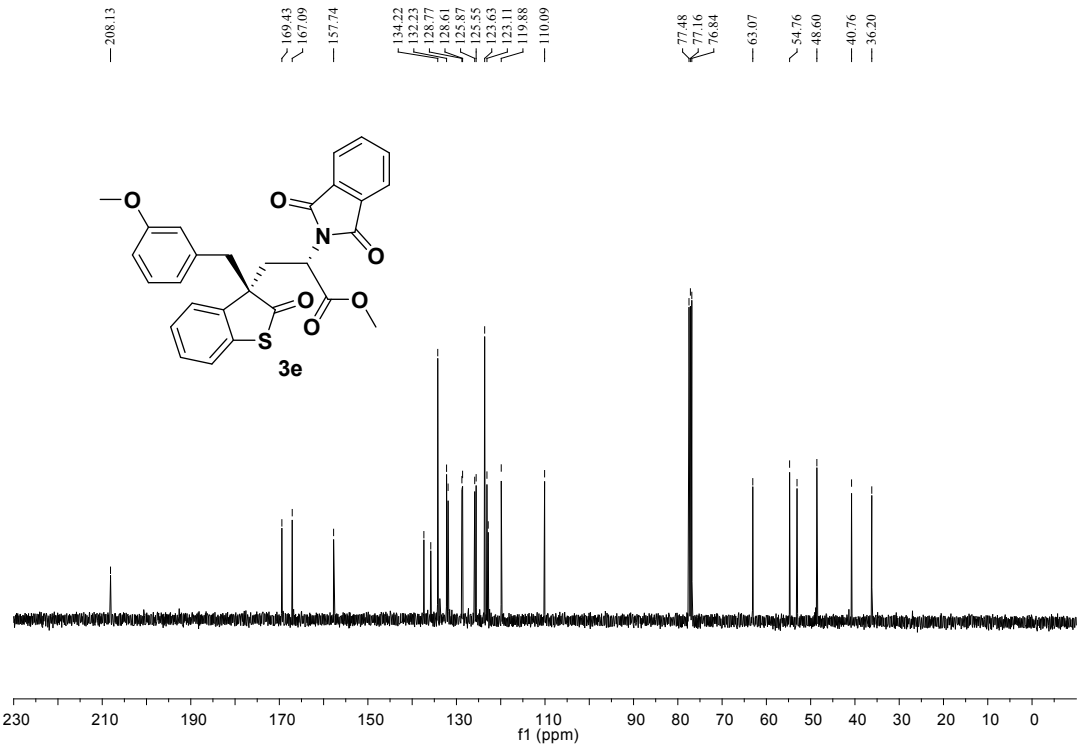
1 Det.A Ch1/210nm

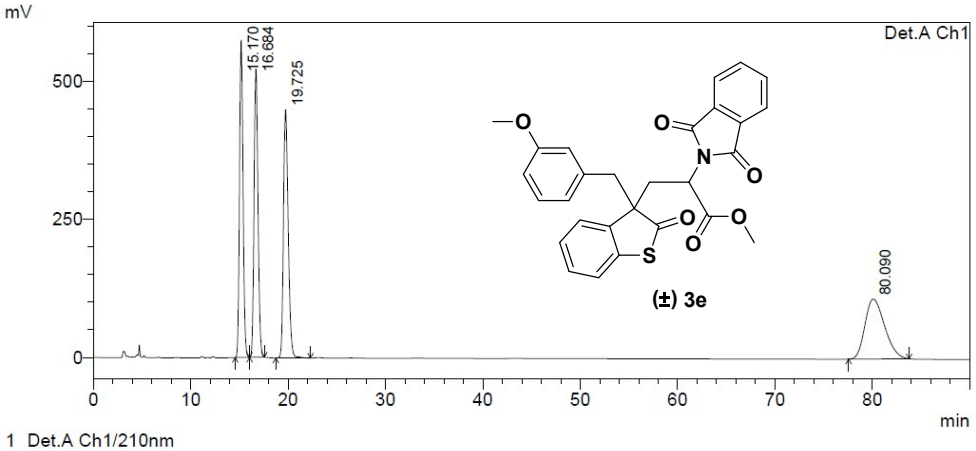
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.184	1788604	100286	5.073	9.550
2	19.015	33467463	949841	94.927	90.450
Total		35256067	1050127	100.000	100.000


7.84
7.83
7.83
7.82
7.73
7.72
7.71
7.71
7.26
7.25
7.23
6.83
6.82
6.81
6.81
6.73
6.72
6.70
6.65
6.63
4.44
4.44
4.41
4.41
3.71
3.65
3.23
3.19
3.15
3.12
3.02
3.01
2.98
2.97
-0.00
3e
1.90
1.90
3.33
1.96
1.02
0.97
0.92
0.91
3.00
2.95
0.99
2.16
0.95
f1 (ppm)


208.13
169.43
167.09
157.74
134.22
132.23
128.77
128.61
125.87
125.55
123.63
123.11
119.88
110.09
77.48
77.16
76.84
63.07
54.76
48.60
40.76
36.20
3e
f1 (ppm)

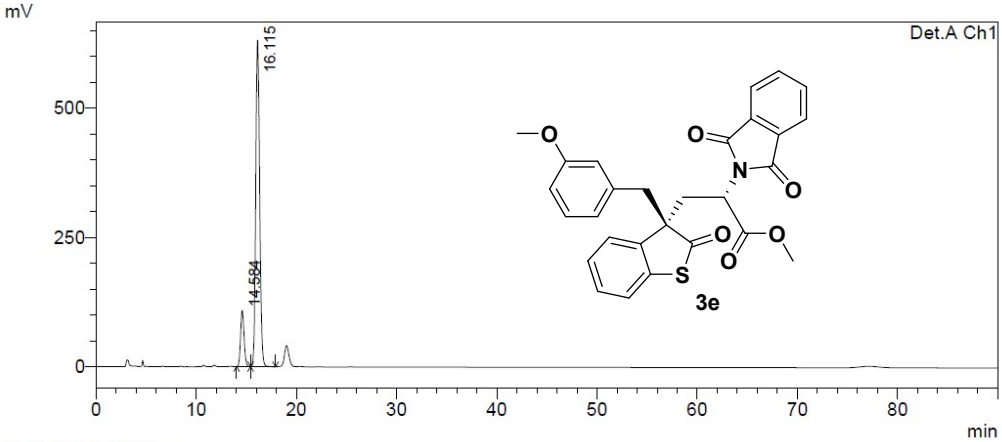


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.170	14555334	574771	24.372	34.724
2	16.684	14612351	522399	24.467	31.560
3	19.725	15300208	449585	25.619	27.161
4	80.090	15254397	108514	25.542	6.556
Total		59722290	1655268	100.000	100.000

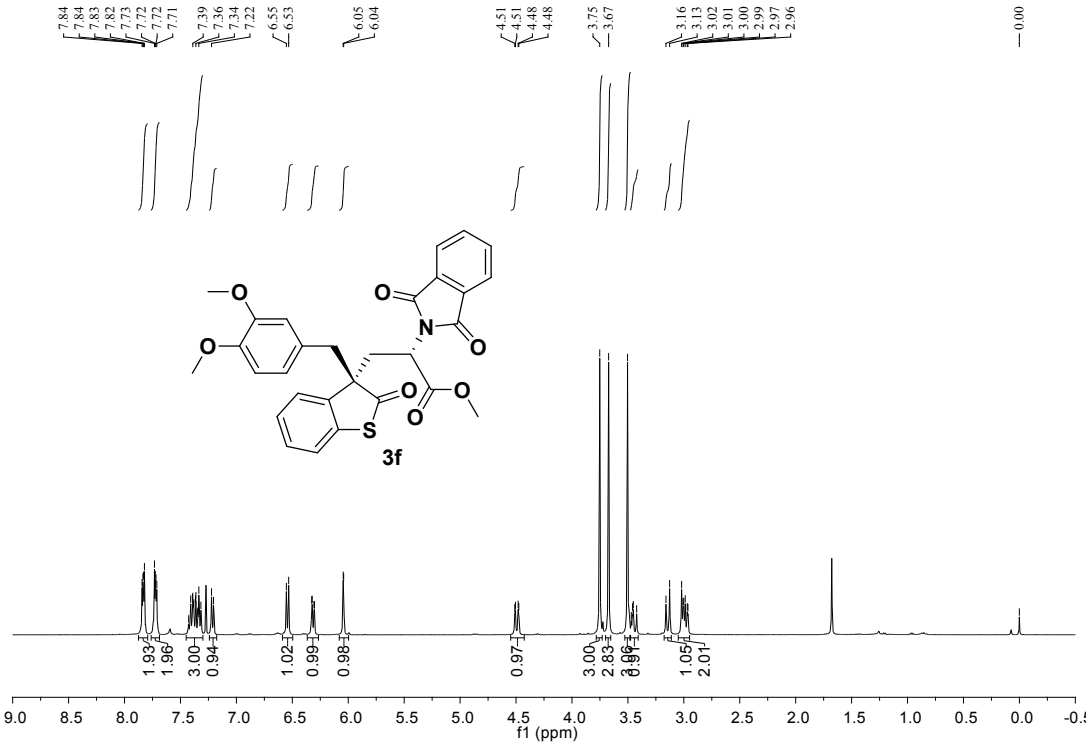


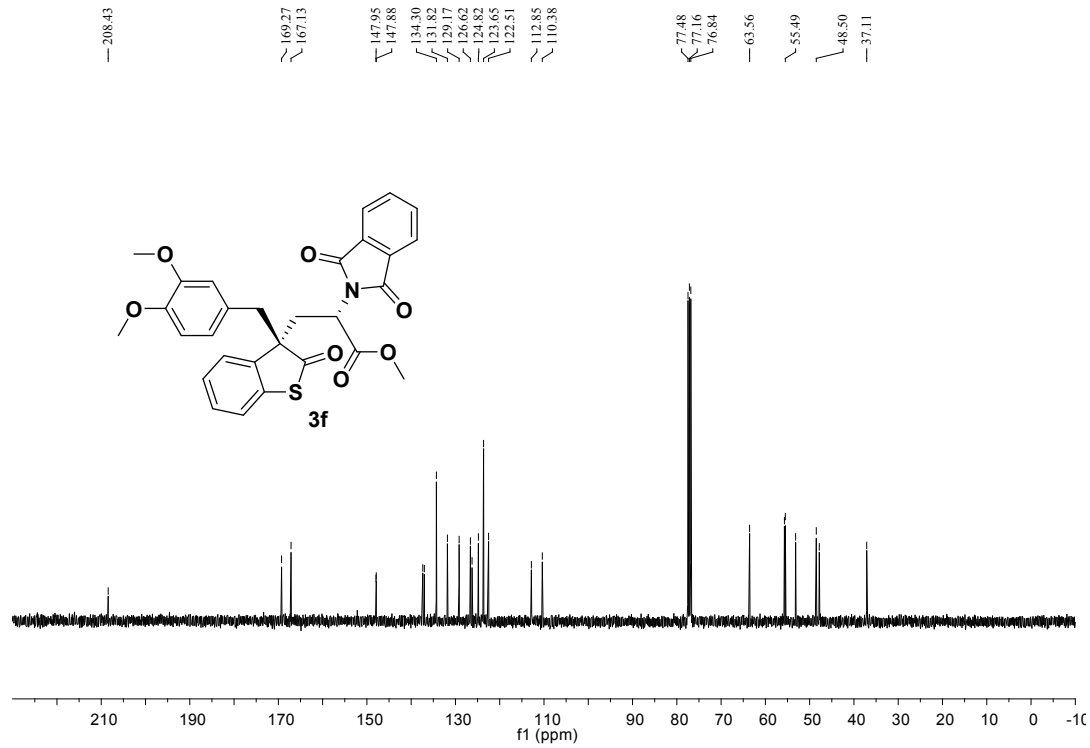
1 Det.A Ch1/210nm

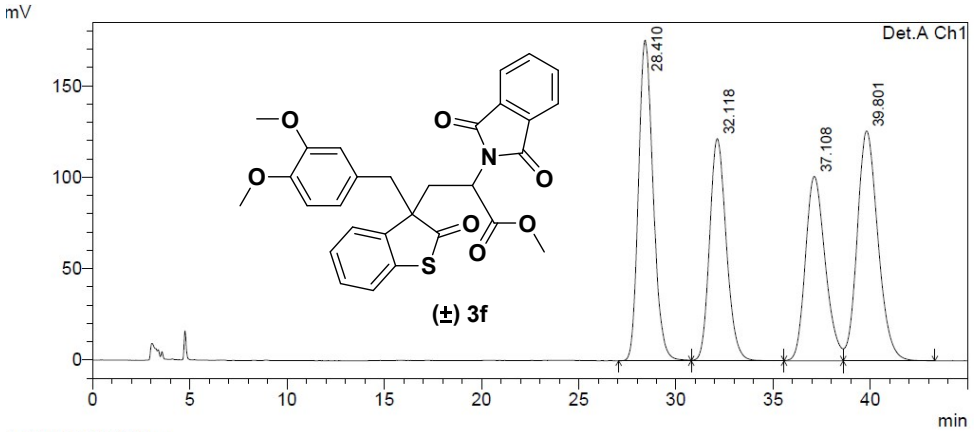
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.584	2621842	108450	13.143	14.651
2	16.115	17326120	631777	86.857	85.349
Total		19947962	740227	100.000	100.000


7.84
7.84
7.83
7.82
7.73
7.72
7.72
7.71
7.39
7.36
7.34
7.22
6.55
6.53
6.05
6.04
4.51
4.51
4.48
4.48
3.75
3.67
3.16
3.13
3.02
3.01
3.00
2.99
2.97
2.96
0.00
3f
1.93
1.96
3.00
0.94
1.02
0.99
0.98
0.97
3.00
2.83
3.06
0.91
1.05
2.01
f1 (ppm)


208.43
169.27
167.13
147.95
147.88
134.30
131.82
129.17
126.62
124.82
123.65
122.51
112.85
110.38
77.48
77.16
76.84
63.56
55.49
48.50
37.11
3f
f1 (ppm)

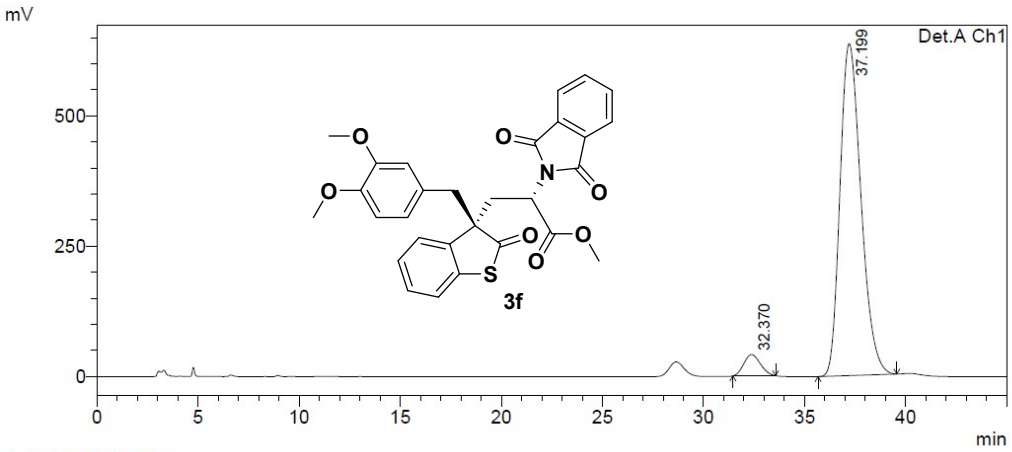


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.410	9208129	175355	27.928	33.500
2	32.118	7262087	121552	22.026	23.222
3	37.108	7159561	100827	21.715	19.262
4	39.801	9340646	125713	28.330	24.016
Total		32970423	523446	100.000	100.000

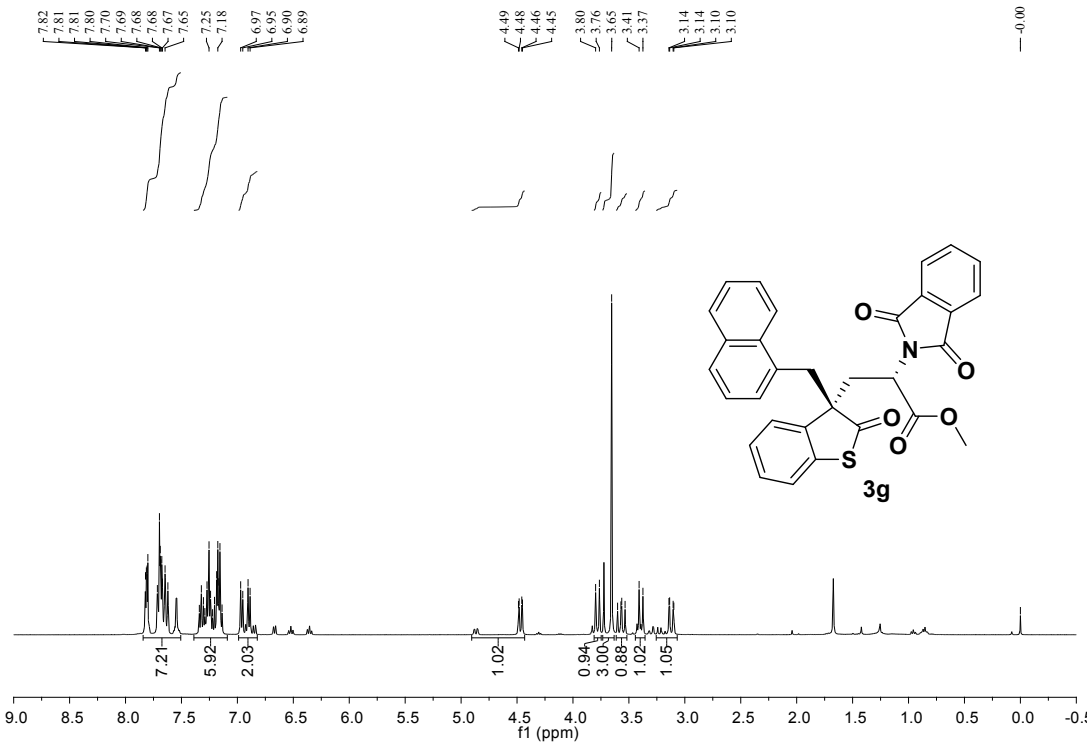


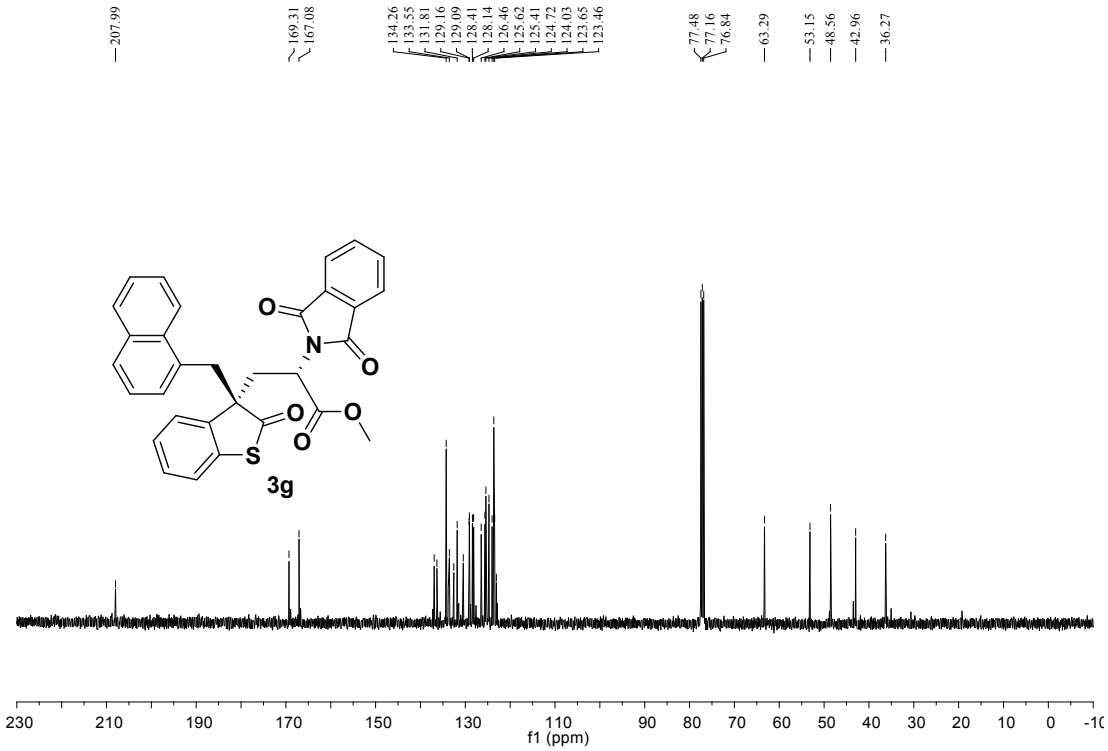
1 Det.A Ch1/210nm

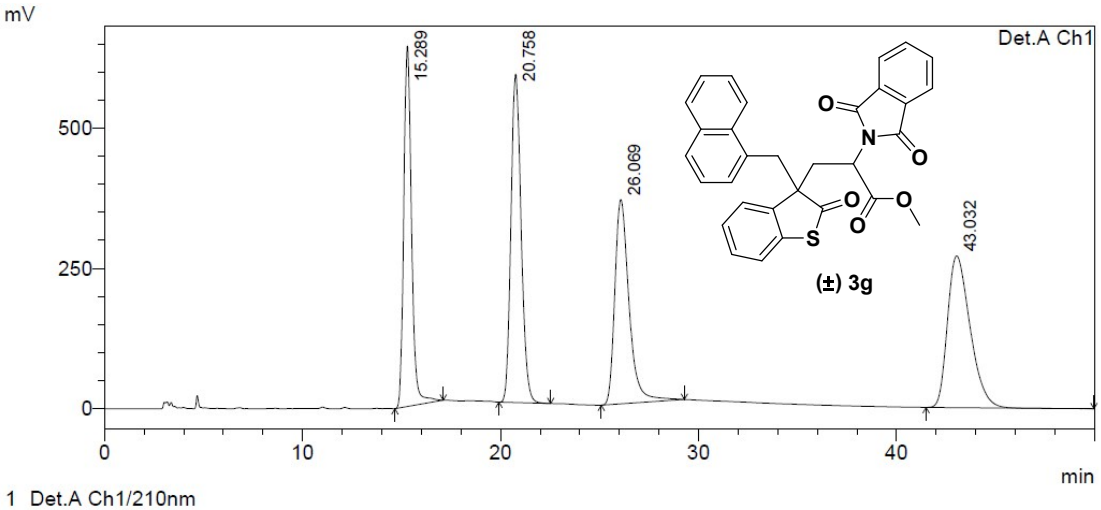
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.370	2309559	40731	4.786	6.013
2	37.199	45949159	636623	95.214	93.987
Total		48258718	677354	100.000	100.000


7.82
7.81
7.81
7.80
7.70
7.69
7.68
7.68
7.67
7.65
7.25
7.18
6.97
6.95
6.90
6.89
4.49
4.48
4.46
4.45
3.80
3.76
3.65
3.41
3.37
3.14
3.14
3.10
3.10
-0.00
O
N
O
O
O
O
S
3g
7.21
5.92
2.03
1.02
0.94
3.00
0.88
1.02
1.05
f1 (ppm)


207.99
169.31
167.08
134.26
133.55
131.81
129.16
129.09
128.41
128.14
126.46
125.62
125.41
124.72
124.03
123.65
123.46
77.48
77.16
76.84
63.29
53.15
48.56
42.96
36.27
O
N
O
O
O
O
S
3g
f1 (ppm)

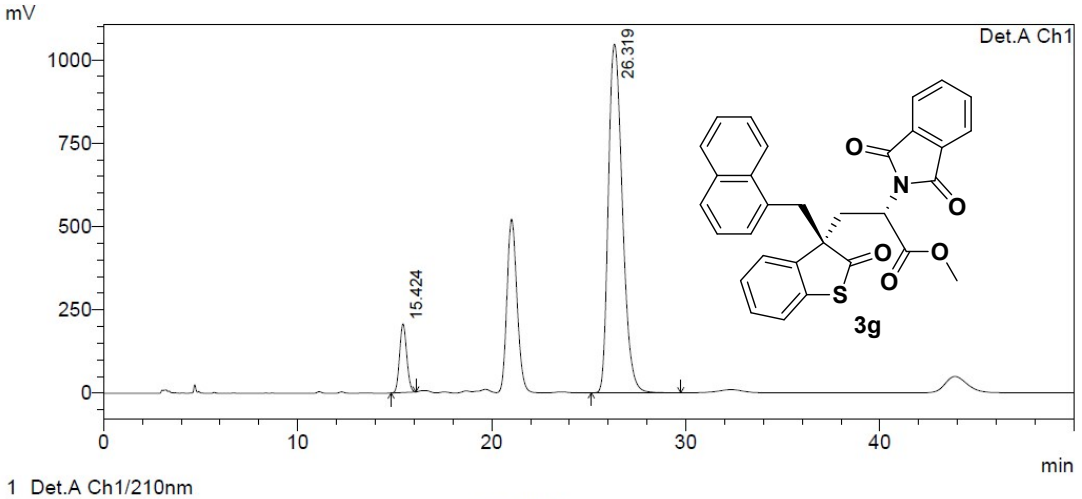


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.289	17527958	641839	22.433	34.495
2	20.758	20968865	584919	26.837	31.436
3	26.069	18221904	363784	23.322	19.551
4	43.032	21414773	270128	27.408	14.518
Total		78133501	1860669	100.000	100.000

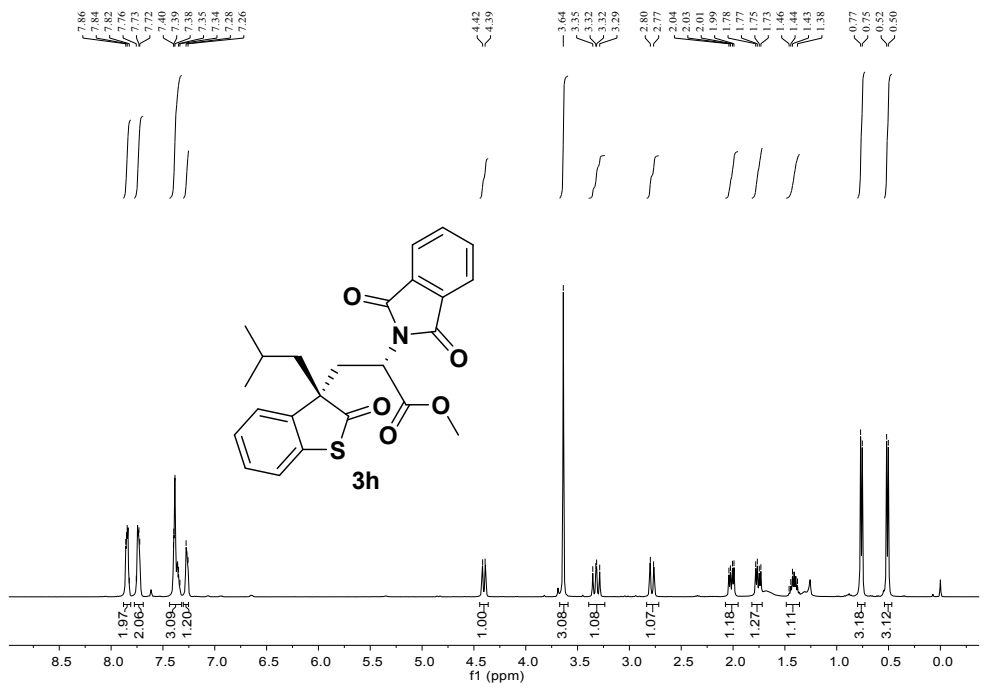


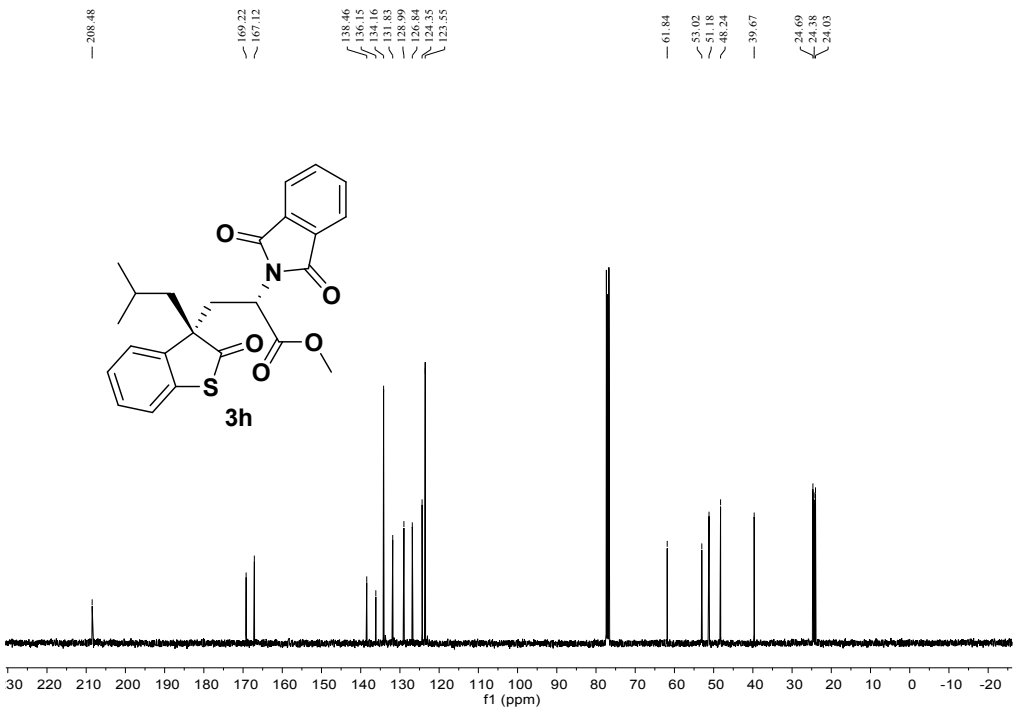
1 Det.A Ch1/210nm

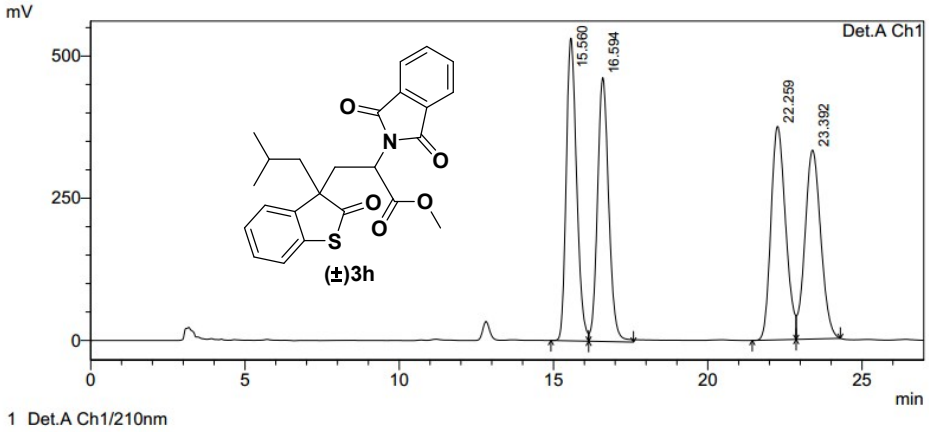
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.424	5254005	205804	9.070	16.437
2	26.319	52674906	1046265	90.930	83.563
Total		57928911	1252070	100.000	100.000


7.86
7.84
7.82
7.76
7.73
7.72
7.40
7.39
7.38
7.35
7.34
7.28
7.26
4.42
4.39
3.64
3.35
3.32
3.32
3.29
2.80
2.77
2.04
2.03
2.01
1.99
1.78
1.77
1.75
1.73
1.46
1.44
1.43
1.38
0.77
0.75
0.52
0.50
O
N
O
O
O
O
S
3h
1.97
2.06
3.09
1.20
1.00
3.08
1.08
1.07
1.18
1.27
1.11
3.18
3.12
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


208.48
169.22
167.12
138.46
136.15
134.16
131.83
128.99
126.84
124.35
123.55
61.84
53.02
51.18
48.24
39.67
24.69
24.38
24.03
O
N
O
O
O
O
S
3h
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

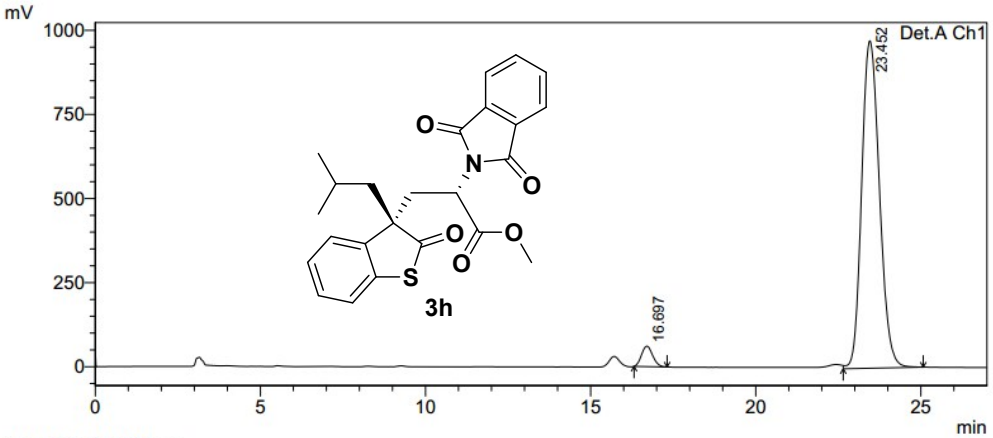


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.560	12424441	532238	25.690	31.242
2	16.594	11766726	463896	24.330	27.231
3	22.259	12349870	375259	25.536	22.028
4	23.392	11821082	332190	24.443	19.499
Total		48362119	1703583	100.000	100.000

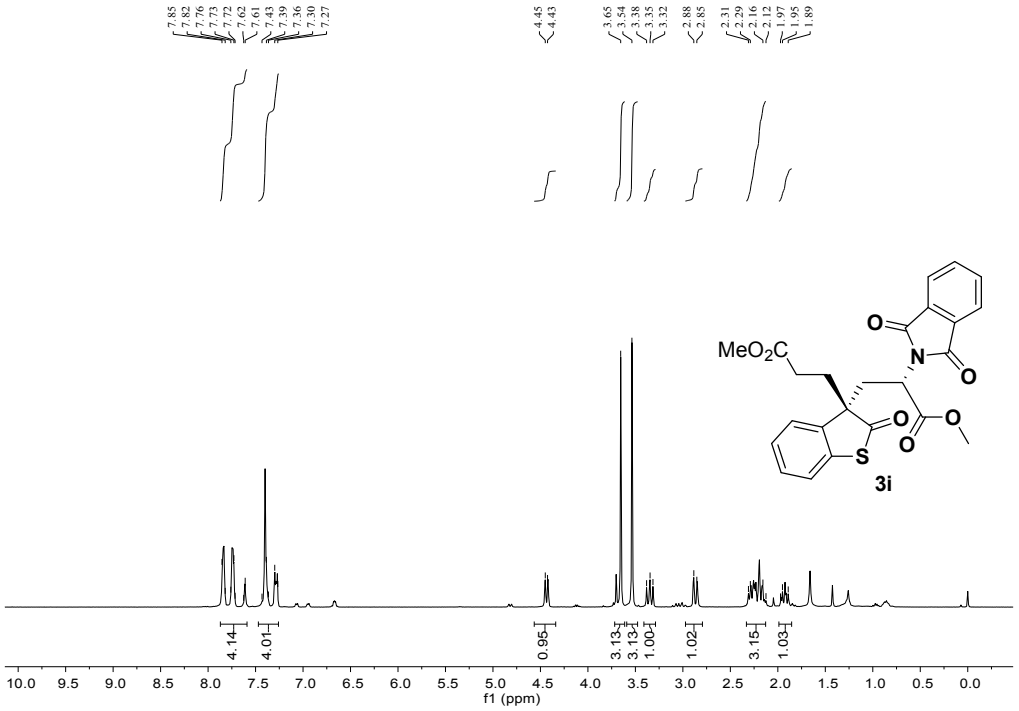


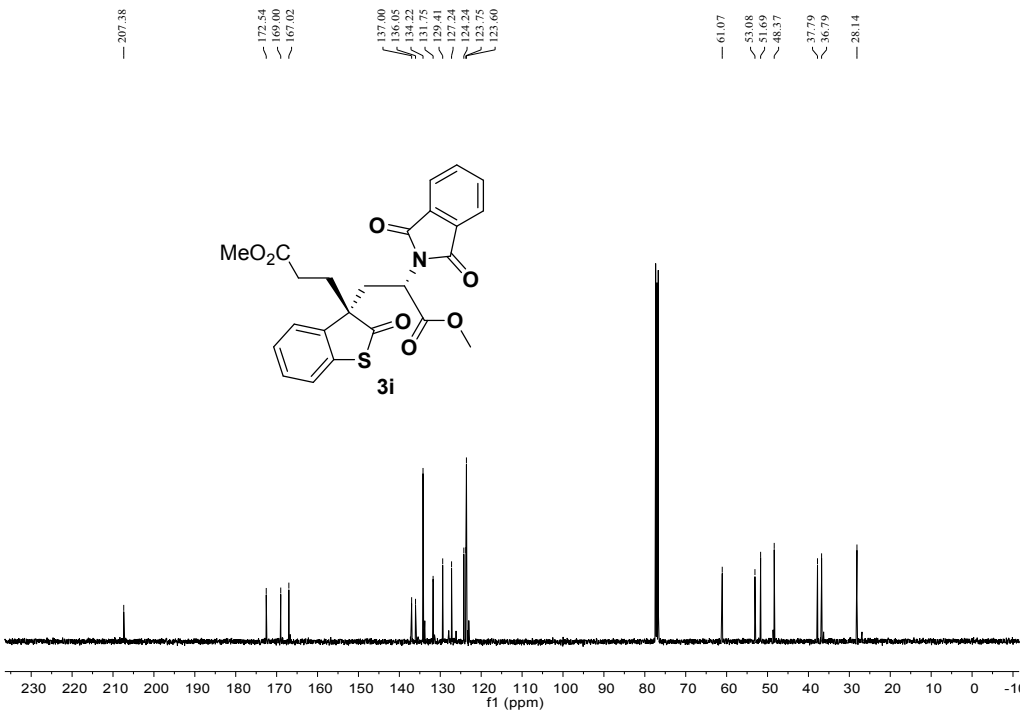
1 Det.A Ch1/210nm

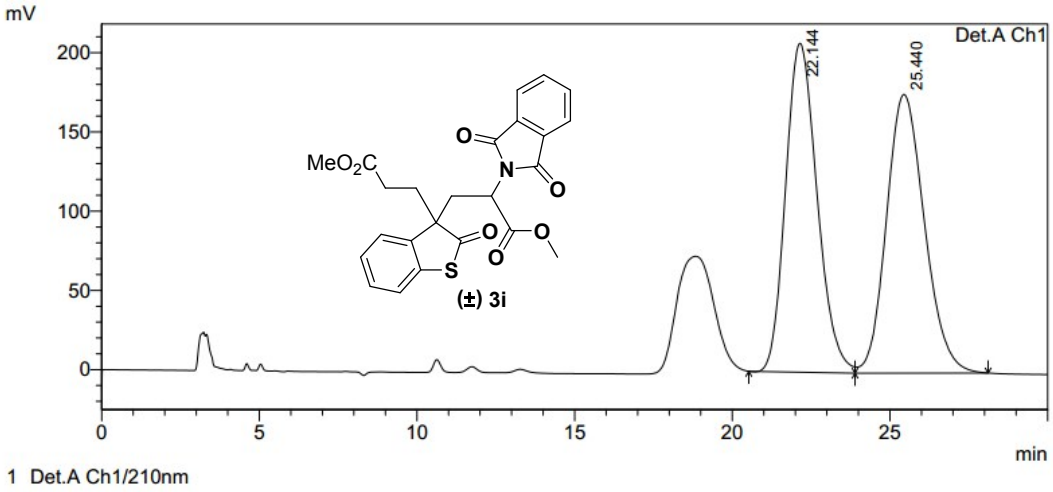
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.697	1427990	60951	3.775	5.892
2	23.452	36402727	973510	96.225	94.108
Total		37830717	1034461	100.000	100.000


7.85
7.82
7.76
7.73
7.72
7.62
7.61
7.43
7.39
7.36
7.30
7.27
4.45
4.43
3.65
3.54
3.38
3.35
3.32
2.88
2.85
2.31
2.29
2.16
2.12
1.97
1.95
1.89
MeO2C
O
N
O
O
O
O
S
3i
4.14
4.01
0.95
3.13
3.13
1.00
1.02
3.15
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


207.38
172.54
169.00
167.02
137.00
136.05
134.22
131.75
129.41
127.24
124.24
123.75
123.60
61.07
53.08
51.69
48.37
37.79
36.79
28.14
MeO2C
O
N
O
O
O
O
S
3i
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

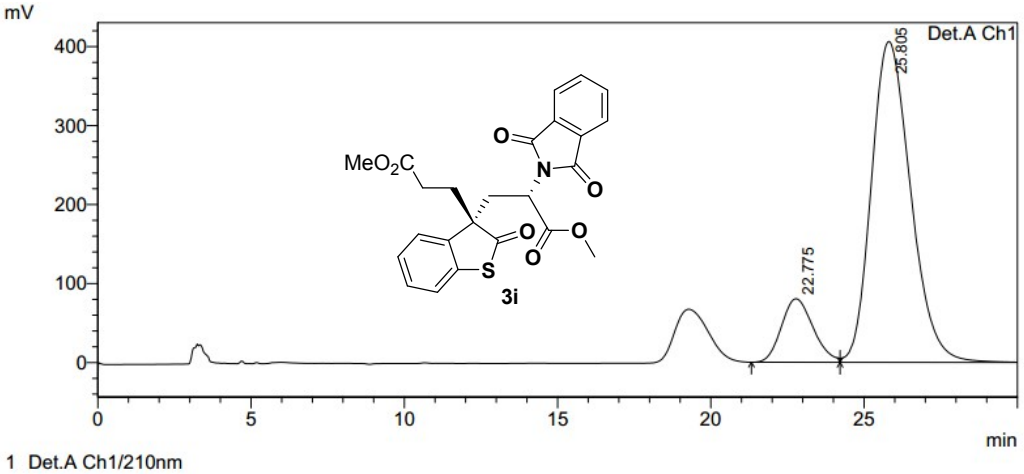


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.144	14424159	207504	49.447	54.126
2	25.440	14746936	175871	50.553	45.874
Total		29171095	383375	100.000	100.000

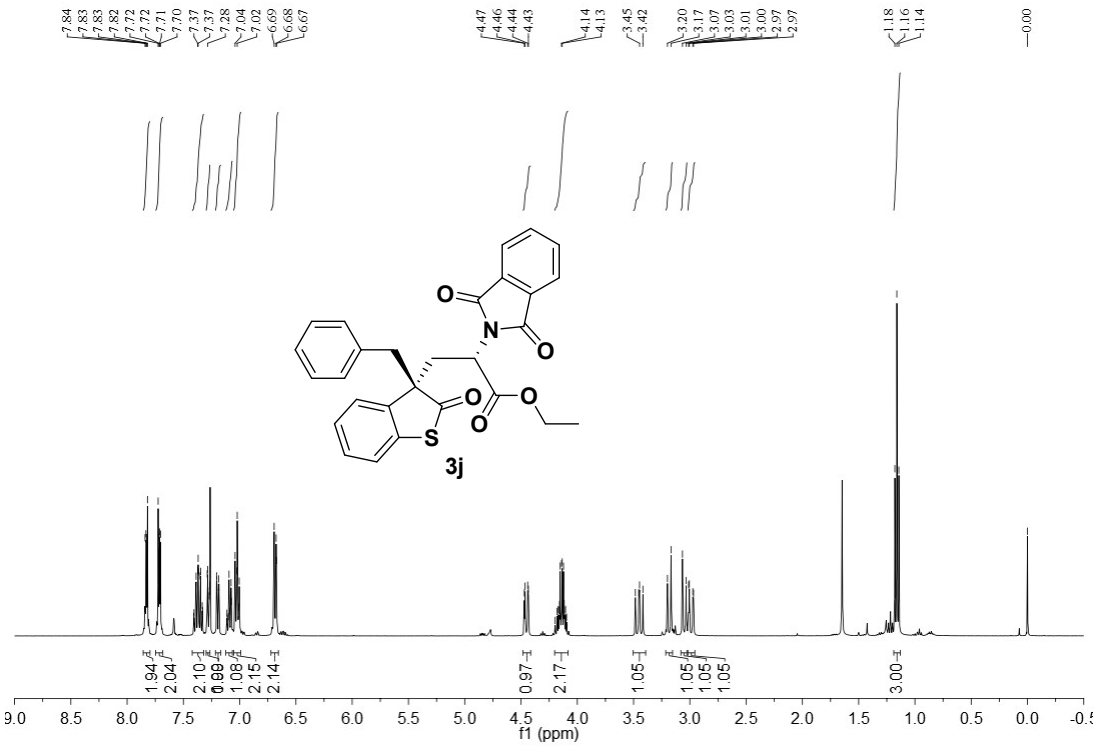


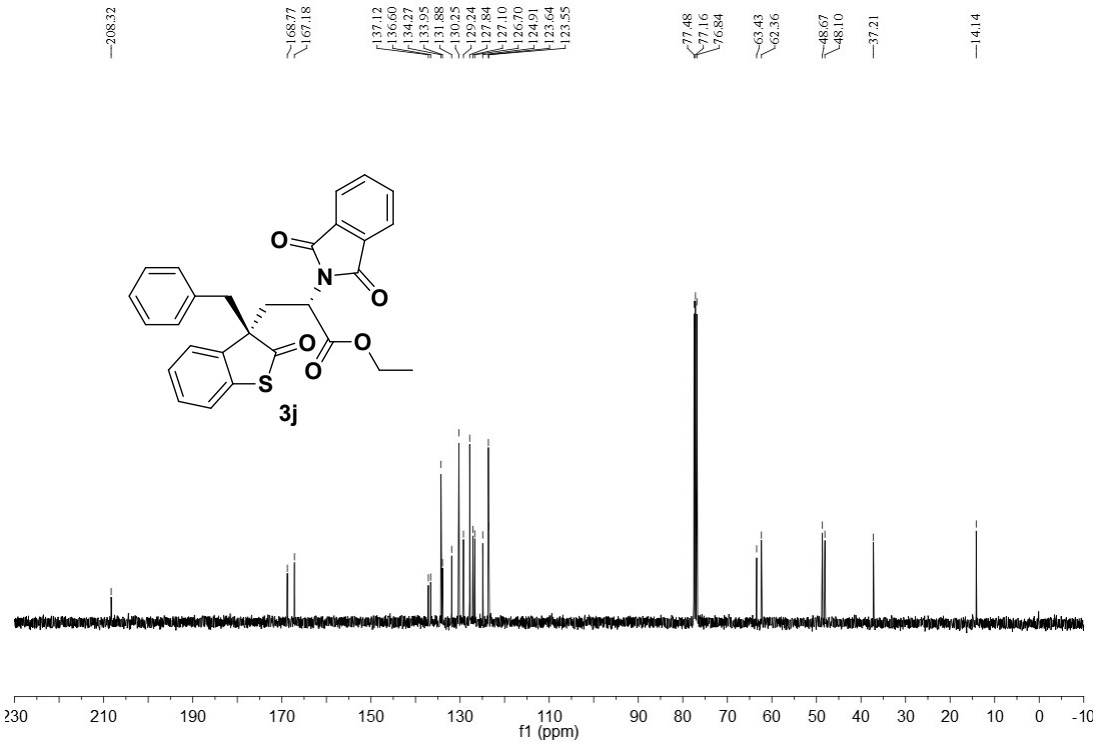
1 Det.A Ch1/210nm

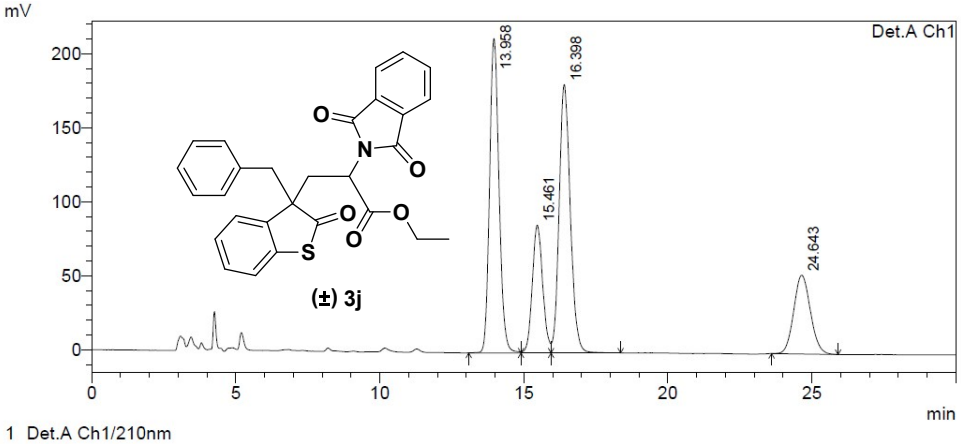
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.775	5777051	80441	13.758	16.529
2	25.805	36214877	406236	86.242	83.471
Total		41991928	486676	100.000	100.000


7.84
7.83
7.83
7.82
7.72
7.72
7.71
7.70
7.37
7.37
7.28
7.04
7.02
6.69
6.68
6.67
4.47
4.46
4.44
4.43
4.14
4.13
3.45
3.42
3.20
3.17
3.07
3.03
3.01
3.00
2.97
2.97
1.18
1.16
1.14
0.00
O
N
O
O
O
O
S
3j
1.94
2.04
2.10
1.08
2.15
2.14
0.97
2.17
1.05
1.05
1.05
3.00
f1 (ppm)

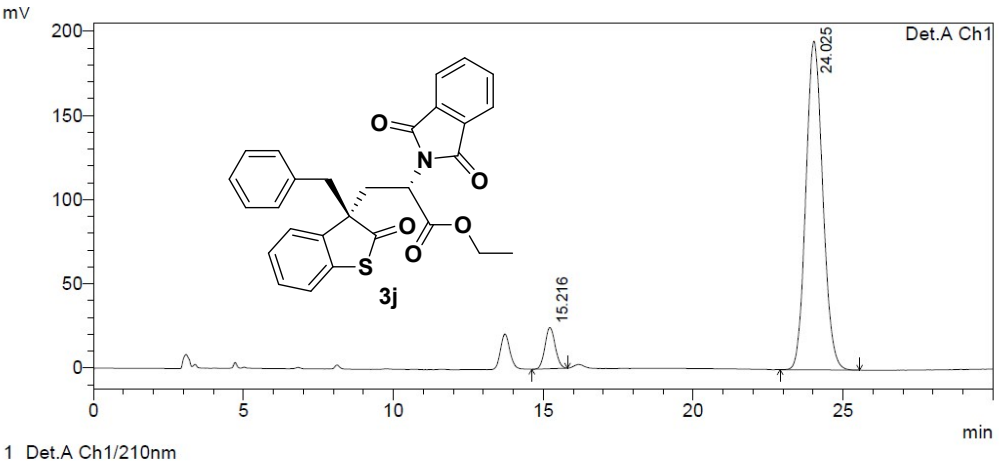

208.32
168.77
167.18
137.12
136.60
134.27
133.95
131.88
130.25
129.24
127.84
127.10
126.70
124.91
123.64
123.55
77.48
77.16
76.84
63.43
62.36
48.67
48.10
37.21
14.14
O
N
O
O
O
O
S
3j
f1 (ppm)



PeakTable

Detector A Ch1 210nm

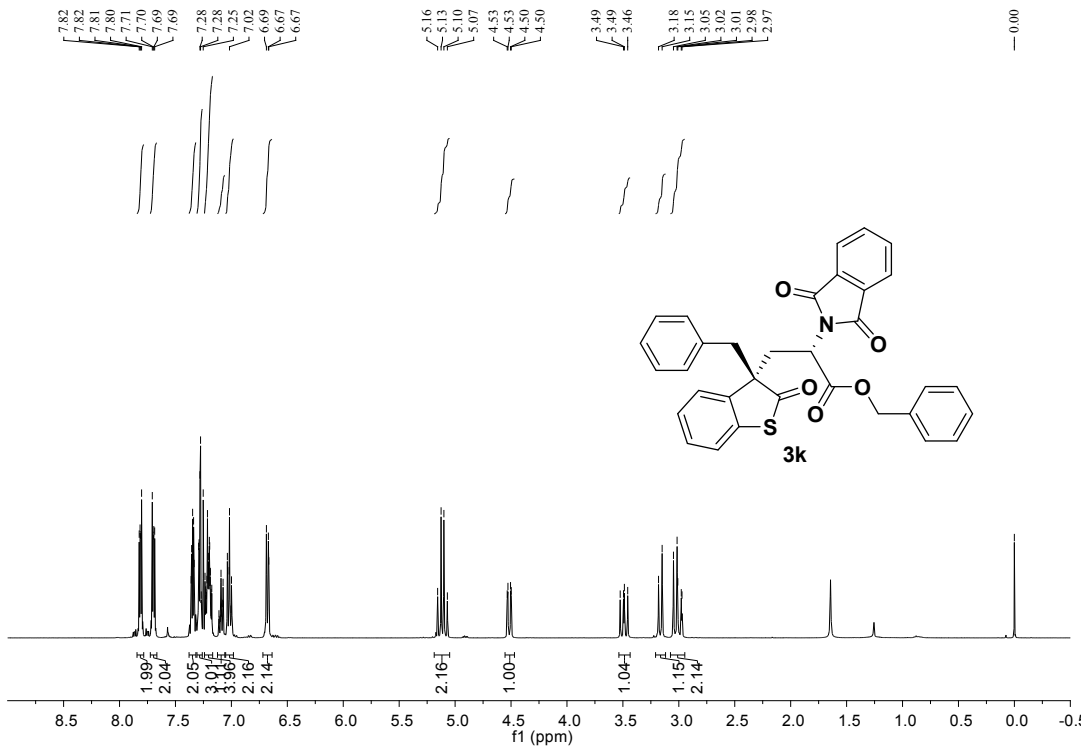
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.958	4848979	212388	34.492	39.827
2	15.461	2167101	86366	15.415	16.195
3	16.398	4892579	181239	34.802	33.986
4	24.643	2149779	53281	15.292	9.991
Total		14058439	533274	100.000	100.000

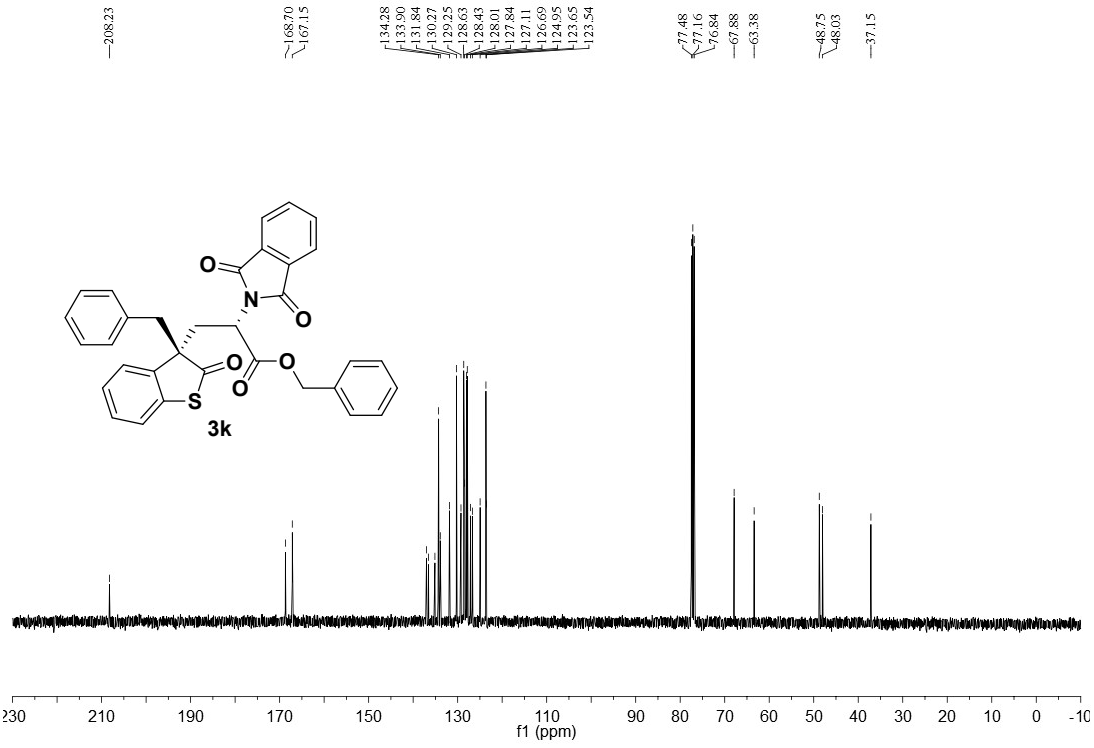


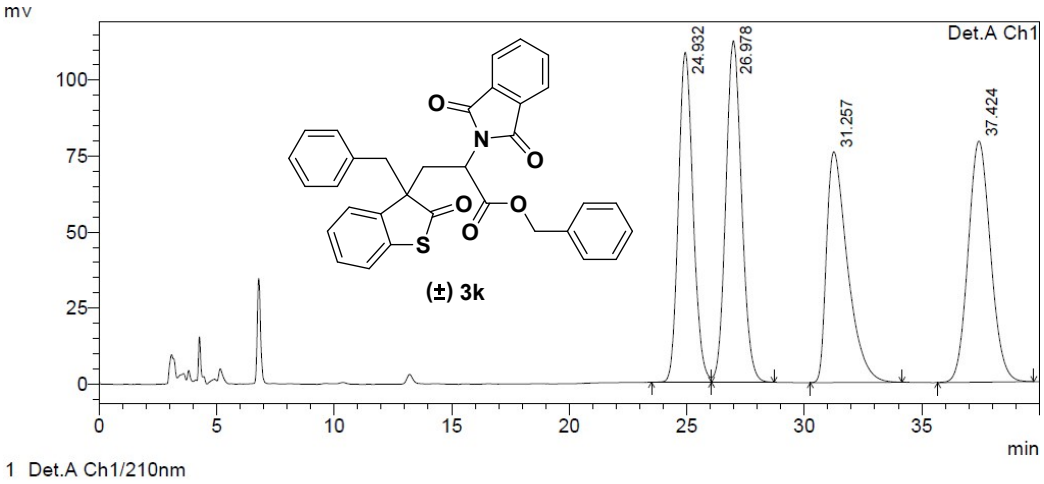
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.216	581034	24448	7.052	11.132
2	24.025	7658826	195162	92.948	88.868
Total		8239860	219610	100.000	100.000


7.82
7.82
7.81
7.80
7.71
7.70
7.69
7.69
7.28
7.28
7.25
7.02
6.69
6.67
6.67
5.16
5.13
5.10
5.07
4.53
4.53
4.50
4.50
3.49
3.49
3.46
3.18
3.15
3.05
3.02
3.01
2.98
2.97
0.00
O
N
O
O
O
O
S
3k
1.99
2.04
2.05
3.01
3.96
2.16
2.14
2.16
1.00
1.04
1.15
2.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

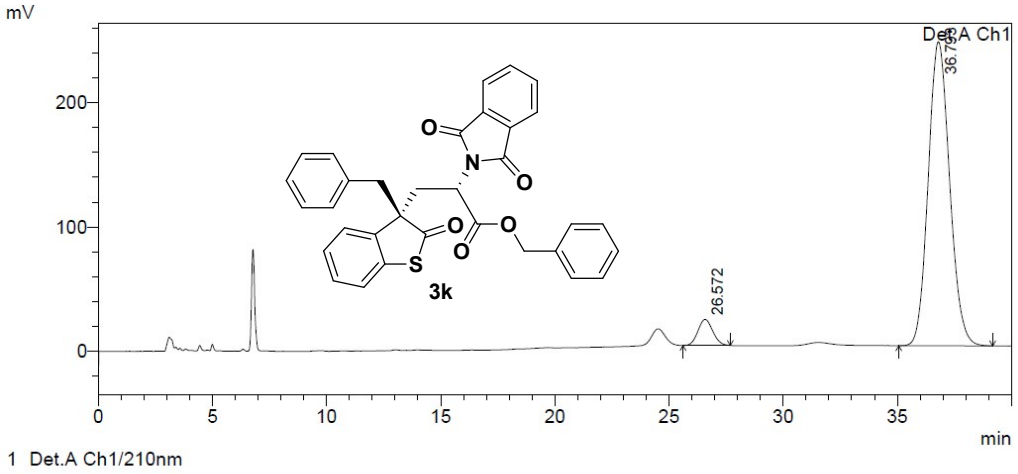

208.23
168.70
167.15
134.28
133.90
131.84
130.27
129.25
128.63
128.43
128.01
127.84
127.11
126.69
124.95
123.65
123.54
77.48
77.16
76.84
67.88
63.38
48.75
48.03
37.15
O
N
O
O
O
O
S
3k
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



PeakTable

Detector A Ch1 210nm

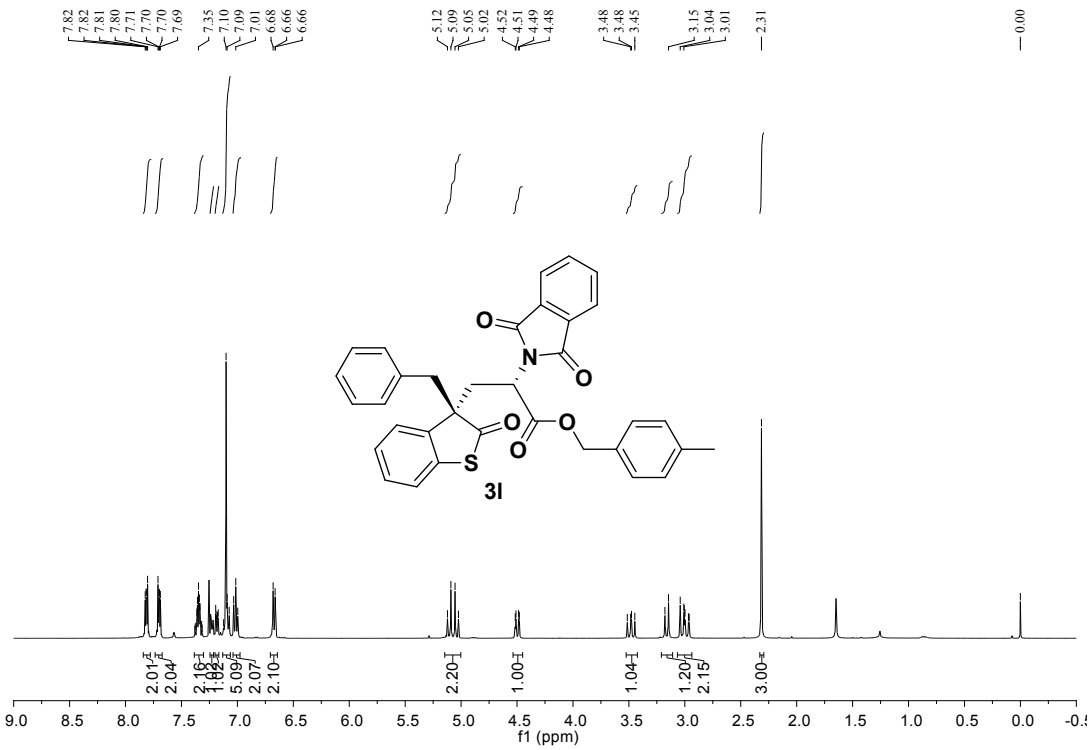
Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.932	4715219	108625	23.608	28.858
2	26.978	5270119	112435	26.386	29.870
3	31.257	4724958	75981	23.656	20.185
4	37.424	5262921	79374	26.350	21.087
Total		19973217	376417	100.000	100.000

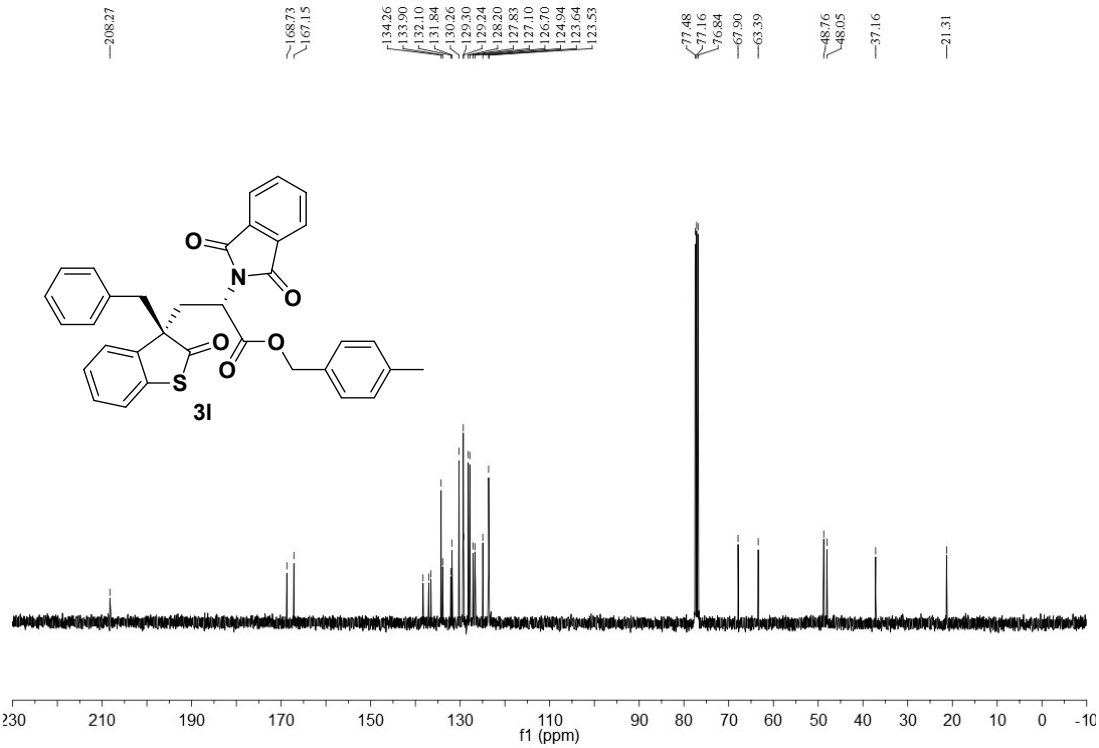


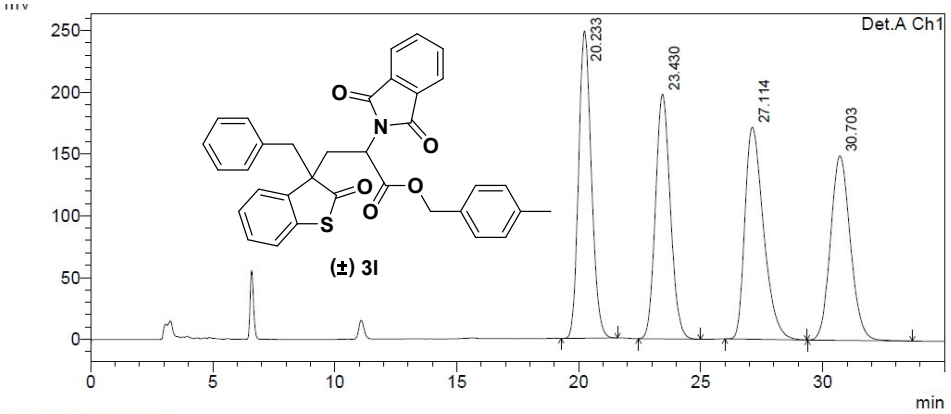
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.572	946161	20931	5.598	7.885
2	36.793	15956106	244516	94.402	92.115
Total		16902267	265447	100.000	100.000


7.82
7.82
7.81
7.80
7.71
7.70
7.70
7.69
7.35
7.10
7.09
7.01
6.68
6.66
6.66
5.12
5.09
5.05
5.02
4.52
4.51
4.49
4.48
3.48
3.48
3.45
3.15
3.04
3.01
2.31
0.00
3l
2.01
2.04
2.16
1.02
5.09
2.07
2.10
2.20
1.00
1.04
1.20
2.15
3.00
f1 (ppm)


208.27
168.73
167.15
134.26
133.90
132.10
131.84
130.26
129.30
129.24
128.20
127.83
127.10
126.70
124.94
123.64
123.53
77.48
77.16
76.84
67.90
63.39
48.76
48.05
37.16
21.31
3l
f1 (ppm)

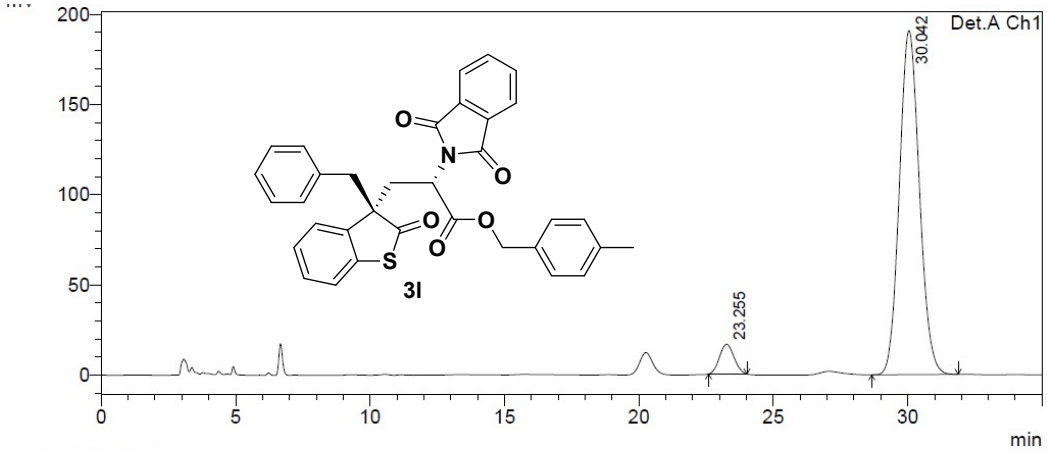


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.233	9039126	248539	25.827	32.386
2	23.430	8391100	198040	23.976	25.806
3	27.114	9123326	171588	26.068	22.359
4	30.703	8444690	149259	24.129	19.449
Total		34998242	767425	100.000	100.000

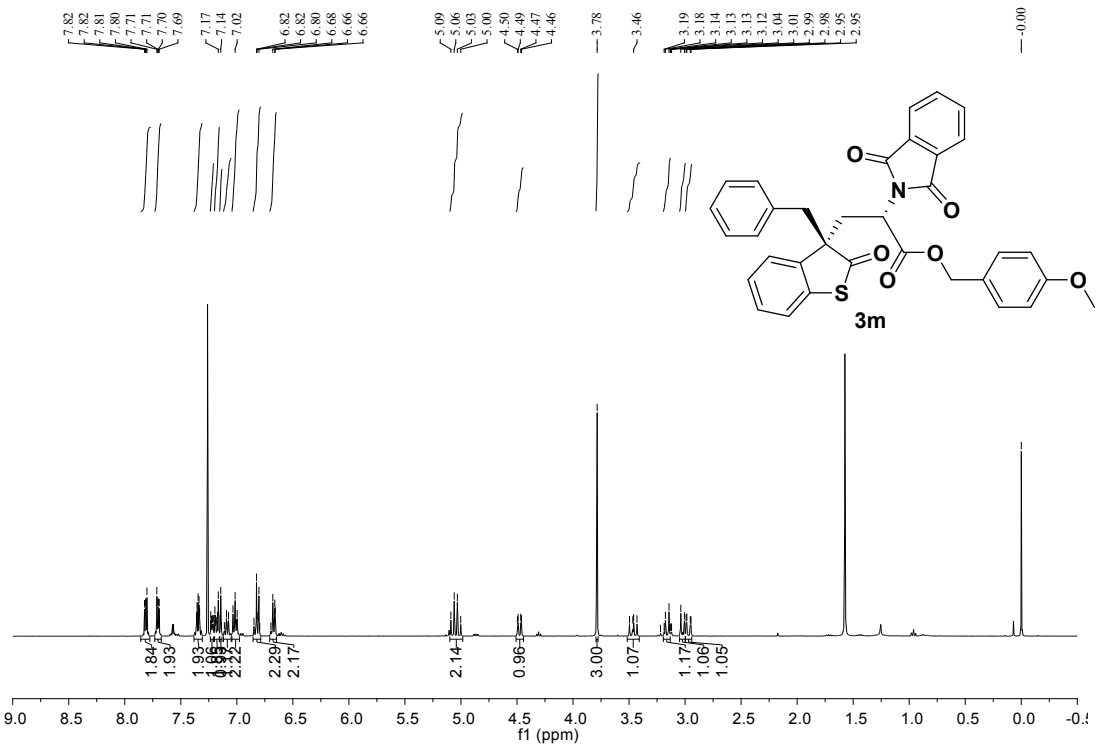


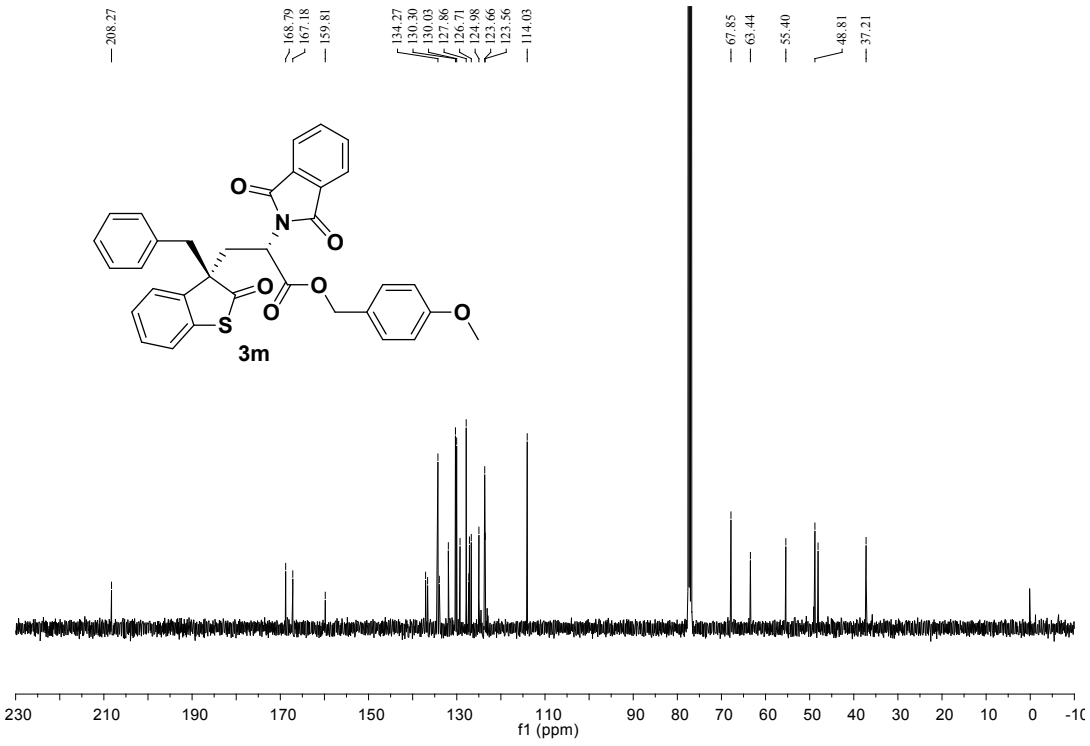
1 Det.A Ch1/210nm

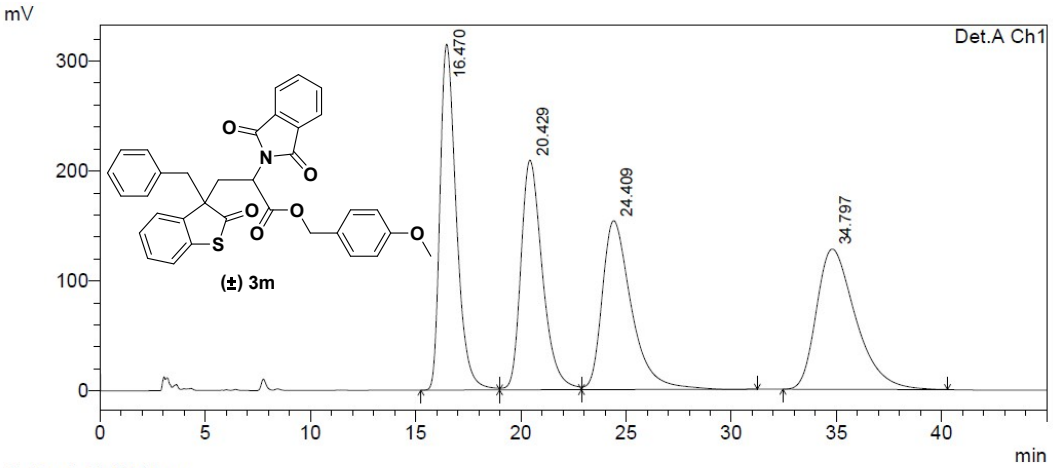
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.255	615927	16481	5.868	7.955
2	30.042	9880024	190684	94.132	92.045
Total		10495951	207165	100.000	100.000


7.82
7.82
7.81
7.80
7.71
7.71
7.71
7.70
7.69
7.17
7.14
7.02
6.82
6.82
6.80
6.68
6.66
6.66
5.09
5.06
5.03
5.00
4.50
4.49
4.47
4.46
3.78
3.46
3.19
3.18
3.14
3.13
3.13
3.12
3.04
3.01
2.99
2.98
2.95
2.95
-0.00
O
N
O
O
O
O
S
3m
1.84
1.93
1.93
2.29
2.17
2.14
0.96
3.00
1.07
1.17
1.06
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


208.27
168.79
167.18
159.81
134.27
130.30
130.03
127.86
126.71
124.98
123.66
123.56
114.03
67.85
63.44
55.40
48.81
37.21
O
N
O
O
O
O
S
3m
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

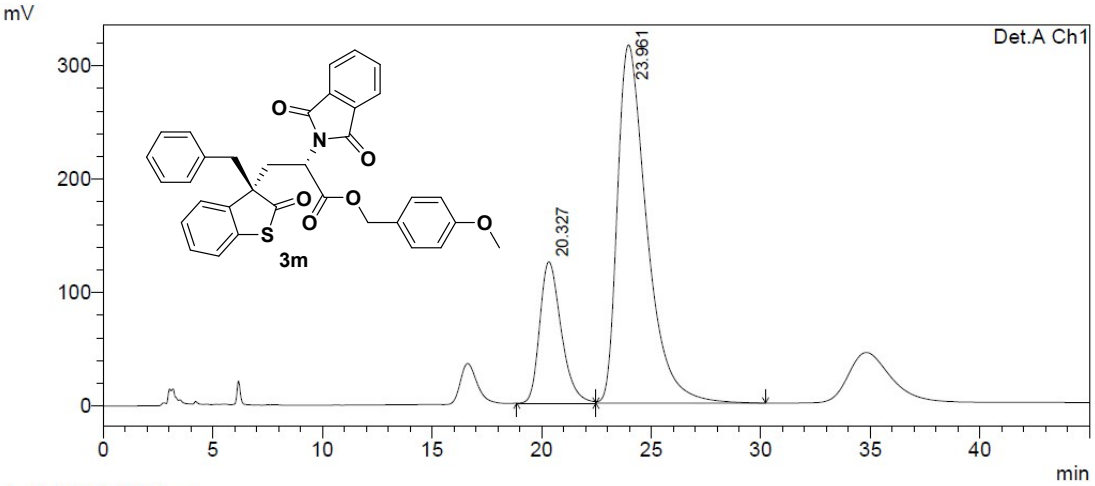


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.470	16912259	314508	26.804	39.098
2	20.429	14855531	208847	23.544	25.963
3	24.409	14813025	153525	23.477	19.085
4	34.797	16516362	127535	26.176	15.854
Total		63097176	804415	100.000	100.000

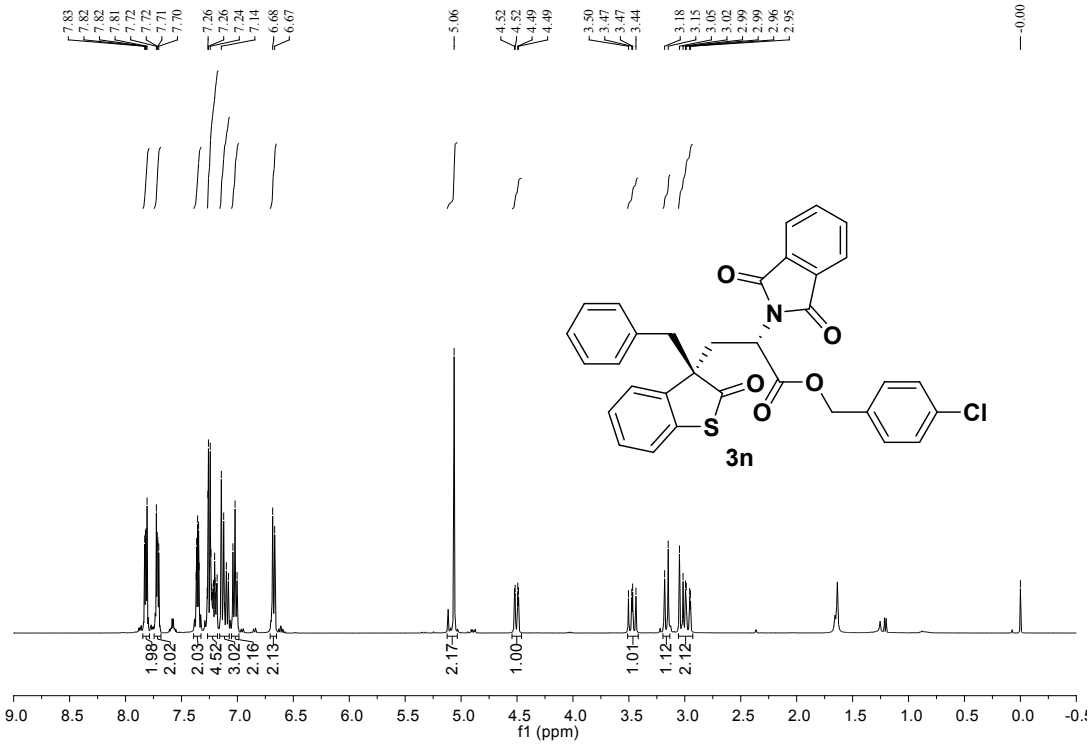


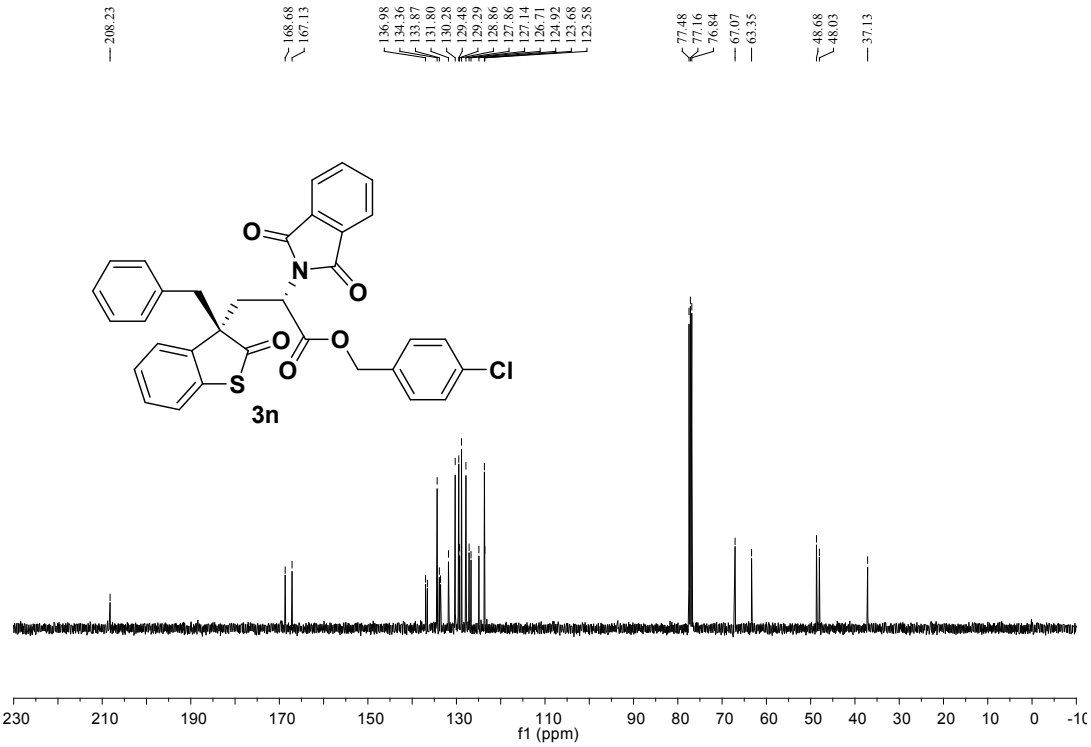
1 Det.A Ch1/210nm

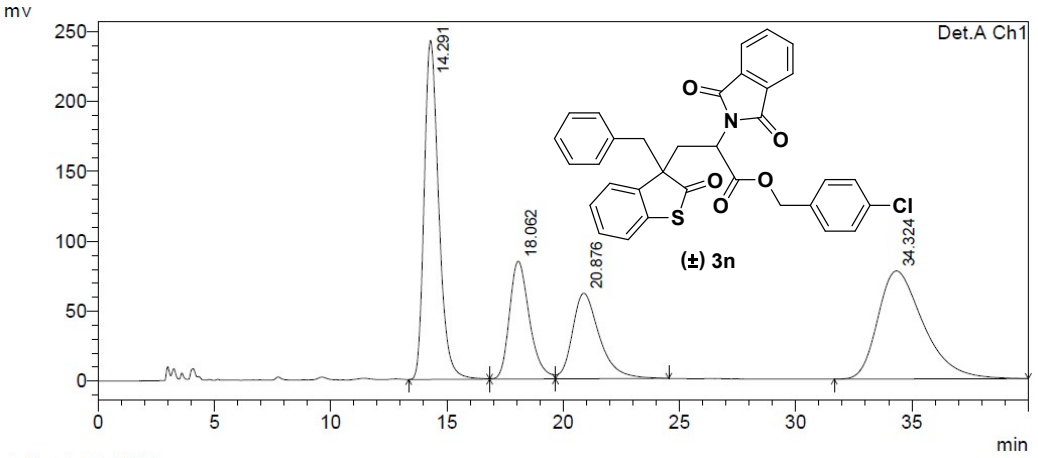
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.327	8512940	124714	22.370	28.306
2	23.961	29541795	315881	77.630	71.694
Total		38054735	440595	100.000	100.000


7.83
7.82
7.82
7.81
7.72
7.72
7.71
7.70
7.26
7.26
7.24
7.14
6.68
6.67
5.06
4.52
4.52
4.49
4.49
3.50
3.47
3.47
3.44
3.18
3.15
3.05
3.02
2.99
2.99
2.96
2.95
-0.00
1.98
2.02
2.03
4.52
3.02
2.16
2.13
2.17
1.00
1.01
1.12
2.12
O
N
O
O
O
O
S
Cl
3n
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


208.23
168.68
167.13
136.98
134.36
133.87
131.80
130.28
129.48
129.29
128.86
127.86
127.14
126.71
124.92
123.68
123.58
77.48
77.16
76.84
67.07
63.35
48.68
48.03
37.13
O
N
O
O
O
O
S
Cl
3n
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

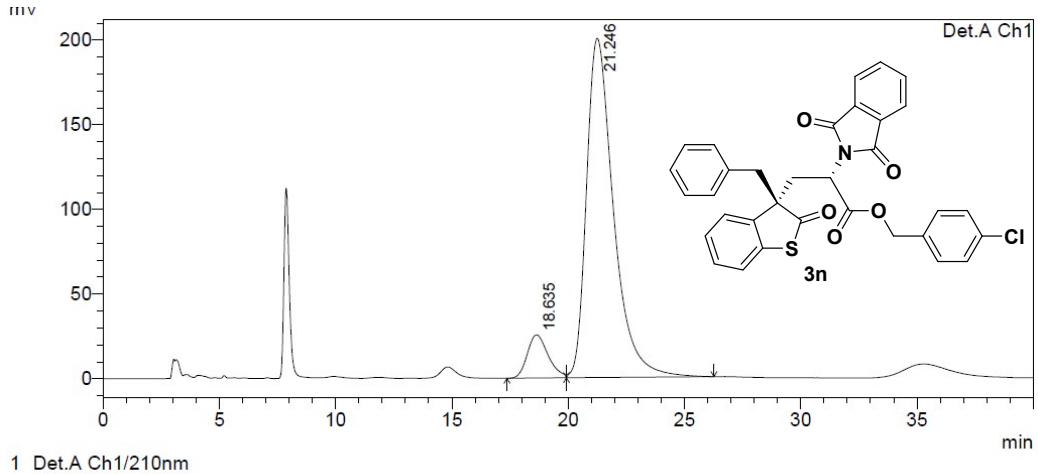


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.291	10534905	242536	33.927	52.118
2	18.062	5033719	84356	16.211	18.127
3	20.876	4948059	61175	15.935	13.146
4	34.324	10535177	77296	33.928	16.610
Total		31051859	465364	100.000	100.000

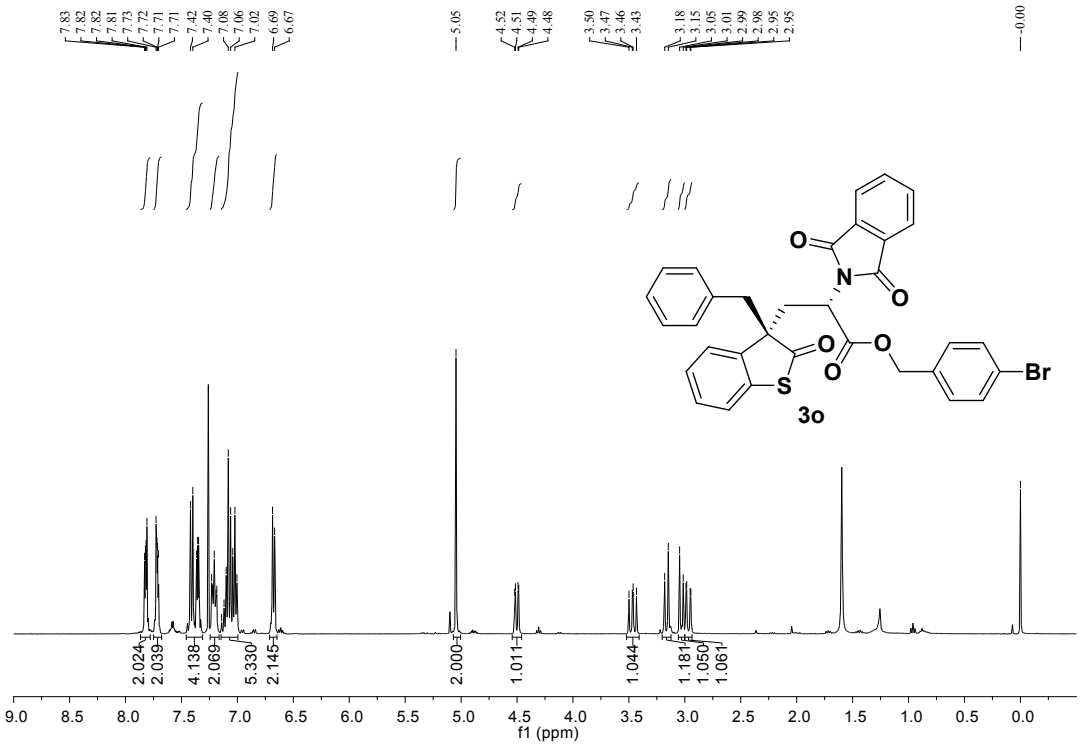


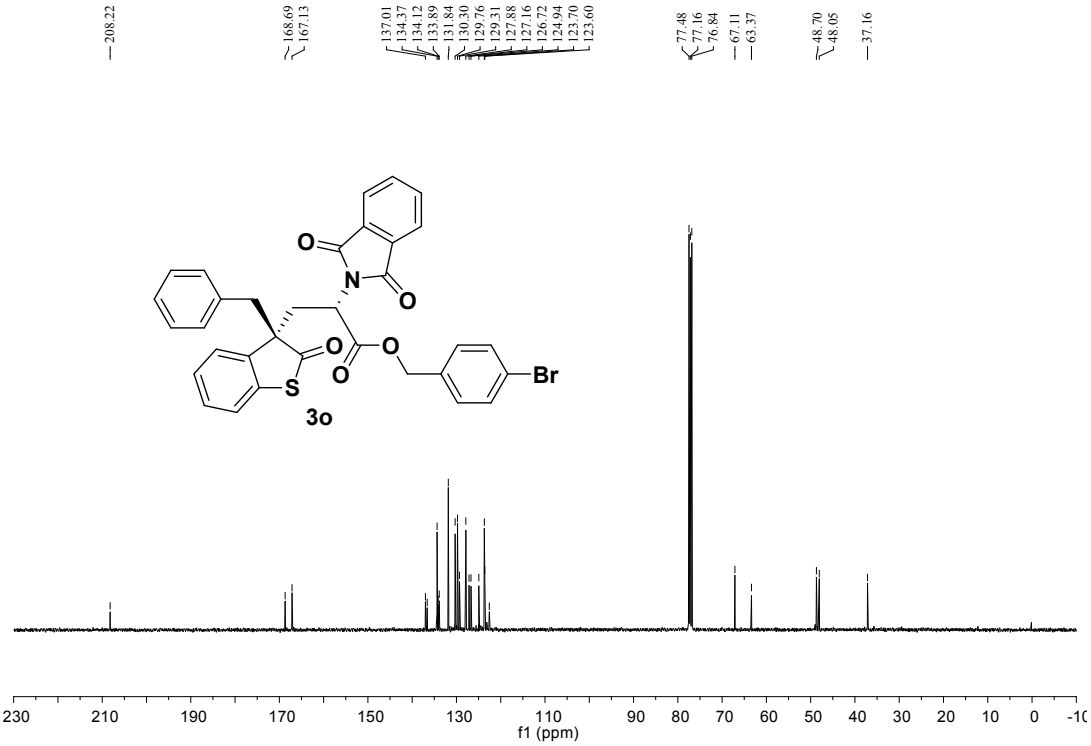
1 Det.A Ch1/210nm

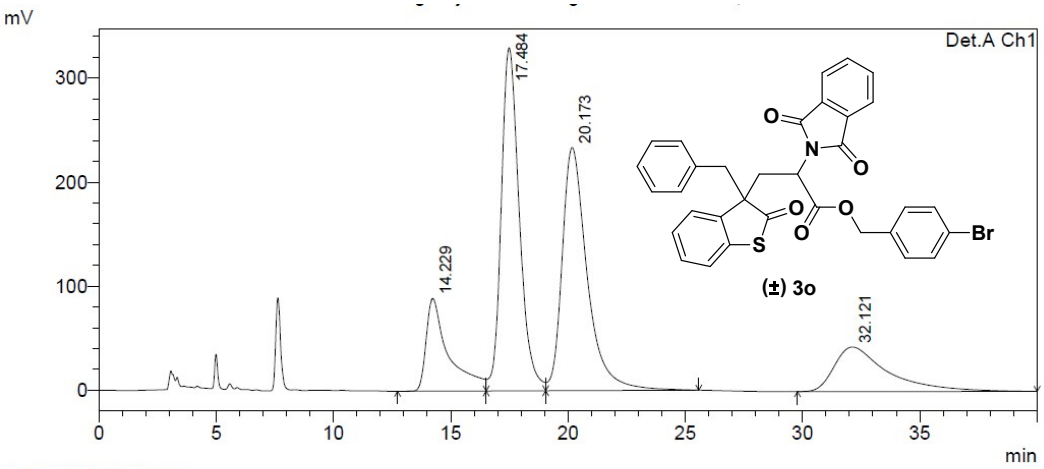
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.635	1582269	25542	8.889	11.305
2	21.246	16217467	200405	91.111	88.695
Total		17799735	225947	100.000	100.000


7.83
7.82
7.82
7.81
7.73
7.72
7.71
7.71
7.42
7.40
7.08
7.06
7.02
6.69
6.67
5.05
4.52
4.51
4.49
4.48
3.50
3.47
3.46
3.43
3.18
3.15
3.05
3.01
2.99
2.98
2.95
2.95
0.00
O
N
O
O
O
O
S
Br
3o
2.024
2.039
4.138
2.069
5.330
2.145
2.000
1.011
1.044
1.181
1.050
1.061
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


208.22
168.69
167.13
137.01
134.37
134.12
133.89
131.84
130.30
129.76
129.31
127.88
127.16
126.72
124.94
123.70
123.60
77.48
77.16
76.84
67.11
63.37
48.70
48.05
37.16
O
N
O
O
O
O
S
Br
3o
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

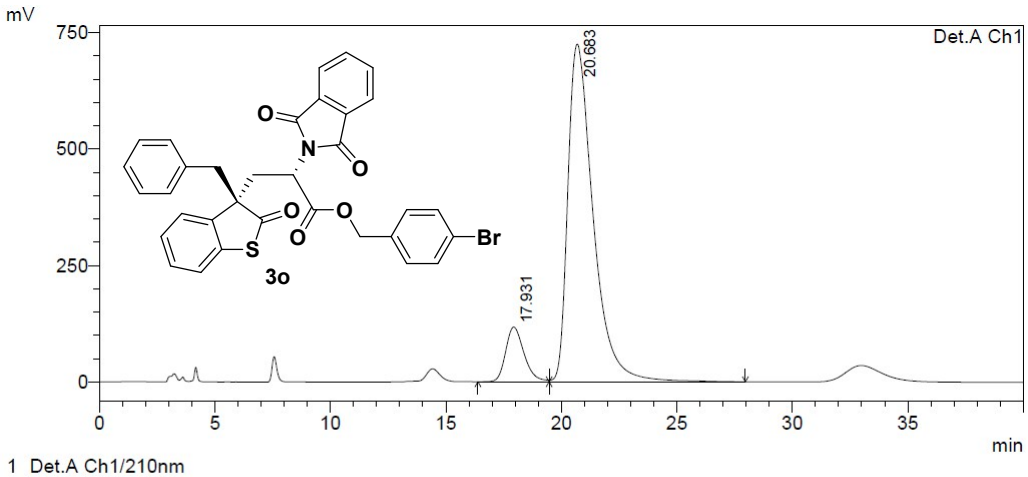


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.229	5929856	89258	12.417	12.832
2	17.484	17668767	329762	36.997	47.409
3	20.173	17360607	233680	36.352	33.596
4	32.121	6797754	42867	14.234	6.163
Total		47756983	695567	100.000	100.000

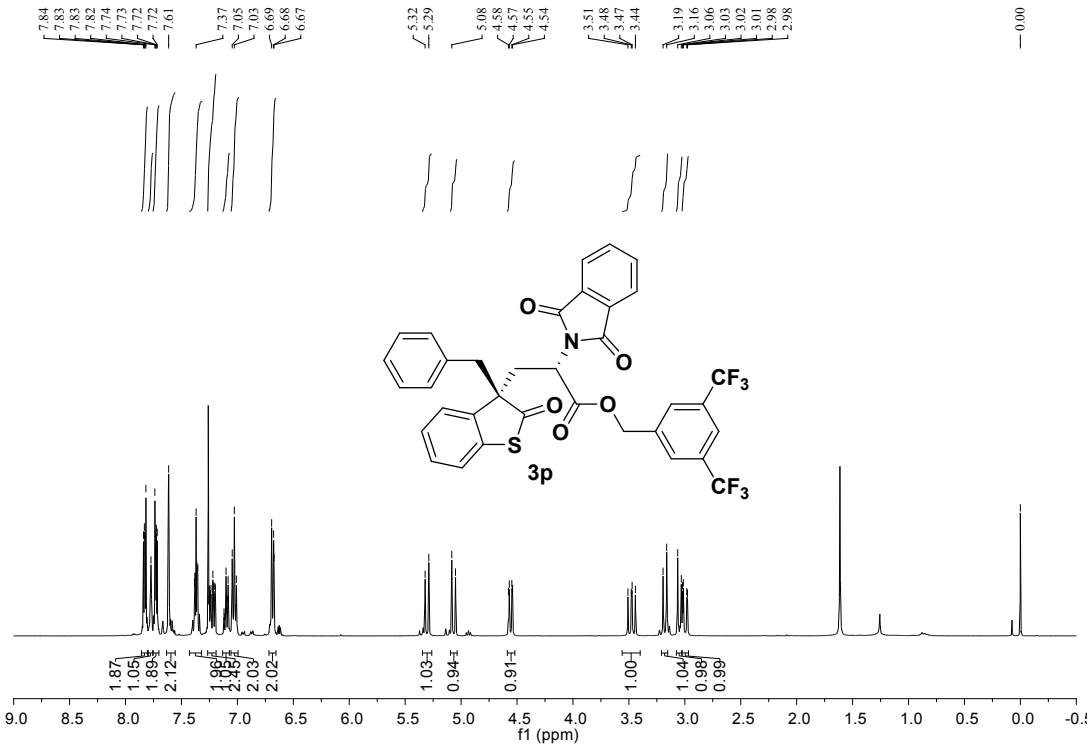


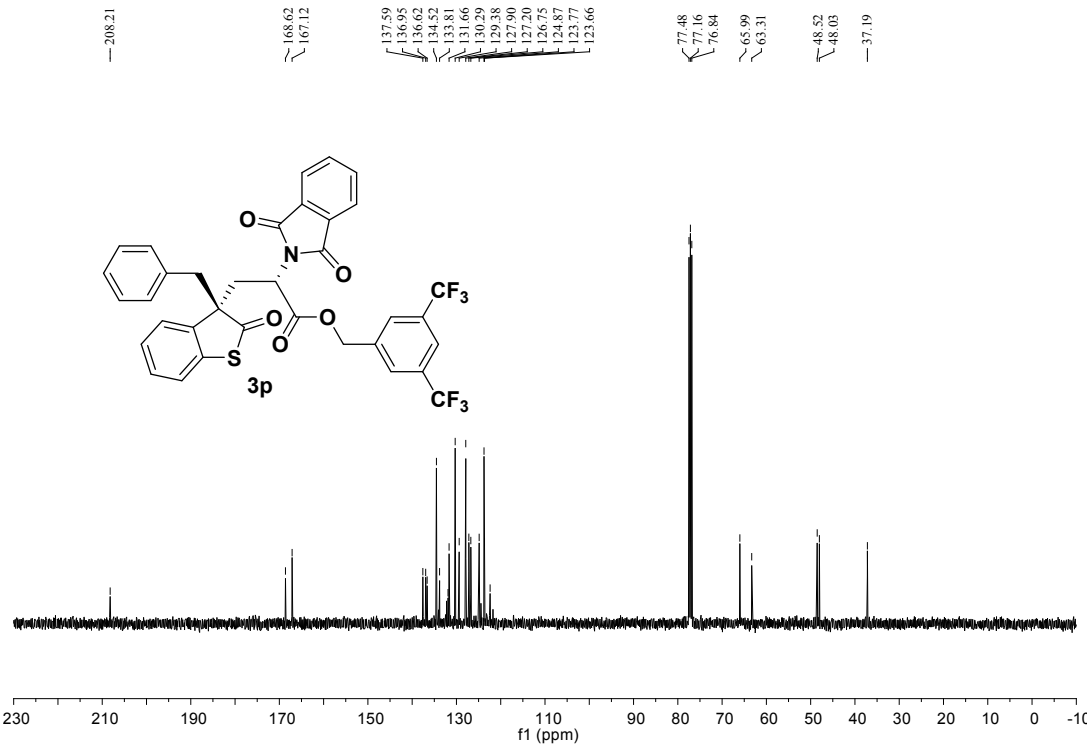
1 Det.A Ch1/210nm

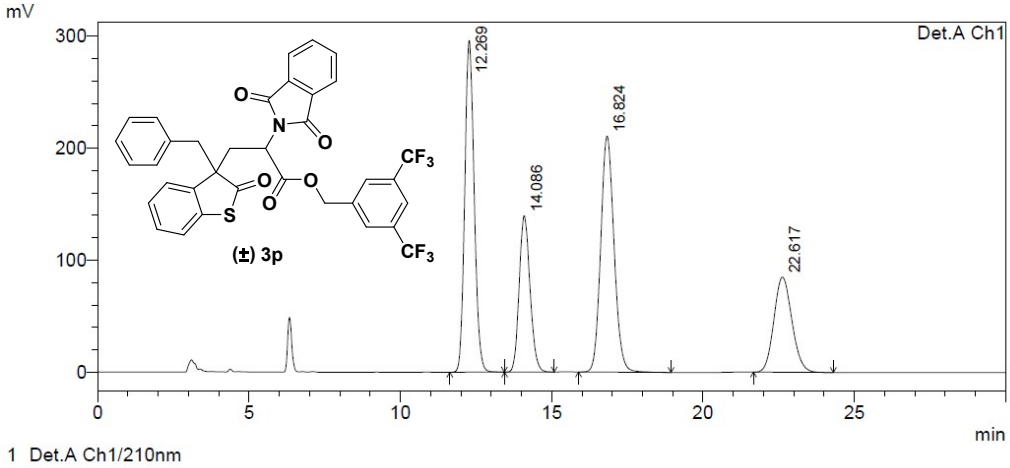
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.931	6513397	117469	10.536	13.946
2	20.683	55308554	724833	89.464	86.054
Total		61821950	842302	100.000	100.000


7.84
7.83
7.83
7.82
7.74
7.73
7.72
7.72
7.61
7.37
7.05
7.03
6.69
6.68
6.67
5.32
5.29
5.08
4.58
4.57
4.55
4.54
3.51
3.48
3.47
3.44
3.19
3.16
3.06
3.03
3.02
3.01
2.98
2.98
0.00
O
N
O
O
O
O
O
S
CF3
CF3
3p
1.87
1.05
1.89
2.12
1.96
2.45
2.03
2.02
1.03
0.94
0.91
1.00
1.04
0.98
0.99
f1 (ppm)

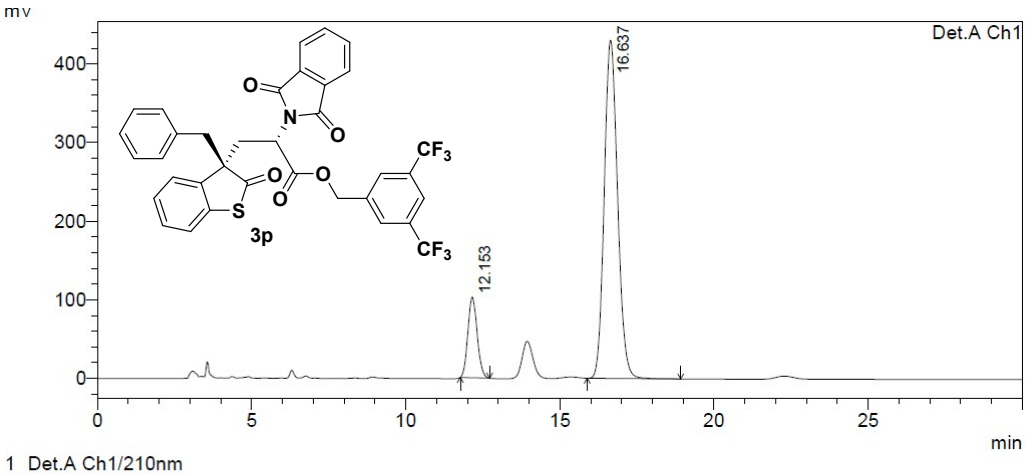

208.21
168.62
167.12
137.59
136.95
136.62
134.52
133.81
131.66
130.29
129.38
127.90
127.20
126.75
124.87
123.77
123.66
77.48
77.16
76.84
65.99
63.31
48.52
48.03
37.19
O
N
O
O
O
O
O
S
CF3
CF3
3p
f1 (ppm)



PeakTable

Detector A Ch1 210nm

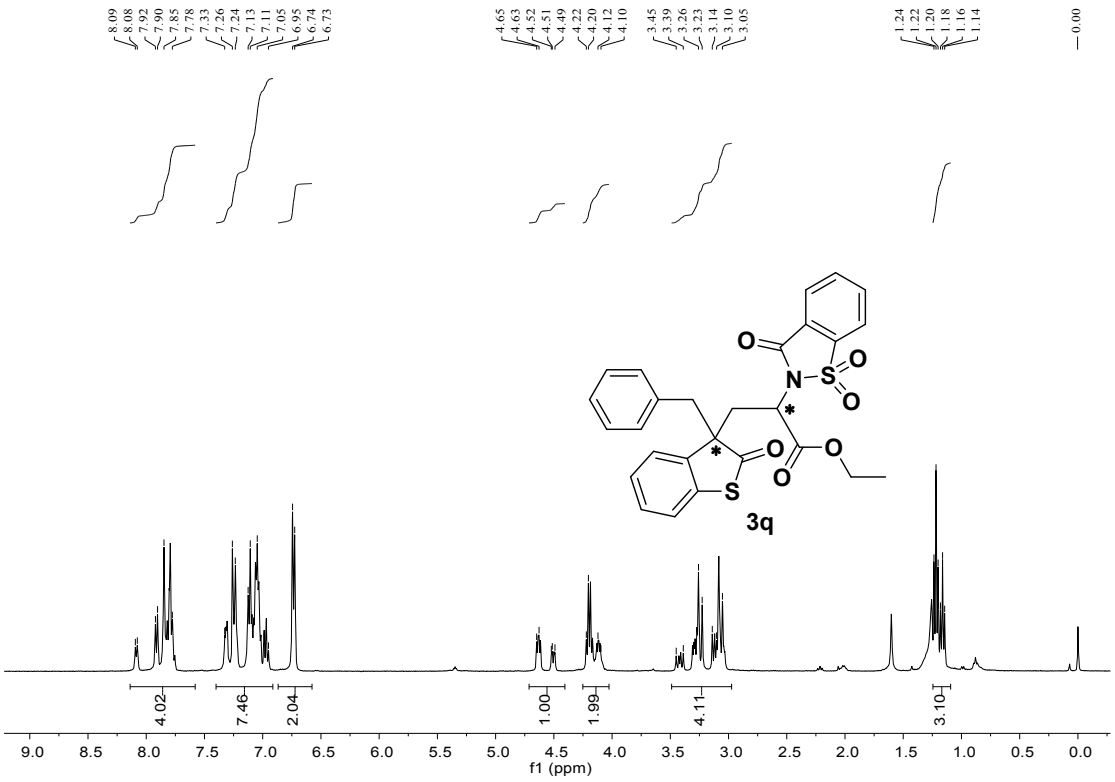
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.269	6440749	296399	32.366	40.496
2	14.086	3486416	139614	17.520	19.075
3	16.824	6451274	210833	32.419	28.805
4	22.617	3521052	85082	17.694	11.624
Total		19899491	731928	100.000	100.000

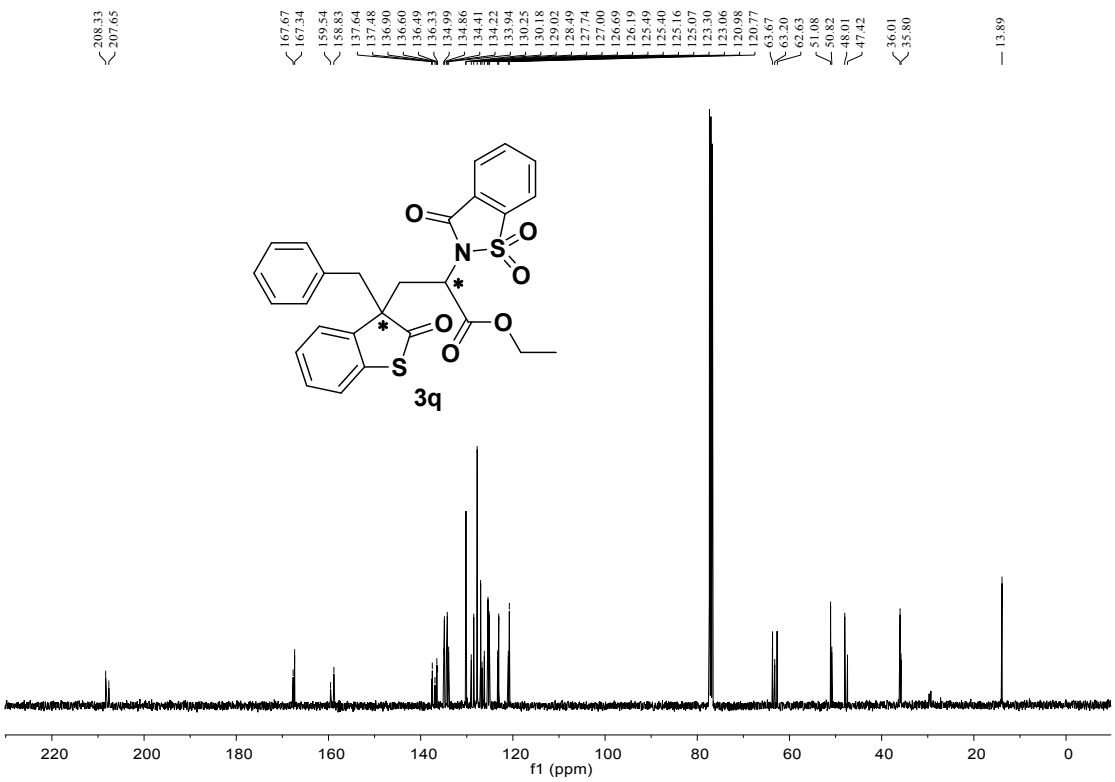


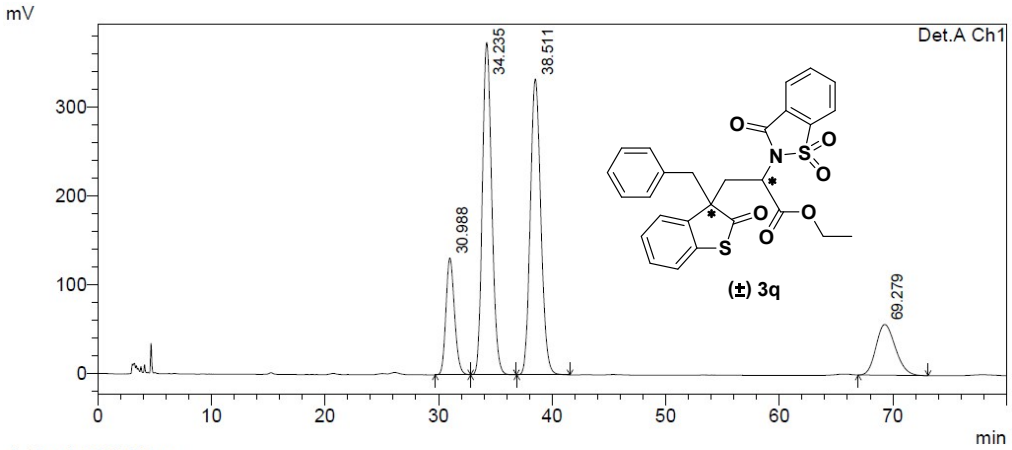
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.153	2158412	102633	14.277	19.257
2	16.637	12959555	430319	85.723	80.743
Total		15117968	532952	100.000	100.000


8.09
8.08
7.92
7.90
7.85
7.78
7.33
7.26
7.24
7.13
7.11
7.05
6.95
6.74
6.73
4.65
4.63
4.52
4.51
4.49
4.22
4.20
4.12
4.10
3.45
3.39
3.26
3.23
3.14
3.10
3.05
1.24
1.22
1.20
1.18
1.16
1.14
0.00
3q
4.02
7.46
2.04
1.00
1.99
4.11
3.10
f1 (ppm)


208.33
207.65
167.67
167.34
159.54
158.83
137.64
137.48
136.90
136.60
136.49
136.33
134.99
134.86
134.41
134.22
133.94
130.25
130.18
129.02
128.49
127.74
127.00
126.69
126.19
125.49
125.40
125.16
125.07
123.30
123.06
120.98
120.77
63.67
63.20
62.63
51.08
50.82
48.01
47.42
36.01
35.80
13.89
3q
f1 (ppm)

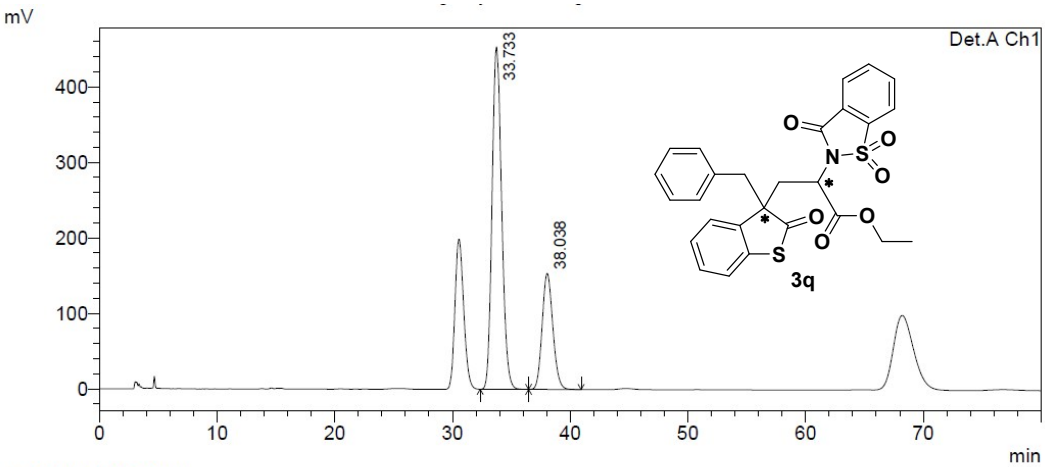


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.988	6918482	131615	12.186	14.681
2	34.235	21516957	374384	37.899	41.761
3	38.511	21559176	333361	37.973	37.185
4	69.279	6779754	57129	11.942	6.372
Total		56774369	896489	100.000	100.000

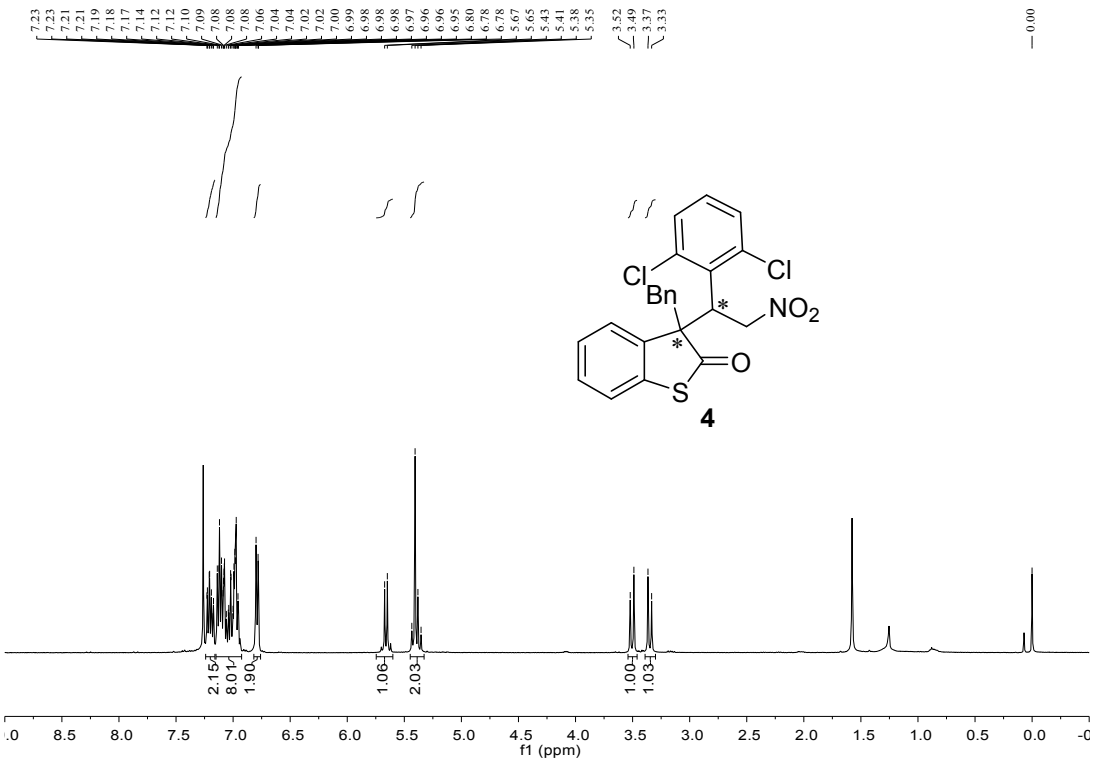


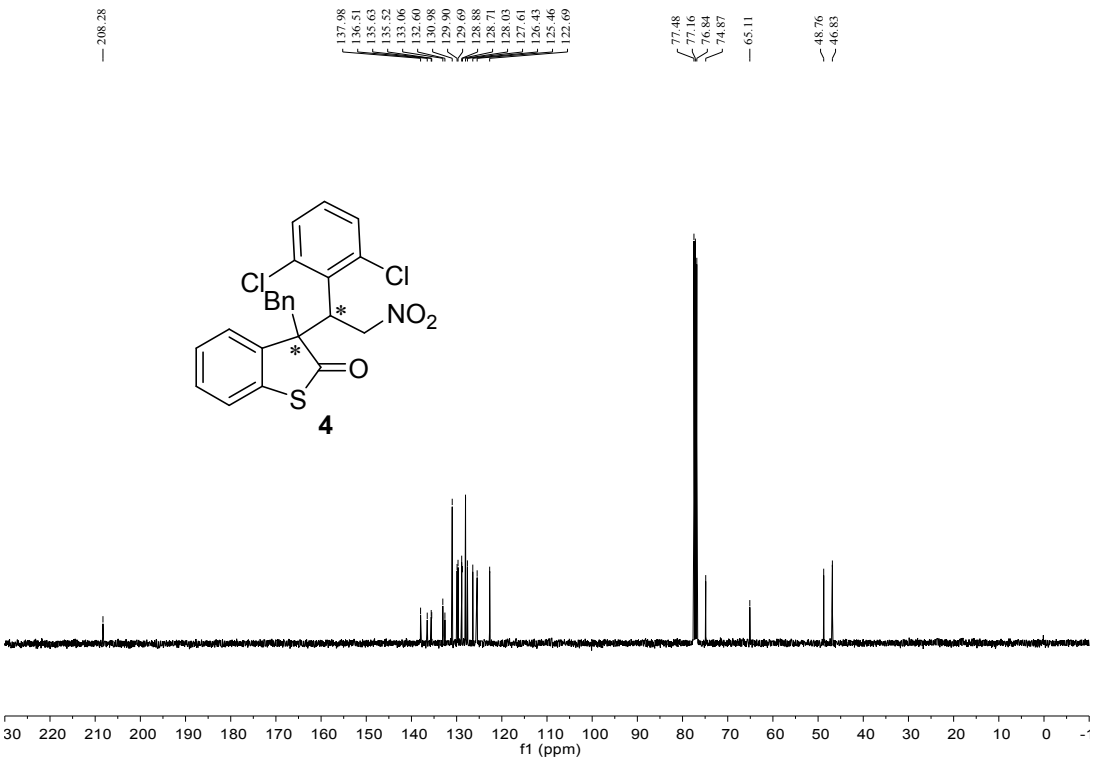
1 Det.A Ch1/210nm

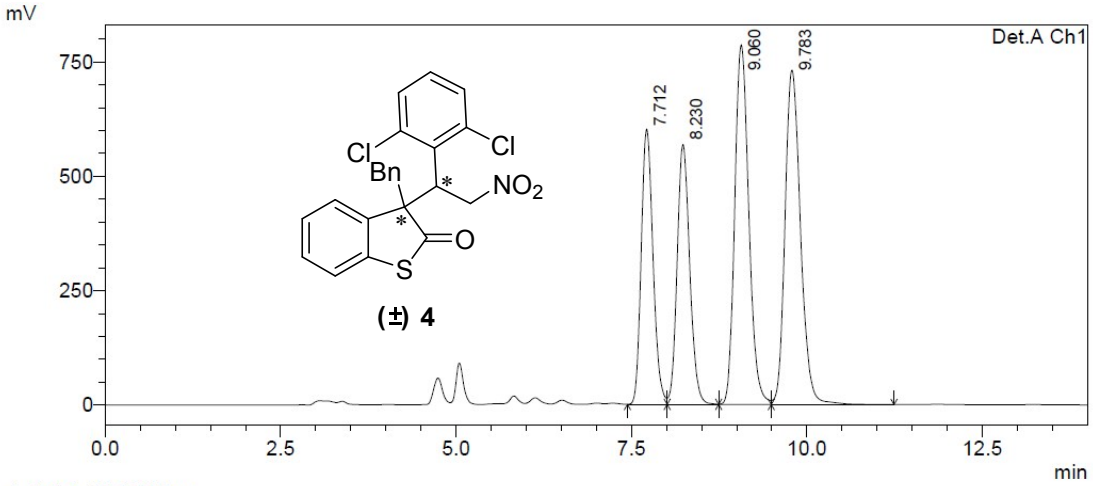
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	33.733	25772137	453588	72.577	74.688
2	38.038	9737852	153723	27.423	25.312
Total		35509989	607311	100.000	100.000


Cl
Cl
Bn
NO2
O
S
4
2.15
8.01
1.90
1.06
2.03
1.00
1.03
f1 (ppm)


Cl
Cl
Bn
NO2
O
S
4
f1 (ppm)

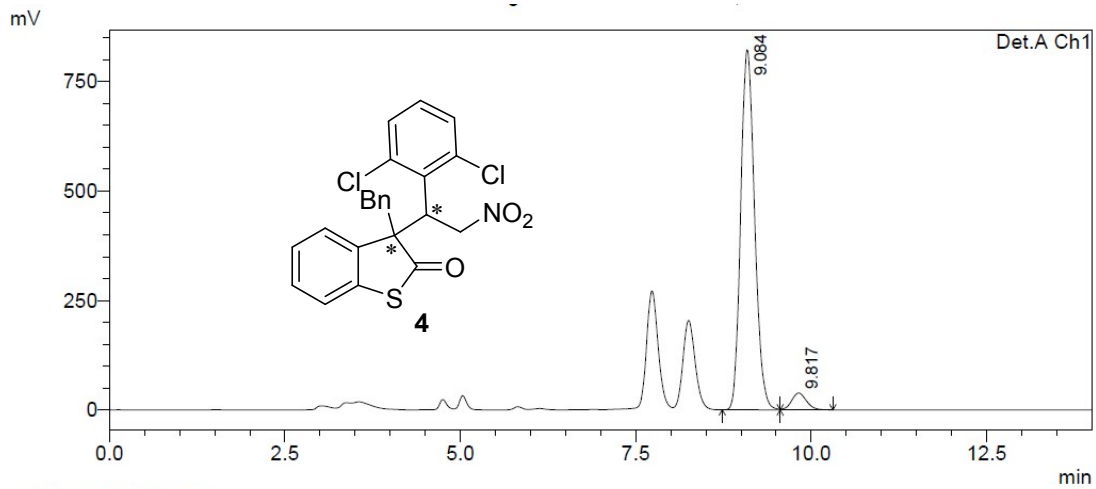


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.712	7019454	602131	19.340	22.406
2	8.230	7083704	568333	19.517	21.148
3	9.060	10964552	786239	30.209	29.257
4	9.783	11227939	730648	30.935	27.188
Total		36295649	2687352	100.000	100.000

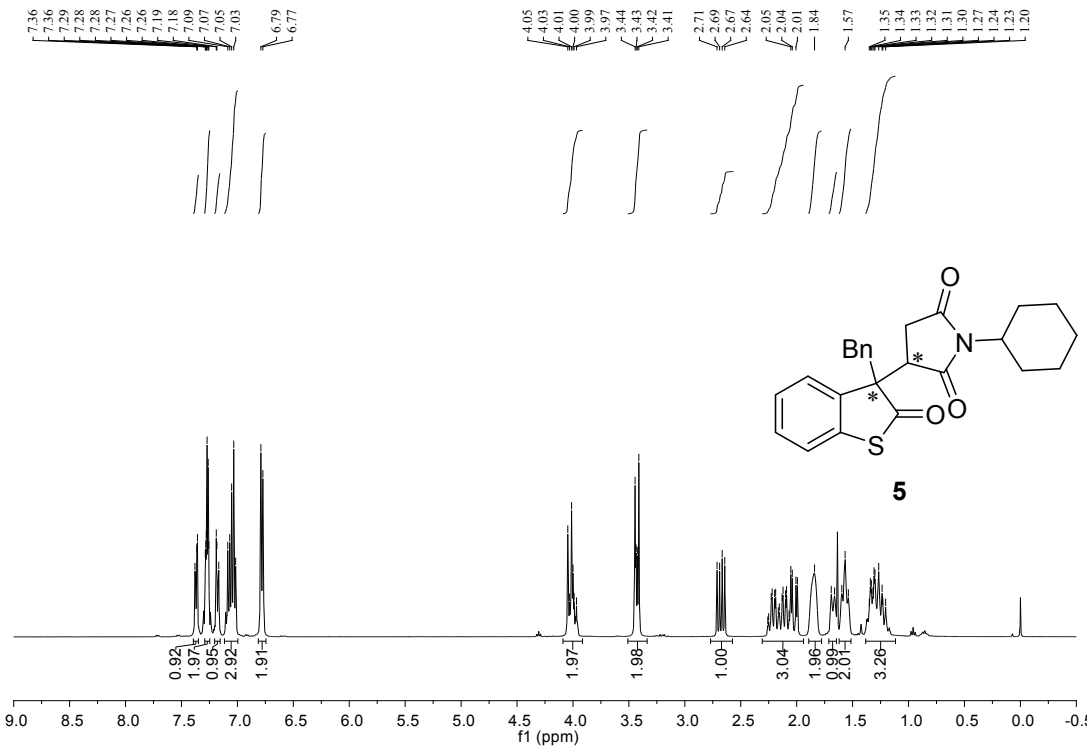


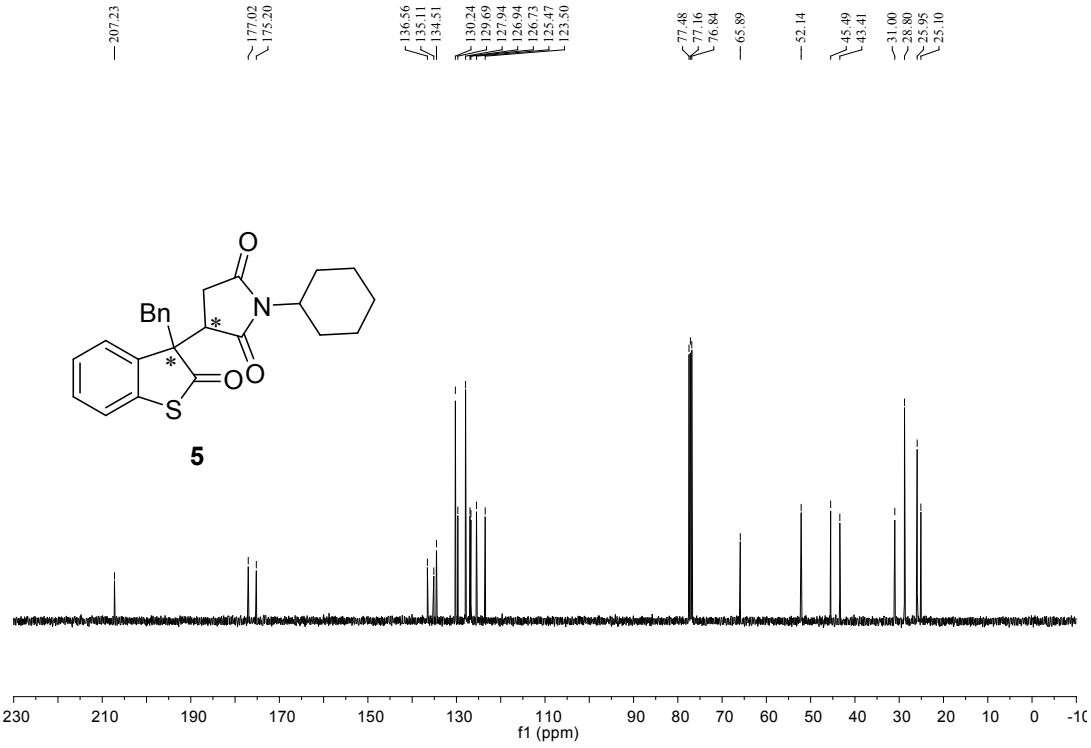
1 Det.A Ch1/210nm

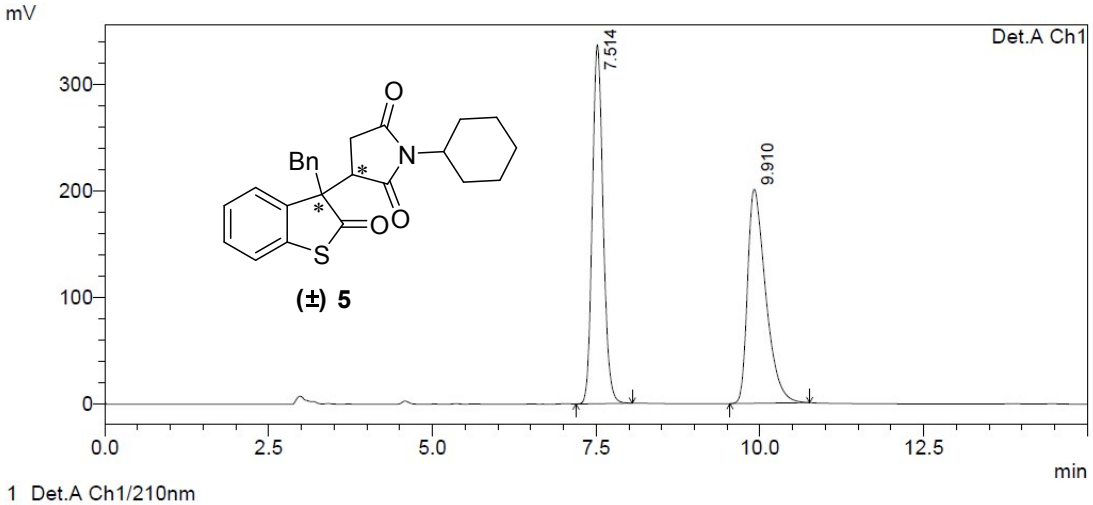
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.084	11361376	822062	95.280	95.520
2	9.817	562828	38553	4.720	4.480
Total		11924204	860615	100.000	100.000


7.36
7.36
7.29
7.28
7.28
7.27
7.26
7.26
7.19
7.18
7.09
7.07
7.05
7.03
6.79
6.77
4.05
4.03
4.01
4.00
3.99
3.97
3.44
3.43
3.42
3.41
2.71
2.69
2.67
2.64
2.05
2.04
2.01
1.84
1.57
1.35
1.34
1.33
1.32
1.31
1.30
1.27
1.24
1.23
1.20
Bn
N
O
S
5
0.92
1.97
0.95
2.92
1.91
1.97
1.98
1.00
3.04
1.96
0.99
2.01
3.26
f1 (ppm)


207.23
177.02
175.20
136.56
135.11
134.51
130.24
129.69
127.94
126.94
126.73
125.47
123.50
77.48
77.16
76.84
65.89
52.14
45.49
43.41
31.00
28.80
25.95
25.10
Bn
N
O
S
5
f1 (ppm)

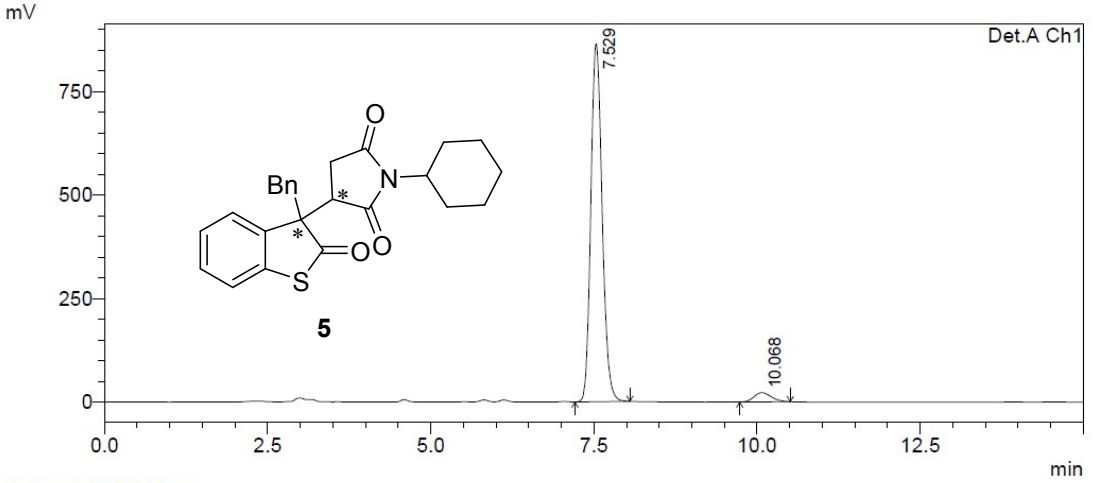


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.514	3864000	336732	49.942	62.649
2	9.910	3873010	200759	50.058	37.351
Total		7737010	537491	100.000	100.000

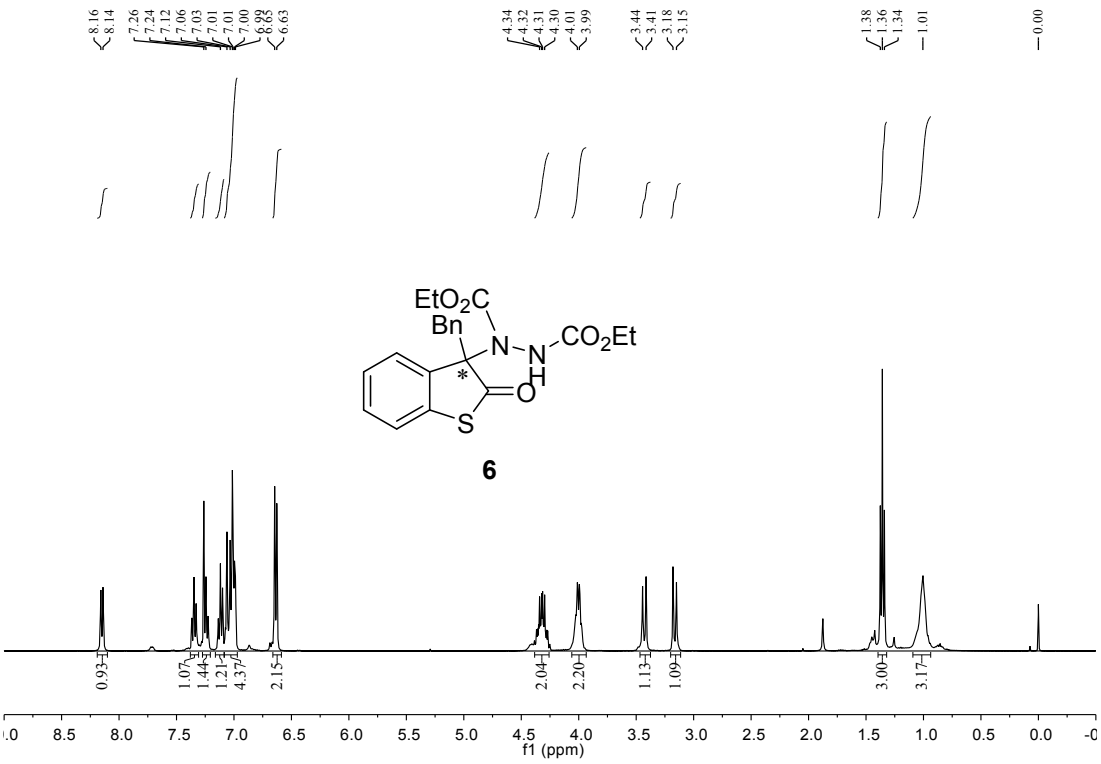


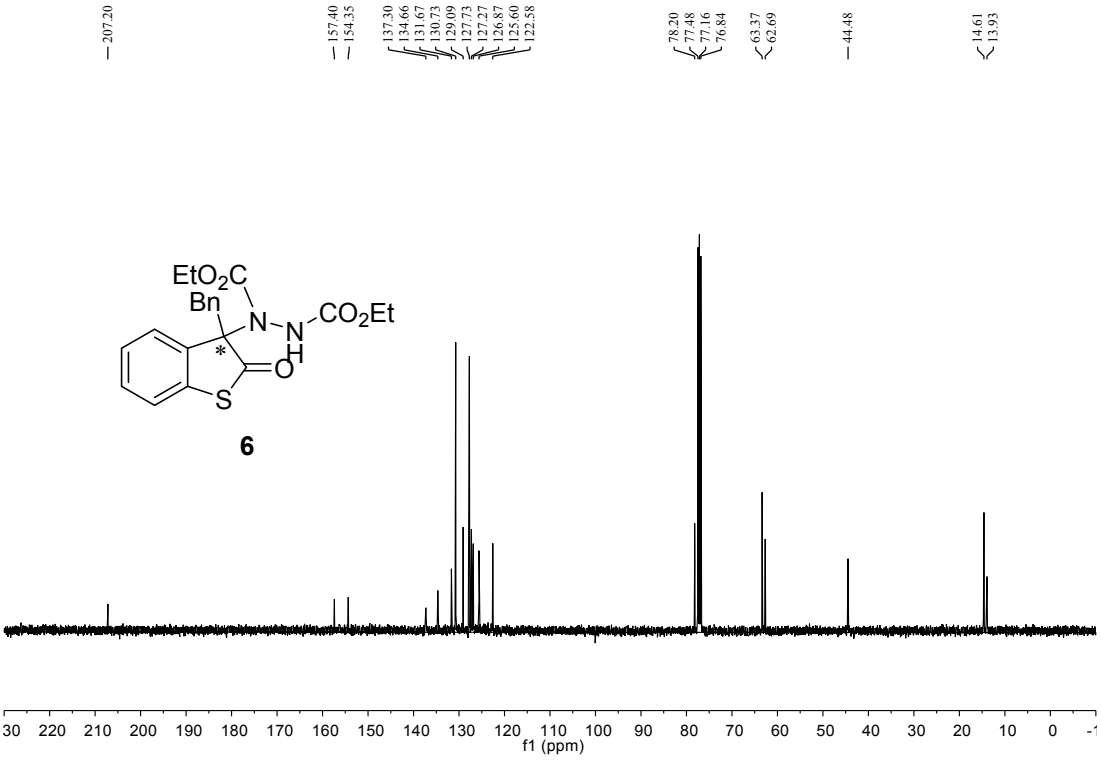
1 Det.A Ch1/210nm

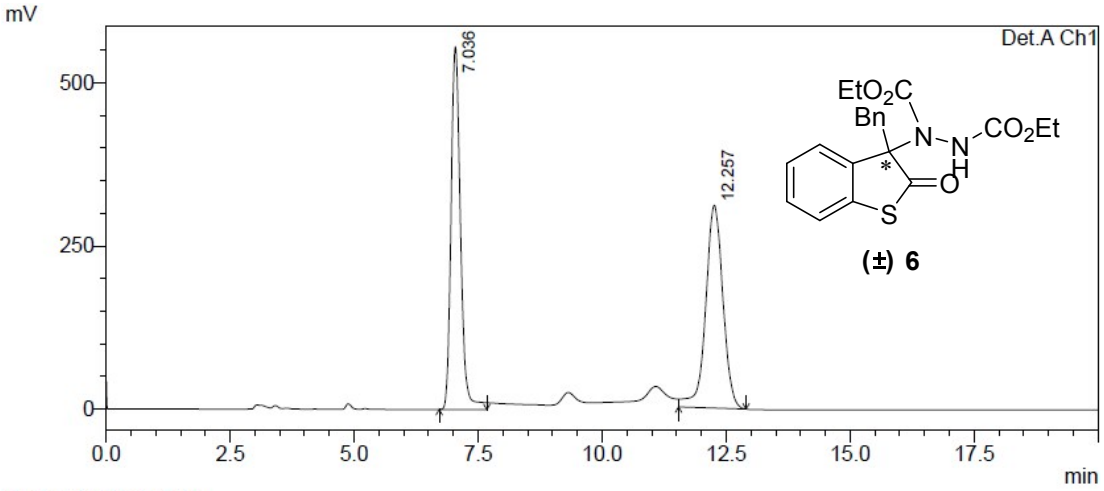
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.529	10435033	865075	96.223	97.479
2	10.068	409620	22369	3.777	2.521
Total		10844653	887444	100.000	100.000


8.16
8.14
7.26
7.24
7.12
7.06
7.03
7.01
7.01
7.00
6.65
6.63
4.34
4.32
4.31
4.30
4.01
3.99
3.44
3.41
3.18
3.15
1.38
1.36
1.34
1.01
0.00
EtO2C
Bn
N
N
CO2Et
H
O
S
*
6
0.93
1.07
1.44
1.21
4.37
2.15
2.04
2.20
1.13
1.09
3.00
3.17
f1 (ppm)


207.20
157.40
154.35
137.30
134.66
131.67
130.73
129.09
127.73
127.27
126.87
125.60
122.58
78.20
77.48
77.16
76.84
63.37
62.69
44.48
14.61
13.93
EtO2C
Bn
N
N
CO2Et
H
O
S
*
6
f1 (ppm)

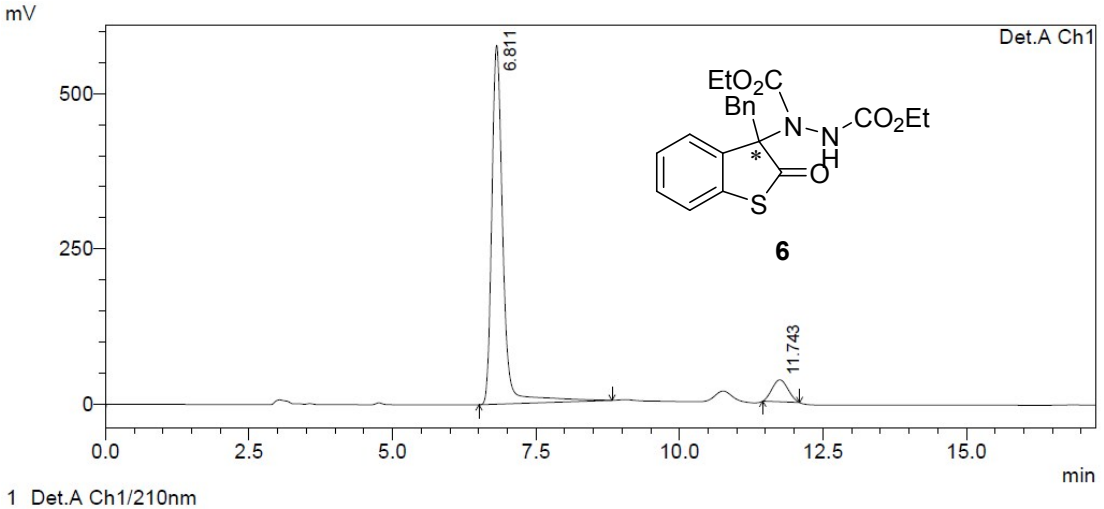


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.036	7407177	557024	49.482	64.156
2	12.257	7562316	311204	50.518	35.844
Total		14969493	868227	100.000	100.000

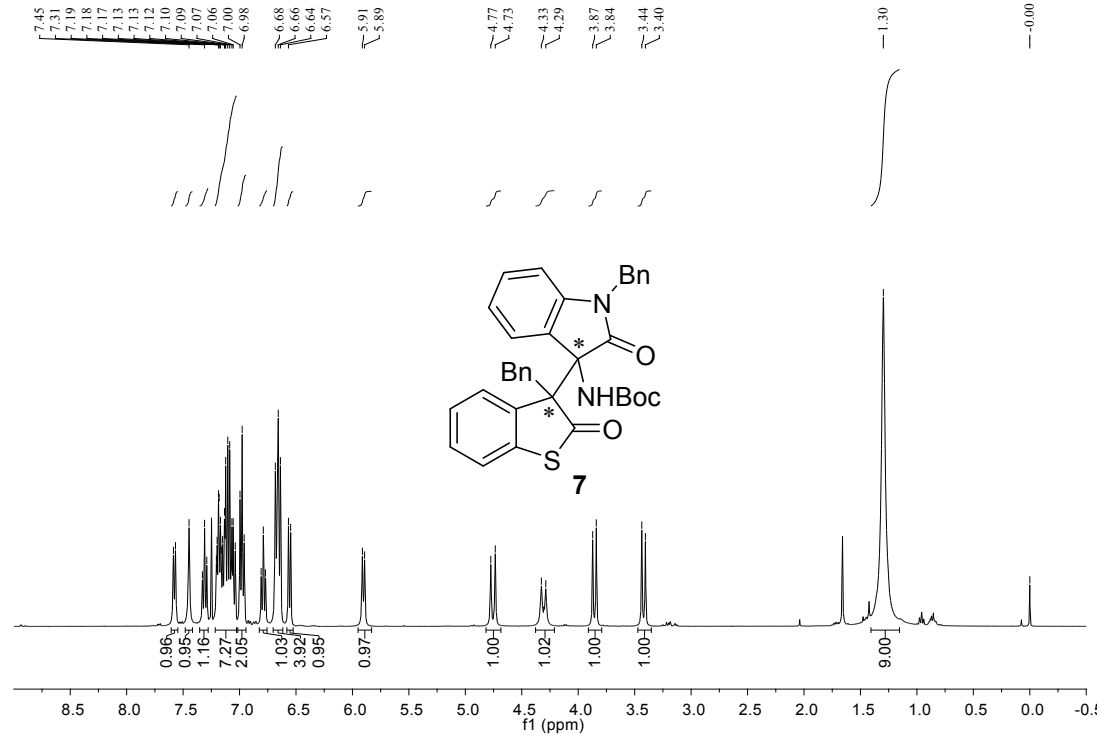


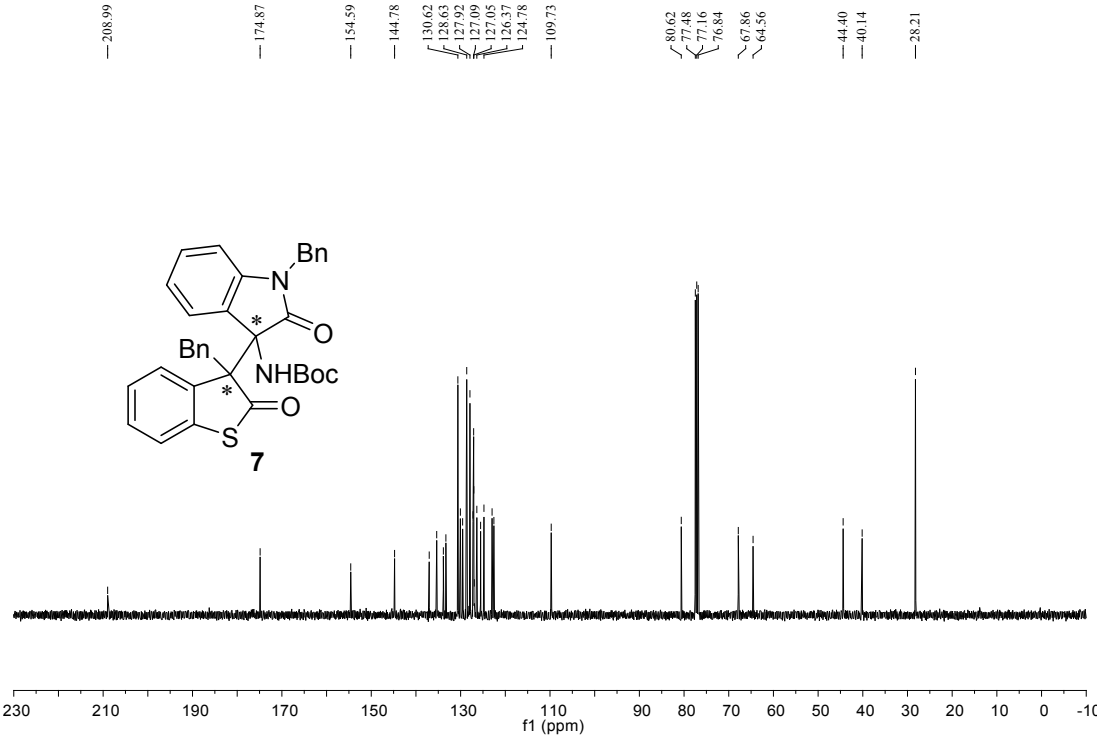
1 Det.A Ch1/210nm

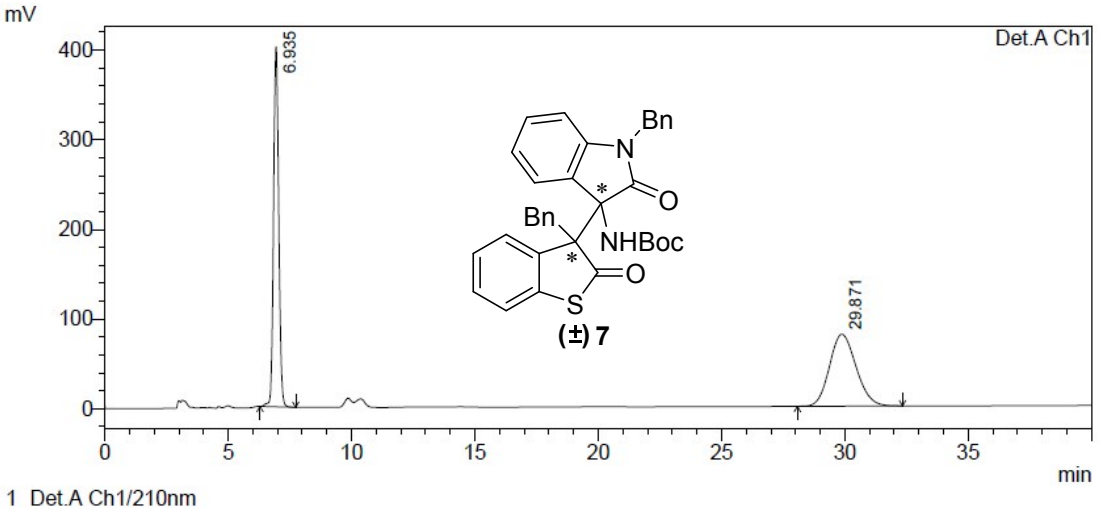
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.811	7856815	577791	92.031	94.240
2	11.743	680288	35316	7.969	5.760
Total		8537103	613107	100.000	100.000


7.45
7.31
7.19
7.18
7.17
7.13
7.13
7.12
7.10
7.09
7.07
7.06
7.00
6.98
6.68
6.66
6.64
6.57
5.91
5.89
4.77
4.73
4.33
4.29
3.87
3.84
3.44
3.40
1.30
-0.00
Bn
N
O
*
Bn
NHBoc
*
O
S
7
0.96
0.95
1.16
7.27
2.05
1.03
3.92
0.95
0.97
1.00
1.02
1.00
1.00
9.00
f1 (ppm)


208.99
174.87
154.59
144.78
130.62
128.63
127.92
127.09
127.05
126.37
124.78
109.73
80.62
77.48
77.16
76.84
67.86
64.56
44.40
40.14
28.21
Bn
N
O
*
Bn
NHBoc
*
O
S
7
f1 (ppm)

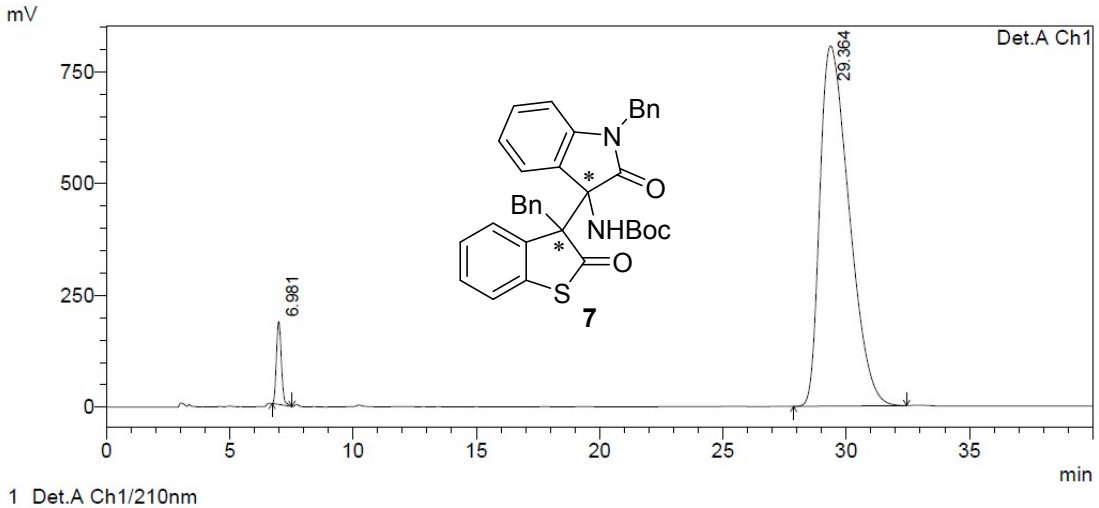


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.935	5858522	401600	49.355	83.342
2	29.871	6011575	80272	50.645	16.658
Total		11870097	481872	100.000	100.000



1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.981	2605131	185847	3.773	18.741
2	29.364	66440975	805813	96.227	81.259
Total		69046106	991660	100.000	100.000