Supporting Information for:

Copper-Catalyzed Enantioselective Carbenoid Insertion into S–H Bonds

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General. All reactions and manipulations were performed using standard Schlenk techniques. THF was distilled from sodium benzophenone ketyl. CH_2Cl_2, $CHCl_3$, DCE were distilled over CaH_2 under nitrogen atmosphere. CuCl and $CuPF_6(MeCN)_4$ were prepared according to the literature procedure.[1] Spirobox ligands [2] were prepared according to the previous procedure. Mercaptans, $CuBr_2$ and $Cu(OTf)_2$ were purchased from Aldrich and used directly. NMR spectra were recorded with a Bruker AV 300 spectrometer at 300/400 MHz (^{1}H NMR), 75/100 MHz (^{13}C NMR) or a Varian Mercury Plus 400 spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR). Chemical shifts were reported in ppm down field from internal Me_4Si. Optical rotations were measured using a Perkin Elmer Model 341 polarimeter. HRMS were recorded on IonSpec FT-ICR mass spectrometer with ESI resource. HPLC analyses were performed on a Hewlett Packard Model HP 1100 Series or Waters 2996 chromatography. SFC (Super Fluent Chromatography) analyses were performed on Agilent 1200 Series.

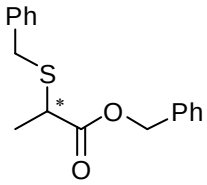
[1] R. N. Keller, H. Wycoff, D. *Inorg. Synth.* **1946**, *2*, 1–4.
[2] B. Liu, S.-F. Zhu, W. Zhang, C. Chen, Q.-L. Zhou, *J. Am. Chem. Soc.* **2007**, *129*, 5834–5835.

1. Typical Procedure for Cu-Catalyzed S–H Insertion

A solution of CuCl (1.0 mg, 0.01 mmol, 5 mol%), $NaBAr_F$ (11.3 mg, 0.012 mmol, 6 mol%) and (S_a,*S*,*S*)-**4a** (6.1 mg, 0.012 mmol, 6 mol%) in $CHCl_3$ (2 mL) was stirred for 2 hours under an argon atmosphere. The solution was heated to 80 ^oC, mercaptan (0.2 mmol, 1 equiv.) and diazo compound (0.2 mmol, 1 equiv.) were added subsequently. The resulting solution was stirred at 80 ^oC for 0.5~2 hours until the diazo compound disappeared. The product was purified by flash chromatography with ethyl acetate/petroleum ether (1:20, v/v).

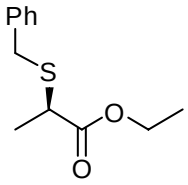
2. Analytical Data for S–H Insertion Products

(+)-benzyl 2-(benzylthio)propionate (3a)



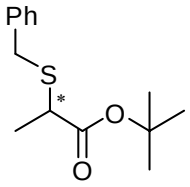
Colorless oil; 82% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39–7.22 (m, 10H), 5.18 (d, *J* = 12.4 Hz, 1H), 5.12 (d, *J* = 12.4 Hz, 1H), 3.79 (d, *J* = 12.4 Hz, 1H), 3.73(d, *J* = 12.4 Hz, 1H), 3.32 (q, *J* = 7.2 Hz, 1H), 1.40 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 137.5, 135.8, 129.1, 128.6, 128.5, 128.4, 128.3, 127.2, 66.8, 40.4, 35.9, 16.9; HRMS (ESI) Calcd for $(C_{17}H_{18}O_2S + Na)^+$: 309.0920, Found 309.0925; 81% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 14.28 min for major isomer, t_R = 15.47 min for minor isomer]; $[\alpha]_D^{20}$ = +170.6 (*c* 1.0, MeOH).

(*R*)-ethyl 2-(benzylthio)propionate (3b) [3]



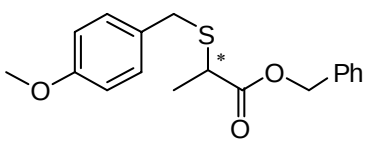
Colorless oil; 91% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28–7.15 (m, 5H), 4.16–4.05 (m, 2H), 3.80 (d, *J* = 13.2 Hz, 1H), 3.72 (d, *J* = 13.2 Hz, 1H), 3.21 (q, *J* = 7.2 Hz, 2H), 1.31 (d, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H); 73 % ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 7.78 min for minor isomer, t_R = 8.79 min for major isomer]; $[\alpha]_D^{20}$ = +170.6 (*c* 1.0, MeOH), $[\alpha]_D^{30}$ = +146.7 (*c* 1.0, CH_2Cl_2) [lit: $[\alpha]_D^{20}$ = +228 (*c* 1.0, CH_2Cl_2) for (*R*) with 95% ee].

(+)-*tert*-butyl 2-(benzylthio)propionate (3c)



Colorless oil; 62% yield; ^1H NMR (300 MHz, $CDCl_3$) δ 7.36–7.22 (m, 5H), 3.88 (d, *J* = 13.2 Hz, 1H), 3.78 (d, *J* = 13.2 Hz, 1H), 3.17 (q, *J* = 7.2 Hz, 1H), 1.56 (s, 9H), 1.33 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.3, 137.8, 129.1, 128.5, 127.1, 81.2, 41.2, 35.9, 28.1, 16.9; HRMS (ESI) Calcd for $(C_{14}H_{20}O_2S + Na)^+$: 275.1076, Found 275.1073; 83% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 4.75 min for minor isomer, t_R = 5.36 min for major isomer]; $[\alpha]_D^{20}$ = +215.8 (*c* 1.0, MeOH).

(+)-benzyl 2-(4-methoxybenzylthio)propionate (3d)

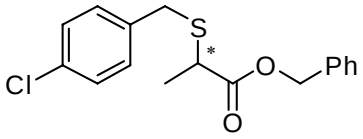


Colorless oil; 73% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39–7.33 (m, 5H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 5.20 (d, *J* = 12.4 Hz, 1H), 5.13 (d, *J* = 12.4 Hz, 1H),

[3] A. M. Ponce, L. E. Overman, *J. Am. Chem. Soc.* **2000**, *122*, 8672–8676.

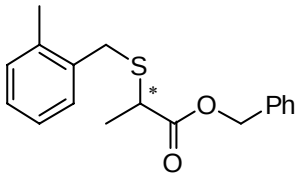
3.79–3.67 (m, 5H), 3.32 (q, J = 7.2 Hz, 1H), 1.40 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 158.7, 135.9, 130.2, 129.4, 128.6, 128.4, 128.3, 113.9, 66.8, 55.3, 40.3, 35.3, 16.9; HRMS (ESI) Calcd for $(C_{18}H_{20}O_3S + Na)^+$: 339.1025, Found 339.1022; 85% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 34.12 min for major isomer, t_R = 38.73 min for minor isomer]; $[\alpha]_D^{20}$ = +167.6 (*c* 1.0, MeOH).

(+)-benzyl 2-(4-chlorobenzylthio)propionate (3e)



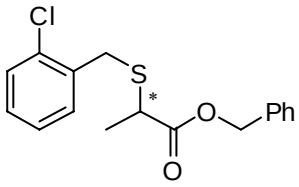
Colorless oil; 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.26 (m, 5H), 7.17–7.07 (m, 4H), 5.11 (d, J = 12.0 Hz, 1H), 5.04 (d, J = 12.0 Hz, 1H), 3.67 (d, J = 13.2 Hz, 1H), 3.59 (d, J = 13.2 Hz, 1H), 3.21 (q, J = 7.2 Hz, 1H), 1.32 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 135.0, 134.7, 131.9, 129.3, 127.6, 127.4, 127.3, 65.8, 39.2, 34.1, 15.7; HRMS (ESI) Calcd for $(C_{17}H_{17}ClO_2S + Na)^+$: 343.0530, Found 343.0532; 83% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 215 nm, t_R = 18.68 min for minor isomer, t_R = 20.48 min for major isomer]; $[\alpha]_D^{20}$ = +152.5 (*c* 1.0, MeOH).

(+)-benzyl 2-(2-methylbenzylthio)propionate (3f)



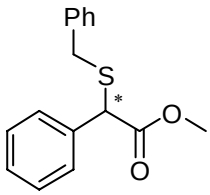
Colorless oil; 87% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31–6.98 (m, 9H), 5.13 (d, J = 12.3 Hz, 1H), 5.07 (d, J = 12.3 Hz, 1H), 3.72 (d, J = 12.6 Hz, 1H), 3.67 (d, J = 12.6 Hz, 1H), 3.31 (q, J = 7.2 Hz, 1H), 2.23 (s, 3H), 1.36 (d, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.9, 136.9, 135.8, 135.0, 130.6, 129.9, 128.7, 128.4, 128.3, 127.5, 125.9, 66.9, 40.8, 33.8, 19.1, 17.0; HRMS (ESI) Calcd for $(C_{18}H_{20}O_2S + Na)^+$: 323.1076, Found 323.1080; 68% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 13.79 min for minor isomer, t_R = 17.71 min for major isomer]; $[\alpha]_D^{20}$ = +121.0 (*c* 1.0, MeOH).

(+)-benzyl 2-(2-chlorobenzylthio)propionate (3g)



Colorless oil; 70% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29–7.07 (m, 9H), 5.11 (d, J = 12.3 Hz, 1H), 5.06 (d, J = 12.3 Hz, 1H), 3.82 (s, 2H), 3.33 (q, J = 7.2 Hz, 1H), 1.36 (d, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.8, 135.7, 135.3, 134.2, 130.9, 129.9, 128.6, 128.4, 128.3, 126.8, 66.9, 40.9, 33.5, 16.9; HRMS (ESI) Calcd for $(C_{17}H_{17}ClO_2S + Na)^+$: 343.0530, Found 343.0524; 78% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 10.89 min for minor isomer, t_R = 11.78 min for major isomer]; $[\alpha]_D^{20}$ = +144.7 (*c* 1.0, MeOH).

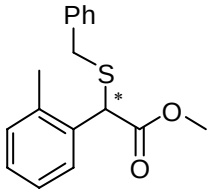
(-)-methyl 2-(benzylthio)-2-phenylacetate (3h)



Colorless oil; 59% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.25 (m, 10H), 4.42 (s, 1H), 3.78–3.59 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 137.1, 135.8, 129.1, 128.7, 128.6, 128.2, 127.3, 52.7, 51.5, 36.2; HRMS (ESI) Calcd for $(C_{16}H_{15}O_2S + Na)^+$: 295.0763, Found 295.0766; 44% ee [SFC condition: Chiralcel OD-H column, sc CO_2/*i*-PrOH = 95:5, P_{CO2} = 100 bar, 2.0 mL/min,

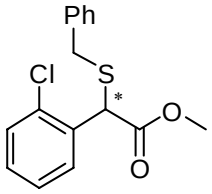
oven 40 °C, wavelength = 220 nm, t_R = 10.56 min for major isomer, t_R = 12.02 min for minor isomer]; $[\alpha]_D^{20}$ = -56.2 (*c* 1.0, MeOH).

(-)-methyl 2-(benzylthio)-2-o-tolylacetate (3i)



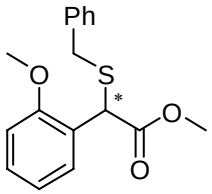
Colorless oil; 64% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.33–7.10 (m, 8H), 4.58 (s, 1H), 3.83–3.66 (m, 5H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 136.2, 135.2, 132.8, 129.6, 128.0, 127.5, 127.2, 127.0, 126.2, 125.4, 52.0, 46.4, 35.5, 18.1; HRMS (ESI) Calcd for $(C_{17}H_{18}O_2S + Na)^+$: 309.0920, Found 309.0923; 77% ee [SFC condition: Chiralpak AD-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 220 nm, t_R = 5.63 min for minor isomer, t_R = 6.89 min for major isomer]; $[\alpha]_D^{20}$ = -30.6 (*c* 1.0, MeOH).

(-)-methyl 2-(benzylthio)-2-(2-chlorophenyl)acetate (3j)



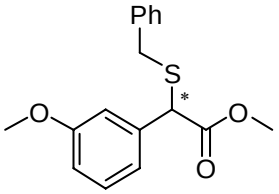
Colorless oil; 83% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65–7.62 (m, 1H), 7.35–7.19 (m, 8H), 4.97 (s, 1H), 3.87–3.69 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.8, 136.9, 133.8, 130.2, 129.6, 129.3, 129.1, 128.6, 127.4, 127.2, 52.9, 47.6, 36.8; HRMS (ESI) Calcd for $(C_{16}H_{15}ClO_2S + Na)^+$: 329.0374, Found 329.0377; 73% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 18.65 min for major isomer, t_R = 26.86 min for minor isomer]; $[\alpha]_D^{20}$ = -10.4 (*c* 1.0, MeOH).

(-)-methyl 2-(benzylthio)-2-(2-methoxyphenyl)acetate (3k)



Colorless oil; 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51–7.48 (m, 1H), 7.31–7.23 (m, 6H), 6.98–6.83 (m, 2H), 4.92 (s, 1H), 3.86–3.68 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 155.5, 136.3, 128.3, 128.2, 128.1, 127.4, 126.1, 123.4, 119.8, 109.7, 54.6, 51.6, 43.5, 35.5; HRMS (ESI) Calcd for $(C_{17}H_{18}O_3S + Na)^+$: 325.0869, Found 325.0861; 77% ee [SFC condition: Chiralcel OJ-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 220 nm, t_R = 8.34 min for major isomer, t_R = 10.34 min for minor isomer]; $[\alpha]_D^{20}$ = -35.3 (*c* 1.0, MeOH).

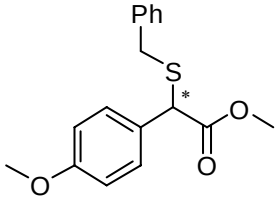
(-)-methyl 2-(benzylthio)-2-(3-methoxyphenyl)acetate (3l)



Colorless oil; 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25–7.14 (m, 6H), 6.90–6.88 (m, 2H), 6.77–6.75 (m, 1H), 4.32 (s, 1H), 3.71–3.52 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 158.8, 136.2, 136.1, 128.6, 128.0, 127.5, 126.2, 119.9, 112.9, 54.2, 51.7, 50.5, 35.2; HRMS (ESI) Calcd for$(C_{17}H_{18}O_3S + Na)^+$: 325.0869, Found 325.0873; 52% ee [SFC condition: Chiralcel AD-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 220 nm, t_R = 7.68 min for minor isomer, t_R = 8.03 min for major isomer]; $[\alpha]_D^{20}$ = -67.4 (*c* 1.0, MeOH).

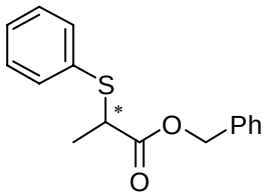
(-)-methyl 2-(benzylthio)-2-(4-methoxyphenyl)acetate (3m)

Colorless oil; 61% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26–7.16 (m, 7H), 6.78 (d, *J* = 8.8 Hz,



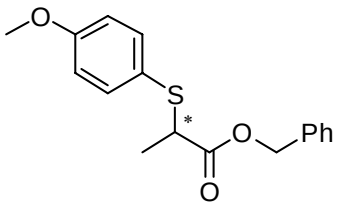
2H), 4.31 (s, 1H), 3.71–3.50 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 159.5, 137.3, 129.8, 129.1, 128.6, 127.7, 127.3, 114.1, 55.3, 52.7, 50.9, 36.2; HRMS (ESI) Calcd for$(C_{17}H_{18}O_3S + Na)^+$: 325.0869, Found 325.0861; 61% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 30.23 min for major isomer, t_R = 43.09 min for minor isomer]; $[\alpha]_D^{20}$ = -95.1 (*c* 1.0, MeOH).

(+)-benzyl 2-(phenylthio)propionate (3n)



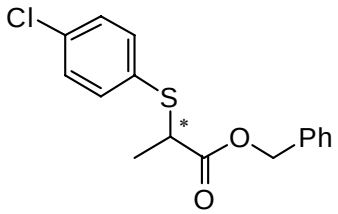
Colorless oil; 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.23 (m, 10H), 5.11 (d, *J* = 12.4 Hz, 1H), 5.07 (d, *J* = 12.4 Hz, 1H), 3.83 (q, *J* = 7.2 Hz, 1H), 1.49 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 135.5, 133.2, 133.0, 129.0, 128.5, 128.3, 128.1, 66.9, 45.2, 17.4; HRMS (ESI) Calcd for $(C_{16}H_{16}O_2S + Na)^+$: 295.0763, Found 295.0766; 69% ee [SFC condition: Chiralcel OJ-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 210 nm, t_R = 6.83 min for minor isomer, t_R = 7.57 min for major isomer]; $[\alpha]_D^{20}$ = +85.6 (*c* 1.0, MeOH).

(+)-benzyl 2-(4-methoxyphenylthio)propionate (3o)



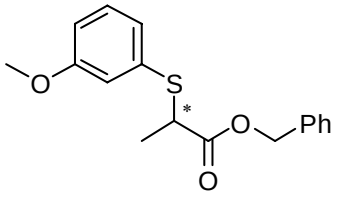
Colorless oil; 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.29 (m, 7H), 6.80–6.78 (m, 2H), 5.14–5.07 (m, 2H), 3.80 (s, 1H), 3.69 (q, *J* = 5.6 Hz, 1H), 1.45 (d, *J* = 5.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 160.2, 136.6, 135.6, 128.5, 128.3, 128.2, 122.8, 114.5, 66.7, 55.3, 45.9, 17.1; HRMS (ESI) Calcd for $(C_{17}H_{18}O_3S + Na)^+$: 325.0869, Found 325.0867; 72% ee [SFC condition: Chiralcel OJ-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 235 nm, t_R = 8.63 min for minor isomer, t_R = 9.42 min for major isomer]; $[\alpha]_D^{20}$ = +51.0 (*c* 1.0, MeOH).

(+)-benzyl 2-(4-chlorophenylthio)propionate (3p)



Colorless oil; 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.19 (m, 9H), 5.13 (d, *J* = 12.0 Hz, 1H), 5.06 (d, *J* = 12.0 Hz, 1H), 3.79 (q, *J* = 7.2, 1H), 1.49 (d, *J* = 7.2, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.2, 135.4, 134.6, 134.4, 131.4, 129.1, 128.5, 128.3, 67.0, 45.3, 17.2; HRMS (ESI) Calcd for $(C_{16}H_{15}ClO_2S + Na)^+$: 329.0374, Found 329.0380; 62% ee [SFC condition: Chiralcel OJ-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 220 nm, t_R = 6.54 min for minor isomer, t_R = 7.17 min for major isomer]; $[\alpha]_D^{20}$ = +74.3 (*c* 1.0, MeOH).

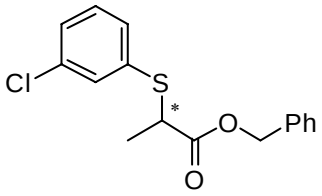
(+)-benzyl 2-(3-methoxyphenylthio)propionate (3q)



Colorless oil; 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.25 (m, 5H), 7.18–7.14 (m, 1H), 6.98–6.96 (m, 2H), 6.79 (d, *J* = 9.2 Hz, 1H), 5.12 (d, *J* = 12.4 Hz, 1H), 5.08 (d, *J* = 12.4 Hz, 1H), 3.86 (q, *J* = 7.2 Hz, 1H), 3.72 (s, 3H), 1.50 (d, *J* = 7.2 Hz, 3H); ^{13}C

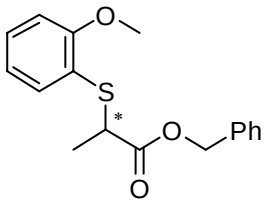
NMR (100 MHz, $CDCl_3$) δ 171.5, 158.6, 134.5, 133.4, 128.7, 127.5, 127.2, 127.1, 123.8, 116.6, 112.9, 65.9, 54.2, 44.1, 16.4; HRMS (ESI) Calcd for $(C_{17}H_{18}O_3S + Na)^+$: 325.0869, Found 325.0874; 62% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 18.02 min for major isomer, t_R = 20.07 min for minor isomer]; $[\alpha]_D^{20}$ = +75.0 (*c* 1.0, MeOH).

(+)-benzyl 2-(3-chlorophenylthio)propionate (3r)



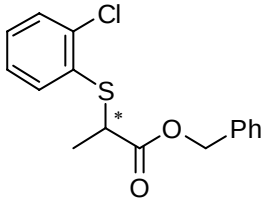
Colorless oil; 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32–7.06 (m, 9H), 5.05 (d, *J* = 12.0 Hz, 1H), 5.00 (d, *J* = 12.0 Hz, 1H), 3.77 (q, *J* = 7.2 Hz, 1H), 1.36 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 134.3, 134.2, 133.5, 131.1, 129.5, 128.9, 127.5, 127.3, 127.2, 127.0, 66.0, 43.9, 16.2; HRMS (ESI) Calcd for $(C_{16}H_{15}ClO_2S + Na)^+$: 329.0374, Found 329.0371; 60% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 9.72 min for major isomer, t_R = 10.80 min for minor isomer]; $[\alpha]_D^{20}$ = +58.2 (*c* 1.0, MeOH).

(+)-benzyl 2-(2-methoxyphenylthio)propionate (3s)



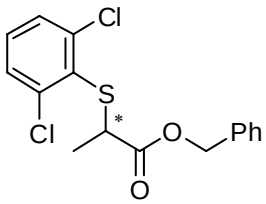
Colorless oil; 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.12 (m, 7H), 6.78–6.75 (m, 2H), 4.98 (d, *J* = 12.4 Hz, 1H), 4.94 (d, *J* = 12.4 Hz, 1H), 3.92 (q, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 1.42 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 158.1, 134.6, 133.7, 128.8, 127.4, 127.1, 120.0, 119.8, 109.8, 65.7, 54.7, 42.1, 16.0; HRMS (ESI) Calcd for $(C_{17}H_{18}O_3S + Na)^+$: 325.0869, Found 325.0863; 60% ee [HPLC condition: Chiralcel OD-H column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 286 nm, t_R = 9.05 min for major isomer, t_R = 10.36 min for minor isomer]; $[\alpha]_D^{20}$ = +126.5 (*c* 1.0, MeOH).

(+)-benzyl 2-(2-chlorophenylthio)propionate (3t)



Colorless oil; 92% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.01 (m, 9H), 5.00 (s, 2H), 3.88 (q, *J* = 7.2 Hz, 1H), 1.47 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 135.6, 134.4, 132.8, 131.7, 128.9, 127.9, 127.4, 127.2, 126.1, 66.0, 42.9, 16.0; HRMS (ESI) Calcd for $(C_{16}H_{15}ClO_2S + Na)^+$: 329.0374, Found 329.0376; 60% ee [HPLC condition: Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm, t_R = 10.65 min for minor isomer, t_R = 12.30 min for major isomer]; $[\alpha]_D^{20}$ = +77.4 (*c* 1.0, MeOH).

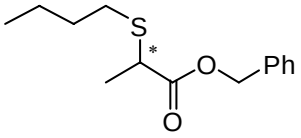
(+)-benzyl 2-(2,6-dichlorophenylthio)propionate (3u)



Colorless oil; 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.11 (m, 8H), 5.10 (d, *J* = 12.4 Hz, 1H), 5.00 (d, *J* = 12.4 Hz, 1H), 3.92 (q, *J* = 7.2 Hz, 1H), 1.54 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 141.8, 135.3, 131.4, 130.6, 128.6, 128.4, 128.2, 128.1, 67.2, 44.2, 16.4; HRMS (ESI) Calcd for $(C_{16}H_{14}Cl_2O_2S + Na)^+$: 362.9984, Found 362.9978; 67% ee [HPLC condition: Chiralcel OJ-H column,

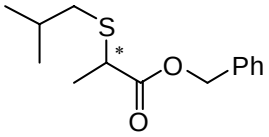
n-Hexane/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 15.26 min for minor isomer, t_R = 19.85 min for major isomer]; $[\alpha]_D^{20}$ = +97.5 (*c* 1.0, MeOH).

(+)-benzyl 2-(butylthio)propionate (3v)



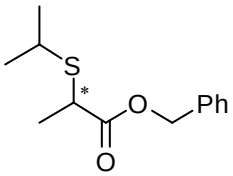
Colorless oil; 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.32 (m, 5H), 5.21 (d, *J* = 12.4 Hz, 1H), 5.15 (d, *J* = 12.4 Hz, 1H), 3.44 (q, *J* = 7.2 Hz, 1H), 2.63–2.51 (m, 2H), 1.56–1.26 (m, 7H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 134.8, 127.5, 127.2, 127.1, 65.7, 40.0, 30.3, 30.0, 20.9, 16.2, 12.6; HRMS (ESI) Calcd for $(C_{14}H_{20}O_2S + Na)^+$: 275.1076, Found 275.1076; 17% ee [The ee value was determined by converting the title product into the corresponding amide as the following procedure: the product was dissolved in ethanol and treated with aq. NaOH (1.25 M) under 0 °C for *ca.* 2 hours. After an acidic workup the crude acid was obtained and was reacted with aniline (1.1 eq) in the presences of DMAP (6 mol%) and DCC (1.1 eq) in THF for 30 min. The reaction mixture was filtered through celite. The filtrate was diluted with Et_2O, washed with 3 N HCl, saturated $NaHCO_3$ and dried with Na_2SO_4. The desired amide was obtained after a flash chromatography on Al_2O_3 column. HPLC condition for the corresponding amide: Chiralcel OD-H column, *n*-Hexane/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, wavelength = 230 nm, t_R = 11.69 min for major isomer, t_R = 12.68 min for minor isomer]; $[\alpha]_D^{20}$ = +48.4 (*c* 1.0, MeOH).

(+)-benzyl 2-(isobutylthio)propionate (3w)



Colorless oil; 84% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36–7.34 (m, 5H), 5.21 (d, *J* = 12.3 Hz, 1H), 5.13 (d, *J* = 12.3 Hz, 1H), 3.41 (q, *J* = 7.2 Hz, 1H), 2.52–2.38 (m, 2H), 1.81–1.67 (m, 1H), 1.45 (d, *J* = 7.2 Hz, 3H), 0.94–0.91 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.1. 134.8, 127.5, 127.2, 65.7, 40.3, 39.1, 27.3, 21.0, 20.8, 16.2; HRMS (ESI) Calcd for $(C_{14}H_{20}O_2S + Na)^+$: 275.1076, Found 275.1077; 32% ee [The ee value was determined by converting the title product into the corresponding amide as the procedure described above. SFC condition for the corresponding amide: Chiralpak AD-H column, sc CO_2/*i*-PrOH = 85:15, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 254 nm, t_R = 4.28 min for major isomer, t_R = 4.91 min for minor isomer]; $[\alpha]_D^{20}$ = +56.7 (*c* 1.0, MeOH).

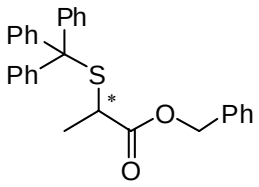
(+)-benzyl 2-(isopropylthio)propionate (3x)



Colorless oil; 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.32 (m, 5H), 5.20 (d, *J* = 12.4 Hz, 1H), 5.15 (d, *J* = 12.4 Hz, 1H), 3.51 (q, *J* = 7.2 Hz, 1H), 3.06–2.99 (m, 1H), 1.45 (d, *J* = 6.8 Hz, 3H), 1.27 (d, *J* = 6.8 Hz, 3H), 1.19 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 134.8, 127.5, 127.2, 127.1, 65.7, 39.3, 34.4, 22.5, 22.1, 16.5; HRMS (ESI) Calcd for $(C_{13}H_{18}O_2S + Na)^+$: 261.0920, Found 261.0920; 61% ee [HPLC condition : Chiralcel OJ-H column, *n*-Hexane/*i*-PrOH = 99:1, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 10.94 min for major isomer, t_R = 13.51 min for minor isomer]; $[\alpha]_D^{20}$ = +55.7 (*c* 1.0, MeOH).

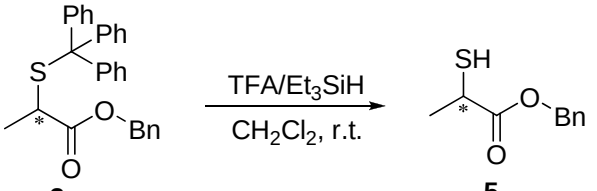
(+)-benzyl 2-(tritylthio)propionate (3y)

Viscous oil; 57% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.42 (m, 6H), 7.34–7.33 (m, 3H),



7.25–7.16 (m, 11H), 4.98 (d, J = 12.4 Hz, 1H), 4.84 (d, J = 12.4 Hz, 1H), 2.99 (q, J = 7.2 Hz, 1H), 1.16 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 143.2, 134.5, 128.6, 127.4, 127.2, 126.9, 125.7, 67.1, 65.8, 41.3, 17.6; HRMS (ESI) Calcd for $(C_{29}H_{26}O_2S + Na)^+$: 461.1546, Found 461.1540; 77% ee [SFC condition: Chiralcel OJ-H column, sc CO_2/*i*-PrOH = 80:20, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 220 nm, t_R = 7.07 min for major isomer, t_R = 12.61 min for minor isomer]; $[\alpha]_D^{20}$ = +136.7 (*c* 1.0, MeOH).

3. Preparation of (+)-benzyl 2-mercaptopropionate (5) [4]



3y
77% ee

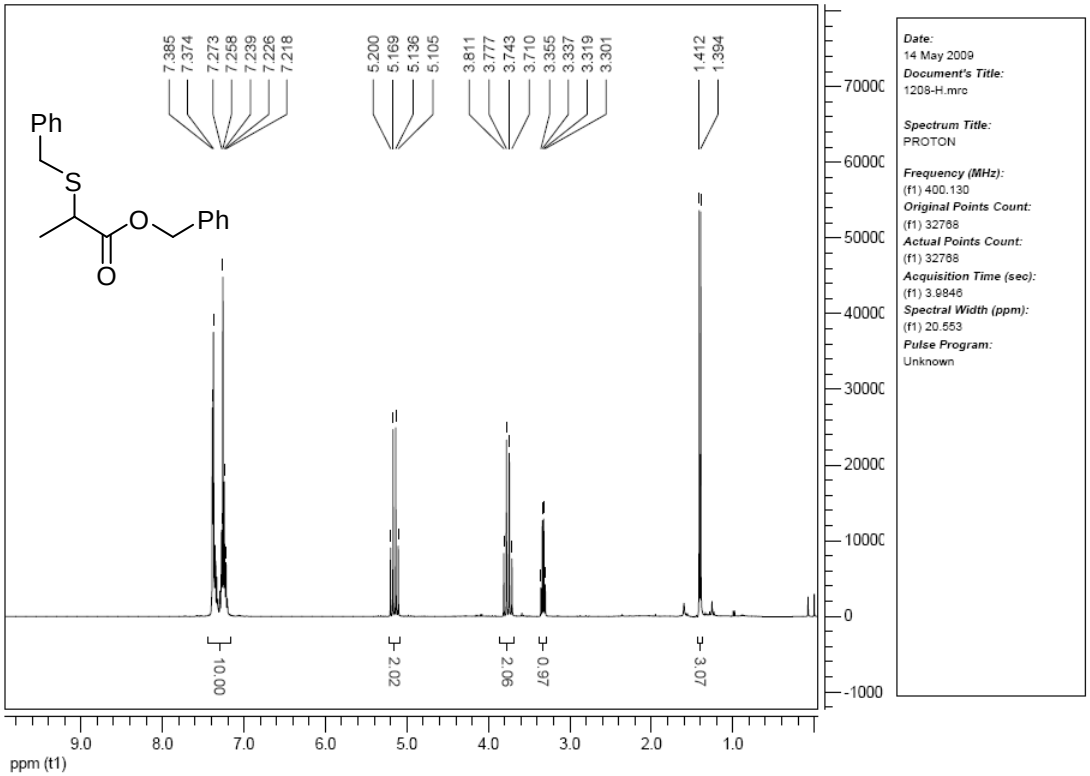
5
81% yield, 77% ee

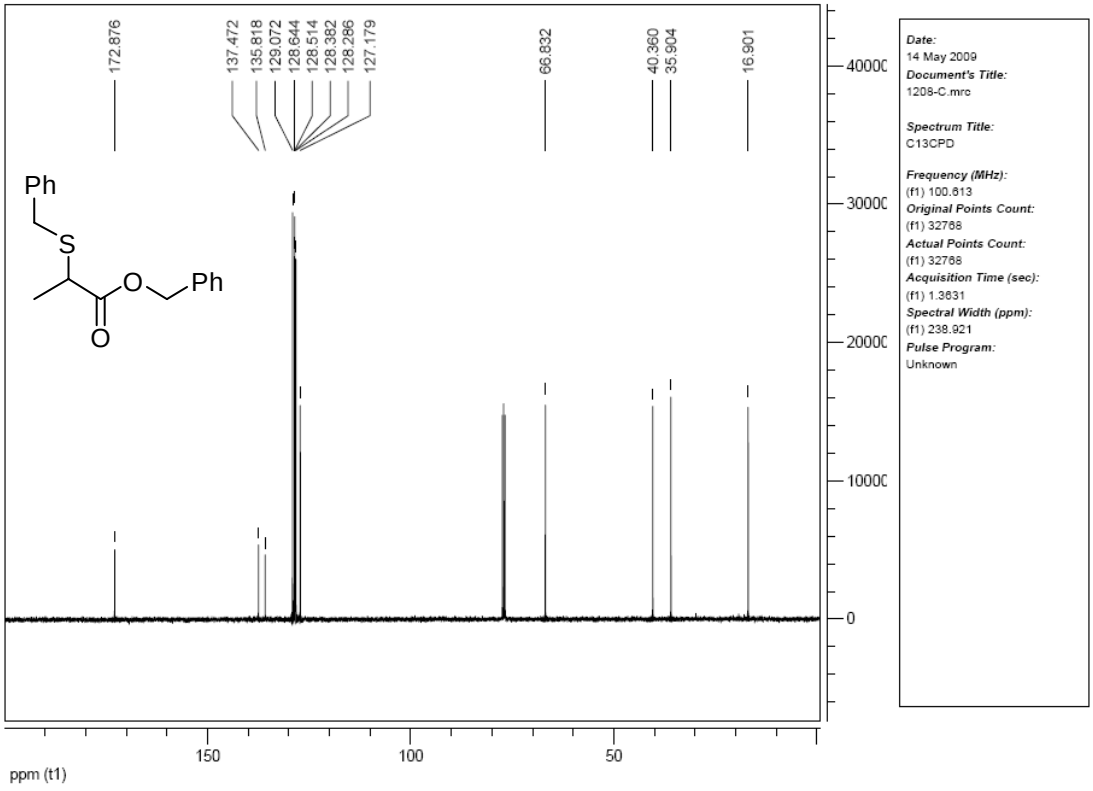
Benzyl 2-(tritylthio)propionate (**3y**) was dissolved in methylene chloride, trifluoroacetic acid and Et_3SiH (1.0 equiv.) were added subsequently. After stirring for 1 h at room temperature (TLC monitoring), the reaction mixture was concentrated and chromatographed on SiO_2 to give benzyl 2-mercaptopropionate (**5**) as a colorless oil in 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.34 (m, 5H), 5.19 (d, J = 12.4 Hz, 1H), 5.15 (d, J = 12.4 Hz, 1H), 3.58–3.51 (m, 1H), 2.17 (d, J = 8.4 Hz, 1H), 1.54 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 135.5, 128.6, 128.4, 128.2, 67.1, 35.7, 21.1. The ee value of **5** was determined by converting the title product into benzyl 2-(benzoylthio)propionate. 77% ee [SFC condition for benzyl 2-(benzoylthio)propionate: Chiralcel OJ-H column, sc CO_2/*i*-PrOH = 90:10, P_{CO2} = 100 bar, 2.0 mL/min, oven 40 °C, wavelength = 254 nm, t_R = 11.03 min for minor isomer, t_R = 11.81 min for major isomer]; $[\alpha]_D^{30}$ = +16.2 (*c* 1.0, MeOH).

[4] Y. Tanabe, H. Yamamoto, M. Murakami, K. Yanagi, Y. Kubota, H. Okumura, Y. Sanemitsu, G. Suzukamo, *J. Chem. Soc., Perkin Trans. 1* **1995**, 935.

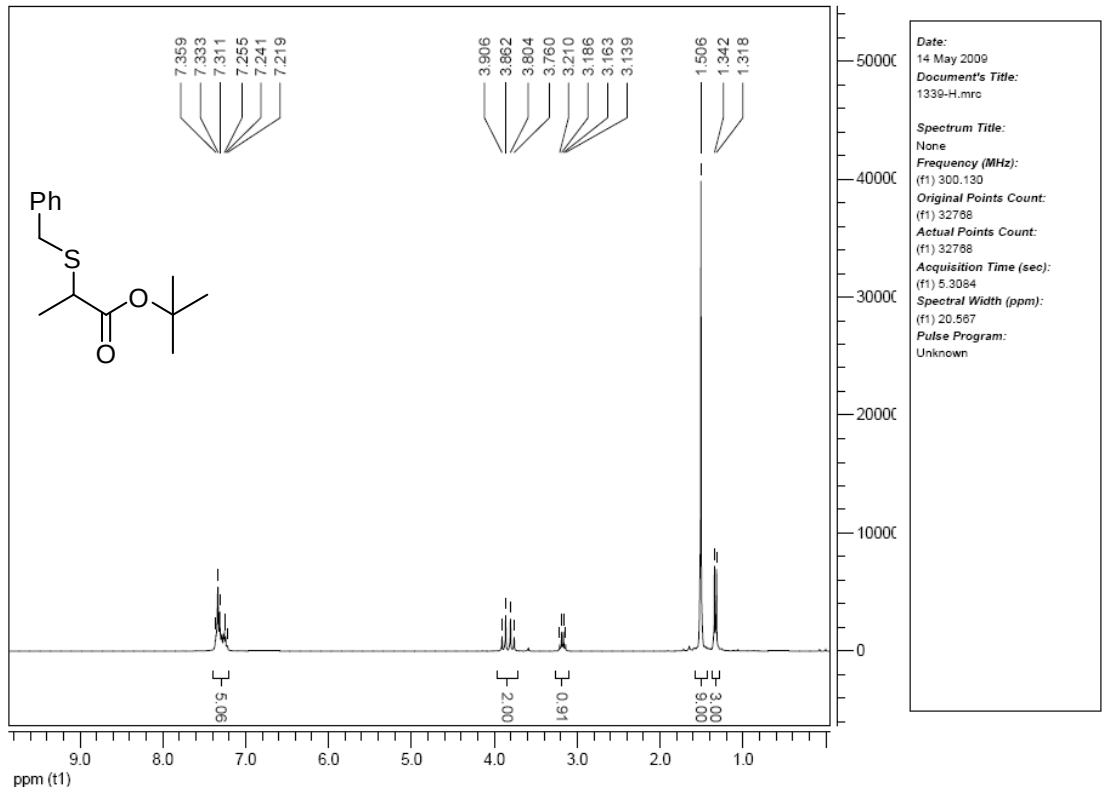
4. NMR Spectra of New S–H Insertion Products

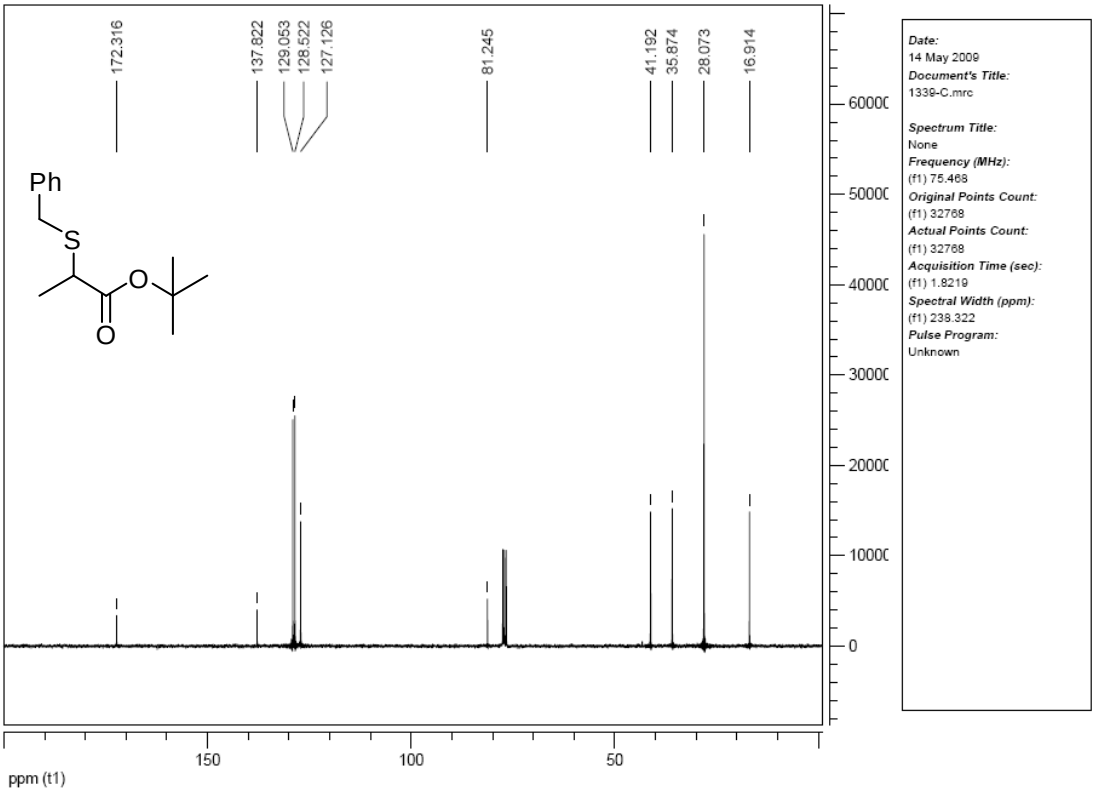
Benzyl 2-(benzylthio)propionate (3a)



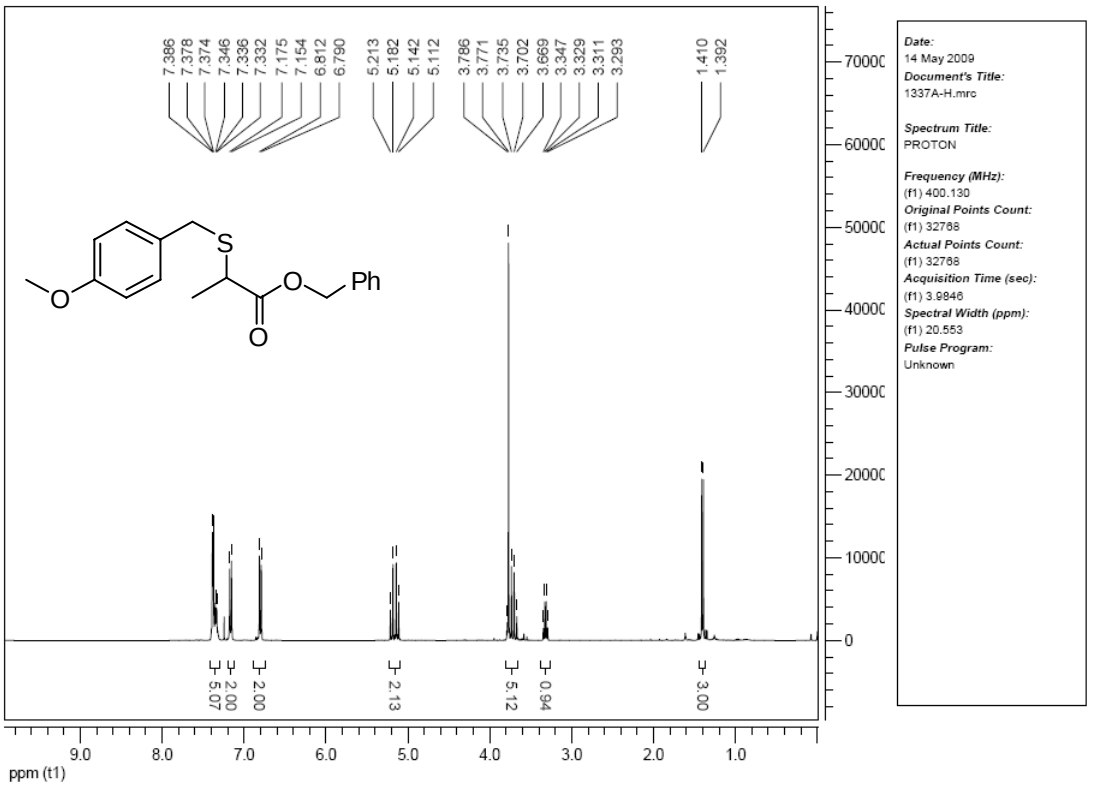


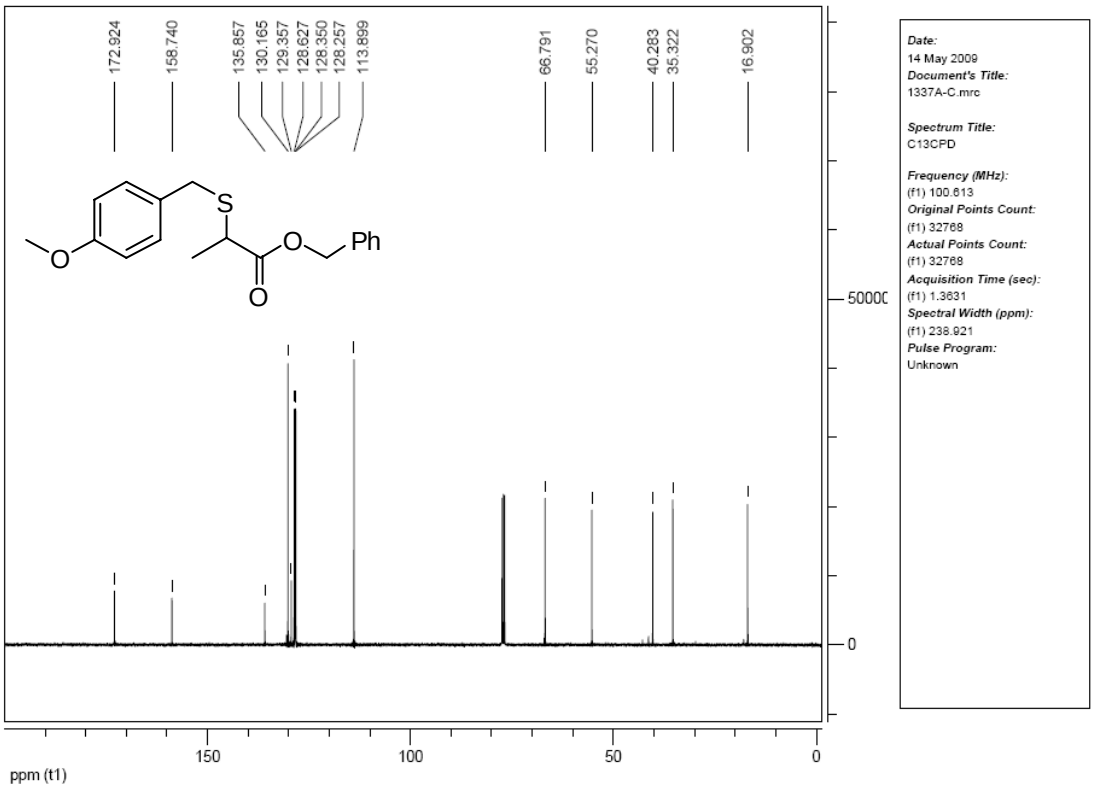
tert-Butyl 2-(benzylthio)propionate (3c)



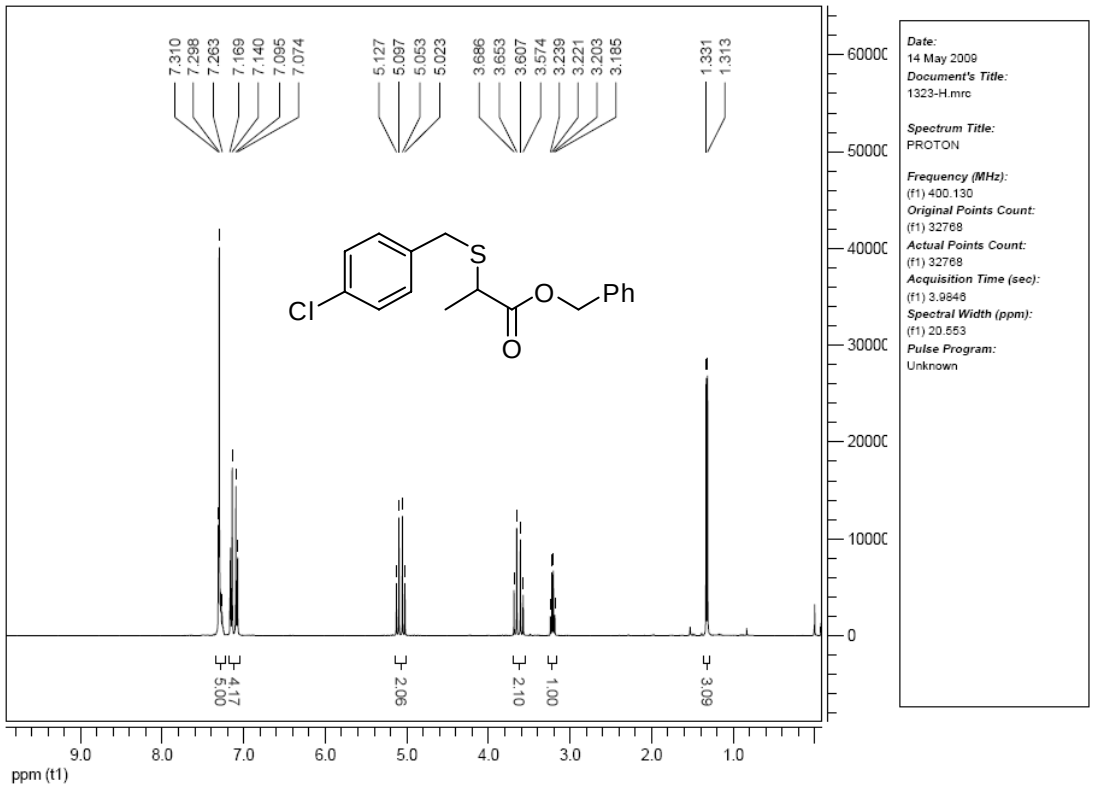


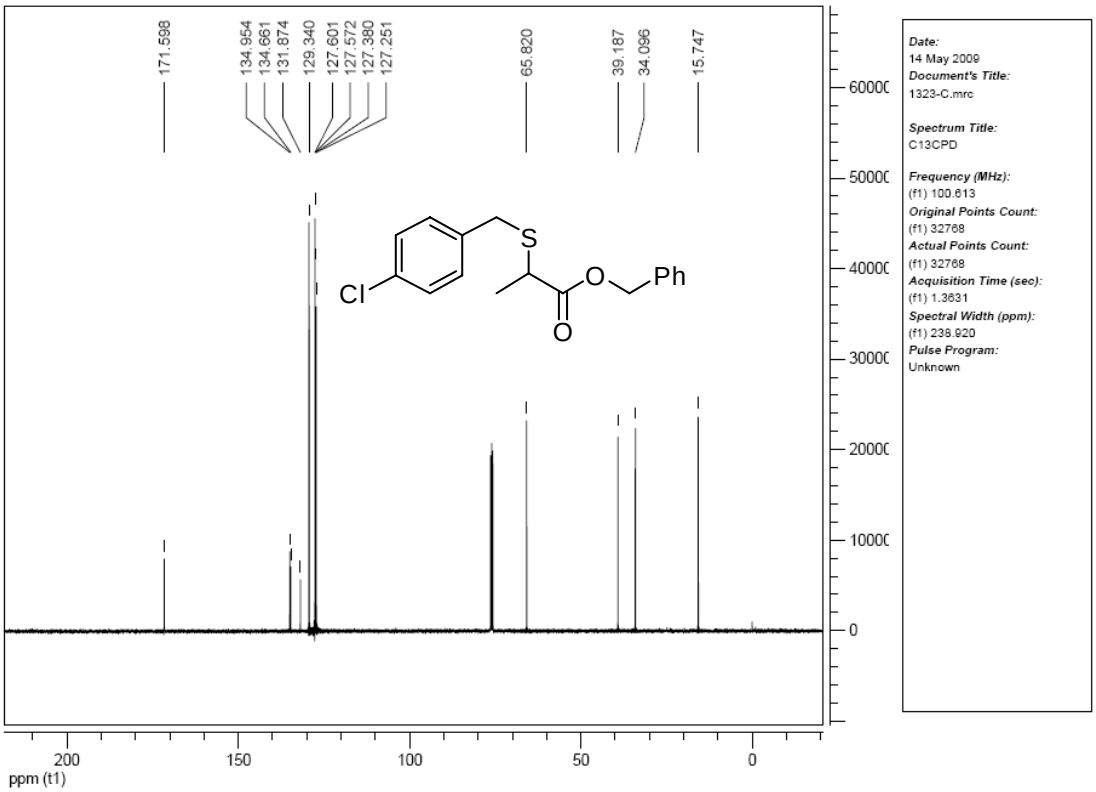
Benzyl 2-(4-methoxybenzylthio)propionate (3d)



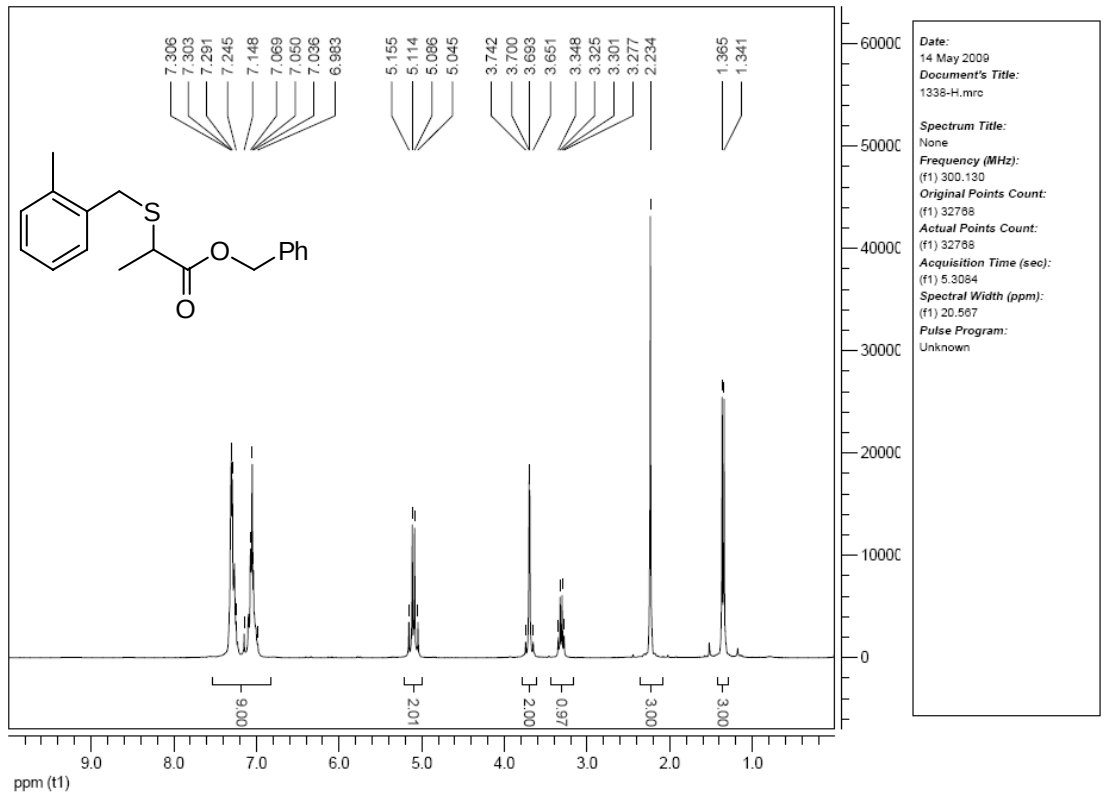


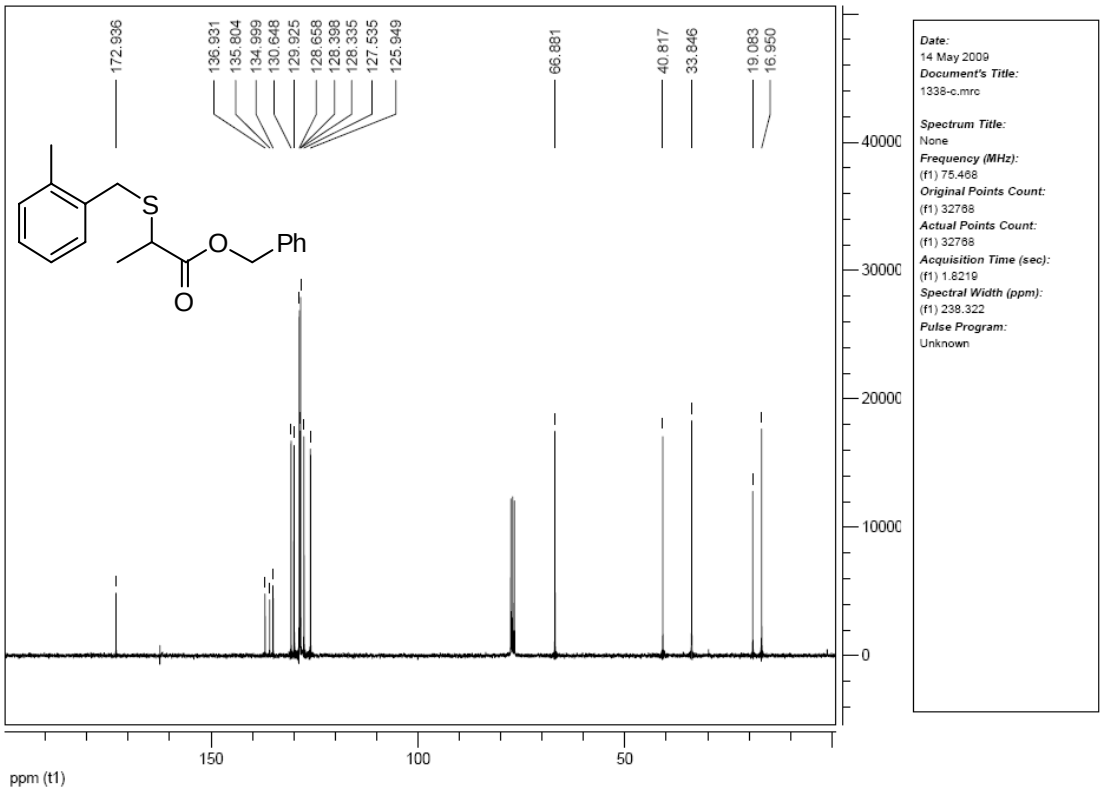
Benzyl 2-(4-chlorobenzylthio)propionate (3e)



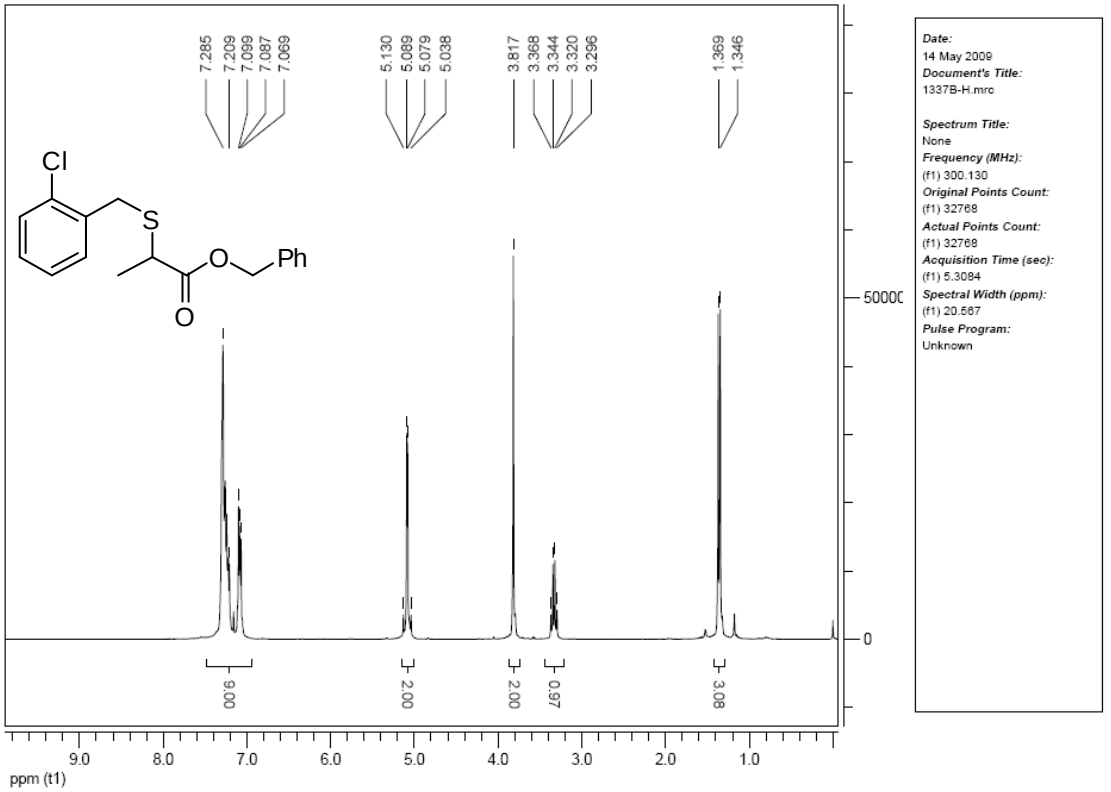


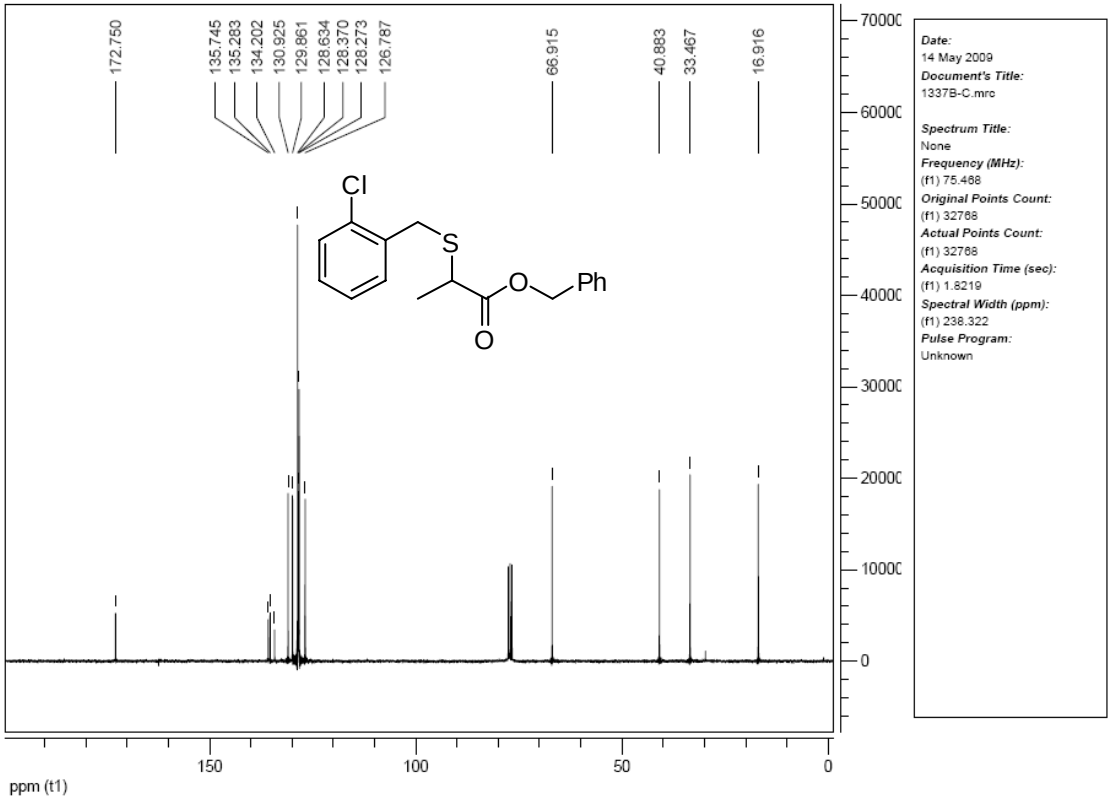
Benzyl 2-(2-methylbenzylthio)propionate (3f)



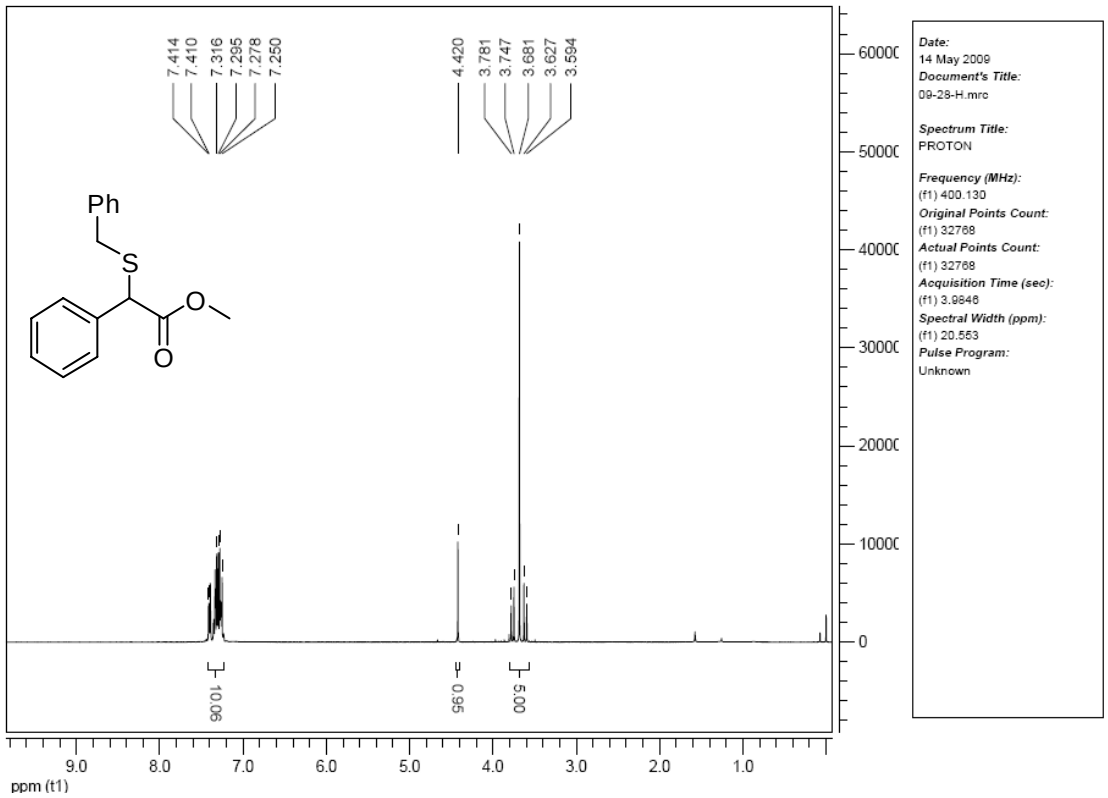


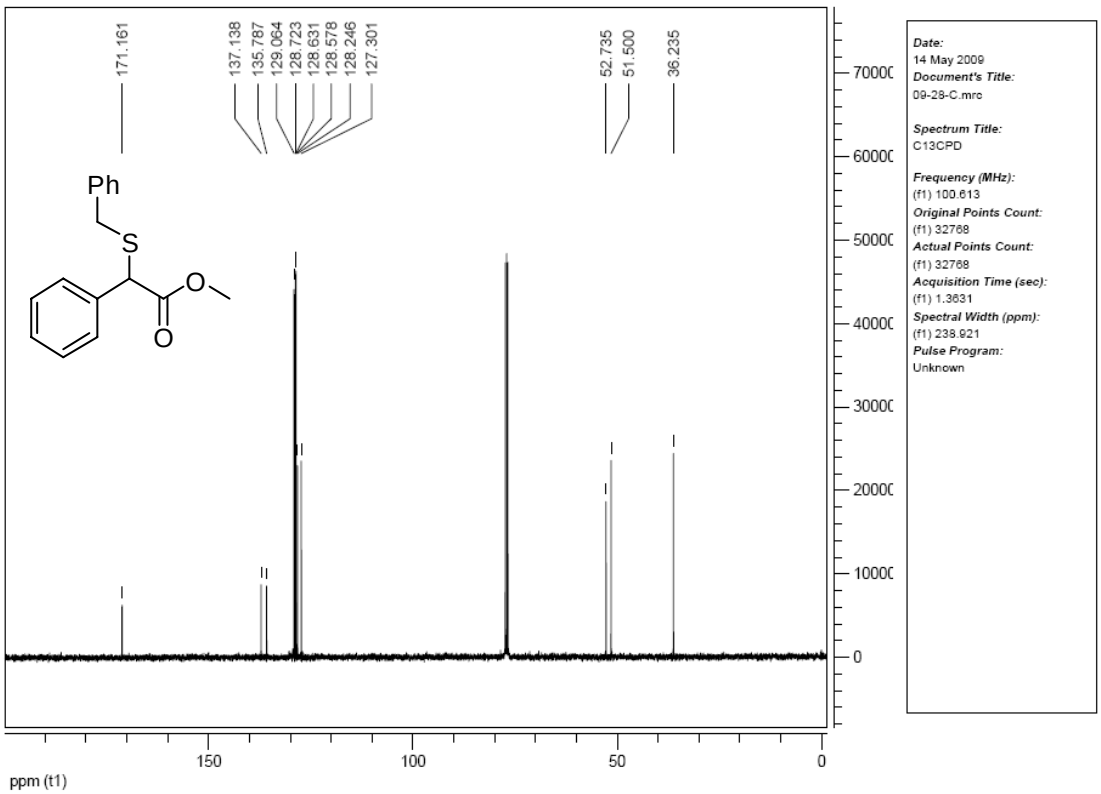
Benzyl 2-(2-chlorobenzylthio)propionate (3g)



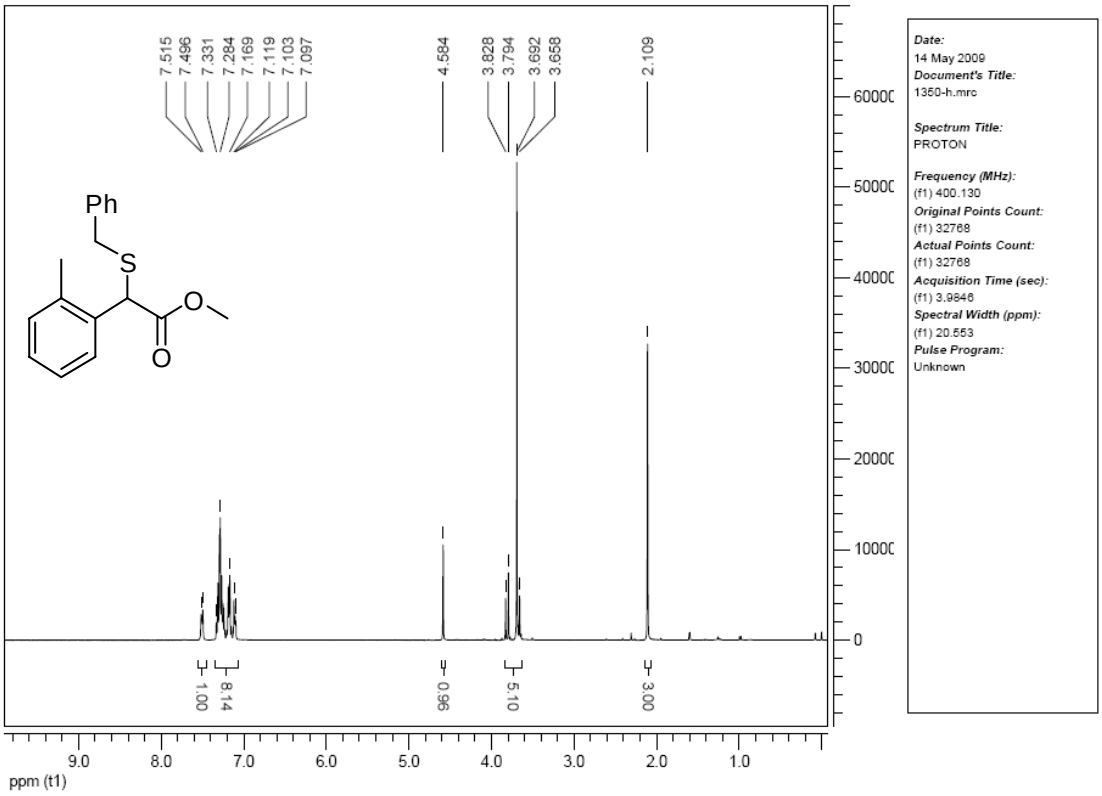


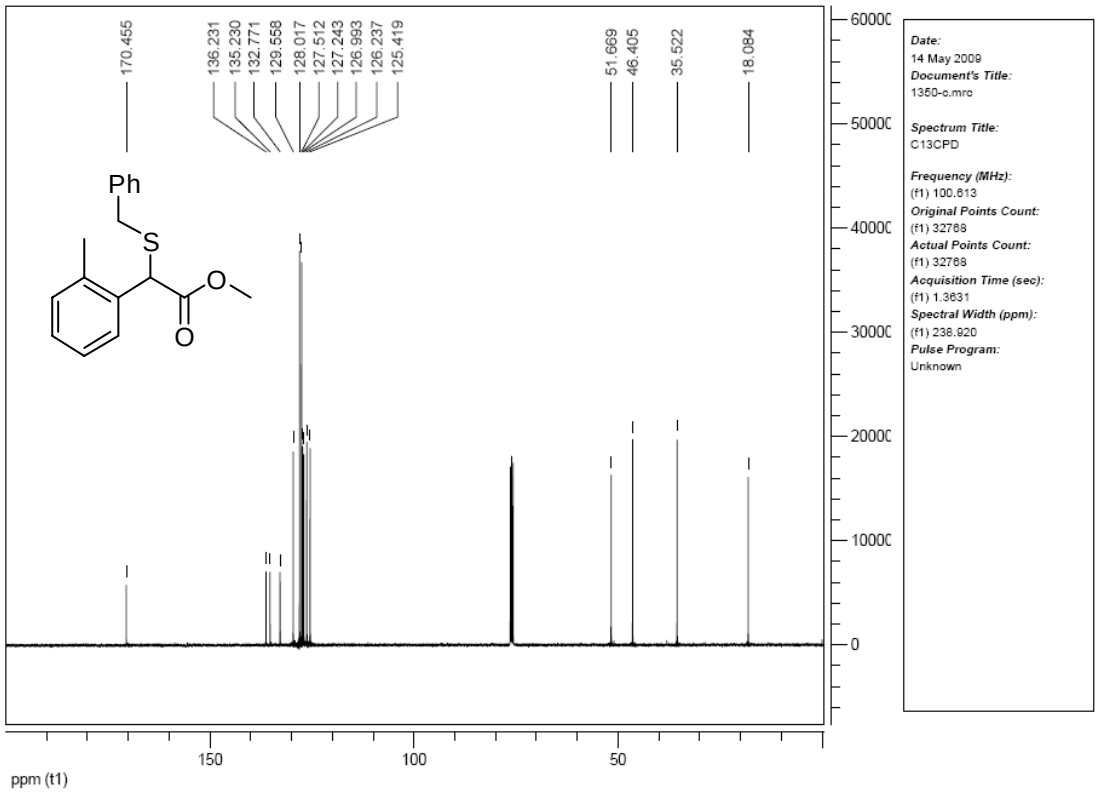
Methyl 2-(benzylthio)-2-phenylacetate (3h)



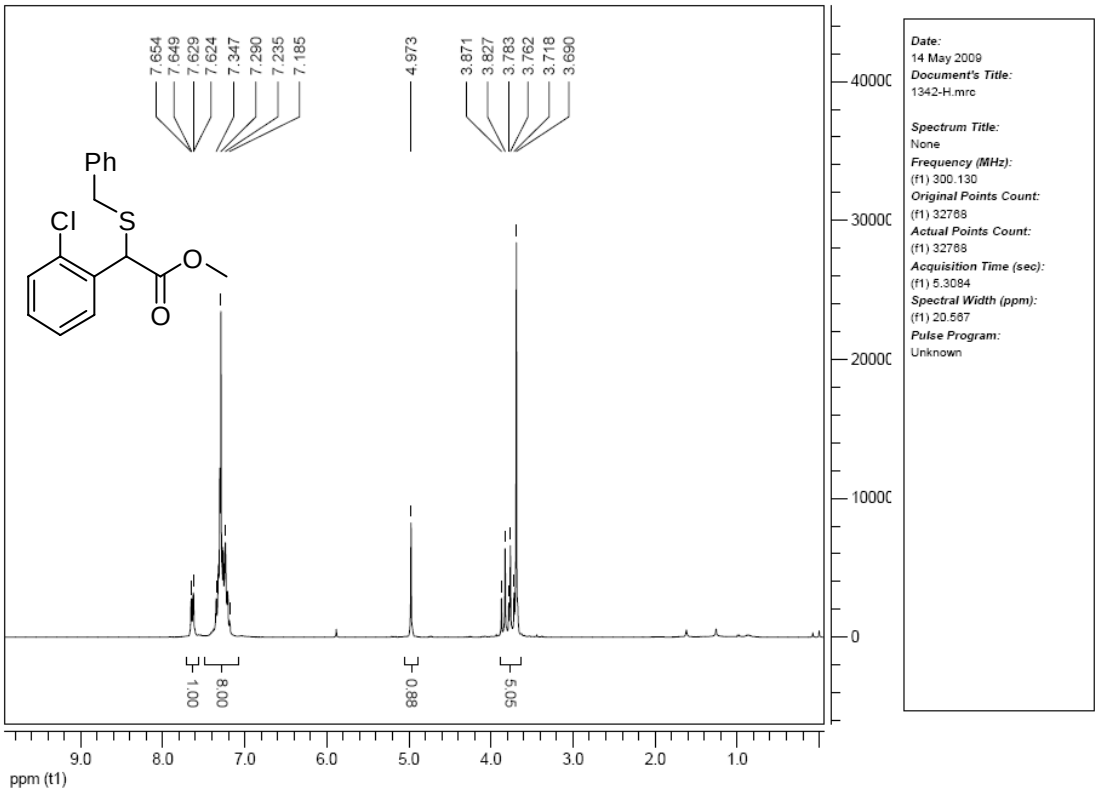


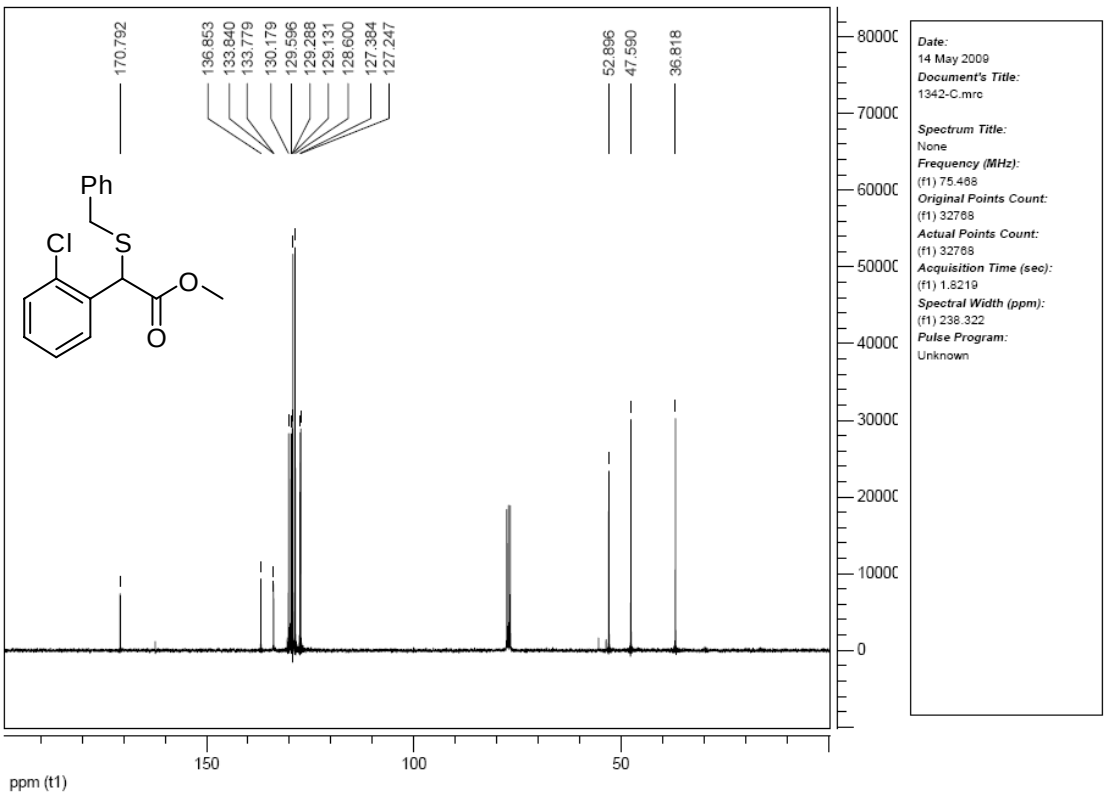
Methyl 2-(benzylthio)-2-o-tolylacetate (3i)



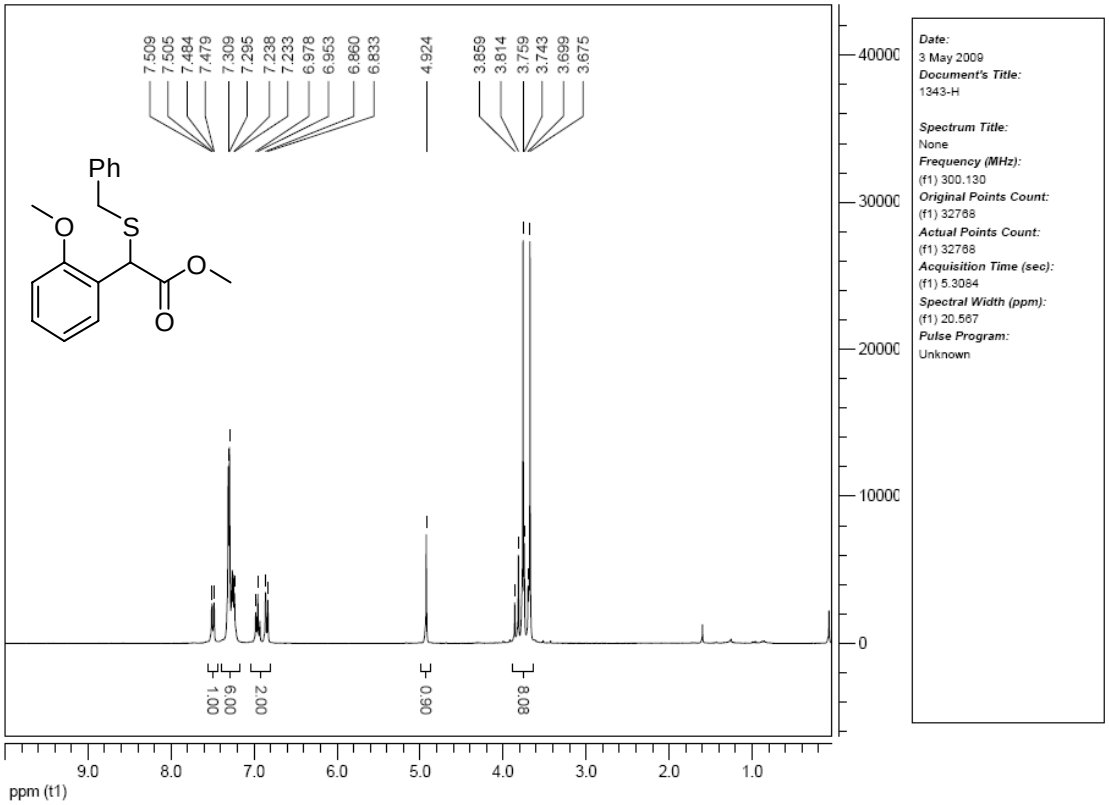


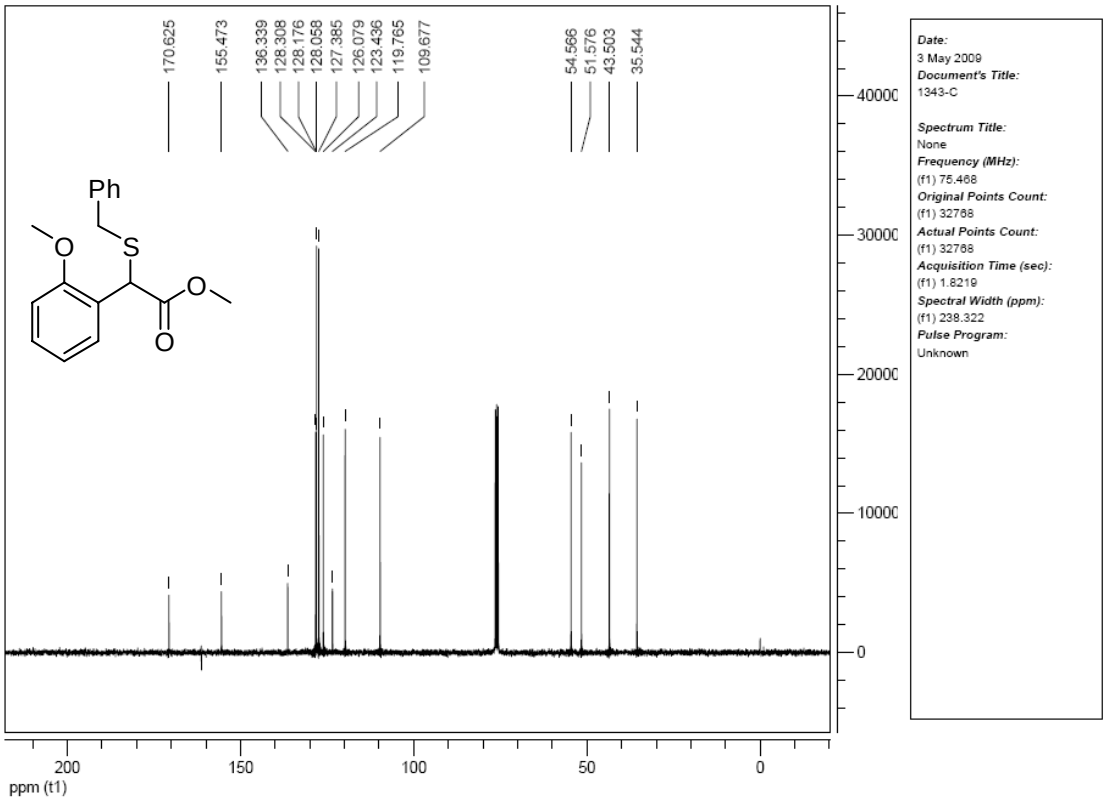
Methyl 2-(benzylthio)-2-(2-chlorophenyl)acetate (3j)



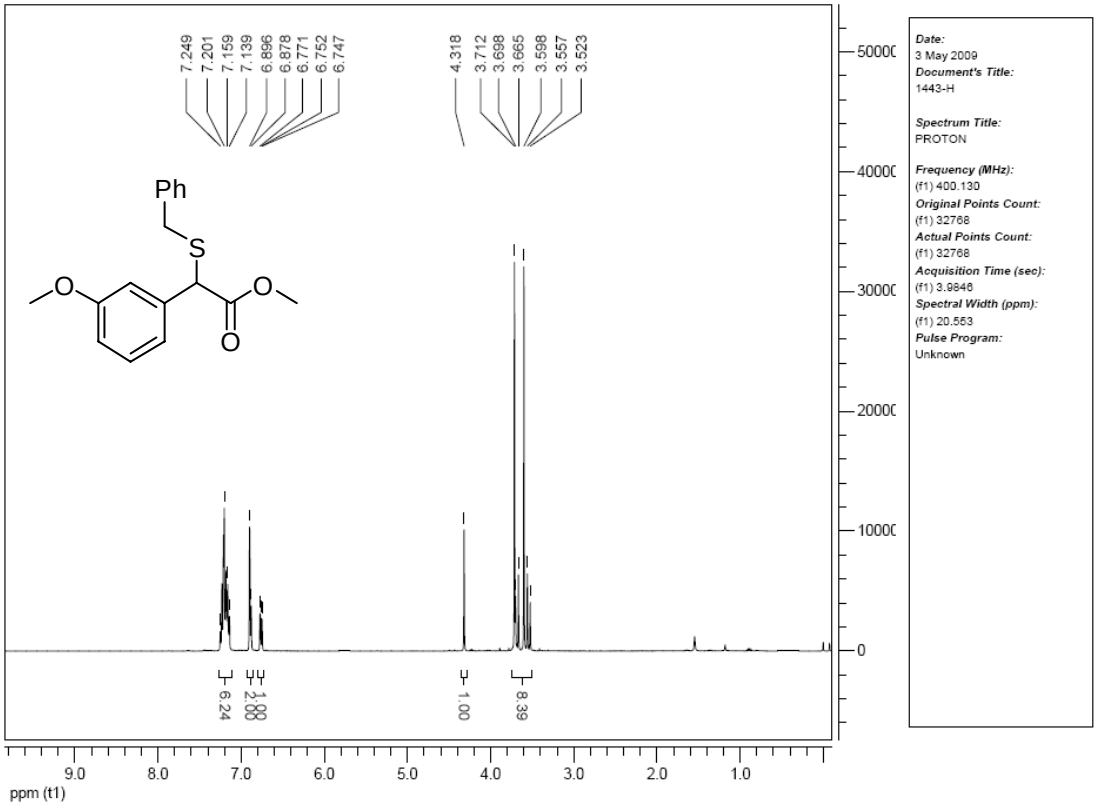


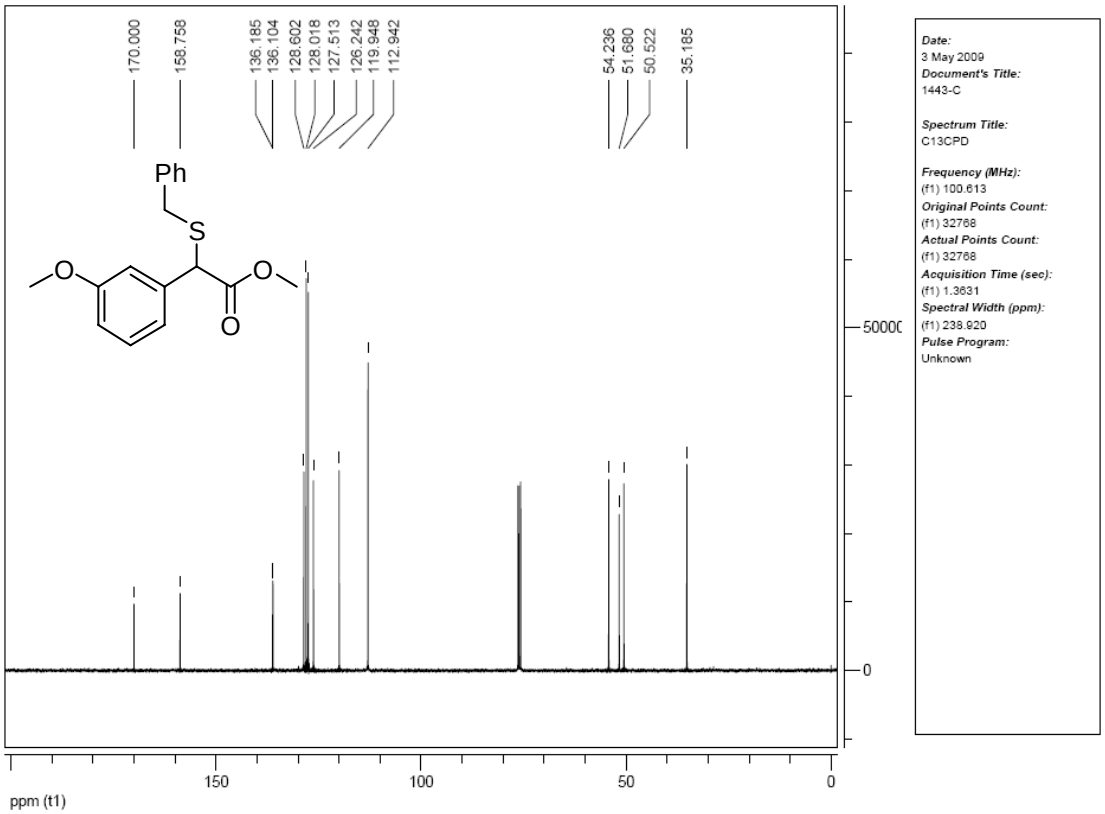
Methyl 2-(benzylthio)-2-(2-methoxyphenyl)acetate (3k)



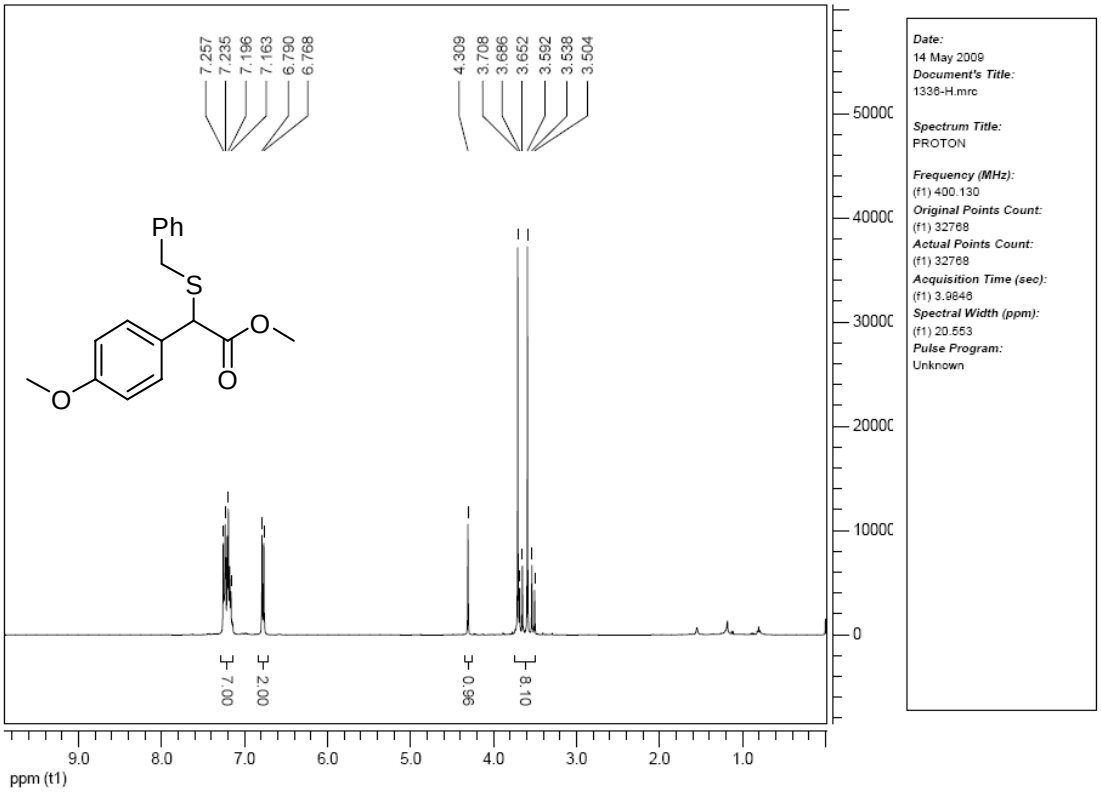


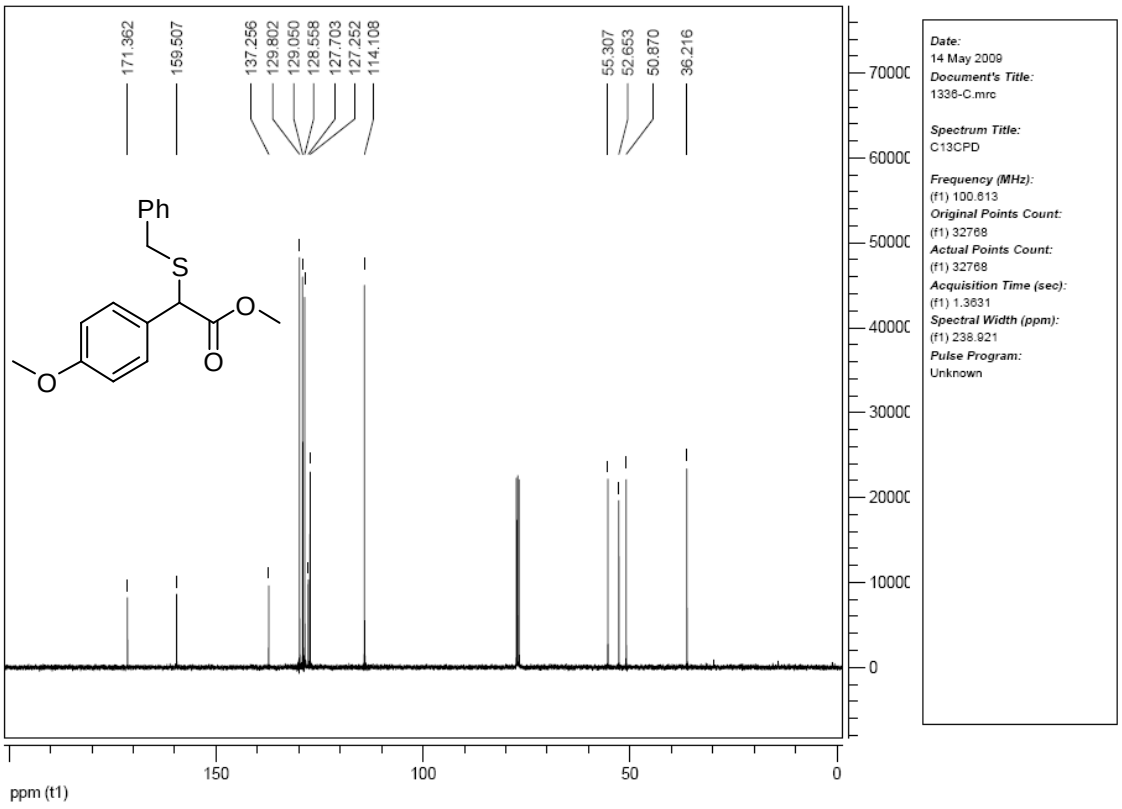
Methyl 2-(benzylthio)-2-(3-methoxyphenyl)acetate (3l)



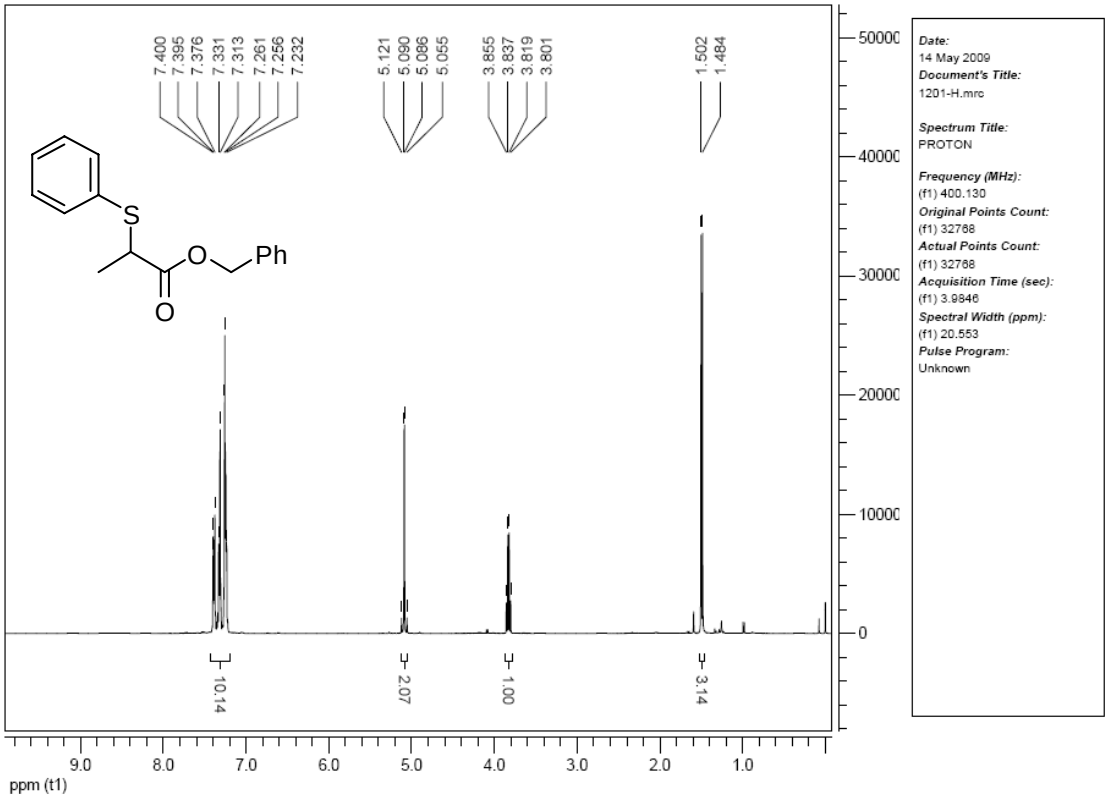


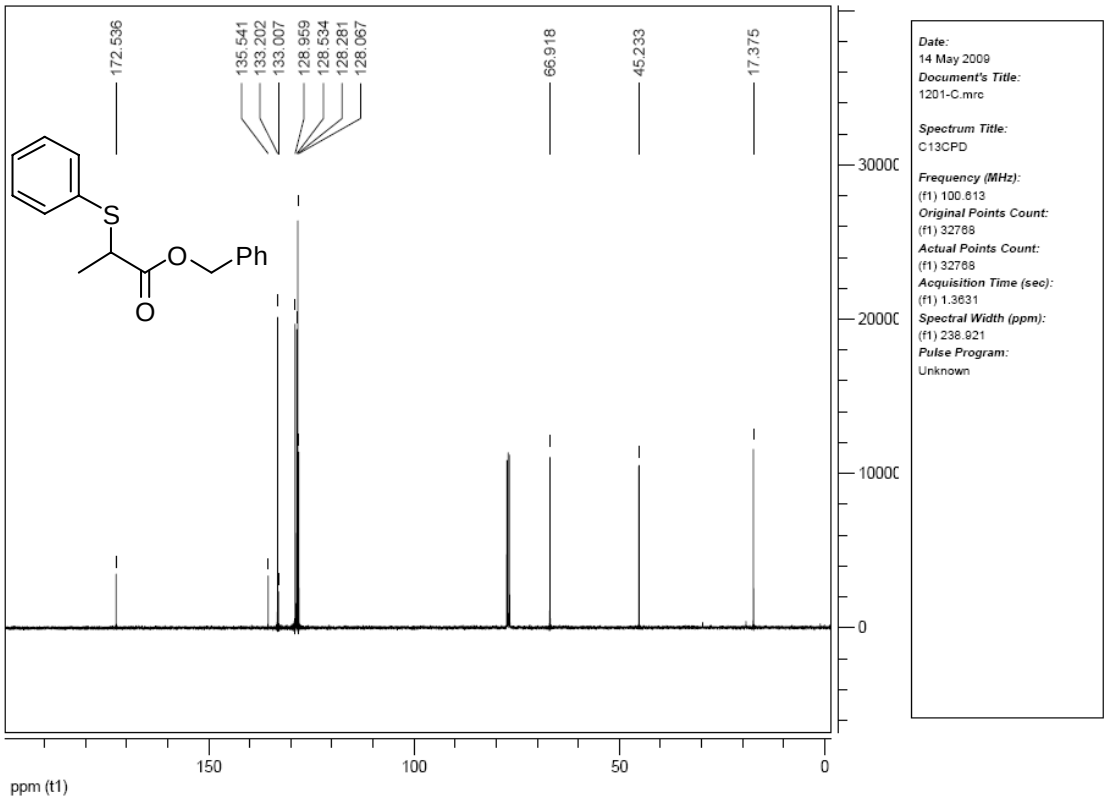
Methyl 2-(benzylthio)-2-(4-methoxyphenyl)acetate (3m)



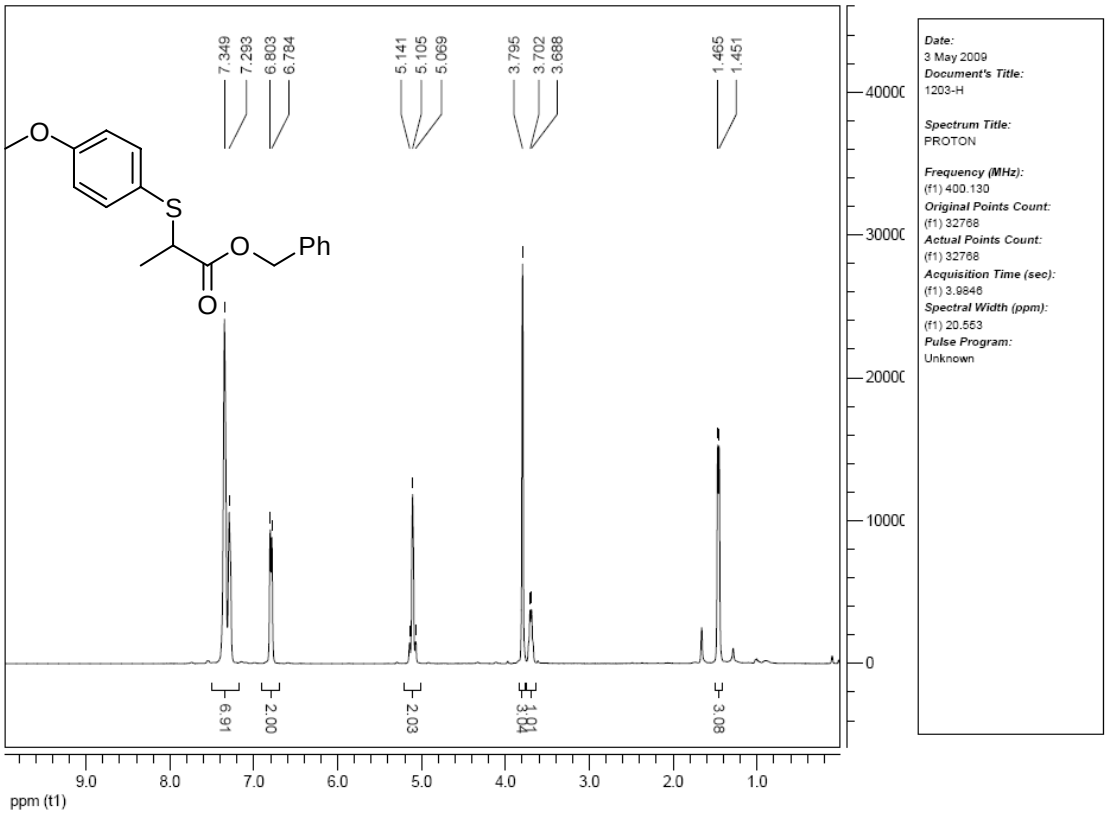


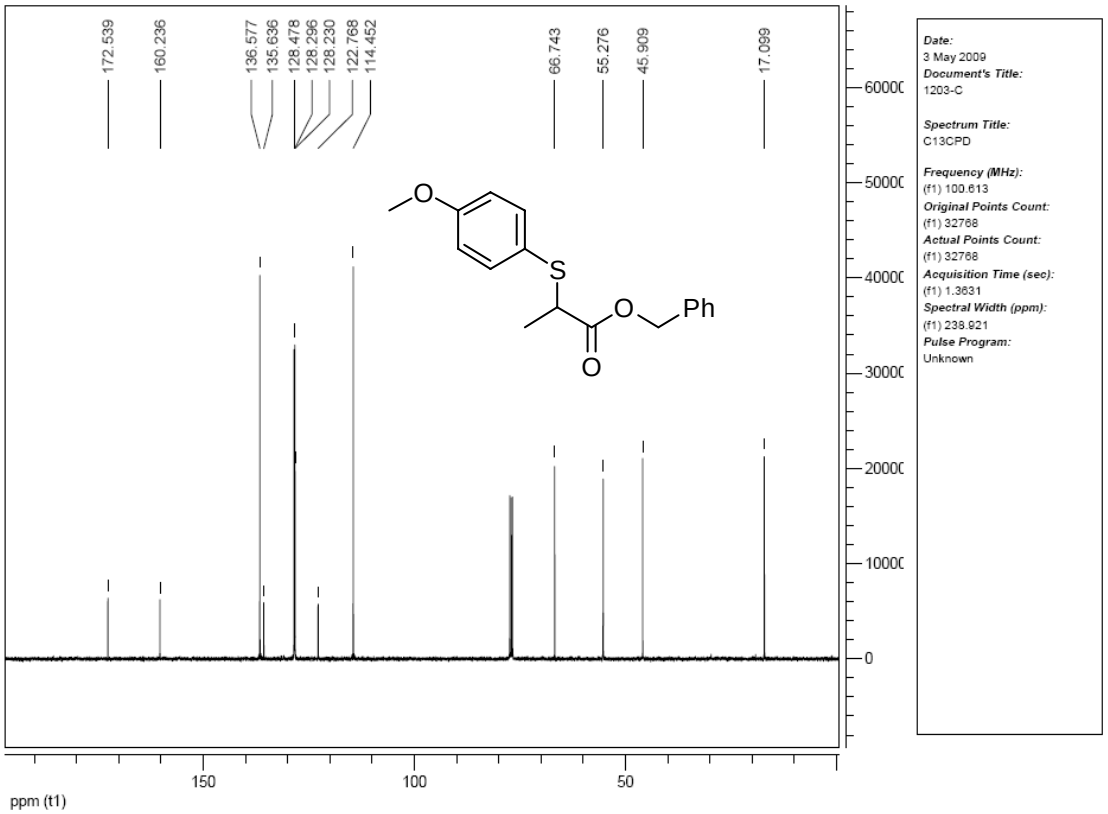
Benzyl 2-(phenylthio)propionate (3n)



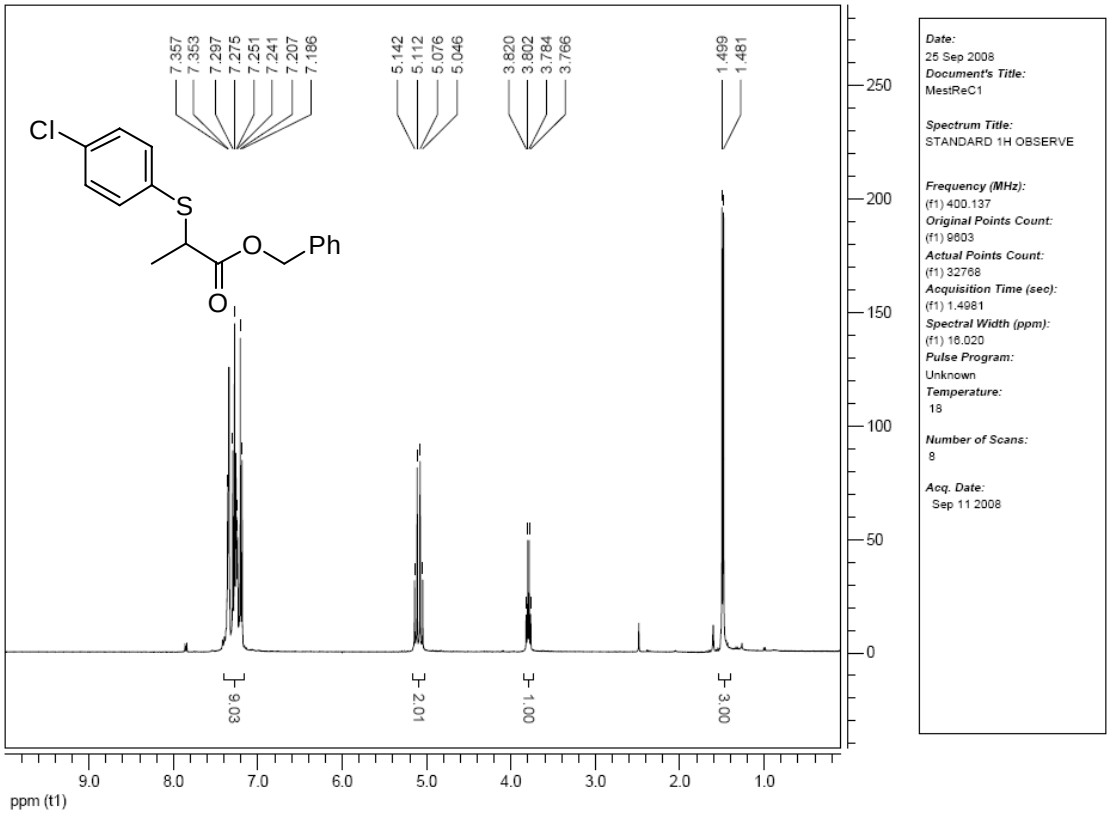


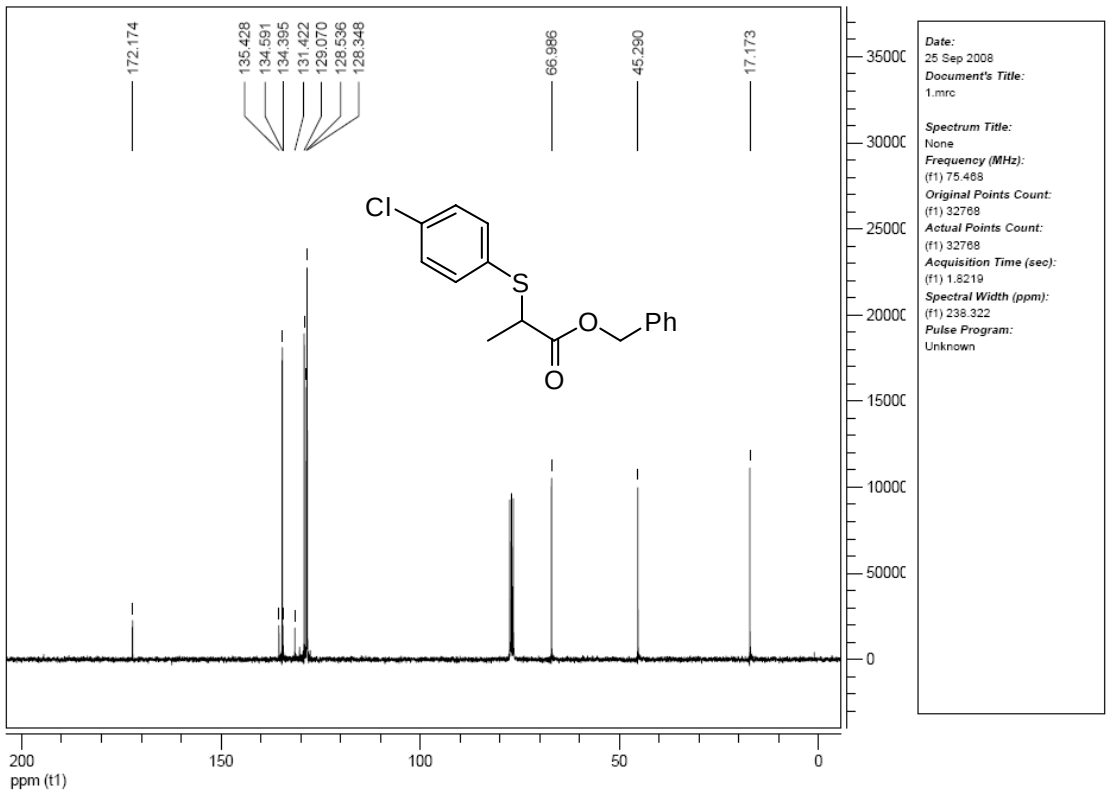
Benzyl 2-(4-methoxyphenylthio)propionate (3o)



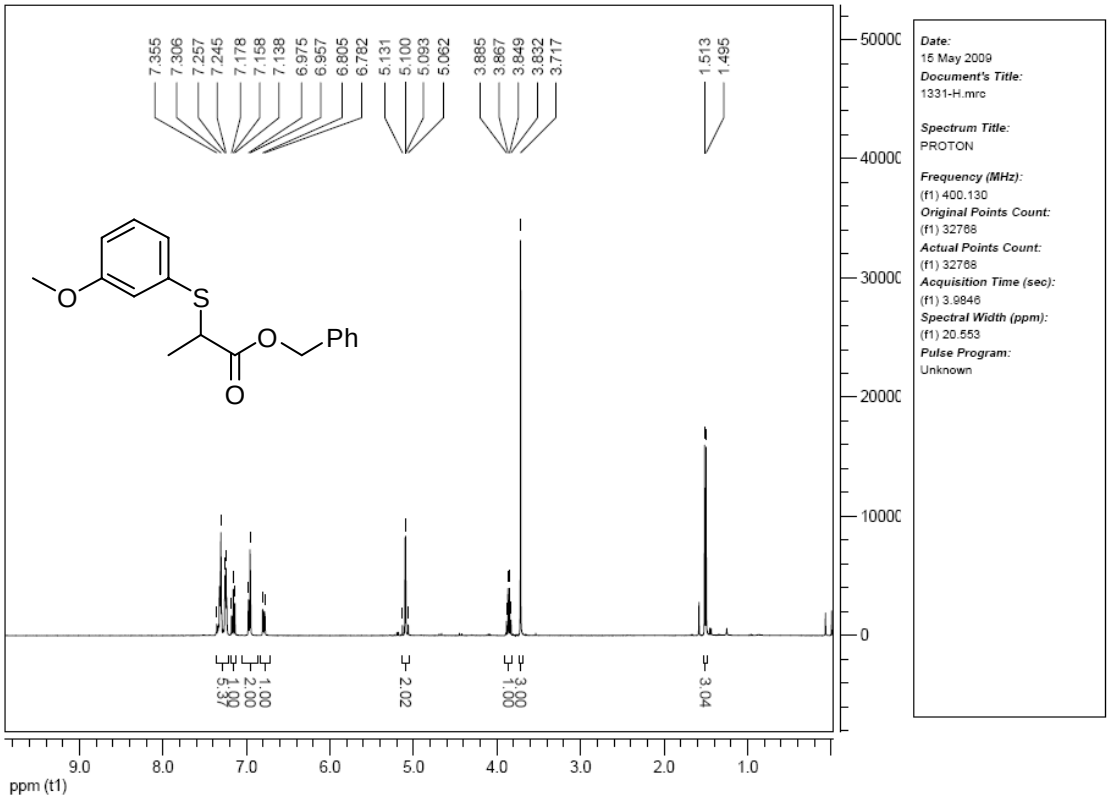


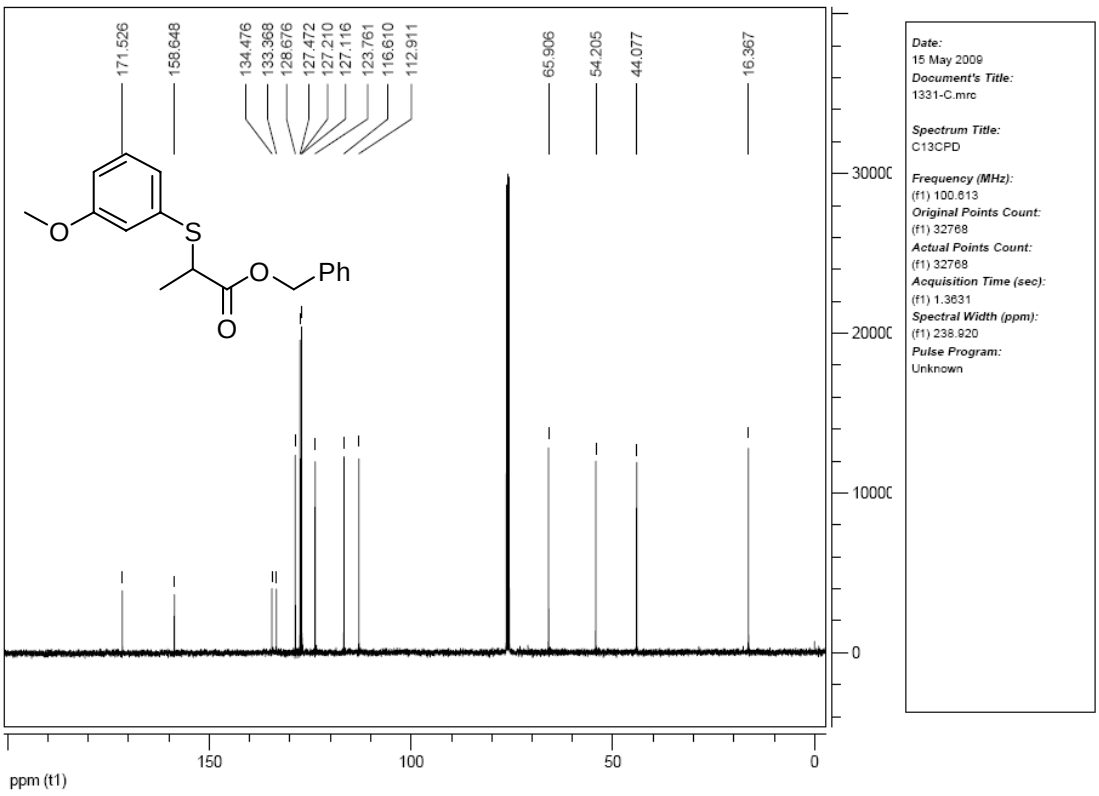
Benzyl 2-(4-chlorophenylthio)propionate (3p)



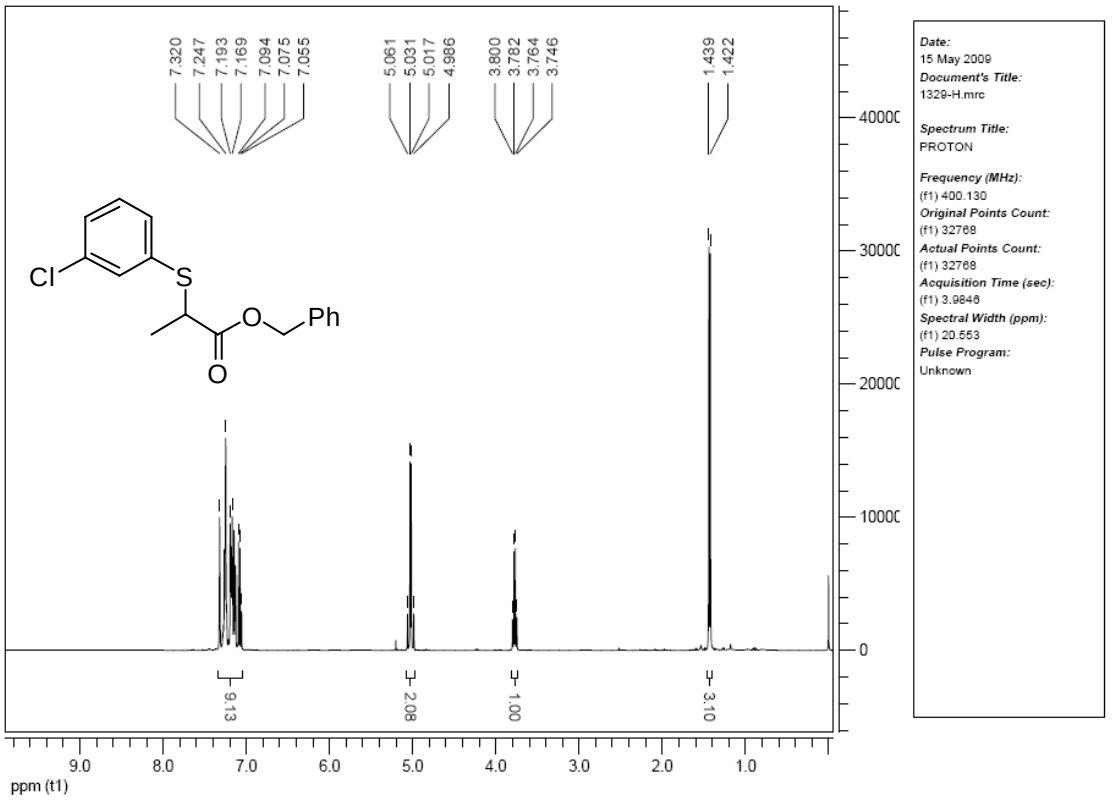


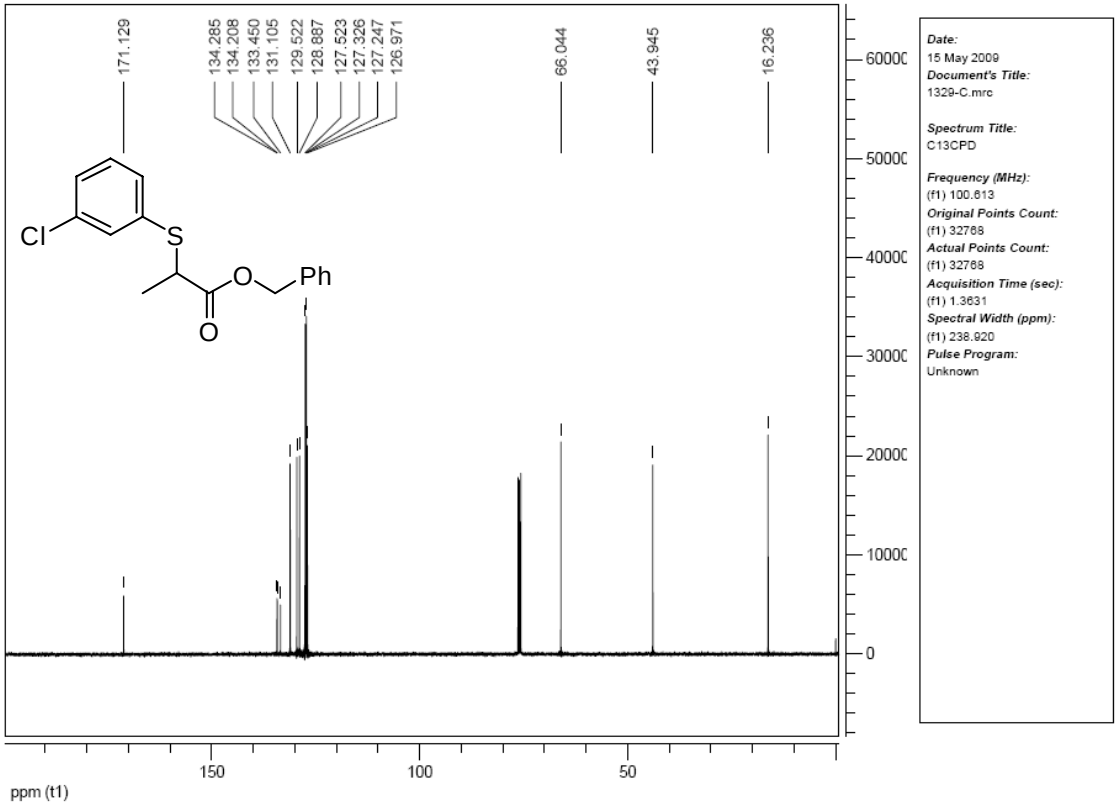
Benzyl 2-(3-methoxyphenylthio)propionate (3q)



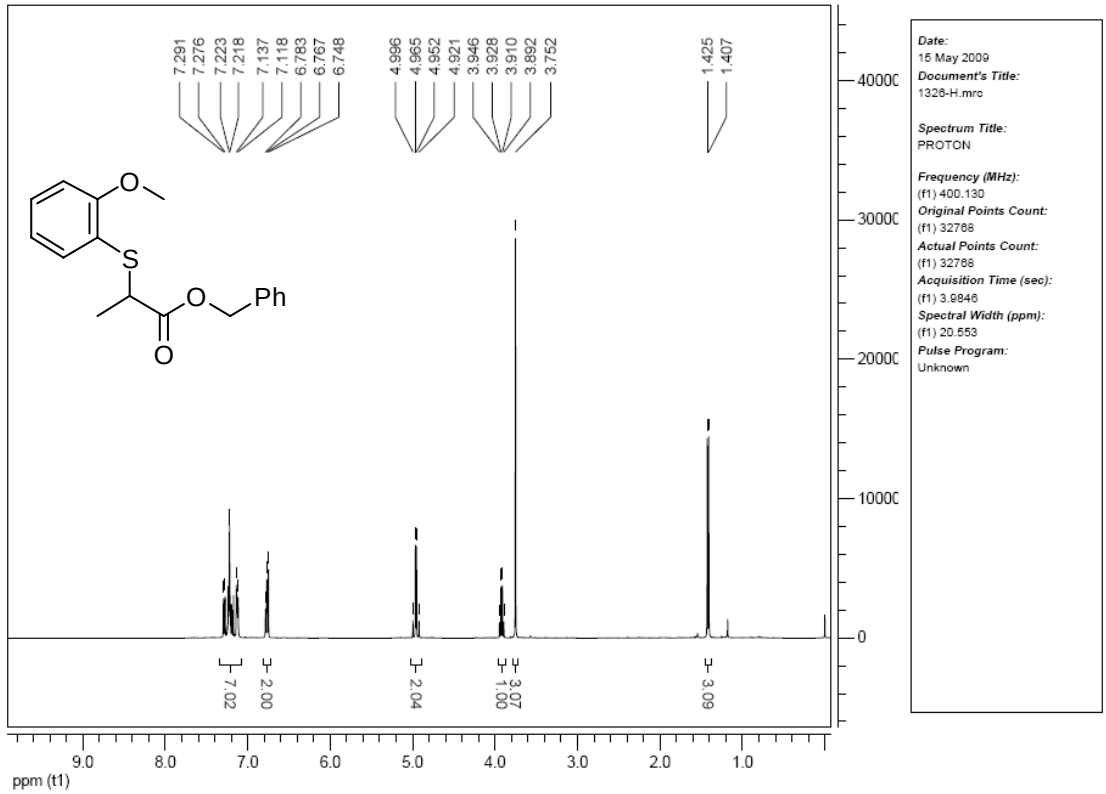


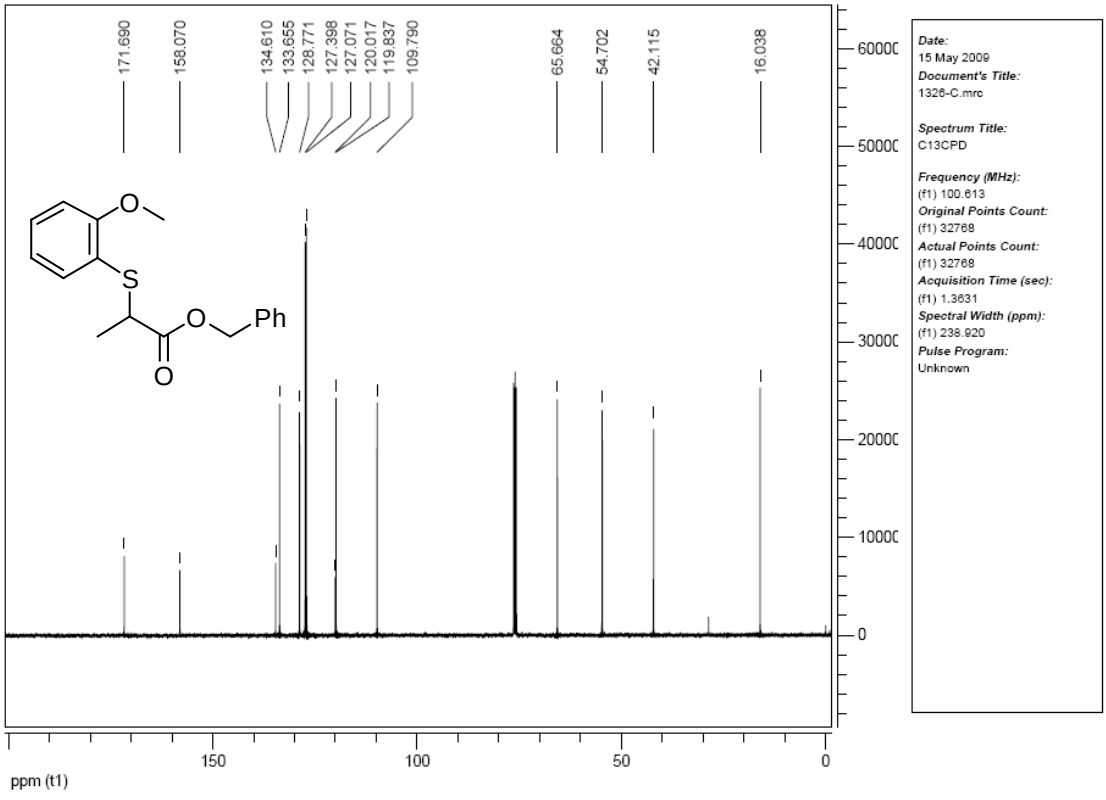
Benzyl 2-(3-chlorophenylthio)propionate (3r)



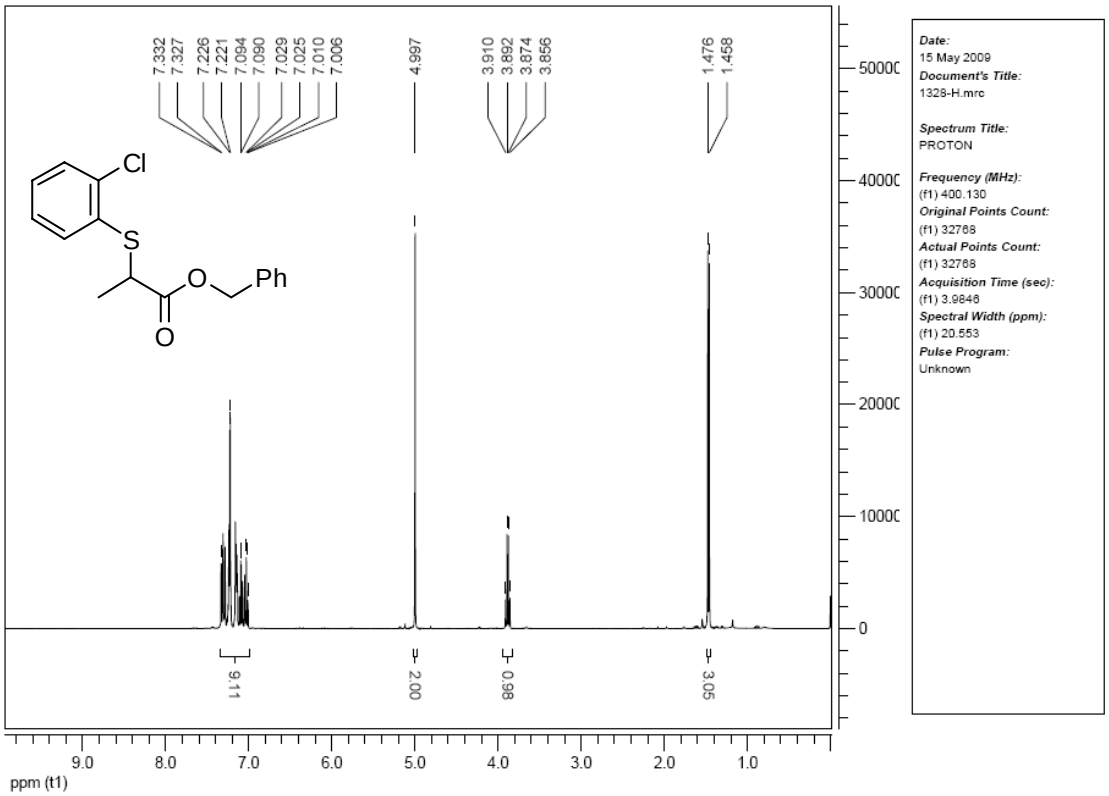


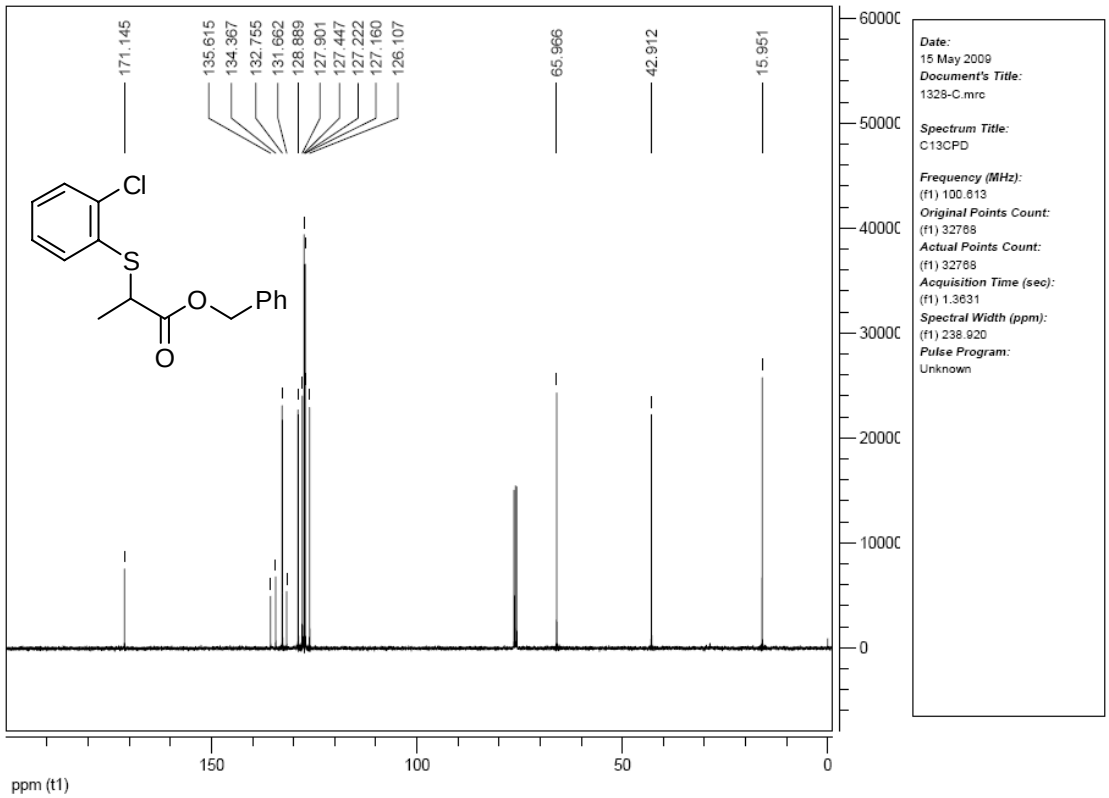
Benzyl 2-(2-methoxyphenylthio)propionate (3s)



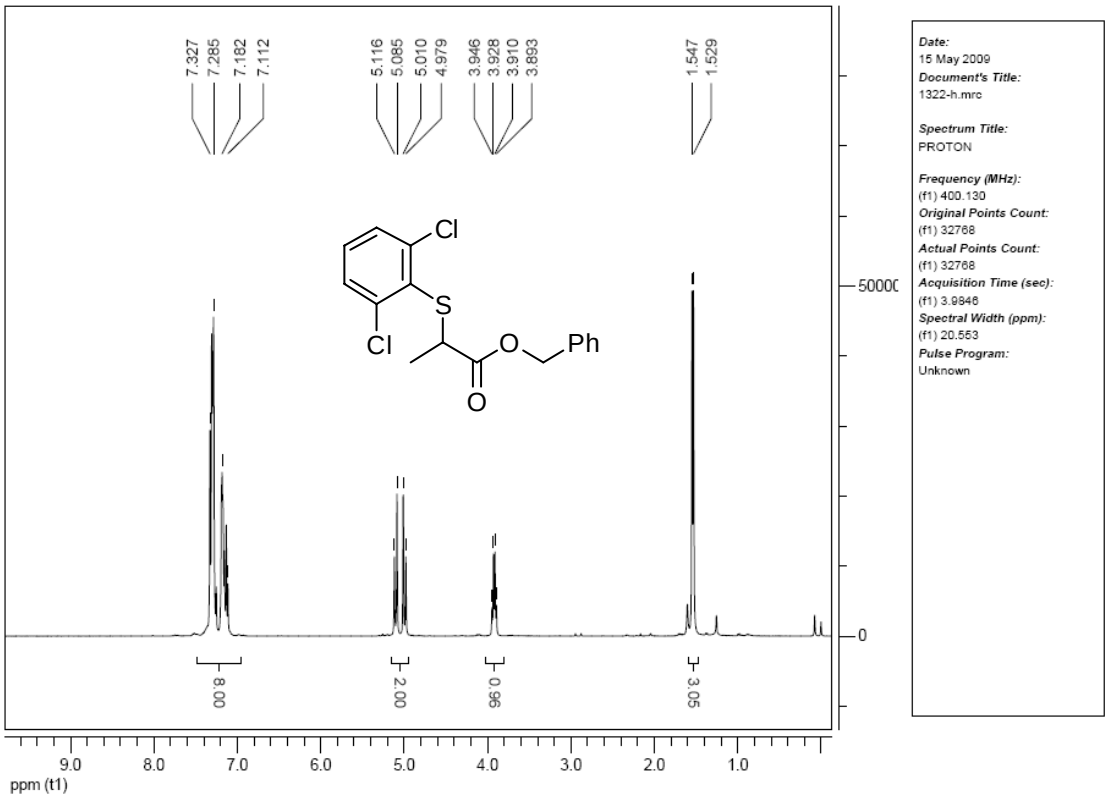


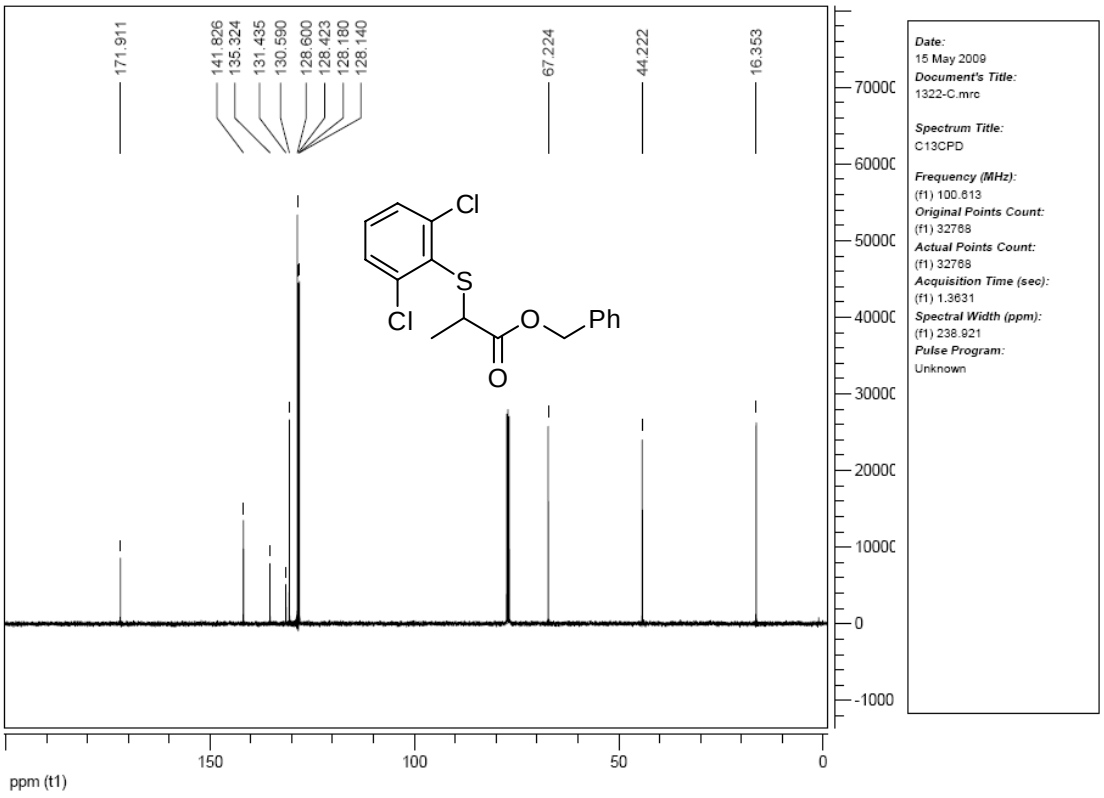
Benzyl 2-(2-chlorophenylthio)propionate (3t)



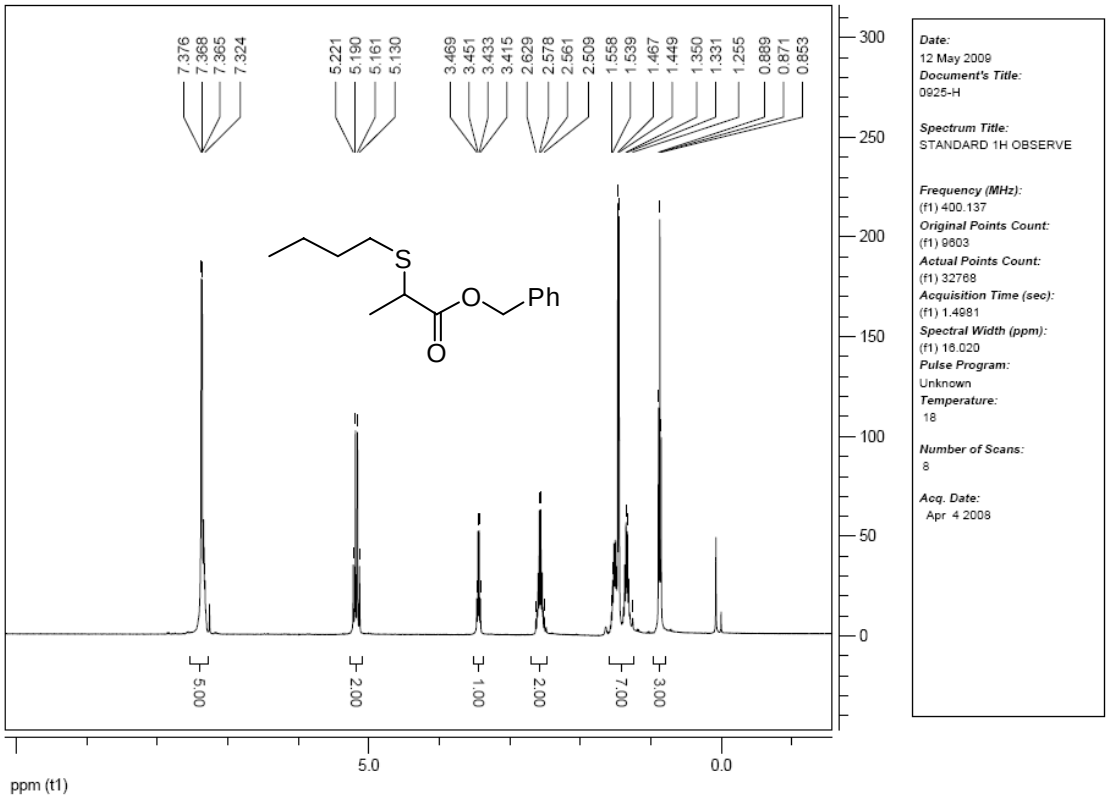


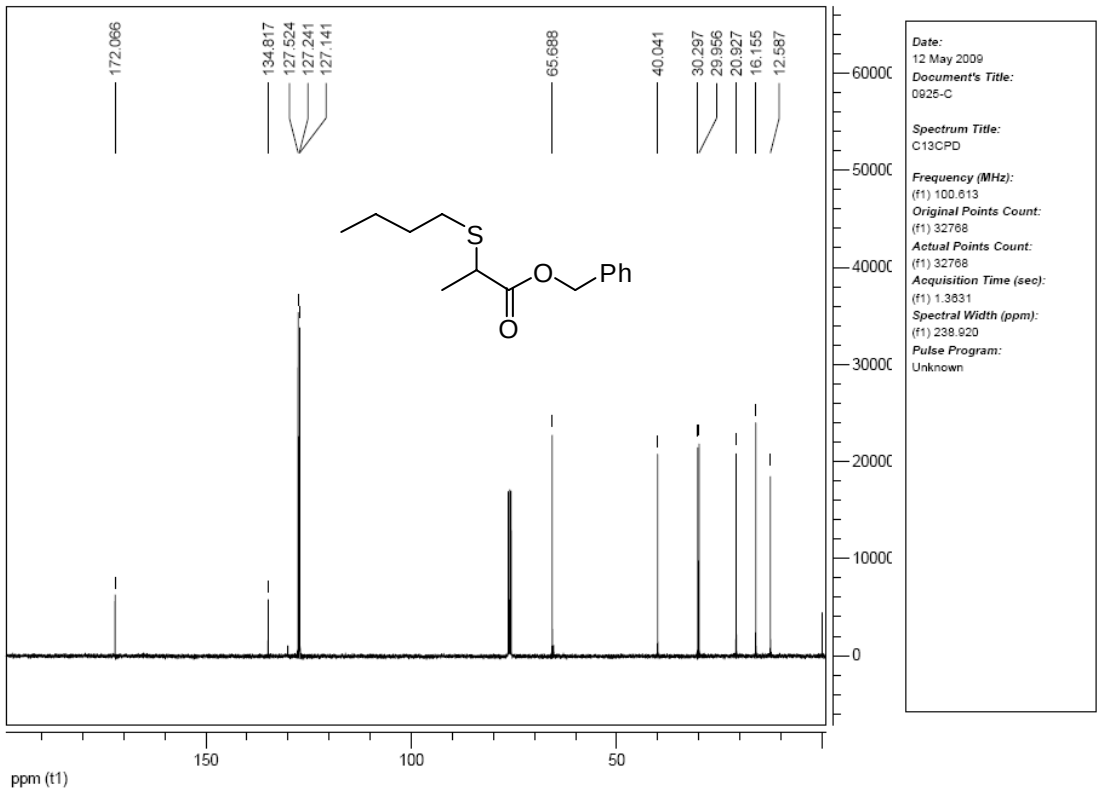
Benzyl 2-(2,6-dichlorophenylthio)propionate (3u)



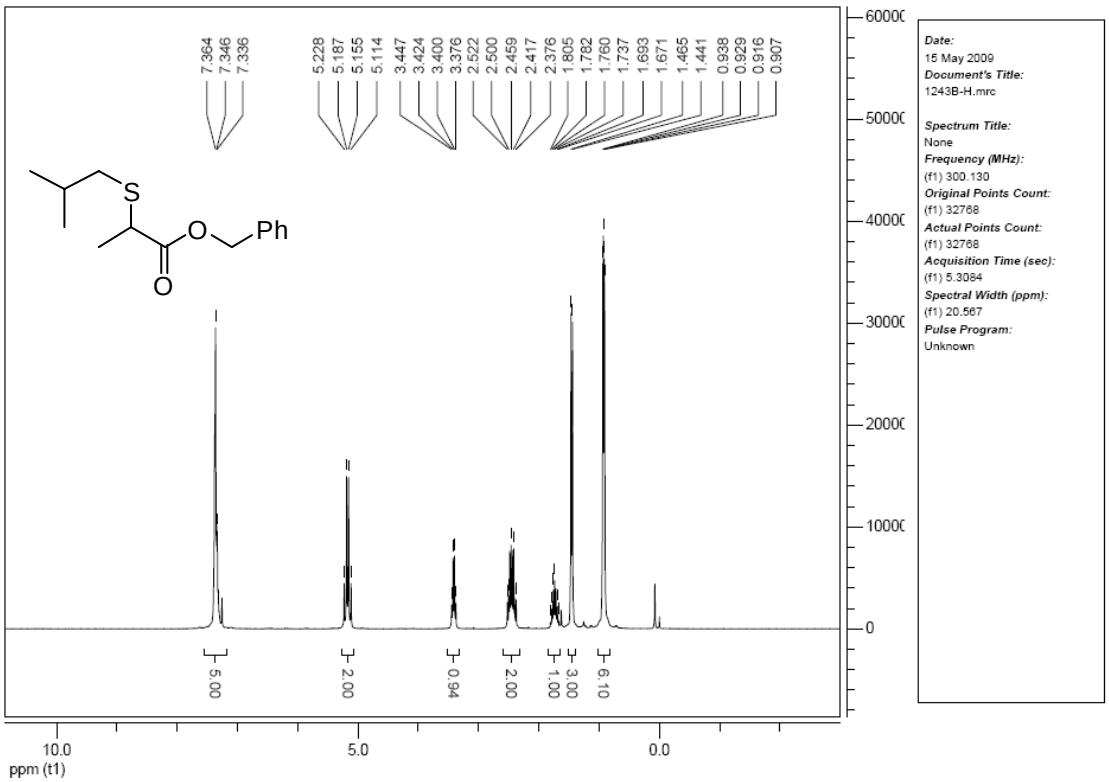


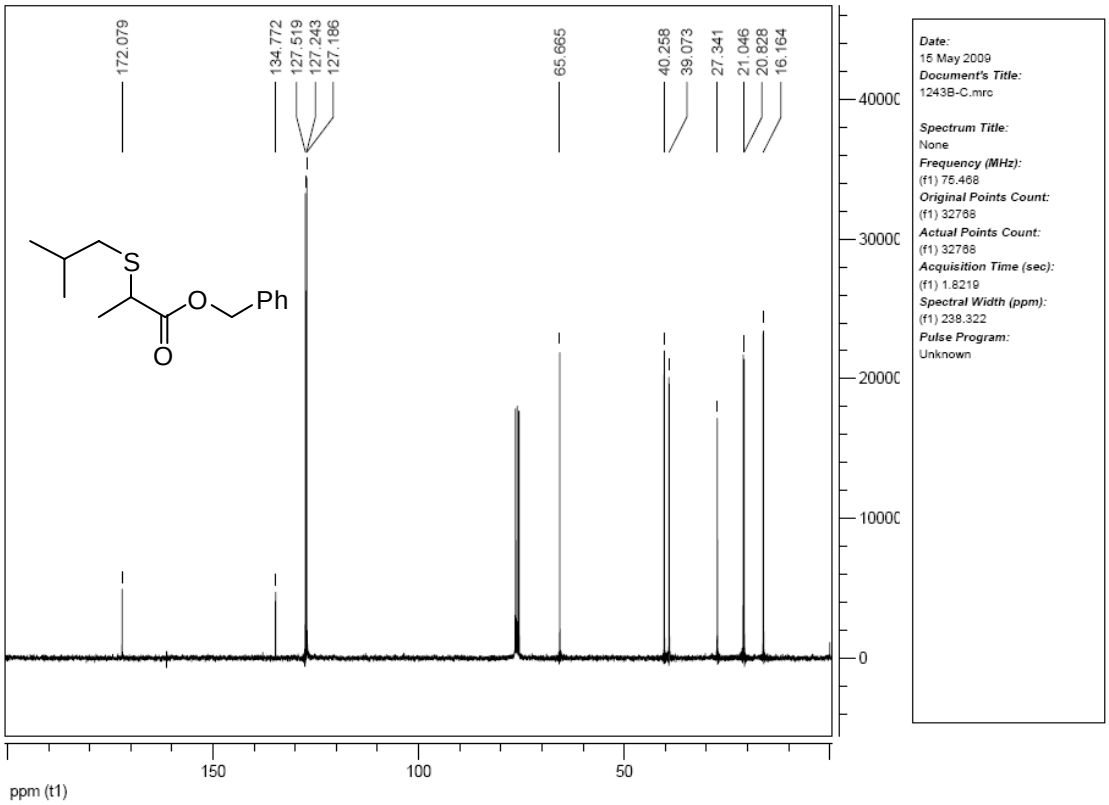
Benzyl 2-(butylthio)propionate (3v)



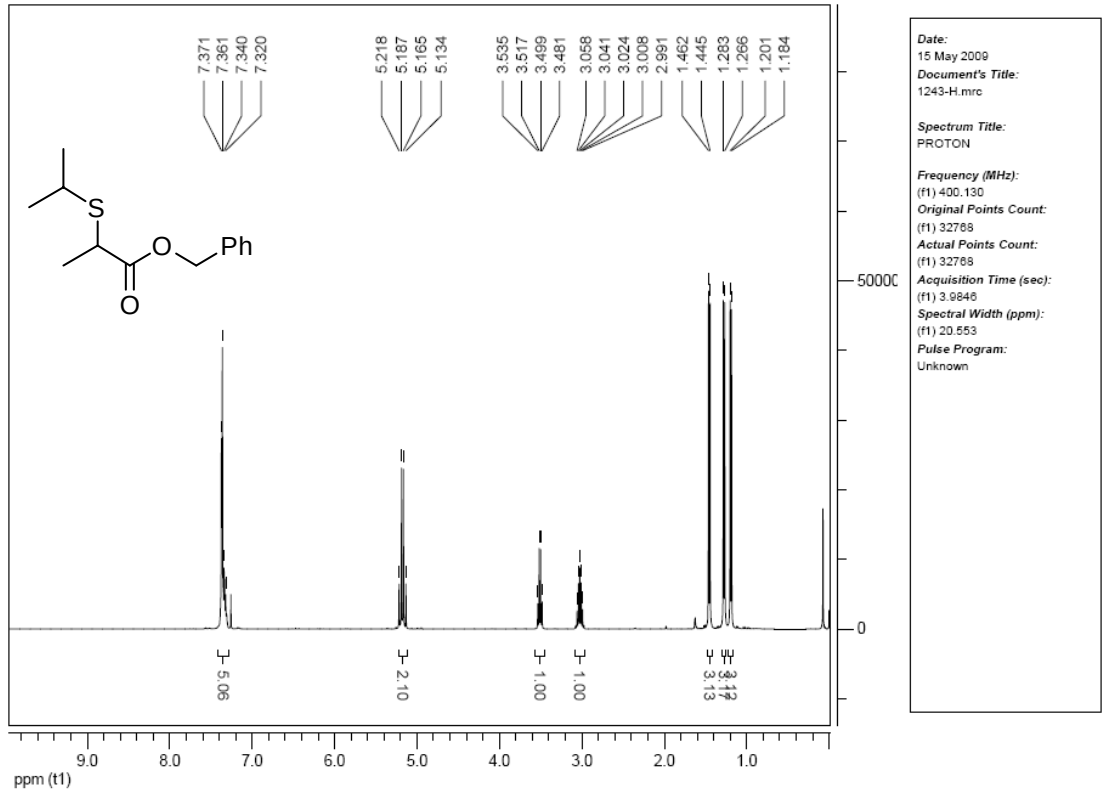


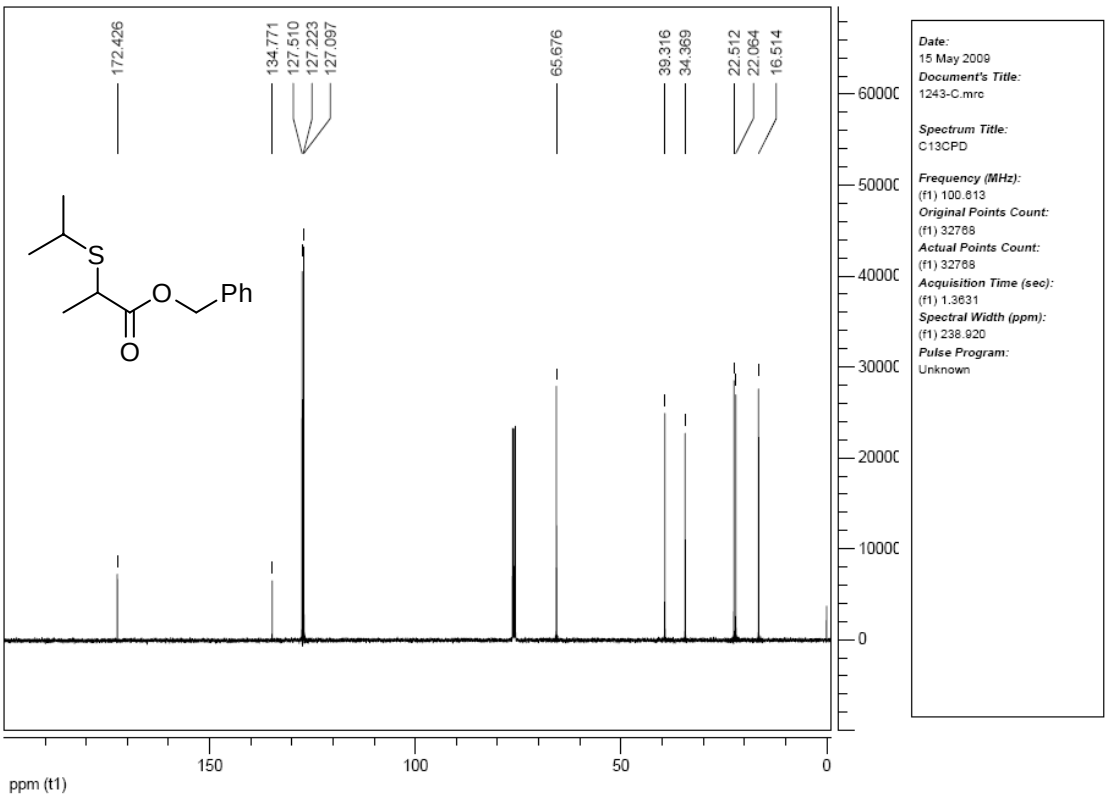
Benzyl 2-(isobutylthio)propionate (3w)



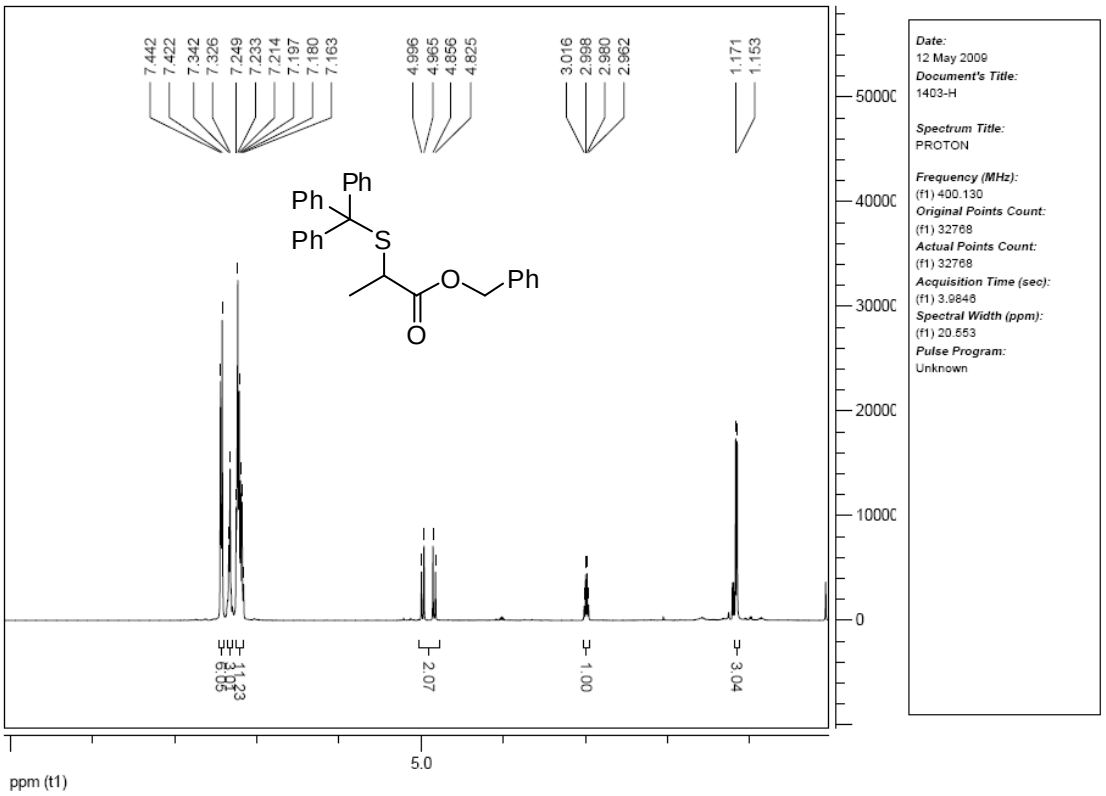


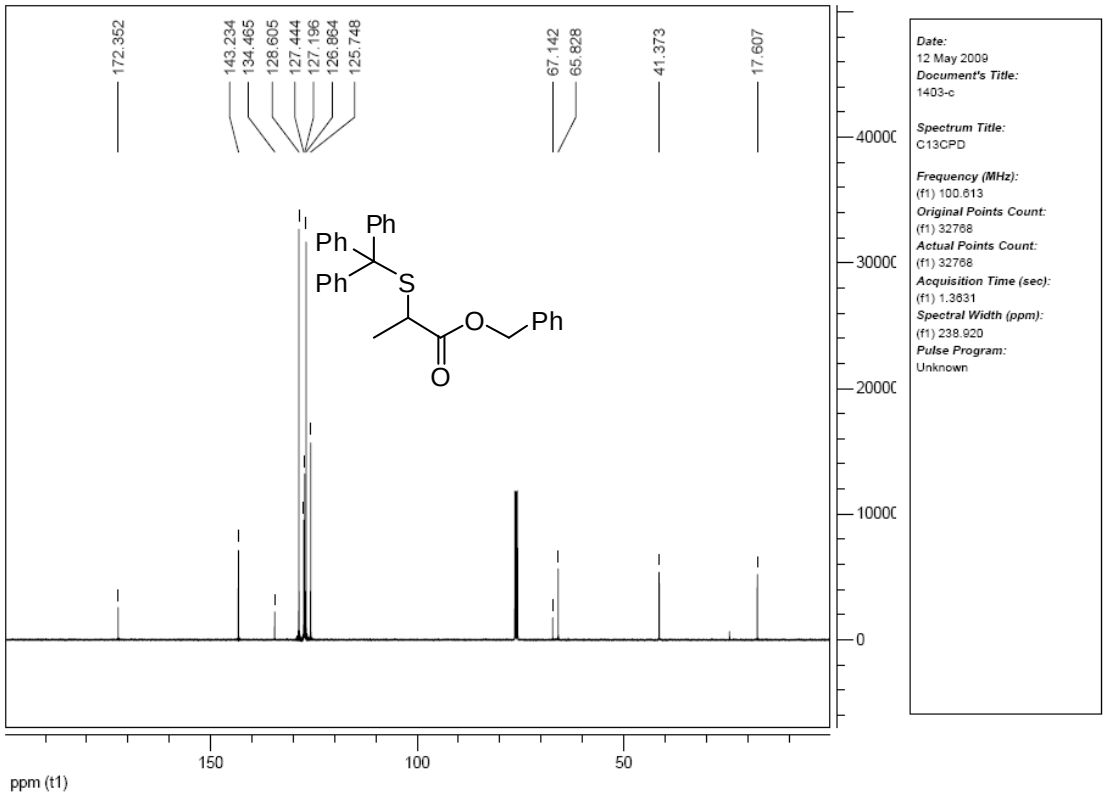
Benzyl 2-(isopropylthio)propionate (3x)





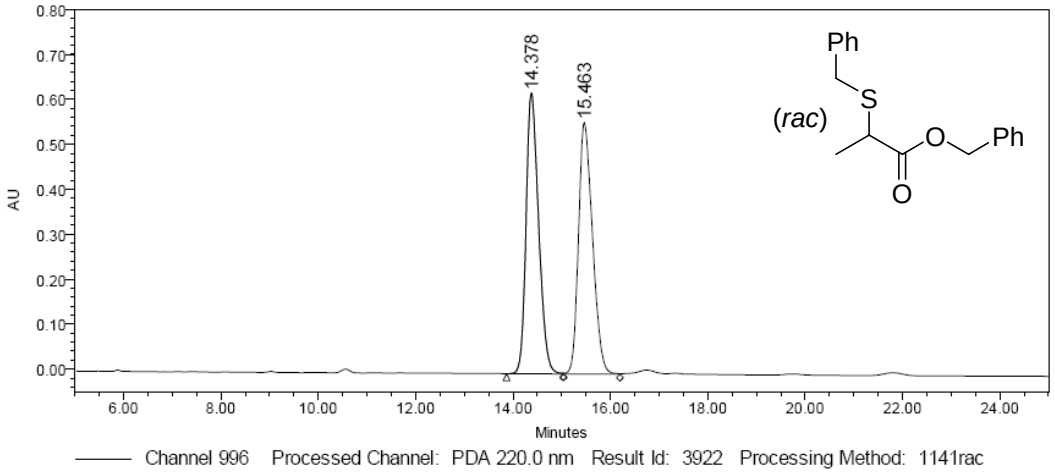
Benzyl 2-(tritylthio)propionate (3y)



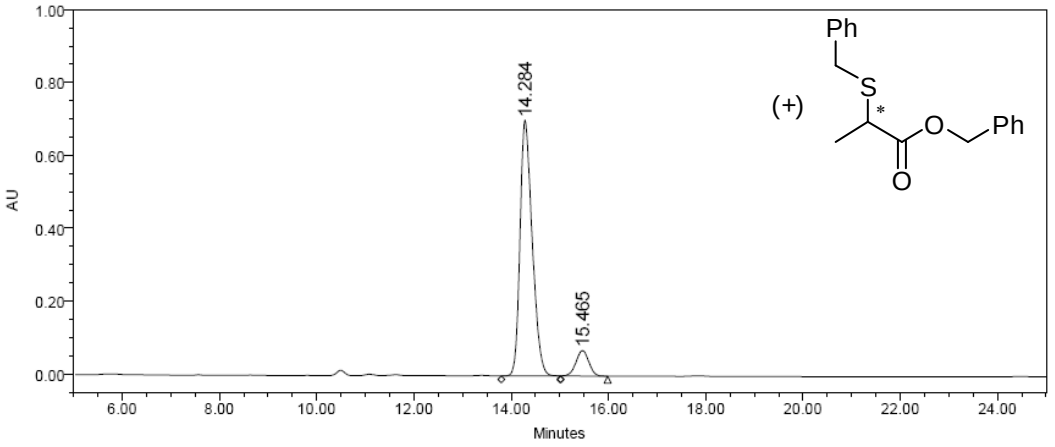


5. HPLC and SFC Charts for S–H insertion Products

(+)-Benzyl 2-(benzylthio)propionate (3a)



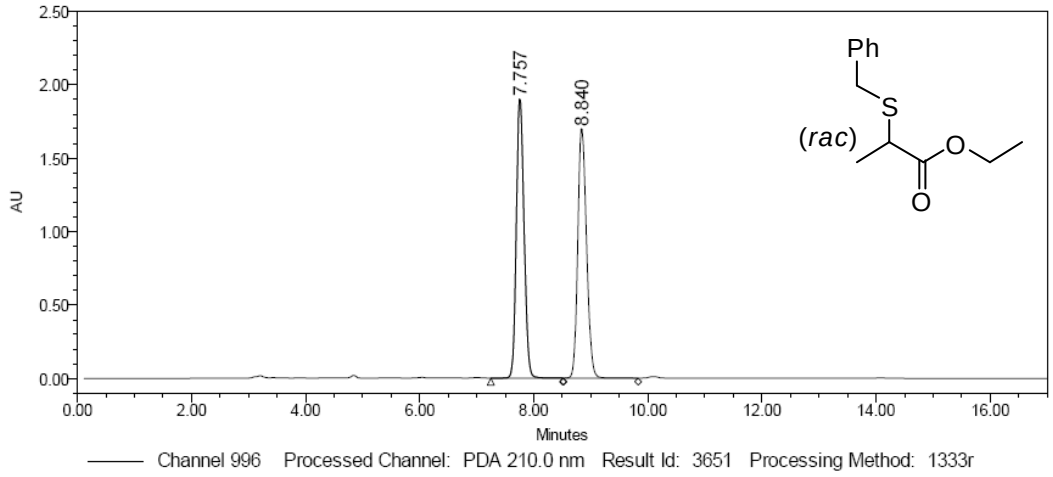
Channel 996 Processed Channel: PDA 220.0 nm Result Id: 3922 Processing Method: 1141rac

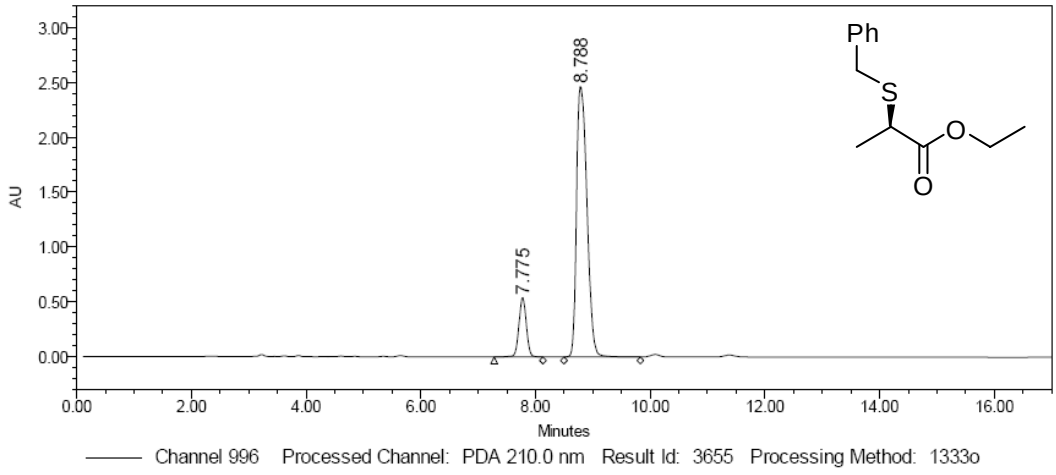


Channel 996 Processed Channel: PDA 220.0 nm Result Id: 3926 Processing Method: 1141opt

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 220.0 nm	14.284	12235642	90.50	702233
2	PDA 220.0 nm	15.465	1283800	9.50	69724

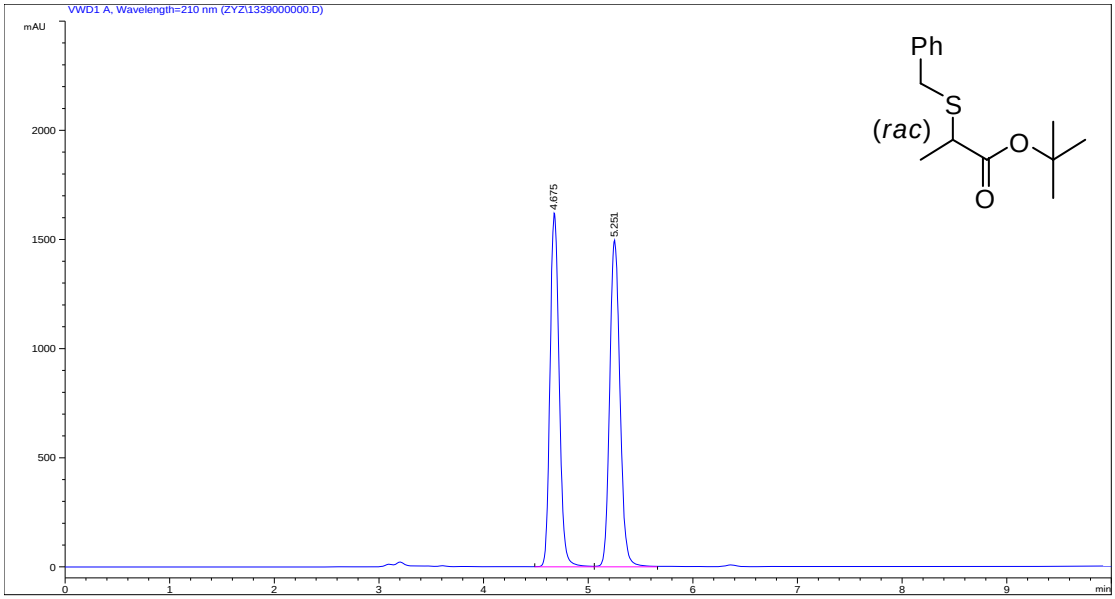
(*R*)-Ethyl 2-(benzylthio)propionate (3b)

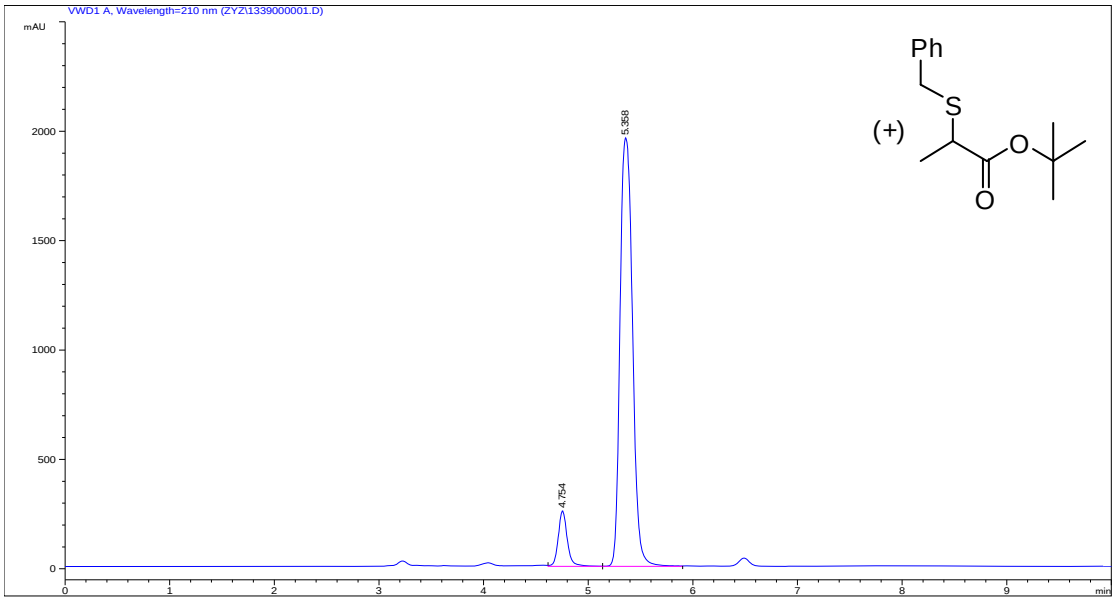




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	7.775	4802436	13.31	541278
2	PDA 210.0 nm	8.788	31276126	86.69	2481210

(+)-*tert*-Butyl 2-(benzylthio)propionate (3c)

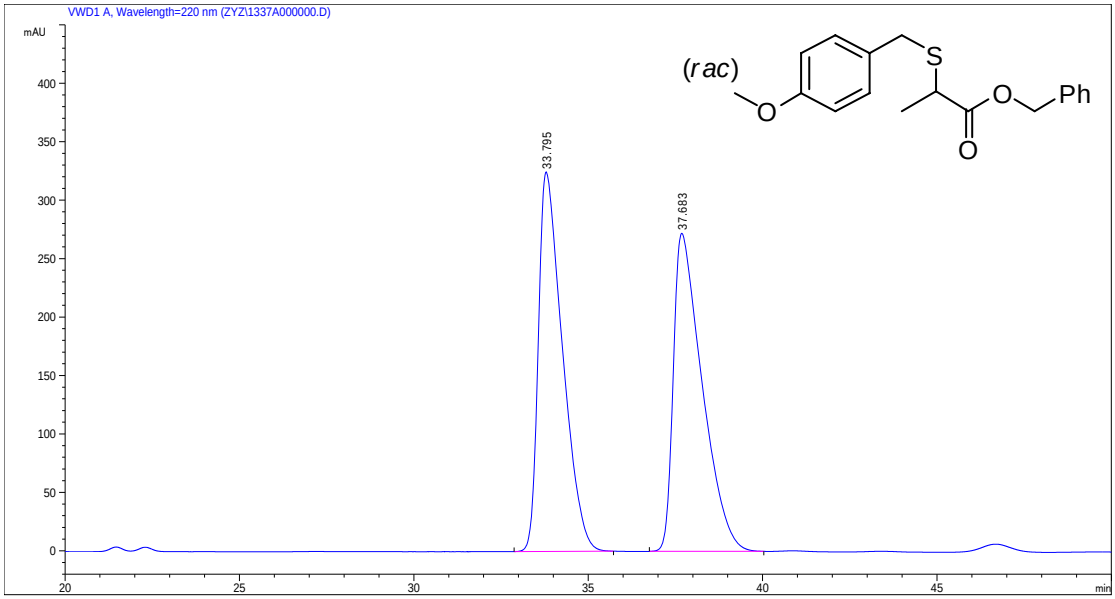


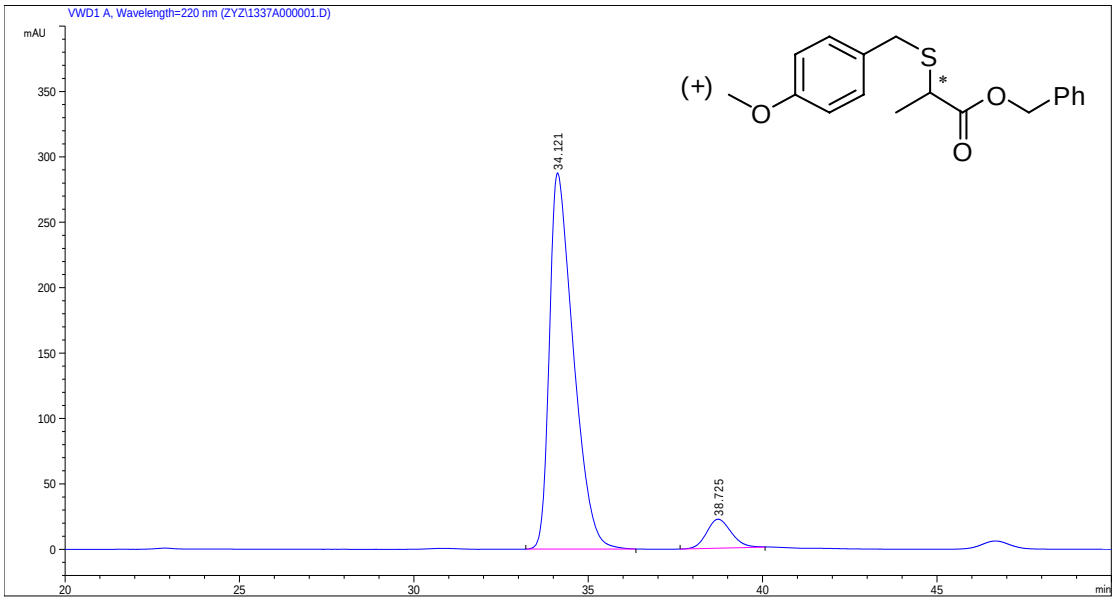


Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.754	VV	0.0907	1527.44092	253.56578	8.6250
2	5.358	VV	0.1328	1.61821e4	1958.29248	91.3750

(+)-Benzyl 2-(4-methoxybenzylthio)propionate (3d)

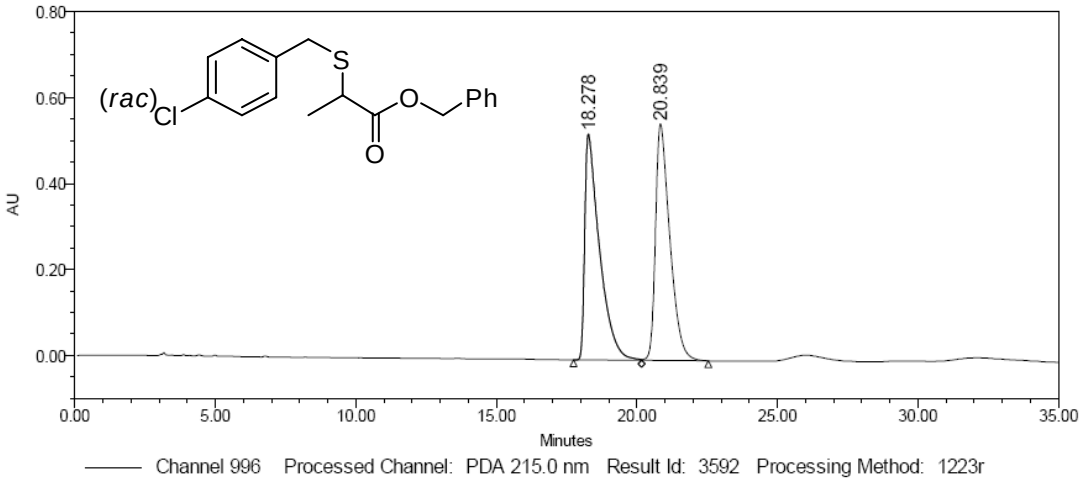


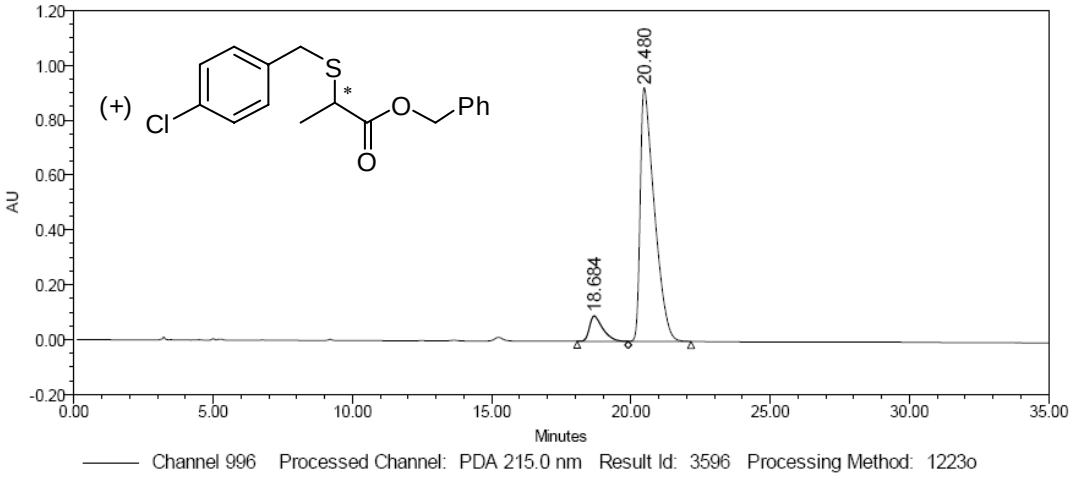


Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	34.121	BB	0.7086	1.37386e4	287.69446	92.6446
2	38.725	BB	0.7455	1090.75757	22.18112	7.3554

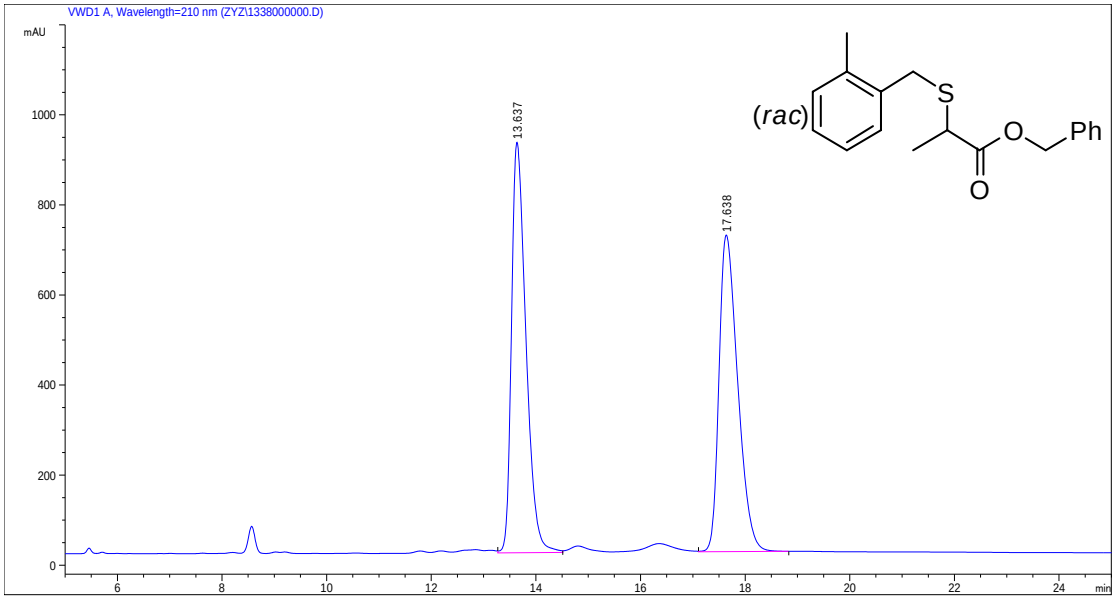
(+)-Benzyl 2-(4-chlorobenzylthio)propionate (3e)

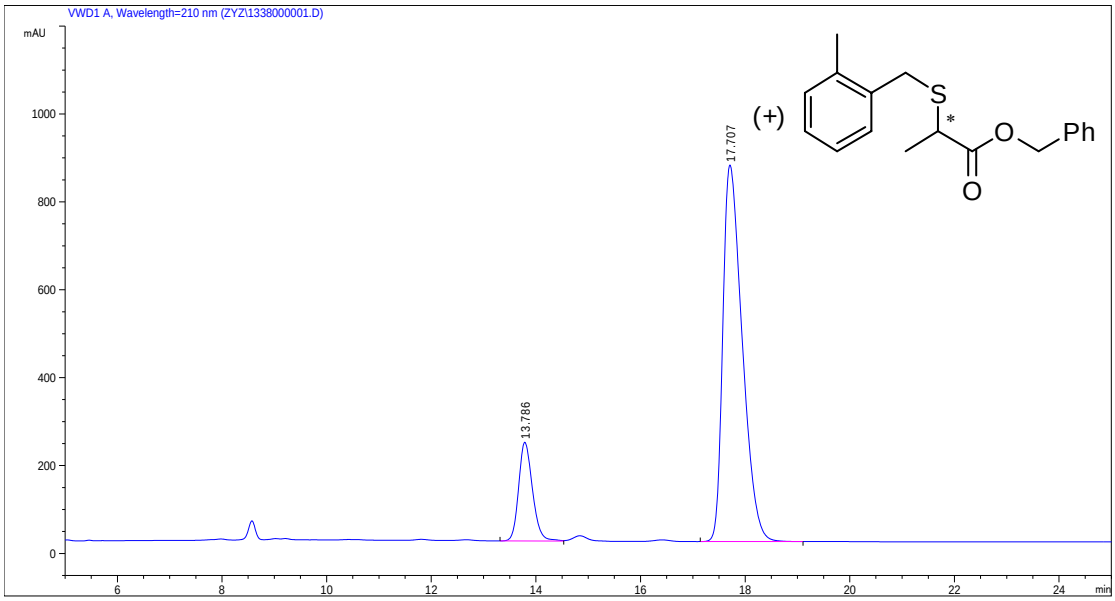




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 215.0 nm	18.684	3083402	8.62	92495
2	PDA 215.0 nm	20.480	32668773	91.38	925162

(+)-Benzyl 2-(2-methylbenzylthio)propionate (3f)

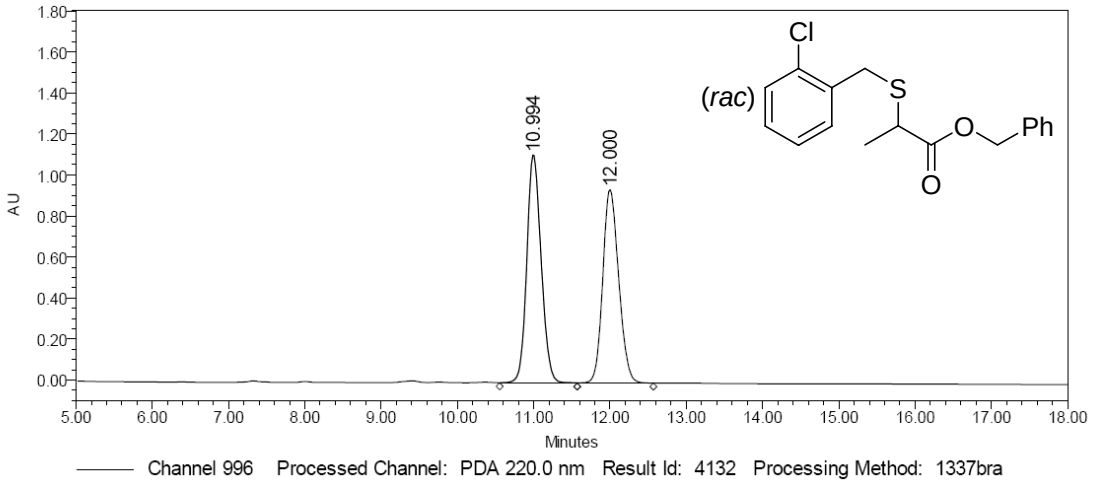


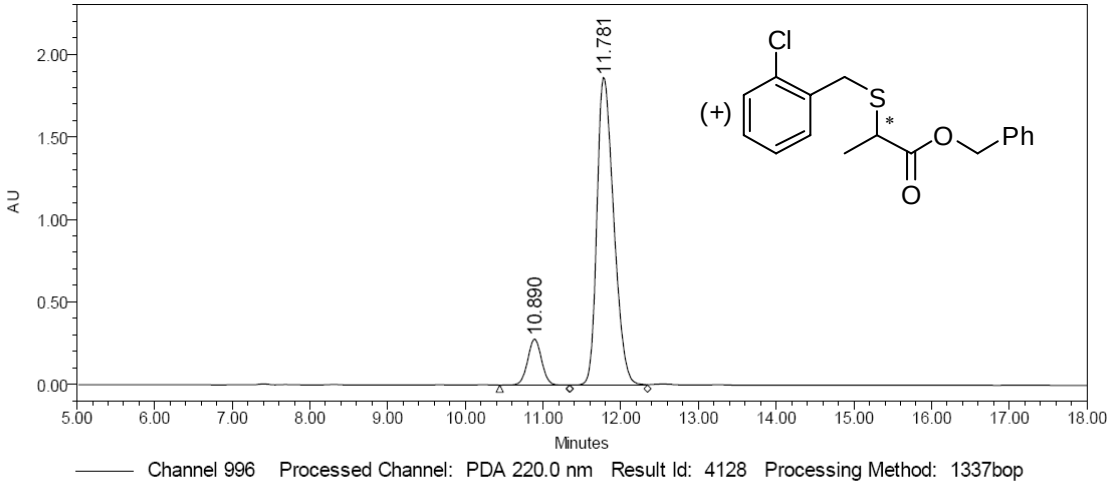


Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.786	BV	0.2832	4135.66553	224.66208	15.7884
2	17.707	BB	0.3964	2.20587e4	856.96472	84.2116

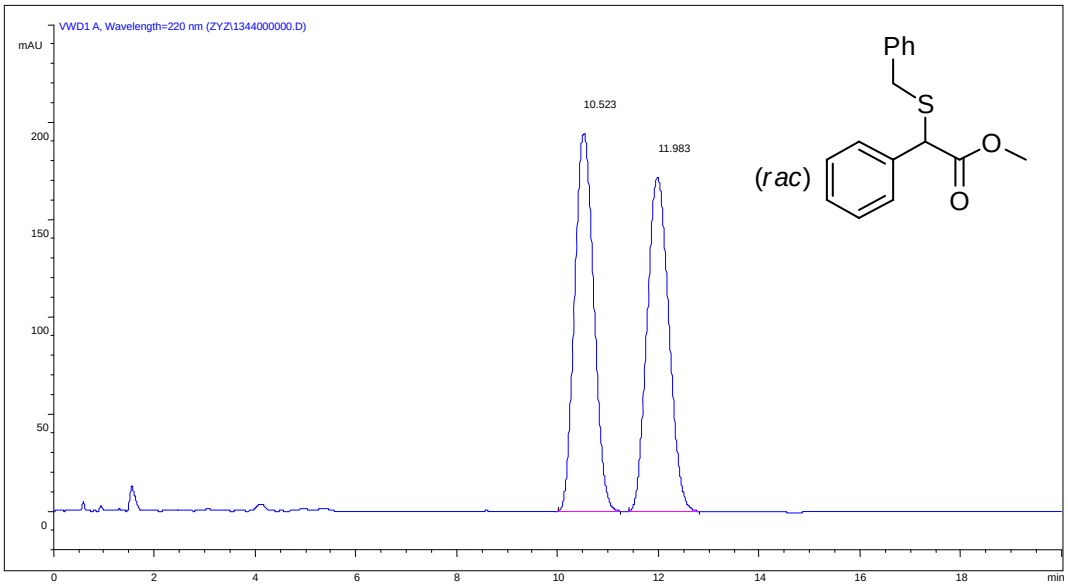
(+)-Benzyl 2-(2-chlorobenzylthio)propionate (3g)

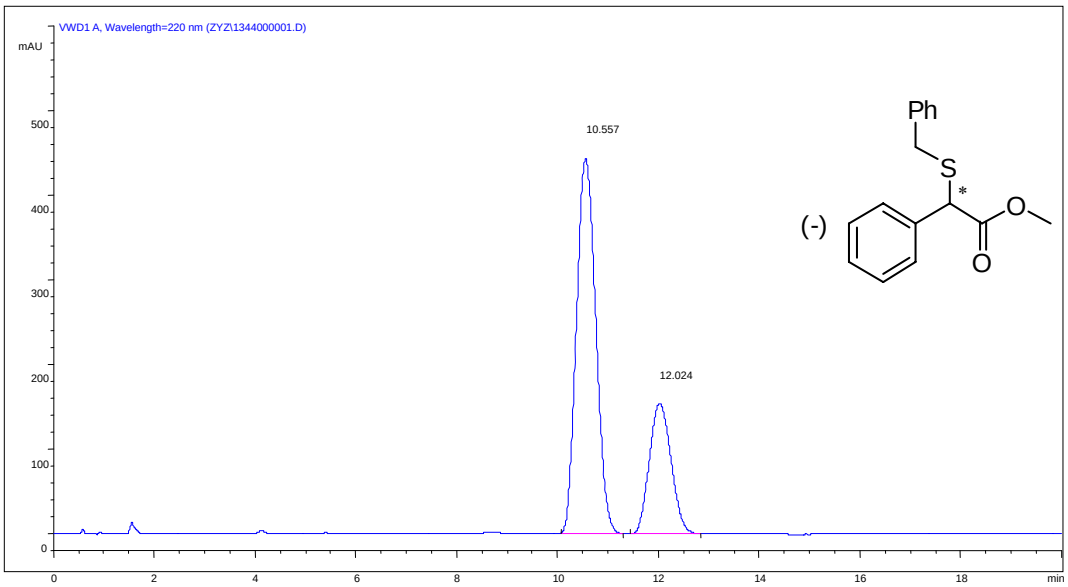




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 220.0 nm	10.890	3473753	11.04	279164
2	PDA 220.0 nm	11.781	27993104	88.96	1870289

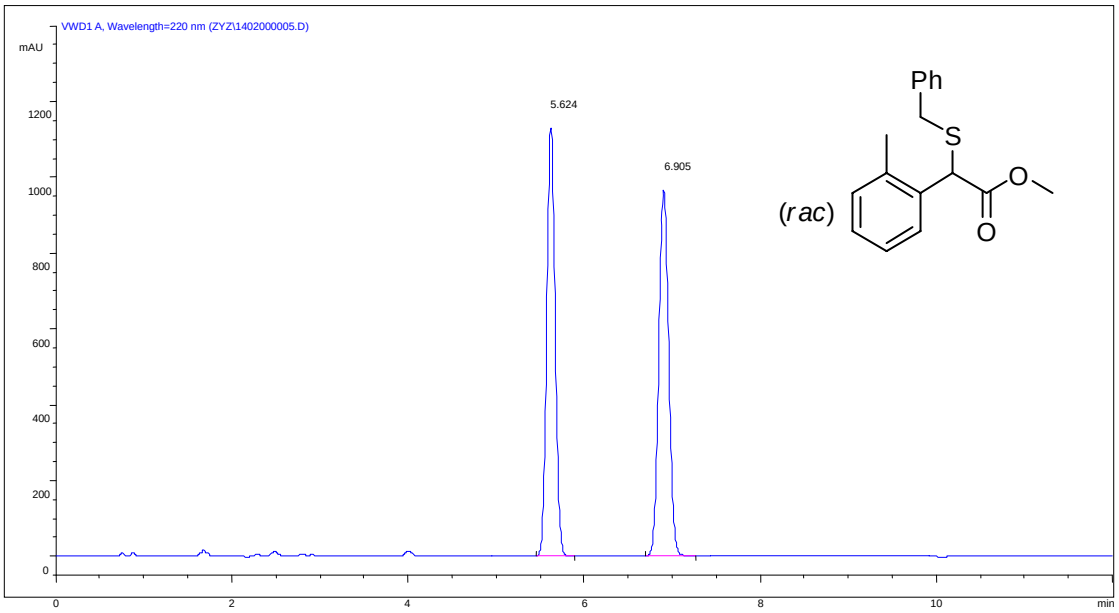
(-)-Methyl 2-(benzylthio)-2-phenylacetate (3h)

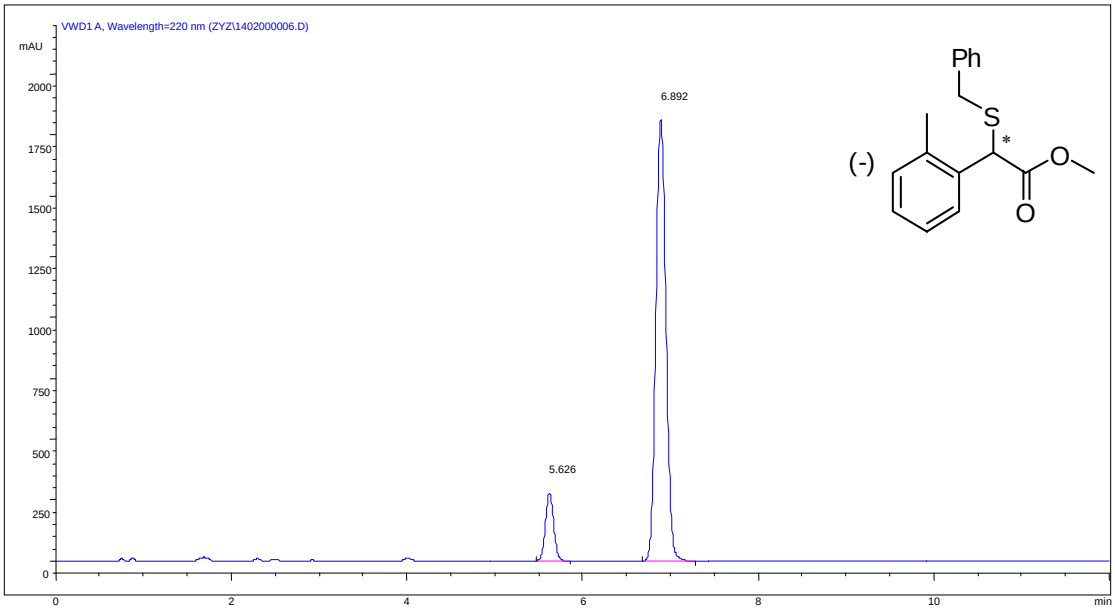




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	10.557	BB	0.4186	1.17970e4	71.8774
2	12.024	BB	0.4721	4615.64453	28.1226

(-)-Methyl 2-(benzylthio)-2-o-tolylacetate (3i)

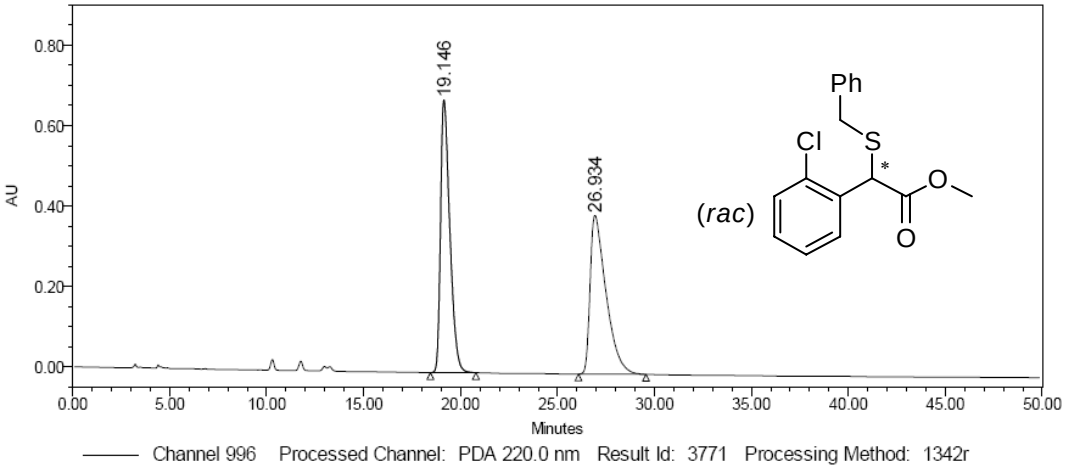


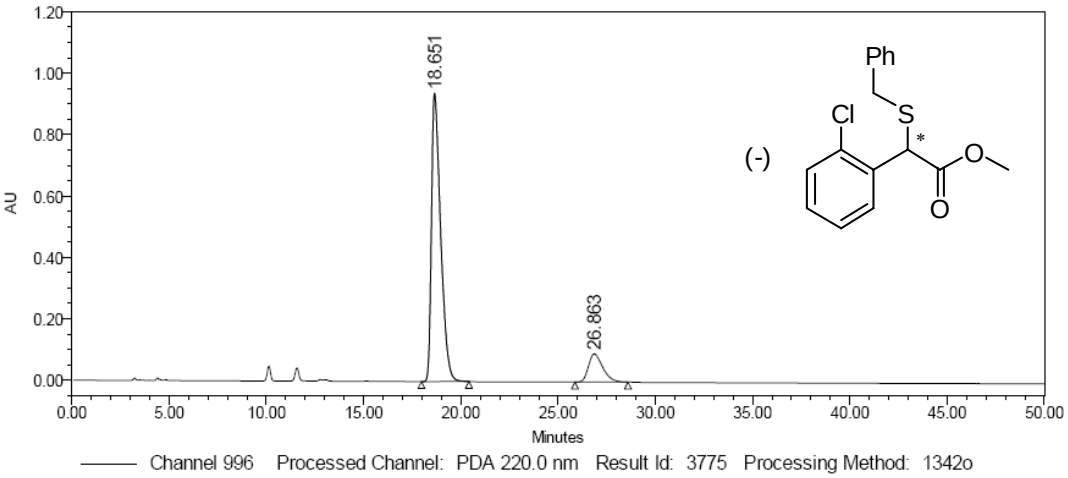


Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	5.626	BB	0.1032	1830.85364	11.3029
2	6.892	BB	0.1245	1.43672e4	88.6971

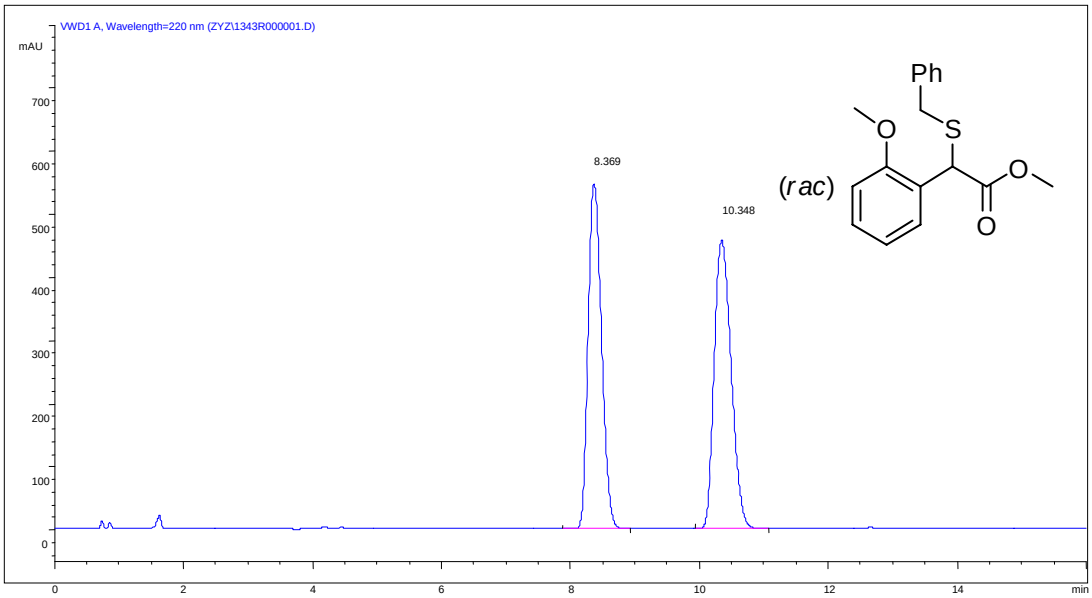
(-)-Methyl 2-(benzylthio)-2-(2-chlorophenyl)acetate (3j)

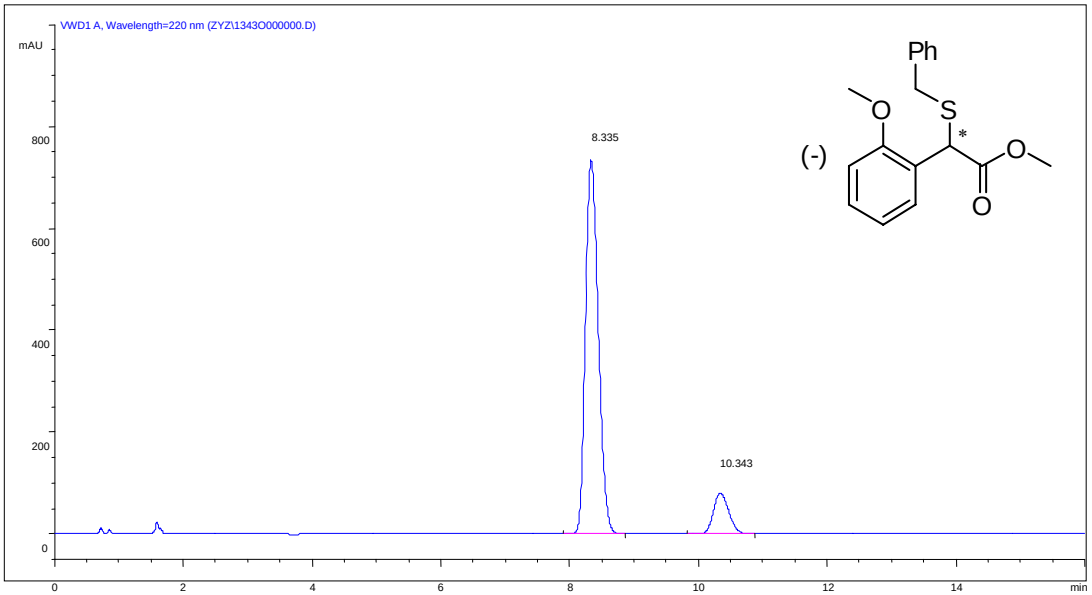




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 220.0 nm	18.651	30730602	86.68	938963
2	PDA 220.0 nm	26.863	4721589	13.32	91867

(-)-Methyl 2-(benzylthio)-2-(2-methoxyphenyl)acetate (3k)

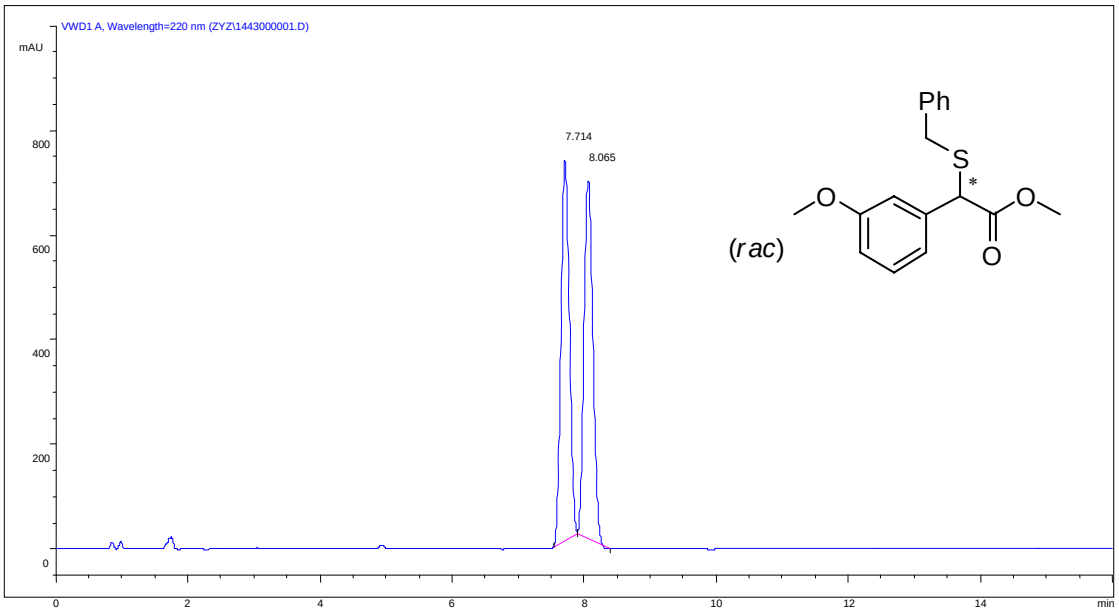


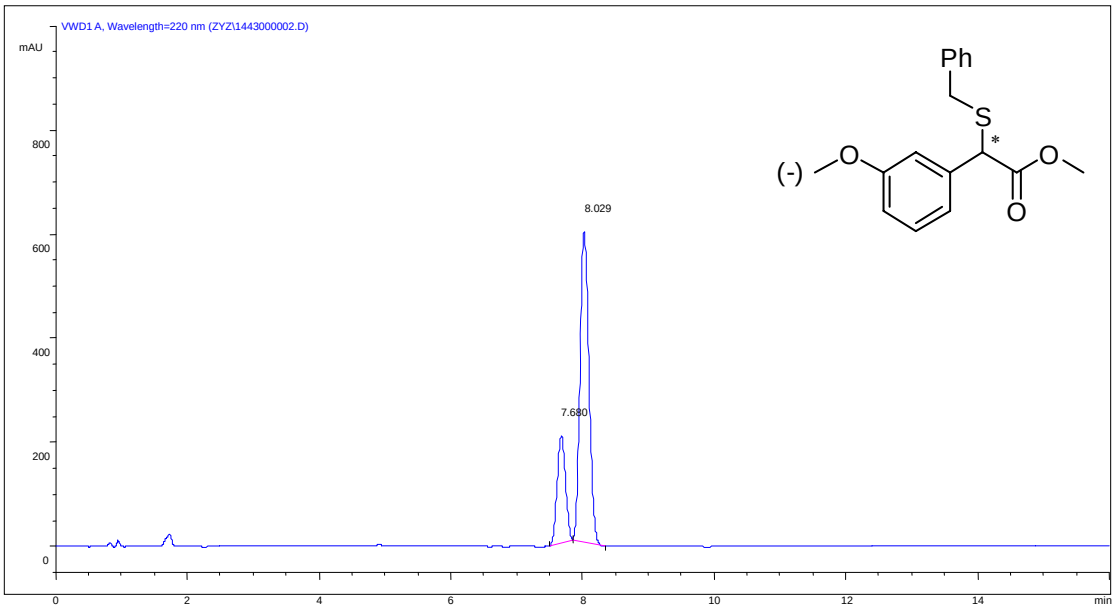


Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	8.335	VB	0.2190	1.01872e4	88.3502
2	10.343	VV	0.2609	1343.27637	11.6498

(-)-Methyl 2-(benzylthio)-2-(3-methoxyphenyl)acetate (3l)

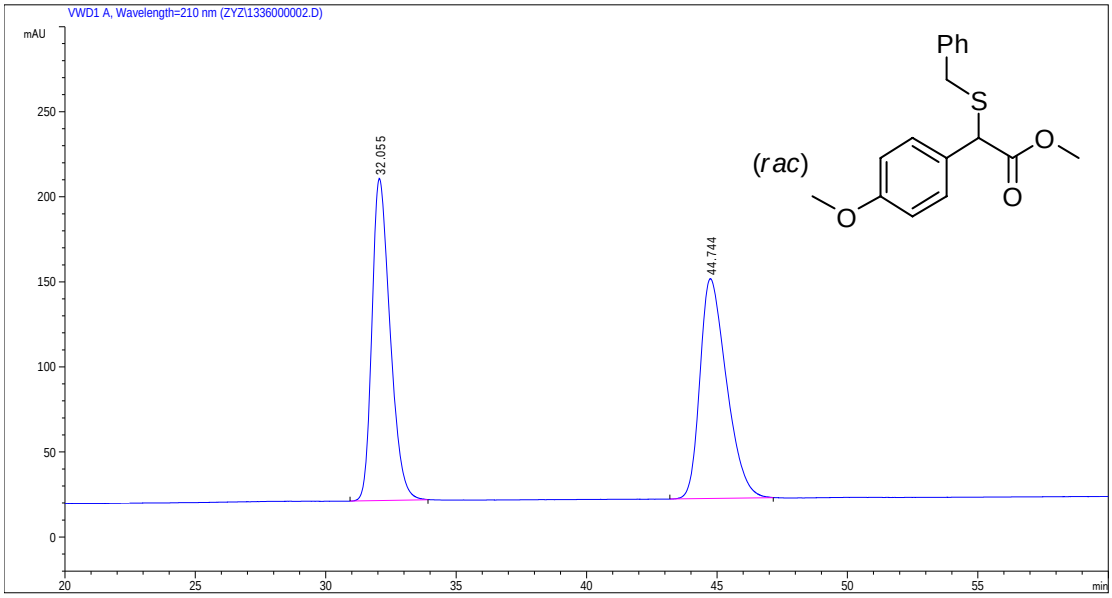


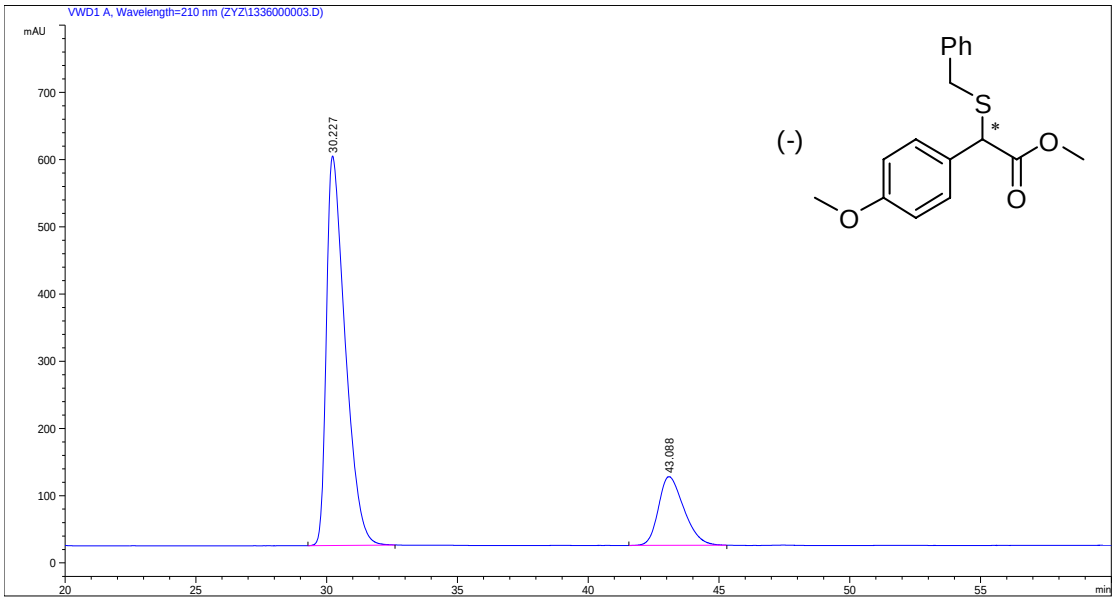


Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	7.680	BB	0.1395	1790.57605	24.1509
2	8.029	BB	0.1482	5623.53613	75.8491

(-)-Methyl 2-(benzylthio)-2-(4-methoxyphenyl)acetate (3m)

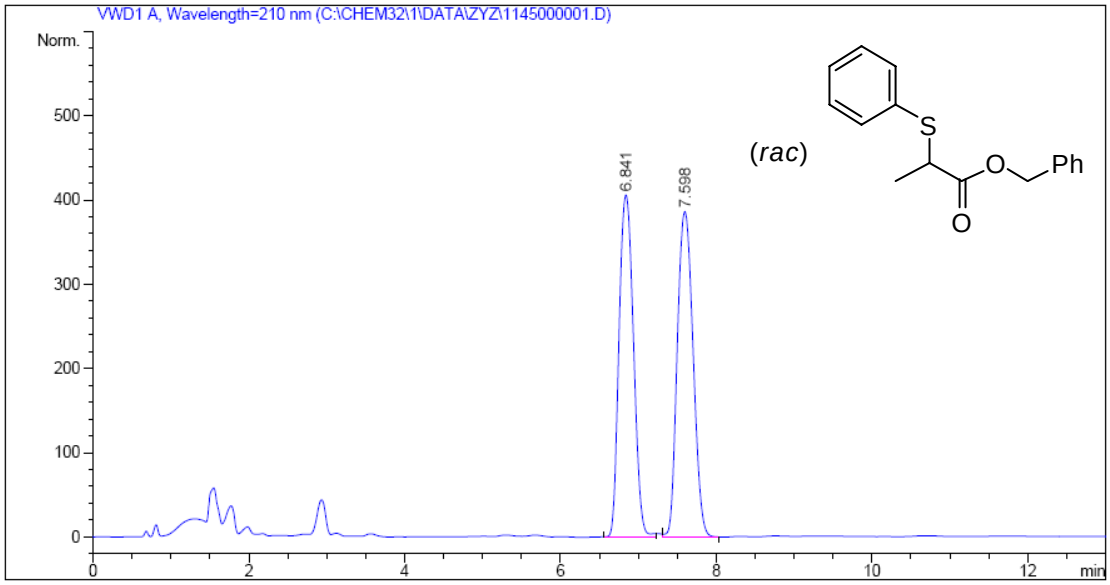


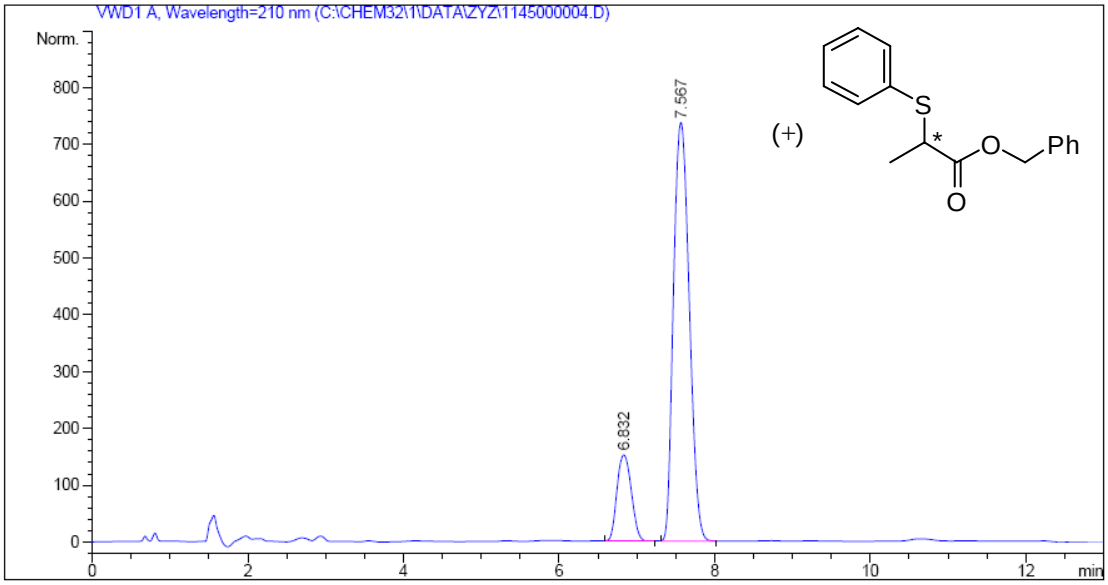


Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	30.227	BB	0.7478	2.88943e4	579.41577	80.7311
2	43.088	BB	1.0093	6896.48682	102.29810	19.2689

(+)-Benzyl 2-(phenylthio)propionate (3n)

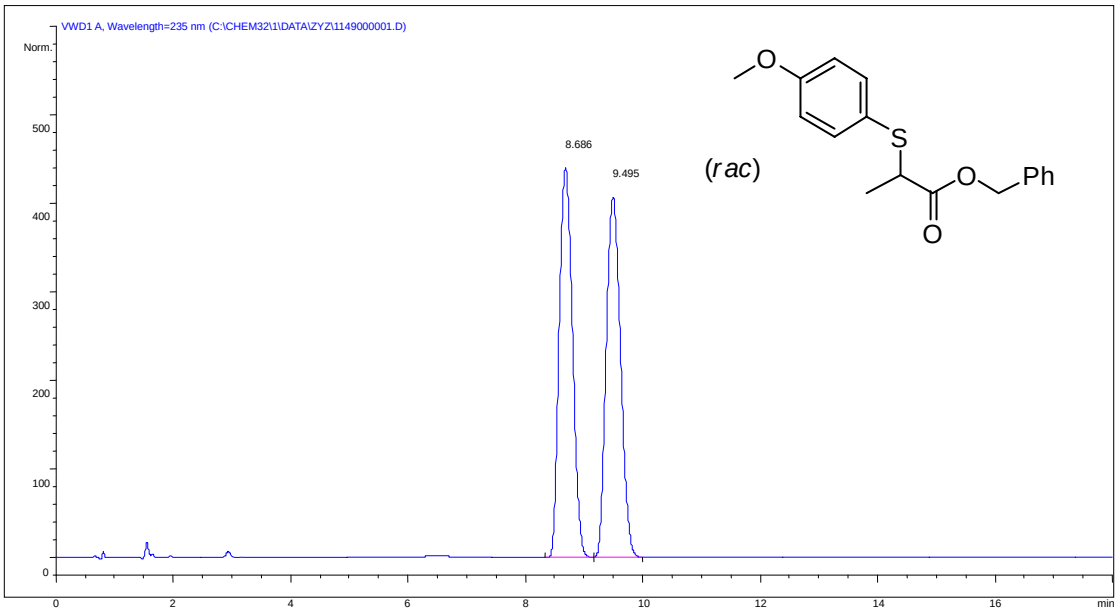


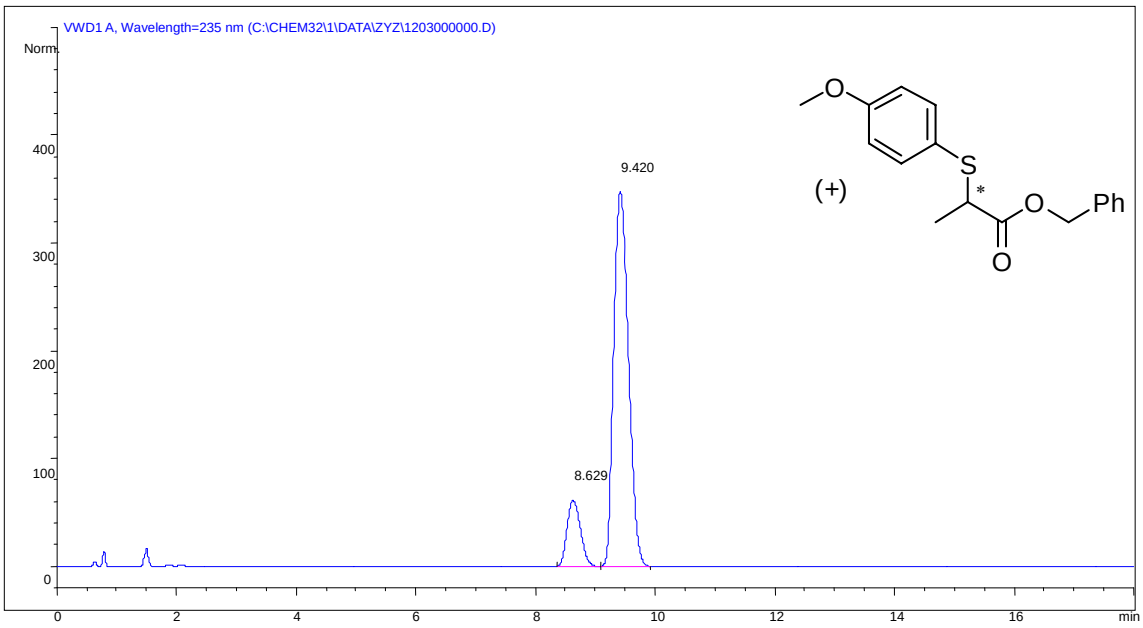


Uncalibrated Peaks:

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Area %
1	6.832	BB	0.2091	1937.87048		15.7010
2	7.567	BB	0.2302	1.04045e4		84.2990

(+)-benzyl 2-(4-methoxyphenylthio)propionate (3o)



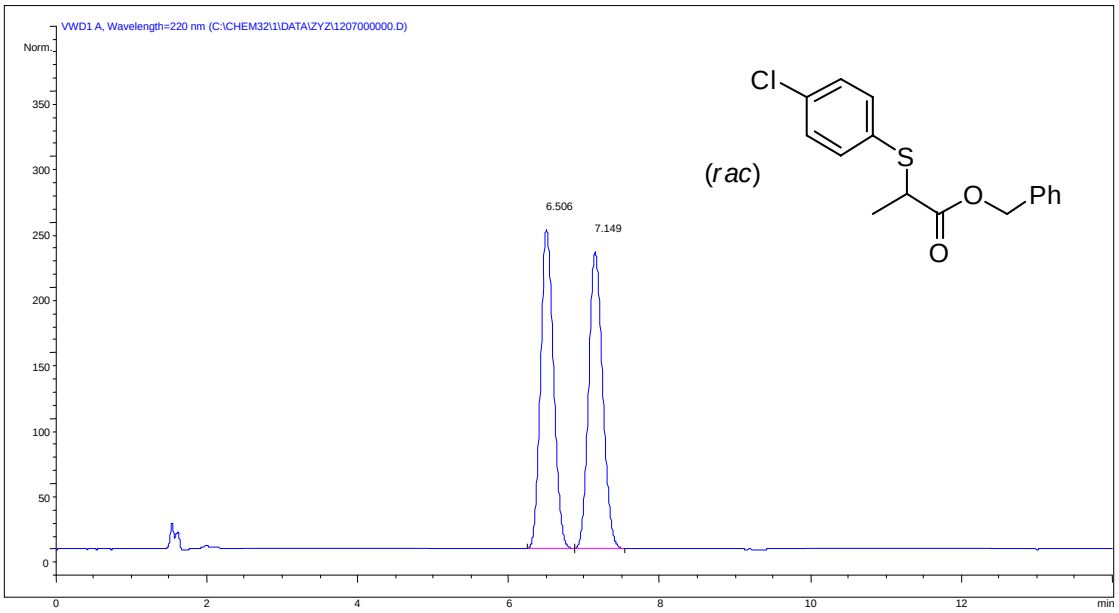


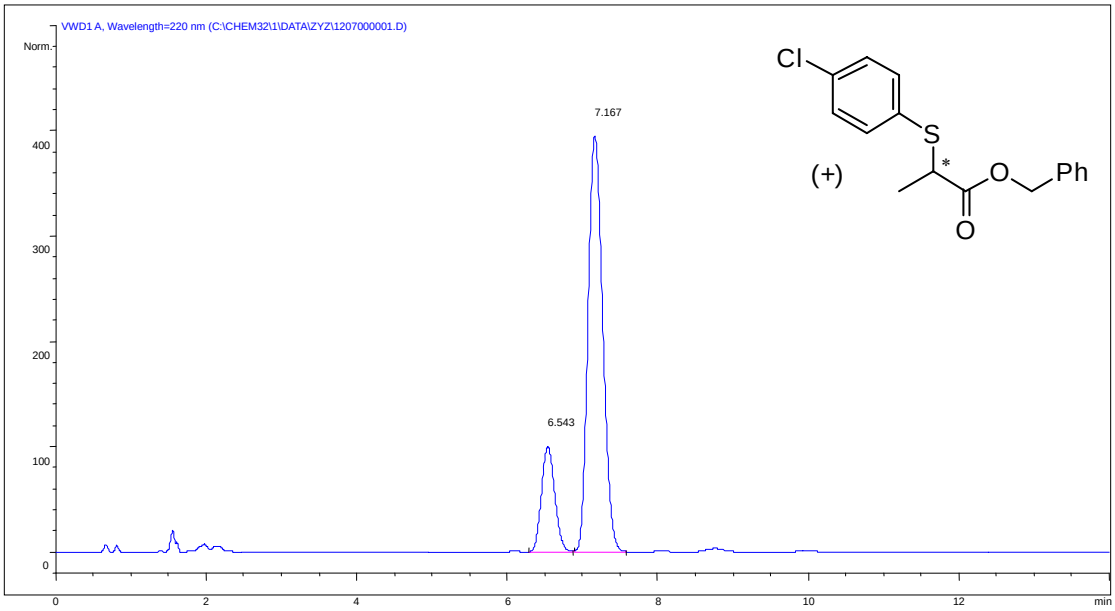
Signal 1: VWD1 A, Wavelength=235 nm

Uncalibrated Peaks:

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	8.629	BB	0.2526	960.95837	13.9023
2	9.420	BB	0.2759	5951.26123	86.0977

(+)-Benzyl 2-(4-chlorophenylthio)propionate (3p)

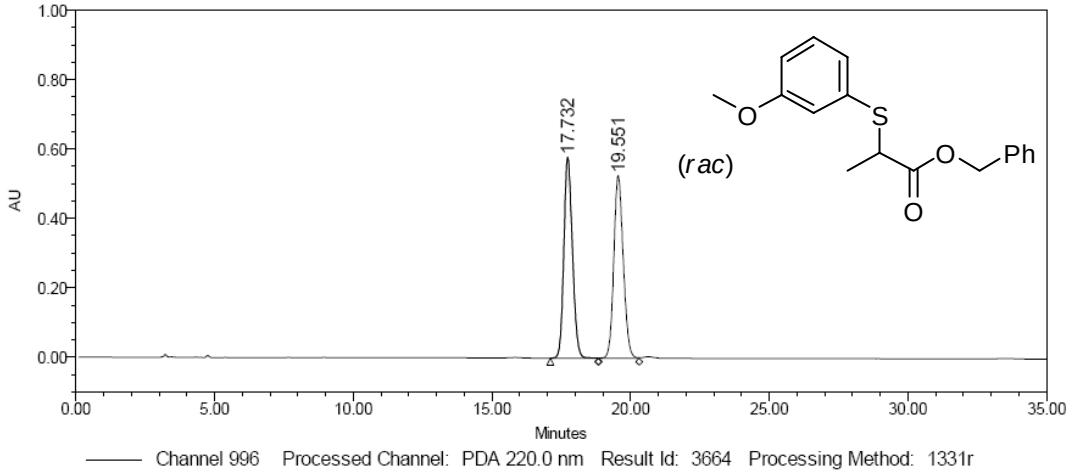


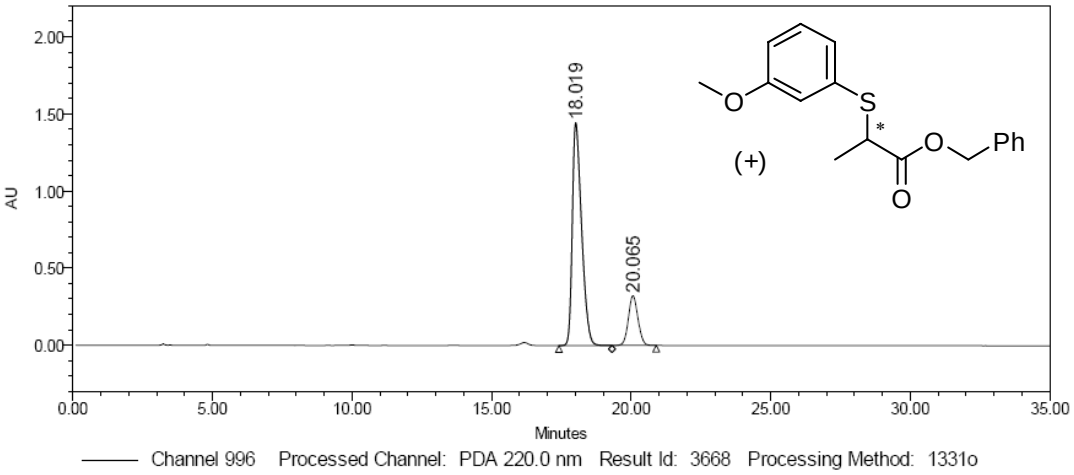


Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	6.543	BB	0.1946	1236.89978	18.7225
2	7.167	BB	0.2127	5369.60156	81.2775

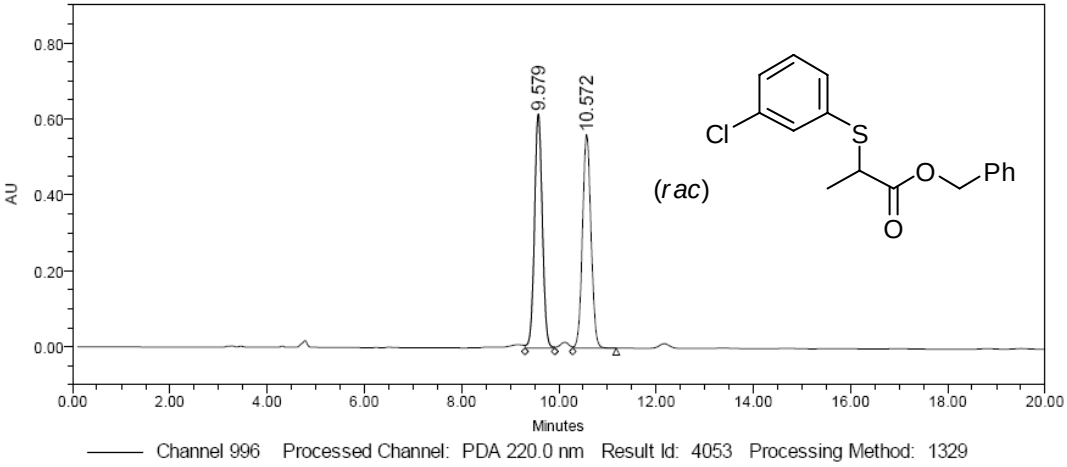
(+)-Benzyl 2-(3-methoxyphenylthio)propionate (3q)

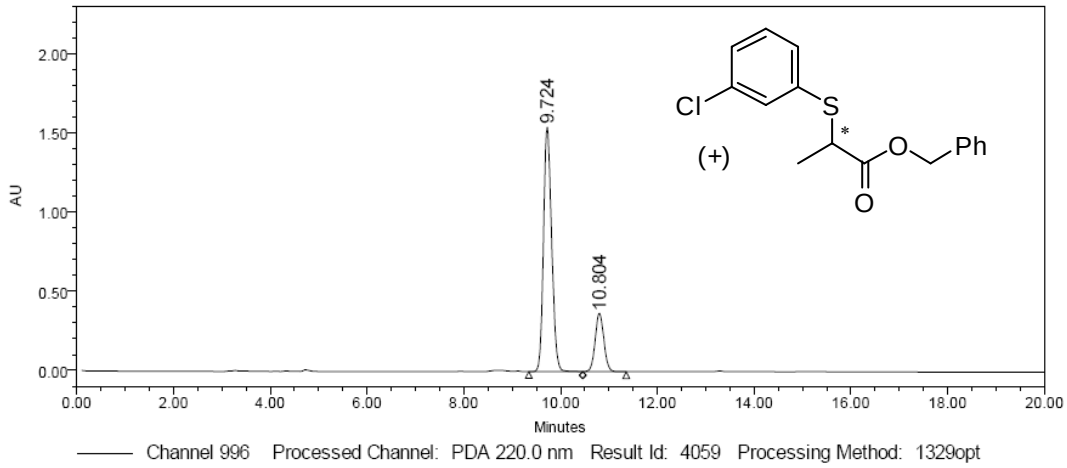




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 220.0 nm	18.019	33407660	81.30	1444894
2	PDA 220.0 nm	20.065	7686691	18.70	322040

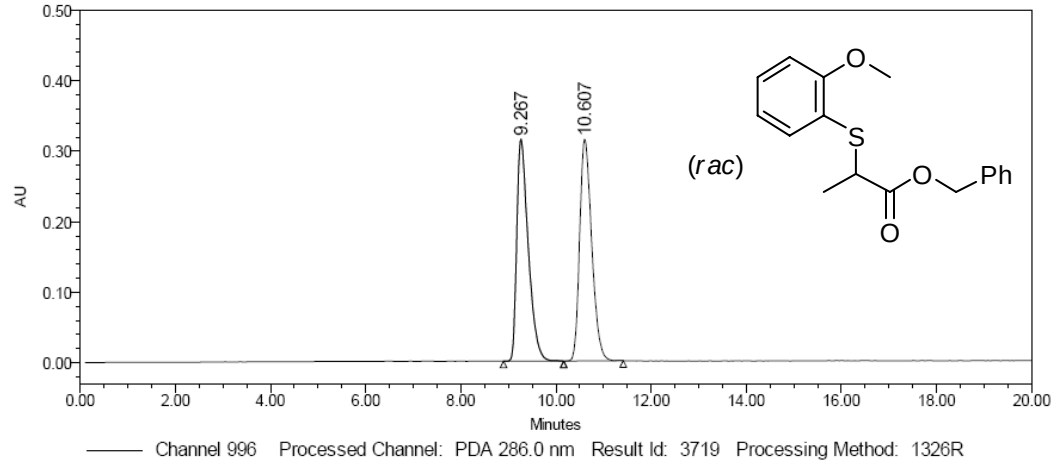
(+)-Benzyl 2-(3-chlorophenylthio)propionate (3r)

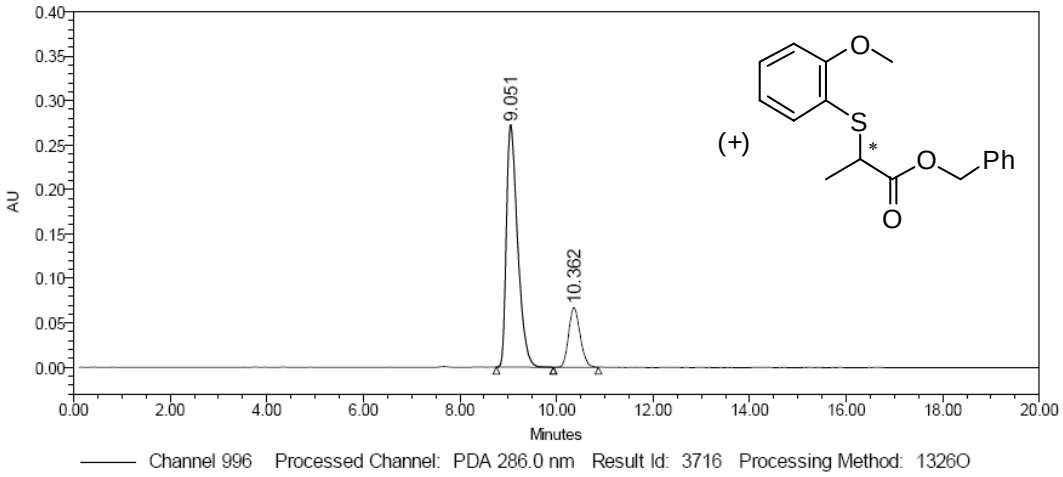




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 220.0 nm	9.724	18086085	79.78	1541075
2	PDA 220.0 nm	10.804	4583959	20.22	367586

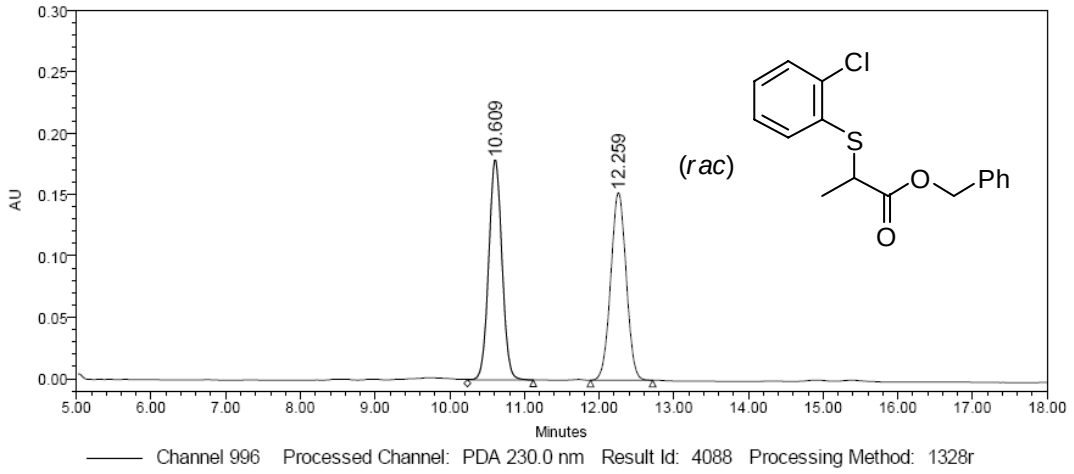
(+)-Benzyl 2-(2-methoxyphenylthio)propionate (3s)

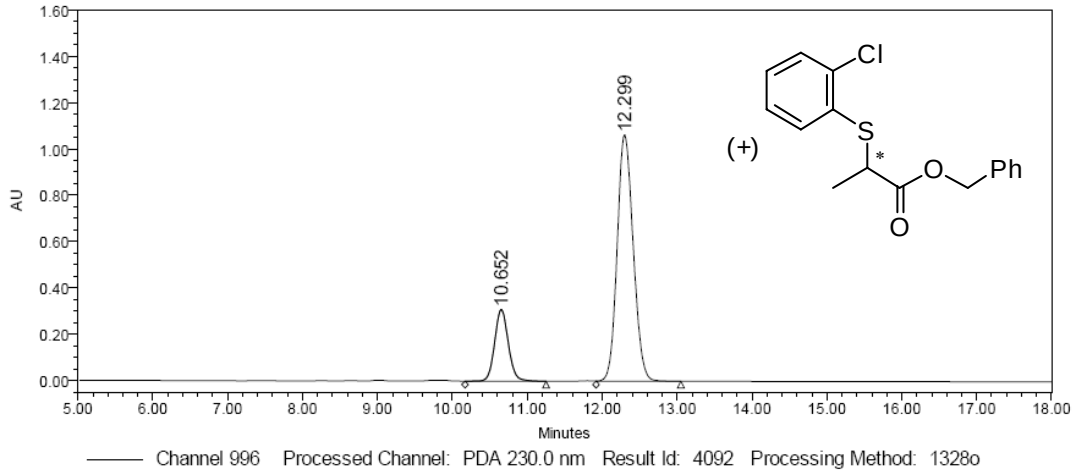




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 286.0 nm	9.051	4409879	79.90	272965
2	PDA 286.0 nm	10.362	1109446	20.10	67157

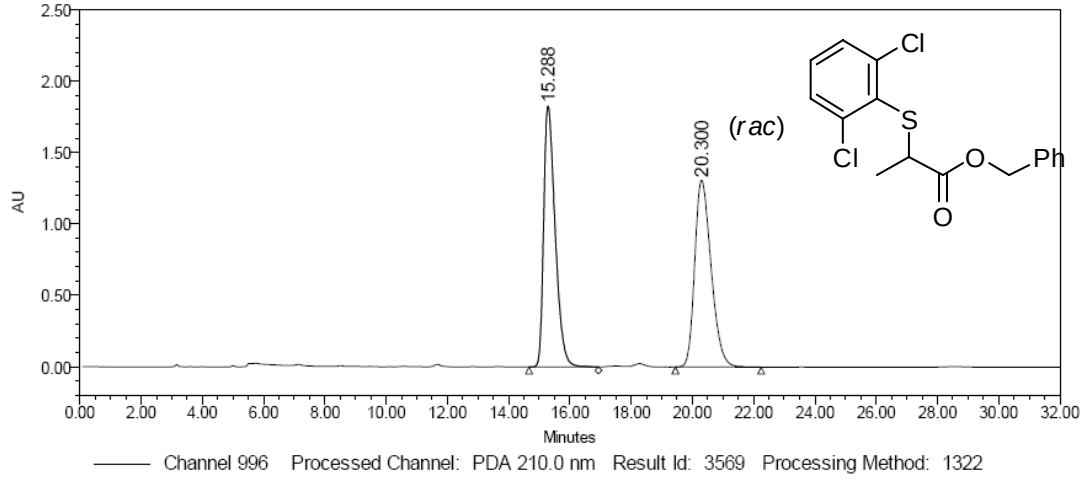
(+)-Benzyl 2-(2-chlorophenylthio)propionate (3t)

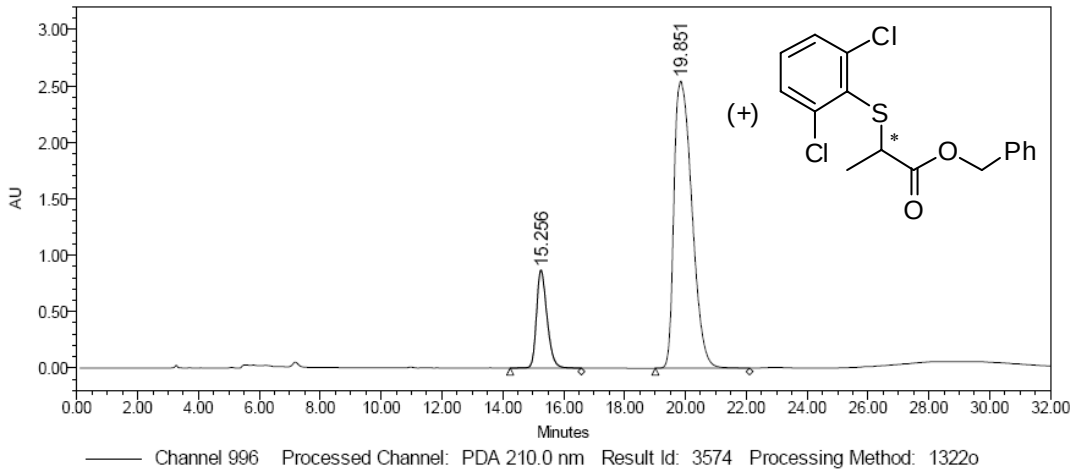




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 230.0 nm	10.652	3892385	19.77	309703
2	PDA 230.0 nm	12.299	15794814	80.23	1063973

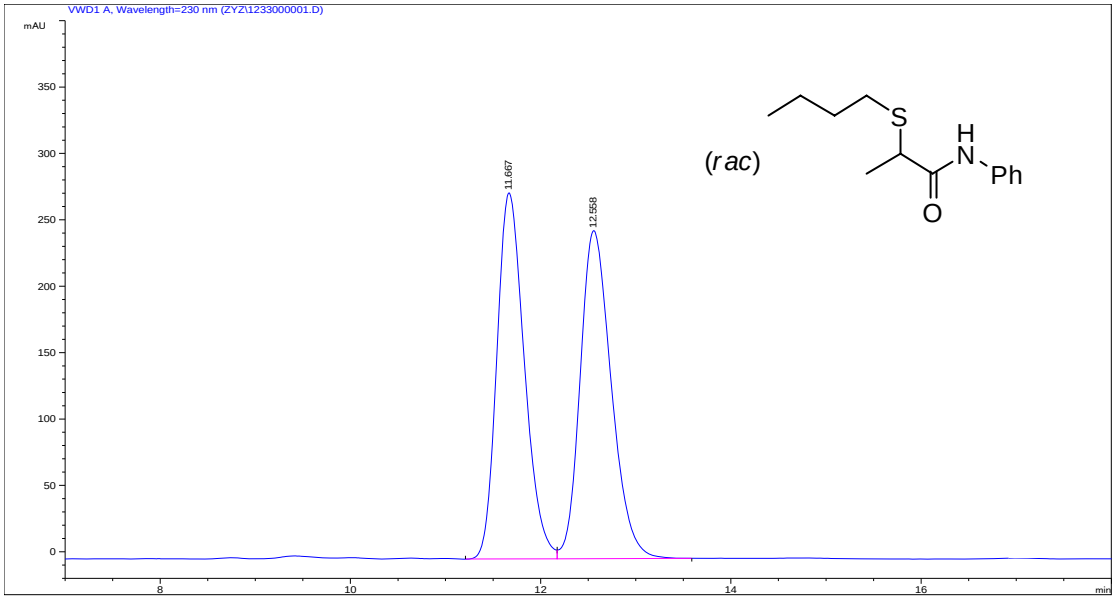
(+)-Benzyl 2-(2,6-dichlorophenylthio)propionate (3u)

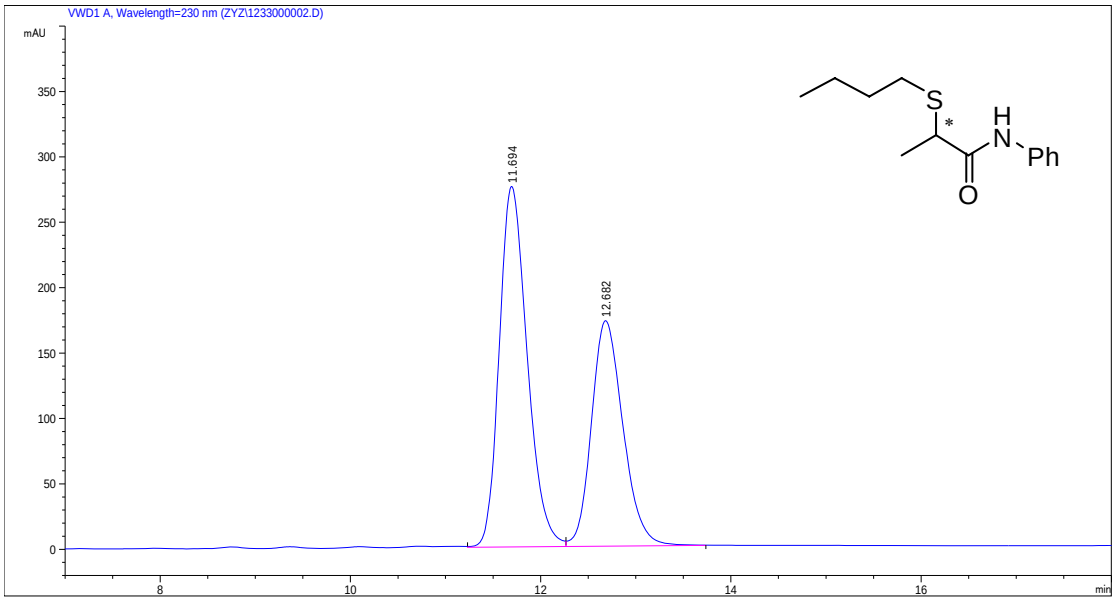




	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	15.256	20908889	16.71	868938
2	PDA 210.0 nm	19.851	104247080	83.29	2542674

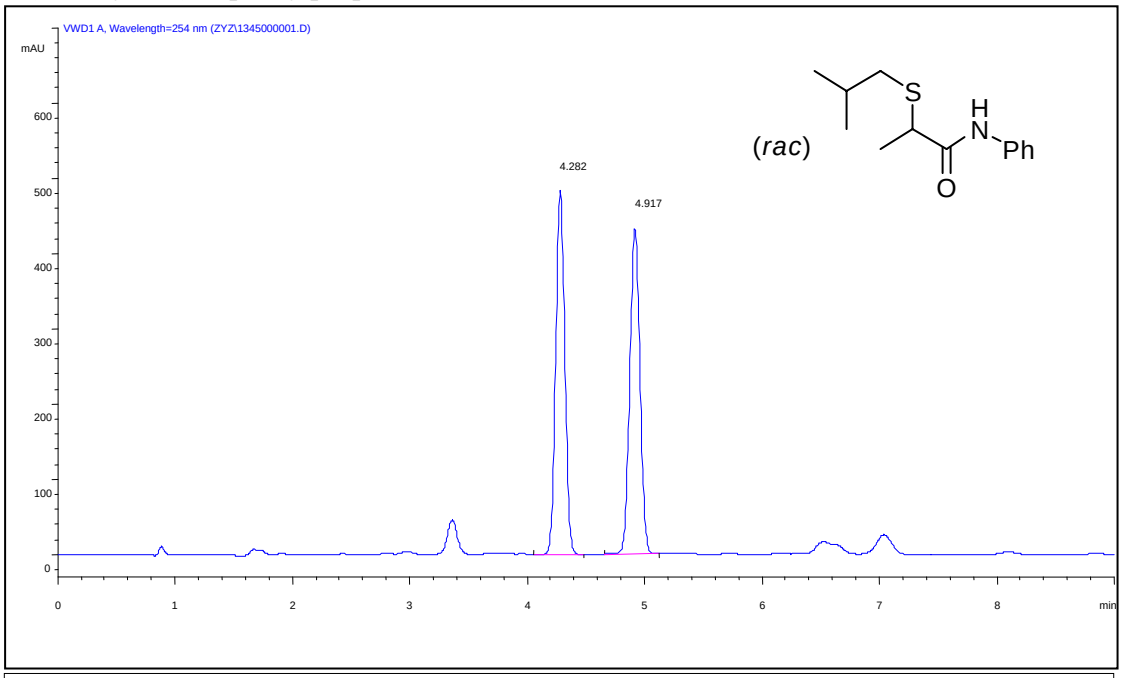
2-(Butylthio)-N-phenylpropanamide (3v)

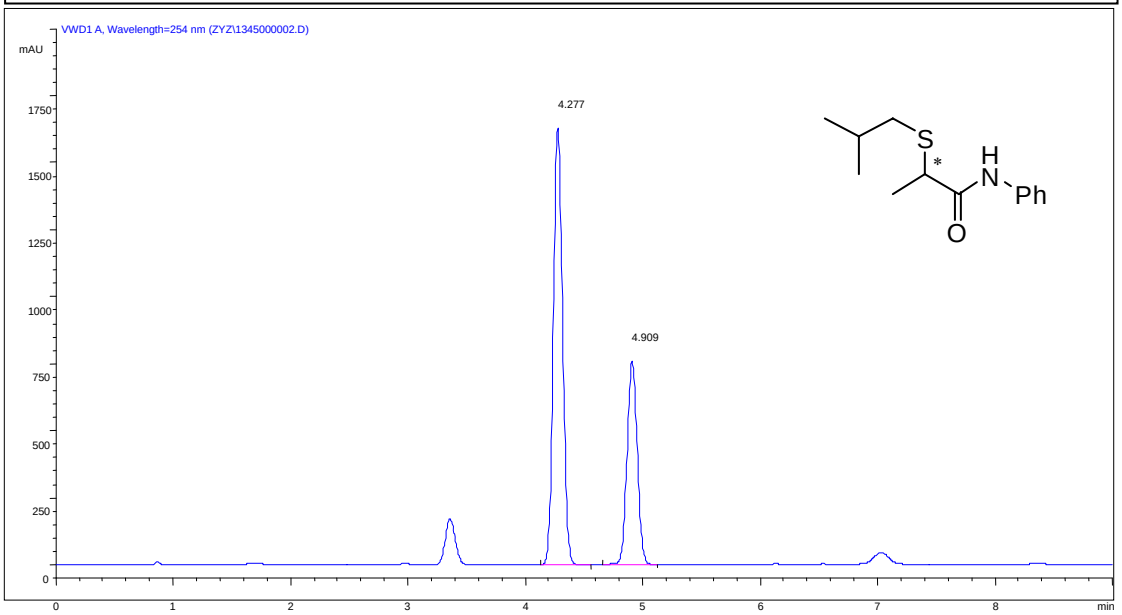




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.694	VV	0.3149	5615.97607	275.63489	58.5500
2	12.682	VB	0.3564	3975.78467	172.42783	41.4500

2-(Isobutylthio)-N-phenylpropanamide (3w)



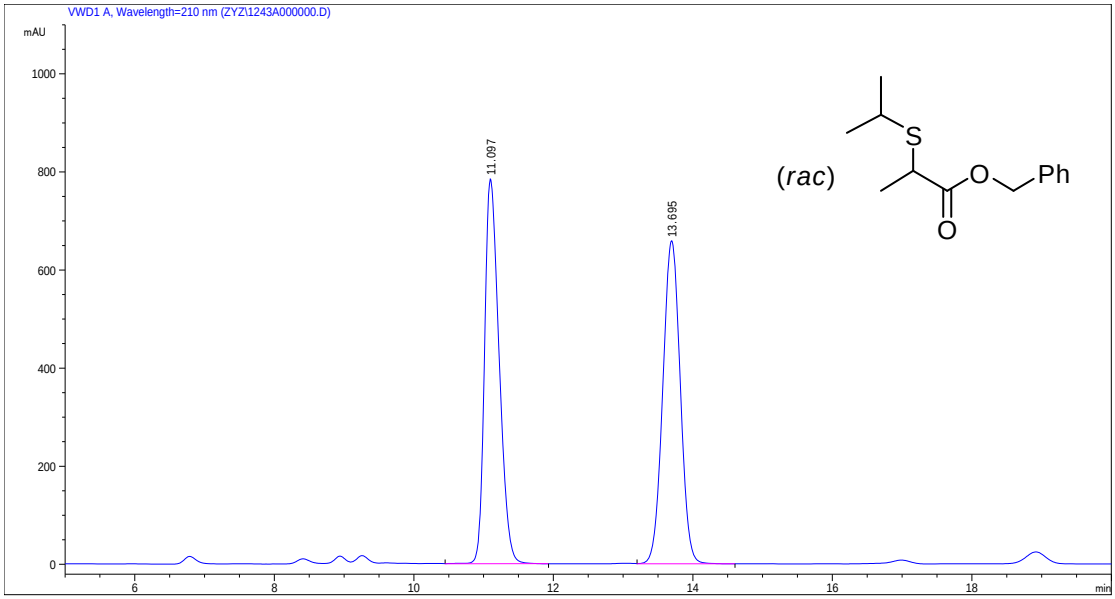


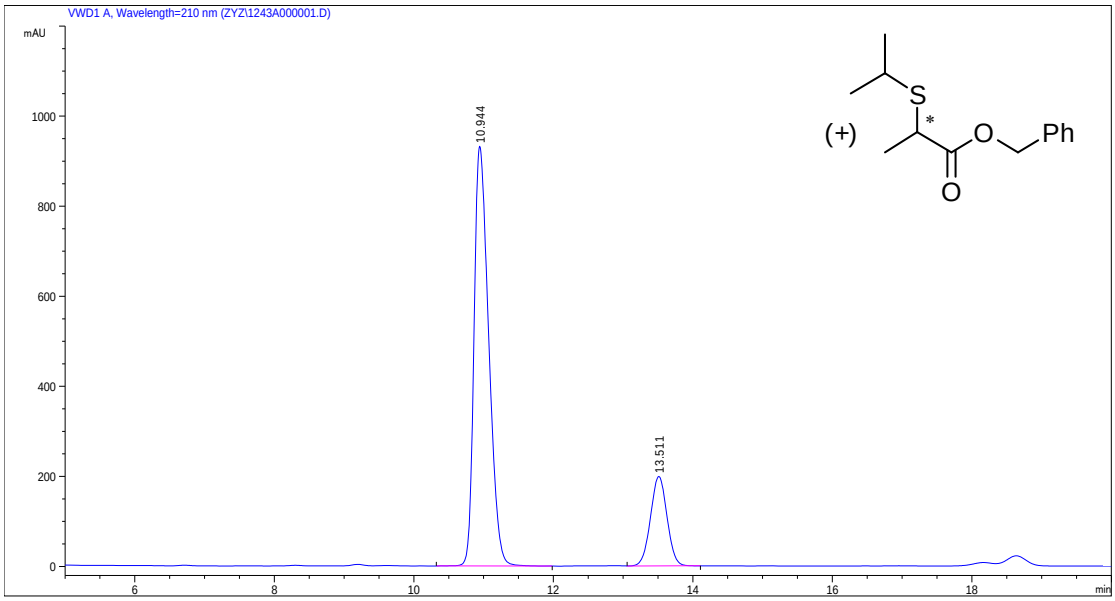
Signal 1: VWD1 A, Wavelength=254 nm

Uncalibrated Peaks:

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	4.277	BB	0.0876	8983.45703	65.9656
2	4.909	BB	0.0957	4634.93750	34.0344

(+)-Benzyl 2-(isopropylthio)propionate (3x)

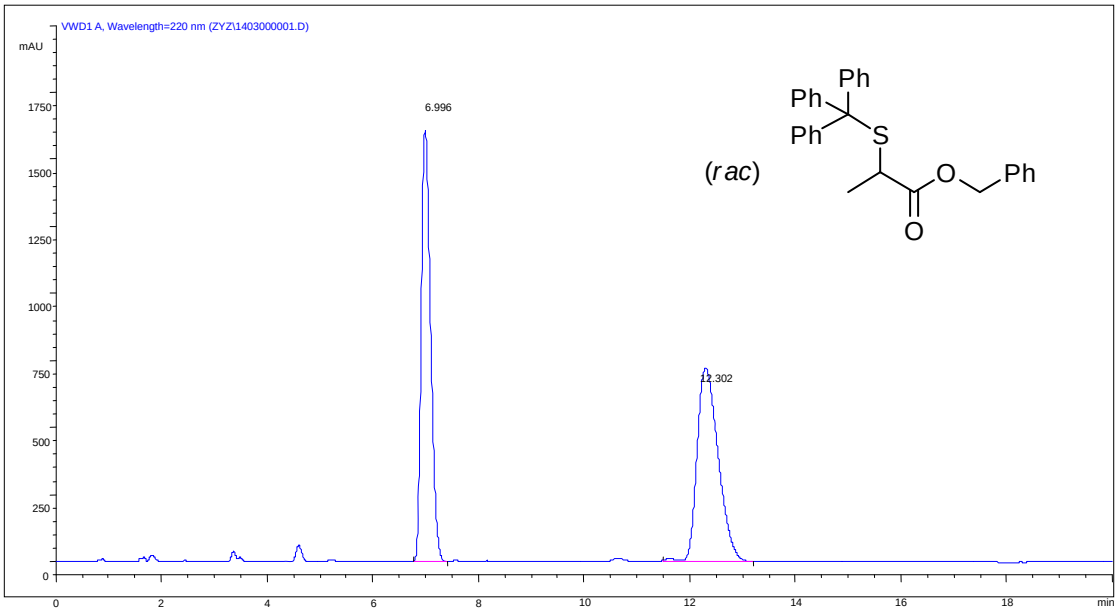


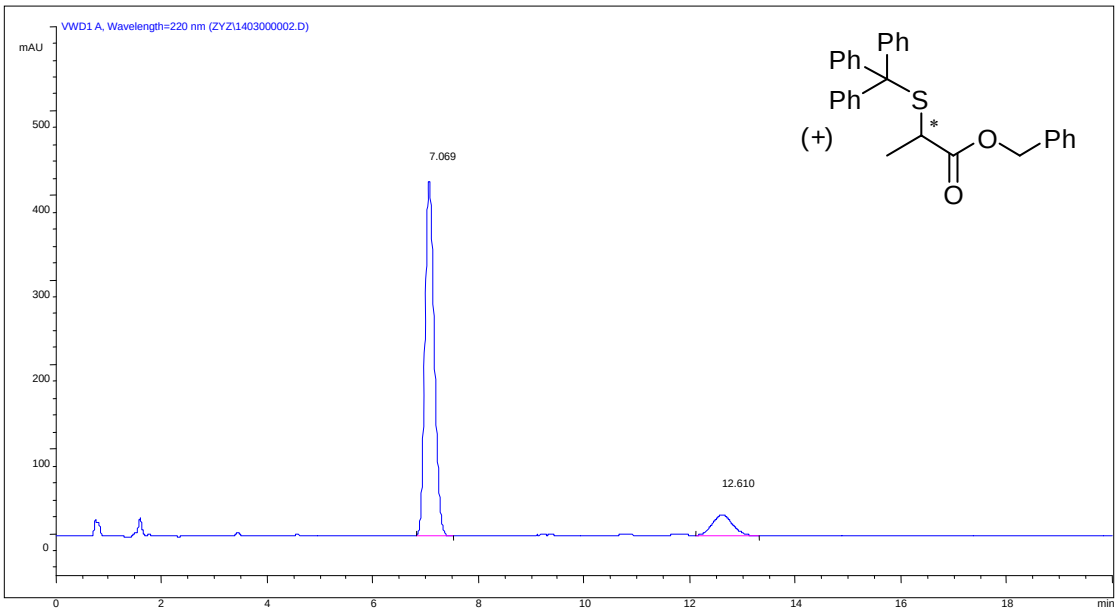


Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.944	BB	0.2268	1.35780e4	931.71515	80.6082
2	13.511	VB	0.2558	3266.45288	198.72371	19.3918

(+)-Benzyl 2-(tritylthio)propionate (3y)

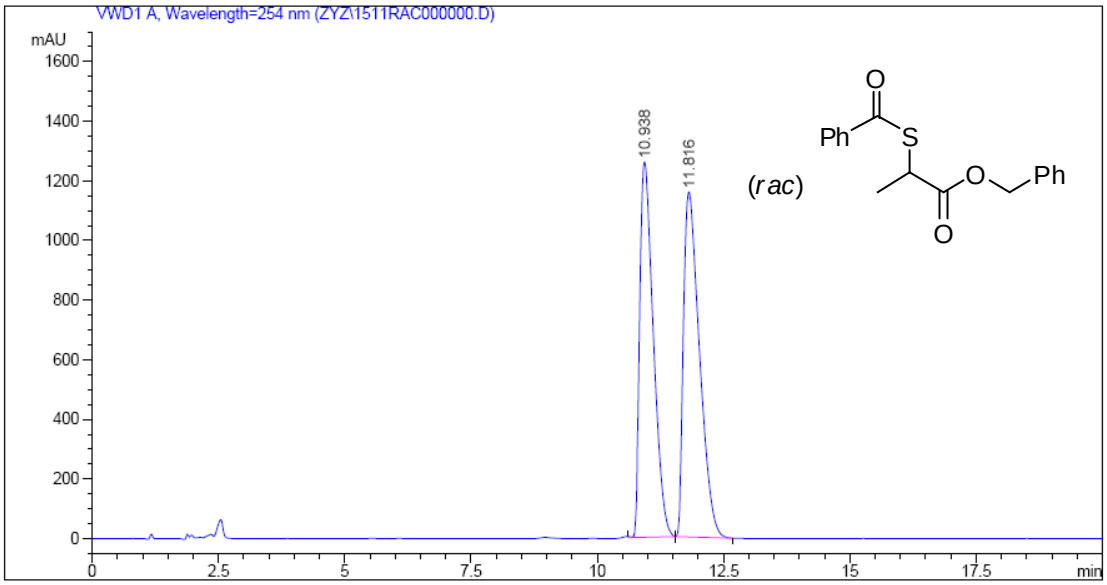


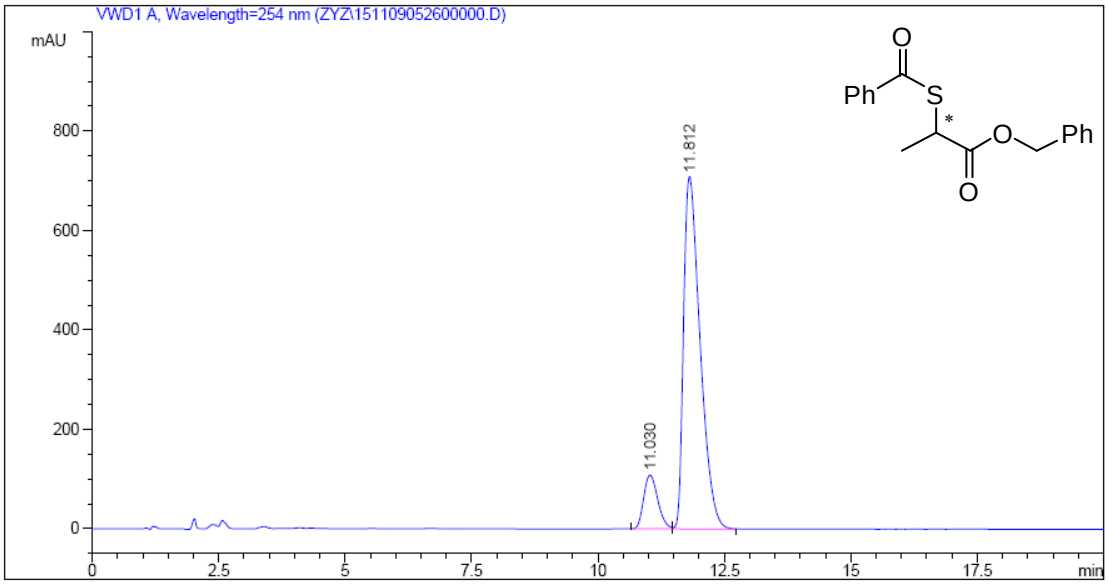


Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	7.069	BB	0.1905	5130.22949	88.5245
2	12.610	BB	0.4210	665.03790	11.4755

Benzyl 2-(benzoylthio)propionate





Signal 1: VWD1 A, Wavelength=254 nm

Uncalibrated Peaks:

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Area %
1	11.030	BV	0.3039	2091.11401		11.4962
2	11.812	VB	0.3464	1.60984e4		88.5038