Supplementary Information for

Highly enantioselective S–H bond insertion cooperatively catalyzed by dirhodium complexes and chiral spiro phosphoric acids

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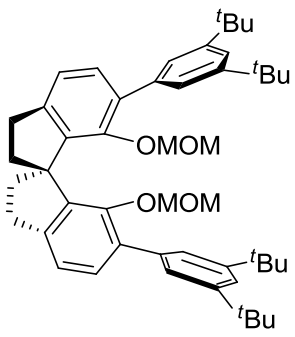
Contents:

1. General Information

Unless otherwise noted, all solvents used in the reactions were distilled from appropriate drying agents prior to use. Dirhodium (II) carboxylates (Sigma-Aldrich) were used without further purification. All the mercaptans were obtained commercially and purified by distillation or recrystallization before used. The chiral spiro phosphoric acids (SPAs)[1] and α-diazoesters[2] were synthesized according to the literatures. All reactions and manipulations which are sensitive to moisture or air were performed in an argon-filled glovebox (VAC DRI-LAB HE 493) or using standard Schlenk techniques. Melting points were measured on a RY–I apparatus and uncorrected. ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded with a Brucker AV 400 spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR) and 162 MHz (^{31}P NMR) in $CDCl_3$. Chemical shifts were reported in ppm down field from internal Me_4Si. Optical rotations were determined by a Perkin Elmer 341 MC polarimeter. HRMS were recorded on an IonSpec FT-ICR mass spectrometer with ESI resource. Enantiomeric excesses (ee) of the S–H insertion products and related chiral compounds were determined by High Performance Liquid Chromatography (HPLC) or Supercritical Fluid Chromatography (SFC). HPLC analysis was performed on a Hewlett Packard Model HP 1100 Series chromatography. SFC analyses were performed on Mettler-Toledo Model Analytix SFC.

2. Analytical Data for SPA (*R*)-1e and Intermediates

(*R*)-7,7'-Bis(methoxymethoxy)-6,6'-bis(3,5-ditertbutylphenyl)-1,1'-spirobiindane

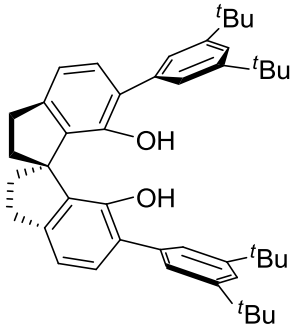


White solid, **m.p.**: 183−184 °C, **TLC** R_f = 0.66 (PE/EA = 15:1, v/v), 91% yield. **[α]$_D^{25}$** +172 (*c* 0.5, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.45−7.41 (m, 4H, ArH), 7.41−7.38 (m, 2H, ArH), 7.24 (d, *J* = 7.6 Hz, 2H, ArH), 7.10 (d, *J* = 7.6 Hz, 2H, ArH), 4.39 (d, *J* = 5.2 Hz, 2H, OCH_2), 4.30 (d, *J* = 4.8 Hz, 2H, OCH_2), 3.18−3.10 (m, 4H, $2CH_2$), 2.77 (s, 6H, $2OCH_3$), 2.68−2.58 (m, 2H, CH_2), 2.42−2.32 (m, 2H, CH_2), 1.40 (s, 36H, $4C(CH_3)_3$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.8 (2C, Ar-C), 150.4 (2C, Ar-C), 144.8 (2C, Ar-C), 142.3 (2C, Ar-C), 138.9 (2C, Ar-C), 133.8 (1C, Ar-C), 133.6 (2C, Ar-C), 130.4 (2C, Ar-C), 128.7 (1C, Ar-C), 128.5 (1C, Ar-C), 128.4 (1C, Ar-C), 123.6 (2C, Ar-C), 120.3 (2C, Ar-C), 119.9 (2C, Ar-C), 98.2 (2C, $2OCH_2$), 60.1 (1C), 56.0 (2C, $2OCH_3$), 39.2 (2C, $2CH_2$), 34.8 (4C, $4\underline{C}(CH_3)_3$), 31.5 (12C, $4C(\underline{C}H_3)_3$), 31.1(2C, $2Ar\underline{C}H_2$). **HRMS (ESI)** calcd for $[C_{49}H_{64}O_4Na, M + Na]^+$: 739.4697, Found 739.4691.

(*R*)-6,6'-Bis(3,5-ditertbutylphenyl)-1,1'-spirobiindane-7,7'-diol

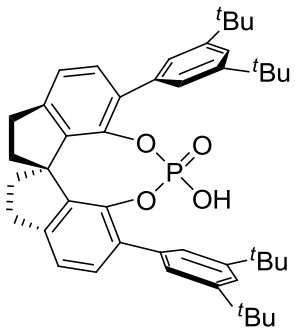
1 (a) F. Xu, D. Huang, C. Han, W. Shen, X. Lin and Y. Wang, *J. Org. Chem.*, 2010, **75**, 8677; (b) I. Čorić, S. Müller and B. List, *J. Am. Chem. Soc*., 2010, **132**, 17370; (c) C.-H. Xing, Y.-X. Liao, J. Ng and Q.-S. Hu, *J. Org. Chem.*, 2011, **76**, 4125; (d) B. Xu, S.-F. Zhu, X.-L. Xie, J.-J. Shen and Q.-L. Zhou, *Angew. Chem., Int. Ed*., 2011, **50**, 11483.

2 (a) M. Regitz, *Angew. Chem., Int. Ed.*, 1967, **6**, 733; (b) H. M. L. Davies and R. J. Townsend, *J. Org. Chem.*, 2001**, 66**, 6595.



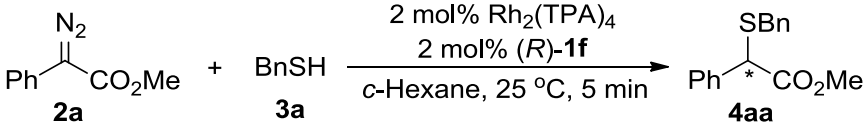
White solid, **m.p.**: 187−188 °C, **TLC** R_f = 0.48 (PE/EA = 15:1, v/v), 87% yield. **[α]$_D^{25}$** +211 (*c* 1.0, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38−7.35 (m, 2H, ArH), 7.28−7.24 (m, 4H, ArH), 7.18 (d, *J* = 7.6 Hz, 2H, ArH), 6.93 (d, *J* = 7.6 Hz, 2H, ArH), 5.13 (s, 2H, 2ArOH), 3.12−3.05 (m, 4H, $2CH_2$), 2.53−2.43 (m, 2H, CH_2), 2.39−2.31 (m, 2H, CH_2), 1.31 (s, 36H, $4C(CH_3)_3$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.0 (4C, Ar-C), 149.4 (2C, Ar-C), 144.9 (2C, Ar-C), 136.5 (2C, Ar-C), 132.6 (2C, Ar-C), 130.2 (2C, Ar-C), 127.7 (2C, Ar-C), 123.5 (4C, Ar-C), 121.4 (2C, Ar-C), 117.0 (2C, Ar-C), 58.7 (1C), 37.8 (2C, $2CH_2$), 34.9 (4C, $4\underline{C}(CH_3)_3$), 31.5 (12C, $4C(\underline{C}H_3)_3$), 31.2 (2C, $2Ar\underline{C}H_2$). **HRMS (ESI)** calcd for $[C_{45}H_{56}O_2Na, M + Na]^+$: 651.4173, Found 651.4174.

(*R*)-6,6'-Bis(3,5-ditertbutylphenyl)-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate ((*R*)-1e)



White solid, **m.p.**: 178−180 °C, **TLC** R_f = 0.75 (CH_2Cl_2/MeOH = 10:1, v/v), 70 % yield. **[α]$_D^{25}$** +310 (*c* 1.1, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.30−7.16 (m, 8H, ArH), 7.09 (d, *J* = 7.6 Hz, 2H, ArH), 3.12–2.96 (m, 2H, CH_2), 2.88–2.76 (m, 2H, CH_2), 2.32–2.22 (m, 2H, CH_2), 2.21–2.09 (m, 2H, CH_2), 1.18 (s, 36H, $4C(CH_3)_3$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.4 (4C, Ar-C), 145.1 (2C, Ar-C), 142.3 (1C, Ar-C), 142.2 (1C, Ar-C), 140.6 (1C, Ar-C), 140.5 (1C, Ar-C), 137.3 (2C, Ar-C), 135.2 (2C, Ar-C), 130.5 (2C, Ar-C), 124.2 (4C, Ar-C), 122.6 (2C, Ar-C), 120.4 (2C, Ar-C), 60.1 (1C), 38.6 (2C, $2CH_2$), 34.8 (4C, $4\underline{C}(CH_3)_3$), 31.4 (12C, $4C(\underline{C}H_3)_3$), 30.3 (2C, $2Ar\underline{C}H_2$); **^{31}P NMR** (162 MHz, $CDCl_3$): δ –11.6 (s). **HRMS (ESI)** calcd for $[C_{45}H_{55}O_4PNa, M + Na]^+$: 713.3730, Found 713.3736.

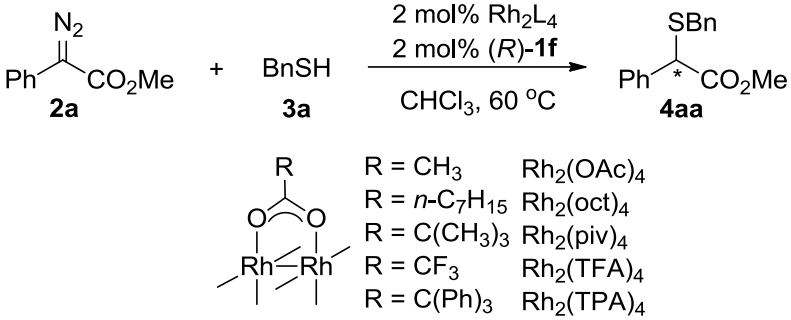
3. Typical Procedure for S–H Insertions and Comparison of Dirhodium Complexes



The $Rh_2(TPA)_4$ (5.3 mg, 0.004 mmol, 2 mol%) and (*R*)-**1f** (2.9 mg, 0.004 mmol, 2 mol%) were introduced into an oven-dried Schlenk tube in an argon-filled glovebox. After *c*-hexane (2 mL) was injected into the Schlenk tube, the mixture was stirred at 25 °C. A solution of methyl α-diazo-α-phenylacetate **2a** (42.2 mg, 0.24 mmol) and benzyl mercaptan (24.8 mg, 0.2 mmol) in *c*-hexane (1 mL) was added by a syringe pump in 5 minute. The reaction was completed immediately after the addition. The reaction mixture was concentrated and purified by a flash chromatography on silica gel (PE/EA = 15:1, v/v) to give methyl 2-(benzylthio)-2-phenylacetate **4aa** as a

colorless oil.

Table S1 Comparison of Dirhodium Complexes[a]

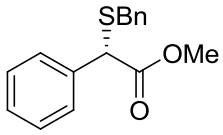


Entry	Rh_2L_4	yield (%)[b]	ee (%)[c]
1	$Rh_2(OAc)_4$	82	72
2	$Rh_2(oct)_4$	76	65
3	$Rh_2(piv)_4$	66	61
4	$Rh_2(TFA)_4$	74	45
5	$Rh_2(TPA)_4$	80	73

[a] Reaction conditions: Rh_2L_4/**1**/**2a**/**3a** = 0.004:0.004:0.2:0.2 (mmol) in 3 mL solvent. Reaction time: 5 min. [b] Isolated yield. [c] Determined by HPLC using Chiralcel OD-H column.

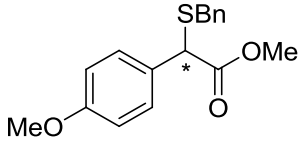
4. Analytical Data for S−H Insertion Products

(*S*)-Methyl 2-(benzylthio)-2-phenylacetate (4aa)[3]



Colorless oil, **TLC** R_f = 0.66 (PE/EA = 15:1, v/v), 92% yield, 94% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 6.43 min for (*R*) isomer, t_R = 6.85 min for (*S*) isomer]. **$[\alpha]_D^{27}$** +140 (*c* 0.90, EtOH) [lit[3]: $[\alpha]_D^{25}$ –143 (*c* 2.73, EtOH) for (*R*) isomer]. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.44–7.37 (m, 2H, ArH), 7.37–7.20 (m, 8H, ArH), 4.42 (s, 1H, CH), 3.76 (d, *J* = 13.5 Hz, 1H, 1/2SCH_2), 3.68 (s, 3H, OCH_3), 3.61 (d, *J* = 13.5 Hz, 1H, 1/2SCH_2).

(+)-Methyl 2-(benzylthio)-2-(4-methoxyphenyl)-acetate (4ba)[4]

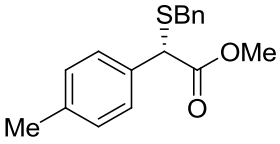


Colorless oil, **TLC** R_f = 0.48 (PE/EA = 10:1, v/v), 96% yield, 96% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 0.5 mL/min, wavelength = 220 nm, t_R = 22.76 min for minor isomer, t_R = 23.53 min for major isomer]. **$[\alpha]_D^{22}$** +143 (*c* 1.0, MeOH)

3 (a) W. A. Bonner, *J. Org. Chem.*, 1967, **32**, 2496; (b) W. A. Bonner, *J. Org. Chem.*, 1968, **33**, 1831.
4 Y.-Z. Zhang, S.-F. Zhu, Y. Cai, H.-X. Mao and Q.-L. Zhou, *Chem. Commun.*, 2009, 5362.

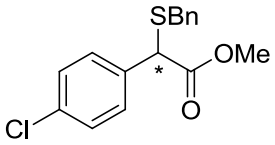
[lit[4]: $[\alpha]_D^{20}$ –95.1 (*c* 1.0, MeOH) with 61% ee]. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.34–7.24 (m, 7H, ArH), 6.86 (d, *J* = 8.8 Hz, 2H, ArH), 4.39 (s, 1H, CH), 3.80 (s, 3H, $ArOCH_3$), 3.75 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2), 3.68 (s, 3H, OCH_3), 3.60 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2).

(*S*)-Methyl 2-(benzylthio)-2-*p*-tolylacetate (4ca)



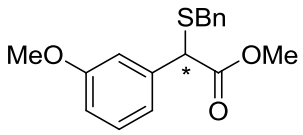
Colorless crystal solid, **m.p.**: 66–67 ºC, TLC R_f = 0.52 (PE/EA = 15:1, v/v), 96% yield, 95% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 7.23 min for minor isomer, t_R = 7.81 min for major isomer]. **$[\alpha]_D^{26}$** +148 (*c* 1.1, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.32–7.20 (m, 7H, ArH), 7.13 (d, *J* = 8.0 Hz, 2H, ArH), 4.39 (s, 1H, CH), 3.74 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2), 3.65 (s, 3H, OCH_3), 3.59 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 2.32 (s, 3H, $ArCH_3$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.2 (1C, C=O), 138.0 (1C, Ar-C), 137.1 (1C, Ar-C), 132.6 (1C, Ar-C), 129.3 (2C, Ar-C), 129.0 (2C, Ar-C), 128.5 (2C, Ar-C), 128.4 (2C, Ar-C), 127.1 (1C, Ar-C), 52.6 (1C, SCH), 51.1 (1C, OCH_3), 36.1 (1C, SCH_2), 21.1 (1C, CH_3). **HRMS (ESI)** calcd for $[C_{17}H_{18}O_2SNa, M + Na]^+$: 309.0920, Found: 309.0916.

(+)-Methyl 2-(benzylthio)-2-(4-chlorophenyl)-acetate (4da)



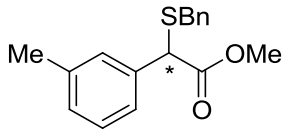
Colorless oil, **TLC** R_f = 0.71 (PE/EA = 10:1, v/v), 90% yield, 93% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 7.21 min for major isomer, t_R = 7.63 min for minor isomer]. **$[\alpha]_D^{22}$** +165 (*c* 1.0, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.27–7.13 (m, 9H, ArH), 4.29 (s, 1H, CH), 3.68 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.59 (s, 3H, OCH_3), 3.51 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.7 (1C, C=O), 136.8 (1C, Ar-C), 134.3 (1C, Ar-C), 134.0 (1C, Ar-C), 129.9 (2C, Ar-C), 128.9 (2C, Ar-C), 128.8 (2C, Ar-C), 128.5 (2C, Ar-C), 127.3 (1C, Ar-C), 52.7 (1C, CH), 50.6 (1C, OCH_3), 36.2 (1C, SCH_2). **HRMS (ESI)** calcd for $[C_{16}H_{15}ClO_2SNa, M + Na]^+$: 329.0373, Found: 329.0375.

(+)-Methyl 2-(benzylthio)-2-(3-methoxyphenyl)-acetate (4ea)[4]



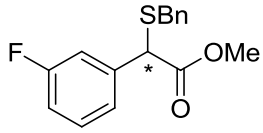
Colorless oil, **TLC** R_f = 0.54 (PE/EA = 10:1, v/v), 90% yield, 91% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 10.28 min for minor isomer, t_R = 11.76 min for major isomer]. **$[\alpha]_D^{24}$** +129 (*c* 1.0, MeOH) [lit[4]: $[\alpha]_D^{20}$ –67.4 (*c* 1.0, MeOH) with 52% ee]. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.33–7.21 (m, 6H, ArH), 6.98–6.94 (m, 2H, ArH), 6.86–6.81 (m, 1H, ArH), 4.39 (s, 1H, CH), 3.79 (s, 3H, $ArOCH_3$), 3.76 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.68 (s, 3H, OCH_3), 3.62 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2).

(+)-Methyl 2-(benzylthio)-2-*m*-tolylacetate (4fa)



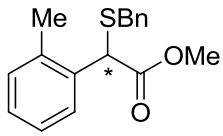
Colorless oil, **TLC** R_f = 0.50 (PE/EA = 15:1, v/v), 80% yield, 91% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 7.30 min for minor isomer, t_R = 8.05 min for major isomer]. **[α]$_D^{26}$** +123 (*c* 1.0, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.40–7.24 (m, 8H, ArH), 7.16 (d, *J* = 7.2 Hz, 1H, ArH), 4.45 (s, 1H, CH), 3.82 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.73 (s, 3H, OCH_3), 3.67 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2), 2.39 (s, 3H, $ArCH_3$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.2 (1C, C=O), 138.4 (1C, Ar-C), 137.1 (1C, Ar-C), 135.5 (1C, Ar-C), 129.1 (1C, Ar-C), 129.0 (2C, Ar-C), 128.5 (2C, Ar-C), 128.4 (2C, Ar-C), 127.2 (1C, Ar-C), 125.6 (1C, Ar-C), 52.6 (1C, SCH), 51.5 (1C, OCH_3), 36.2 (1C, SCH_2), 21.3 (1C, CH_3). **HRMS (ESI)** calcd for [$C_{17}H_{18}O_2SNa$, M + Na]$^+$: 309.0920, Found: 309.0915.

(+)-Methyl 2-(benzylthio)-2-(3-fluorophenyl)-acetate (4ga)



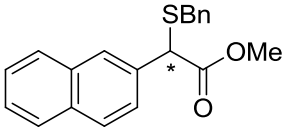
Colorless oil, **TLC** R_f = 0.46 (PE/EA = 15:1, v/v), 77% yield, 90% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 210 nm, t_R = 7.22 min for major isomer, t_R = 7.70 min for minor isomer]. **[α]$_D^{26}$** +120 (*c* 0.84, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.34–7.24 (m, 6H, ArH), 7.19–7.12 (m, 2H, ArH), 7.02–6.96 (m, 1H, ArH), 4.39 (s, 1H, CH), 3.77 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.69 (s, 3H, OCH_3), 3.62 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.6 (1C, C=O), 162.8 (d, *J* = 245.4 Hz, 1C, Ar-C), 138.2 (d, *J* = 7.5 Hz, 1C, Ar-C), 136.8 (1C, Ar-C), 130.1 (d, *J* = 8.2 Hz, 1C, Ar-C), 129.0 (2C, Ar-C), 128.6 (2C, Ar-C), 127.4 (1C, Ar-C), 124.3 (d, *J* = 3.0 Hz, 1C, Ar-C), 115.6 (d, *J* = 22.6 Hz, 1C, Ar-C), 115.2 (d, *J* = 21.2 Hz, 1C, Ar-C), 52.8 (1C, SCH), 50.9 (1C, OCH_3), 36.2 (1C, SCH_2). **HRMS (ESI)** calcd for [$C_{16}H_{15}FO_2SNa$, M + Na]$^+$: 313.0669, Found: 313.0668.

(+)-Methyl 2-(benzylthio)-2-*o*-tolylacetate (4ha)[4]



Colorless oil, **TLC** R_f = 0.68 (PE/EA = 15:1, v/v), 90% yield, 58% ee [**HPLC** condition: Chiralcel AD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 5.56 min for major isomer, t_R = 6.32 min for minor isomer]. **[α]$_D^{27}$** +23.2 (*c* 0.83, MeOH) [lit[4]: $[\alpha]_D^{20}$ –30.6 (*c* 1.0, MeOH) with 77% ee]. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54–7.48 (m, 1H, ArH), 7.34–7.28 (m, 5H, ArH), 7.22–7.14 (m, 2H, ArH), 7.13–7.08 (m, 2H, ArH), 4.59 (s, 1H, CH), 3.81 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.70 (s, 3H, OCH_3), 3.68 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 2.11 (s, 3H, $ArCH_3$).

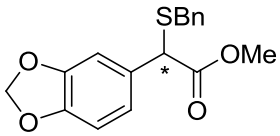
(+)-Methyl 2-(benzylthio)-2-(naphthalen-2-yl)-acetate (4ia)



Yellow solid, **m.p.**: 77–78 °C, **TLC** R_f = 0.45 (PE/EA = 15:1, v/v), 91% yield, 92% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 10.59 min for minor isomer, t_R =

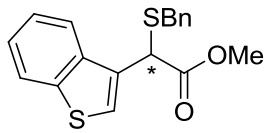
12.36 min for major isomer]. **[α]$_D^{24}$** +167 (*c* 0.45, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.85–7.77 (m, 4H, ArH), 7.57 (dd, J_1 = 7.6 Hz and J_2 = 1.6 Hz, 1H, ArH), 7.51–7.44 (m, 2H, ArH), 7.34–7.23 (m, 5H, ArH), 4.59 (s, 1H, CH), 3.77 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.69 (s, 3H, OCH_3), 3.60 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.0 (1C, C=O), 137.1 (1C, Ar-C), 133.1 (1C, Ar-C), 129.0 (3C, Ar-C), 128.6 (1C, Ar-C), 128.5 (3C, Ar-C), 128.0 (1C, Ar-C), 127.8 (1C, Ar-C), 127.6 (1C, Ar-C), 127.3 (1C, Ar-C), 126.4 (2C, Ar-C), 126.1 (1C, Ar-C), 52.7 (1C, SCH), 51.7 (1C, OCH_3), 36.1 (1C, SCH_2). **HRMS (ESI)** calcd for [$C_{20}H_{18}O_2SNa$, M + Na]$^+$: 345.0920, Found: 345.0925.

(+)-Methyl 2-(benzo[d][1,3]dioxol-5-yl)-2-(benzylthio)-acetate (4ja)



Colorless oil, **TLC** R_f = 0.50 (PE/EA = 10:1, v/v), 89% yield, 94% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 14.50 min for minor isomer, t_R = 15.86 min for major isomer]. **[α]$_D^{24}$** +170 (*c* 0.61, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.37–7.25 (m, 5H, ArH), 7.01 (d, *J* = 1.6 Hz, 1H, ArH), 6.83 (dd, J_1 = 8.0 Hz and J_2 = 2.0 Hz, 1H, ArH), 6.77 (d, *J* = 8.0 Hz, 1H, ArH), 6.00–5.96 (m, 2H, OCH_2O), 4.38 (s, 1H, CH), 3.78 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.71 (s, 3H, OCH_3), 3.64 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.0 (1C, C=O), 147.9 (1C, Ar-C), 147.5 (1C, Ar-C), 137.1 (1C, Ar-C), 129.3 (1C, Ar-C), 129.0 (2C, Ar-C), 128.5 (2C, Ar-C), 127.2 (1C, Ar-C), 122.2 (1C, Ar-C), 108.8 (1C, Ar-C), 108.1 (1C, Ar-C), 101.2 (1C, OCH_2O), 52.6 (1C, SCH), 51.2 (1C, OCH_3), 36.1 (1C, SCH_2). **HRMS (ESI)** calcd for [$C_{17}H_{16}O_4SNa$, M + Na]$^+$: 339.0662, Found: 339.0662.

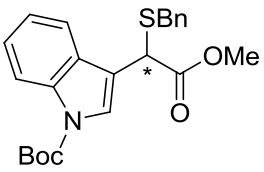
(+)-Methyl 2-(benzo[b]thiophen-3-yl)-2-(benzylthio)-acetate (4ka)



Yellow solid, **m.p.**: 65–66 °C, **TLC** R_f = 0.50 (PE/EA = 15:1, v/v), 91% yield, 87% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 0.5 mL/min, wavelength = 220 nm, t_R = 23.18 min for minor isomer, t_R = 24.02 min for major isomer]. **[α]$_D^{27}$** +8.4 (*c* 0.50, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.84–7.80 (m, 1H, ArH), 7.65 (s, 1H, ArH), 7.56–7.51 (m, 1H, ArH), 7.36–7.22 (m, 7H, ArH), 4.80 (s, 1H, CH), 3.87 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2), 3.73 (s, 3H, OCH_3), 3.68 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.8 (1C, C=O), 140.2 (1C, Ar-C), 137.1 (1C, Ar-C), 136.9 (1C, Ar-C), 129.1 (2C, Ar-C), 128.8 (1C, Ar-C), 128.5 (2C, Ar-C), 127.3 (1C, Ar-C), 126.0 (1C, Ar-C), 124.6 (1C, Ar-C), 124.2 (1C, Ar-C), 122.8 (1C, Ar-C), 121.8 (1C, Ar-C), 52.7 (1C, SCH), 44.3 (1C, OCH_3), 36.3 (1C, SCH_2). **HRMS (ESI)** calcd for [$C_{18}H_{16}O_2S_2Na$, M + Na]$^+$: 351.0484, Found: 351.0487.

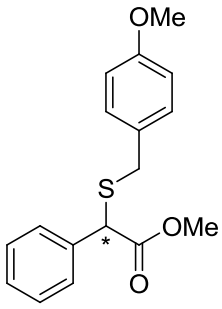
(+)-*tert*-Butyl 3-(1-(benzylthio)-2-methoxy-2-oxoethyl)-1H-indole-1-carboxylate (4la)

Yellow oil, **TLC** R_f = 0.46 (PE/EA = 15:1, v/v), 96% yield, 90% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min,



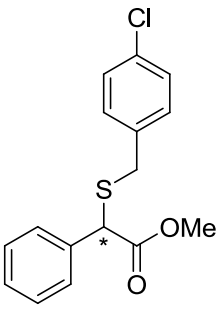
wavelength = 220 nm, t_R = 6.39 min for minor isomer, t_R = 7.03 min for major isomer]. **[α]$_D^{26}$** +18.3 (*c* 1.0, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.13 (brd, *J* = 8.0 Hz, 1H, ArH), 7.73 (s, 1H, ArH), 7.41 (d, *J* = 8.0 Hz, 1H, ArH), 7.33–7.21 (m, 6H, ArH), 7.19 (t, *J* = 7.2 Hz, 1H, ArH), 4.66 (s, 1H, CH), 3.86 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.74 (s, 3H, OCH_3), 3.71 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 1.65 (s, 9H, $C(CH_3)_3$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.9 (1C, $\underline{C}O_2Me$), 149.3 (1C, $\underline{C}O_2{}^t$Bu), 137.0 (1C, Ar-C), 135.4 (1C, Ar-C), 129.1 (2C, Ar-C), 128.5 (1C, Ar-C), 128.4 (2C, Ar-C), 127.2 (1C, CH), 125.1 (1C, Ar-C), 124.7 (1C, CH), 122.6 (1C, Ar-C), 119.4 (1C, Ar-C), 115.2 (1C, Ar-C), 114.2 (1C, Ar-C), 83.9 (1C, $O\underline{C}(CH_3)_3$), 52.6 (1C, SCH), 42.3 (1C, OCH_3), 36.2 (1C, SCH_2), 28.1 (3C, $OC(\underline{C}H_3)_3$). **HRMS (ESI)** calcd for $[C_{23}H_{25}NO_4SNa, M + Na]^+$: 434.1397, Found: 434.1392.

(+)-Methyl 2-(4-methoxybenzylthio)-2-phenylacetate (4ab)



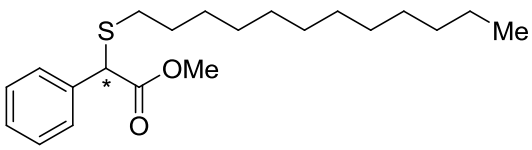
Colorless oil, **TLC** R_f = 0.42 (PE/EA = 15:1, v/v), 97% yield, 93% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 9.52 min for minor isomer, t_R = 10.98 min for major isomer]. **[α]$_D^{26}$** +120 (*c* 1.2, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47–7.43 (m, 2H, ArH), 7.42–7.31 (m, 3H, ArH), 7.24 (d, *J* = 8.4 Hz, 2H, ArH), 6.89 (d, *J* = 8.4 Hz, 2H, ArH), 4.47 (s, 1H, CH), 3.84 (s, 3H, $ArOCH_3$), 3.77 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2), 3.73 (s, 3H, OCH_3), 3.62 (d, *J* = 13.2 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.1 (1C, C=O), 158.7 (1C, Ar-C), 135.8 (1C, Ar-C), 130.1 (2C, Ar-C), 128.9 (1C, Ar-C), 128.6 (2C, Ar-C), 128.5 (2C, Ar-C), 128.1 (1C, Ar-C), 113.8 (2C, Ar-C), 55.2 (1C, $ArOCH_3$), 52.6 (1C, SCH), 51.3 (1C, OCH_3), 35.5 (1C, SCH_2). **HRMS (ESI)** calcd for $[C_{17}H_{18}O_3SNa, M + Na]^+$: 325.0869, Found: 325.0866.

(+)-Methyl 2-(4-chlorobenzylthio)-2-phenylacetate (4ac)



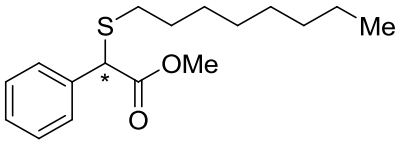
Colorless oil, **TLC** R_f = 0.70 (PE/EA = 15:1, v/v), 94% yield, 94% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 7.02 min for minor isomer, t_R = 8.34 min for major isomer]. **[α]$_D^{26}$** +150 (*c* 0.5, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.41–7.36 (m, 2H, ArH), 7.36–7.29 (m, 3H, ArH), 7.28–7.24 (m, 2H, ArH), 7.22–7.17 (m, 2H, ArH), 4.39 (s, 1H, CH), 3.72 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2), 3.68 (s, 3H, OCH_3), 3.56 (d, *J* = 13.6 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.9 (1C, C=O), 135.6 (1C, Ar-C), 135.5 (1C, Ar-C), 133.0 (1C, Ar-C), 130.3 (2C, Ar-C), 128.7 (2C, Ar-C), 128.6 (2C, Ar-C), 128.5 (2C, Ar-C), 128.2 (1C, Ar-C), 52.7 (1C, SCH), 51.4 (1C, OCH_3), 35.4 (1C, SCH_2). **HRMS (ESI)** calcd for $[C_{16}H_{15}ClO_2SNa, M + Na]^+$: 329.0373, Found: 329.0372.

(+)-Methyl 2-(dodecylthio)-2-phenylacetate (4ad)



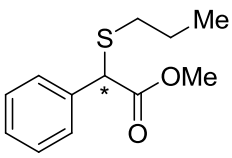
Colorless oil, **TLC** R_f = 0.60 (PE/EA = 20:1, v/v), 86% yield, 93% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 4.04 min for minor isomer, t_R = 4.57 min for major isomer]. **[α]$_D^{29}$** +63.2 (*c* 0.5, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.2 Hz, 2H, ArH), 7.37–7.26 (m, 3H, ArH), 4.58 (s, 1H, CH), 3.73 (s, 3H, OCH_3), 2.55–2.45 (m, 2H, CH_2), 1.58–1.50 (m, 2H, CH_2), 1.38–1.18 (m, 18H, $9CH_2$), 0.88 (t, *J* = 6.8 Hz, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.4 (1C, C=O), 136.2 (1C, Ar-C), 128.6 (2C, Ar-C), 128.4 (2C, Ar-C), 128.1 (1C, Ar-C), 52.6 (1C, SCH), 52.1 (1C, OCH_3), 32.0 (1C, CH_2), 31.9 (1C, CH_2), 29.6 (2C, $2CH_2$), 29.5 (1C, CH_2), 29.4 (1C, CH_2), 29.3 (1C, CH_2), 29.1 (1C, CH_2), 28.9 (1C, CH_2), 28.8 (1C, CH_2), 22.7 (1C, CH_2), 14.1 (1C, CH_3). **HRMS (ESI)** calcd for $[C_{21}H_{34}O_2SNa, M + Na]^+$: 373.2172, Found: 373.2170.

(+)-Methyl 2-(octylthio)-2-phenylacetate (4ae)



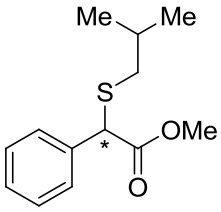
Colorless oil, **TLC** R_f = 0.74 (PE/EA = 15:1, v/v), 87% yield, 93% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 4.28 min for minor isomer, t_R = 5.00 min for major isomer]. **[α]$_D^{25}$** +83.0 (*c* 0.64, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48–7.42 (m, 2H, ArH), 7.37–7.25 (m, 3H, ArH), 4.58 (s, 1H, CH), 3.73 (s, 3H, OCH_3), 2.56–2.44 (m, 2H, CH_2), 1.59–1.49 (m, 2H, CH_2), 1.37–1.17 (m, 10H, $5CH_2$), 0.87 (t, *J* = 7.2 Hz, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.4 (1C, C=O), 136.1 (1C, Ar-C), 128.6 (2C, Ar-C), 128.4 (2C, Ar-C), 128.0 (1C, Ar-C), 52.6 (1C, SCH), 52.1 (1C, OCH_3), 31.9 (1C, CH_2), 31.7 (1C, CH_2), 29.0 (2C, $2CH_2$), 28.9 (1C, CH_2), 28.7 (1C, CH_2), 22.6 (1C, CH_2), 14.0 (1C, CH_3). **HRMS (ESI)** calcd for $[C_{17}H_{26}O_2SNa, M + Na]^+$: 317.1546, Found: 317.1549.

(+)-Methyl 2-phenyl-2-(propylthio)acetate (4af)



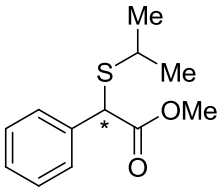
Colorless oil, **TLC** R_f = 0.64 (PE/EA = 15:1, v/v), 86% yield, 93% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 4.41 min for minor isomer, t_R = 5.07 min for major isomer]. **[α]$_D^{24}$** +90.4 (*c* 0.85, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.41–7.36 (m, 2H, ArH), 7.29–7.17 (m, 3H, ArH), 4.51 (s, 1H, CH), 3.65 (s, 3H, OCH_3), 2.48–2.36 (m, 2H, CH_2), 1.56–1.45 (m, 2H, CH_2), 0.88 (t, *J* = 7.6 Hz, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.4 (1C, C=O), 136.1 (1C, Ar-C), 128.6 (2C, Ar-C), 128.4 (2C, Ar-C), 128.0 (1C, Ar-C), 52.6 (1C, SCH), 52.1 (1C, OCH_3), 33.9 (1C, SCH_2), 22.3 (1C, CH_2), 13.4 (1C, CH_3). **HRMS (ESI)** calcd for $[C_{12}H_{16}O_2SNa, M + Na]^+$: 247.0763, Found: 247.0766.

(+)-Methyl 2-(isobutylthio)-2-phenylacetate (4ag)



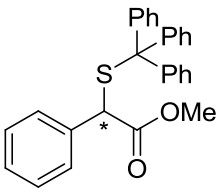
Colorless oil, **TLC** R_f = 0.66 (PE/EA = 15:1, v/v), 89% yield, 87% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 4.34 min for minor isomer, t_R = 5.44 min for major isomer]. **[α]$_D^{26}$** +85.5 (*c* 0.95, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49–7.43 (m, 2H, ArH), 7.37–7.25 (m, 3H, ArH), 4.55 (s, 1H, CH), 3.73 (s, 3H, OCH_3), 2.40 (d, *J* = 6.8 Hz, 2H, SCH_2), 1.77 (sept, *J* = 6.8 Hz, 1H, C<u>H</u>$(CH_3)_2$), 0.95 (t, *J* = 6.8 Hz, 6H, CH(C<u>H</u>$_3)_2$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.4 (1C, C=O), 136.2 (1C, Ar-C), 128.6 (2C, Ar-C), 128.4 (2C, Ar-C), 128.0 (1C, Ar-C), 52.6 (1C, SCH), 52.5 (1C, OCH_3), 40.8 (1C, SCH_2), 28.1 (1C, <u>C</u>H$(CH_3)_2$), 21.9 (2C, CH(<u>C</u>H$_3)_2$). **HRMS (ESI)** calcd for $[C_{13}H_{18}O_2SNa, M + Na]^+$: 261.0920, Found: 261.0923.

(+)-Methyl 2-(isopropylthio)-2-phenylacetate (4ah)



Colorless oil, **TLC** R_f = 0.52 (PE/EA = 20:1, v/v), 89% yield, 78% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 95:5, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 4.46 min for minor isomer, t_R = 4.95 min for major isomer]. **[α]$_D^{27}$** +90.1 (*c* 0.57, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50–7.45 (m, 2H, ArH), 7.37–7.26 (m, 3H, ArH), 4.65 (s, 1H, CH), 3.72 (s, 3H, OCH_3), 2.89 (sept, *J* = 6.8 Hz, 1H, C<u>H</u>$(CH_3)_2$), 1.27 (d, *J* = 5.2 Hz, 3H, CH_3), 1.25 (d, *J* = 5.2 Hz, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.6 (1C, C=O), 136.4 (1C, Ar-C), 128.6 (2C, Ar-C), 128.4 (2C, Ar-C), 128.0 (1C, Ar-C), 52.7 (1C, SCH), 51.3 (1C, OCH_3), 35.6 (1C, SCH), 23.0 (2C, CH(<u>C</u>H$_3)_2$). **HRMS (ESI)** calcd for $[C_{12}H_{16}O_2SNa, M + Na]^+$: 247.0763, Found: 247.0767.

(+)-Methyl 2-phenyl-2-(tritylthio)-acetate (4ai)[5]

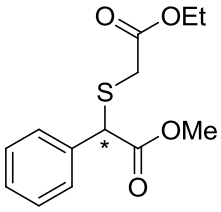


Colorless oil, **TLC** R_f = 0.42 (PE/EA = 15:1, v/v), 88% yield, 94% ee [**HPLC** condition: Chiralcel AD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 5.59 min for major isomer, t_R = 9.43 min for minor isomer]. **[α]$_D^{27}$** +130 (*c* 1.0, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.42–7.38 (m, 5H, ArH), 7.27–7.14 (m, 15H, ArH), 4.06 (s, 1H, CH), 3.40 (s, 3H, OCH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.4 (1C, C=O), 143.9 (3C, Ar-C), 136.7 (1C, Ar-C), 129.7 (6C, Ar-C), 128.6 (2C, Ar-C), 128.1 (2C, Ar-C), 127.9 (6C, Ar-C), 127.8 (1C, Ar-C), 126.8 (3C, Ar-C), 69.2 (1C, <u>C</u>Ph_3), 52.5 (1C, SCH), 52.3 (1C, OCH_3). **HRMS (ESI)** calcd for $[C_{28}H_{24}O_2SNa, M + Na]^+$: 447.1389, Found: 447.1383.

(+)-Methyl 2-(2-ethoxy-2-oxoethylthio)-2-phenylacetate (4aj)

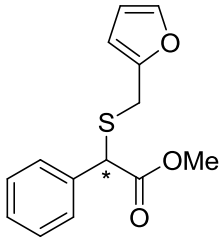
Colorless oil, **TLC** R_f = 0.52 (PE/EA = 6:1, v/v), 83% yield, 98% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 7.57 min for minor isomer, t_R = 9.40 min for

5 (*S*)-**1f** was used as the catalyst.



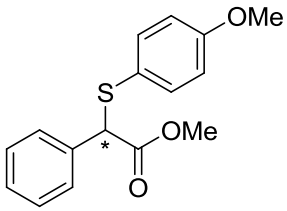
major isomer]. **[α]$_D^{26}$** +172 (*c* 1.0, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.46–7.41 (m, 2H, ArH), 7.37–7.29 (m, 3H, ArH), 4.88 (s, 1H, CH), 4.14 (q, *J* = 7.2 Hz, 2H, OCH_2CH_3), 3.71 (s, 3H, OCH_3), 3.25 (d, *J* = 15.2 Hz, 1H, 1/2SCH_2), 3.06 (d, *J* = 15.2 Hz, 1H, 1/2SCH_2), 1.26 (t, *J* = 7.2 Hz, 1H, OCH_2CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.6 (1C, C=O), 169.7 (1C, C=O), 135.1 (1C, Ar-C), 128.7 (2C, Ar-C), 128.6 (2C, Ar-C), 128.4 (1C, Ar-C), 61.4 (1C, OCH_2CH_3), 52.8 (1C, SCH), 52.2 (1C, OCH_3), 32.9 (1C, SCH_2), 14.0 (1C, OCH_2CH_3). **HRMS (ESI)** calcd for [$C_{13}H_{16}O_4SNa$, M + Na]$^+$: 291.0662, Found: 291.0665.

(+)-Methyl 2-(furan-2-ylmethylthio)-2-phenylacetate (4ak)



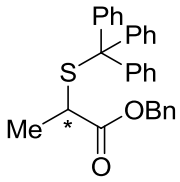
Colorless oil, **TLC** R_f = 0.40 (PE/EA = 15:1, v/v), 85% yield, 96% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 6.41 min for minor isomer, t_R = 6.88 min for major isomer]. **[α]$_D^{26}$** +144 (*c* 0.95, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.46–7.41 (m, 2H, ArH), 7.38–7.30 (m, 4H, ArH), 6.31 (dd, J_1 = 2.8 Hz and J_2 = 2.0 Hz, 1H, ArH), 6.16 (d, *J* = 3.2 Hz, 1H, ArH), 4.58 (s, 1H, CH), 3.77 (d, *J* = 14.8 Hz, 1H, 1/2SCH_2), 3.71 (s, 3H, OCH_3), 3.61 (d, *J* = 14.8 Hz, 1H, 1/2SCH_2); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.9 (1C, C=O), 150.6 (1C, Ar-C), 142.4 (1C, Ar-C), 135.5 (1C, Ar-C), 128.7 (2C, Ar-C), 128.6 (2C, Ar-C), 128.3 (1C, Ar-C), 110.4 (1C, Ar-C), 108.0 (1C, Ar-C), 52.8 (1C, SCH), 51.8 (1C, OCH_3), 28.2 (1C, SCH_2). **HRMS (ESI)** calcd for [$C_{14}H_{14}O_3SNa$, M + Na]$^+$: 285.0556, Found: 285.0548.

(–)-Methyl 2-(4-methoxyphenylthio)-2-phenylacetate (4al)[5]



Colorless oil, **TLC** R_f = 0.50 (PE/EA = 10:1, v/v), 91% yield, 77% ee [**HPLC** condition: Chiralcel OD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 6.19 min for major isomer, t_R = 7.94 min for minor isomer]. **[α]$_D^{27}$** –76.4 (*c* 0.95, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.41–7.36 (m, 2H, ArH), 7.34–7.27 (m, 5H, ArH), 6.81–6.76 (m, 2H, ArH), 4.76 (s, 1H, CH), 3.77 (s, 3H, $ArOCH_3$), 3.66 (s, 3H, OCH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 171.0 (1C, C=O), 160.2 (1C, Ar-C), 136.2 (2C, Ar-C), 135.7 (1C, Ar-C), 128.5 (4C, Ar-C), 128.1 (1C, Ar-C), 123.5 (1C, Ar-C), 114.4 (2C, Ar-C), 57.3 (1C, $ArOCH_3$), 55.2 (1C, OCH_3), 52.5 (1C, SCH). **HRMS (ESI)** calcd for [$C_{16}H_{16}O_3SNa$, M + Na]$^+$: 311.0712, Found: 311.0708.

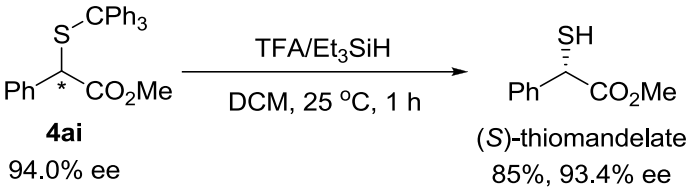
(–)-Benzyl 2-(tritylthio)-propanoate (6)[4,5]



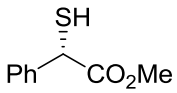
Colorless oil, **TLC** R_f = 0.46 (PE/EA = 15:1, v/v), 62% yield, 96% ee [**HPLC** condition: Chiralcel AD-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 6.66 min for major isomer, t_R = 7.24 min for minor isomer]. **[α]$_D^{27}$** –155.8 (*c* 1.05, MeOH) [lit[4]: $[\alpha]_D^{20}$ +136 (*c* 1.0, MeOH) for 77% ee]. **^{1}H NMR**

(300 MHz, $CDCl_3$): δ 7.47–7.39 (m, 6H, ArH), 7.38–7.28 (m, 3H, ArH), 7.26–7.14 (m, 11H, ArH), 4.98 (d, *J* = 12.3 Hz, 1H, 1/2CH_2), 4.84 (d, *J* = 12.3 Hz, 1H, 1/2CH_2), 2.99 (q, *J* = 7.2 Hz, 1H, CH), 1.16 (d, *J* = 7.2 Hz, 2H, CH_3).

5. Synthesis of Optically Active Unprotected α-Thiol Ester

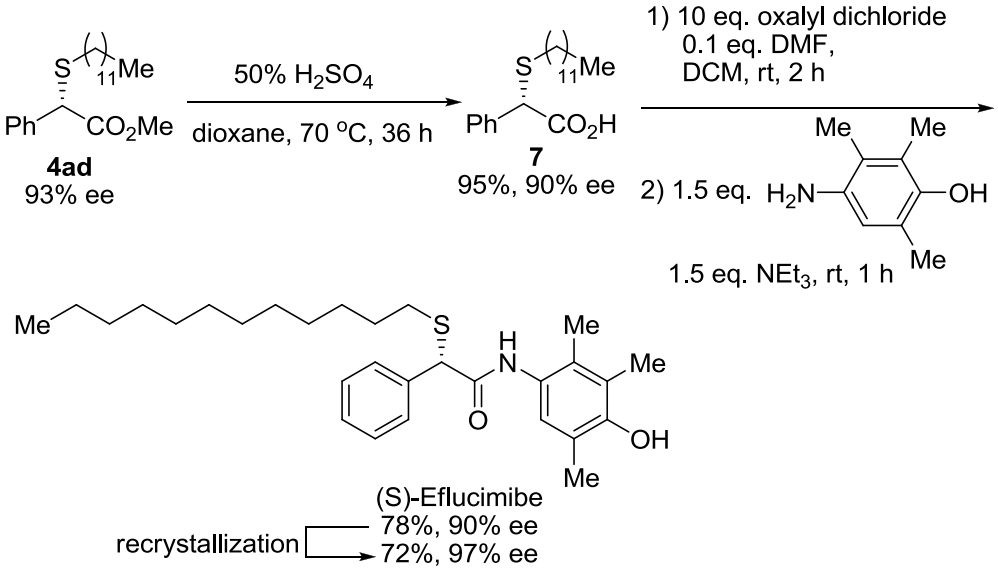


(*S*)-Thiomandelate[3b,6]



Methyl 2-phenyl-2-(tritylthio) acetate (**4ai**, 35 mg, 0.083 mmol) was dissolved in CH_2Cl_2 (2 mL), trifluoroacetic acid (TFA, 1 mL) and Et_3SiH (20 mg, 0.166 mmol) were added susequently. After stirring for 1 h at 25 °C (TLC monitoring), the reaction finished and the mixture was concentrated and purified through a silica gel chromatography to give methyl (*S*)-thiomandelate as a colorless oil. **TLC** R_f = 0.50 (PE/EA = 15:1, v/v), 18 mg, 85% yield, 93.4% ee [**HPLC** condition: Chiralcel OJ-H column, *n*-hexane/*i*-propanol = 90:10, flow rate = 1.0 mL/min, wavelength = 220 nm, t_R = 16.22 min for major isomer, t_R = 19.26 min for minor isomer]. **$[\alpha]_D^{28}$** +93.8 (*c* 0.50, EtOH) [lit[3b]: $[\alpha]_D^{25}$ +115 (*c* 2.0, 95% EtOH) for (*S*) with 93% ee]. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.46–7.41 (m, 2H, ArH), 7.38–7.28 (m, 3H, ArH), 4.70 (d, *J* = 7.6 Hz, 1H, CH), 3.75 (s, 3H, OCH_3), 2.60 (d, *J* = 7.6 Hz, 1H, SH).

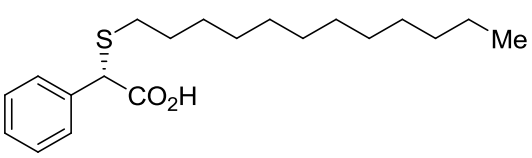
6. Synthesis of (*S*)-Eflucimibe



(*S*)-2-(Dodecylthio)-2-phenylacetic acid (7)

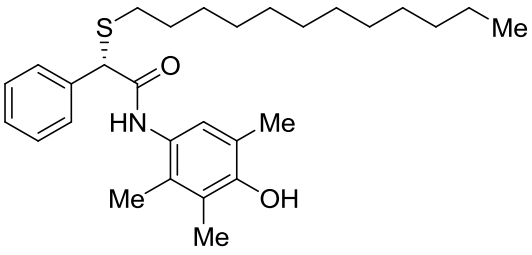
(*S*)-Methyl 2-(dodecylthio)-2- phenylacetate (**4ae**, 35 mg, 0.1 mmol) was intruduced

6 B. Strijtveen and R. M. Kellogg, *J. Org. Chem.*, 1986, **51**, 3664.



into a 25 mL Schlenk flask. After dioxane (4 mL) was added, the solution was stirred in ice-bath. After 50% H_2SO_4 aqueous solution (4 mL) was added dropwise, the resulting mixture was stirred in 70 °C oil-bath for 36 h till the **4ae** disappeared (monitoring by TLC). The mixture was extracted by EtOAc (10 mL × 3). The organic layers were combined, washed by brine, dried over Mg_2SO_4, concentrated and purified by flash chromatography on silica to afford (*S*)-2-(dodecylthio)-2-phenylacetic acid (**7**) as colorless oil. **TLC** R_f = 0.65 (PE/EA = 2:1, v/v), 32 mg, 95% yield, 90% ee [**SFC** condition: Chiralcel AD-3 column, carbon dioxide/*i*-propanol = 85:15, flow rate = 2.0 mL/min, wavelength = 220 nm, t_R = 8.44 min for (*R*)-isomer, t_R = 10.09 min for (*S*) isomer]. **[α]$_D^{28}$** +34.6 (*c* 0.5, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47 (d, *J* = 6.8 Hz, 2H, ArH), 7.38–7.28 (m, 3H, ArH), 4.57 (s, 1H, CH), 2.62–2.50 (m, 2H, CH_2), 1.61–1.51 (m, 2H, CH_2), 1.38–1.18 (m, 18H, $9CH_2$), 0.88 (t, *J* = 6.8 Hz, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.5 (1C, C=O), 135.5 (1C, Ar-C), 128.7 (2C, Ar-C), 128.5 (2C, Ar-C), 128.3 (1C, Ar-C), 52.0 (1C, SCH), 32.2 (1C, CH_2), 31.9 (1C, CH_2), 29.6 (2C, $2CH_2$), 29.5 (1C, CH_2), 29.4 (1C, CH_2), 29.3 (1C, CH_2), 29.1 (1C, CH_2), 28.9 (1C, CH_2), 28.8 (1C, CH_2), 22.7 (1C, CH_2), 14.1 (1C, CH_3). **HRMS (ESI)** calcd for $[C_{20}H_{33}O_2S, M + H]^+$: 337.2196, Found: 337.2199.

(*S*)-Eflucimibe

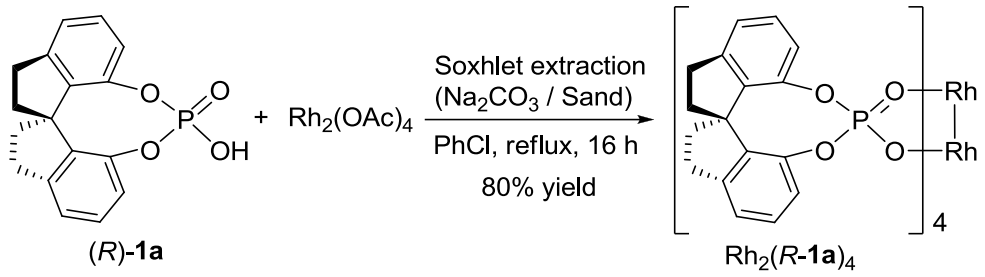


(*S*)-2-(Dodecylthio)-2-phenylacetic acid (**7**, 30 mg, 0.089 mmol) was dissolved with dry CH_2Cl_2 (4 mL) and introduced into a 20 mL Schlenk tube under N_2 protection. Drops of DMF (5 μL) was added and the mixture was stirred in an ice-bath. Then oxalyl chloride (127 mg, 1 mmol) was added carefully. After stirred for 1 h at room temperature, the mixture was concentrated under vacuum and cooled by ice-bath before a dry CH_2Cl_2 solution of 4-amino-2,3,6-trimethylphenol (23 mg, 0.15 mmol) was added. After NEt_3 (15 mg, 0.15 mmol) was added, the mixture was stirred at room temperature for 1 h, concentrated and purified by flash chlomatography on silica to afford yellow-solid product. After a recrystallization with ^{i}PrOH, (*S*)-Eflucimible was obtained as white crystal solid, **m.p.**: 127–128 °C; **TLC** R_f = 0.55 (PE/EA = 4:1, v/v), 72% yield, 97% ee [**SFC** condition: Chiralcel AD-3 column, carbon dioxide/*i*-propanol = 70:30, flow rate = 2.0 mL/min, wavelength = 254 nm, t_R = 10.46 min for (*R*)-isomer, t_R = 11.47 min for (*S*)-isomer]. **[α]$_D^{28}$** –29.1 (*c* 0.7, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.44 (s, 1H, NH), 7.48 (d, *J* = 7.2 Hz, 2H, ArH), 7.37 (t, *J* = 7.2 Hz, 2H, ArH), 7.31 (t, *J* = 7.2 Hz, 2H, ArH), 7.04 (s, 1H, ArH), 7.04 (s, 1H, ArH), 5.38 (s, 1H, OH), 4.72 (s, 1H, SCH), 2.77–2.63 (m, 2H, CH_2), 2.10 (s, 3H, $ArCH_3$), 2.08 (s, 3H, $ArCH_3$), 2.04 (s, 3H, $ArCH_3$), 1.73–1.61 (m, 2H, CH_2), 1.45–1.35 (m, 2H, CH_2), 1.33–1.21 (m, 16H, $8CH_2$), 0.89 (t, *J* = 6.8 Hz, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.0 (1C, C=O),

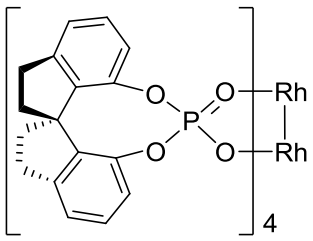
150.6 (1C, Ar-C), 137.0 (1C, Ar-C), 129.2 (1C, Ar-C), 128.9 (2C, Ar-C), 128.1 (1C, Ar-C), 127.9 (2C, Ar-C), 126.8 (1C, Ar-C), 124.1 (1C, Ar-C), 123.2 (1C, Ar-C), 121.4 (1C, Ar-C), 55.6 (1C, SCH), 33.0 (1C, CH_2), 31.9 (1C, CH_2), 29.6 (2C, $2CH_2$), 29.5 (1C, CH_2), 29.4 (1C, CH_2), 29.3 (1C, CH_2), 29.1 (2C, CH_2), 28.8 (1C, CH_2), 22.7 (1C, CH_2), 15.9 (1C, CH_3), 14.09 (1C, CH_3), 14.06 (1C, CH_2), 12.3 (1C, CH_2). **HRMS (ESI)** calcd for $[C_{29}H_{44}NO_2S, M + H]^+$: 470.3087, Found: 470.3094.

7. Synthesis of Rh_2(*R*-1a)$_4$

According to the reported procedure,[7] (*R*)-1,1'-spirobiindanyl-7,7'-diyl phosphoric aicd ((*R*)-**1a**, 125 mg, 0.4 mmol), $Rh_2(OAc)_4$ (25 mg, 0.05 mmol) and 30 mL dry chlorobenzene were introduced into a 100 mL two-necked flask. The mixture was refluxed for 16 hours at 170–180 ℃ using a Soxhlet apparatus filled with sand and Na_2CO_3 for the removal of acetic acid. The mixture was then concentrated under vacuum and purified by column chromatography on silica gel using CH_2Cl_2 as mobile phase. The obtained crude product (75 mg) was recrystallized in a mixed solvent of CH_2Cl_2 and MeOH to give Rh_2(*R*-**1a**)$_4$ as a green needle crystal.



Tetrakis[(*R*)-1,1'-Spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II)



Green-blue needle crystal, **m.p.**: decomposed over 300 °C. **TLC** R_f = 0.50 (CH_2Cl_2), 80% yield. **[α]$_D^{28}$** –338 (*c* 0.60, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.13–6.95 (m, 24H, ArH), 3.59 (s, 2H, OH), 3.12–2.95 (m, 8H, $4CH_2$), 2.86–2.68 (m, 16H, $4CH_2 + 2CH_3O + H_2O$), 2.26–2.12 (m, 8H, $4CH_2$), 2.06–1.88 (m, 8H, $4CH_2$); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 146.3 (4C, Ar-C), 145.9 (4C, Ar-C), 139.3 (4C, Ar-C), 128.7 (4C, Ar-C), 122.3 (4C, Ar-C), 122.2 (4C, Ar-C), 59.0 (4C, C), 51.7 (MeOH), 38.3 (8C, $8CH_2$), 30.5 (8C, $8CH_2$); **^{31}P NMR** (162 MHz, $CDCl_3$): δ 5.30 (s) (methanol in coordination sphere). **HRMS (ESI)** calcd for $[C_{68}H_{60}NO_{16}P_4Rh_2, M + NH_4]^+$: 1476.0967, Found: 1476.0935.

7 R. Hrdina, L. Guénée, D. Moraleda and J. Lacour, *Organometallics*, 2013, **32**, 473.

8. X-ray Diffraction Analysis

1. Crystallographic data for (*S*)-4ca.

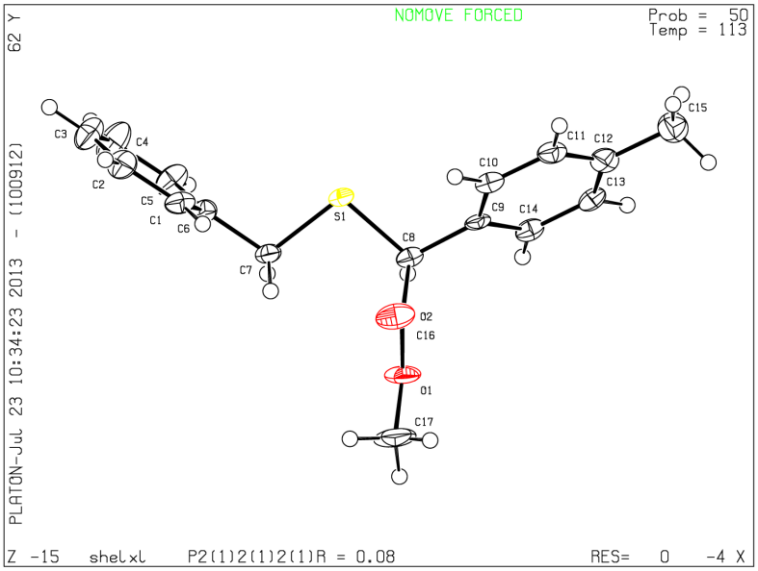


Table S2 Crystal data and structure refinement for (*S*)-4ca

Empirical formula	C17 H18 O2 S
Moiety formula	$C_{17}H_{18}O_2S$
Formula weight	286.37
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 5.6730(11) Å alpha = 90°. b = 8.3677(17) Å beta = 90°. c = 31.795(6) Å gamma = 90°.
Volume	1509.3(5) $Å^3$
Z	4
Calculated density	1.260 Mg/m^3
Absorption coefficient	0.213 mm^{-1}
F(000)	608
Crystal size	0.20 x 0.180 x 0.12 mm
Theta range for data collection	2.56 to 25.02°.
Limiting indices	-6<=h<=6, -9<=k<=9, -33<=l<=37

Reflections collected / unique	7898 / 2603 [R(int) = 0.1418]
Completeness to theta = 25.242	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9749 and 0.9586
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2603 / 0 / 183
Goodness-of-fit on F^2	1.131
Final R indices [I>2sigma(I)]	R_1 = 0.0834, wR_2 = 0.1875
R indices (all data)	R_1 = 0.0925, wR_2 = 0.1904
Absolute structure parameter	-0.1(2)
Extinction coefficient	0.00175(11)
Largest diff. peak and hole	0.505 and -0.391 e.Å^{-3}

2. Crystallographic data for Rh$_2$(*R*-1a)$_4$(MeOH)$_2$.

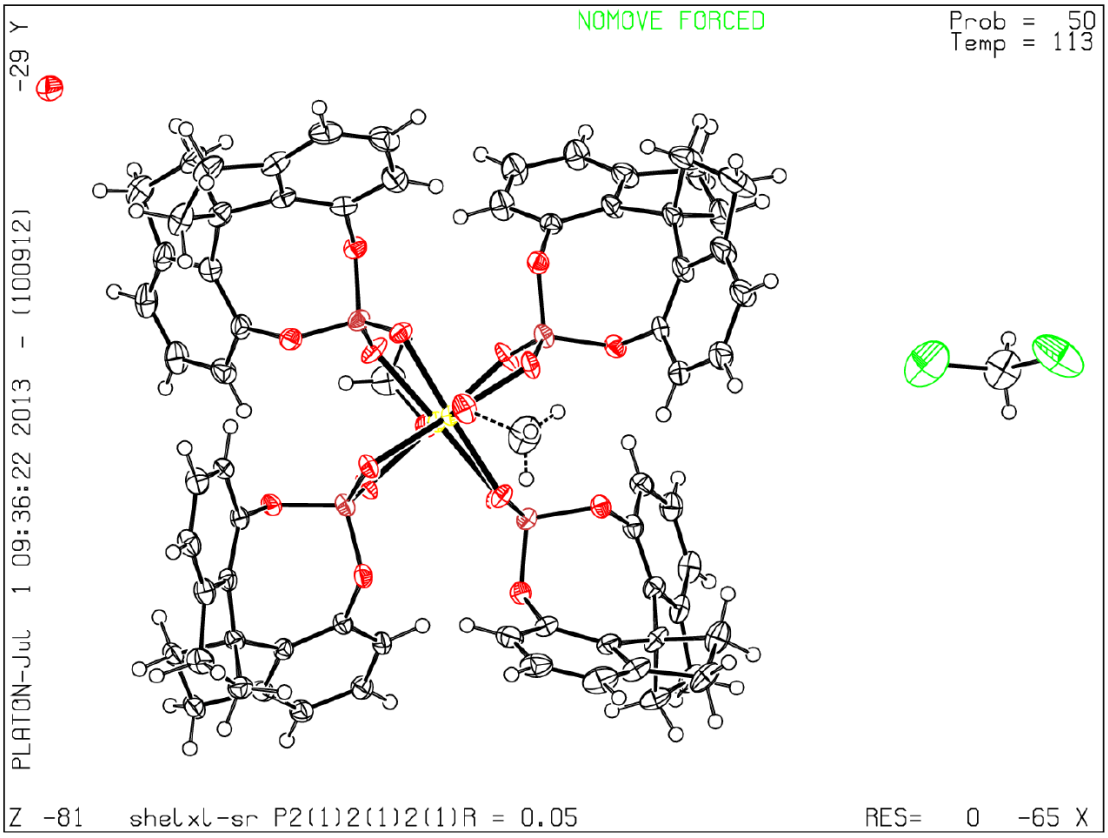


Table S3 Crystal data and structure refinement for Rh$_2$(*R*-1a)$_4$(MeOH)$_2$

Empirical formula	C70 H66 Cl2 O19 P4 Rh2

Moiety formula	$C_{68}H_{56}O_{16}P_4Rh_2$, $2(CH_3O)$, CH_2Cl_2, H_2O
Formula weight	1611.83
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 16.527(3) Å alpha = 90°. b = 18.866(4) Å beta = 90°. c = 26.157(5) Å gamma = 90°.
Volume	8156(3) $Å^3$
Z	4
Calculated density	1.313 Mg/m^3
Absorption coefficient	0.610 mm^{-1}
F(000)	3288
Crystal size	0.260 x 0.160 x 0.140 mm
Theta range for data collection	1.33 to 29.97°.
Limiting indices	-22<=h<=23, -26<=k<=26, -36<=l<=36
Reflections collected / unique	110127 / 23721 [R(int) = 0.0642]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9194 and 0.8575
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	203721 / 32 / 887
Goodness-of-fit on F^2	1.097
Final R indices [I>2sigma(I)]	R_1 = 0.0481, wR_2 = 0.1192
R indices (all data)	R_1 = 0.0514, wR_2 = 0.1213
Absolute structure parameter	-0.010(18)
Extinction coefficient	0.00175(11)
Largest diff. peak and hole	0.645 and -0.996 $e.Å^{-3}$

Table S4 Selected bond lengths [A], angles [deg] and torsion angles [deg] for Rh_2(*R*-1a)$_4$

Rh(1)-O(1)	2.037(3)	Rh(1)-O(10)	2.051(3)
Rh(1)-O(14)	2.055(2)	Rh(1)-O(5)	2.061(2)
Rh(1)-O(18)	2.271(3)	Rh(1)-Rh(2)	2.5222(5)
Rh(2)-O(13)	2.046(2)	Rh(2)-O(9)	2.052(2)
Rh(2)-O(2)	2.061(2)	Rh(2)-O(6)	2.066(2)
Rh(2)-O(17)	2.309(3)	P(1)-O(1)	1.517(3)
P(1)-O(2)	1.504(3)	P(1)-O(3)	1.593(3)
P(1)-O(4)	1.589(3)	O(3)-C(1)	1.414(4)
O(4)-C(10)	1.416(5)	O(1)-Rh(1)-O(10)	177.61(11)
O(1)-Rh(1)-O(14)	88.58(13)	O(10)-Rh(1)-O(14)	92.58(12)
O(1)-Rh(1)-O(5)	90.99(12)	O(10)-Rh(1)-O(5)	87.82(12)
O(14)-Rh(1)-O(5)	179.17(11)	O(1)-Rh(1)-O(18)	88.26(10)
O(10)-Rh(1)-O(18)	89.67(10)	O(14)-Rh(1)-O(18)	89.23(10)
O(5)-Rh(1)-O(18)	90.05(10)	O(1)-Rh(1)-Rh(2)	91.48(8)
O(10)-Rh(1)-Rh(2)	90.63(7)	O(14)-Rh(1)-Rh(2)	89.28(8)
O(5)-Rh(1)-Rh(2)	91.43(8)	O(18)-Rh(1)-Rh(2)	178.50(7)
O(13)-Rh(2)-O(9)	89.11(11)	O(13)-Rh(2)-O(2)	88.81(11)
O(9)-Rh(2)-O(2)	177.85(11)	O(13)-Rh(2)-O(6)	179.40(11)
O(9)-Rh(2)-O(6)	90.78(11)	O(2)-Rh(2)-O(6)	91.30(10)
O(13)-Rh(2)-O(17)	86.89(10)	O(9)-Rh(2)-O(17)	88.96(11)
O(2)-Rh(2)-O(17)	90.41(11)	O(6)-Rh(2)-O(17)	92.51(10)
O(13)-Rh(2)-Rh(1)	91.49(8)	O(9)-Rh(2)-Rh(1)	90.56(7)
O(2)-Rh(2)-Rh(1)	90.01(7)	O(6)-Rh(2)-Rh(1)	89.10(7)
O(17)-Rh(2)-Rh(1)	178.32(7)	O(2)-P(1)-O(1)	119.07(15)
O(2)-P(1)-O(4)	111.64(15)	O(1)-P(1)-O(4)	103.65(16)
O(2)-P(1)-O(3)	105.09(15)	O(1)-P(1)-O(3)	111.38(17)
O(4)-P(1)-O(3)	105.34(14)	O(1)-Rh(1)-Rh(2)-O(13)	-99.52(12)
O(10)-Rh(1)-Rh(2)-O(13)	81.62(12)	O(14)-Rh(1)-Rh(2)-O(13)	-10.96(12)
O(5)-Rh(1)-Rh(2)-O(13)	169.46(11)	O(18)-Rh(1)-Rh(2)-O(13)	-20(3)
O(1)-Rh(1)-Rh(2)-O(9)	171.36(12)	O(10)-Rh(1)-Rh(2)-O(9)	-7.51(11)

O(14)-Rh(1)-Rh(2)-O(9)	-100.08(12)	O(5)-Rh(1)-Rh(2)-O(9)	80.33(11)
O(18)-Rh(1)-Rh(2)-O(9)	-109(3)	O(1)-Rh(1)-Rh(2)-O(2)	-10.71(12)
O(10)-Rh(1)-Rh(2)-O(2)	170.42(12)	O(14)-Rh(1)-Rh(2)-O(2)	77.85(12)
O(5)-Rh(1)-Rh(2)-O(2)	-101.74(11)	O(18)-Rh(1)-Rh(2)-O(2)	69(3)
O(1)-Rh(1)-Rh(2)-O(6)	80.59(12)	O(10)-Rh(1)-Rh(2)-O(6)	-98.27(12)
O(14)-Rh(1)-Rh(2)-O(6)	169.15(11)	O(5)-Rh(1)-Rh(2)-O(6)	-10.44(11)

3. Crystallographic data for (*R*)-1a.

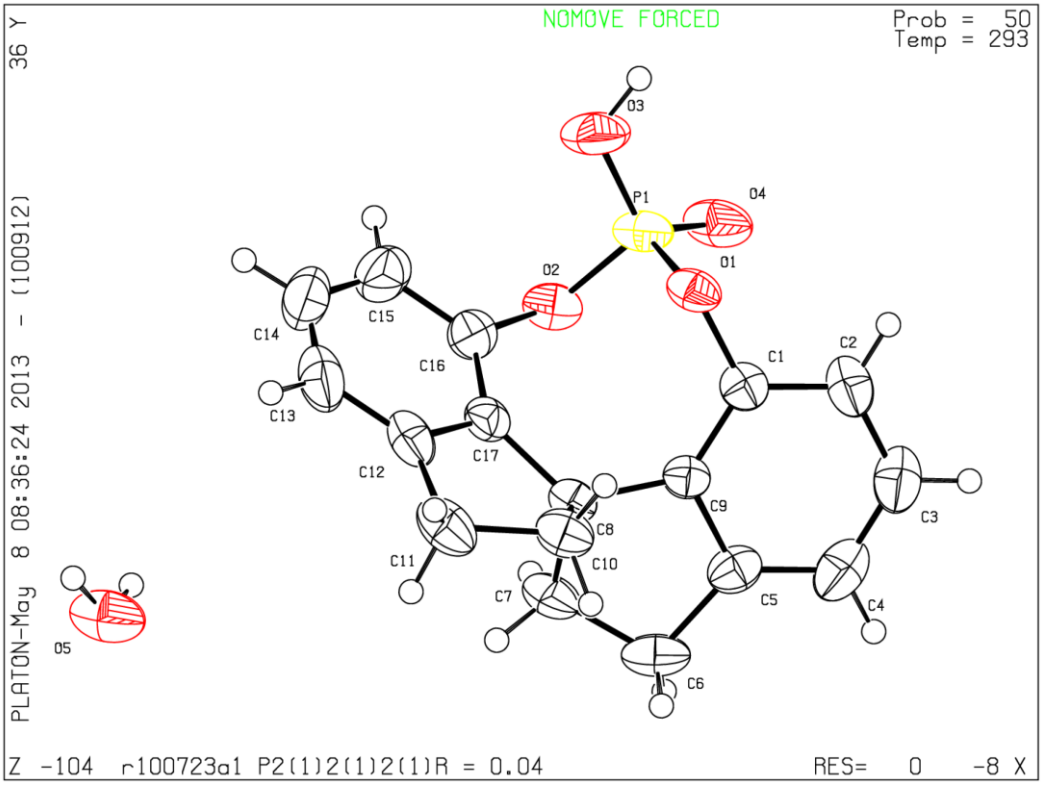


Table S5 Crystal data and structure refinement for (*R*)-1a

Empirical formula	C17 H17 O5 P	
Moiety formula	$C_{17}H_{15}O_4P$, H_2O	
Formula weight	332.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 6.6316(13) Å	alpha = 90°.
	b = 9.2654(19) Å	beta = 90°.
	c = 26.038(5) Å	gamma = 90°.
Volume	1599.9(6) $Å^3$	
Z	4	
Calculated density	1.379 Mg/m^3	
Absorption coefficient	0.195 mm^{-1}	
F(000)	696	

Crystal size	0.20 x 0.10 x 0.06 mm
Theta range for data collection	1.56 to 25.02°.
Limiting indices	-7<=h<=7, -11<=k<=10, -25<=l<=30
Reflections collected / unique	10910 / 2807 [R(int) = 0.0438]
Completeness to theta = 25.02	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9884 and 0.9621
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2807 / 4 / 221
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R_1 = 0.0397, wR_2 = 0.0908
R indices (all data)	R_1 = 0.0458, wR_2 = 0.0962
Absolute structure parameter	0.00(10)
Extinction coefficient	0.104(6)
Largest diff. peak and hole	0.248 and -0.241 e.Å^{-3}

Table S6 Selected bond lengths [A], angles [deg] and torsion angles [deg] for (*R*)-1a

P(1)-O(4)	1.4818(18)	P(1)-O(3)	1.4974(19)
P(1)-O(2)	1.5835(17)	P(1)-O(1)	1.5919(16)
O(1)-C(1)	1.411(3)	O(2)-C(16)	1.415(3)
O(3)-H(3)	0.912(10)	O(4)-P(1)-O(3)	119.49(11)
O(4)-P(1)-O(2)	105.55(10)	O(3)-P(1)-O(2)	109.17(11)
O(4)-P(1)-O(1)	111.57(10)	O(3)-P(1)-O(1)	105.29(11)
O(2)-P(1)-O(1)	104.90(8)	C(1)-O(1)-P(1)	116.05(14)
C(16)-O(2)-P(1)	118.39(14)	P(1)-O(3)-H(3)	117(3)
O(4)-P(1)-O(1)-C(1)	-49.28(16)	O(3)-P(1)-O(1)-C(1)	179.67(15)
O(2)-P(1)-O(1)-C(1)	64.52(15)	O(4)-P(1)-O(2)-C(16)	175.89(16)
O(3)-P(1)-O(2)-C(16)	-54.50(18)	O(1)-P(1)-O(2)-C(16)	57.92(18)

4. Crystallographic data for (*S*)-1b.

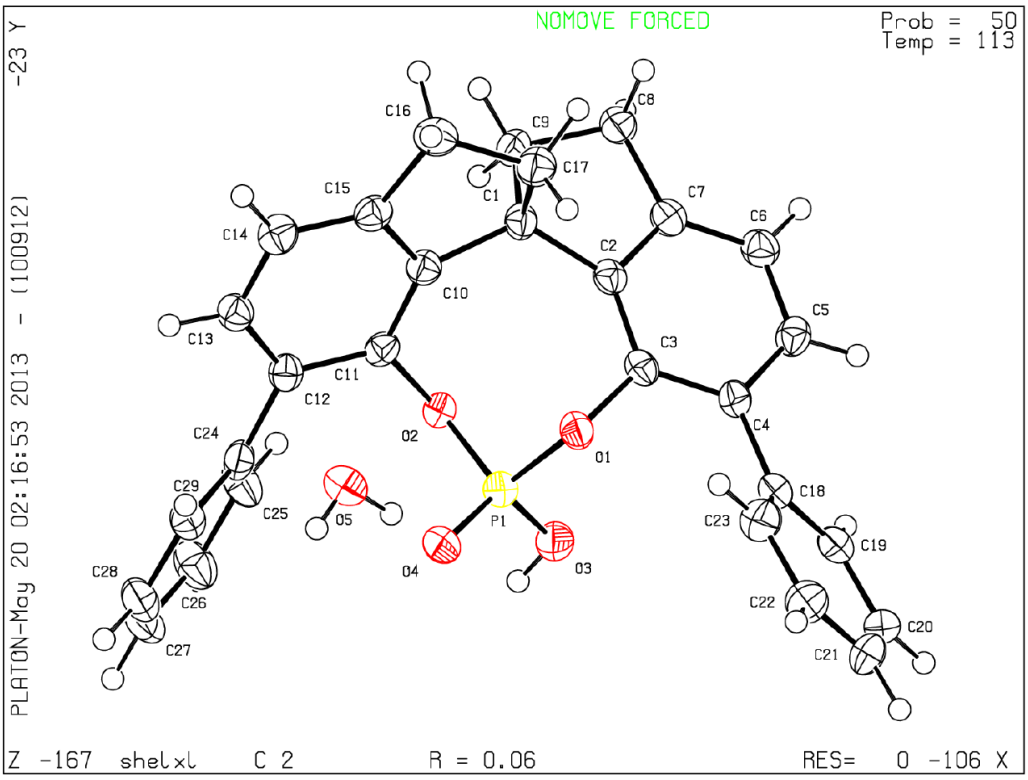


Table S7 Crystal data and structure refinement for (*S*)-1b

Empirical formula	C29 H25 O5 P	
Moiety formula	$C_{29}H_{23}O_4P$, H_2O	
Formula weight	484.46	
Temperature	113(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 25.330(4) Å	alpha = 90°.
	b = 6.6640(8) Å	beta = 121.291° (16).
	c = 16.090(2) Å	gamma = 90°.
Volume	2320.9(6) $Å^3$	
Z	4	
Calculated density	1.386 Mg/m^3	
Absorption coefficient	0.159 mm^{-1}	
F(000)	1016	

Crystal size	0.160 x 0.140 x 0.120 mm
Theta range for data collection	1.481 to 28.160°.
Limiting indices	-32<=h<=33, -8<=k<=6, -21<=l<=21
Reflections collected / unique	10436 / 4627 [R(int) = 0.0672]
Completeness to theta = 25.02	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.981 and 0.679
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4627 / 1 / 326
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R_1 = 0.0630, wR_2 = 0.1290
R indices (all data)	R_1 = 0.0814, wR_2 = 0.1415
Absolute structure parameter	-0.05(13)
Extinction coefficient	0.0069(9)
Largest diff. peak and hole	0.276 and -0.439 e.Å^{-3}

Table S8 Selected bond lengths [A], angles [deg] and torsion angles [deg] for (*S*)-1b

P(1)-O(4)	1.471(3)	P(1)-O(3)	1.500(4)
P(1)-O(2)	1.593(3)	P(1)-O(1)	1.592(3)
O(1)-C(3)	1.413(5)	O(2)-C(11)	1.406(5)
O(3)-H(3)	0.8400	O(4)-P(1)-O(3)	119.6(2)
O(4)-P(1)-O(1)	106.52(18)	O(3)-P(1)-O(1)	107.63(18)
O(4)-P(1)-O(2)	112.60(17)	O(3)-P(1)-O(2)	104.0(2)
O(1)-P(1)-O(2)	105.51(16)	C(3)-O(1)-P(1)	119.4(3)
C(11)-O(2)-P(1)	116.0(3)	P(1)-O(3)-H(3)	109.5
O(4)-P(1)-O(1)-C(3)	-178.2(3)	O(3)-P(1)-O(1)-C(3)	52.3(4)
O(2)-P(1)-O(1)-C(3)	-58.3(3)	O(4)-P(1)-O(2)-C(11)	50.0(3)
O(3)-P(1)-O(2)-C(11)	-178.9(3)	O(1)-P(1)-O(2)-C(11)	-65.8(3)
C(3)-C(4)-C(18)-C(23)	-43.6(7)	C(11)-C(12)-C(24)-C(25)	-51.3(7)

5. Crystallographic data for (*R*)-1f.

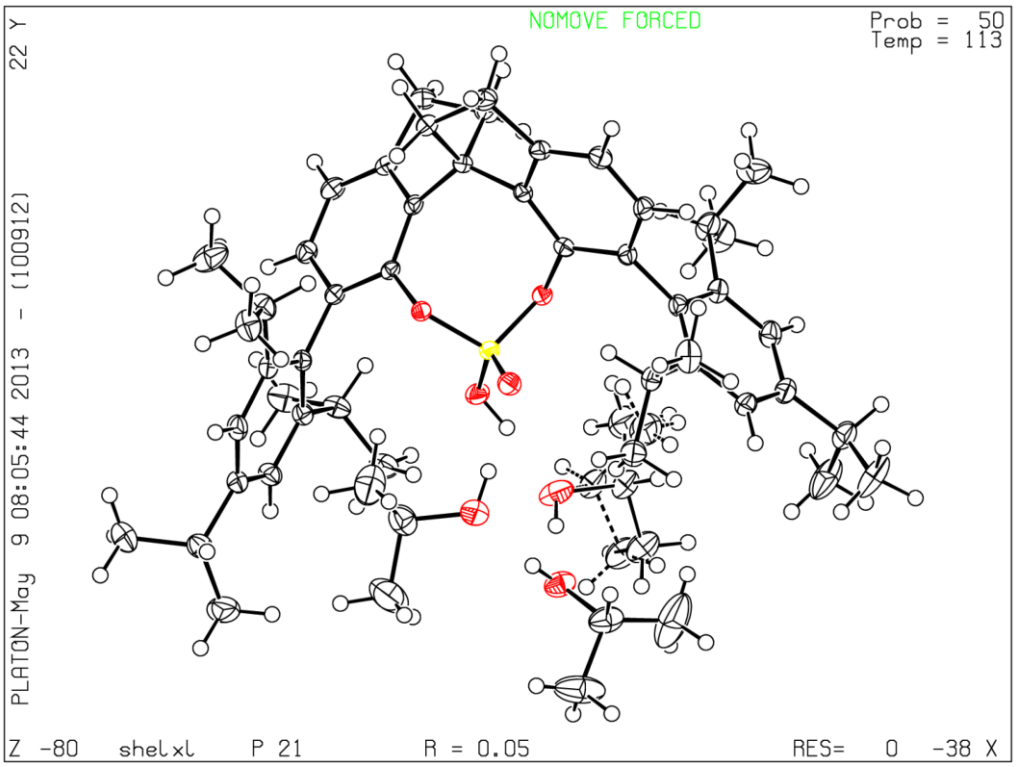


Table S9 Crystal data and structure refinement for (*R*)-1f

Empirical formula	C56 H83 O7 P	
Moiety formula	$C_{47}H_{59}O_4P$, $3(C_3H_8O)$	
Formula weight	899.19	
Temperature	113(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 11.7790(13) Å	alpha = 90°.
	b = 17.451(2) Å	beta = 110.544(4)°.
	c = 13.8490(16) Å	gamma = 90°.
Volume	2665.7(5) $Å^3$	
Z	2	
Calculated density	1.120 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	980	

Crystal size	0.260 x 0.240 x 0.180 mm
Theta range for data collection	1.570 to 33.146°.
Limiting indices	-18<=h<=18, -26<=k<=26, -21<=l<=21
Reflections collected / unique	45085 / 20147 [R(int) = 0.0516]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.982 and 0.813
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20147 / 14 / 619
Goodness-of-fit on F^2	0.993
Final R indices [I>2sigma(I)]	R_1 = 0.0524, wR_2 = 0.0955
R indices (all data)	R_1 = 0.0624, wR_2 = 0.0999
Absolute structure parameter	0.02(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.431 and -0.382 e.Å^{-3}

Table S10 Selected bond lengths [A], angles [deg] and torsion angles [deg] for (*R*)-1f

P(1)-O(3)	1.4674(14)	P(1)-O(4)	1.5325(14)
P(1)-O(1)	1.5875(13)	P(1)-O(2)	1.6053(13)
O(1)-C(3)	1.401(2)	O(2)-C(11)	1.407(2)
O(4)-H(4)	0.89(3)	O(3)-P(1)-O(4)	118.29(8)
O(3)-P(1)-O(1)	107.88(8)	O(4)-P(1)-O(1)	106.49(7)
O(3)-P(1)-O(2)	114.12(8)	O(4)-P(1)-O(2)	102.89(8)
O(1)-P(1)-O(2)	106.35(6)	C(3)-O(1)-P(1)	122.63(11)
C(11)-O(2)-P(1)	116.77(11)	P(1)-O(4)-H(4)	113.4(16)
O(3)-P(1)-O(1)-C(3)	175.81(13)	O(4)-P(1)-O(1)-C(3)	-56.24(14)
O(2)-P(1)-O(1)-C(3)	52.99(14)	O(3)-P(1)-O(2)-C(11)	-49.92(14)
O(4)-P(1)-O(2)-C(11)	-179.36(12)	O(1)-P(1)-O(2)-C(11)	68.89(13)
C(3)-C(4)-C(18)-C(19)	67.3(2)	C(11)-C(12)-C(33)-C(38)	78.6(2)

9. DFT Calculation Details and Results

All of the DFT calculations were performed with the Gaussian 09 program package.[8] The geometry optimization of all the minima and transition states involved were performed at the B3LYP levels of theory[9] with a basis set consisting of the LANL2DZ basis set[10a] for rhodium and the 6-31G(d) basis set[10b] for the other atoms. IRC[11] calculations were carried out to confirm that each transition state is connected with its corresponding reactant and product. Single point energy calculations using B3LYP//6-311+G(d,p) basis set for all non-transition metal atoms were also performed as well as M06-2X//6-31G(d) methods.[12] Solvent effects were computed with the PCM[13] model in cyclohexane using the gas phase optimized structures. Unless specifically mentioned, all discussed relative energies in this paper are referred to ΔG_{sol} in cyclohexane solvent. The zero-point energy-corrected enthalpies (ΔH_{sol}) in the cyclohexane solvent, and the Gibbs free energies in the gas phase (ΔG_{gas}) at 298K were also given. Computed structures are illustrated using CYLVIEW drawings.[14]

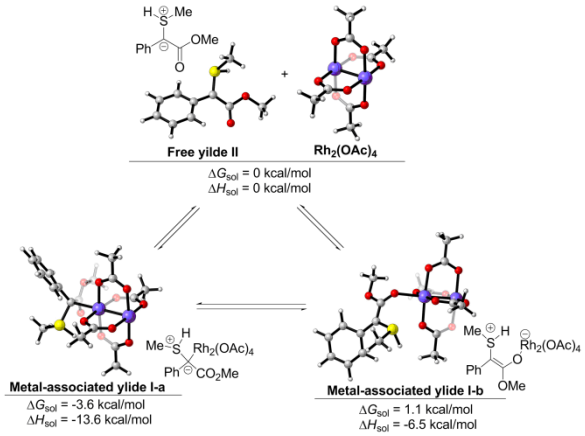


Fig. S1 DFT calculations on the energies of three possible ylide intermediates; keyword 5D was used for the free ylide **II** in this surface.

8 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision B.01*, Gaussian, Inc., Wallingford CT, 2009.

9 (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

10 (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299; (b) W. J. Hehre, L. Radom, P. V. R. Schleyer and J. A. Pople, *Ab Initio Molecular Orbital Theory*, Wiley, New York, 1986; for the transition states **TS IV-R** and **TS IV-S**, the M06-2X-G(d)//6-31G(d) basis set has also been performed.

11 (a) K. Fukui, *J. Phys. Chem.*, 1970, **74**, 4161; (b) C. Gonzalez and H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154; (c) C. Gonzalez and H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523.

12 (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215; (b) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157.

13 (a) V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995; (b) M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.*, 2003, **24**, 669; (c) Y. Takano and K. N. Houk, *J. Chem. Theory Comput.*, 2005, **1**, 70.

14 C. Y. Legault, *CYLView*, *version 1.0b* nd, Canada, 2009; http://www.cylview.org.

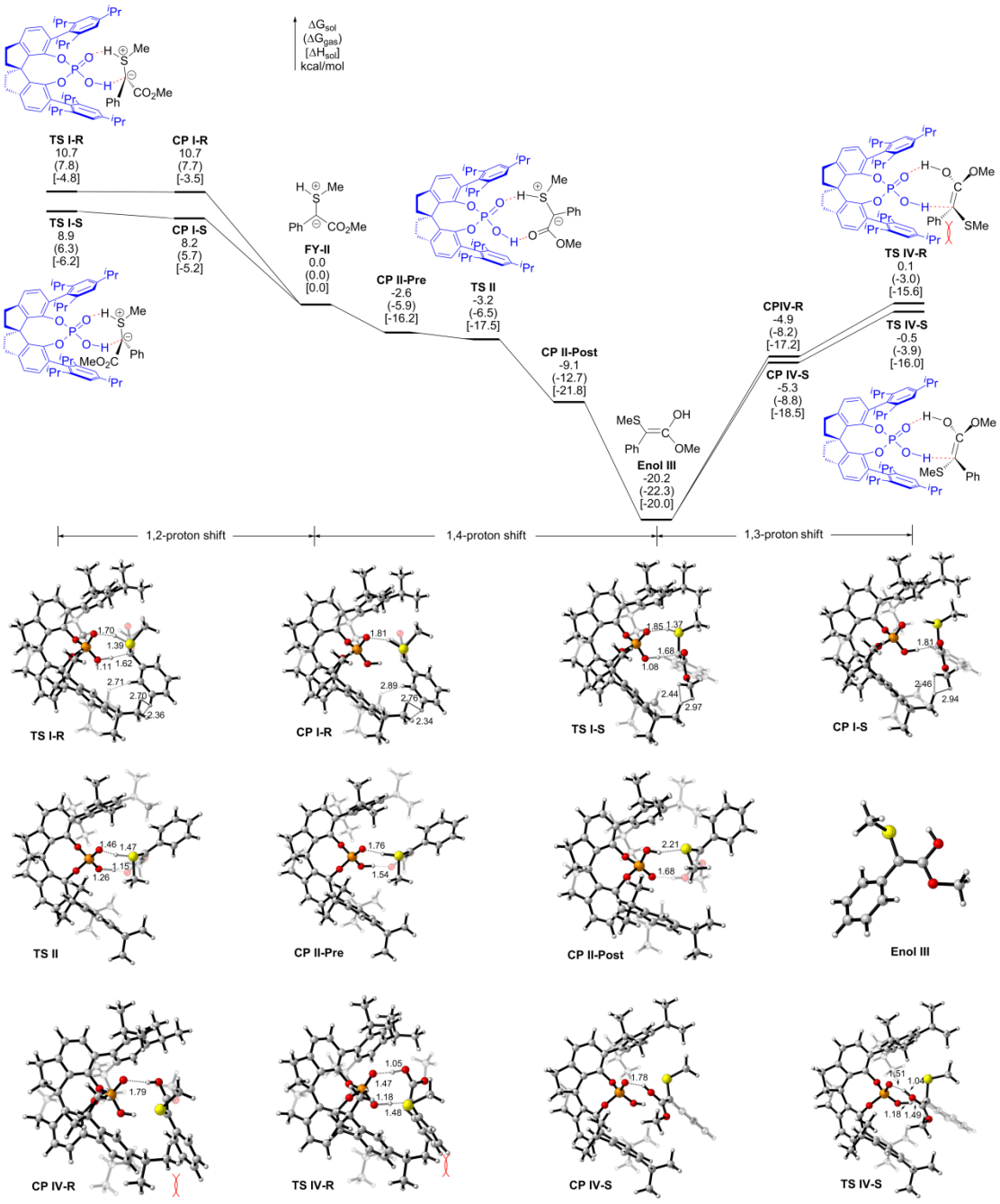


Fig. S2 The computed energy surfaces at the B3LYP/6-31+G(d) level for the phosphoric acid catalyzed proton shifts.

The direct proton shifts and the proton shifts promoted by other protonic sources, such as a trace amount of water or the thiol were also calculated (Fig. S3).[15] The DFT calculations show that all the free activation energies are higher than those of proton shift processes promoted by the spiro phosphoric acid (*R*)-**1f**. These results support that phosphoric acid (*R*)-**1f** acts as the real catalyst for the proton shift processes.

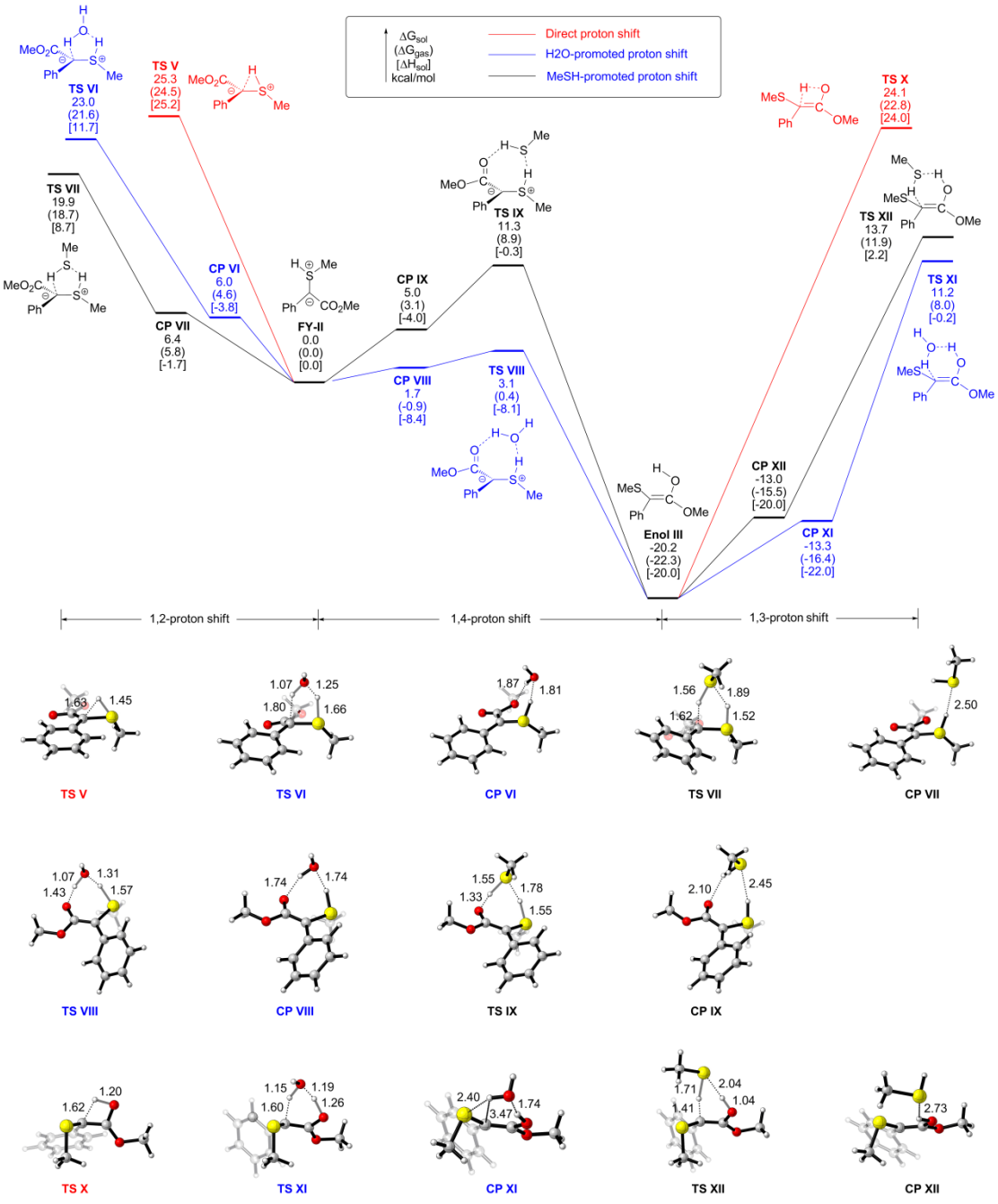


Fig. S3 The direct proton shifts and the proton shifts promoted by other protonic sources computed by the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) method.

15 The direct [1,4]-proton shift from **FY II** to **Enol III** was hard to addressed due to the long migration distance; the [1,3]-proton shift of **Enol III** could be promoted by two H_2O molecules with activation energies of 8.8/(4.8)/[-13.0].

Table S11 Sum of computed energies of stationary points

Thermal correction to Enthalpy (*c*H, in Hartree); Thermal correction to Gibbs Free Energy (*c*G, in Hartree); Single-point Energy in gas phase (E_{gas}, in Hartree); Single-point Energy in solution of cyclohexane (E_{sol}, in Hartree)

Structure	*c*H	*c*G	E_{gas}	E_{sol}
Rh_2OAc_4	0.231211	0.163126	-1133.39781533	-1133.40832129
Rh-CY-I-a	0.449086	0.341246	-2070.47453794	-2070.48457345
Rh-OY-I-a	0.449041	0.337529	-2070.46152416	-2070.47302977
FY II (5d)	0.212699	0.15712	-937.043352803	-937.049223022
FY-II	0.212613	0.157061	-937.043387743	-937.049253141
Enol III	0.215311	0.15949	-937.081408981	-937.083850381
(*R*)-1f	1.014702	0.875364	-2469.50624223	-2469.51093569
H_2O	0.024947	0.003501	-76.4583531777	-76.4615308212
MeSH	0.050952	0.022198	-438.743200525	-438.744623141
CP I-R	1.228757	1.056567	-3406.56142591	-3406.56722091
TS I-R	1.224701	1.054541	-3406.55932261	-3406.56519530
CP I-S	1.228183	1.054686	-3406.56286176	-3406.56933200
TS I-S	1.226040	1.055151	-3406.56228524	-3406.56877690
CP II-Pre	1.22877	1.055556	-3406.58211574	-3406.58742898
TS II	1.222533	1.050303	-3406.57792965	-3406.58322899
CP II-Post	1.230966	1.05629	-3406.5936998	-3406.59860378
CP IV-R	1.231566	1.056282	-3406.58657023	-3406.59186304
TS IV-R	1.225113	1.055208	-3406.57713907	-3406.5827806
TS IV-R (M06-2X)	1.225113	1.055208	-3404.63859557	-3404.64482395
CP IV-S	1.231574	1.057626	-3406.58888743	-3406.59385591
TS IV-S	1.225697	1.055378	-3406.57882905	-3406.58399383
TS IV-S (M06-2X)	1.225697	1.055378	-3404.64194574	-3404.64763179
TS V	0.209131	0.153773	-937.001042632	-937.00557992
CP VI	0.240262	0.178773	-1013.51264816	-1013.51950199
TS VI	0.235443	0.176533	-1013.48324114	-1013.49004577
CP VII	0.26552	0.194072	-1375.79213522	-1375.79850966
TS VII	0.260388	0.193983	-1375.77155342	-1375.77686092
CP VIII	0.240385	0.179423	-1013.52208356	-1013.52694452
TS VIII	0.235737	0.176874	-1013.51736248	-1013.52212144
CP IX	0.265728	0.195707	-1375.79809813	-1375.80234467
TS IX	0.259661	0.193842	-1375.78691068	-1375.79046304
TS X	0.209538	0.154123	-937.004178671	-937.007863696
CP XI	0.242651	0.179546	-1013.546865	-1013.55094119
TS XI	0.236025	0.177291	-1013.50565514	-1013.50961988
CP XII	0.268141	0.195061	-1375.82707752	-1375.83035436
TS XII	0.263335	0.197436	-1375.78578764	-1375.79020915

Coordinates for the minima

$Rh_2(OAc)_4$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.001499	-0.003918	-1.192219
2	45	0	-0.002478	-0.004025	1.194276
3	8	0	1.455400	1.456069	1.139472
4	6	0	1.867680	1.865490	0.006592
5	8	0	1.458953	1.456389	-1.128597
6	8	0	1.460880	-1.461400	-1.128877
7	6	0	1.868813	-1.871440	0.006267
8	8	0	1.456950	-1.461680	1.139213
9	8	0	-1.459511	1.452867	-1.135720
10	6	0	-1.867481	1.866490	-0.002313
11	8	0	-1.463028	1.452981	1.132383
12	8	0	-1.454942	-1.464353	-1.136060
13	6	0	-1.870583	-1.870465	-0.002732
14	8	0	-1.459070	-1.464119	1.132062
15	6	0	-2.902849	2.967918	-0.004882
16	1	0	-2.389212	3.935925	-0.041773
17	1	0	-3.500376	2.930331	0.908125
18	6	0	-2.972325	-2.905373	-0.004986
19	1	0	-3.940423	-2.390919	-0.023920
20	1	0	-2.901564	-3.532412	-0.896221
21	1	0	-2.924481	-3.513056	0.900893
22	6	0	2.943778	-2.934377	-0.001868
23	1	0	2.615828	-3.781479	-0.612058
24	1	0	3.849443	-2.528229	-0.464739
25	1	0	3.166159	-3.265648	1.013338
26	6	0	2.939015	2.932211	-0.001734
27	1	0	3.823091	2.554349	-0.525465
28	1	0	2.579114	3.805052	-0.555758
29	1	0	3.204913	3.219916	1.016259
30	1	0	-3.539758	2.886853	-0.888316

Metal-associated ylide I-a (Rh-CY-I-a)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.029369	-0.579240	0.378231
2	6	0	-2.085231	-1.928882	-0.244379
3	8	0	-2.361930	-1.877077	-1.562543
4	6	0	-2.245567	-3.123437	-2.263237
5	45	0	0.234353	-0.040723	0.065477
6	45	0	2.606702	0.504986	-0.238455
7	8	0	2.684496	-0.919430	-1.727345
8	6	0	1.637393	-1.580956	-1.996505
9	8	0	0.495963	-1.454162	-1.442850
10	8	0	0.848263	-1.443640	1.495496
11	6	0	2.100192	-1.602401	1.723715
12	8	0	3.040357	-0.966389	1.172461
13	8	0	-0.179115	1.397565	-1.357252
14	6	0	0.781211	2.047876	-1.886697
15	8	0	2.017246	1.917313	-1.627545
16	8	0	0.208739	1.412235	1.568274
17	6	0	1.278648	2.061679	1.831960
18	8	0	2.404652	1.908720	1.277133
19	8	0	-1.859480	-2.981767	0.341325
20	6	0	-3.011547	0.496945	-0.013568
21	1	0	-2.936878	-3.865947	-1.854790
22	1	0	-1.223493	-3.498674	-2.189387
23	1	0	-2.497655	-2.894890	-3.299498
24	6	0	-4.196178	0.211873	-0.716964
25	6	0	-5.107884	1.220555	-1.029709
26	6	0	-4.873547	2.534992	-0.627476
27	6	0	-3.711449	2.830392	0.087643
28	6	0	-2.790333	1.828456	0.386276
29	1	0	-4.400811	-0.801497	-1.041066
30	1	0	-6.009576	0.970811	-1.583442
31	1	0	-5.586885	3.318972	-0.867844
32	1	0	-3.512463	3.850614	0.406434
33	1	0	-1.881482	2.073516	0.924588
34	16	0	-2.012789	-0.737650	2.182601
35	1	0	-0.983689	-1.619046	2.285214
36	6	0	-3.391211	-1.834456	2.709281
37	1	0	-3.329315	-2.772784	2.160261
38	1	0	-3.302937	-1.990130	3.787802
39	6	0	0.400346	3.053967	-2.951834

40	1	0	0.345612	2.541440	-3.919505
41	1	0	-0.582957	3.478295	-2.737617
42	1	0	1.155674	3.839493	-3.020010
43	6	0	1.162723	3.133168	2.896317
44	1	0	0.657207	4.007048	2.468978
45	1	0	0.554911	2.773731	3.731017
46	1	0	2.151826	3.433649	3.245651
47	6	0	2.462126	-2.652683	2.752258
48	1	0	2.023290	-2.386650	3.720125
49	1	0	2.041674	-3.618427	2.453939
50	1	0	3.545296	-2.732562	2.852204
51	6	0	1.747204	-2.638512	-3.075624
52	1	0	1.612737	-3.629383	-2.627837
53	1	0	0.953469	-2.497738	-3.815395
54	1	0	2.723574	-2.589537	-3.559847
55	1	0	-4.318667	-1.302729	2.487054

Metal-associated ylide I-b (Rh-OY-I-b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.812848	0.157607	-0.375981
2	45	0	-2.835932	-0.296282	0.868834
3	8	0	-3.008775	-2.065207	-0.187257
4	6	0	-2.142020	-2.337191	-1.076313
5	8	0	-1.121337	-1.638369	-1.375016
6	8	0	-1.982884	1.140519	-1.765784
7	6	0	-3.242230	1.188717	-1.588411
8	8	0	-3.885653	0.681107	-0.616012
9	8	0	0.236089	-0.875011	1.114484
10	6	0	-0.416210	-1.336026	2.110407
11	8	0	-1.666725	-1.248578	2.293349
12	8	0	-0.641172	1.918692	0.713807
13	6	0	-1.536023	2.203333	1.575904
14	8	0	-2.554170	1.500248	1.858796
15	6	0	2.199960	0.884850	-1.125492
16	8	0	2.656162	2.153145	-1.043010
17	8	0	1.053811	0.655002	-1.580323
18	6	0	1.727297	3.185783	-1.420527
19	1	0	1.409372	3.058546	-2.458568
20	1	0	0.853944	3.167955	-0.766246

21	1	0	2.282733	4.117766	-1.302634
22	6	0	0.383830	-2.082911	3.159262
23	1	0	0.571029	-3.105361	2.808679
24	1	0	1.348951	-1.594617	3.318704
25	1	0	-0.173465	-2.136703	4.096045
26	6	0	-2.364169	-3.602762	-1.878565
27	1	0	-3.043742	-3.378905	-2.709329
28	1	0	-1.421743	-3.965917	-2.293550
29	1	0	-2.833408	-4.368087	-1.255993
30	6	0	-1.369833	3.515521	2.313163
31	1	0	-0.336829	3.621677	2.656297
32	1	0	-1.577314	4.343076	1.625191
33	1	0	-2.058455	3.570758	3.157722
34	6	0	-4.045820	1.951146	-2.620368
35	1	0	-4.081465	3.008422	-2.331772
36	1	0	-3.568734	1.881252	-3.600319
37	1	0	-5.068978	1.571776	-2.660280
38	6	0	3.132337	-0.106098	-0.691815
39	6	0	4.469723	0.102864	-0.104071
40	6	0	4.968991	-0.740853	0.909769
41	6	0	5.316360	1.141505	-0.548382
42	6	0	6.238794	-0.556827	1.457563
43	1	0	4.352271	-1.547050	1.301384
44	6	0	6.579016	1.330044	0.007988
45	1	0	4.969408	1.806019	-1.329459
46	6	0	7.054517	0.482730	1.012027
47	1	0	6.583997	-1.225945	2.241915
48	1	0	7.202339	2.142801	-0.356787
49	1	0	8.043767	0.629100	1.436530
50	16	0	2.455336	-1.681825	-0.853801
51	6	0	3.760668	-2.742992	-1.585845
52	1	0	3.820410	-2.480378	-2.643551
53	1	0	4.720266	-2.569490	-1.096802
54	1	0	2.494195	-2.269306	0.379539
55	1	0	3.447264	-3.785192	-1.476318

FY II (5d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402198	0.763400	-0.542878
2	6	0	-2.021366	0.913585	-0.655725
3	6	0	-1.129461	-0.022009	-0.091523
4	6	0	-1.692632	-1.135163	0.567021
5	6	0	-3.074844	-1.291078	0.657964
6	6	0	-3.943102	-0.342624	0.114357
7	6	0	0.340080	0.139176	-0.178559
8	6	0	1.274726	-0.956680	-0.142554
9	8	0	2.594252	-0.523939	-0.239336
10	6	0	3.560256	-1.577964	-0.284363
11	8	0	1.016867	-2.149440	-0.064966
12	1	0	3.401116	-2.218072	-1.156957
13	1	0	3.505413	-2.198099	0.614900
14	1	0	4.532794	-1.085282	-0.348605
15	1	0	-1.034948	-1.884866	0.987676
16	1	0	-3.474481	-2.163997	1.168825
17	1	0	-5.019706	-0.466993	0.193159
18	1	0	-4.056511	1.508149	-0.989940
19	1	0	-1.633314	1.769648	-1.202104
20	16	0	0.934930	1.741576	-0.256154
21	6	0	1.992910	2.153820	1.212960
22	1	0	1.318504	2.251792	2.065595
23	1	0	2.710200	1.348303	1.366251
24	1	0	1.982895	1.687961	-1.119926
25	1	0	2.493983	3.106495	1.013800

FY II

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.401198	0.756354	-0.553233
2	6	0	-2.020684	0.906046	-0.667124
3	6	0	-1.128932	-0.022695	-0.092436
4	6	0	-1.691427	-1.128685	0.577770
5	6	0	-3.073241	-1.284798	0.669416
6	6	0	-3.941459	-0.342841	0.115250

7	6	0	0.340291	0.138730	-0.180573
8	6	0	1.274401	-0.956776	-0.144555
9	8	0	2.594755	-0.523524	-0.238429
10	6	0	3.560619	-1.578316	-0.285589
11	8	0	1.016176	-2.149395	-0.070245
12	1	0	3.401957	-2.215645	-1.160193
13	1	0	3.504559	-2.200818	0.611851
14	1	0	4.533354	-1.085802	-0.347451
15	1	0	-1.033420	-1.872975	1.007704
16	1	0	-3.472665	-2.152391	1.189440
17	1	0	-5.018042	-0.467128	0.194690
18	1	0	-4.055854	1.495814	-1.008519
19	1	0	-1.632333	1.756121	-1.222685
20	16	0	0.934547	1.742125	-0.255007
21	6	0	1.988347	2.155204	1.217553
22	1	0	1.311486	2.253607	2.068065
23	1	0	2.705219	1.349917	1.373457
24	1	0	1.985385	1.687532	-1.115150
25	1	0	2.489853	3.107770	1.019438

Enol III

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.598148	-0.516498	-0.099709
2	6	0	0.539025	0.347156	-0.168603
3	6	0	-0.885280	-0.053392	-0.102048
4	6	0	-1.863244	0.654812	-0.826687
5	6	0	-1.320197	-1.125059	0.702865
6	6	0	-3.209118	0.299642	-0.763041
7	1	0	-1.557766	1.490875	-1.448211
8	6	0	-2.666453	-1.481715	0.759844
9	1	0	-0.596443	-1.679929	1.288194
10	6	0	-3.621271	-0.773744	0.028388
11	1	0	-3.938081	0.863819	-1.339729
12	1	0	-2.970541	-2.313563	1.390749
13	1	0	-4.670892	-1.050990	0.078292
14	16	0	0.969853	2.067776	-0.403198
15	6	0	0.630161	2.783426	1.256315
16	1	0	-0.420074	2.629219	1.515126
17	1	0	1.271431	2.333431	2.017833

18	1	0	0.833177	3.856295	1.191388
19	8	0	2.892380	-0.144050	-0.153007
20	1	0	2.885099	0.833590	-0.263452
21	8	0	1.427606	-1.842055	0.021780
22	6	0	2.563145	-2.697201	-0.168519
23	1	0	3.329424	-2.511415	0.588715
24	1	0	2.171779	-3.710161	-0.066558
25	1	0	2.995841	-2.561307	-1.164191

(*R*)-1f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.054271	-0.217263	-0.337382
2	8	0	1.200449	0.821593	-0.841346
3	8	0	-0.967742	0.666707	0.555877
4	8	0	-0.477057	-0.957025	-1.494183
5	8	0	0.697322	-1.044990	0.878445
6	1	0	1.541962	-1.463377	0.623255
7	6	0	0.049035	3.548335	0.004380
8	6	0	1.327319	2.843306	0.451293
9	6	0	1.892252	1.634090	0.059497
10	6	0	3.155700	1.215781	0.524461
11	6	0	3.841469	2.081995	1.389497
12	1	0	4.829698	1.795147	1.734750
13	6	0	3.270516	3.271621	1.844244
14	1	0	3.806317	3.896007	2.554782
15	6	0	2.005468	3.632684	1.394442
16	6	0	1.156462	4.815916	1.803267
17	1	0	1.508429	5.744002	1.331467
18	1	0	1.170477	4.987919	2.885441
19	6	0	-0.238904	4.413244	1.280590
20	1	0	-0.887733	5.268522	1.069532
21	1	0	-0.744857	3.786288	2.023689
22	6	0	-1.219648	2.835225	-0.465962
23	6	0	-1.760825	1.590377	-0.148500
24	6	0	-3.071522	1.231092	-0.515358
25	6	0	-3.800744	2.164404	-1.269771
26	1	0	-4.821325	1.917828	-1.545099
27	6	0	-3.239421	3.366109	-1.703154
28	1	0	-3.811196	4.036372	-2.340231

29	6	0	-1.946885	3.691815	-1.308501
30	6	0	-1.119155	4.903856	-1.679143
31	1	0	-1.466760	5.805571	-1.155988
32	1	0	-1.164248	5.126281	-2.751324
33	6	0	0.297024	4.495062	-1.216478
34	1	0	0.934727	5.347884	-0.963451
35	1	0	0.797137	3.925637	-2.008168
36	6	0	3.729473	-0.121279	0.149121
37	6	0	4.097259	-0.391773	-1.192312
38	6	0	4.601205	-1.657065	-1.516701
39	1	0	4.882991	-1.860528	-2.547094
40	6	0	4.759170	-2.669080	-0.570830
41	6	0	4.411826	-2.377550	0.751325
42	1	0	4.545402	-3.143195	1.510616
43	6	0	3.909652	-1.129226	1.141567
44	6	0	4.026614	0.662147	-2.297016
45	1	0	3.546541	1.554239	-1.887167
46	6	0	3.183603	0.201924	-3.501481
47	1	0	2.174194	-0.085131	-3.193282
48	1	0	3.641442	-0.652111	-4.014706
49	1	0	3.099919	1.014747	-4.232922
50	6	0	5.443520	1.080760	-2.740276
51	1	0	5.992166	0.238375	-3.178033
52	1	0	6.030290	1.458484	-1.895342
53	1	0	5.388228	1.872403	-3.497239
54	6	0	5.301464	-4.035262	-0.969829
55	1	0	5.495797	-4.000291	-2.050430
56	6	0	4.271786	-5.154097	-0.722824
57	1	0	3.334737	-4.955079	-1.254015
58	1	0	4.037338	-5.252084	0.343914
59	1	0	4.661055	-6.119390	-1.067541
60	6	0	6.638224	-4.347966	-0.271094
61	1	0	7.039528	-5.307436	-0.618480
62	1	0	6.514130	-4.414236	0.816367
63	1	0	7.383926	-3.571910	-0.475373
64	6	0	3.638597	-0.897497	2.633912
65	1	0	3.079197	0.035671	2.738282
66	6	0	2.791881	-2.003287	3.295296
67	1	0	3.298581	-2.975020	3.284371
68	1	0	1.817787	-2.118250	2.811631
69	1	0	2.608677	-1.746465	4.345173
70	6	0	4.968858	-0.735987	3.400788
71	1	0	5.587659	0.064977	2.982884
72	1	0	5.558154	-1.659960	3.361295

73	1	0	4.778449	-0.503599	4.455399
74	6	0	-3.702379	-0.071475	-0.114260
75	6	0	-4.044788	-1.037387	-1.096530
76	6	0	-4.690756	-2.209731	-0.691464
77	1	0	-4.951046	-2.945276	-1.447940
78	6	0	-5.004421	-2.472623	0.643931
79	6	0	-4.656411	-1.509856	1.590126
80	1	0	-4.899687	-1.694545	2.634315
81	6	0	-4.016245	-0.313909	1.245044
82	6	0	-3.754961	-0.852828	-2.588066
83	1	0	-3.097826	0.013479	-2.700851
84	6	0	-3.008935	-2.053216	-3.202112
85	1	0	-3.618080	-2.965216	-3.191121
86	1	0	-2.076690	-2.241805	-2.666372
87	1	0	-2.764600	-1.838862	-4.249962
88	6	0	-5.050663	-0.570439	-3.376366
89	1	0	-5.582185	0.307703	-2.993278
90	1	0	-5.740491	-1.421447	-3.320712
91	1	0	-4.824302	-0.393510	-4.435005
92	6	0	-5.696790	-3.763001	1.062705
93	1	0	-5.850500	-3.707933	2.149412
94	6	0	-4.818292	-4.997708	0.784565
95	1	0	-3.845818	-4.910728	1.281162
96	1	0	-4.633477	-5.119538	-0.289261
97	1	0	-5.307433	-5.910916	1.145237
98	6	0	-7.083452	-3.913754	0.409631
99	1	0	-7.586074	-4.818107	0.773553
100	1	0	-7.003843	-3.994101	-0.680962
101	1	0	-7.722863	-3.053078	0.634762
102	6	0	-3.726665	0.691868	2.359784
103	1	0	-3.221632	1.556160	1.920441
104	6	0	-2.783392	0.111552	3.430815
105	1	0	-1.845335	-0.228613	2.982400
106	1	0	-3.239650	-0.737866	3.952903
107	1	0	-2.548374	0.873538	4.184531
108	6	0	-5.030181	1.217569	2.993716
109	1	0	-5.596234	0.413401	3.478220
110	1	0	-5.680544	1.675143	2.239749
111	1	0	-4.807623	1.974078	3.756350

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.119720
2	1	0	0.000000	0.761560	-0.478879
3	1	0	0.000000	-0.761560	-0.478879

MeSH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.164837	0.019531	0.000001
2	1	0	1.535761	0.522717	0.895818
3	1	0	1.535748	0.522847	-0.895748
4	16	0	-0.667732	-0.087180	0.000000
5	1	0	-0.907919	1.241913	-0.000001
6	1	0	1.531101	-1.009784	-0.000081

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.141491	-0.606865	0.255101
2	8	0	0.911720	-1.795424	0.577949
3	8	0	-1.332857	-1.298265	-0.605340
4	8	0	-0.535814	0.031754	1.540360
5	8	0	0.519027	0.326096	-0.840183
6	1	0	0.562022	1.305739	-0.585330
7	6	0	-0.518060	-4.286113	-0.568365
8	6	0	0.796600	-3.633019	-0.975981
9	6	0	1.517426	-2.584563	-0.408667
10	6	0	2.862881	-2.348020	-0.752227
11	6	0	3.419081	-3.161363	-1.754983
12	1	0	4.461863	-3.011165	-2.015451
13	6	0	2.671969	-4.121704	-2.434584
14	1	0	3.120898	-4.691867	-3.244083
15	6	0	1.357743	-4.349269	-2.045059

16	6	0	0.357705	-5.331231	-2.615342
17	1	0	0.618337	-6.366581	-2.354802
18	1	0	0.307996	-5.287049	-3.709453
19	6	0	-0.961085	-4.893603	-1.942584
20	1	0	-1.682108	-5.708586	-1.827496
21	1	0	-1.438919	-4.106525	-2.537149
22	6	0	-1.681464	-3.575453	0.114019
23	6	0	-2.143756	-2.263972	0.020795
24	6	0	-3.416549	-1.900479	0.503215
25	6	0	-4.156796	-2.889723	1.172462
26	1	0	-5.146154	-2.628944	1.534997
27	6	0	-3.653372	-4.169662	1.398581
28	1	0	-4.231512	-4.893049	1.968196
29	6	0	-2.415565	-4.507257	0.866361
30	6	0	-1.670570	-5.819974	0.969329
31	1	0	-2.134709	-6.594633	0.343073
32	1	0	-1.655148	-6.212068	1.992768
33	6	0	-0.265354	-5.445527	0.454011
34	1	0	0.274973	-6.285784	0.007679
35	1	0	0.342529	-5.058681	1.279996
36	6	0	3.732725	-1.325327	-0.082664
37	6	0	4.058360	-1.457108	1.290664
38	6	0	4.972161	-0.562111	1.857661
39	1	0	5.232639	-0.674021	2.907948
40	6	0	5.592270	0.448530	1.123631
41	6	0	5.247296	0.570072	-0.225270
42	1	0	5.713063	1.348893	-0.823674
43	6	0	4.333718	-0.289944	-0.847243
44	6	0	3.517340	-2.577308	2.180535
45	1	0	2.822575	-3.181598	1.593593
46	6	0	2.733541	-2.030255	3.388722
47	1	0	1.907594	-1.390207	3.065293
48	1	0	3.378653	-1.448045	4.057842
49	1	0	2.314586	-2.857655	3.974639
50	6	0	4.647489	-3.523466	2.634760
51	1	0	5.382467	-3.004750	3.261316
52	1	0	5.180554	-3.945825	1.775519
53	1	0	4.237191	-4.353918	3.222407
54	6	0	6.655428	1.324453	1.774801
55	1	0	6.616750	1.123435	2.854356
56	6	0	6.408933	2.829424	1.579410
57	1	0	5.412366	3.121765	1.927555
58	1	0	6.494661	3.112896	0.523753
59	1	0	7.150003	3.415507	2.135978

60	6	0	8.064837	0.934513	1.285314
61	1	0	8.832984	1.525508	1.799015
62	1	0	8.169029	1.111154	0.207987
63	1	0	8.268172	-0.125901	1.469896
64	6	0	4.054657	-0.084282	-2.339791
65	1	0	3.285478	-0.798103	-2.643811
66	6	0	3.502940	1.317302	-2.655861
67	1	0	4.214824	2.110409	-2.403212
68	1	0	2.577453	1.512636	-2.109190
69	1	0	3.284126	1.399518	-3.727514
70	6	0	5.310845	-0.364102	-3.190504
71	1	0	5.710647	-1.368975	-3.013969
72	1	0	6.111111	0.351111	-2.966041
73	1	0	5.076554	-0.275378	-4.258194
74	6	0	-4.043540	-0.555788	0.283142
75	6	0	-4.338464	0.288155	1.382793
76	6	0	-5.022836	1.484727	1.152672
77	1	0	-5.244335	2.127870	2.000177
78	6	0	-5.410444	1.891312	-0.124804
79	6	0	-5.117012	1.040861	-1.190759
80	1	0	-5.430776	1.332438	-2.191423
81	6	0	-4.449778	-0.177550	-1.019233
82	6	0	-3.940625	-0.053218	2.819998
83	1	0	-3.298109	-0.937328	2.793397
84	6	0	-3.117258	1.071839	3.474422
85	1	0	-3.715065	1.978153	3.629219
86	1	0	-2.261470	1.322873	2.845232
87	1	0	-2.747988	0.747242	4.455130
88	6	0	-5.171630	-0.386246	3.686414
89	1	0	-5.745820	-1.223755	3.275567
90	1	0	-5.848446	0.473841	3.756215
91	1	0	-4.865005	-0.654192	4.705026
92	6	0	-6.140377	3.206968	-0.357115
93	1	0	-6.175467	3.365631	-1.444160
94	6	0	-5.393845	4.403920	0.260664
95	1	0	-4.340454	4.405071	-0.036557
96	1	0	-5.427172	4.370441	1.356422
97	1	0	-5.855105	5.348752	-0.051872
98	6	0	-7.595763	3.142658	0.145272
99	1	0	-8.123632	4.081068	-0.065272
100	1	0	-7.629685	2.974880	1.228645
101	1	0	-8.145846	2.325901	-0.335238
102	6	0	-4.247889	-1.070504	-2.244752
103	1	0	-3.720991	-1.974297	-1.928282

104	6	0	-3.377913	-0.398527	-3.323500
105	1	0	-2.402311	-0.112512	-2.918507
106	1	0	-3.859349	0.499846	-3.728603
107	1	0	-3.211078	-1.086545	-4.161675
108	6	0	-5.598985	-1.529290	-2.829277
109	1	0	-6.187521	-0.681622	-3.199583
110	1	0	-6.200817	-2.048180	-2.074791
111	1	0	-5.440012	-2.216263	-3.669661
112	6	0	3.855653	4.778272	-0.632125
113	6	0	2.848368	3.900226	-0.234095
114	6	0	1.496389	4.149220	-0.538203
115	6	0	1.204778	5.314489	-1.274340
116	6	0	2.215361	6.177138	-1.695299
117	6	0	3.547953	5.921295	-1.370860
118	6	0	0.423765	3.233408	-0.040847
119	6	0	-0.934332	3.217375	-0.569135
120	8	0	-0.972065	3.473086	-1.906695
121	6	0	-2.269938	3.421236	-2.511522
122	8	0	-1.948435	2.934225	0.067204
123	1	0	-2.885454	4.265385	-2.182781
124	1	0	-2.782342	2.491591	-2.258316
125	1	0	-2.090807	3.487112	-3.586118
126	1	0	0.176190	5.539810	-1.529413
127	1	0	1.953758	7.063983	-2.267597
128	1	0	4.334419	6.599557	-1.690922
129	1	0	4.887330	4.559160	-0.372260
130	1	0	3.115113	2.999056	0.311982
131	16	0	0.501415	2.972458	1.703634
132	6	0	-0.664513	4.085282	2.603184
133	1	0	-0.252514	5.094513	2.544818
134	1	0	-1.640440	4.019645	2.124685
135	1	0	-0.186584	1.789798	1.819800
136	1	0	-0.701653	3.753363	3.644213

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.089537	0.575031	0.269581
2	8	0	-0.992462	1.743853	0.602123
3	8	0	1.258430	1.306219	-0.602585

4	8	0	0.549716	0.016808	1.581092
5	8	0	-0.543470	-0.423571	-0.748028
6	1	0	-0.513669	-1.500834	-0.472031
7	6	0	0.385948	4.279638	-0.499584
8	6	0	-0.920741	3.614320	-0.911677
9	6	0	-1.616678	2.537651	-0.364196
10	6	0	-2.961809	2.291017	-0.705058
11	6	0	-3.544439	3.129269	-1.672056
12	1	0	-4.588005	2.969829	-1.924775
13	6	0	-2.821639	4.121376	-2.330867
14	1	0	-3.289710	4.710684	-3.115477
15	6	0	-1.504727	4.352478	-1.953288
16	6	0	-0.526286	5.363800	-2.509223
17	1	0	-0.799561	6.388408	-2.220545
18	1	0	-0.488230	5.347376	-3.604659
19	6	0	0.805768	4.929639	-1.861588
20	1	0	1.515189	5.752610	-1.732209
21	1	0	1.289738	4.165776	-2.480950
22	6	0	1.570778	3.577216	0.153622
23	6	0	2.057917	2.276619	0.025546
24	6	0	3.347749	1.936400	0.480954
25	6	0	4.077694	2.930290	1.155002
26	1	0	5.079926	2.686086	1.492621
27	6	0	3.549598	4.192571	1.417748
28	1	0	4.120943	4.917779	1.991940
29	6	0	2.294953	4.510153	0.914379
30	6	0	1.522534	5.802859	1.058703
31	1	0	1.960953	6.603011	0.446067
32	1	0	1.512170	6.169307	2.091737
33	6	0	0.119760	5.409358	0.552017
34	1	0	-0.444155	6.247341	0.131290
35	1	0	-0.469895	4.990245	1.375479
36	6	0	-3.805891	1.219799	-0.081314
37	6	0	-4.122060	1.268628	1.299096
38	6	0	-5.008281	0.321304	1.823782
39	1	0	-5.262375	0.369682	2.880520
40	6	0	-5.610538	-0.663099	1.040743
41	6	0	-5.277695	-0.700465	-0.316530
42	1	0	-5.734458	-1.453720	-0.953958
43	6	0	-4.391185	0.214995	-0.897907
44	6	0	-3.604375	2.356137	2.241788
45	1	0	-2.928279	3.005741	1.682324
46	6	0	-2.799634	1.771785	3.418232
47	1	0	-1.948426	1.185846	3.059815

48	1	0	-3.420869	1.127635	4.052376
49	1	0	-2.412990	2.580474	4.050583
50	6	0	-4.756984	3.248382	2.746203
51	1	0	-5.476580	2.679452	3.346406
52	1	0	-5.303338	3.700214	1.910598
53	1	0	-4.366174	4.057948	3.374862
54	6	0	-6.646412	-1.597833	1.653520
55	1	0	-6.588004	-1.467421	2.742975
56	6	0	-6.383250	-3.083059	1.355514
57	1	0	-5.371120	-3.379832	1.650302
58	1	0	-6.501713	-3.301982	0.287623
59	1	0	-7.096351	-3.715508	1.897702
60	6	0	-8.071402	-1.199873	1.218577
61	1	0	-8.820084	-1.835031	1.707854
62	1	0	-8.194413	-1.308677	0.134197
63	1	0	-8.286603	-0.156962	1.475205
64	6	0	-4.125082	0.101796	-2.403135
65	1	0	-3.409691	0.878167	-2.681605
66	6	0	-3.482983	-1.240244	-2.796368
67	1	0	-4.128896	-2.093084	-2.560721
68	1	0	-2.529273	-1.383708	-2.282413
69	1	0	-3.290661	-1.260061	-3.876253
70	6	0	-5.409221	0.344450	-3.222186
71	1	0	-5.867987	1.311372	-2.985843
72	1	0	-6.160491	-0.430587	-3.029312
73	1	0	-5.185460	0.328585	-4.295677
74	6	0	4.014896	0.615283	0.235100
75	6	0	4.369875	-0.219684	1.324176
76	6	0	5.120546	-1.372474	1.077750
77	1	0	5.389086	-2.006486	1.918443
78	6	0	5.517968	-1.746577	-0.206410
79	6	0	5.154153	-0.912125	-1.263904
80	1	0	5.469438	-1.178994	-2.271072
81	6	0	4.418308	0.264068	-1.075755
82	6	0	3.963179	0.081968	2.767914
83	1	0	3.271702	0.928270	2.755868
84	6	0	3.207154	-1.097192	3.408394
85	1	0	3.859815	-1.965016	3.563341
86	1	0	2.376753	-1.400548	2.768670
87	1	0	2.809097	-0.802871	4.387376
88	6	0	5.176989	0.468963	3.636233
89	1	0	5.700928	1.345119	3.239531
90	1	0	5.901918	-0.352361	3.689630
91	1	0	4.859158	0.701275	4.660174

92	6	0	6.335772	-3.006801	-0.455316
93	1	0	6.335676	-3.179465	-1.540905
94	6	0	5.718830	-4.250653	0.210510
95	1	0	4.656226	-4.344034	-0.035153
96	1	0	5.800194	-4.200586	1.302900
97	1	0	6.240100	-5.159342	-0.114370
98	6	0	7.802601	-2.819914	-0.020382
99	1	0	8.392886	-3.717915	-0.241140
100	1	0	7.869341	-2.630505	1.057834
101	1	0	8.264833	-1.971316	-0.536750
102	6	0	4.138640	1.143496	-2.295184
103	1	0	3.575296	2.019319	-1.964247
104	6	0	3.272870	0.423657	-3.346644
105	1	0	2.322175	0.096328	-2.914563
106	1	0	3.785413	-0.454529	-3.758156
107	1	0	3.052523	1.096767	-4.184488
108	6	0	5.446541	1.669524	-2.919679
109	1	0	6.065574	0.853488	-3.310961
110	1	0	6.044512	2.217406	-2.182800
111	1	0	5.227165	2.348562	-3.752858
112	6	0	-3.659843	-4.688287	-0.836458
113	6	0	-2.702573	-3.758918	-0.429441
114	6	0	-1.329301	-4.036248	-0.536809
115	6	0	-0.955551	-5.284764	-1.067384
116	6	0	-1.911823	-6.206092	-1.491806
117	6	0	-3.271165	-5.915390	-1.374729
118	6	0	-0.313724	-3.045149	-0.032390
119	6	0	1.090077	-3.141245	-0.481090
120	8	0	1.159758	-3.385441	-1.812368
121	6	0	2.479801	-3.433545	-2.372400
122	8	0	2.085296	-2.946919	0.205919
123	1	0	3.019232	-4.315284	-2.011305
124	1	0	3.045532	-2.538065	-2.110518
125	1	0	2.332297	-3.500906	-3.451279
126	1	0	0.095601	-5.534038	-1.163084
127	1	0	-1.590132	-7.159188	-1.904289
128	1	0	-4.018076	-6.634855	-1.699605
129	1	0	-4.713831	-4.445666	-0.740369
130	1	0	-3.025136	-2.800936	-0.030797
131	16	0	-0.470290	-2.831386	1.745238
132	6	0	0.633919	-3.982776	2.658204
133	1	0	0.221848	-4.986411	2.535487
134	1	0	1.638826	-3.909197	2.246736
135	1	0	0.204004	-1.619778	1.880278

136	1	0	0.604835	-3.694173	3.711951

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.030495	0.569646	-0.206246
2	8	0	1.197295	1.592427	-0.476977
3	8	0	-1.087221	1.393720	0.728452
4	8	0	-0.593798	0.104323	-1.500994
5	8	0	0.469269	-0.529919	0.806757
6	1	0	0.199471	-1.497384	0.536561
7	6	0	0.161777	4.176777	0.918856
8	6	0	1.360812	3.287115	1.237922
9	6	0	1.918667	2.201432	0.560875
10	6	0	3.219410	1.745935	0.854396
11	6	0	3.886305	2.362941	1.927652
12	1	0	4.898324	2.041808	2.150499
13	6	0	3.287149	3.344642	2.713291
14	1	0	3.813561	3.757548	3.570227
15	6	0	2.023306	3.802897	2.363874
16	6	0	1.186507	4.865339	3.042471
17	1	0	1.602506	5.869147	2.877993
18	1	0	1.132679	4.722822	4.127997
19	6	0	-0.183595	4.702171	2.352343
20	1	0	-0.773087	5.623855	2.328408
21	1	0	-0.774967	3.940293	2.873007
22	6	0	-1.094465	3.729278	0.185318
23	6	0	-1.741004	2.496909	0.162003
24	6	0	-3.030749	2.356648	-0.387132
25	6	0	-3.613849	3.502816	-0.954526
26	1	0	-4.617842	3.419520	-1.358627
27	6	0	-2.937182	4.718881	-1.039573
28	1	0	-3.400644	5.568668	-1.534526
29	6	0	-1.671713	4.824557	-0.475327
30	6	0	-0.737654	6.014549	-0.450366
31	1	0	-1.086039	6.782016	0.254992
32	1	0	-0.654797	6.502085	-1.428481
33	6	0	0.592016	5.382680	0.014624
34	1	0	1.248532	6.084010	0.538250
35	1	0	1.140977	4.994596	-0.851019

36	6	0	3.970618	0.712425	0.063916
37	6	0	4.358598	0.984564	-1.271366
38	6	0	5.232767	0.101023	-1.915700
39	1	0	5.544473	0.323370	-2.933884
40	6	0	5.754548	-1.031688	-1.291946
41	6	0	5.326992	-1.303144	0.010992
42	1	0	5.703416	-2.188213	0.518037
43	6	0	4.444036	-0.465093	0.701707
44	6	0	3.919772	2.233031	-2.037220
45	1	0	3.273926	2.827947	-1.388068
46	6	0	3.096505	1.872089	-3.288793
47	1	0	2.218777	1.275398	-3.023897
48	1	0	3.692785	1.301441	-4.011024
49	1	0	2.751236	2.783555	-3.792459
50	6	0	5.121622	3.128376	-2.399961
51	1	0	5.811552	2.624475	-3.086800
52	1	0	5.688650	3.413057	-1.506356
53	1	0	4.777747	4.046811	-2.891388
54	6	0	6.802406	-1.887367	-1.994998
55	1	0	6.907860	-1.490637	-3.014134
56	6	0	6.398138	-3.366502	-2.120760
57	1	0	5.458229	-3.475487	-2.672122
58	1	0	6.269473	-3.832389	-1.136616
59	1	0	7.171417	-3.931766	-2.654781
60	6	0	8.175285	-1.752970	-1.306294
61	1	0	8.941314	-2.316600	-1.852798
62	1	0	8.141962	-2.139550	-0.280702
63	1	0	8.491320	-0.705300	-1.256839
64	6	0	4.039482	-0.859179	2.125053
65	1	0	3.282090	-0.149840	2.469472
66	6	0	3.397261	-2.257796	2.179920
67	1	0	4.118430	-3.046450	1.932867
68	1	0	2.558985	-2.344927	1.486105
69	1	0	3.024964	-2.461009	3.191139
70	6	0	5.229851	-0.789700	3.103499
71	1	0	5.682841	0.207082	3.132925
72	1	0	6.016695	-1.500040	2.822201
73	1	0	4.903279	-1.041828	4.119705
74	6	0	-3.821938	1.081159	-0.363424
75	6	0	-4.196981	0.446767	-1.578265
76	6	0	-5.045829	-0.666224	-1.525797
77	1	0	-5.351547	-1.129222	-2.461454
78	6	0	-5.541861	-1.177652	-0.322226
79	6	0	-5.142371	-0.549405	0.856656

80	1	0	-5.520998	-0.930100	1.802758
81	6	0	-4.303053	0.571264	0.867102
82	6	0	-3.759263	0.956428	-2.955559
83	1	0	-3.040193	1.764992	-2.805110
84	6	0	-3.040576	-0.114565	-3.798118
85	1	0	-3.674934	-0.991873	-3.976694
86	1	0	-2.112444	-0.430409	-3.315864
87	1	0	-2.777079	0.298270	-4.779363
88	6	0	-4.957117	1.532326	-3.739664
89	1	0	-5.474114	2.318556	-3.178770
90	1	0	-5.695418	0.754284	-3.968717
91	1	0	-4.620191	1.961296	-4.690982
92	6	0	-6.534694	-2.333397	-0.284418
93	1	0	-6.711722	-2.568521	0.773930
94	6	0	-5.996373	-3.611259	-0.951091
95	1	0	-5.059955	-3.935455	-0.484358
96	1	0	-5.809283	-3.457081	-2.020806
97	1	0	-6.721340	-4.428725	-0.859531
98	6	0	-7.888742	-1.924481	-0.897278
99	1	0	-8.618306	-2.738232	-0.805401
100	1	0	-7.785320	-1.686387	-1.962754
101	1	0	-8.297883	-1.040246	-0.396791
102	6	0	-4.008939	1.232761	2.214141
103	1	0	-3.373236	2.103768	2.037826
104	6	0	-3.239360	0.295520	3.163395
105	1	0	-2.287233	-0.008910	2.718740
106	1	0	-3.817303	-0.606766	3.397131
107	1	0	-3.023405	0.804945	4.110520
108	6	0	-5.300108	1.755873	2.875361
109	1	0	-5.989350	0.940378	3.124378
110	1	0	-5.830245	2.450426	2.214176
111	1	0	-5.063696	2.285795	3.806051
112	6	0	-0.352435	-5.955794	2.660917
113	6	0	-0.147906	-5.263642	1.467827
114	6	0	-0.550380	-3.922753	1.328331
115	6	0	-1.175474	-3.311804	2.430760
116	6	0	-1.400886	-4.009992	3.616000
117	6	0	-0.985583	-5.336646	3.739903
118	6	0	-0.361825	-3.150897	0.058426
119	6	0	0.680554	-3.432796	-0.924113
120	8	0	1.786239	-3.999232	-0.368467
121	6	0	2.888928	-4.181060	-1.265891
122	8	0	0.632048	-3.146467	-2.117370
123	1	0	3.248689	-3.217068	-1.632314

124	1	0	2.599723	-4.803249	-2.117564
125	1	0	3.662750	-4.673823	-0.676249
126	1	0	-1.483236	-2.272231	2.357090
127	1	0	-1.887171	-3.508914	4.449243
128	1	0	-1.148808	-5.879965	4.666914
129	1	0	-0.024233	-6.989236	2.742075
130	1	0	0.344186	-5.760567	0.639068
131	16	0	-1.888875	-2.665314	-0.694832
132	6	0	-2.323643	-3.800479	-2.079011
133	1	0	-3.155084	-3.346208	-2.622593
134	1	0	-1.445446	-3.922290	-2.711278
135	1	0	-2.638119	-4.746528	-1.634571
136	1	0	-1.455979	-1.594601	-1.427080

TS I-S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.035070	0.563763	-0.197842
2	8	0	1.189927	1.591456	-0.477930
3	8	0	-1.092480	1.394955	0.734473
4	8	0	-0.607329	0.113805	-1.497932
5	8	0	0.454996	-0.541754	0.799772
6	1	0	0.172689	-1.545546	0.520163
7	6	0	0.154945	4.177703	0.914791
8	6	0	1.355603	3.289570	1.232821
9	6	0	1.912360	2.202456	0.556494
10	6	0	3.214473	1.749558	0.848970
11	6	0	3.883454	2.369672	1.919131
12	1	0	4.896323	2.049980	2.140416
13	6	0	3.285243	3.352602	2.703875
14	1	0	3.813163	3.768132	3.558637
15	6	0	2.020106	3.808541	2.356126
16	6	0	1.183871	4.871598	3.034495
17	1	0	1.598295	5.875533	2.866763
18	1	0	1.132896	4.731452	4.120498
19	6	0	-0.187649	4.705418	2.348014
20	1	0	-0.778428	5.626304	2.323830
21	1	0	-0.776762	3.943664	2.871423
22	6	0	-1.102585	3.728051	0.184905
23	6	0	-1.747155	2.494481	0.165659

24	6	0	-3.037445	2.352277	-0.382349
25	6	0	-3.623286	3.496698	-0.950321
26	1	0	-4.627754	3.411446	-1.352911
27	6	0	-2.948589	4.713685	-1.038175
28	1	0	-3.414074	5.562150	-1.533529
29	6	0	-1.682105	4.821527	-0.476609
30	6	0	-0.749010	6.012377	-0.455746
31	1	0	-1.096414	6.780811	0.249090
32	1	0	-0.668677	6.498356	-1.434871
33	6	0	0.582188	5.382361	0.007453
34	1	0	1.239355	6.085270	0.528191
35	1	0	1.129454	4.993048	-0.858710
36	6	0	3.965172	0.714420	0.060231
37	6	0	4.350069	0.982170	-1.276802
38	6	0	5.224001	0.097435	-1.919885
39	1	0	5.533513	0.316798	-2.939400
40	6	0	5.748429	-1.032505	-1.293293
41	6	0	5.323669	-1.299989	0.011399
42	1	0	5.702441	-2.182620	0.521021
43	6	0	4.441331	-0.460323	0.700977
44	6	0	3.908001	2.227484	-2.045860
45	1	0	3.263169	2.823790	-1.397044
46	6	0	3.081709	1.861393	-3.293908
47	1	0	2.204722	1.265860	-3.024127
48	1	0	3.676308	1.288015	-4.015409
49	1	0	2.735029	2.770861	-3.800233
50	6	0	5.108014	3.122799	-2.414742
51	1	0	5.796546	2.617451	-3.101942
52	1	0	5.677252	3.410852	-1.523609
53	1	0	4.761892	4.039384	-2.908043
54	6	0	6.796803	-1.888767	-1.994920
55	1	0	6.900949	-1.494751	-3.015241
56	6	0	6.394666	-3.368862	-2.116303
57	1	0	5.455642	-3.480889	-2.668628
58	1	0	6.265287	-3.831649	-1.130772
59	1	0	7.169281	-3.934952	-2.647533
60	6	0	8.170088	-1.750636	-1.307699
61	1	0	8.936576	-2.314488	-1.853357
62	1	0	8.138158	-2.134560	-0.281071
63	1	0	8.484491	-0.702349	-1.261197
64	6	0	4.040164	-0.849908	2.126517
65	1	0	3.284796	-0.138500	2.470932
66	6	0	3.395169	-2.246940	2.185655
67	1	0	4.113107	-3.037601	1.935522

68	1	0	2.553339	-2.330624	1.495923
69	1	0	3.026747	-2.448826	3.198629
70	6	0	5.233077	-0.779802	3.101703
71	1	0	5.687677	0.216373	3.127019
72	1	0	6.018129	-1.492245	2.820673
73	1	0	4.908634	-1.028388	4.119492
74	6	0	-3.825520	1.074822	-0.358292
75	6	0	-4.199669	0.439623	-1.573158
76	6	0	-5.044213	-0.676748	-1.520449
77	1	0	-5.349433	-1.140193	-2.456115
78	6	0	-5.537012	-1.190752	-0.316559
79	6	0	-5.138992	-0.561376	0.862072
80	1	0	-5.515306	-0.943889	1.808349
81	6	0	-4.303816	0.562437	0.872305
82	6	0	-3.765766	0.952076	-2.950726
83	1	0	-3.048523	1.762189	-2.800411
84	6	0	-3.045862	-0.115441	-3.796669
85	1	0	-3.678103	-0.994208	-3.975869
86	1	0	-2.115600	-0.429376	-3.317307
87	1	0	-2.785744	0.300091	-4.777685
88	6	0	-4.966807	1.525681	-3.731674
89	1	0	-5.485233	2.309268	-3.168459
90	1	0	-5.703106	0.745735	-3.960853
91	1	0	-4.632902	1.957433	-4.682808
92	6	0	-6.523119	-2.352185	-0.277925
93	1	0	-6.705312	-2.581813	0.780746
94	6	0	-5.971198	-3.630524	-0.932533
95	1	0	-5.035072	-3.943882	-0.457645
96	1	0	-5.778894	-3.481915	-2.002140
97	1	0	-6.690214	-4.453125	-0.839808
98	6	0	-7.876010	-1.956877	-0.901986
99	1	0	-8.600495	-2.775072	-0.809230
100	1	0	-7.767931	-1.725051	-1.968386
101	1	0	-8.294427	-1.072271	-0.409904
102	6	0	-4.011098	1.224237	2.219474
103	1	0	-3.377027	2.096395	2.043239
104	6	0	-3.240158	0.288443	3.169091
105	1	0	-2.286874	-0.012959	2.724941
106	1	0	-3.815328	-0.615842	3.401600
107	1	0	-3.026987	0.798494	4.116532
108	6	0	-5.303756	1.744682	2.879964
109	1	0	-5.991504	0.927715	3.128372
110	1	0	-5.834867	2.438286	2.218546
111	1	0	-5.069017	2.274956	3.810884

112	6	0	-0.487830	-6.020583	2.529964
113	6	0	-0.280307	-5.284075	1.364495
114	6	0	-0.523681	-3.899549	1.328024
115	6	0	-0.989684	-3.284442	2.502454
116	6	0	-1.215350	-4.022554	3.664157
117	6	0	-0.962420	-5.394766	3.684355
118	6	0	-0.334360	-3.081292	0.082201
119	6	0	0.694606	-3.397045	-0.914008
120	8	0	1.781070	-3.994665	-0.358931
121	6	0	2.882971	-4.201054	-1.252885
122	8	0	0.649176	-3.108891	-2.105059
123	1	0	3.266150	-3.244584	-1.614959
124	1	0	2.581446	-4.814022	-2.106916
125	1	0	3.642368	-4.713679	-0.661550
126	1	0	-1.168888	-2.212868	2.504786
127	1	0	-1.576331	-3.520111	4.557950
128	1	0	-1.128318	-5.970415	4.591211
129	1	0	-0.285347	-7.088796	2.533016
130	1	0	0.092062	-5.783027	0.475331
131	16	0	-1.884808	-2.617840	-0.668760
132	6	0	-2.300156	-3.748892	-2.057842
133	1	0	-3.144687	-3.307215	-2.591095
134	1	0	-1.424609	-3.847438	-2.697768
135	1	0	-2.592760	-4.705447	-1.620799
136	1	0	-1.460284	-1.523531	-1.382459

CP II-Pre

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.603631	4.295971	-1.829225
2	6	0	4.406627	3.621034	-1.595370
3	6	0	3.610774	3.903045	-0.465943
4	6	0	4.084300	4.887152	0.425958
5	6	0	5.292677	5.543310	0.201840
6	6	0	6.060010	5.260111	-0.929705
7	6	0	2.323399	3.215437	-0.236374
8	6	0	1.732184	2.857239	0.992956
9	8	0	2.511233	3.040702	2.092608
10	6	0	1.933157	2.662753	3.346529
11	8	0	0.563573	2.397309	1.116300

12	1	0	1.017360	3.226668	3.545297
13	1	0	1.704849	1.593078	3.369411
14	1	0	2.692373	2.898284	4.093976
15	1	0	3.497102	5.131582	1.303394
16	1	0	5.628539	6.294539	0.912831
17	1	0	6.997627	5.780260	-1.106015
18	1	0	6.188488	4.053314	-2.713261
19	1	0	4.087222	2.856858	-2.299166
20	16	0	1.385779	2.794015	-1.645164
21	6	0	-0.209050	3.715583	-1.606843
22	1	0	0.011946	4.756512	-1.848967
23	1	0	-0.643679	3.617107	-0.612920
24	1	0	-0.864338	3.278852	-2.365585
25	1	0	0.874532	1.550796	-1.332571
26	1	0	-0.126756	1.024114	1.257654
27	15	0	-0.483928	-0.683212	-0.045924
28	8	0	-1.947115	-0.943024	-0.695976
29	8	0	-0.043012	-2.103122	0.596456
30	8	0	0.399280	-0.132811	-1.111812
31	8	0	-0.666542	0.159865	1.267831
32	6	0	-2.348266	-3.983329	-0.212693
33	6	0	-3.118216	-2.781210	0.333488
34	6	0	-3.020632	-1.416402	0.066641
35	6	0	-3.999852	-0.502751	0.504755
36	6	0	-5.055311	-1.016488	1.275490
37	1	0	-5.837160	-0.335349	1.594575
38	6	0	-5.111330	-2.357237	1.654900
39	1	0	-5.913196	-2.709579	2.298967
40	6	0	-4.136036	-3.231448	1.190880
41	6	0	-3.975978	-4.706906	1.484301
42	1	0	-4.725812	-5.306158	0.949081
43	1	0	-4.094045	-4.935602	2.549659
44	6	0	-2.550885	-4.993937	0.967546
45	1	0	-2.399832	-6.032732	0.658949
46	1	0	-1.819393	-4.769272	1.752178
47	6	0	-0.890851	-3.965312	-0.662575
48	6	0	0.192255	-3.200591	-0.241503
49	6	0	1.515568	-3.519595	-0.602711
50	6	0	1.693214	-4.616479	-1.462218
51	1	0	2.705603	-4.895403	-1.738017
52	6	0	0.613533	-5.322213	-1.995921
53	1	0	0.786430	-6.126946	-2.706267
54	6	0	-0.676990	-4.984994	-1.603459
55	6	0	-1.996234	-5.572861	-2.057014

56	1	0	-2.157322	-6.574919	-1.635611
57	1	0	-2.052905	-5.678620	-3.146484
58	6	0	-3.021923	-4.557554	-1.504601
59	1	0	-4.004065	-4.996732	-1.304835
60	1	0	-3.160929	-3.741202	-2.222648
61	6	0	-3.993402	0.958944	0.153370
62	6	0	-4.231742	1.368438	-1.181506
63	6	0	-4.343481	2.735980	-1.463213
64	1	0	-4.541237	3.046316	-2.487167
65	6	0	-4.244571	3.716555	-0.476259
66	6	0	-3.992400	3.291791	0.830640
67	1	0	-3.902824	4.035267	1.618092
68	6	0	-3.855778	1.941331	1.169979
69	6	0	-4.423554	0.382937	-2.335115
70	1	0	-4.315827	-0.631091	-1.942823
71	6	0	-3.351448	0.562527	-3.427115
72	1	0	-2.346177	0.446323	-3.010621
73	1	0	-3.419600	1.550290	-3.899302
74	1	0	-3.480751	-0.188020	-4.216553
75	6	0	-5.843165	0.479606	-2.928903
76	1	0	-6.029996	1.463624	-3.374708
77	1	0	-6.606125	0.311631	-2.160581
78	1	0	-5.980914	-0.272611	-3.715184
79	6	0	-4.454004	5.187377	-0.814504
80	1	0	-4.530754	5.259107	-1.908459
81	6	0	-3.276110	6.075838	-0.376068
82	1	0	-2.334972	5.739958	-0.824901
83	1	0	-3.147343	6.065588	0.712442
84	1	0	-3.444628	7.116064	-0.679133
85	6	0	-5.780427	5.708383	-0.226309
86	1	0	-5.958105	6.747775	-0.528128
87	1	0	-5.765438	5.675199	0.869649
88	1	0	-6.627846	5.103399	-0.566524
89	6	0	-3.576662	1.591432	2.634065
90	1	0	-3.286314	0.538111	2.678035
91	6	0	-2.409628	2.406235	3.227431
92	1	0	-2.679469	3.460441	3.365307
93	1	0	-1.520926	2.367884	2.593580
94	1	0	-2.147080	2.008980	4.215452
95	6	0	-4.830726	1.780003	3.513058
96	1	0	-5.672570	1.170586	3.170040
97	1	0	-5.157672	2.826963	3.507991
98	1	0	-4.615400	1.502182	4.552090
99	6	0	2.694004	-2.739489	-0.099099

100	6	0	3.524198	-2.027048	-1.004227
101	6	0	4.615406	-1.310904	-0.501304
102	1	0	5.242052	-0.760775	-1.198687
103	6	0	4.924478	-1.270623	0.860334
104	6	0	4.109171	-1.998010	1.726530
105	1	0	4.348652	-1.997011	2.787734
106	6	0	3.004874	-2.734242	1.283131
107	6	0	3.298177	-2.018918	-2.518422
108	1	0	2.352258	-2.524871	-2.726664
109	6	0	3.167610	-0.596776	-3.093722
110	1	0	4.080953	-0.007962	-2.948243
111	1	0	2.334078	-0.074807	-2.619113
112	1	0	2.975242	-0.643830	-4.172783
113	6	0	4.412573	-2.796808	-3.248001
114	1	0	4.492312	-3.828280	-2.886134
115	1	0	5.389890	-2.322022	-3.100021
116	1	0	4.216556	-2.829587	-4.326811
117	6	0	6.104581	-0.468198	1.391968
118	1	0	6.138408	-0.631389	2.478372
119	6	0	5.922954	1.043195	1.156387
120	1	0	4.984662	1.410358	1.584993
121	1	0	5.909123	1.284332	0.087386
122	1	0	6.748371	1.605121	1.610283
123	6	0	7.444261	-0.961426	0.813244
124	1	0	8.281955	-0.407160	1.253434
125	1	0	7.486317	-0.816943	-0.272900
126	1	0	7.596348	-2.027815	1.014411
127	6	0	2.226393	-3.548541	2.317528
128	1	0	1.377704	-4.021499	1.816919
129	6	0	1.654821	-2.671945	3.448347
130	1	0	1.012947	-1.882282	3.047129
131	1	0	2.451150	-2.201370	4.037294
132	1	0	1.056957	-3.282848	4.136087
133	6	0	3.094955	-4.688277	2.887933
134	1	0	3.965521	-4.297580	3.427724
135	1	0	3.463999	-5.342780	2.090324
136	1	0	2.514172	-5.300026	3.589435

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.085063	4.501749	-1.863340
2	6	0	3.911588	3.780340	-1.648016
3	6	0	3.095950	4.026651	-0.526365
4	6	0	3.513522	5.028582	0.372453
5	6	0	4.694664	5.736771	0.163035
6	6	0	5.488352	5.482929	-0.957251
7	6	0	1.833293	3.287146	-0.310781
8	6	0	1.268246	2.930581	0.902078
9	8	0	1.999724	3.114960	2.022249
10	6	0	1.388608	2.761051	3.271682
11	8	0	0.051058	2.480924	1.013390
12	1	0	0.476904	3.340056	3.441198
13	1	0	1.152131	1.693912	3.305432
14	1	0	2.136434	3.000829	4.028485
15	1	0	2.905484	5.248243	1.242203
16	1	0	4.988787	6.502774	0.876386
17	1	0	6.405673	6.041735	-1.121290
18	1	0	5.689923	4.286391	-2.740689
19	1	0	3.627828	3.012009	-2.361041
20	16	0	0.955369	2.747350	-1.751337
21	6	0	-0.676660	3.585527	-1.762734
22	1	0	-0.507139	4.640377	-1.986435
23	1	0	-1.155754	3.453602	-0.793685
24	1	0	-1.271513	3.123530	-2.555054
25	1	0	0.569312	1.379750	-1.384225
26	1	0	-0.194930	1.371749	1.189331
27	15	0	-0.393168	-0.645246	0.010262
28	8	0	-1.806031	-1.067323	-0.689918
29	8	0	0.216921	-2.035195	0.589209
30	8	0	0.426748	-0.048881	-1.113907
31	8	0	-0.608493	0.188653	1.273121
32	6	0	-1.877041	-4.136602	-0.281918
33	6	0	-2.781940	-3.041096	0.280083
34	6	0	-2.830169	-1.667788	0.042764
35	6	0	-3.915714	-0.882080	0.480530
36	6	0	-4.918861	-1.527506	1.221893
37	1	0	-5.777397	-0.945892	1.541595
38	6	0	-4.829361	-2.873529	1.574916
39	1	0	-5.596133	-3.327515	2.197806

40	6	0	-3.754741	-3.621920	1.110505
41	6	0	-3.434496	-5.076733	1.374134
42	1	0	-4.105612	-5.743366	0.814451
43	1	0	-3.539698	-5.342593	2.432318
44	6	0	-1.979934	-5.191409	0.872474
45	1	0	-1.710958	-6.199445	0.542717
46	1	0	-1.286969	-4.905836	1.672200
47	6	0	-0.425064	-3.950890	-0.713339
48	6	0	0.567067	-3.084796	-0.262220
49	6	0	1.922145	-3.269565	-0.602447
50	6	0	2.224098	-4.327335	-1.475646
51	1	0	3.264241	-4.502157	-1.733515
52	6	0	1.229739	-5.124995	-2.043879
53	1	0	1.493830	-5.895517	-2.764107
54	6	0	-0.093806	-4.925336	-1.668442
55	6	0	-1.337605	-5.639278	-2.153053
56	1	0	-1.395875	-6.662284	-1.755655
57	1	0	-1.369482	-5.725818	-3.245338
58	6	0	-2.471692	-4.751573	-1.593959
59	1	0	-3.403532	-5.297195	-1.416091
60	1	0	-2.689367	-3.939225	-2.296848
61	6	0	-4.065894	0.578438	0.160792
62	6	0	-4.300626	0.994742	-1.172753
63	6	0	-4.543450	2.350183	-1.429062
64	1	0	-4.736225	2.664568	-2.452870
65	6	0	-4.580689	3.310904	-0.418195
66	6	0	-4.339797	2.880034	0.888736
67	1	0	-4.360091	3.607517	1.695823
68	6	0	-4.075790	1.542603	1.203376
69	6	0	-4.356308	0.022423	-2.351338
70	1	0	-4.150373	-0.983143	-1.977477
71	6	0	-3.284422	0.337780	-3.412317
72	1	0	-2.281917	0.307354	-2.974515
73	1	0	-3.440426	1.326714	-3.861305
74	1	0	-3.322004	-0.399545	-4.223493
75	6	0	-5.763790	-0.018721	-2.979968
76	1	0	-6.044224	0.949276	-3.411775
77	1	0	-6.522153	-0.283272	-2.234639
78	1	0	-5.802052	-0.764373	-3.783556
79	6	0	-4.918594	4.762534	-0.734887
80	1	0	-4.950497	4.854615	-1.829600
81	6	0	-3.856246	5.750403	-0.220074
82	1	0	-2.863175	5.511446	-0.616100
83	1	0	-3.789511	5.735381	0.873961

84	1	0	-4.105194	6.774974	-0.521400
85	6	0	-6.315832	5.137107	-0.201782
86	1	0	-6.577116	6.164806	-0.482257
87	1	0	-6.350507	5.068384	0.892062
88	1	0	-7.084348	4.466994	-0.602079
89	6	0	-3.819645	1.185338	2.669760
90	1	0	-3.444518	0.159213	2.704905
91	6	0	-2.742356	2.078023	3.315730
92	1	0	-3.090991	3.110210	3.443040
93	1	0	-1.832110	2.099176	2.713818
94	1	0	-2.491688	1.694503	4.312302
95	6	0	-5.114565	1.251873	3.505820
96	1	0	-5.893931	0.589630	3.115510
97	1	0	-5.522198	2.270155	3.515915
98	1	0	-4.915269	0.961794	4.544745
99	6	0	3.008823	-2.390262	-0.058049
100	6	0	3.795825	-1.594074	-0.931284
101	6	0	4.800992	-0.785026	-0.390594
102	1	0	5.393343	-0.171191	-1.064331
103	6	0	5.065887	-0.732079	0.979753
104	6	0	4.298381	-1.543314	1.814489
105	1	0	4.505964	-1.532655	2.882447
106	6	0	3.280721	-2.373746	1.332480
107	6	0	3.615799	-1.593290	-2.451666
108	1	0	2.730990	-2.187174	-2.692289
109	6	0	3.363279	-0.185959	-3.021070
110	1	0	4.205750	0.490617	-2.835888
111	1	0	2.464932	0.244637	-2.573598
112	1	0	3.214328	-0.238685	-4.106734
113	6	0	4.822126	-2.250474	-3.153088
114	1	0	4.997477	-3.269103	-2.788860
115	1	0	5.742113	-1.678840	-2.981447
116	1	0	4.657372	-2.300929	-4.236484
117	6	0	6.148260	0.170895	1.555542
118	1	0	6.165731	-0.004537	2.640399
119	6	0	5.828432	1.661291	1.333822
120	1	0	4.842535	1.924342	1.731337
121	1	0	5.829598	1.918037	0.268400
122	1	0	6.577096	2.293253	1.827304
123	6	0	7.545917	-0.182422	1.013085
124	1	0	8.313011	0.441652	1.487486
125	1	0	7.607410	-0.016490	-0.069069
126	1	0	7.793052	-1.232688	1.204285
127	6	0	2.557106	-3.272269	2.336315

128	1	0	1.771084	-3.817359	1.807983
129	6	0	1.875907	-2.469346	3.460820
130	1	0	1.176659	-1.735339	3.050303
131	1	0	2.609724	-1.938907	4.079718
132	1	0	1.317046	-3.143169	4.122254
133	6	0	3.516160	-4.331493	2.916994
134	1	0	4.328564	-3.867837	3.489124
135	1	0	3.970285	-4.933713	2.122030
136	1	0	2.977328	-5.008410	3.591505

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.709312	3.764656	-1.747948
2	6	0	4.419867	3.241318	-1.658657
3	6	0	3.507911	3.703200	-0.690942
4	6	0	3.944932	4.724203	0.176402
5	6	0	5.234010	5.244506	0.087188
6	6	0	6.127679	4.768691	-0.874222
7	6	0	2.130310	3.159968	-0.615233
8	6	0	1.408430	3.020287	0.534126
9	8	0	1.992476	3.203903	1.742234
10	6	0	1.149940	3.316823	2.894836
11	8	0	0.089108	2.765588	0.516449
12	1	0	0.366850	4.065829	2.745761
13	1	0	0.690365	2.355440	3.145021
14	1	0	1.814647	3.622071	3.704469
15	1	0	3.265408	5.113564	0.925595
16	1	0	5.537509	6.035376	0.768990
17	1	0	7.132100	5.177804	-0.943911
18	1	0	6.388482	3.383370	-2.506683
19	1	0	4.111138	2.467750	-2.354069
20	16	0	1.371356	2.544281	-2.120721
21	6	0	0.083569	3.790327	-2.505735
22	1	0	0.543682	4.776806	-2.599794
23	1	0	-0.683119	3.792023	-1.729786
24	1	0	-0.358185	3.503280	-3.464581
25	1	0	0.566175	0.624829	-1.391344
26	1	0	-0.158796	1.890336	0.925658
27	15	0	-0.549927	-0.667781	0.032208

28	8	0	-1.929711	-0.903353	-0.785605
29	8	0	-0.123615	-2.111938	0.595997
30	8	0	0.446374	-0.340929	-1.150449
31	8	0	-0.625625	0.291873	1.169402
32	6	0	-2.401991	-3.941609	-0.484536
33	6	0	-3.211476	-2.760215	0.048038
34	6	0	-3.069569	-1.385013	-0.123580
35	6	0	-4.050174	-0.474207	0.316179
36	6	0	-5.181108	-1.009591	0.953930
37	1	0	-5.960050	-0.325918	1.277293
38	6	0	-5.303691	-2.372929	1.220219
39	1	0	-6.164840	-2.746976	1.768345
40	6	0	-4.307936	-3.239096	0.784940
41	6	0	-4.192788	-4.731012	1.006126
42	1	0	-4.888545	-5.288443	0.363477
43	1	0	-4.419973	-5.018485	2.038965
44	6	0	-2.725342	-5.007005	0.619420
45	1	0	-2.549658	-6.031111	0.277157
46	1	0	-2.073924	-4.827635	1.482480
47	6	0	-0.905014	-3.925588	-0.790828
48	6	0	0.151372	-3.198524	-0.249751
49	6	0	1.497663	-3.536121	-0.493759
50	6	0	1.733089	-4.617695	-1.357871
51	1	0	2.759918	-4.917592	-1.540569
52	6	0	0.695082	-5.280296	-2.014439
53	1	0	0.917977	-6.069708	-2.727996
54	6	0	-0.619146	-4.920666	-1.740793
55	6	0	-1.896271	-5.461663	-2.347207
56	1	0	-2.117189	-6.475747	-1.986324
57	1	0	-1.843107	-5.523069	-3.440211
58	6	0	-2.953473	-4.446439	-1.859776
59	1	0	-3.958682	-4.870832	-1.777209
60	1	0	-3.004338	-3.598524	-2.552470
61	6	0	-3.916394	1.010960	0.151131
62	6	0	-3.938004	1.595908	-1.137753
63	6	0	-3.822359	2.986483	-1.252905
64	1	0	-3.842161	3.436024	-2.243458
65	6	0	-3.700035	3.823018	-0.143106
66	6	0	-3.708769	3.226108	1.119244
67	1	0	-3.627193	3.857170	2.000104
68	6	0	-3.810158	1.843068	1.296999
69	6	0	-4.152572	0.779261	-2.412611
70	1	0	-4.170182	-0.279763	-2.142352
71	6	0	-3.017059	0.966038	-3.435888

72	1	0	-2.049255	0.696552	-3.002696
73	1	0	-2.958349	2.001439	-3.792368
74	1	0	-3.186183	0.327313	-4.311365
75	6	0	-5.522455	1.099767	-3.045110
76	1	0	-5.581355	2.146720	-3.365339
77	1	0	-6.337928	0.922266	-2.335106
78	1	0	-5.695478	0.470370	-3.926662
79	6	0	-3.596994	5.333221	-0.313119
80	1	0	-3.430129	5.524808	-1.382259
81	6	0	-2.405533	5.934325	0.454964
82	1	0	-1.471860	5.417519	0.209788
83	1	0	-2.551075	5.860552	1.539408
84	1	0	-2.289060	6.997210	0.211952
85	6	0	-4.913381	6.032181	0.080150
86	1	0	-4.846254	7.113657	-0.090329
87	1	0	-5.139795	5.872888	1.141361
88	1	0	-5.757300	5.646122	-0.502078
89	6	0	-3.819655	1.305930	2.731195
90	1	0	-3.796681	0.214347	2.689396
91	6	0	-2.581729	1.739221	3.539063
92	1	0	-2.530549	2.828009	3.659149
93	1	0	-1.667610	1.396677	3.048756
94	1	0	-2.618814	1.300178	4.543751
95	6	0	-5.112090	1.714052	3.467902
96	1	0	-6.008519	1.378202	2.934497
97	1	0	-5.182313	2.803310	3.573367
98	1	0	-5.133732	1.279300	4.474632
99	6	0	2.635230	-2.780038	0.127423
100	6	0	3.565103	-2.081784	-0.689289
101	6	0	4.594580	-1.360526	-0.076211
102	1	0	5.294687	-0.817627	-0.705249
103	6	0	4.749995	-1.302394	1.310507
104	6	0	3.850605	-2.029131	2.089187
105	1	0	3.973596	-2.019989	3.169951
106	6	0	2.800712	-2.769638	1.534730
107	6	0	3.520700	-2.103210	-2.219769
108	1	0	2.576819	-2.558233	-2.529886
109	6	0	3.558896	-0.699483	-2.849446
110	1	0	4.502589	-0.180153	-2.646563
111	1	0	2.742442	-0.078198	-2.475184
112	1	0	3.455442	-0.774627	-3.938734
113	6	0	4.666689	-2.966077	-2.789124
114	1	0	4.649494	-3.985966	-2.389068
115	1	0	5.643732	-2.534686	-2.540419

116	1	0	4.596304	-3.028756	-3.882051
117	6	0	5.849685	-0.472619	1.958975
118	1	0	5.779043	-0.639280	3.043009
119	6	0	5.644894	1.033934	1.707175
120	1	0	4.655221	1.366616	2.037634
121	1	0	5.731583	1.278413	0.642362
122	1	0	6.400366	1.620180	2.244555
123	6	0	7.255086	-0.920873	1.516436
124	1	0	8.026351	-0.347599	2.044767
125	1	0	7.404315	-0.762418	0.441812
126	1	0	7.417682	-1.984543	1.723595
127	6	0	1.924630	-3.588199	2.484295
128	1	0	1.121281	-4.048765	1.903741
129	6	0	1.261844	-2.722553	3.572866
130	1	0	0.685727	-1.904775	3.130600
131	1	0	2.004868	-2.288166	4.252157
132	1	0	0.582154	-3.333059	4.180229
133	6	0	2.732947	-4.741383	3.113799
134	1	0	3.557927	-4.361684	3.728014
135	1	0	3.163074	-5.391323	2.343505
136	1	0	2.090799	-5.354854	3.758003

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.278935	0.639944	-0.202174
2	8	0	-1.483545	1.226306	0.708100
3	8	0	0.647188	1.904361	-0.588331
4	8	0	0.472042	-0.206132	0.925372
5	8	0	-0.663004	-0.090234	-1.436309
6	1	0	-0.648990	-1.878089	-1.294277
7	6	0	-0.958873	4.270053	0.606605
8	6	0	-2.083178	3.446855	-0.013009
9	6	0	-2.408776	2.096770	0.099961
10	6	0	-3.644520	1.594751	-0.352026
11	6	0	-4.513718	2.507443	-0.974906
12	1	0	-5.482505	2.145954	-1.303988
13	6	0	-4.158937	3.834808	-1.207260
14	1	0	-4.834641	4.495311	-1.744841
15	6	0	-2.937874	4.297275	-0.733179

16	6	0	-2.327954	5.674238	-0.876376
17	1	0	-2.831174	6.405626	-0.228731
18	1	0	-2.402576	6.058412	-1.900103
19	6	0	-0.868580	5.437799	-0.433947
20	1	0	-0.387986	6.329630	-0.020912
21	1	0	-0.270666	5.101917	-1.288873
22	6	0	0.429983	3.744634	0.956001
23	6	0	1.218268	2.753270	0.375405
24	6	0	2.585163	2.616775	0.688073
25	6	0	3.106290	3.490896	1.657678
26	1	0	4.163644	3.421430	1.891301
27	6	0	2.308891	4.406747	2.341344
28	1	0	2.736769	5.025217	3.126379
29	6	0	0.968397	4.521137	1.995170
30	6	0	-0.088992	5.420771	2.596376
31	1	0	0.061597	6.469457	2.304677
32	1	0	-0.082674	5.396498	3.692127
33	6	0	-1.390708	4.849382	1.996229
34	1	0	-2.192806	5.588594	1.910498
35	1	0	-1.759350	4.027945	2.621268
36	6	0	-4.112146	0.178274	-0.178480
37	6	0	-4.416686	-0.317104	1.114832
38	6	0	-5.011941	-1.577366	1.232638
39	1	0	-5.260391	-1.949327	2.225100
40	6	0	-5.338587	-2.364181	0.124353
41	6	0	-5.003529	-1.868732	-1.135735
42	1	0	-5.227027	-2.463724	-2.015650
43	6	0	-4.391820	-0.621067	-1.315675
44	6	0	-4.183391	0.489691	2.392845
45	1	0	-3.732757	1.446568	2.118650
46	6	0	-3.201541	-0.215135	3.348205
47	1	0	-2.236693	-0.388945	2.861821
48	1	0	-3.594391	-1.180820	3.688690
49	1	0	-3.026570	0.401383	4.238371
50	6	0	-5.512564	0.814800	3.103485
51	1	0	-6.021345	-0.093879	3.445774
52	1	0	-6.198060	1.349680	2.436629
53	1	0	-5.331836	1.445269	3.982641
54	6	0	-6.094936	-3.673658	0.329105
55	1	0	-5.740664	-4.103432	1.277553
56	6	0	-5.862062	-4.722819	-0.768410
57	1	0	-4.796018	-4.917891	-0.928407
58	1	0	-6.292418	-4.409161	-1.726649
59	1	0	-6.341614	-5.668995	-0.493068

60	6	0	-7.604972	-3.396991	0.492350
61	1	0	-8.151757	-4.324698	0.700997
62	1	0	-8.017576	-2.957902	-0.423984
63	1	0	-7.795121	-2.696375	1.312384
64	6	0	-4.074889	-0.178842	-2.747204
65	1	0	-3.509292	0.755198	-2.696004
66	6	0	-3.186619	-1.193060	-3.492951
67	1	0	-3.686367	-2.160579	-3.619847
68	1	0	-2.249159	-1.355672	-2.959067
69	1	0	-2.947378	-0.812362	-4.493314
70	6	0	-5.360808	0.089964	-3.555514
71	1	0	-5.998781	0.840217	-3.076252
72	1	0	-5.956354	-0.823890	-3.668580
73	1	0	-5.111934	0.450982	-4.560733
74	6	0	3.503724	1.624767	0.036674
75	6	0	4.164563	0.643349	0.824413
76	6	0	5.099408	-0.198775	0.213452
77	1	0	5.602572	-0.943706	0.823996
78	6	0	5.411840	-0.112974	-1.145095
79	6	0	4.745849	0.852752	-1.898466
80	1	0	4.982126	0.939771	-2.956753
81	6	0	3.804556	1.727651	-1.343870
82	6	0	3.924434	0.469979	2.327581
83	1	0	3.107027	1.132275	2.623857
84	6	0	3.493116	-0.960494	2.697842
85	1	0	4.265602	-1.701976	2.468389
86	1	0	2.586269	-1.253805	2.164270
87	1	0	3.284117	-1.024261	3.772666
88	6	0	5.169694	0.872216	3.145065
89	1	0	5.484497	1.900218	2.934233
90	1	0	6.019305	0.216918	2.919644
91	1	0	4.964581	0.794145	4.219732
92	6	0	6.466234	-1.007234	-1.783809
93	1	0	6.458325	-0.791380	-2.861314
94	6	0	6.153635	-2.504351	-1.611811
95	1	0	5.158361	-2.744887	-1.998538
96	1	0	6.175781	-2.801573	-0.556857
97	1	0	6.893925	-3.113811	-2.144772
98	6	0	7.876521	-0.672792	-1.259354
99	1	0	8.633816	-1.282061	-1.767758
100	1	0	7.955261	-0.871306	-0.183720
101	1	0	8.120994	0.382801	-1.422203
102	6	0	3.202278	2.797436	-2.255469
103	1	0	2.482905	3.381580	-1.676695

104	6	0	2.437880	2.184635	-3.444416
105	1	0	1.654311	1.503044	-3.101143
106	1	0	3.108157	1.626833	-4.109376
107	1	0	1.967250	2.975993	-4.040939
108	6	0	4.282093	3.785885	-2.740925
109	1	0	5.038949	3.285983	-3.356703
110	1	0	4.797620	4.256889	-1.896300
111	1	0	3.829478	4.579028	-3.348901
112	1	0	0.834656	-1.054873	0.584687
113	6	0	-0.131504	-3.385558	-0.163107
114	6	0	1.241552	-3.299281	-0.211713
115	6	0	2.118500	-4.059523	0.719733
116	6	0	1.819221	-4.176483	2.091263
117	6	0	3.297516	-4.672878	0.259956
118	6	0	2.650140	-4.887906	2.954153
119	1	0	0.925661	-3.703633	2.483909
120	6	0	4.129763	-5.383825	1.123724
121	1	0	3.566013	-4.585313	-0.787748
122	6	0	3.811675	-5.498895	2.477574
123	1	0	2.391138	-4.956223	4.007984
124	1	0	5.030030	-5.851912	0.732845
125	1	0	4.460905	-6.050900	3.152041
126	16	0	1.970474	-2.456043	-1.615521
127	6	0	1.474489	-3.524409	-3.027424
128	1	0	1.872275	-4.535649	-2.909164
129	1	0	0.386762	-3.562347	-3.124656
130	1	0	1.898403	-3.070236	-3.927915
131	8	0	-0.999134	-2.740472	-0.949638
132	8	0	-0.720536	-4.243975	0.683716
133	6	0	-2.138946	-4.144112	0.881394
134	1	0	-2.365277	-4.885179	1.649489
135	1	0	-2.425673	-3.144898	1.218955
136	1	0	-2.678635	-4.375732	-0.039265

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.156842	0.556077	-0.296801
2	8	0	-1.327352	1.256515	0.598172
3	8	0	0.897650	1.739483	-0.645103

4	8	0	0.451725	-0.470417	0.690094
5	8	0	-0.648406	0.026470	-1.617822
6	1	0	-0.713605	-1.424741	-1.819546
7	6	0	-0.560728	4.252179	0.405314
8	6	0	-1.743246	3.494591	-0.188512
9	6	0	-2.186723	2.186080	-0.003053
10	6	0	-3.492787	1.799495	-0.368764
11	6	0	-4.288174	2.765646	-1.010058
12	1	0	-5.307492	2.498984	-1.267298
13	6	0	-3.805431	4.029066	-1.345299
14	1	0	-4.431192	4.724717	-1.898894
15	6	0	-2.527111	4.387322	-0.936770
16	6	0	-1.788822	5.688908	-1.164285
17	1	0	-2.224517	6.506819	-0.573899
18	1	0	-1.822829	6.007327	-2.212642
19	6	0	-0.358289	5.350039	-0.691763
20	1	0	0.193357	6.217831	-0.317847
21	1	0	0.217148	4.919126	-1.519019
22	6	0	0.770415	3.640049	0.827920
23	6	0	1.494833	2.563048	0.316875
24	6	0	2.836184	2.342081	0.689900
25	6	0	3.390345	3.214240	1.643371
26	1	0	4.429531	3.069744	1.921800
27	6	0	2.646888	4.220429	2.254786
28	1	0	3.094197	4.840646	3.027592
29	6	0	1.333534	4.421687	1.850071
30	6	0	0.336731	5.434959	2.366068
31	1	0	0.582919	6.450465	2.025155
32	1	0	0.306321	5.470876	3.461227
33	6	0	-0.985921	4.938476	1.749283
34	1	0	-1.723076	5.732834	1.598693
35	1	0	-1.438881	4.182335	2.400926
36	6	0	-4.109111	0.463541	-0.064062
37	6	0	-4.321423	0.067820	1.280930
38	6	0	-5.052721	-1.098263	1.539167
39	1	0	-5.230001	-1.386213	2.573095
40	6	0	-5.602286	-1.883180	0.526455
41	6	0	-5.356761	-1.493141	-0.793409
42	1	0	-5.773107	-2.086327	-1.604191
43	6	0	-4.622877	-0.344788	-1.115456
44	6	0	-3.852809	0.886010	2.485497
45	1	0	-3.328841	1.771271	2.120256
46	6	0	-2.858751	0.098289	3.360104
47	1	0	-1.984596	-0.210177	2.779319

48	1	0	-3.322496	-0.798408	3.789207
49	1	0	-2.510240	0.720077	4.193842
50	6	0	-5.046720	1.395107	3.318381
51	1	0	-5.615029	0.569458	3.762244
52	1	0	-5.737411	1.982856	2.703292
53	1	0	-4.694309	2.032860	4.138114
54	6	0	-6.495784	-3.071237	0.864538
55	1	0	-6.479876	-3.183627	1.957284
56	6	0	-5.996027	-4.396077	0.262409
57	1	0	-4.987356	-4.634241	0.616478
58	1	0	-5.971559	-4.355895	-0.833432
59	1	0	-6.657122	-5.223175	0.547243
60	6	0	-7.956215	-2.799778	0.452100
61	1	0	-8.607619	-3.626162	0.761511
62	1	0	-8.046517	-2.691084	-0.635322
63	1	0	-8.330914	-1.878548	0.910987
64	6	0	-4.441242	-0.006249	-2.598940
65	1	0	-3.751743	0.838632	-2.671695
66	6	0	-3.811417	-1.163088	-3.397592
67	1	0	-4.475892	-2.034794	-3.444931
68	1	0	-2.864157	-1.480632	-2.959234
69	1	0	-3.620707	-0.843363	-4.429095
70	6	0	-5.773834	0.406058	-3.258986
71	1	0	-6.247688	1.251507	-2.749890
72	1	0	-6.490773	-0.423856	-3.251688
73	1	0	-5.608220	0.692533	-4.304598
74	6	0	3.715714	1.266089	0.123959
75	6	0	4.262369	0.277938	0.985967
76	6	0	5.189159	-0.632669	0.468957
77	1	0	5.604169	-1.384971	1.135146
78	6	0	5.602960	-0.605570	-0.864627
79	6	0	5.045532	0.367121	-1.693545
80	1	0	5.362216	0.407649	-2.733693
81	6	0	4.113890	1.306009	-1.234000
82	6	0	3.903009	0.168456	2.470900
83	1	0	3.156984	0.933103	2.700299
84	6	0	3.263804	-1.187264	2.820672
85	1	0	3.932729	-2.028057	2.605677
86	1	0	2.340007	-1.337546	2.258405
87	1	0	3.019756	-1.222566	3.889777
88	6	0	5.127543	0.436276	3.369319
89	1	0	5.581725	1.411933	3.161499
90	1	0	5.903765	-0.324520	3.224776
91	1	0	4.836981	0.416298	4.426804

92	6	0	6.647028	-1.578016	-1.398159
93	1	0	6.760103	-1.371350	-2.471576
94	6	0	6.206769	-3.046565	-1.256562
95	1	0	5.240665	-3.215026	-1.743524
96	1	0	6.099632	-3.330784	-0.203113
97	1	0	6.947073	-3.717670	-1.709377
98	6	0	8.021202	-1.350846	-0.738815
99	1	0	8.776824	-2.015564	-1.175353
100	1	0	7.981054	-1.552953	0.338249
101	1	0	8.357753	-0.316719	-0.871405
102	6	0	3.626476	2.371582	-2.216197
103	1	0	2.908924	3.013679	-1.700209
104	6	0	2.894703	1.755001	-3.423474
105	1	0	2.043884	1.148542	-3.100031
106	1	0	3.562958	1.119056	-4.016847
107	1	0	2.520767	2.546778	-4.084589
108	6	0	4.785086	3.280631	-2.674102
109	1	0	5.545428	2.717205	-3.227547
110	1	0	5.279143	3.755506	-1.818839
111	1	0	4.412002	4.073006	-3.334795
112	1	0	0.622435	-1.552144	0.245101
113	6	0	-0.393378	-3.159870	-0.926753
114	6	0	0.886940	-2.869585	-0.365353
115	6	0	1.378627	-3.775952	0.732748
116	6	0	0.631542	-3.888493	1.918646
117	6	0	2.580976	-4.490786	0.643702
118	6	0	1.055810	-4.707326	2.962663
119	1	0	-0.287873	-3.318745	2.024968
120	6	0	3.010052	-5.308182	1.690720
121	1	0	3.196501	-4.390165	-0.243947
122	6	0	2.248432	-5.425671	2.853367
123	1	0	0.459494	-4.773561	3.869193
124	1	0	3.945491	-5.853871	1.594313
125	1	0	2.584596	-6.059831	3.669415
126	16	0	2.076374	-2.271619	-1.604806
127	6	0	2.012643	-3.574358	-2.896922
128	1	0	2.247020	-4.560934	-2.487618
129	1	0	1.036138	-3.597576	-3.389367
130	1	0	2.770556	-3.307503	-3.639707
131	8	0	-1.001580	-2.437490	-1.816156
132	8	0	-1.041983	-4.236983	-0.526007
133	6	0	-2.405439	-4.427135	-0.965441
134	1	0	-2.743115	-5.317992	-0.437226
135	1	0	-3.017527	-3.562161	-0.704267

136	1	0	-2.434781	-4.586897	-2.045498

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.012526	-1.554467	-2.195866
2	1	0	0.779364	-1.063857	0.396637
3	6	0	1.436036	-2.765761	-1.680937
4	6	0	0.953431	-3.253088	-0.484430
5	6	0	1.772568	-4.024380	0.494588
6	6	0	2.815211	-4.889437	0.110652
7	6	0	1.474384	-3.940087	1.868831
8	6	0	3.540002	-5.611359	1.060224
9	1	0	3.056363	-5.002256	-0.938975
10	6	0	2.197473	-4.662133	2.815530
11	1	0	0.654798	-3.305394	2.192294
12	6	0	3.240653	-5.501182	2.417935
13	1	0	4.337000	-6.273389	0.730002
14	1	0	1.943265	-4.567439	3.868358
15	1	0	3.805194	-6.066375	3.154916
16	16	0	-0.828506	-3.252924	-0.256193
17	6	0	-1.239614	-4.928468	-0.884520
18	1	0	-1.009488	-5.008457	-1.950220
19	1	0	-0.689775	-5.689467	-0.324533
20	1	0	-2.312679	-5.071912	-0.732789
21	8	0	0.746502	-2.084033	-2.597551
22	8	0	2.712559	-2.982159	-2.041946
23	6	0	3.227883	-2.277337	-3.184746
24	1	0	4.276089	-2.572946	-3.242103
25	1	0	2.700428	-2.573390	-4.094493
26	1	0	3.148019	-1.197064	-3.047092
27	15	0	-0.302230	0.665736	-0.337402
28	8	0	0.651773	1.922613	-0.694270
29	8	0	-1.499643	1.261381	0.570614
30	8	0	-0.679951	-0.026554	-1.594131
31	8	0	0.450084	-0.210448	0.764000
32	6	0	-1.079589	4.317327	0.194752
33	6	0	0.295518	3.869391	0.679212
34	6	0	1.128784	2.834408	0.259443
35	6	0	2.456004	2.722289	0.717768

36	6	0	2.898662	3.683718	1.641945
37	1	0	3.926827	3.627950	1.984873
38	6	0	2.056209	4.672425	2.145981
39	1	0	2.418787	5.369583	2.897194
40	6	0	0.752500	4.750835	1.672683
41	6	0	-0.343310	5.706694	2.087394
42	1	0	-0.176983	6.710334	1.671530
43	1	0	-0.408029	5.823594	3.175137
44	6	0	-1.598587	5.047547	1.482133
45	1	0	-2.402970	5.755931	1.263414
46	1	0	-1.994282	4.297440	2.176478
47	6	0	-2.161217	3.391920	-0.353550
48	6	0	-2.459665	2.057370	-0.089597
49	6	0	-3.693247	1.487648	-0.457284
50	6	0	-4.575504	2.302233	-1.187681
51	1	0	-5.541691	1.891137	-1.461269
52	6	0	-4.235031	3.592149	-1.593952
53	1	0	-4.917718	4.166999	-2.214779
54	6	0	-3.024197	4.131866	-1.177752
55	6	0	-2.432456	5.490461	-1.486793
56	1	0	-2.966706	6.292527	-0.958901
57	1	0	-2.482719	5.731370	-2.554837
58	6	0	-0.980260	5.348456	-0.977900
59	1	0	-0.534642	6.297539	-0.664393
60	1	0	-0.347477	4.926131	-1.766839
61	6	0	3.411082	1.655328	0.269702
62	6	0	3.888061	1.636616	-1.063735
63	6	0	4.851459	0.686920	-1.424425
64	1	0	5.230603	0.685649	-2.444508
65	6	0	5.367285	-0.242059	-0.519288
66	6	0	4.882956	-0.204149	0.789575
67	1	0	5.267567	-0.915978	1.514284
68	6	0	3.921103	0.720730	1.209483
69	6	0	3.451100	2.656523	-2.116470
70	1	0	2.686499	3.299684	-1.674410
71	6	0	2.821161	1.989790	-3.354101
72	1	0	1.963964	1.368108	-3.077576
73	1	0	3.545705	1.361340	-3.886523
74	1	0	2.472318	2.753252	-4.060148
75	6	0	4.623610	3.573470	-2.520238
76	1	0	5.432430	3.006562	-2.996044
77	1	0	5.044395	4.086453	-1.648236
78	1	0	4.286236	4.335293	-3.233652
79	6	0	6.458885	-1.216309	-0.943874

80	1	0	6.487113	-1.205668	-2.042979
81	6	0	6.182252	-2.663288	-0.499139
82	1	0	5.188333	-2.998975	-0.810672
83	1	0	6.234737	-2.766681	0.590898
84	1	0	6.930205	-3.342312	-0.926219
85	6	0	7.840203	-0.744164	-0.446884
86	1	0	8.631719	-1.416148	-0.800545
87	1	0	7.875485	-0.729951	0.649104
88	1	0	8.065741	0.267640	-0.801410
89	6	0	3.495602	0.689877	2.680738
90	1	0	2.673950	1.398011	2.815565
91	6	0	2.970667	-0.688850	3.121483
92	1	0	3.733123	-1.470905	3.037332
93	1	0	2.109910	-0.993420	2.522335
94	1	0	2.653140	-0.649377	4.170719
95	6	0	4.649917	1.136083	3.602603
96	1	0	5.023660	2.131347	3.338082
97	1	0	5.496293	0.441458	3.543017
98	1	0	4.316122	1.166003	4.646890
99	6	0	-4.131670	0.105161	-0.069454
100	6	0	-4.421082	-0.861521	-1.067773
101	6	0	-4.971879	-2.088241	-0.682043
102	1	0	-5.202642	-2.817689	-1.454358
103	6	0	-5.243271	-2.402713	0.651886
104	6	0	-4.925835	-1.447343	1.616199
105	1	0	-5.128542	-1.675932	2.660206
106	6	0	-4.381038	-0.199791	1.291400
107	6	0	-4.168057	-0.622371	-2.558478
108	1	0	-3.624156	0.319899	-2.664874
109	6	0	-3.282900	-1.717630	-3.182538
110	1	0	-3.789744	-2.690101	-3.200581
111	1	0	-2.350471	-1.829353	-2.625489
112	1	0	-3.038779	-1.456298	-4.219411
113	6	0	-5.488733	-0.498421	-3.346170
114	1	0	-6.124817	0.306111	-2.961046
115	1	0	-6.068455	-1.427999	-3.294339
116	1	0	-5.285568	-0.291159	-4.403929
117	6	0	-5.890219	-3.723008	1.050959
118	1	0	-5.979539	-3.718626	2.145982
119	6	0	-5.027868	-4.939027	0.666944
120	1	0	-4.030266	-4.871708	1.114209
121	1	0	-4.907612	-5.012674	-0.420880
122	1	0	-5.494677	-5.869711	1.011738
123	6	0	-7.313031	-3.853827	0.474187

124	1	0	-7.788609	-4.778916	0.821949
125	1	0	-7.295951	-3.878922	-0.621903
126	1	0	-7.942355	-3.010312	0.778421
127	6	0	-4.134968	0.787941	2.432528
128	1	0	-3.719202	1.706785	2.011785
129	6	0	-3.107435	0.247894	3.445679
130	1	0	-2.162642	0.002385	2.951983
131	1	0	-3.473560	-0.655170	3.948054
132	1	0	-2.905818	0.998116	4.220424
133	6	0	-5.451799	1.181844	3.131440
134	1	0	-5.929622	0.319425	3.610709
135	1	0	-6.167582	1.605662	2.418050
136	1	0	-5.262385	1.931194	3.909866

TS IV-S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.058264	-1.182844	-2.143941
2	1	0	0.549966	-1.501545	0.239445
3	6	0	1.120357	-2.645800	-1.567743
4	6	0	0.515556	-2.889389	-0.298953
5	6	0	1.153103	-3.821357	0.698708
6	6	0	1.868012	-4.979450	0.349809
7	6	0	0.946162	-3.566612	2.065915
8	6	0	2.379959	-5.831698	1.331639
9	1	0	2.030098	-5.220307	-0.694407
10	6	0	1.452404	-4.417725	3.045042
11	1	0	0.368760	-2.694360	2.357468
12	6	0	2.178406	-5.554946	2.682703
13	1	0	2.931140	-6.719898	1.032553
14	1	0	1.279538	-4.191138	4.093925
15	1	0	2.575702	-6.219622	3.445305
16	16	0	-1.306918	-3.031029	-0.363302
17	6	0	-1.502189	-4.724529	-1.034002
18	1	0	-1.166913	-4.784807	-2.073929
19	1	0	-0.957490	-5.449482	-0.422729
20	1	0	-2.570586	-4.953172	-0.992157
21	8	0	0.623840	-1.882733	-2.495993
22	8	0	2.307200	-3.156612	-1.844767
23	6	0	2.979895	-2.723823	-3.051710

24	1	0	3.929214	-3.257477	-3.042460
25	1	0	2.390397	-2.995160	-3.929360
26	1	0	3.142287	-1.645814	-3.025239
27	15	0	-0.187891	0.619152	-0.294390
28	8	0	0.852543	1.816545	-0.661949
29	8	0	-1.341582	1.318541	0.612296
30	8	0	-0.691488	0.081812	-1.604789
31	8	0	0.487234	-0.398201	0.661381
32	6	0	-0.667210	4.334323	0.288567
33	6	0	0.684989	3.777588	0.723460
34	6	0	1.426173	2.688379	0.266385
35	6	0	2.766417	2.498548	0.661103
36	6	0	3.314918	3.431736	1.557196
37	1	0	4.353964	3.311917	1.848552
38	6	0	2.559843	4.466061	2.105718
39	1	0	3.000380	5.137070	2.838944
40	6	0	1.240568	4.621902	1.699309
41	6	0	0.225093	5.638120	2.172039
42	1	0	0.440155	6.637982	1.769687
43	1	0	0.209006	5.735717	3.263652
44	6	0	-1.092399	5.074045	1.603392
45	1	0	-1.854462	5.838357	1.424684
46	1	0	-1.513444	4.339150	2.299124
47	6	0	-1.833315	3.515123	-0.256778
48	6	0	-2.233340	2.200656	-0.021967
49	6	0	-3.515119	1.746598	-0.391213
50	6	0	-4.342308	2.653726	-1.075563
51	1	0	-5.343044	2.330459	-1.342792
52	6	0	-3.906942	3.924340	-1.448051
53	1	0	-4.551475	4.573488	-2.035632
54	6	0	-2.647405	4.347179	-1.043048
55	6	0	-1.952984	5.661126	-1.329694
56	1	0	-2.405599	6.488587	-0.765697
57	1	0	-2.008378	5.937231	-2.389045
58	6	0	-0.507947	5.383630	-0.862180
59	1	0	0.024780	6.283138	-0.538771
60	1	0	0.067476	4.928341	-1.676370
61	6	0	3.623267	1.360795	0.190970
62	6	0	4.014474	1.262550	-1.166399
63	6	0	4.872638	0.224525	-1.550084
64	1	0	5.187860	0.162116	-2.590284
65	6	0	5.367032	-0.716680	-0.644629
66	6	0	4.976796	-0.593341	0.689686
67	1	0	5.348606	-1.309046	1.417510

68	6	0	4.120281	0.420794	1.131534
69	6	0	3.599938	2.285224	-2.224821
70	1	0	2.906427	2.992527	-1.764403
71	6	0	2.862685	1.637957	-3.412175
72	1	0	1.977949	1.088644	-3.076729
73	1	0	3.513088	0.946997	-3.963523
74	1	0	2.533816	2.408344	-4.120160
75	6	0	4.815024	3.103222	-2.707622
76	1	0	5.557122	2.467458	-3.205161
77	1	0	5.313432	3.603723	-1.869961
78	1	0	4.499709	3.871326	-3.424416
79	6	0	6.338528	-1.797648	-1.102463
80	1	0	6.267005	-1.849003	-2.198697
81	6	0	5.998034	-3.192572	-0.547658
82	1	0	4.952473	-3.460070	-0.733839
83	1	0	6.159161	-3.244976	0.535188
84	1	0	6.640027	-3.953467	-1.007704
85	6	0	7.792288	-1.414813	-0.758782
86	1	0	8.494214	-2.169602	-1.134278
87	1	0	7.927751	-1.338591	0.326751
88	1	0	8.061764	-0.447876	-1.197372
89	6	0	3.774094	0.460303	2.622647
90	1	0	3.062304	1.272001	2.788046
91	6	0	3.082127	-0.831083	3.092421
92	1	0	3.726782	-1.710605	2.983434
93	1	0	2.170176	-1.006645	2.518379
94	1	0	2.811551	-0.748697	4.152649
95	6	0	5.018787	0.756556	3.482781
96	1	0	5.502923	1.695123	3.189653
97	1	0	5.766016	-0.040923	3.393539
98	1	0	4.741562	0.834335	4.541034
99	6	0	-4.058665	0.386015	-0.063958
100	6	0	-4.445511	-0.497399	-1.106587
101	6	0	-5.086543	-1.695762	-0.774900
102	1	0	-5.390919	-2.361097	-1.579337
103	6	0	-5.352705	-2.063647	0.546491
104	6	0	-4.943731	-1.190720	1.553259
105	1	0	-5.143640	-1.460941	2.587860
106	6	0	-4.309163	0.027143	1.283170
107	6	0	-4.204385	-0.196024	-2.588630
108	1	0	-3.588378	0.704194	-2.655793
109	6	0	-3.421923	-1.317992	-3.296779
110	1	0	-3.997392	-2.250780	-3.343429
111	1	0	-2.482058	-1.521968	-2.780124

112	1	0	-3.195946	-1.021075	-4.328469
113	6	0	-5.525875	0.076099	-3.336229
114	1	0	-6.092622	0.898204	-2.886054
115	1	0	-6.173249	-0.809342	-3.331799
116	1	0	-5.326978	0.337027	-4.382987
117	6	0	-6.082149	-3.356209	0.889092
118	1	0	-6.161964	-3.399513	1.984026
119	6	0	-5.299335	-4.603140	0.438619
120	1	0	-4.296848	-4.616389	0.879847
121	1	0	-5.190228	-4.629082	-0.652683
122	1	0	-5.819674	-5.519869	0.741931
123	6	0	-7.514984	-3.370063	0.322861
124	1	0	-8.046578	-4.278001	0.633098
125	1	0	-7.509497	-3.345550	-0.773431
126	1	0	-8.086410	-2.503213	0.672403
127	6	0	-3.970501	0.932184	2.467769
128	1	0	-3.498519	1.840036	2.084670
129	6	0	-2.964764	0.268862	3.428096
130	1	0	-2.047929	-0.011143	2.901237
131	1	0	-3.383349	-0.633700	3.889312
132	1	0	-2.698655	0.960227	4.237403
133	6	0	-5.241866	1.379833	3.216774
134	1	0	-5.768582	0.529422	3.665558
135	1	0	-5.941508	1.886888	2.542705
136	1	0	-4.984460	2.074833	4.025632

TS V

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.370755	0.933661	0.073367
2	6	0	-1.993765	1.074379	-0.087917
3	6	0	-1.135395	-0.044807	-0.132313
4	6	0	-1.739711	-1.321792	-0.042233
5	6	0	-3.116898	-1.452022	0.112106
6	6	0	-3.947426	-0.331261	0.175368
7	6	0	0.324066	0.100626	-0.272879
8	6	0	1.284474	-0.956224	-0.024492
9	8	0	2.604778	-0.543134	-0.147217
10	6	0	3.570056	-1.592637	-0.012622
11	8	0	1.026104	-2.118320	0.254651
12	1	0	3.418767	-2.363888	-0.773168

13	1	0	3.506023	-2.058024	0.974614
14	1	0	4.541958	-1.113924	-0.146503
15	1	0	-1.113002	-2.201782	-0.072376
16	1	0	-3.544173	-2.449436	0.183804
17	1	0	-5.021972	-0.442563	0.291965
18	1	0	-3.993698	1.824226	0.107882
19	1	0	-1.587664	2.075316	-0.193232
20	16	0	0.970484	1.801921	-0.503879
21	6	0	2.010629	2.199135	0.964290
22	1	0	1.380970	2.059616	1.847793
23	1	0	2.861275	1.519640	0.988894
24	1	0	1.334691	0.717180	-1.394837
25	1	0	2.330386	3.240177	0.871716

CP VI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.610940	-1.015754	-0.199462
2	6	0	-2.220701	-1.081197	-0.271589
3	6	0	-1.408489	0.028167	0.041311
4	6	0	-2.068880	1.222077	0.403812
5	6	0	-3.459302	1.287690	0.456627
6	6	0	-4.245460	0.171904	0.163458
7	6	0	0.069425	-0.044116	0.003895
8	6	0	0.894787	1.093793	-0.255163
9	8	0	2.283232	0.789568	-0.299350
10	6	0	3.099925	1.889255	-0.733611
11	8	0	0.546042	2.251009	-0.436939
12	1	0	3.001263	2.744116	-0.060026
13	1	0	2.814973	2.205849	-1.740231
14	1	0	4.125357	1.513014	-0.730898
15	1	0	-1.480056	2.101280	0.629646
16	1	0	-3.931532	2.225854	0.739004
17	1	0	-5.329584	0.228633	0.210364
18	1	0	-4.198122	-1.897245	-0.446234
19	1	0	-1.765045	-2.018414	-0.583604
20	16	0	0.758229	-1.621742	0.204727
21	6	0	1.654726	-2.160089	-1.318142
22	1	0	0.904464	-2.363141	-2.084407
23	1	0	2.328682	-1.363808	-1.633539

24	1	0	1.883982	-1.410336	0.975326
25	1	0	2.207544	-3.073257	-1.078359
26	8	0	3.290910	-0.668943	1.844279
27	1	0	2.995988	-0.329466	2.704113
28	1	0	3.118408	0.061346	1.212484

TS VI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.465060	0.948228	-0.402161
2	6	0	2.076881	1.062259	-0.318394
3	6	0	1.267340	-0.029459	0.047405
4	6	0	1.923505	-1.248594	0.325415
5	6	0	3.308329	-1.360812	0.231964
6	6	0	4.094746	-0.264811	-0.129663
7	6	0	-0.213058	0.069147	0.192336
8	6	0	-1.058496	-1.020571	-0.288127
9	8	0	-2.402960	-0.684891	-0.312245
10	6	0	-3.281316	-1.772427	-0.621563
11	8	0	-0.699327	-2.153832	-0.570360
12	1	0	-3.190015	-2.571854	0.119454
13	1	0	-3.060192	-2.186577	-1.609120
14	1	0	-4.288362	-1.351067	-0.601203
15	1	0	1.333681	-2.114105	0.598804
16	1	0	3.776453	-2.318034	0.449850
17	1	0	5.175565	-0.355879	-0.197260
18	1	0	4.052483	1.817008	-0.690482
19	1	0	1.620280	2.022067	-0.540803
20	16	0	-0.907302	1.740966	0.187673
21	6	0	-1.842637	2.066156	-1.356186
22	1	0	-1.133926	2.092030	-2.186992
23	1	0	-2.588570	1.287815	-1.506835
24	1	0	-1.827620	1.207867	1.457798
25	1	0	-2.314109	3.046442	-1.244300
26	8	0	-1.787827	0.360378	2.372729
27	1	0	-1.360817	0.783112	3.141044
28	1	0	-0.999220	-0.082204	1.800107

CP VII

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.043094	-1.389702	0.111769
2	6	0	2.736389	-1.110878	0.507377
3	6	0	1.982285	-0.081793	-0.094468
4	6	0	2.625090	0.682586	-1.092890
5	6	0	3.938788	0.412736	-1.469382
6	6	0	4.659620	-0.628111	-0.880681
7	6	0	0.582050	0.191646	0.288871
8	6	0	-0.063643	1.464270	0.121332
9	8	0	-1.371974	1.470494	0.612887
10	6	0	-2.036967	2.733180	0.496821
11	8	0	0.400432	2.474106	-0.391530
12	1	0	-2.102979	3.050178	-0.547942
13	1	0	-1.505042	3.507296	1.057435
14	1	0	-3.035170	2.580311	0.911989
15	1	0	2.085467	1.497488	-1.556930
16	1	0	4.400536	1.023962	-2.241553
17	1	0	5.682789	-0.835296	-1.182379
18	1	0	4.585647	-2.196250	0.599601
19	1	0	2.301995	-1.706993	1.307209
20	16	0	-0.288919	-1.113936	0.998273
21	6	0	-0.774397	-0.748508	2.746602
22	1	0	0.133961	-0.792276	3.350234
23	1	0	-1.224794	0.242842	2.786081
24	1	0	-1.556870	-0.996794	0.498095
25	1	0	-1.481271	-1.518873	3.069684
26	6	0	-4.297702	-1.804741	-1.948520
27	1	0	-4.916852	-1.304208	-2.695875
28	1	0	-4.901378	-2.558861	-1.438655
29	16	0	-3.747577	-0.621830	-0.656107
30	1	0	-3.028703	0.193877	-1.454221
31	1	0	-3.448719	-2.295051	-2.429266

TS VII

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.664465	-0.035553	1.047642
2	6	0	-2.277710	-0.115448	1.184261
3	6	0	-1.439050	-0.212637	0.062172
4	6	0	-2.047473	-0.239272	-1.207890
5	6	0	-3.431718	-0.174672	-1.342185
6	6	0	-4.251462	-0.067031	-0.216166
7	6	0	0.052478	-0.253009	0.142874
8	6	0	0.751997	-1.353845	-0.538167
9	8	0	2.106344	-1.339902	-0.298494
10	6	0	2.861906	-2.289618	-1.066489
11	8	0	0.252321	-2.137900	-1.323359
12	1	0	2.719886	-2.118441	-2.136150
13	1	0	2.555971	-3.312041	-0.828423
14	1	0	3.904252	-2.126320	-0.788730
15	1	0	-1.424649	-0.322022	-2.091536
16	1	0	-3.871686	-0.200928	-2.335953
17	1	0	-5.331265	-0.010196	-0.323830
18	1	0	-4.284668	0.040044	1.937398
19	1	0	-1.848109	-0.103840	2.182370
20	16	0	0.751104	0.451942	1.631526
21	6	0	1.771946	-0.736954	2.579775
22	1	0	1.105913	-1.473844	3.033224
23	1	0	2.493533	-1.216313	1.922012
24	1	0	1.761099	1.236952	0.814533
25	1	0	2.269694	-0.158388	3.362577
26	6	0	0.866403	3.396463	-0.683640
27	1	0	0.292509	3.600003	-1.590538
28	1	0	1.494208	4.260397	-0.454530
29	16	0	1.946051	1.929886	-0.938517
30	1	0	0.813075	0.871553	-0.733863
31	1	0	0.169321	3.236010	0.144991

CP VIII

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.366755	-1.165426	-0.831085
2	6	0	1.973688	-1.134820	-0.802779
3	6	0	1.271212	-0.154104	-0.073413
4	6	0	2.038616	0.807810	0.614839
5	6	0	3.430914	0.791166	0.564481
6	6	0	4.107954	-0.198116	-0.151470
7	6	0	-0.208071	-0.150303	-0.021282
8	6	0	-1.074984	0.975718	0.010637
9	8	0	-0.436397	2.176358	-0.096489
10	6	0	-1.282727	3.328504	-0.116696
11	8	0	-2.323532	0.949819	0.113531
12	1	0	-1.883698	3.394441	0.794789
13	1	0	-1.956558	3.309259	-0.978717
14	1	0	-0.605894	4.181773	-0.188315
15	1	0	1.531865	1.575810	1.187072
16	1	0	3.991113	1.551173	1.104226
17	1	0	5.194130	-0.212870	-0.181379
18	1	0	3.872623	-1.939432	-1.403360
19	1	0	1.418305	-1.881666	-1.364831
20	16	0	-0.980308	-1.702427	0.122061
21	6	0	-1.822284	-1.794998	1.765524
22	1	0	-1.044653	-1.878220	2.526407
23	1	0	-2.411367	-0.887283	1.897318
24	1	0	-2.155792	-1.555135	-0.610419
25	1	0	-2.458669	-2.684520	1.770940
26	8	0	-3.686067	-0.961036	-1.188635
27	1	0	-3.646362	-0.767943	-2.138500
28	1	0	-3.398583	-0.120270	-0.748000

TS VIII

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.344140	-1.088118	-0.857819
2	6	0	1.950552	-1.075486	-0.845371
3	6	0	1.226348	-0.134735	-0.085758
4	6	0	1.973651	0.800976	0.658105
5	6	0	3.366968	0.799810	0.630388
6	6	0	4.064912	-0.146036	-0.122859
7	6	0	-0.256064	-0.158661	-0.058584
8	6	0	-1.103090	0.963029	-0.023767

9	8	0	-0.463772	2.166244	-0.057232
10	6	0	-1.296392	3.327058	-0.092837
11	8	0	-2.376180	0.981318	0.036277
12	1	0	-1.937545	3.384399	0.791326
13	1	0	-1.929326	3.335810	-0.985603
14	1	0	-0.606094	4.172436	-0.115431
15	1	0	1.451218	1.535965	1.258711
16	1	0	3.910946	1.537568	1.215803
17	1	0	5.151606	-0.148430	-0.136961
18	1	0	3.866801	-1.830244	-1.456735
19	1	0	1.410550	-1.807124	-1.440850
20	16	0	-1.000550	-1.757034	0.041935
21	6	0	-1.653791	-1.900155	1.761819
22	1	0	-0.805147	-1.913306	2.447991
23	1	0	-2.301607	-1.046454	1.967585
24	1	0	-2.385079	-1.496011	-0.659644
25	1	0	-2.213059	-2.837254	1.838022
26	8	0	-3.495807	-0.930412	-1.046424
27	1	0	-3.468246	-0.823556	-2.013017
28	1	0	-3.153531	-0.014534	-0.623015

CP IX

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.510834	-1.564170	-1.089712
2	6	0	2.175989	-1.377420	-0.735153
3	6	0	1.749045	-0.220846	-0.051655
4	6	0	2.726764	0.752004	0.240668
5	6	0	4.055464	0.576276	-0.139812
6	6	0	4.461844	-0.585025	-0.800101
7	6	0	0.337692	-0.041187	0.353769
8	6	0	-0.426680	1.166370	0.393886
9	8	0	0.230607	2.257701	-0.096582
10	6	0	-0.523136	3.472825	-0.105958
11	8	0	-1.596407	1.263784	0.805867
12	1	0	-0.857319	3.738711	0.901080
13	1	0	-1.401394	3.387508	-0.753251
14	1	0	0.157381	4.232651	-0.494259
15	1	0	2.433317	1.653919	0.764845
16	1	0	4.782540	1.349398	0.097531

17	1	0	5.500842	-0.722503	-1.087143
18	1	0	3.802545	-2.471604	-1.613087
19	1	0	1.447909	-2.140035	-1.001190
20	16	0	-0.485069	-1.439738	0.946658
21	6	0	-1.001730	-1.167037	2.701956
22	1	0	-0.098969	-1.214915	3.313094
23	1	0	-1.477182	-0.188527	2.764153
24	1	0	-1.754172	-1.342612	0.430047
25	1	0	-1.692505	-1.968708	2.979324
26	6	0	-3.267037	-0.513437	-2.324236
27	1	0	-2.178417	-0.427587	-2.343187
28	1	0	-3.716811	0.360523	-2.800174
29	16	0	-3.887702	-0.709641	-0.604758
30	1	0	-3.286066	0.390435	-0.090049
31	1	0	-3.565245	-1.408574	-2.874329

TS IX

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.477539	-1.484313	-1.062629
2	6	0	2.121017	-1.302200	-0.799038
3	6	0	1.657810	-0.203786	-0.049007
4	6	0	2.620728	0.711127	0.420252
5	6	0	3.975111	0.538827	0.140456
6	6	0	4.415145	-0.561093	-0.598224
7	6	0	0.212639	-0.046048	0.251793
8	6	0	-0.496629	1.160300	0.261915
9	8	0	0.227931	2.265683	-0.051145
10	6	0	-0.489852	3.500518	-0.147125
11	8	0	-1.736888	1.341138	0.546039
12	1	0	-0.952462	3.765279	0.807401
13	1	0	-1.268054	3.448064	-0.914041
14	1	0	0.260740	4.242877	-0.423661
15	1	0	2.298497	1.564292	1.005479
16	1	0	4.692976	1.264070	0.516228
17	1	0	5.472661	-0.696292	-0.808871
18	1	0	3.799216	-2.344486	-1.644671
19	1	0	1.405151	-2.022859	-1.186514
20	16	0	-0.622025	-1.518909	0.759724
21	6	0	-1.082343	-1.252969	2.521631

22	1	0	-0.164937	-1.229340	3.112109
23	1	0	-1.622464	-0.308845	2.609322
24	1	0	-2.054145	-1.338764	0.189781
25	1	0	-1.710660	-2.091049	2.836272
26	6	0	-3.022370	-0.623470	-2.199456
27	1	0	-1.932176	-0.596953	-2.274598
28	1	0	-3.439240	0.249390	-2.706452
29	16	0	-3.564580	-0.629701	-0.440517
30	1	0	-2.663862	0.524113	0.056181
31	1	0	-3.396679	-1.527670	-2.683828

TS X

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.545426	-0.547861	-0.373344
2	6	0	0.425235	0.352303	-0.668520
3	6	0	-0.961070	-0.036064	-0.316571
4	6	0	-1.998642	0.912052	-0.239195
5	6	0	-1.306996	-1.389047	-0.119731
6	6	0	-3.312336	0.526401	0.022145
7	1	0	-1.765692	1.960521	-0.398162
8	6	0	-2.618485	-1.771333	0.151857
9	1	0	-0.540639	-2.158155	-0.180898
10	6	0	-3.634396	-0.816356	0.225176
11	1	0	-4.089377	1.285571	0.071266
12	1	0	-2.847161	-2.823799	0.302129
13	1	0	-4.658094	-1.114348	0.434343
14	16	0	0.978997	2.044863	-0.389518
15	6	0	0.868732	2.263667	1.437302
16	1	0	-0.154909	2.098470	1.783189
17	1	0	1.548401	1.586372	1.961834
18	1	0	1.159803	3.297199	1.649432
19	8	0	2.301252	-0.670567	-1.404340
20	1	0	1.431309	-0.000087	-1.892214
21	8	0	1.797996	-1.173817	0.744670
22	6	0	2.955968	-2.048151	0.778292
23	1	0	3.867067	-1.451430	0.702776
24	1	0	2.902752	-2.557039	1.739932
25	1	0	2.907994	-2.759666	-0.048453

CP XI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.055691	0.992452	0.019672
2	6	0	-0.288090	-0.140447	-0.067205
3	6	0	1.199637	-0.103474	-0.113544
4	6	0	1.908049	-0.921415	-1.013207
5	6	0	1.949479	0.710953	0.755313
6	6	0	3.300974	-0.915517	-1.053732
7	1	0	1.354216	-1.569575	-1.685878
8	6	0	3.343280	0.721237	0.710594
9	1	0	1.432113	1.342448	1.469005
10	6	0	4.028897	-0.091155	-0.193413
11	1	0	3.818855	-1.554770	-1.764716
12	1	0	3.894987	1.361042	1.395273
13	1	0	5.115313	-0.085723	-0.224430
14	16	0	-1.057819	-1.747869	-0.126271
15	6	0	-0.847762	-2.352083	1.597663
16	1	0	0.212426	-2.338802	1.861607
17	1	0	-1.415755	-1.737773	2.300229
18	1	0	-1.215041	-3.382287	1.627851
19	8	0	-2.383613	1.107977	0.065157
20	1	0	-2.899900	0.283614	-0.137806
21	8	0	-0.437678	2.191445	0.073118
22	6	0	-1.226225	3.376851	-0.076751
23	1	0	-1.943833	3.484464	0.740998
24	1	0	-0.505708	4.196004	-0.054243
25	1	0	-1.764502	3.379274	-1.029563
26	8	0	-4.100686	-0.885822	-0.611005
27	1	0	-3.416538	-1.579568	-0.520495
28	1	0	-4.241003	-0.805663	-1.567992

TS XI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.429457	0.676149	-0.020585
2	6	0	-0.444088	-0.356436	-0.224456
3	6	0	1.021046	-0.030319	-0.213756

4	6	0	1.840731	-0.555717	-1.227104
5	6	0	1.636087	0.737804	0.790073
6	6	0	3.214831	-0.324480	-1.243215
7	1	0	1.386934	-1.158382	-2.010052
8	6	0	3.011716	0.977511	0.773447
9	1	0	1.030588	1.163467	1.583409
10	6	0	3.807816	0.447469	-0.241652
11	1	0	3.822319	-0.742352	-2.042133
12	1	0	3.460841	1.578670	1.560388
13	1	0	4.878637	0.633363	-0.253481
14	16	0	-0.859311	-1.972894	0.510294
15	6	0	-0.571339	-1.721764	2.302610
16	1	0	0.450270	-1.373351	2.477272
17	1	0	-1.288969	-1.012985	2.725633
18	1	0	-0.703180	-2.695976	2.783252
19	8	0	-2.670722	0.513189	-0.276372
20	1	0	-2.680221	-0.332650	-1.207135
21	8	0	-1.014443	1.898743	0.316130
22	6	0	-1.973165	2.970909	0.224040
23	1	0	-2.782911	2.823449	0.942150
24	1	0	-1.410461	3.874484	0.459310
25	1	0	-2.390580	3.027061	-0.783960
26	8	0	-2.202920	-0.968980	-2.094263
27	1	0	-2.403012	-1.904988	-1.917034
28	1	0	-1.201669	-0.783872	-1.562702

CP XII

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101740	1.255442	0.091649
2	6	0	0.472042	0.015083	0.023315
3	6	0	1.928936	-0.223532	-0.118443
4	6	0	2.407533	-1.298693	-0.891400
5	6	0	2.881864	0.583333	0.533837
6	6	0	3.772808	-1.546280	-1.020074
7	1	0	1.694858	-1.943601	-1.396291
8	6	0	4.247366	0.337361	0.399199
9	1	0	2.546859	1.408796	1.151122
10	6	0	4.704018	-0.727996	-0.378132
11	1	0	4.109312	-2.381580	-1.629554

12	1	0	4.957783	0.978184	0.916141
13	1	0	5.768920	-0.920897	-0.477959
14	16	0	-0.642481	-1.378279	0.073519
15	6	0	-0.370121	-2.030358	1.770987
16	1	0	0.686377	-2.273631	1.907245
17	1	0	-0.686135	-1.306263	2.525819
18	1	0	-0.965440	-2.943270	1.866597
19	8	0	-1.412911	1.511831	0.232772
20	1	0	-1.913306	0.665996	0.254187
21	8	0	0.644407	2.371171	0.006638
22	6	0	-0.021784	3.632719	-0.127286
23	1	0	-0.640028	3.850168	0.747798
24	1	0	0.781352	4.366177	-0.211550
25	1	0	-0.645951	3.656904	-1.025675
26	6	0	-4.594711	-1.622928	-0.514073
27	1	0	-3.633809	-1.971021	-0.898044
28	1	0	-5.403819	-1.890001	-1.197156
29	16	0	-4.563466	0.185614	-0.200754
30	1	0	-4.390003	0.573859	-1.482474
31	1	0	-4.781069	-2.096107	0.452797

TS XII

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.652422	1.386407	-0.052416
2	6	0	-0.152670	0.079958	0.228689
3	6	0	1.262483	-0.275303	-0.126786
4	6	0	1.498622	-1.473886	-0.819074
5	6	0	2.365624	0.514040	0.235752
6	6	0	2.795116	-1.869690	-1.142381
7	1	0	0.653983	-2.094108	-1.105877
8	6	0	3.664383	0.118601	-0.090156
9	1	0	2.207563	1.449178	0.763655
10	6	0	3.884109	-1.074201	-0.778998
11	1	0	2.954690	-2.799048	-1.682781
12	1	0	4.504657	0.745441	0.197469
13	1	0	4.895331	-1.381867	-1.031688
14	16	0	-0.781796	-0.663545	1.783399
15	6	0	0.228844	0.190858	3.046020
16	1	0	1.295363	0.053674	2.849003

17	1	0	-0.010118	1.256974	3.102042
18	1	0	-0.017731	-0.278946	4.002932
19	8	0	-1.929699	1.650857	-0.027388
20	1	0	-2.454192	0.774870	-0.245489
21	8	0	0.141235	2.334101	-0.516869
22	6	0	-0.459815	3.506120	-1.116963
23	1	0	-1.007738	4.077038	-0.364565
24	1	0	0.380615	4.082071	-1.502294
25	1	0	-1.134953	3.215472	-1.924085
26	6	0	-3.226015	-2.276660	-0.238746
27	1	0	-3.341286	-1.929480	0.789936
28	1	0	-2.554704	-3.139072	-0.253399
29	16	0	-2.593657	-0.942755	-1.340149
30	1	0	-1.102725	-0.580443	-0.584872
31	1	0	-4.203350	-2.588087	-0.617573

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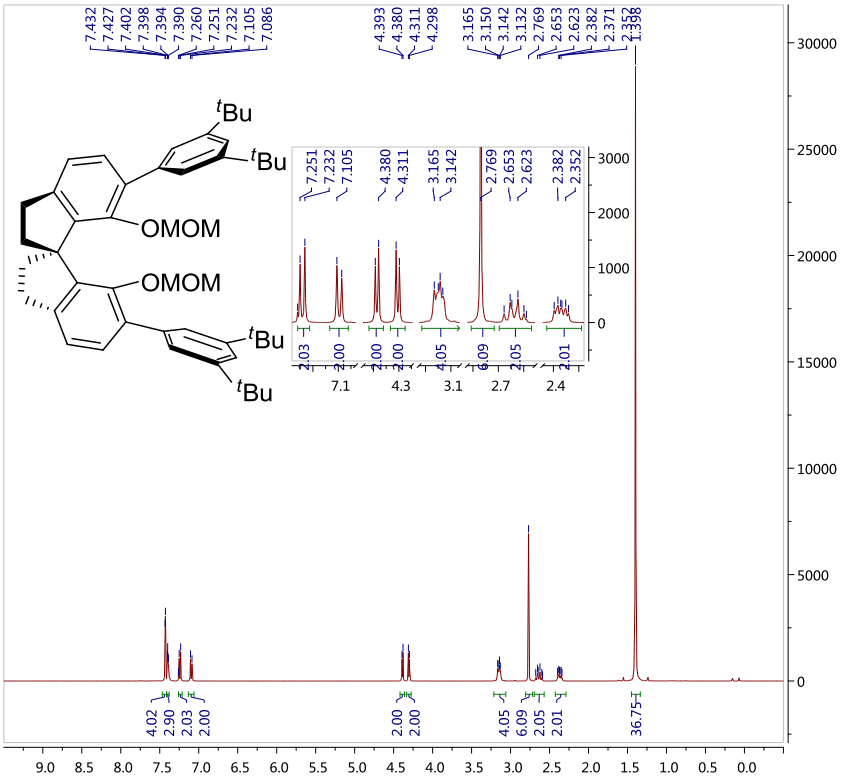
10. NMR Spectra for New Compounds

(*R*)-7,7'-Bis(methoxymethoxy)-6,6'-bis(3,5-*tert*-butylphenyl)-1,1'-spirobiindane



Parameters		
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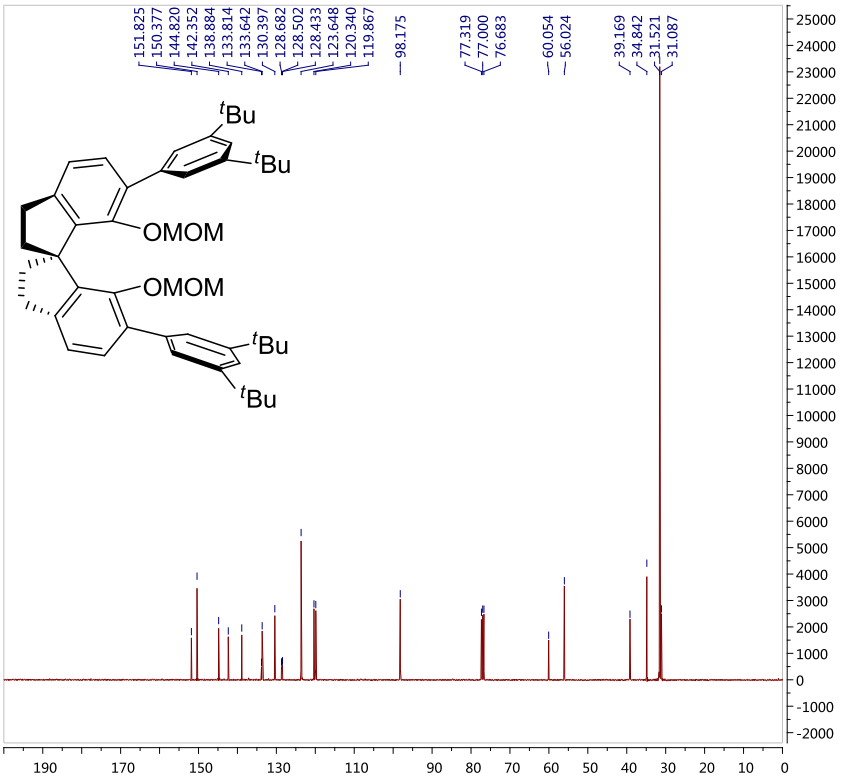
1	Data File Name	Z:/ Data/ NMR/ 2011年/ 2011-5/ xb-13-46-pure-3/ 1/ fid
2	Title	xb-13-46-pure-3
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	294.4
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	20
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2011-05-14T16:06:00
14	Modification Date	2011-05-14T16:06:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H



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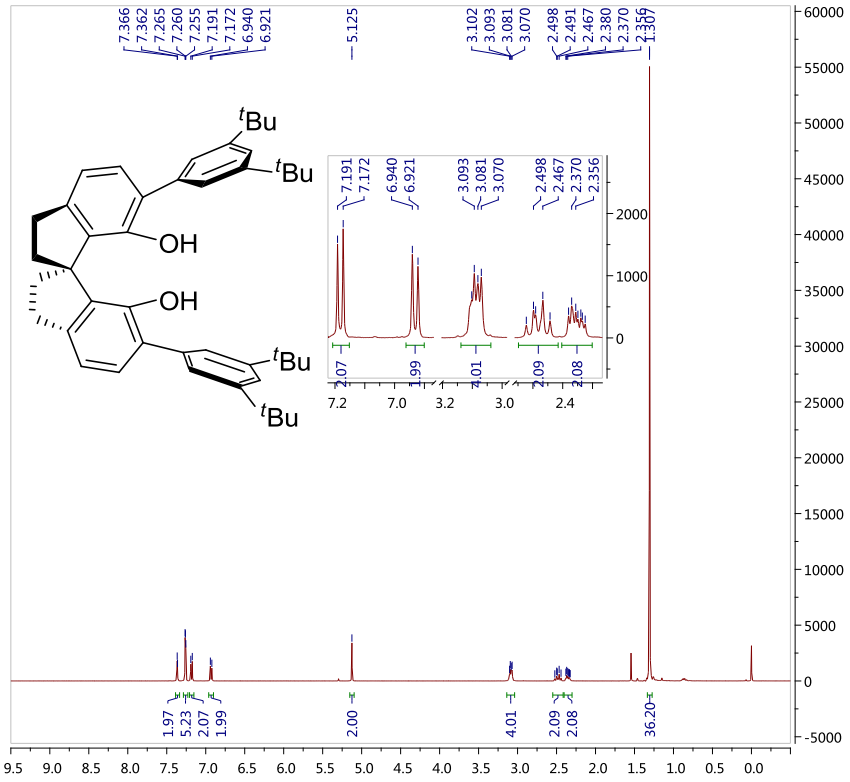
1	Data File Name	Z:/ Data/ NMR/ 2011年/ 2011-5/ xb-13-46-pure-3/ 2/ fid
2	Title	xb-13-46-pure-3
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	295.5
7	Pulse Sequence	zgpg30
8	Number of Scans	329
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2011-05-14T16:12:00
14	Modification Date	2011-05-14T16:15:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(*R*)-6,6'-Bis(3,5-di-*tert*-butylphenyl)-1,1'-spirobiindane-7,7'-diol



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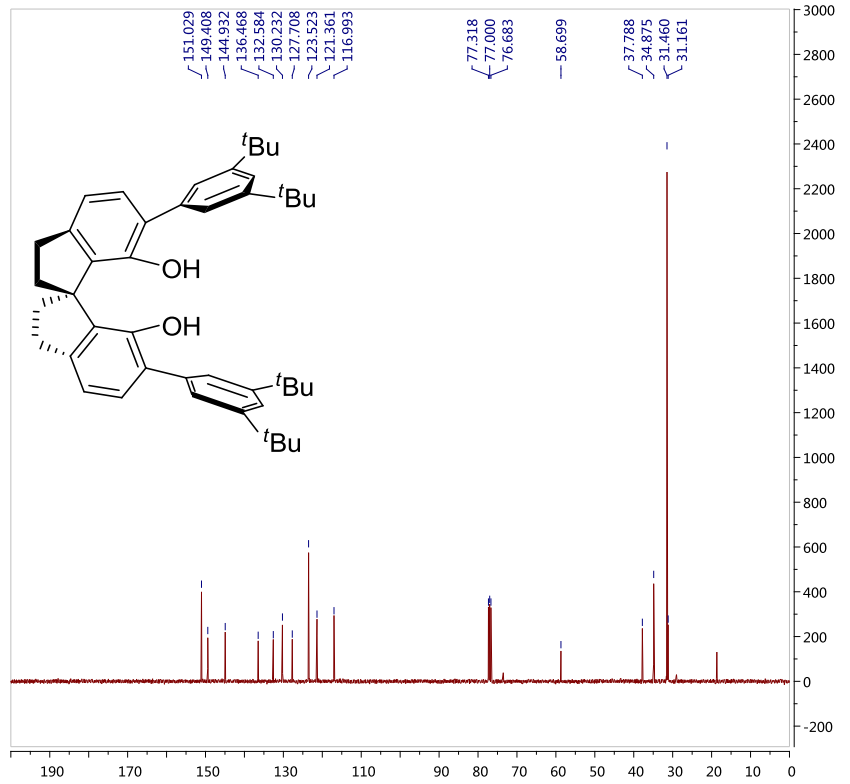
2	Title	xb-13-48-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	290.0
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	1.9923
13	Acquisition Date	2011-05-16T16:12:00
14	Modification Date	2011-05-16T16:12:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1652.8
18	Nucleus	1H



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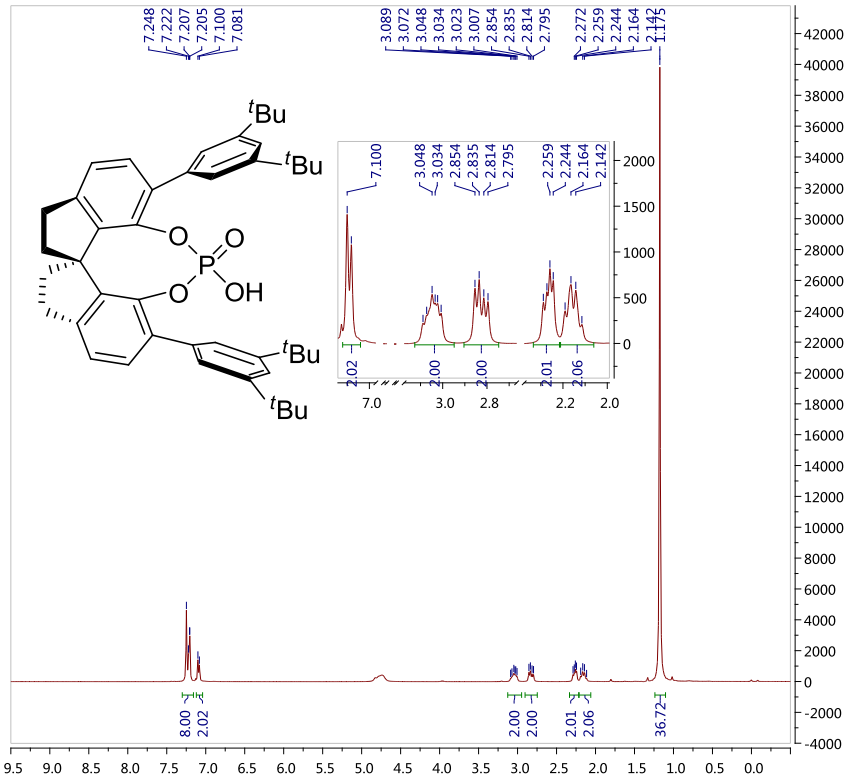
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-4/ xb-13-48-A(20120417)/ 2/ fid
2	Title	xb-13-48-A(20120417)
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	290.8
7	Pulse Sequence	zgpg30
8	Number of Scans	52
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-04-17T19:25:00
14	Modification Date	2012-04-17T19:25:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(*R*)-6,6'-Bis(3,5-di-*tert*-butylphenyl)-1,1'-spirobiindanyl-7,7'-diyl-hydrogenphosphate



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1	Data File Name	Z:/ Data/ NMR/ 2011年/ 2011-5/ xb-14-4-final/ 1/ fid
2	Title	xb-14-4-final
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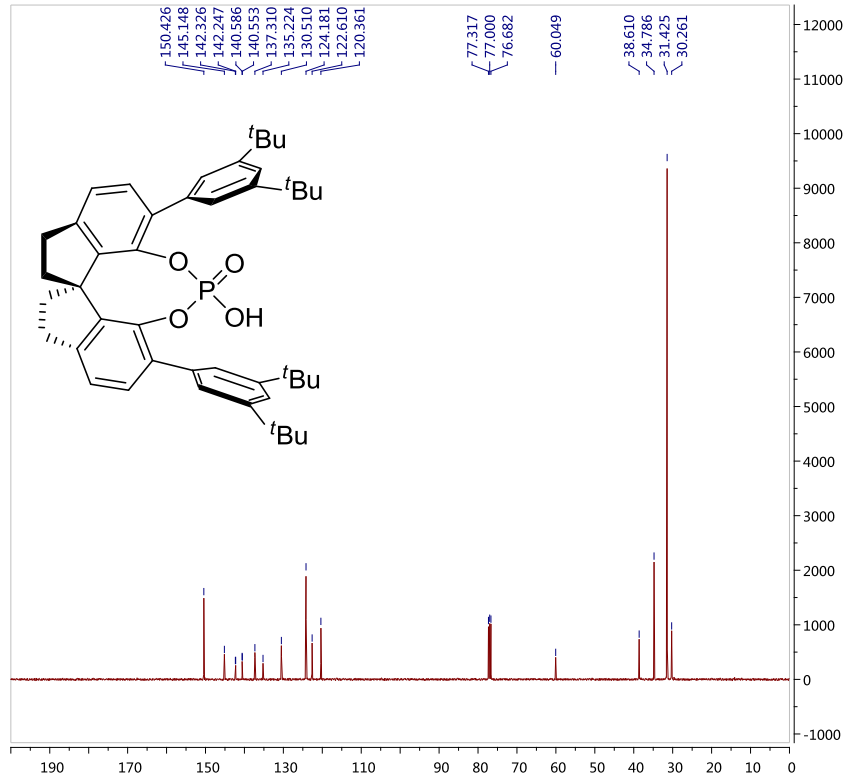
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	291.0
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	32
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	1.9923
13	Acquisition Date	2011-05-30T13:59:00
14	Modification Date	2011-05-30T13:59:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1704.7
18	Nucleus	1H



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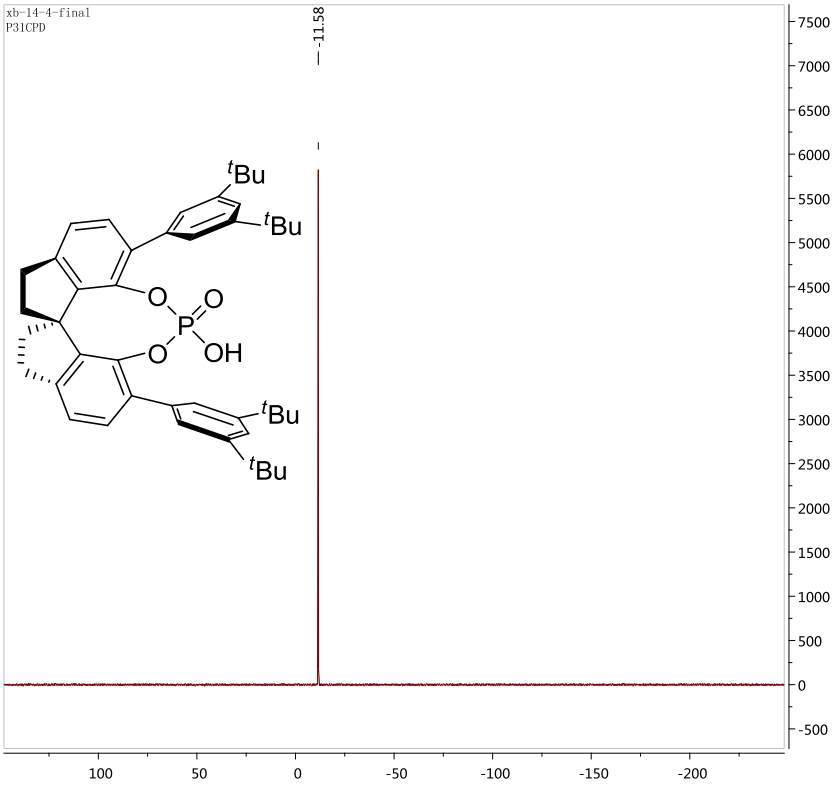
2	Title	xb-14-4-final
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	291.3
7	Pulse Sequence	zgpg30
8	Number of Scans	258
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2011-05-30T14:03:00
14	Modification Date	2011-05-30T14:10:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C



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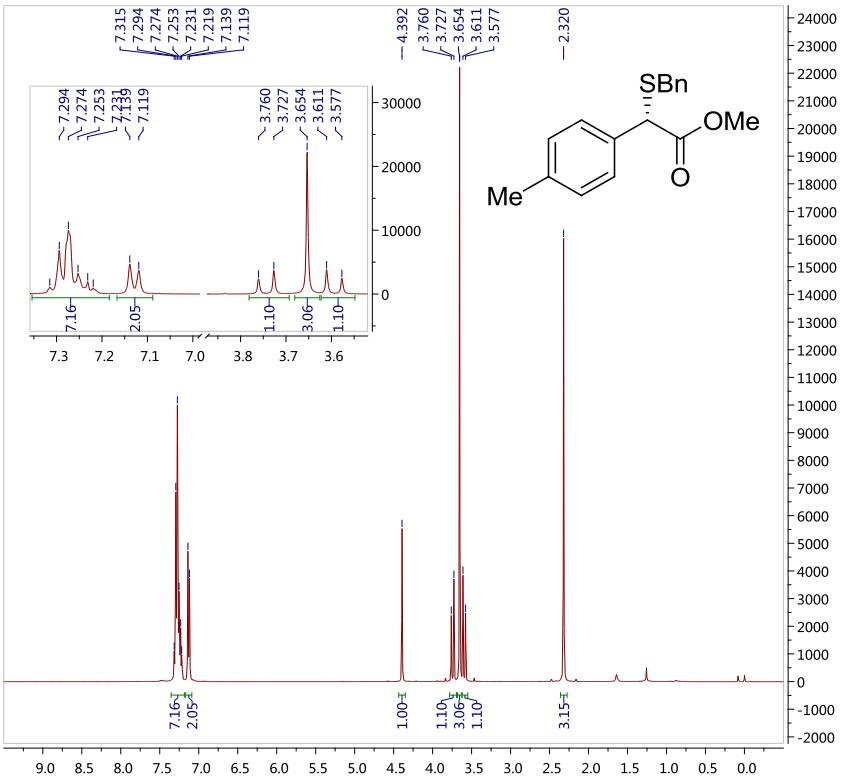
2	Title	xb-14-4-final
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	291.1
7	Pulse Sequence	zgpg30
8	Number of Scans	27
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Time	0.2556
13	Acquisition Date	2011-05-30T14:01:00
14	Modification Date	2011-05-30T14:01:00
15	Spectrometer Frequency	161.98
16	Spectral Width	64102.6
17	Lowest Frequency	-40150.1
18	Nucleus	31P

(*S*)-Methyl 2-(benzylthio)-2-*p*-tolylacetate (4ca)



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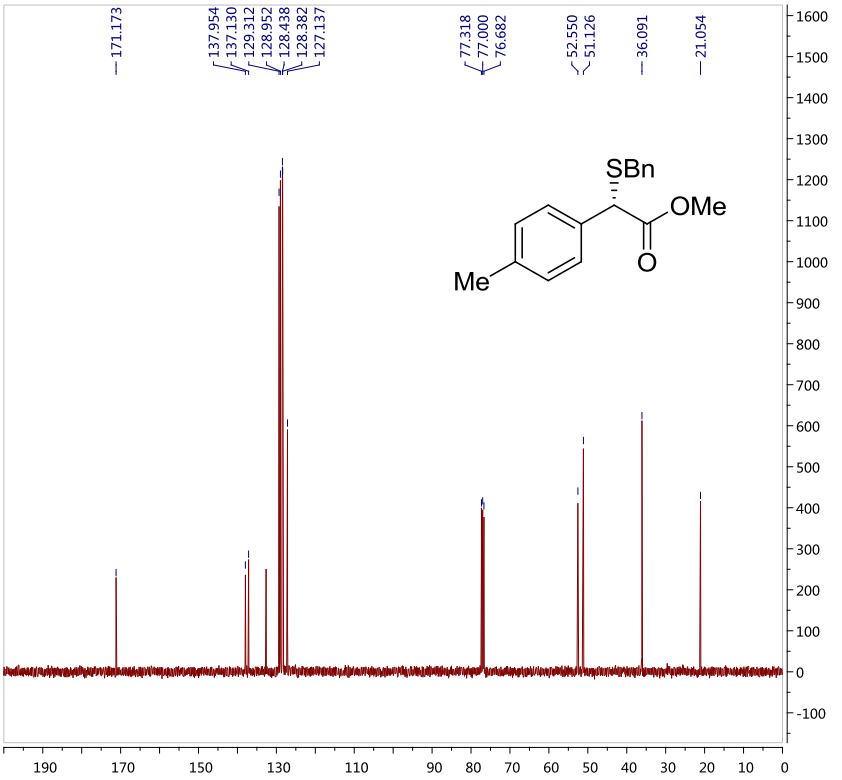
2	Title	xb-18-47-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.9
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	57
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	1.9923
13	Acquisition Date	2012-07-25T16:36:00
14	Modification Date	2012-07-25T16:36:00
15	Spectrometer Frequency	400.23
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.3
18	Nucleus	1H



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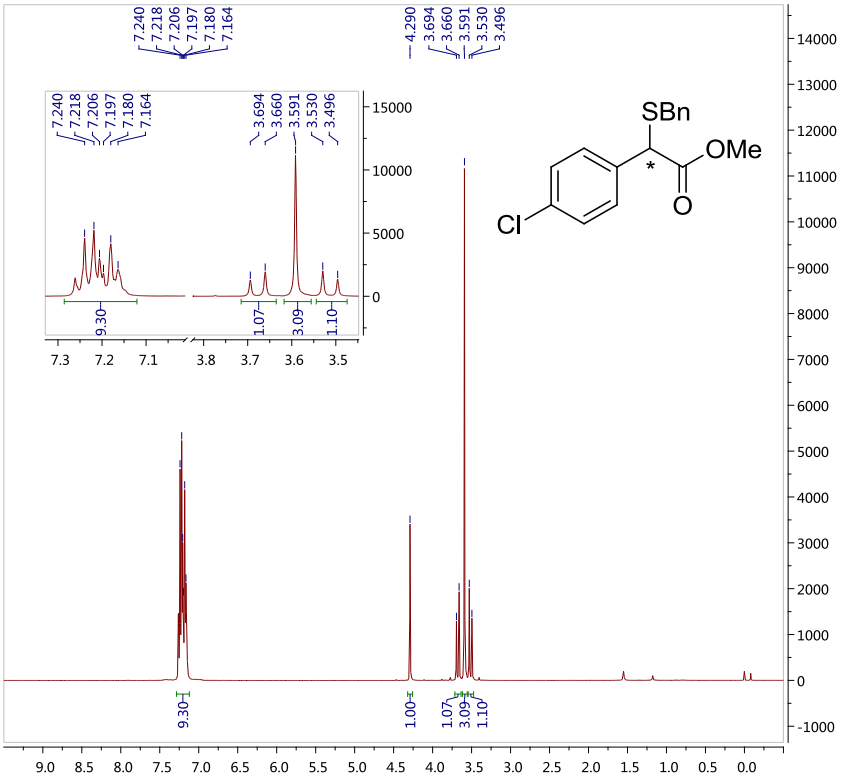
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-47-A/ 2/ fid
2	Title	xb-18-47-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.1
7	Pulse Sequence	zgpg30
8	Number of Scans	90
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-25T16:38:00
14	Modification Date	2012-07-25T16:40:00
15	Spectrometer Frequency	100.64
16	Spectral Width	29761.9
17	Lowest Frequency	-4817.6
18	Nucleus	13C

(+)-Methyl 2-(benzylthio)-2-(4-chlorophenyl)acetate (4da)



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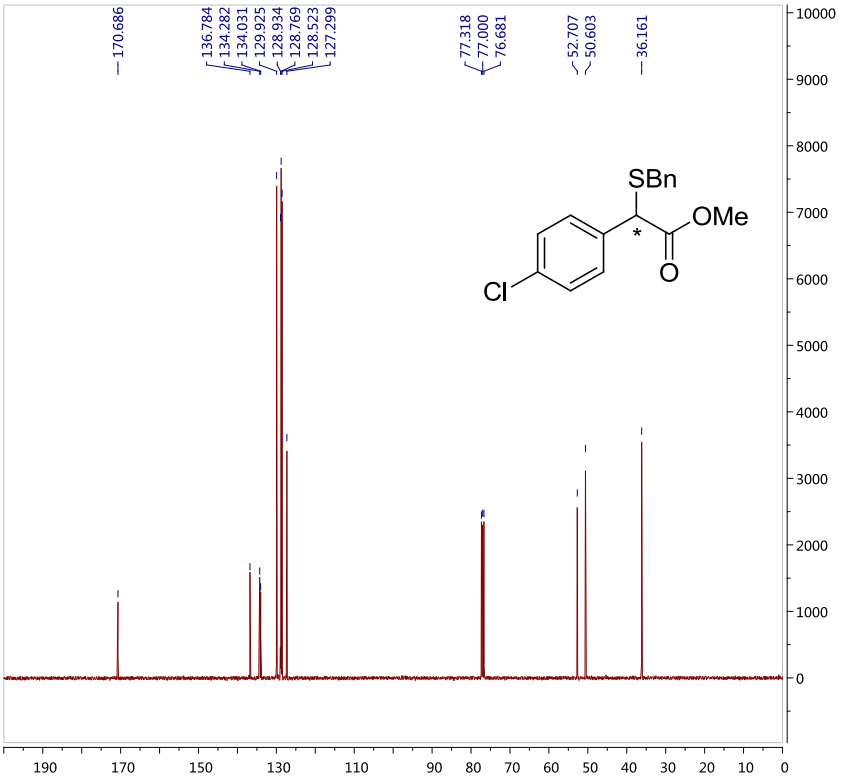
2	Title	xb-18-28-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.8
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	45
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-07-01T19:16:00
14	Modification Date	2012-07-01T19:16:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1692.3
18	Nucleus	1H



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2	Title	xb-18-28-A
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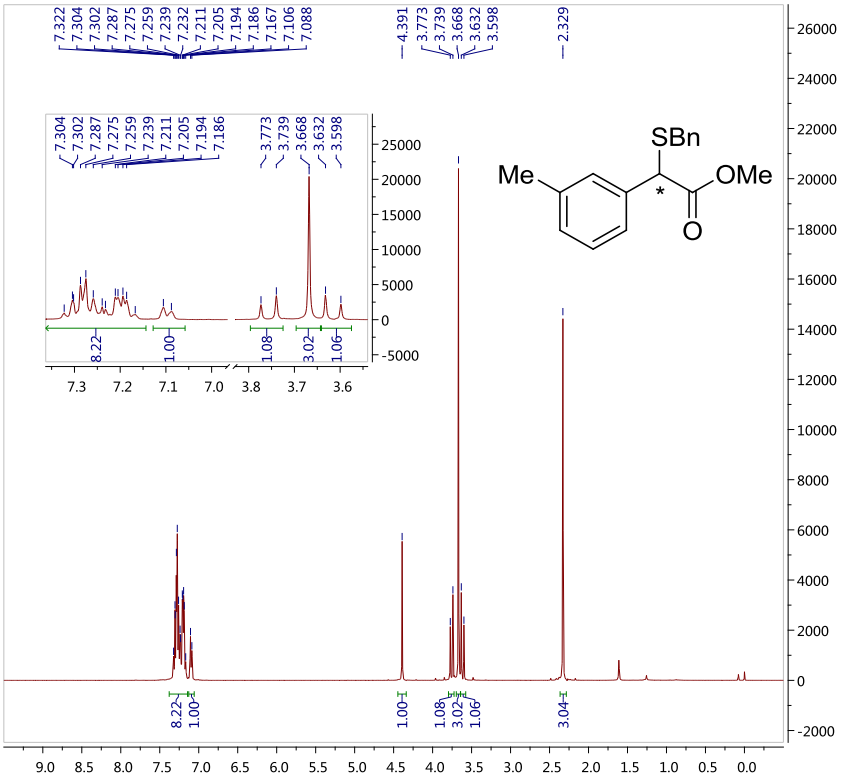
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.3
7	Pulse Sequence	zgpg30
8	Number of Scans	497
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-01T19:18:00
14	Modification Date	2012-07-01T19:30:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-Methyl 2-(benzylthio)-2-*m*-tolylacetate (4fa)



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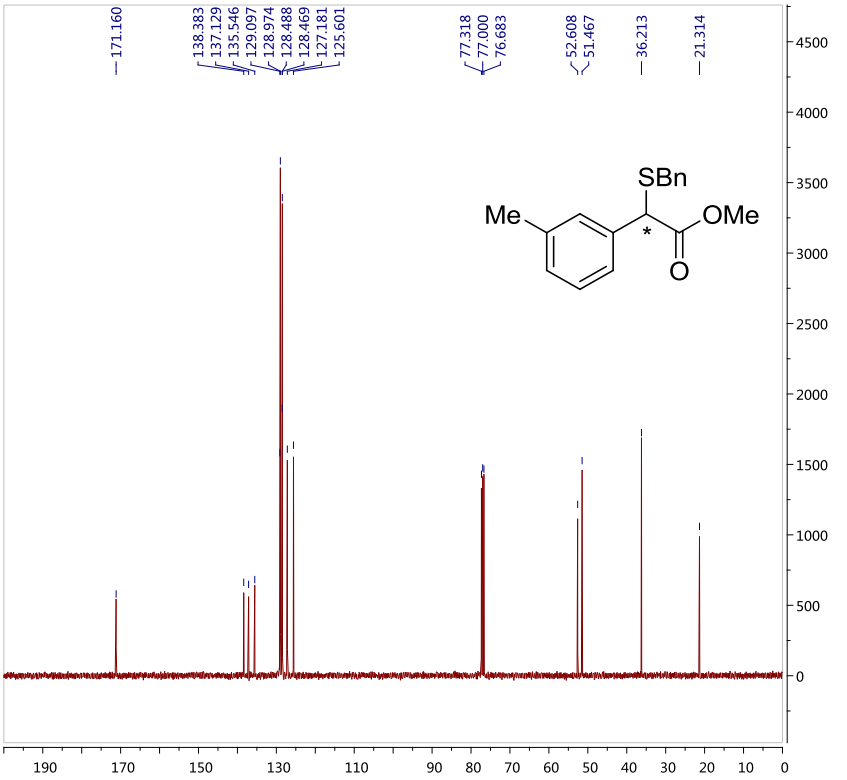
2	Title	xb-18-47-C
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.0
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	72
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	1.9923
13	Acquisition Date	2012-07-25T16:44:00
14	Modification Date	2012-07-25T16:44:00
15	Spectrometer Frequency	400.23
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.3
18	Nucleus	1H



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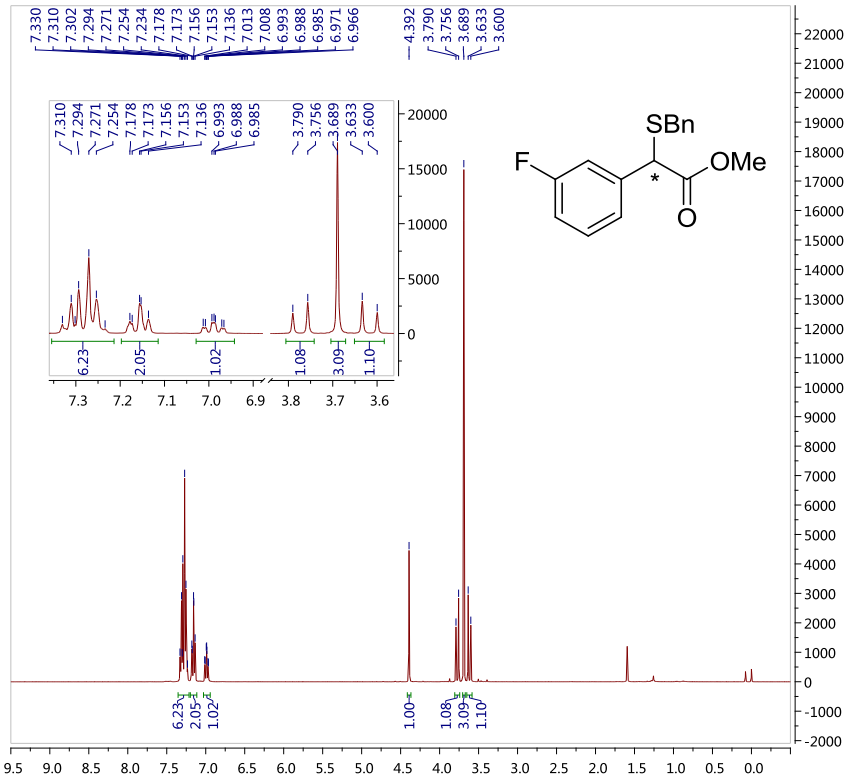
2	Title	xb-18-47-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.3
7	Pulse Sequence	zgpg30
8	Number of Scans	329
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-25T16:46:00
14	Modification Date	2012-07-25T16:54:00
15	Spectrometer Frequency	100.64
16	Spectral Width	29761.9
17	Lowest Frequency	-4817.6
18	Nucleus	13C

(+)-Methyl 2-(benzylthio)-2-(3-fluorophenyl)acetate (4ga)



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2	Title	xb-18-50-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	298.1
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	90
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
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14	Modification Date	2012-07-26T18:42:00
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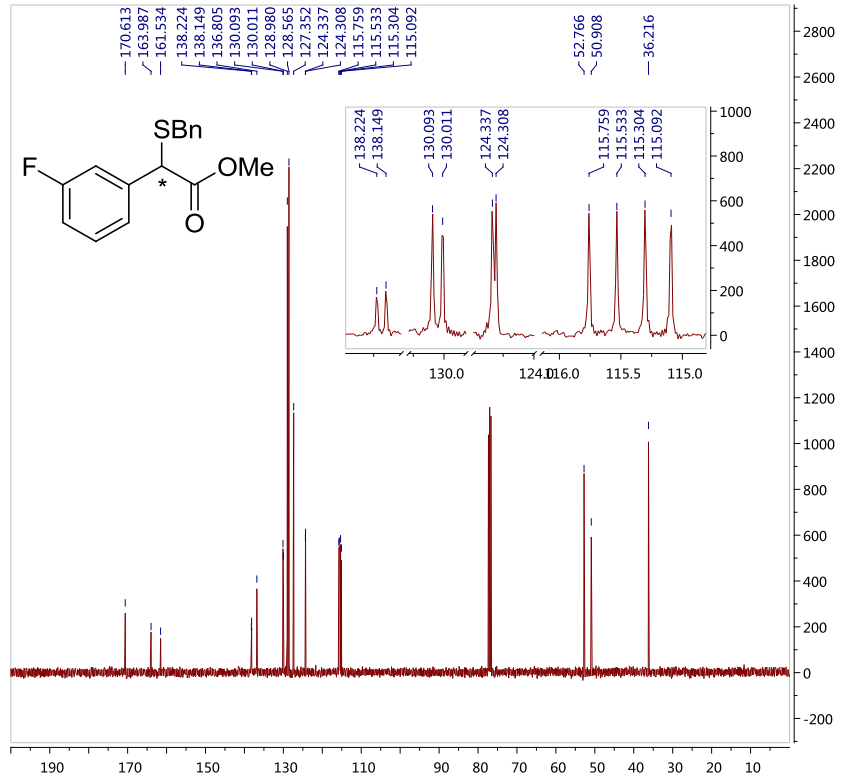
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H



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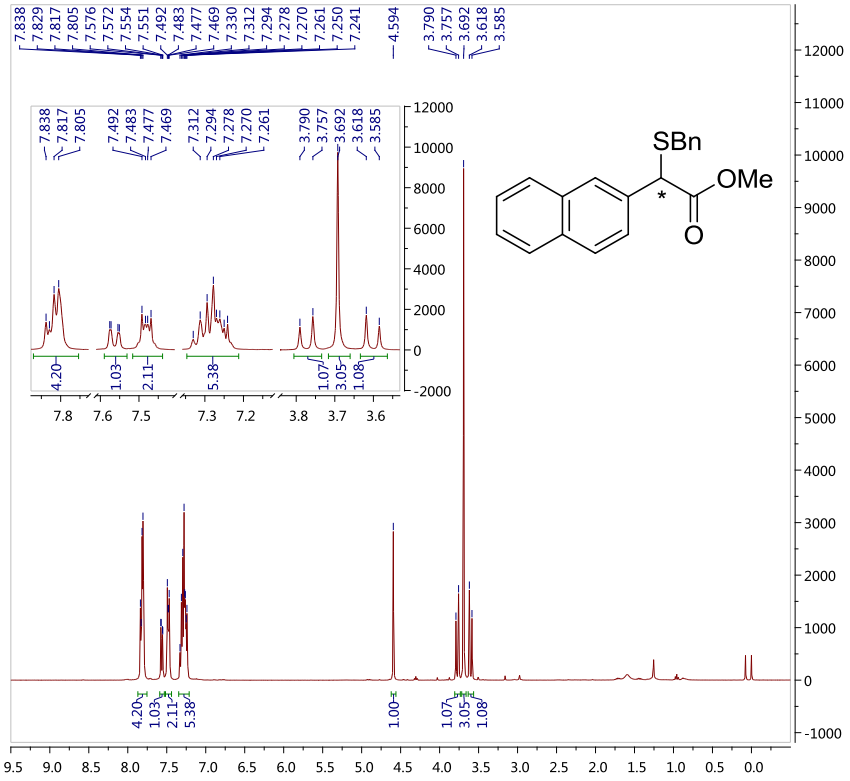
2	Title	xb-18-50-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	298.4
7	Pulse Sequence	zgpg30
8	Number of Scans	175
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2012-07-26T18:44:00
14	Modification Date	2012-07-26T18:47:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(+)-Methyl 2-(benzylthio)-2-(naphthalen-2-yl)acetate (4ia)



Parameters		
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2	Title	xb-18-39-B
3	Comment	PROTON
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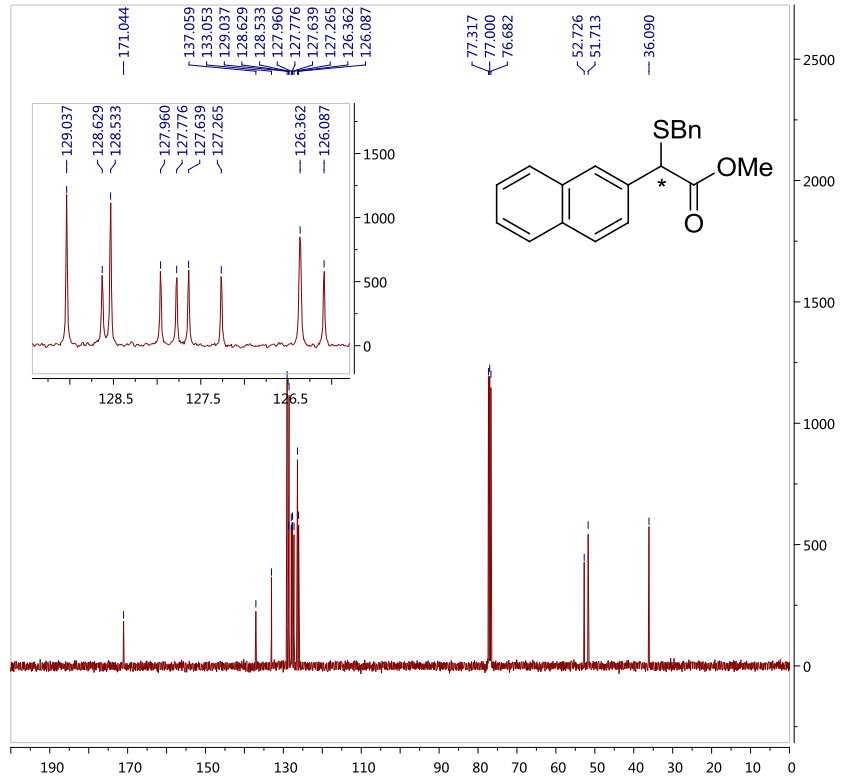
5	Solvent	CDCl3
6	Temperature	292.6
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	144
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-07-13T16:00:00
14	Modification Date	2012-07-13T16:00:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1658.4
18	Nucleus	1H



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2	Title	xb-18-39-B
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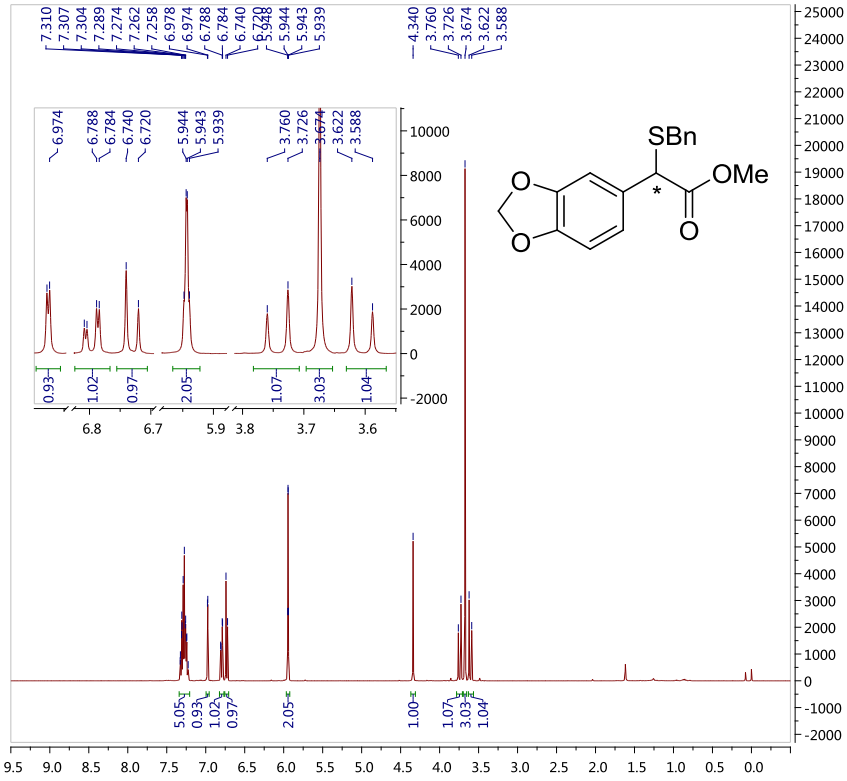
5	Solvent	CDCl3
6	Temperature	293.2
7	Pulse Sequence	zgpg30
8	Number of Scans	269
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-13T16:02:00
14	Modification Date	2012-07-13T16:09:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-Methyl 2-(benzo[d][1,3]dioxol-5-yl)-2-(benzylthio)acetate (4ja)



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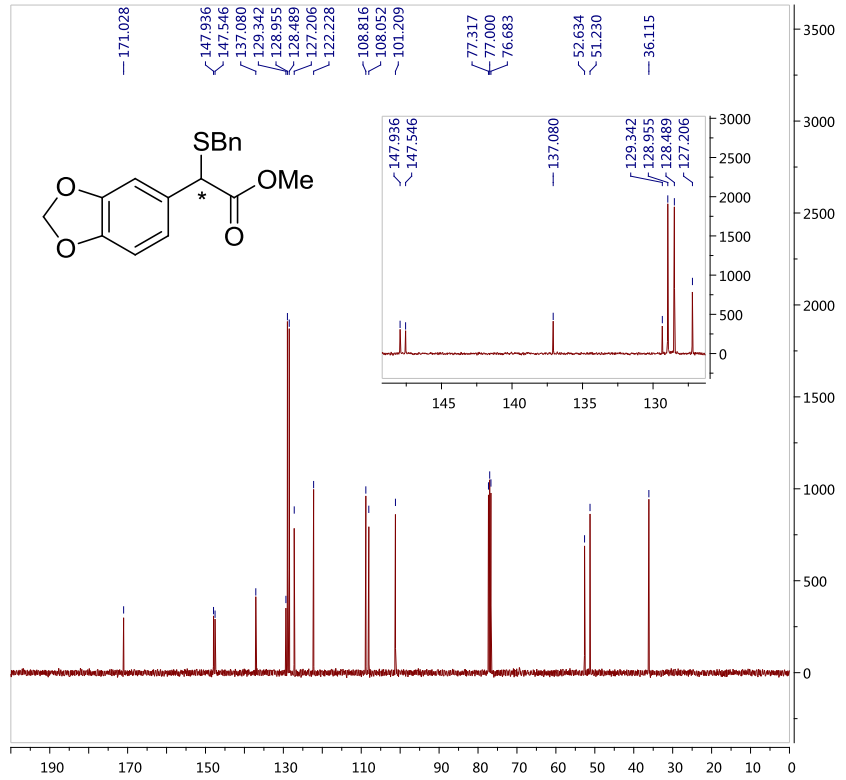
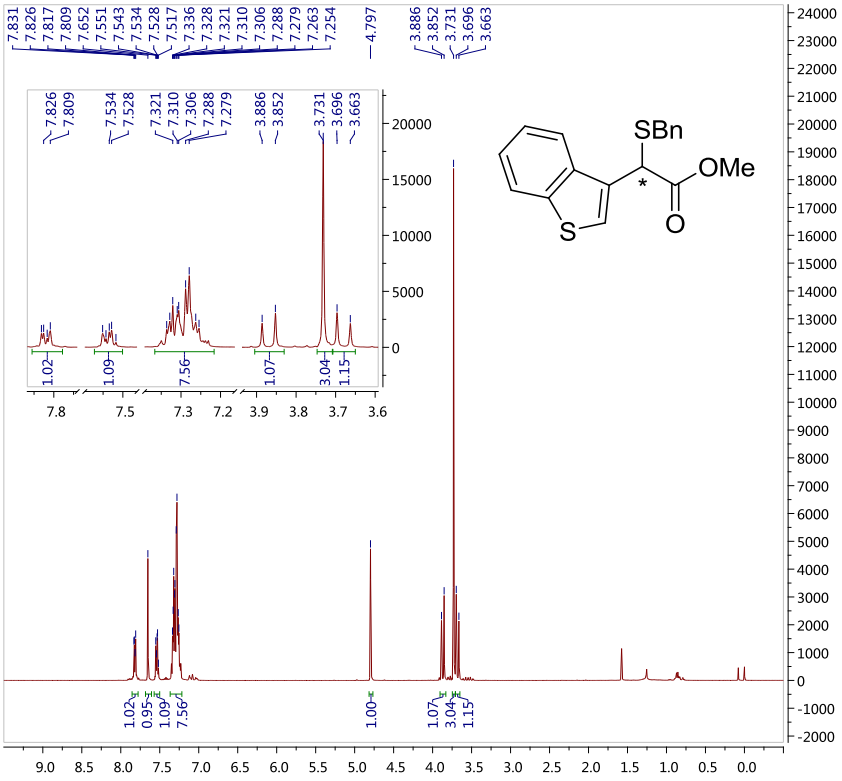
2	Title	xb-18-40-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	297.7
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	72
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2012-07-14T17:48:00
14	Modification Date	2012-07-14T17:48:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H

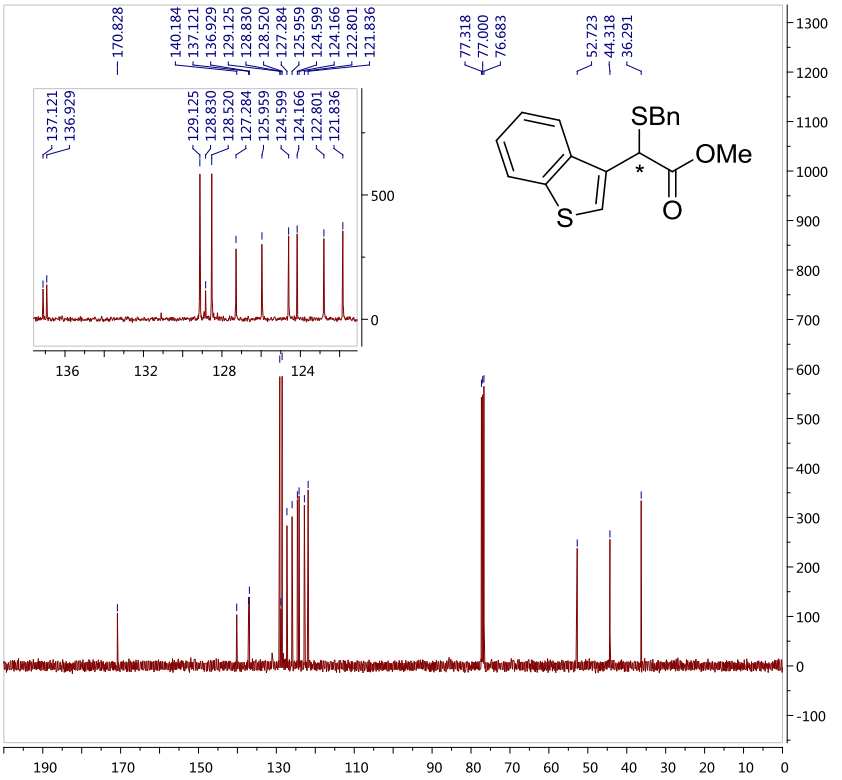


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-40-A/ 2/ fid
2	Title	xb-18-40-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	298.0
7	Pulse Sequence	zgpg30
8	Number of Scans	146
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2012-07-14T17:50:00
14	Modification Date	2012-07-14T17:53:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(+)-methyl 2-(benzo[b]thiophen-3-yl)-2-(benzylthio)acetate (4ka)

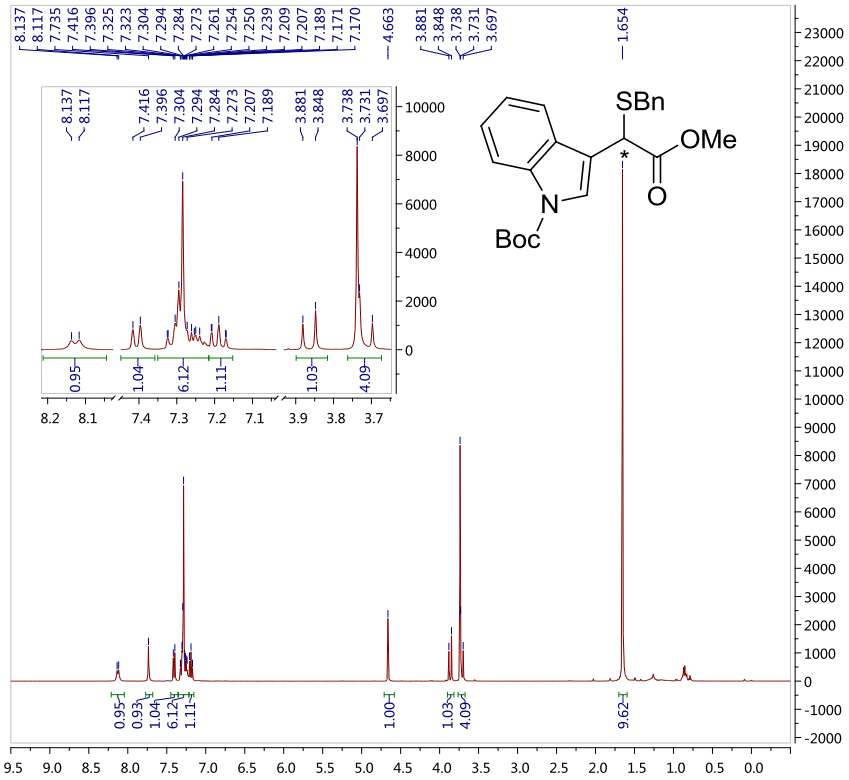


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ xb-19-13-D-rac/ 1/ fid
2	Title	xb-19-13-D-rac
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.0
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	114
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-08-28T16:11:00
14	Modification Date	2012-08-28T16:11:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1662.6
18	Nucleus	1H

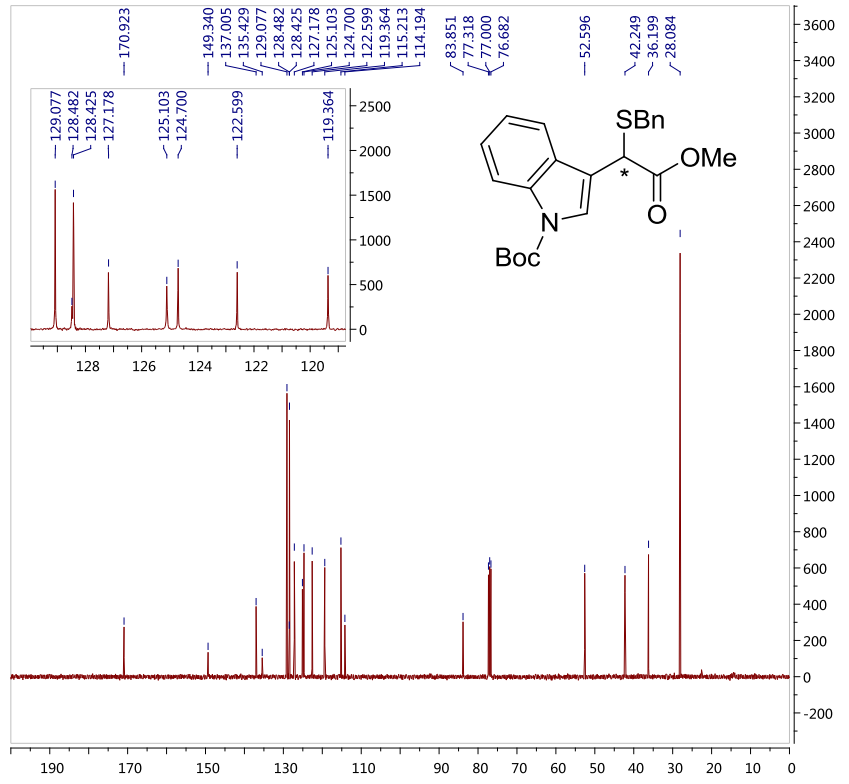


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ xb-19-13-D-rac/ 2/ fid
2	Title	xb-19-13-D-rac
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.3
7	Pulse Sequence	zgpg30
8	Number of Scans	84
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-08-28T16:13:00
14	Modification Date	2012-08-28T16:15:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-*tert*-Butyl 3-(1-(benzylthio)-2-methoxy-2-oxoethyl)-1H-indole-1-carboxylate (4la)

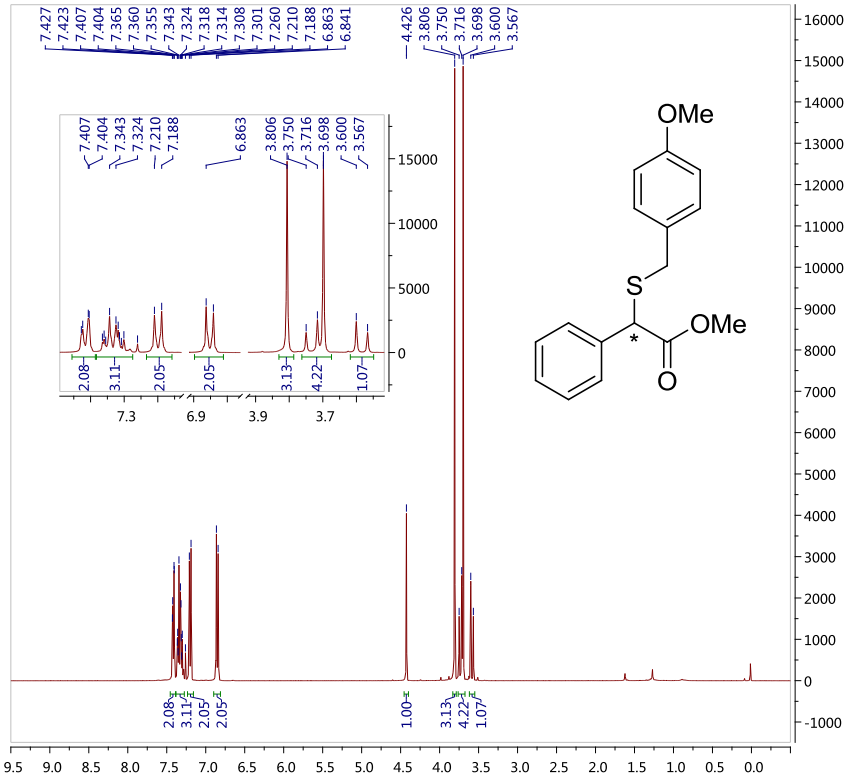


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ xb-19-7-A/ 1/ fid
2	Title	xb-19-7-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.8
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	36
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-08-21T12:19:00
14	Modification Date	2012-08-21T12:19:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1701.6
18	Nucleus	1H

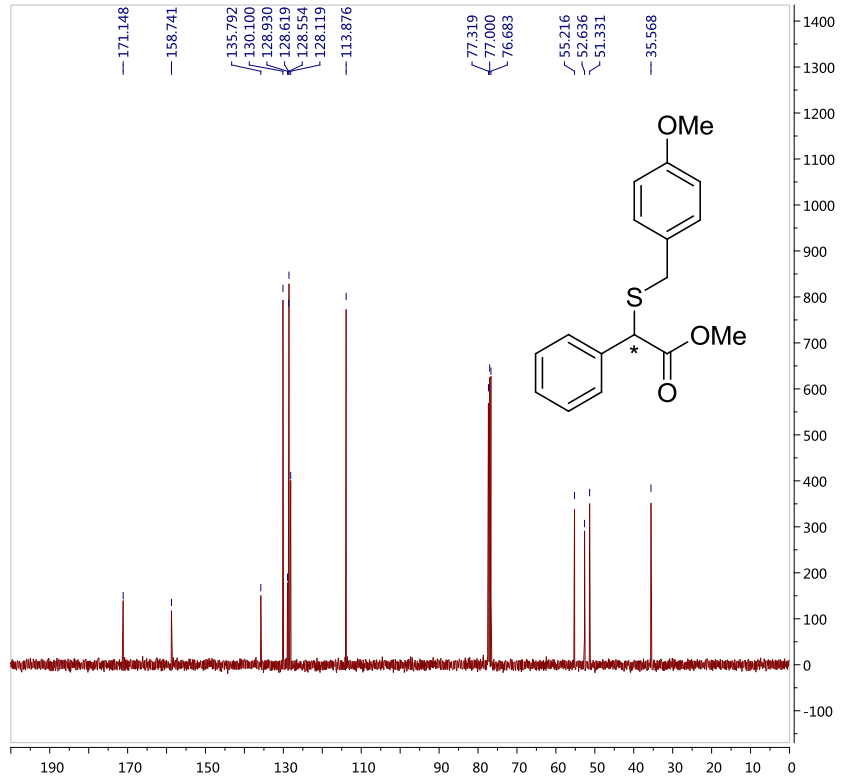


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ xb-19-7-A/ 2/ fid
2	Title	xb-19-7-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	294.0
7	Pulse Sequence	zgpg30
8	Number of Scans	115
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-08-21T12:21:00
14	Modification Date	2012-08-21T12:23:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-Methyl 2-(4-methoxybenzylthio)-2-phenylacetate (4ab)

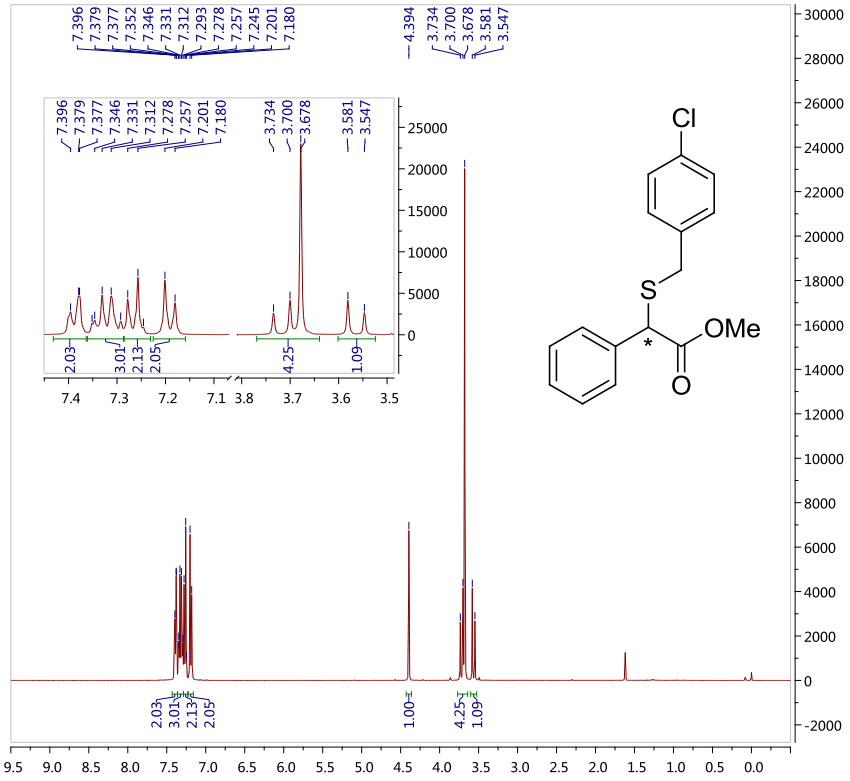


Parameters		
	Parameter	Value
1	Data File Name	C:/ Users/ Asymm-303-2/ Desktop/ xb-19-1-C(20130114)/ 1/ fid
2	Title	xb-19-1-C(20130114)
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	295.6
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	81
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2013-01-14T08:37:00
14	Modification Date	2013-01-14T08:37:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H

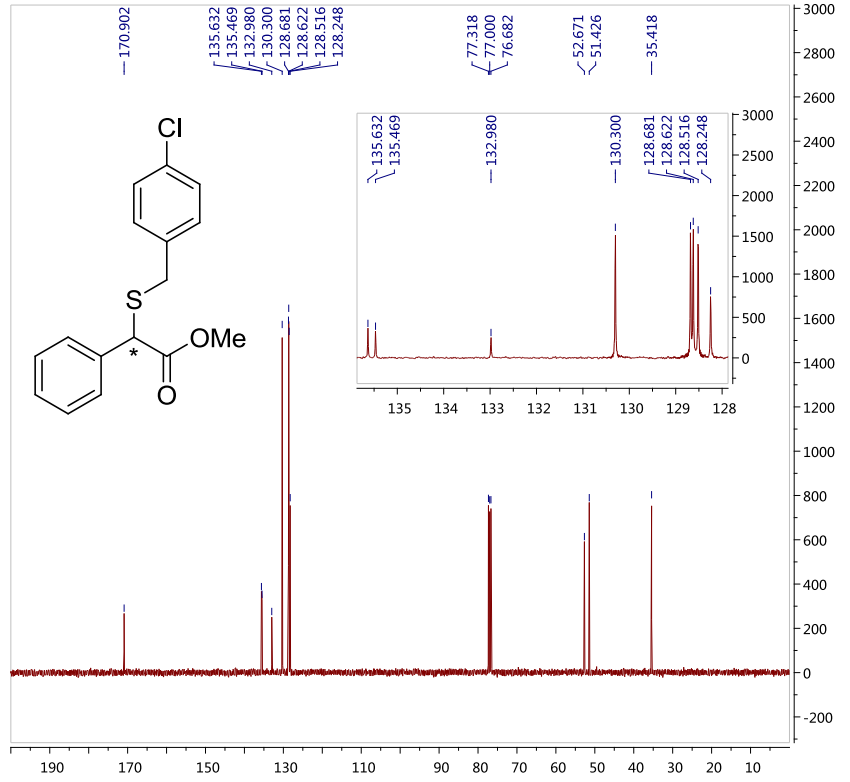


Parameters		
	Parameter	Value
1	Data File Name	C:/ Users/ Asymm-303-2/ Desktop/ xb-19-1-C(20130114)/ 2/ fid
2	Title	xb-19-1-C(20130114)
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	295.9
7	Pulse Sequence	zgpg30
8	Number of Scans	66
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2013-01-14T08:39:00
14	Modification Date	2013-01-14T08:40:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(+)-Methyl 2-(4-chlorobenzylthio)-2-phenylacetate (4ac)

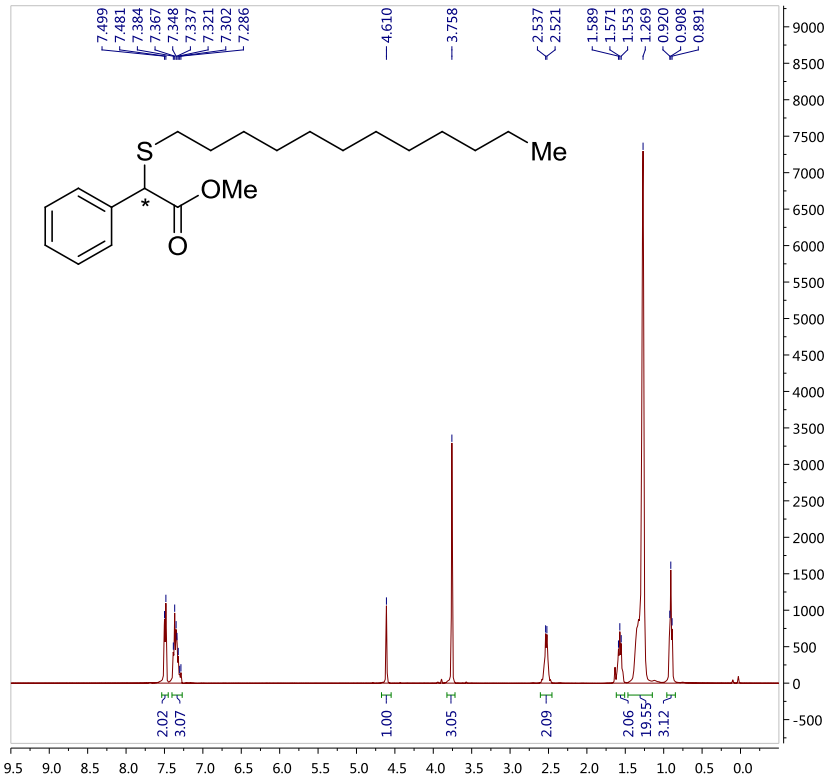


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-19-1-A/ 1/ fid
2	Title	xb-19-1-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.7
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	81
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	1.9923
13	Acquisition Date	2012-07-27T19:50:00
14	Modification Date	2012-07-27T19:50:00
15	Spectrometer Frequency	400.23
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.3
18	Nucleus	1H

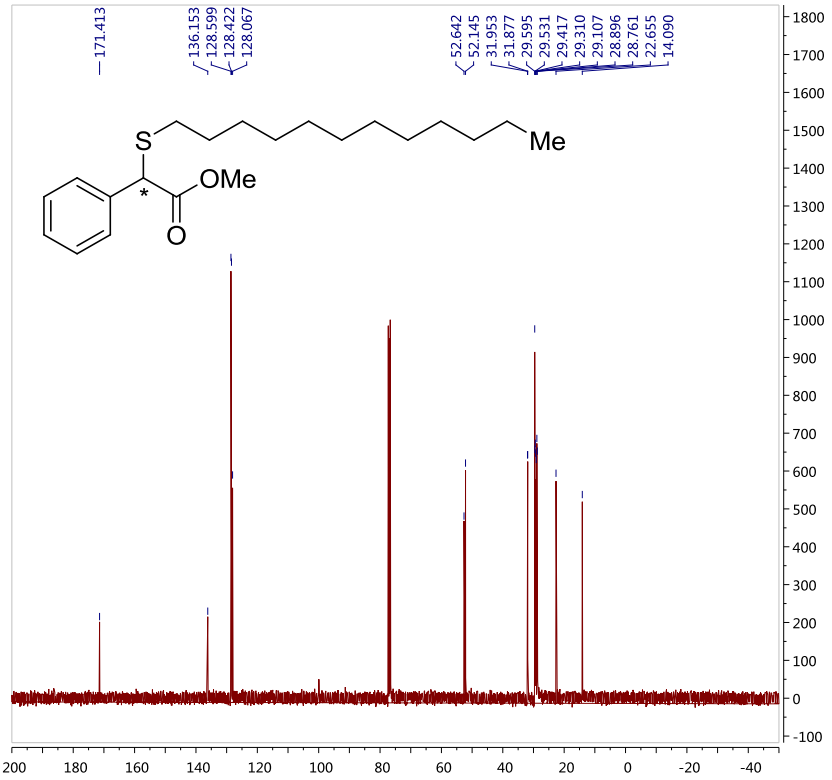


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-19-1-A/ 2/ fid
2	Title	xb-19-1-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	294.0
7	Pulse Sequence	zgpg30
8	Number of Scans	142
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-27T19:52:00
14	Modification Date	2012-07-27T19:55:00
15	Spectrometer Frequency	100.64
16	Spectral Width	29761.9
17	Lowest Frequency	-4817.6
18	Nucleus	13C

(+)-Methyl 2-(dodecylthio)-2-phenylacetate (4ad)

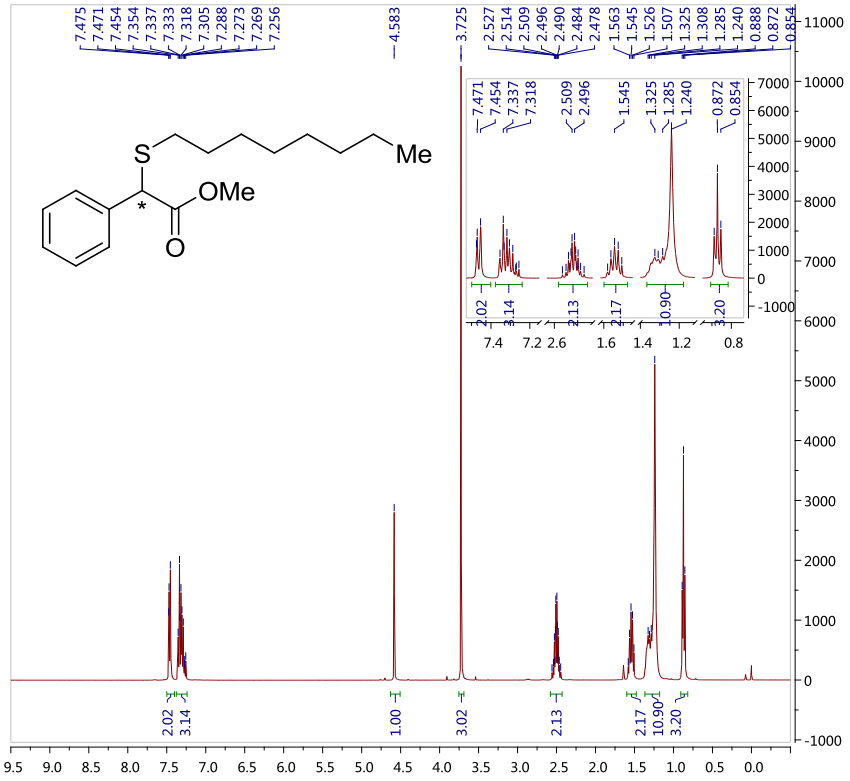


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-5/ xb-22-16-A1/ 1/ fid
2	Title	xb-22-16-A1
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	51
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2013-05-05T14:46:00
19	Modification Date	2013-05-05T14:46:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1640.9
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

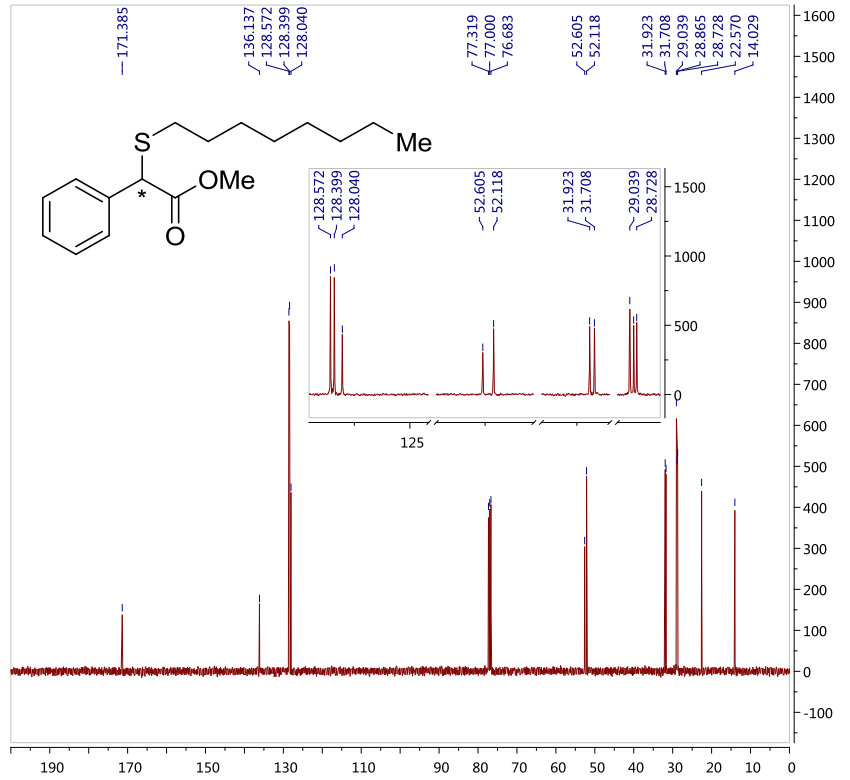


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-5/ xb-22-16-A1/ 2/ fid
2	Title	xb-22-16-A1
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	132
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2013-05-05T14:48:00
19	Modification Date	2013-05-05T14:51:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-Methyl 2-(octylthio)-2-phenylacetate (4ae)

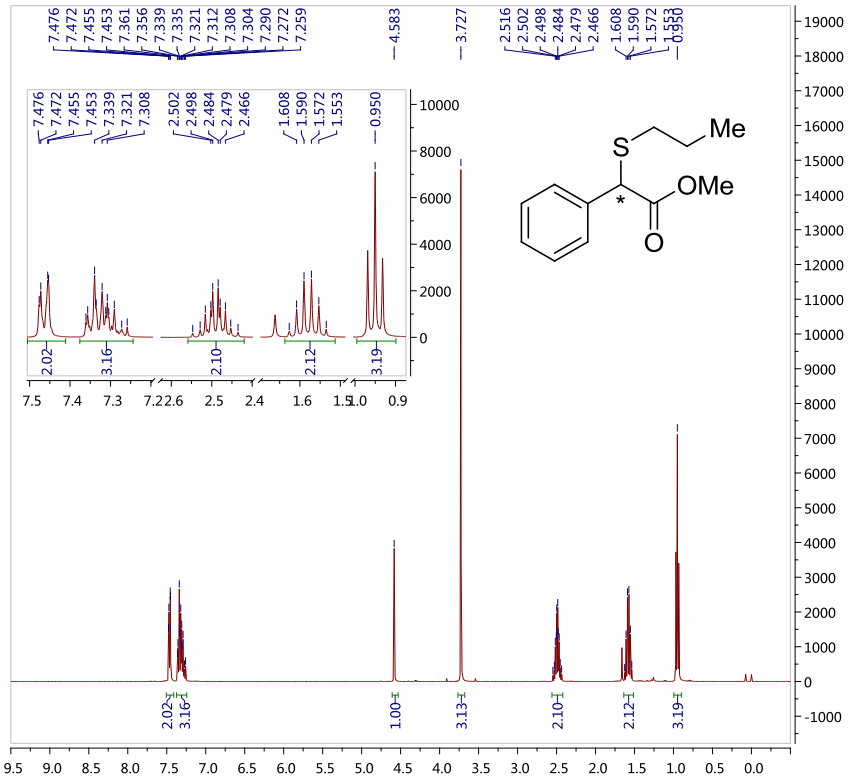


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ XB-18-42-A/ 1/ fid
2	Title	XB-18-42-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	291.7
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-07-17T16:03:00
14	Modification Date	2012-07-17T16:03:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1652.4
18	Nucleus	1H

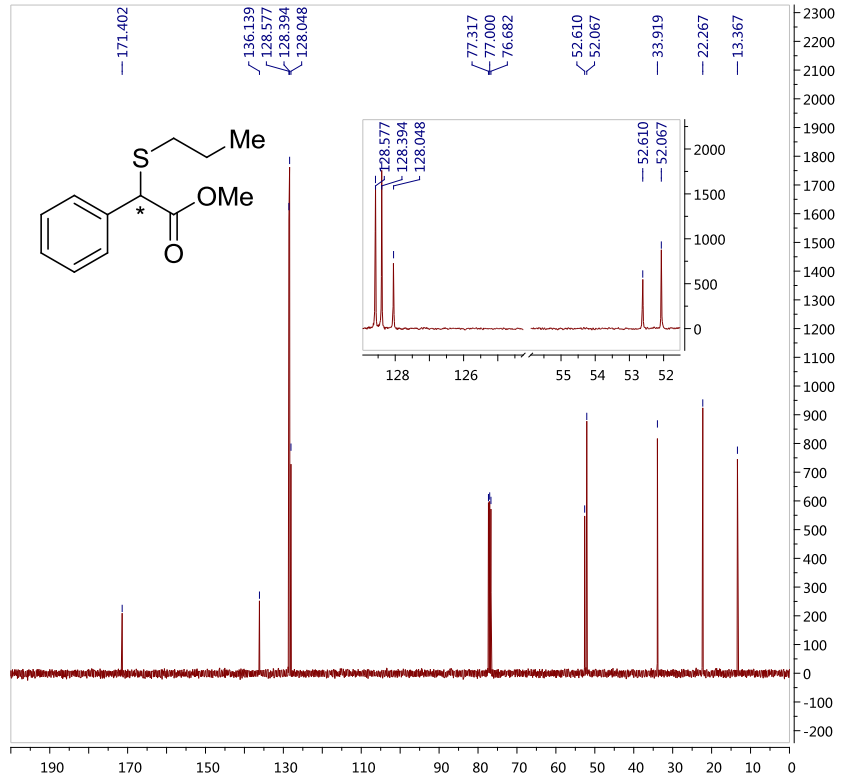


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ XB-18-42-A/ 2/ fid
2	Title	XB-18-42-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.2
7	Pulse Sequence	zgpg30
8	Number of Scans	72
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-17T16:04:00
14	Modification Date	2012-07-17T16:06:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-Methyl 2-phenyl-2-(propylthio)acetate (4af)

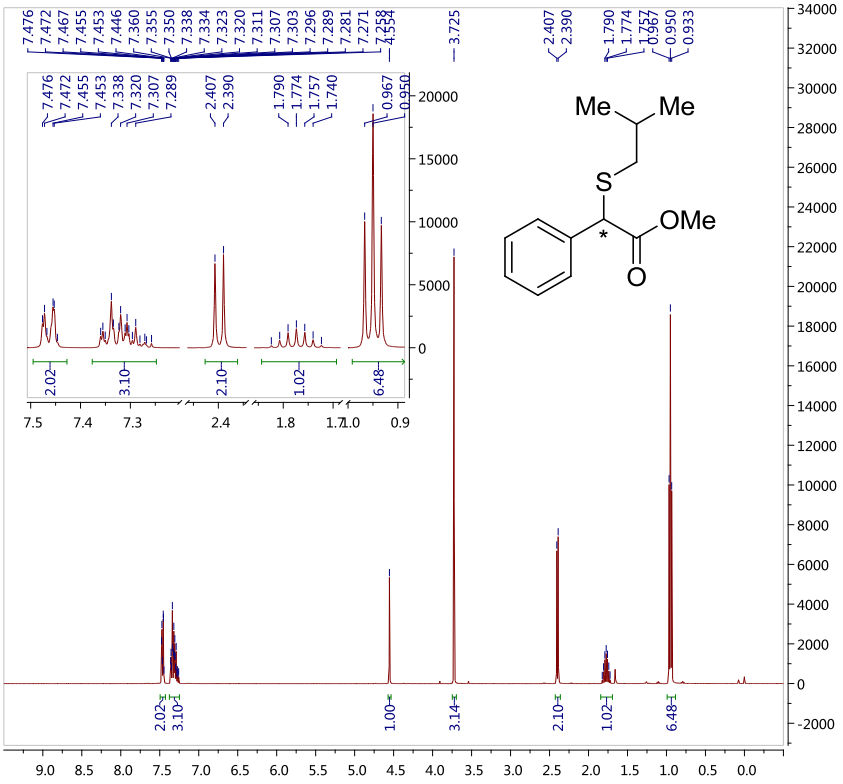


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-36-C/ 1/ fid
2	Title	xb-18-36-C
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.9
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	51
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-07-10T17:55:00
14	Modification Date	2012-07-10T17:55:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1681.4
18	Nucleus	1H

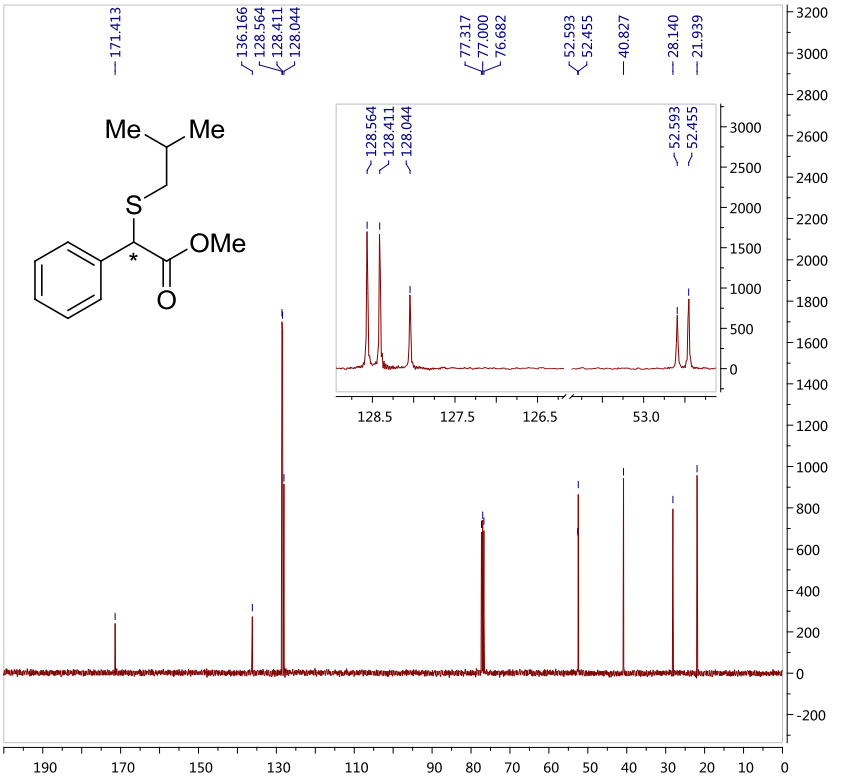


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-36-C/ 2/ fid
2	Title	xb-18-36-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.3
7	Pulse Sequence	zgpg30
8	Number of Scans	133
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-10T17:56:00
14	Modification Date	2012-07-10T17:59:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-Methyl 2-(isobutylthio)-2-phenylacetate (4ag)

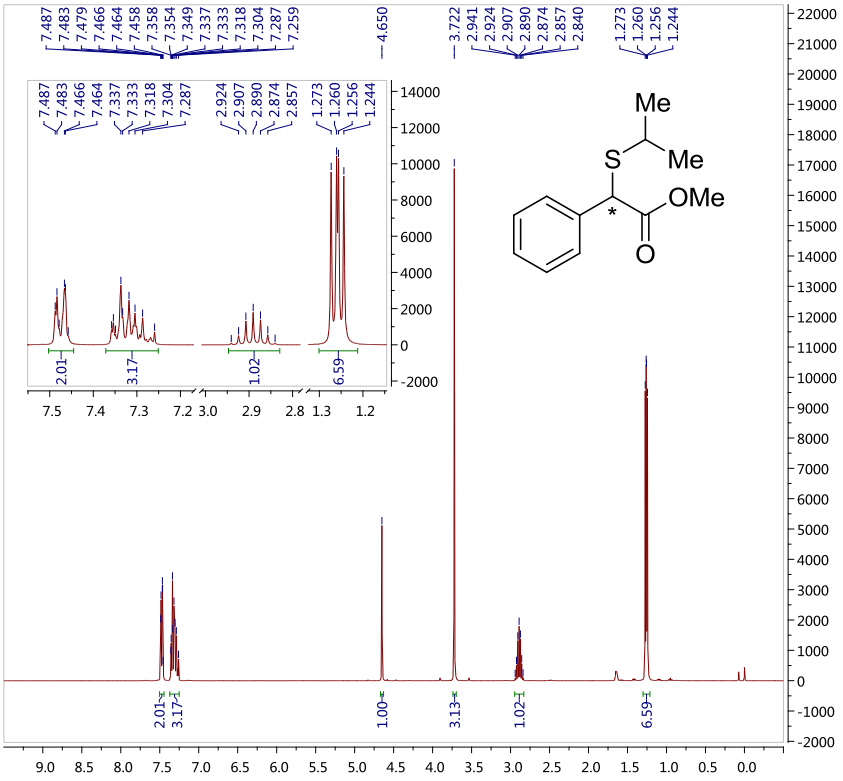


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ xb-19-16-A/ 1/ fid
2	Title	xb-19-16-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	296.6
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	51
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2012-08-30T15:45:00
14	Modification Date	2012-08-30T15:45:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H

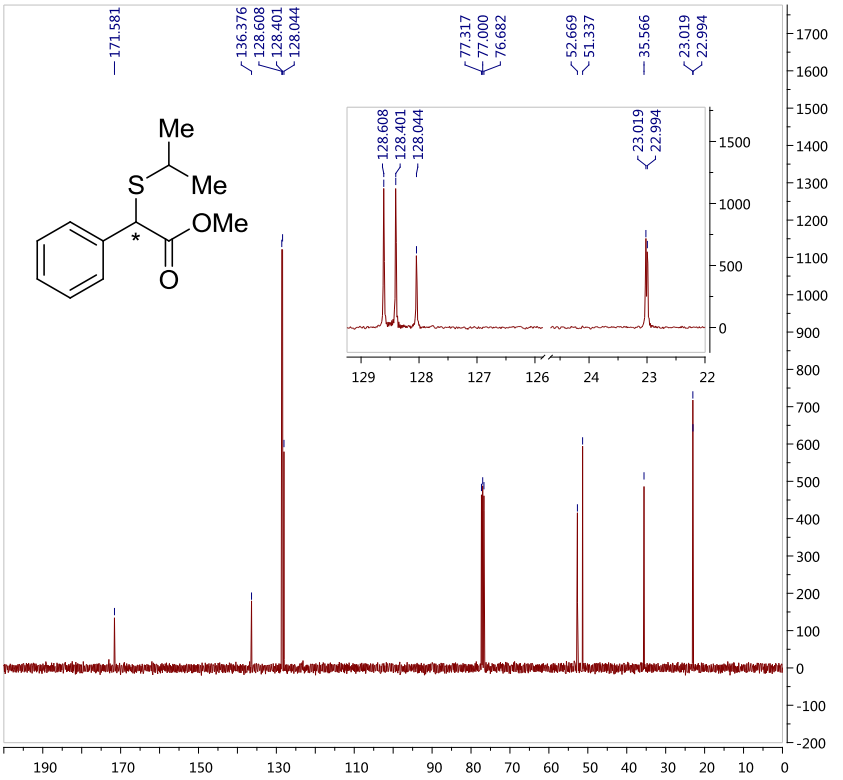


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ xb-19-16-A/ 2/ fid
2	Title	xb-19-16-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	297.1
7	Pulse Sequence	zgpg30
8	Number of Scans	95
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2012-08-30T15:47:00
14	Modification Date	2012-08-30T15:49:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(+)-Methyl 2-(isopropylthio)-2-phenylacetate (4ah)

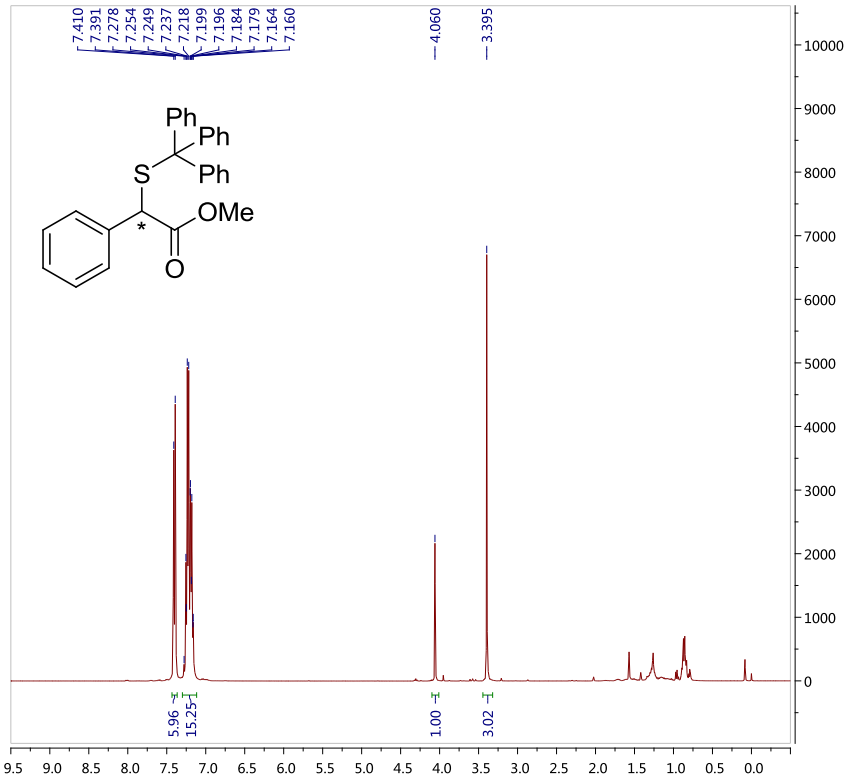


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-44-A/ 1/ fid
2	Title	xb-18-44-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	296.5
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	72
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2012-07-20T17:36:00
14	Modification Date	2012-07-20T17:36:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H

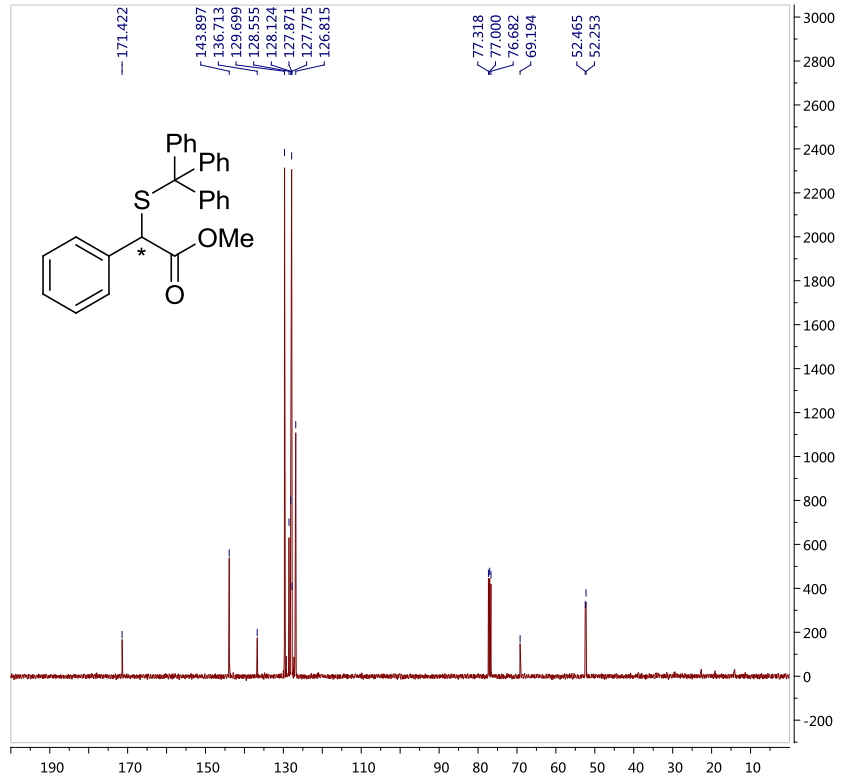


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-44-A/ 2/ fid
2	Title	xb-18-44-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	296.7
7	Pulse Sequence	zgpg30
8	Number of Scans	72
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2012-07-20T17:38:00
14	Modification Date	2012-07-20T17:39:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(+)-Methyl 2-phenyl-2-(tritylthio)acetate (4ai)



Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-36-A/ 1/ fid
2	Title	xb-18-36-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.0
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-07-10T17:48:00
14	Modification Date	2012-07-10T17:48:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1702.7
18	Nucleus	1H



Parameters		
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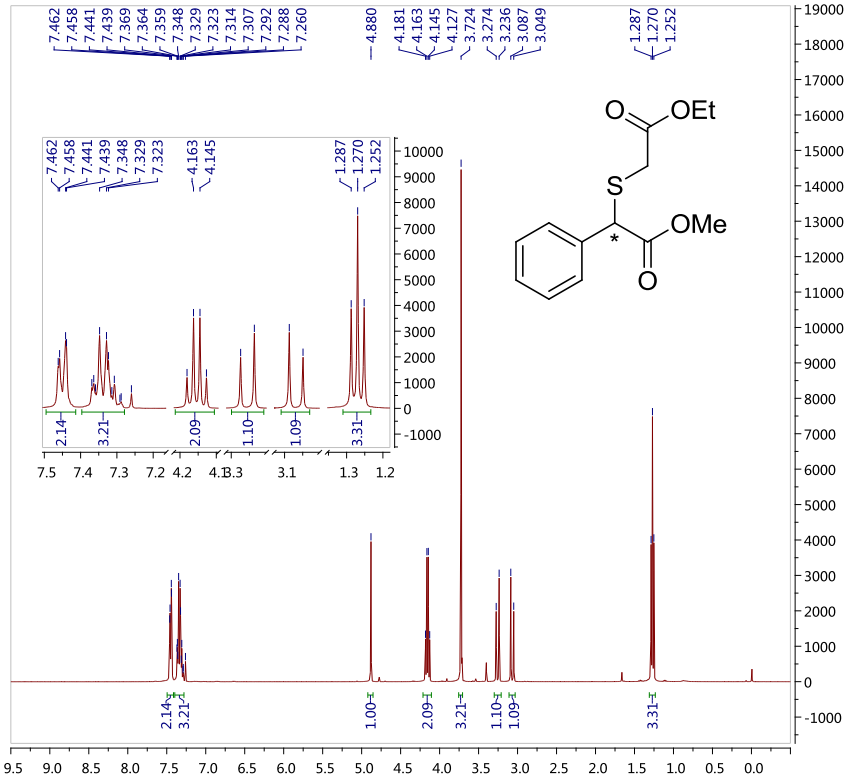
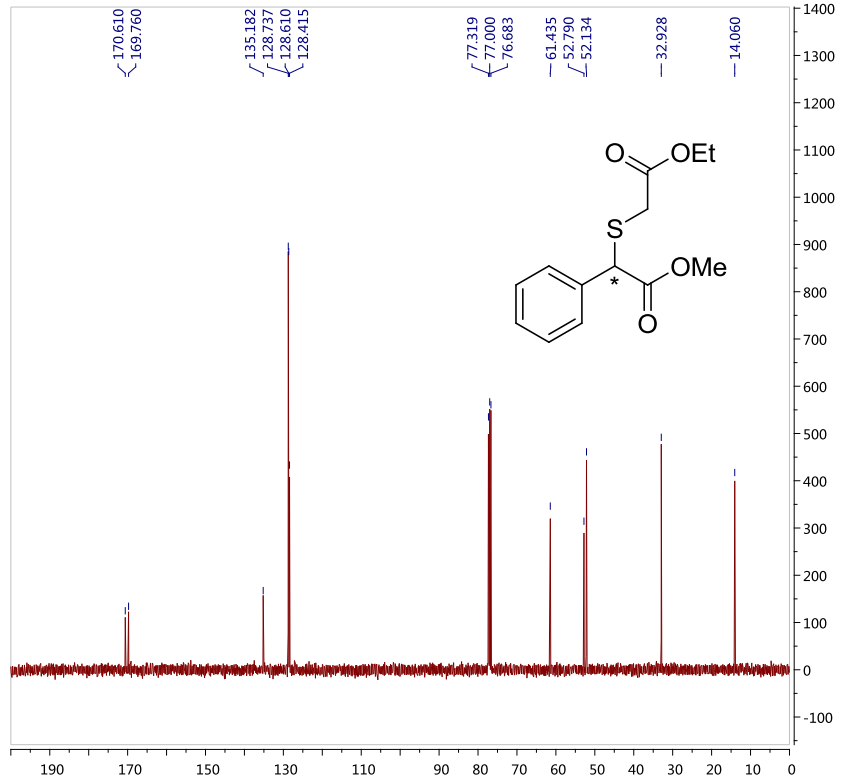
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-36-A/ 2/ fid
2	Title	xb-18-36-A
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	293.3
7	Pulse Sequence	zgpg30
8	Number of Scans	80
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-07-10T17:50:00
14	Modification Date	2012-07-10T17:51:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(+)-Methyl 2-(2-ethoxy-2-oxoethylthio)-2-phenylacetate (4aj)

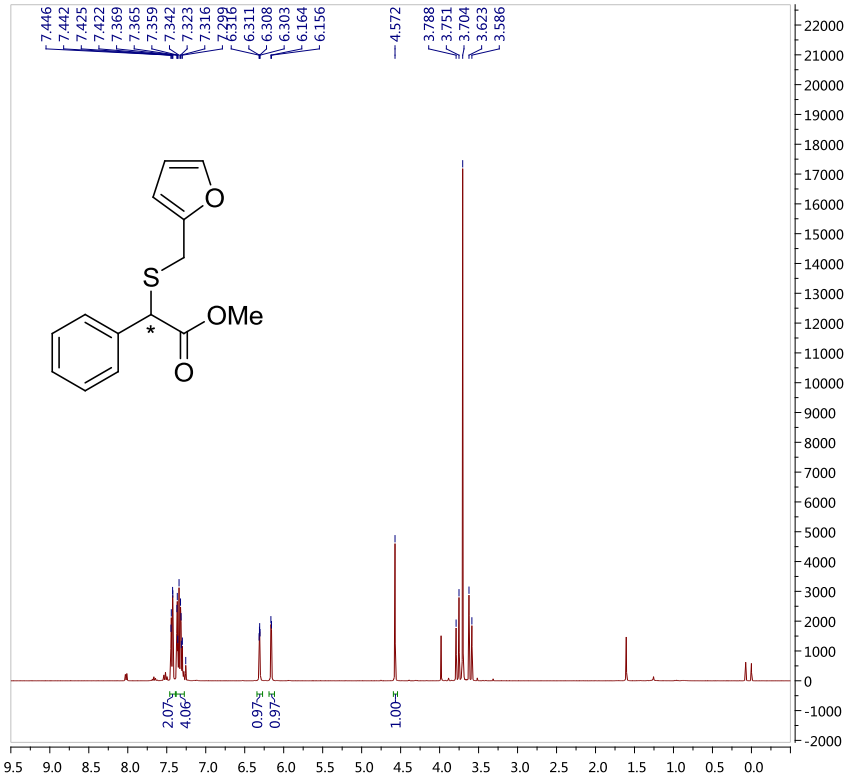


Parameters		
	Parameter	Value
1	Data File Name	C:/ Users/ Asymm-303-2/ Desktop/ xb-19-16-C(20130114)/ 1/ fid
2	Title	xb-19-16-C(20130114)
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	295.8
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	81
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2013-01-14T08:30:00
14	Modification Date	2013-01-14T08:30:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H

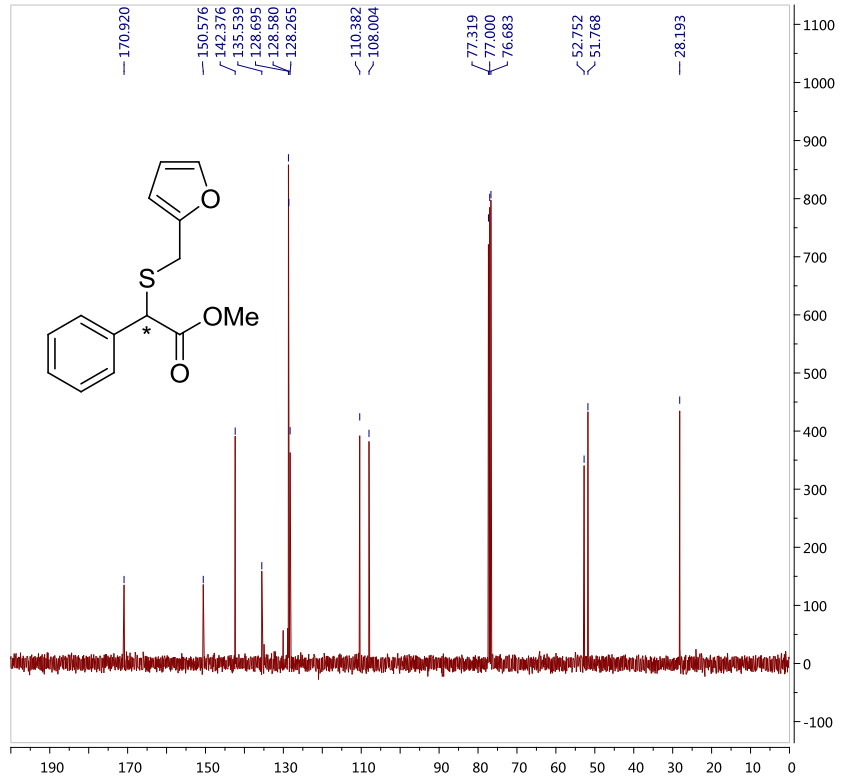


Parameters		
	Parameter	Value
1	Data File Name	C:/ Users/ Asymm-303-2/ Desktop/ xb-19-16-C(20130114)/ 2/ fid
2	Title	xb-19-16-C(20130114)
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	296.1
7	Pulse Sequence	zgpg30
8	Number of Scans	70
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2013-01-14T08:32:00
14	Modification Date	2013-01-14T08:33:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(+)-Methyl 2-(furan-2-ylmethylthio)-2-phenylacetate (4ak)

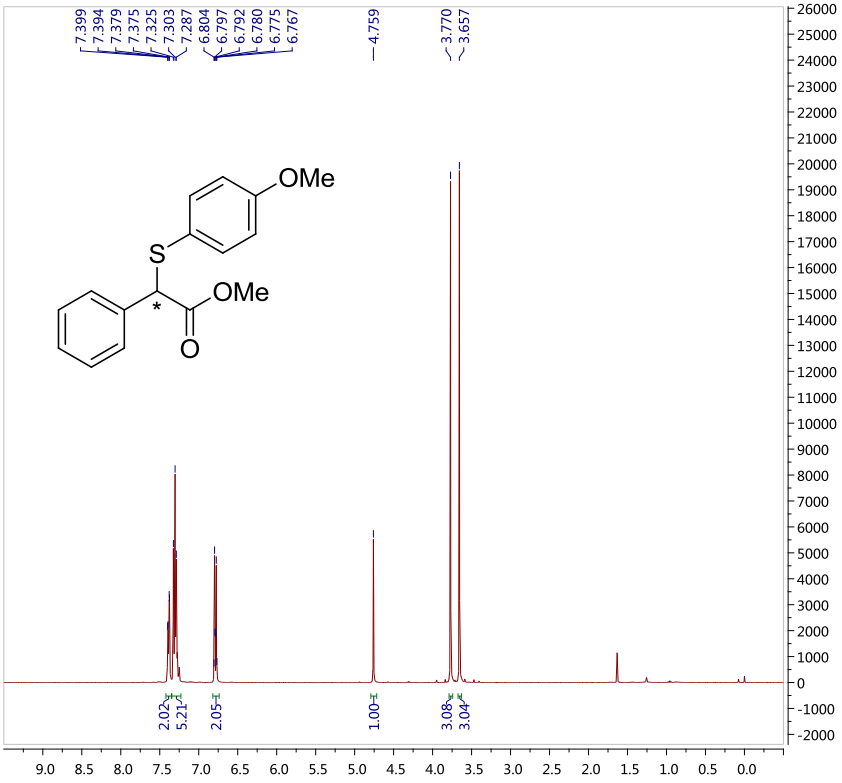


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ XB-19-15-B-rac/ 1/ fid
2	Title	XB-19-15-B-rac
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	295.8
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	101
10	Relaxation Delay	1.0000
11	Pulse Width	13.7000
12	Acquisition Time	1.9999
13	Acquisition Date	2012-08-29T14:09:00
14	Modification Date	2012-08-29T14:09:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1640.9
18	Nucleus	1H

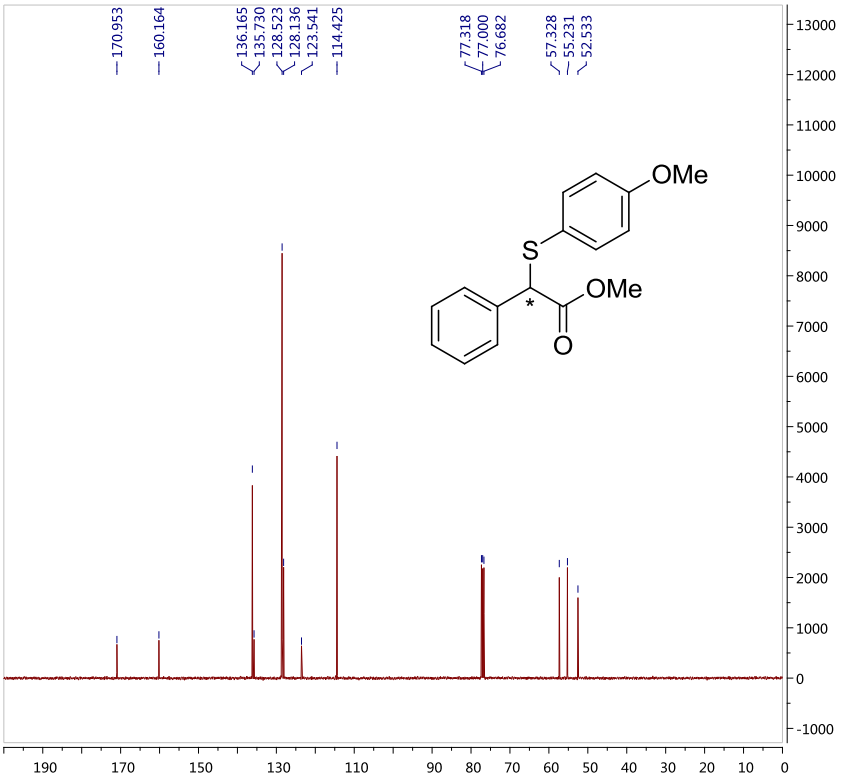


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-8/ XB-19-15-B-rac/ 2/ fid
2	Title	XB-19-15-B-rac
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	296.2
7	Pulse Sequence	zgpg30
8	Number of Scans	91
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	0.4588
13	Acquisition Date	2012-08-29T14:11:00
14	Modification Date	2012-08-29T14:13:00
15	Spectrometer Frequency	100.61
16	Spectral Width	35714.3
17	Lowest Frequency	-7796.3
18	Nucleus	13C

(–)-Methyl 2-(4-methoxyphenylthio)-2-phenylacetate (4al)

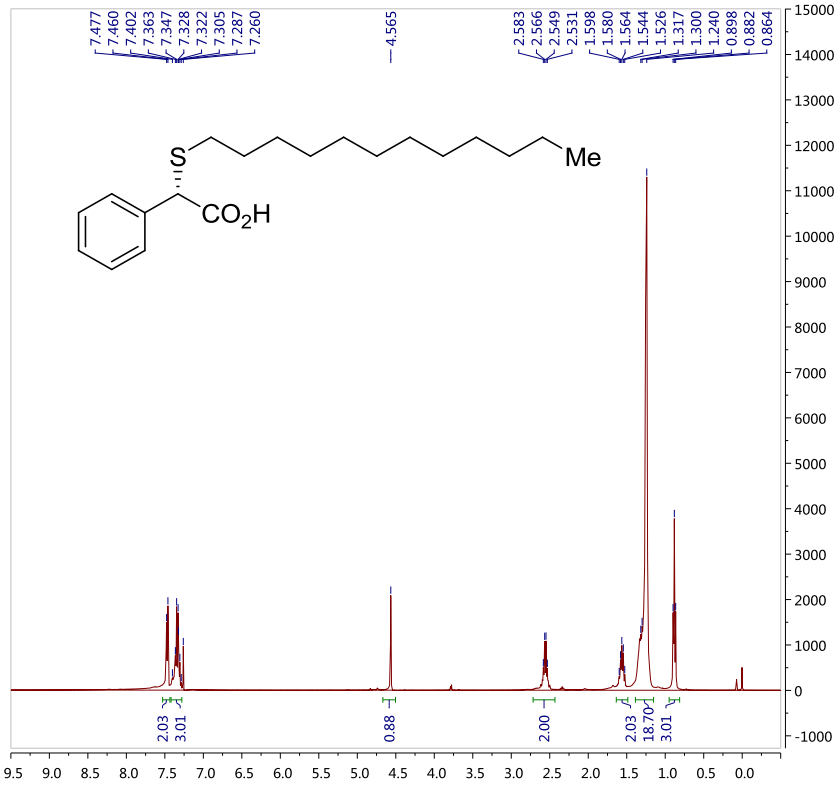


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-31-B/ 1/ fid
2	Title	xb-18-31-B
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.0
7	Pulse Sequence	zg30
8	Number of Scans	8
9	Receiver Gain	101
10	Relaxation Delay	1.0000
11	Pulse Width	13.5000
12	Acquisition Time	2.9999
13	Acquisition Date	2012-09-18T09:45:00
14	Modification Date	2012-09-18T09:45:00
15	Spectrometer Frequency	400.13
16	Spectral Width	8223.7
17	Lowest Frequency	-1654.7
18	Nucleus	1H

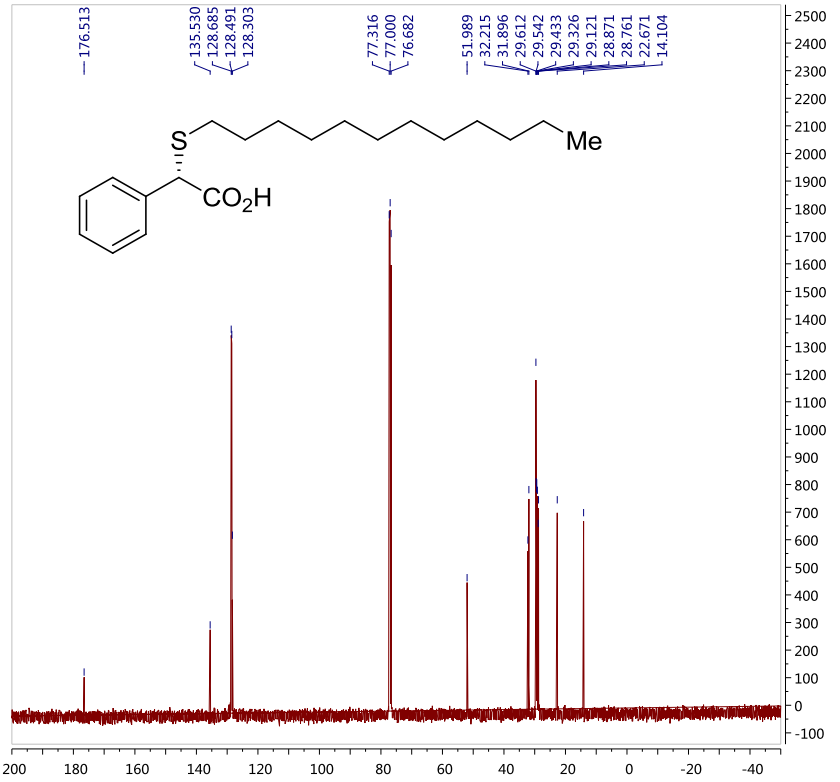


Parameters		
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-7/ xb-18-31-B/ 2/ fid
2	Title	xb-18-31-B
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Solvent	CDCl3
6	Temperature	292.4
7	Pulse Sequence	zgpg30
8	Number of Scans	462
9	Receiver Gain	203
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Time	0.5506
13	Acquisition Date	2012-09-18T09:47:00
14	Modification Date	2012-09-18T09:59:00
15	Spectrometer Frequency	100.61
16	Spectral Width	29761.9
17	Lowest Frequency	-4820.2
18	Nucleus	13C

(*S*)-2-(dodecylthio)-2-phenylacetic acid (7)

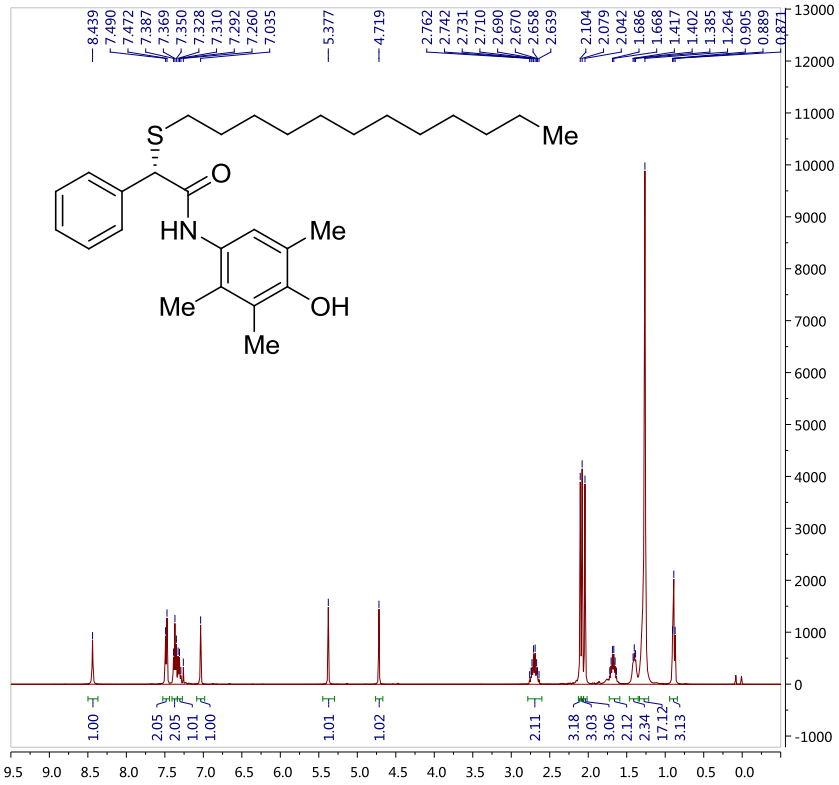


	参数	值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical (第一稿)/ 新增应用-Eflucimibe的合成/ Acid/ nmr/ 1/ fid
2	Title	nmr
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	77
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.0447
18	Acquisition Date	2013-07-04T18:14:03
19	Modification Date	2013-07-04T18:14:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1535.4
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

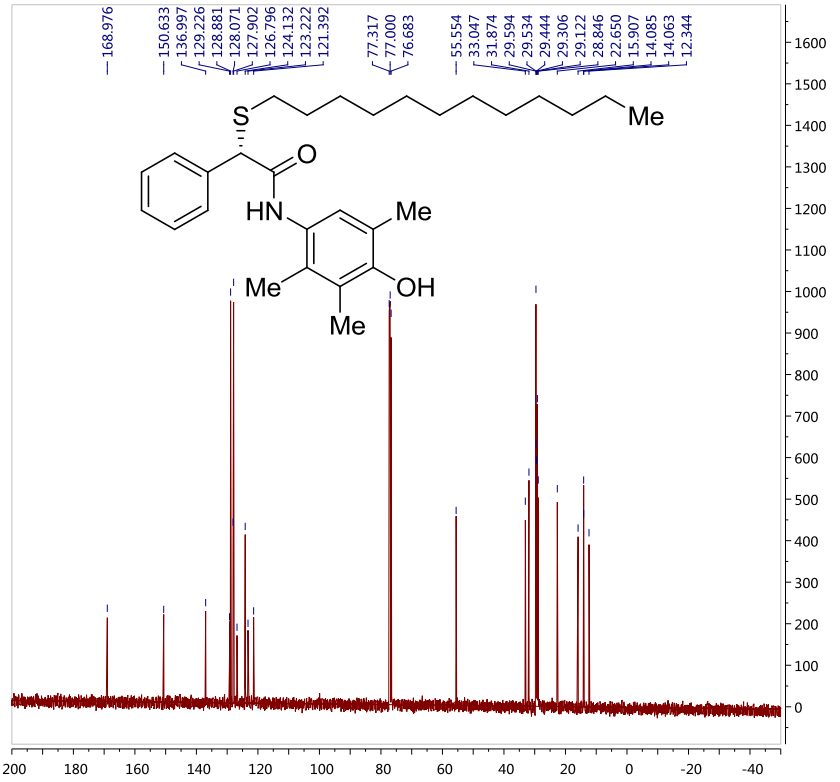


	参数	值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical (第一稿)/ 新增应用-Eflucimibe的合成/ Acid/ nmr/ 2/ fid
2	Title	nmr
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	531
14	Receiver Gain	119
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2013-07-04T18:16:20
19	Modification Date	2013-07-04T18:28:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*S*)-Eflucimible

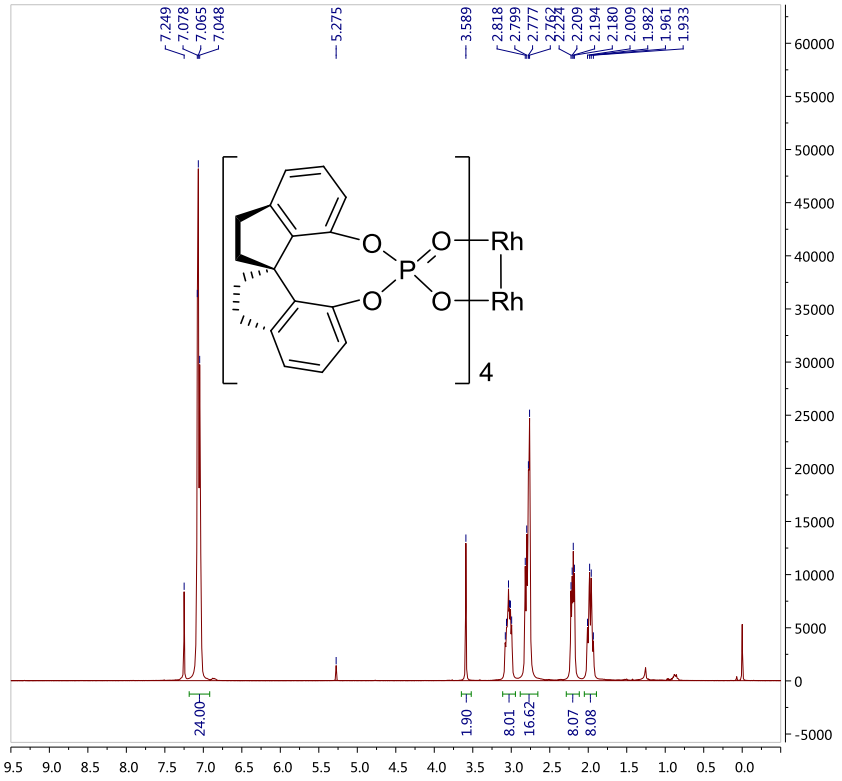


	参数	值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical（第一稿）/ 新增应用-Eflucimibe的合成/ Eflucimible/ nmr/ xb-23-15-1/ 1/ fid
2	Title	xb-23-15-1
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	32
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.0447
18	Acquisition Date	2013-07-05T21:39:33
19	Modification Date	2013-07-05T21:39:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1535.4
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

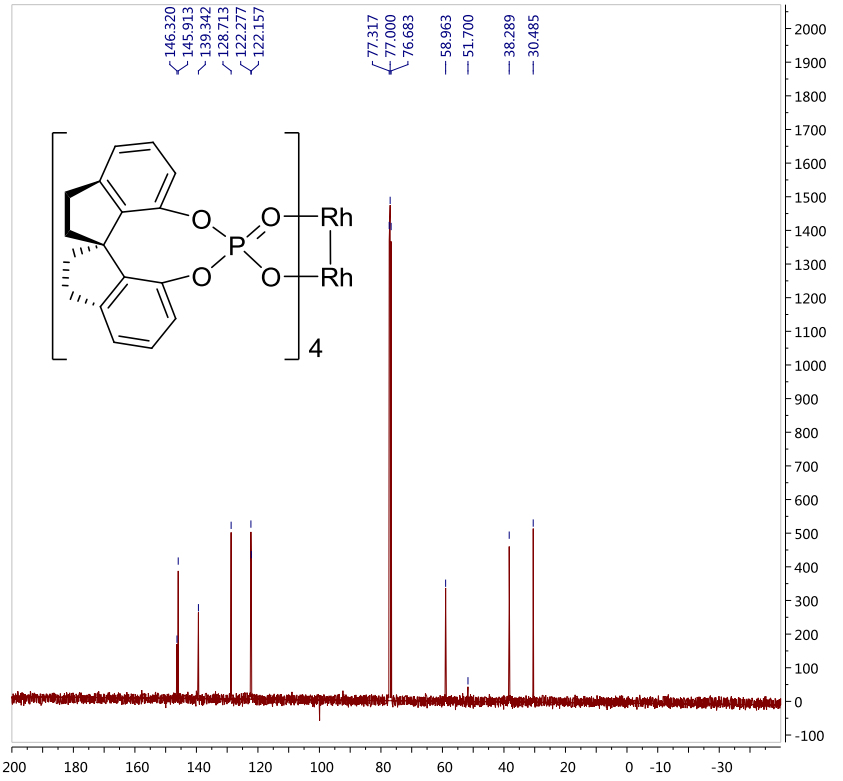


	参数	值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical（第一稿）/ 新增应用-Eflucimibe的合成/ Eflucimible/ nmr/ xb-23-15-1/ 2/ fid
2	Title	xb-23-15-1
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	249
14	Receiver Gain	111
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2013-07-05T21:41:44
19	Modification Date	2013-07-05T21:47:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

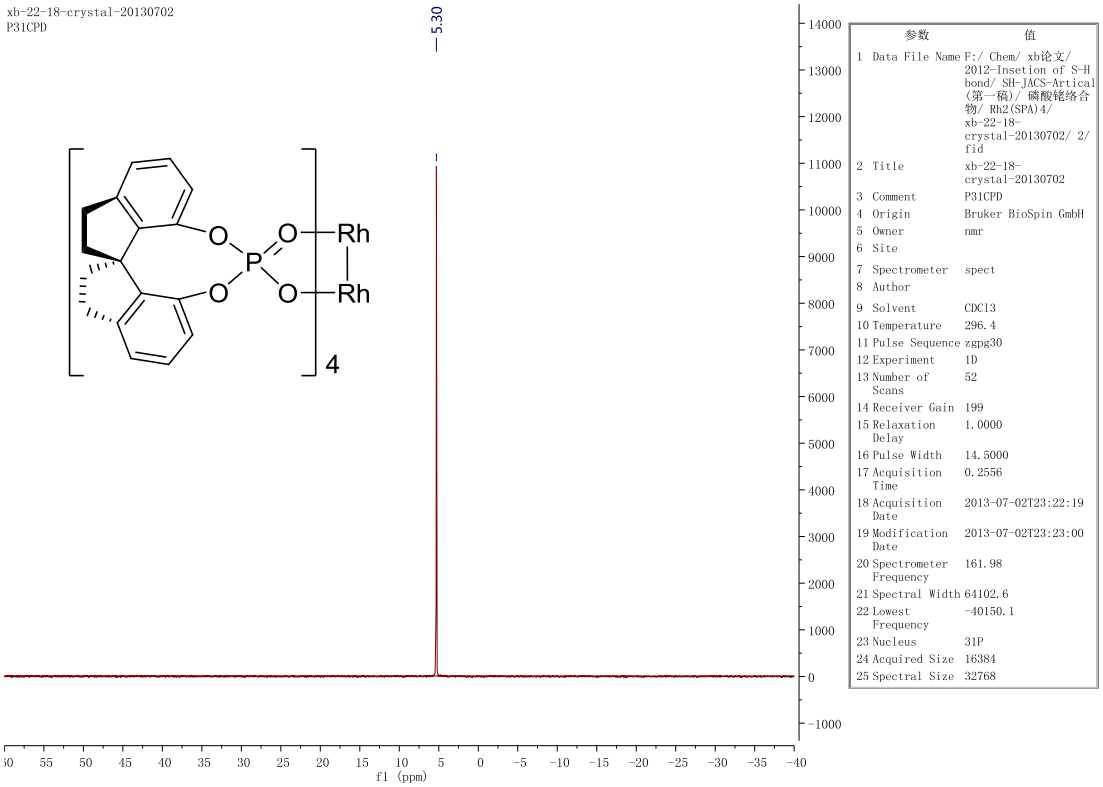
Tetrakis[(*R*)-1,1'-Spirobiindanyl-7,7'-diyl-phosphate] dirhodium (II)



参数		值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical (第一稿)/ 磷酸铑络合物/ Rh2(SPA)4/ xb-22-18-crystal-20130702/ 1/ fid
2	Title	xb-22-18-crystal-20130702
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDC13
10	Temperature	296.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	59
14	Receiver Gain	119
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.0447
18	Acquisition Date	2013-07-02T23:18:01
19	Modification Date	2013-07-02T23:20:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1480.4
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768



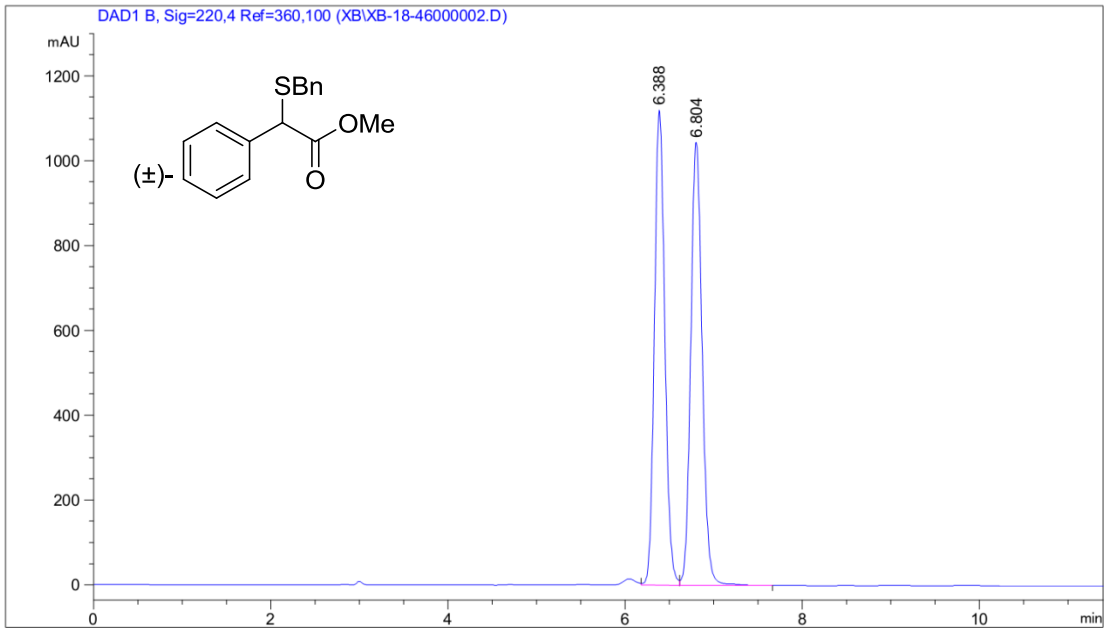
参数		值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical (第一稿)/ 磷酸铑络合物/ Rh2(SPA)4/ xb-22-18-crystal-20130702/ 4/ fid
2	Title	xb-22-18-crystal-20130702
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDC13
10	Temperature	296.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	483
14	Receiver Gain	87
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2013-07-02T23:28:46
19	Modification Date	2013-07-02T23:39:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



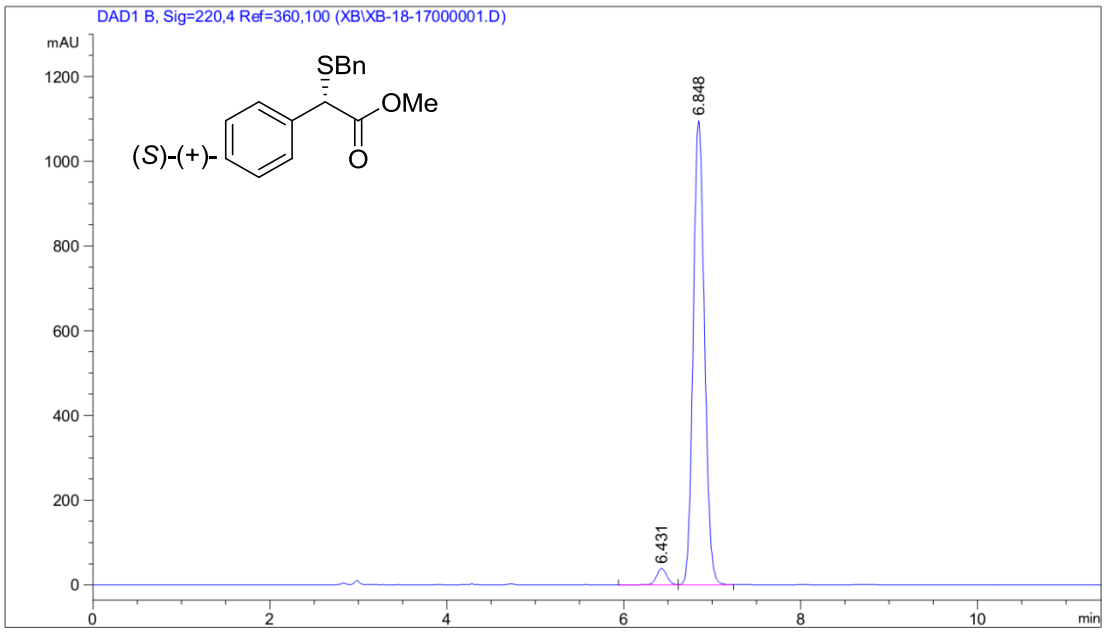
参数		值
1	Data File Name	F:/ Chem/ xb论文/ 2012-Insetion of S-H bond/ SH-JACS-Artical (第一稿)/ 磷酸铑络合物/ Rh2(SPA)4/ xb-22-18-crystal-20130702/ 2/ fid
2	Title	xb-22-18-crystal-20130702
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	52
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	14.5000
17	Acquisition Time	0.2556
18	Acquisition Date	2013-07-02T23:22:19
19	Modification Date	2013-07-02T23:23:00
20	Spectrometer Frequency	161.98
21	Spectral Width	64102.6
22	Lowest Frequency	-40150.1
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768

11. HPLC or SFC Charts of S–H Insertion Products

Methyl 2-(benzylthio)-2-phenylacetate (4aa)

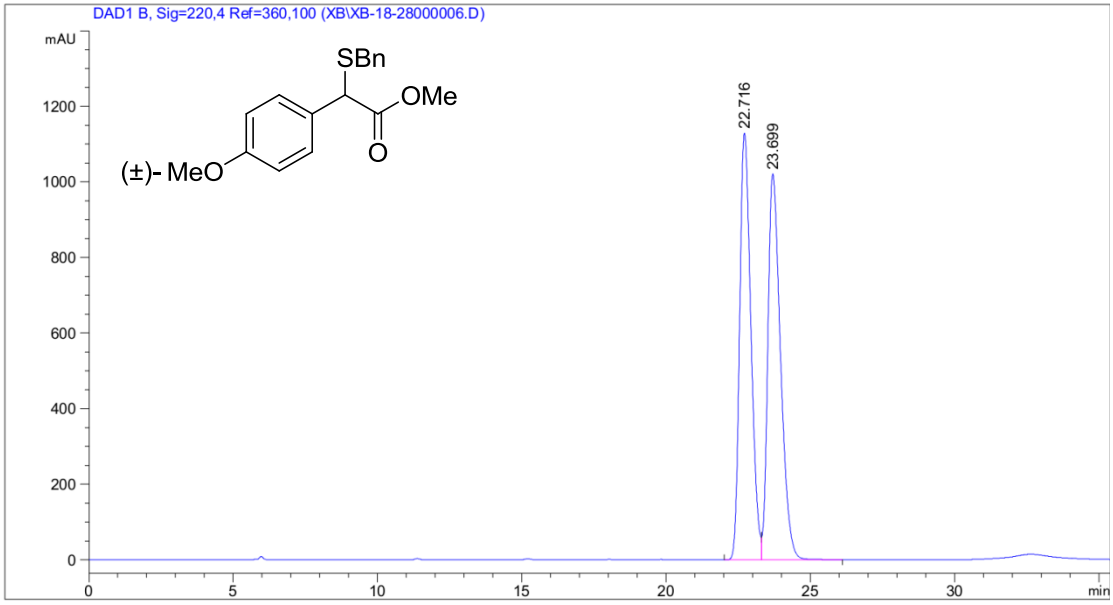


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.388	VV	0.1274	9161.90625	1120.52185	49.4983
2	6.804	VB	0.1404	9347.64355	1044.94666	50.5017

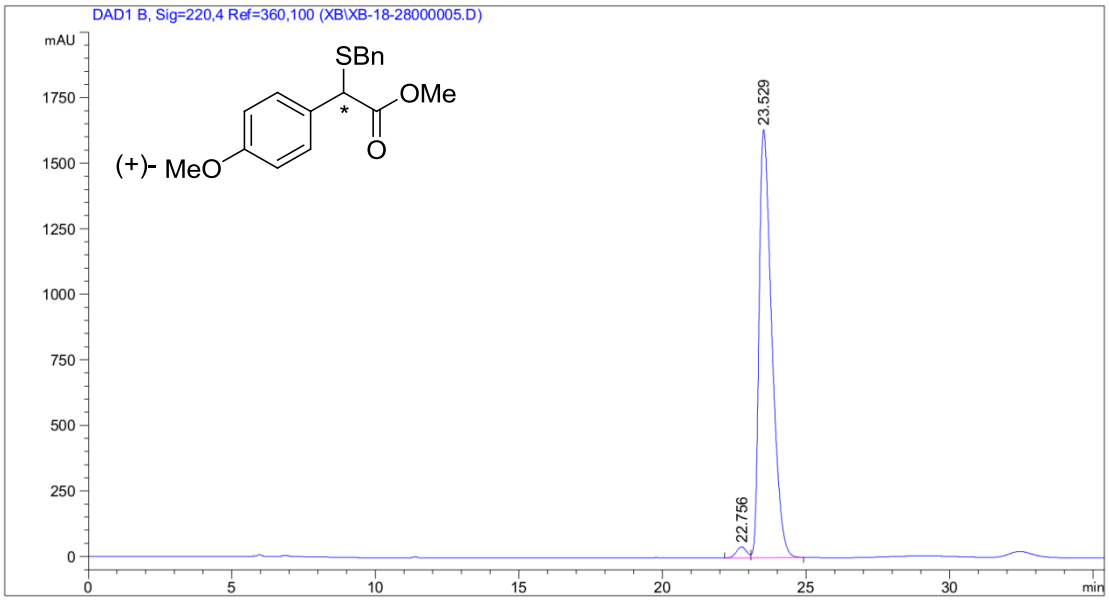


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.431	BV	0.1291	322.33688	38.73292	3.2132
2	6.848	VV	0.1393	9709.35156	1096.54297	96.7868

Methyl 2-(benzylthio)-2-(4-methoxyphenyl)acetate (4ba)

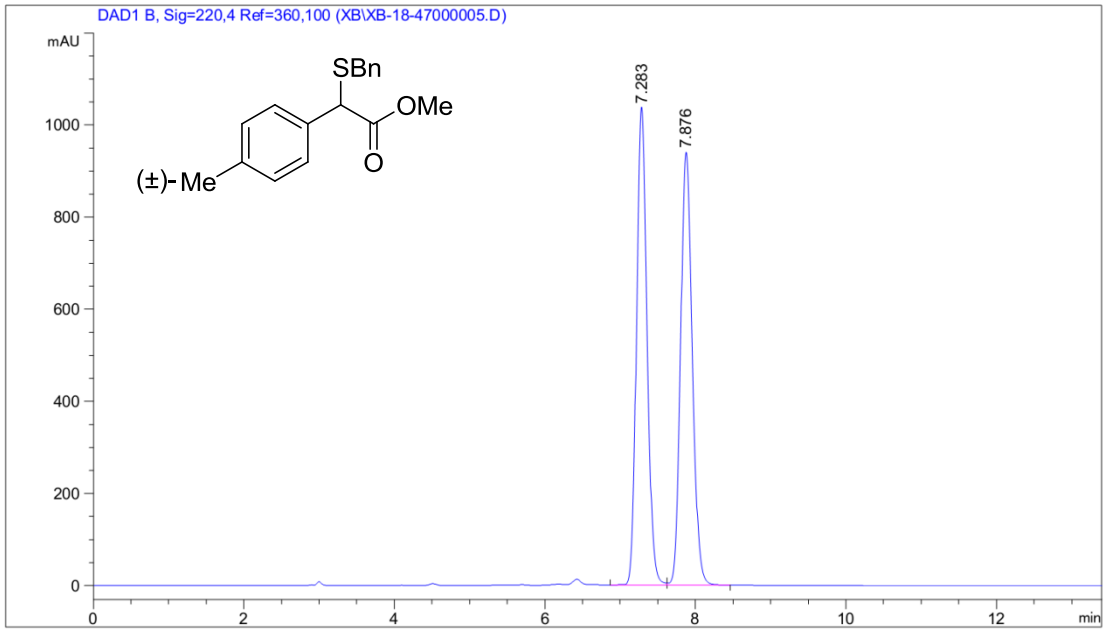


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.716	BV	0.4224	3.06389e4	1129.67126	49.5041
2	23.699	VB	0.4669	3.12528e4	1021.55164	50.4959

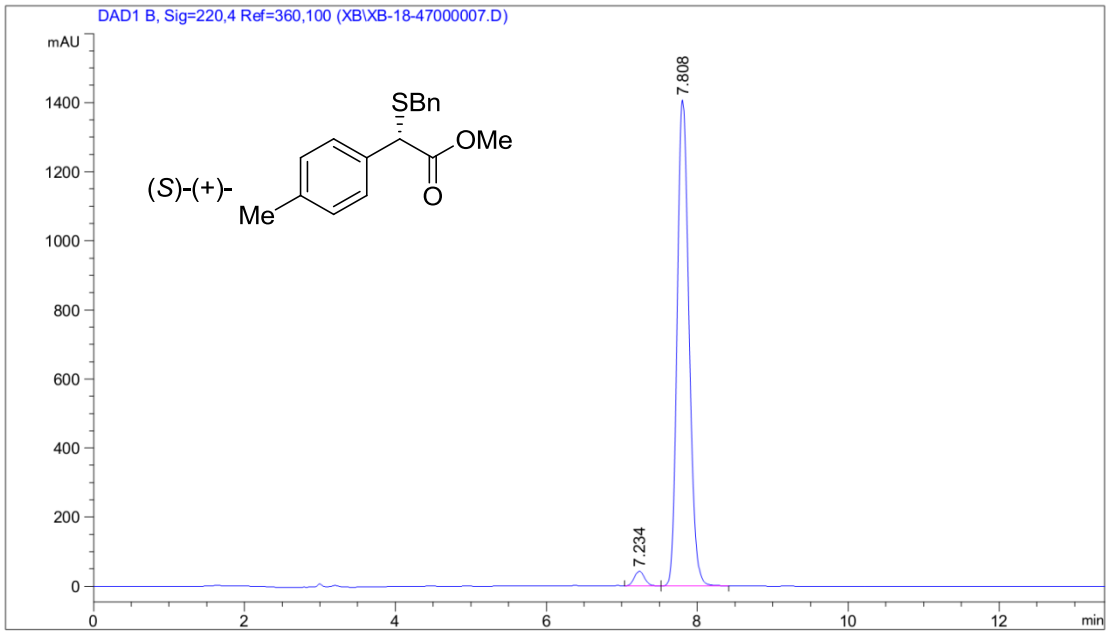


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.756	BV	0.3863	1011.03229	41.19424	1.9744
2	23.529	VB	0.4689	5.01954e4	1631.89587	98.0256

Methyl 2-(benzylthio)-2-*p*-tolylacetate (4ca)

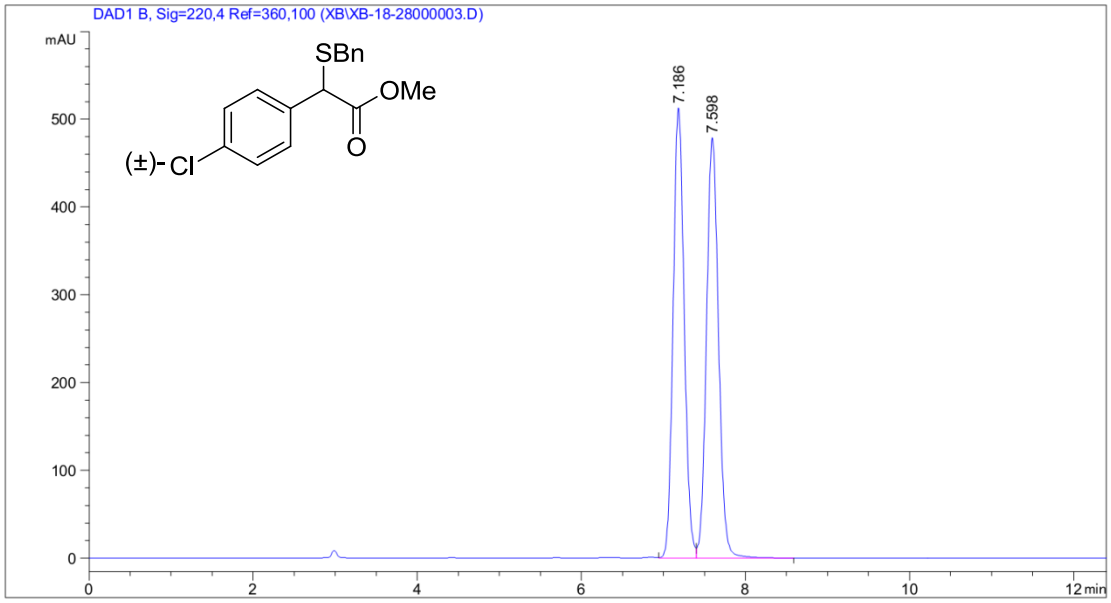


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.283	BV	0.1539	1.01190e4	1036.50195	49.9767
2	7.876	VB	0.1698	1.01284e4	939.21606	50.0233

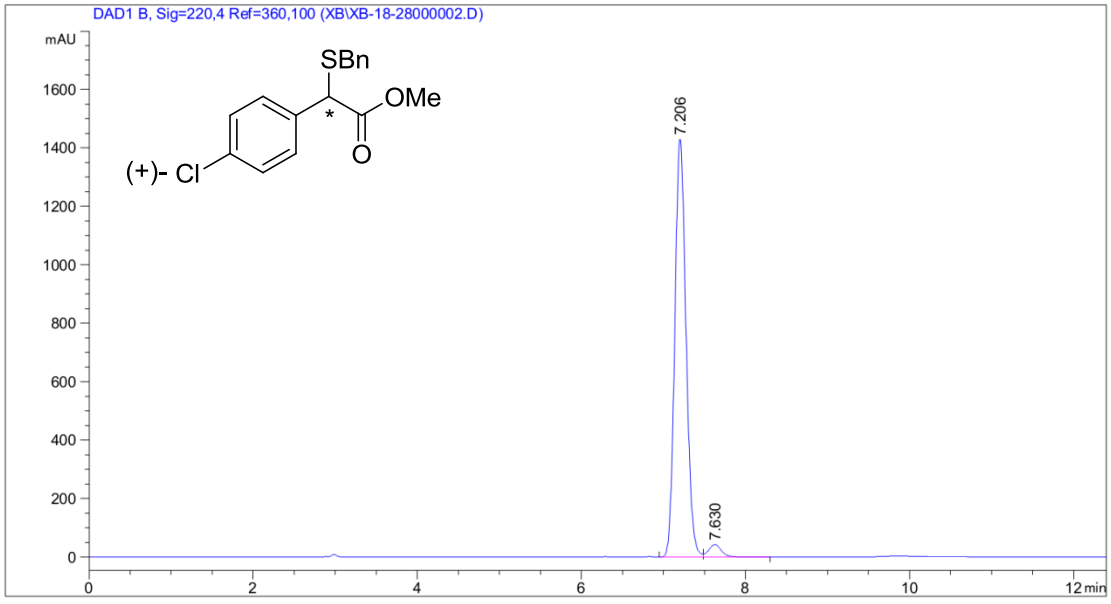


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.234	VB	0.1502	408.92328	42.51991	2.6131
2	7.808	BV	0.1684	1.52400e4	1407.12268	97.3869

Methyl 2-(benzylthio)-2-(4-chlorophenyl)acetate (4da)

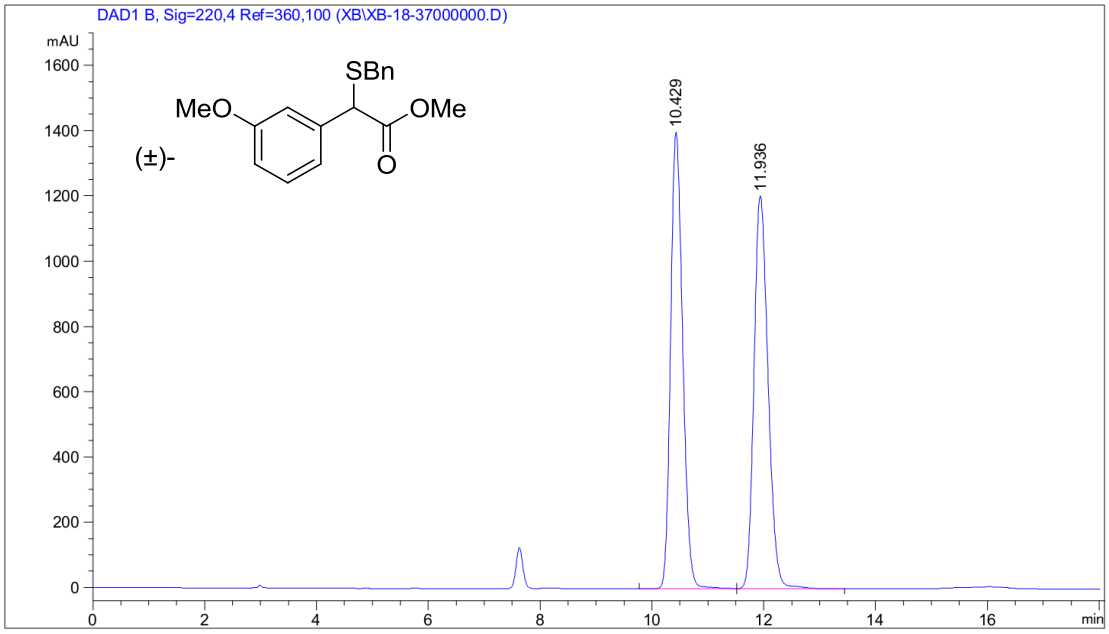


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.186	VV	0.1453	4808.54004	513.46362	49.6272
2	7.598	VB	0.1568	4880.78271	479.34772	50.3728

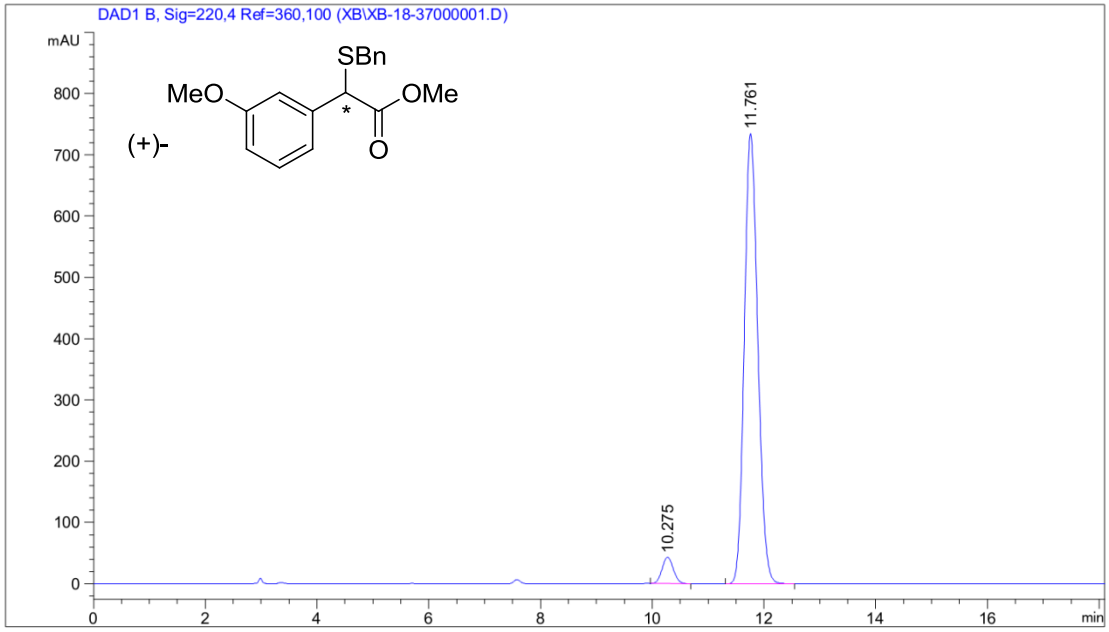


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.206	VV	0.1468	1.35840e4	1430.38940	96.7040
2	7.630	VB	0.1649	462.99091	42.56126	3.2960

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

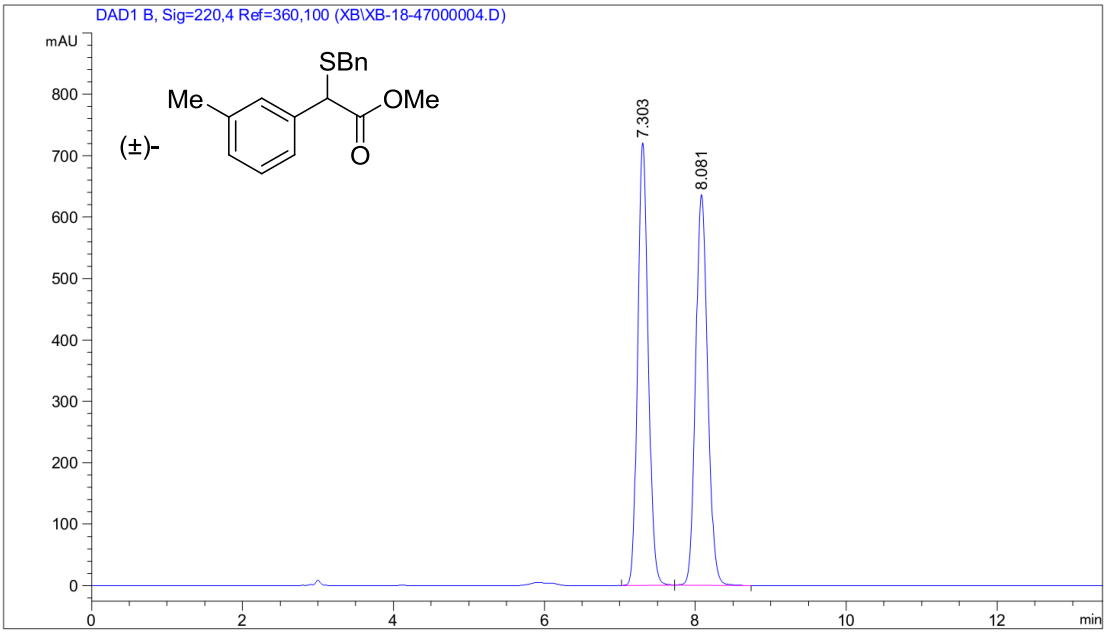


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.429	BB	0.2322	2.08945e4	1399.52051	49.8415
2	11.936	BB	0.2717	2.10273e4	1204.38037	50.1585

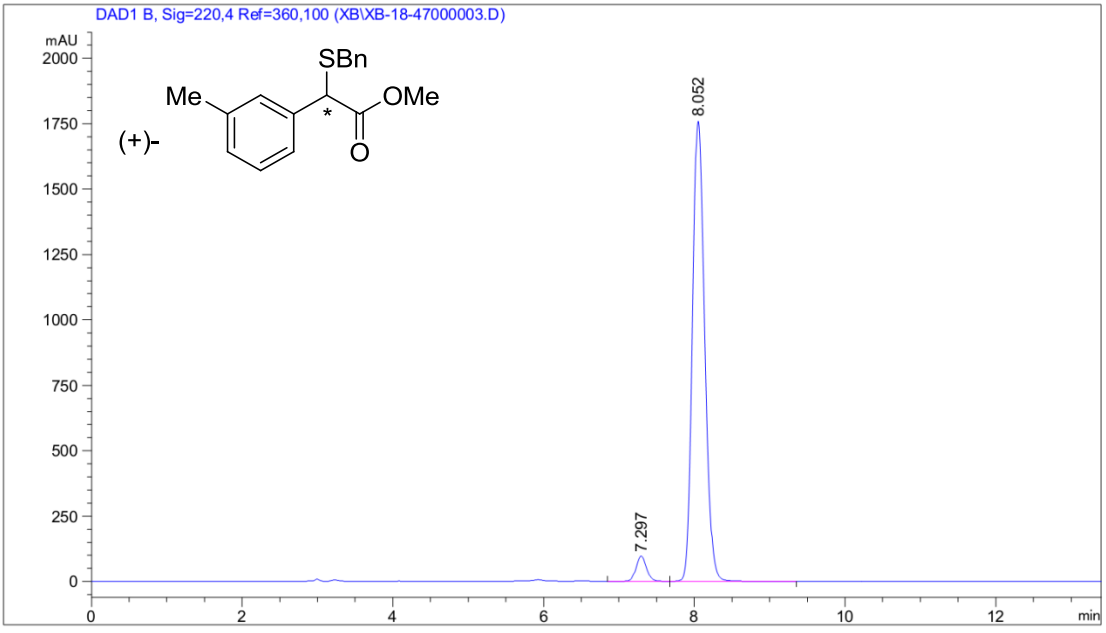


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.275	BB	0.2198	605.67334	43.13449	4.6780
2	11.761	BB	0.2619	1.23417e4	735.04395	95.3220

Methyl 2-(benzylthio)-2-*m*-tolylacetate (4fa)

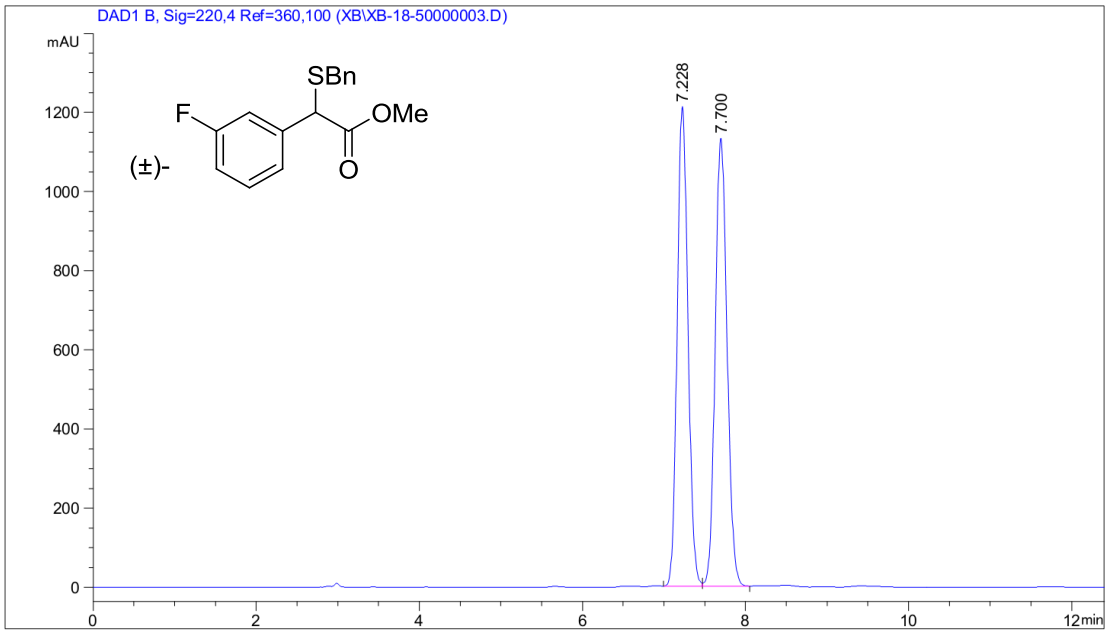


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.303	VB	0.1537	7022.85449	720.91986	49.9048
2	8.081	BB	0.1712	7049.63867	636.36768	50.0952

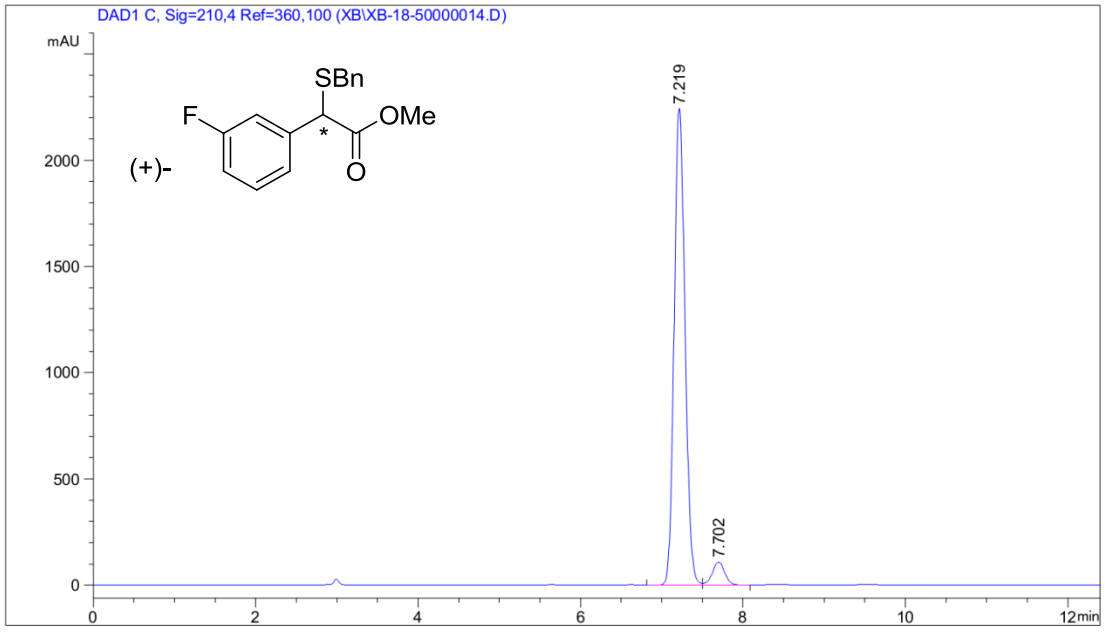


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.297	BB	0.1525	945.08844	96.28322	4.5417
2	8.052	BB	0.1756	1.98638e4	1760.33264	95.4583

Methyl 2-(benzylthio)-2-(3-fluorophenyl)acetate (4ga)

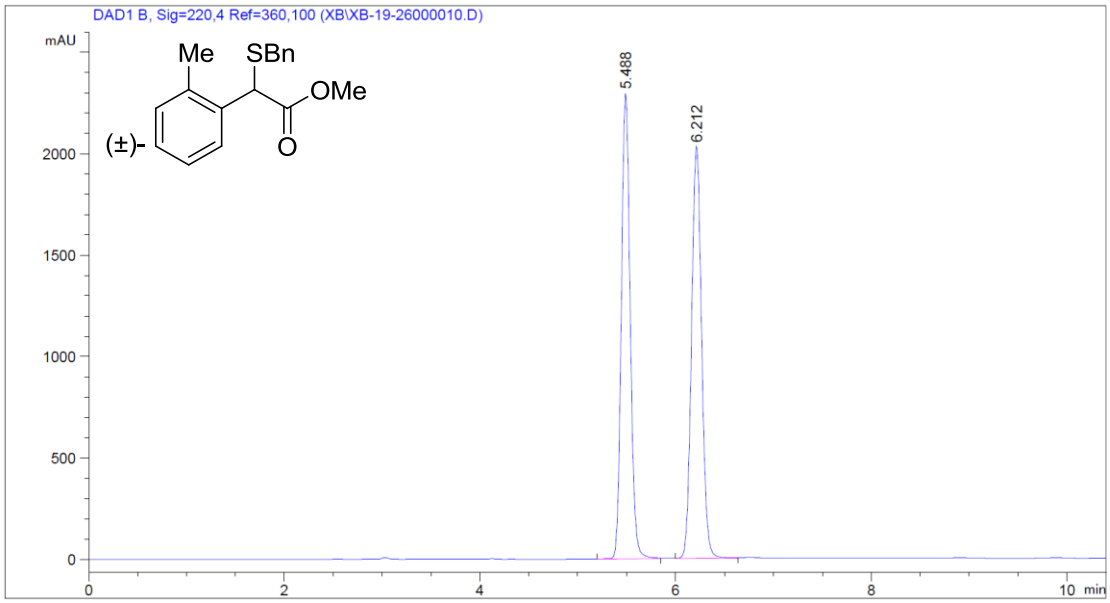


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.228	BV	0.1453	1.11519e4	1212.31604	49.3318
2	7.700	VB	0.1579	1.14540e4	1133.01489	50.6682

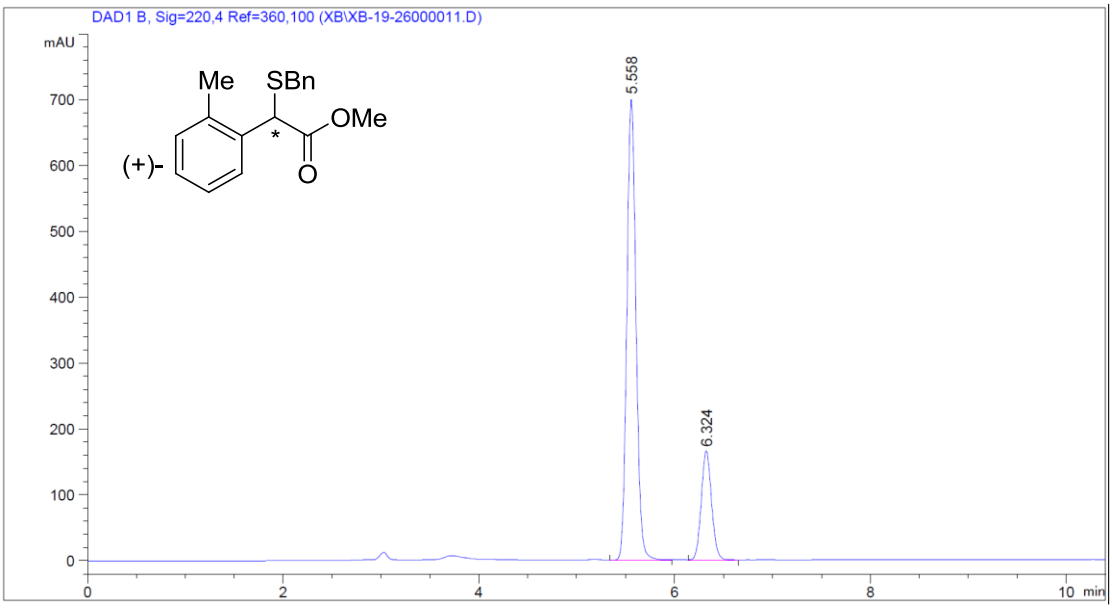


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.219	BV	0.1443	2.08224e4	2242.78613	94.7633
2	7.702	VB	0.1637	1150.66101	108.51464	5.2367

Methyl 2-(benzylthio)-2-*o*-tolylacetate (4ha)

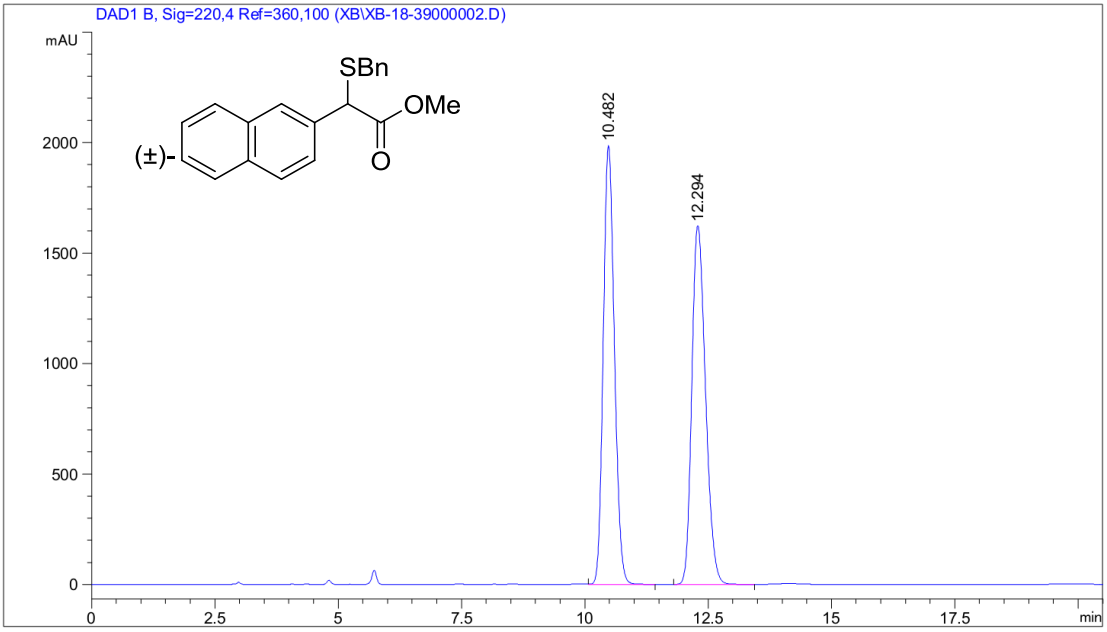


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.488	BV	0.0996	1.44683e4	2293.80615	49.8666
2	6.212	VV	0.1116	1.45457e4	2029.98193	50.1334

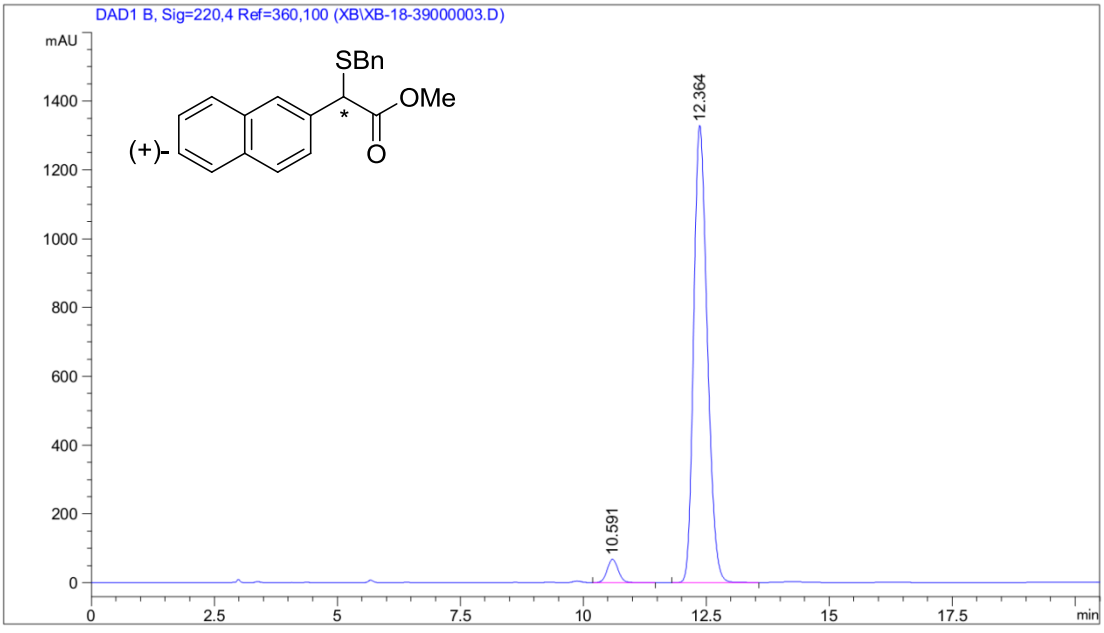


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.558	BV	0.0992	4518.58789	701.22833	78.8349
2	6.324	BB	0.1134	1213.12439	165.74094	21.1651

Methyl 2-(benzylthio)-2-(naphthalen-2-yl)acetate (4ia)

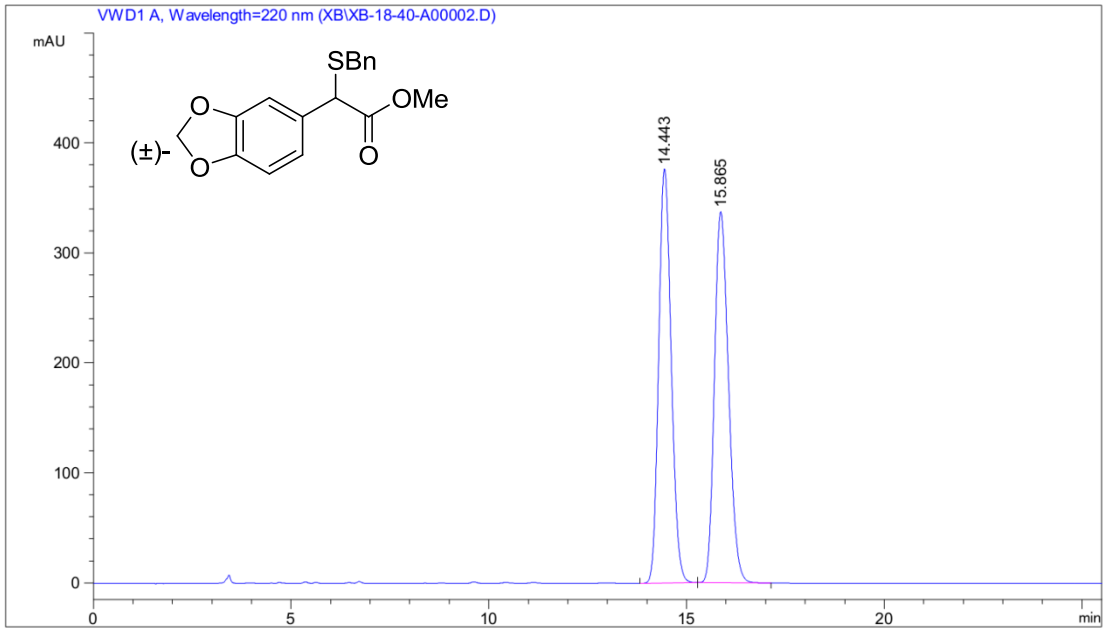


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.482	VV	0.2453	3.12019e4	1986.14172	49.9035
2	12.294	BV	0.2973	3.13227e4	1622.13232	50.0965

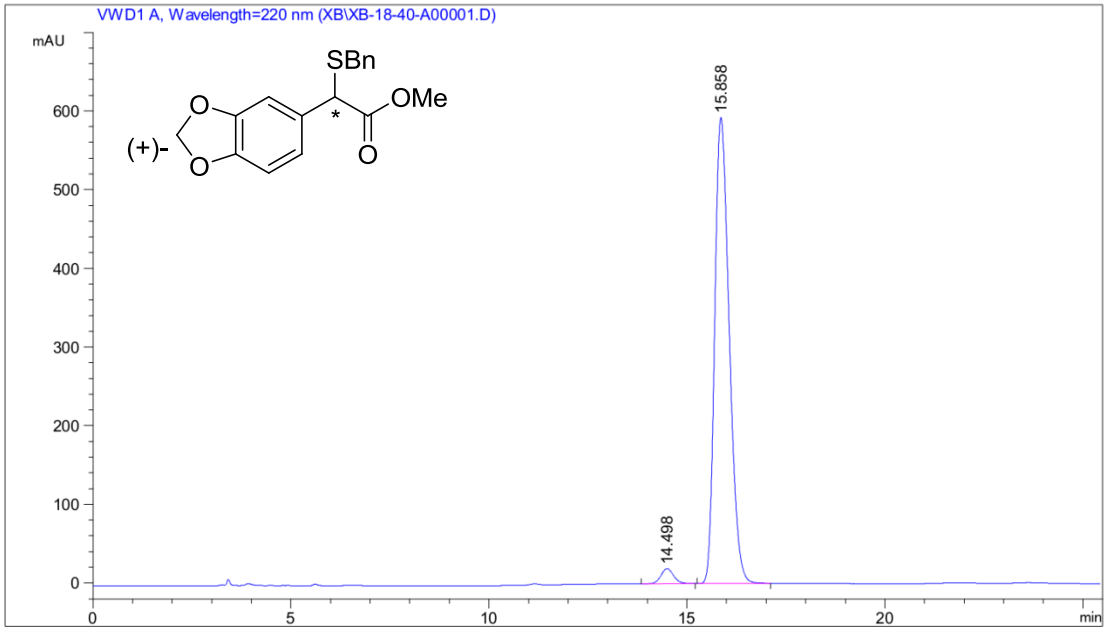


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.591	VB	0.2442	1056.32495	67.63370	3.9702
2	12.364	BV	0.3004	2.55497e4	1328.40381	96.0298

Methyl 2-(benzo[d][1,3]dioxol-5-yl)-2-(benzylthio)acetate (4ja)

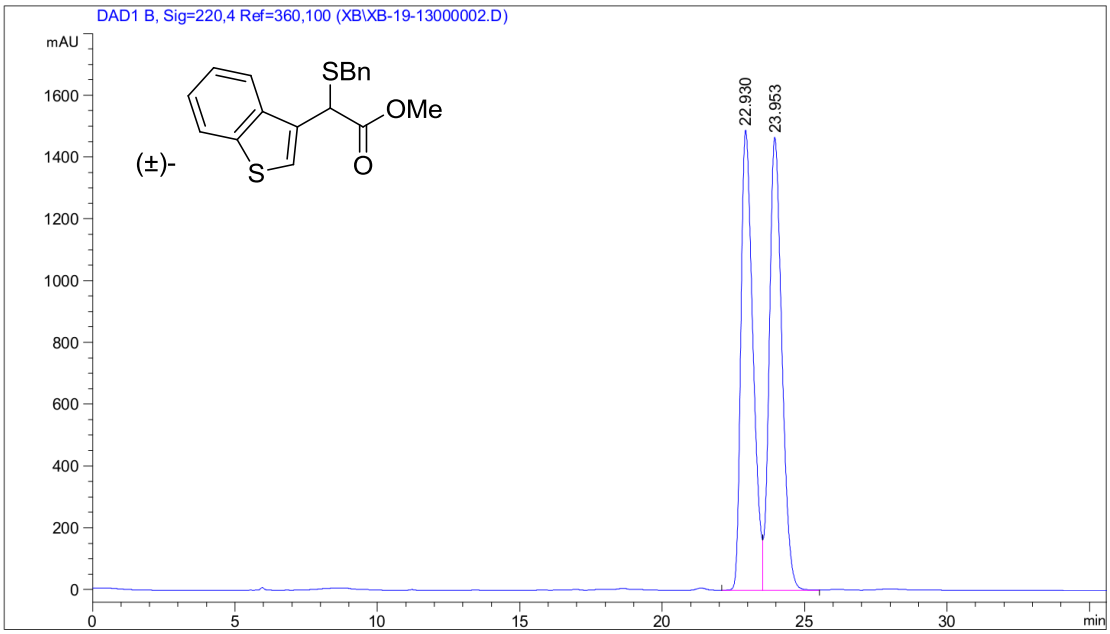


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.443	BB	0.3444	8297.42871	376.60632	49.8838
2	15.865	BB	0.3858	8336.09277	337.39456	50.1162

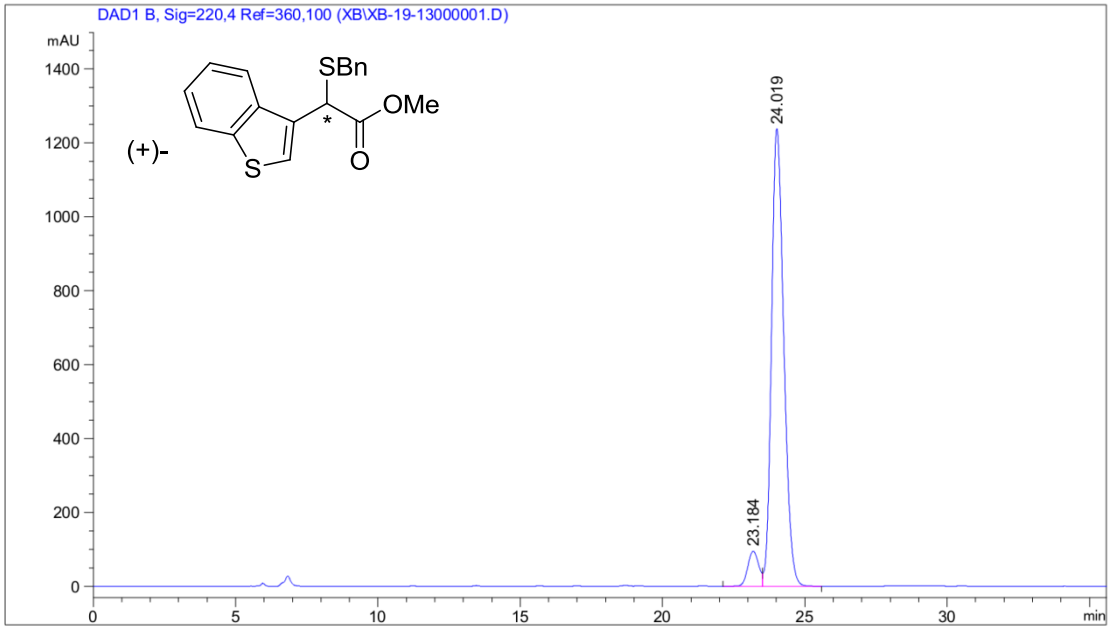


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.498	BB	0.3438	430.00943	19.23573	2.7758
2	15.858	BB	0.3971	1.50615e4	592.30389	97.2242

Methyl 2-(benzo[b]thiophen-3-yl)-2-(benzylthio)acetate (4ka)

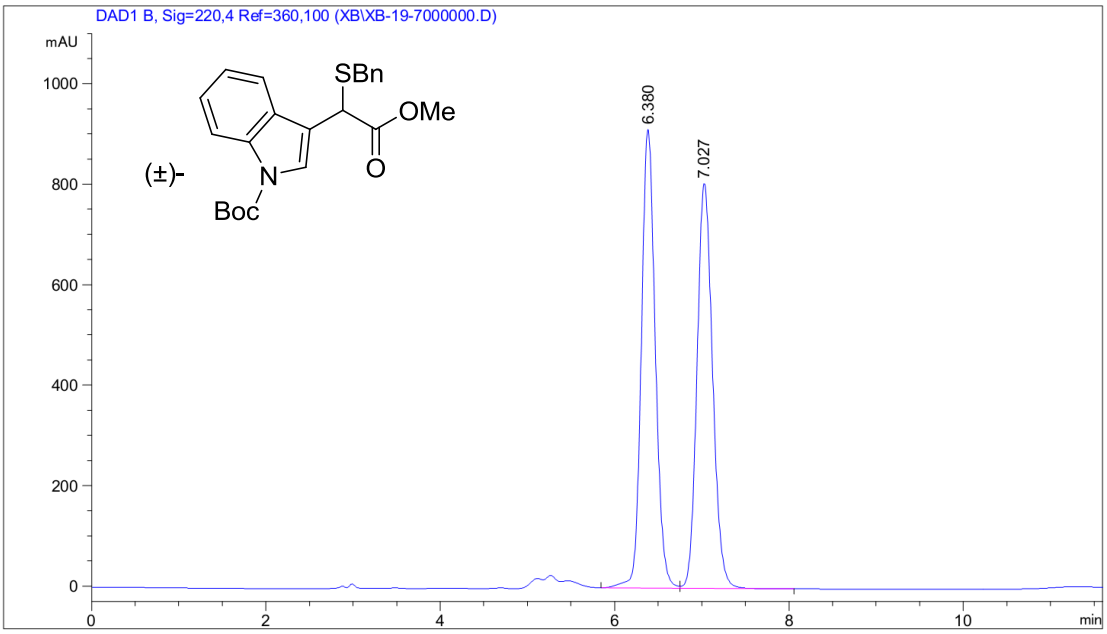


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.930	BV	0.4543	4.36969e4	1489.17297	49.1150
2	23.953	VV	0.4764	4.52717e4	1465.68042	50.8850

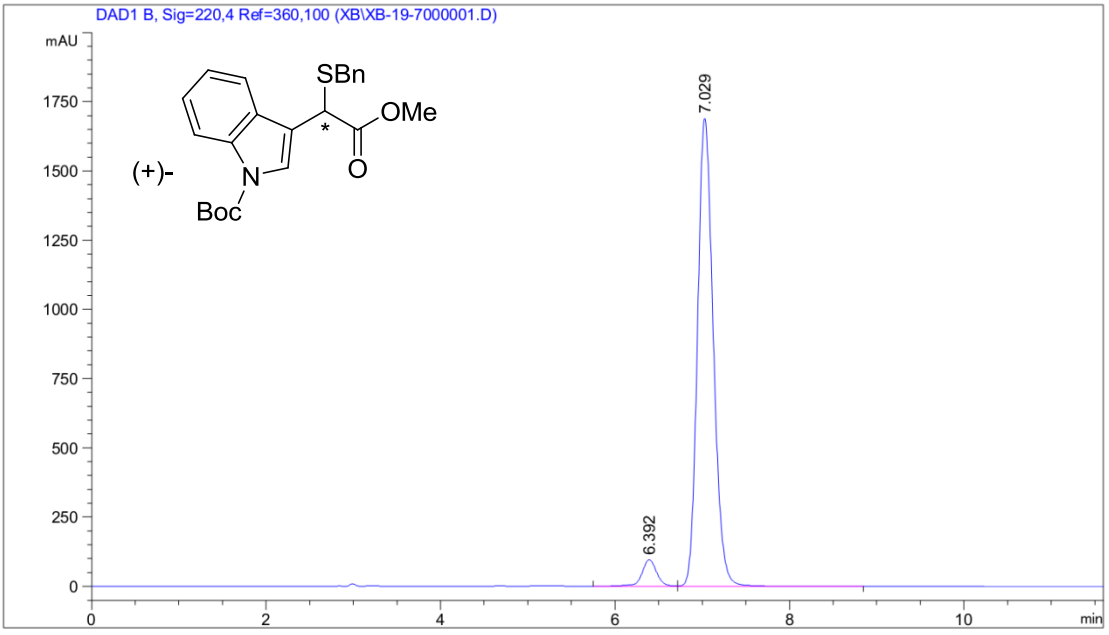


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.184	VV	0.4187	2577.92578	95.56606	6.4842
2	24.019	VV	0.4660	3.71790e4	1239.15613	93.5158

tert-Butyl 3-(1-(benzylthio)-2-methoxy-2-oxoethyl)-1H-indole-1-carboxylate (4la)

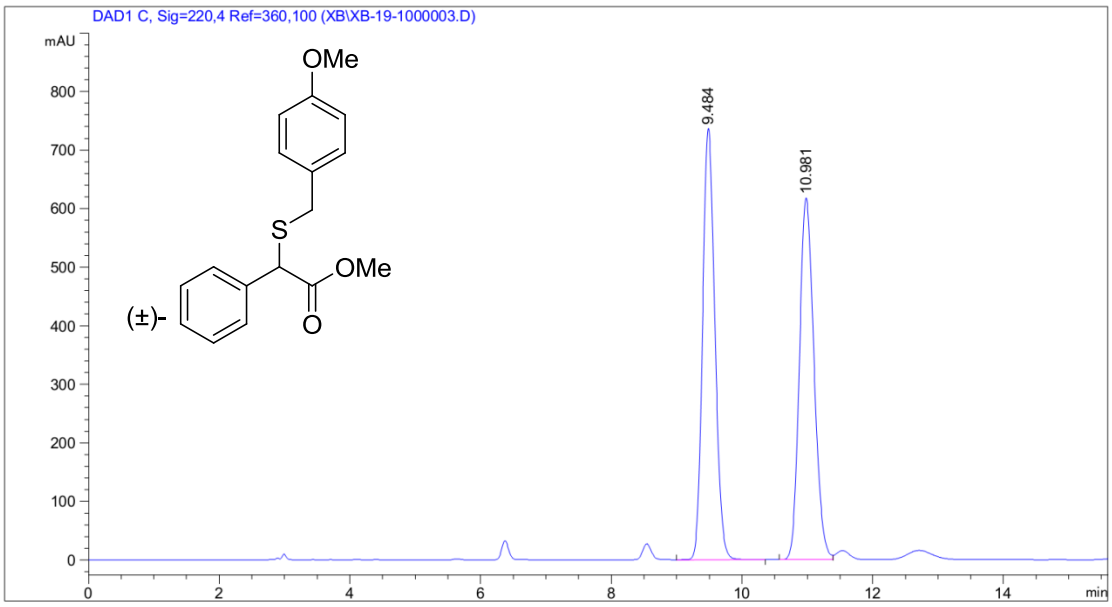


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.380	BV	0.1741	1.01850e4	913.59381	50.4749
2	7.027	VB	0.1927	9993.34863	805.99438	49.5251

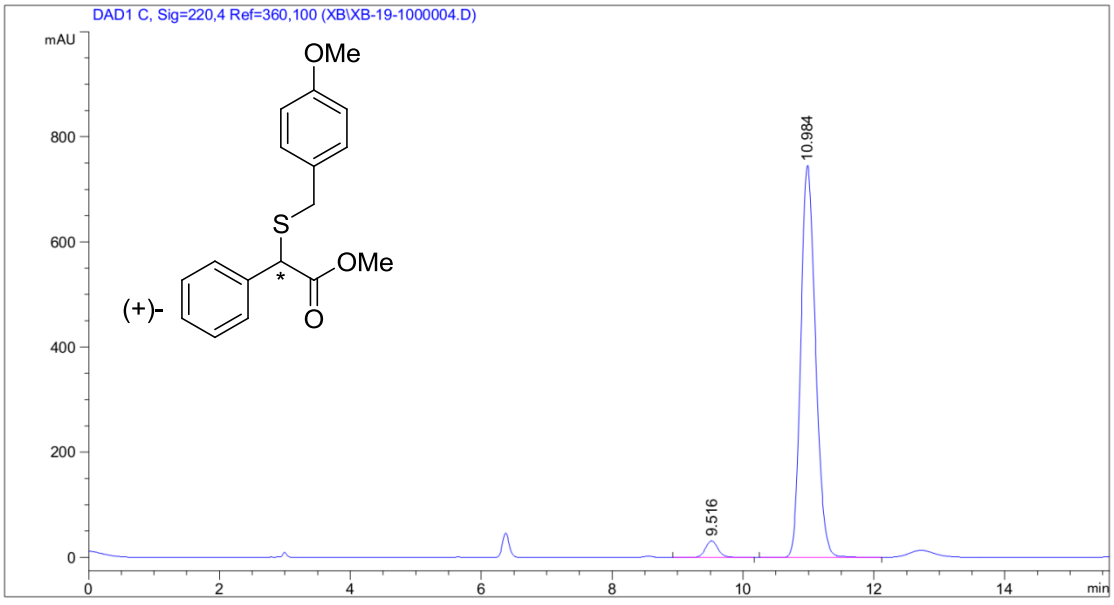


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.392	BV	0.1784	1121.57739	95.94312	5.0391
2	7.029	VB	0.1940	2.11358e4	1689.34387	94.9609

Methyl 2-(4-methoxybenzylthio)-2-phenylacetate (4ab)

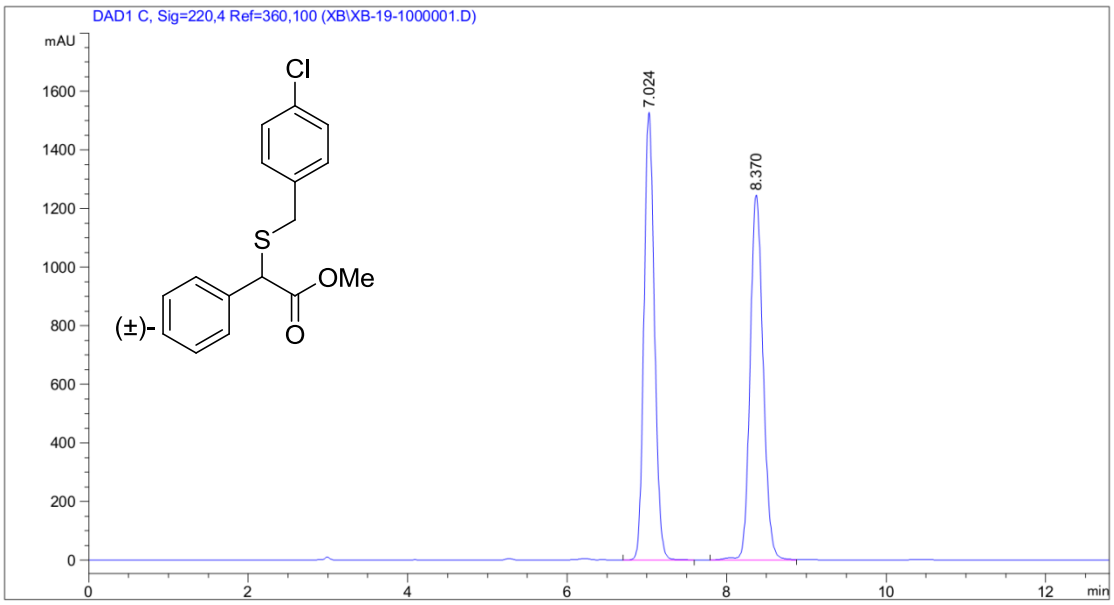


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.484	BB	0.2047	9625.59277	735.38440	49.9992
2	10.981	BV	0.2419	9625.91699	617.32813	50.0008

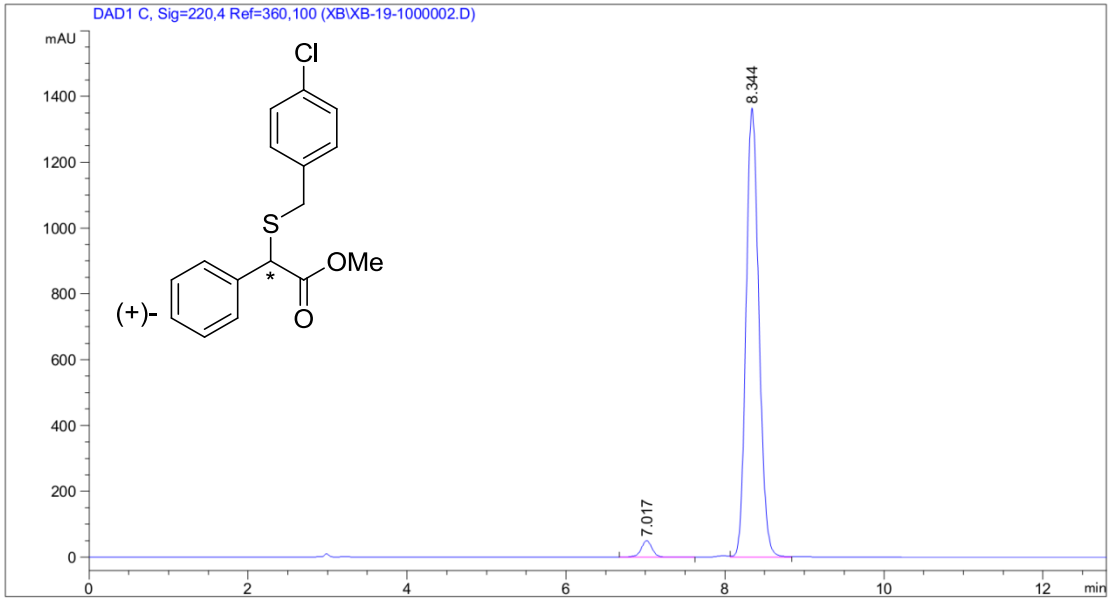


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.516	BB	0.2075	421.39734	31.61955	3.4808
2	10.984	BV	0.2469	1.16848e4	745.41724	96.5192

Methyl 2-(4-chlorobenzylthio)-2-phenylacetate (4ac)

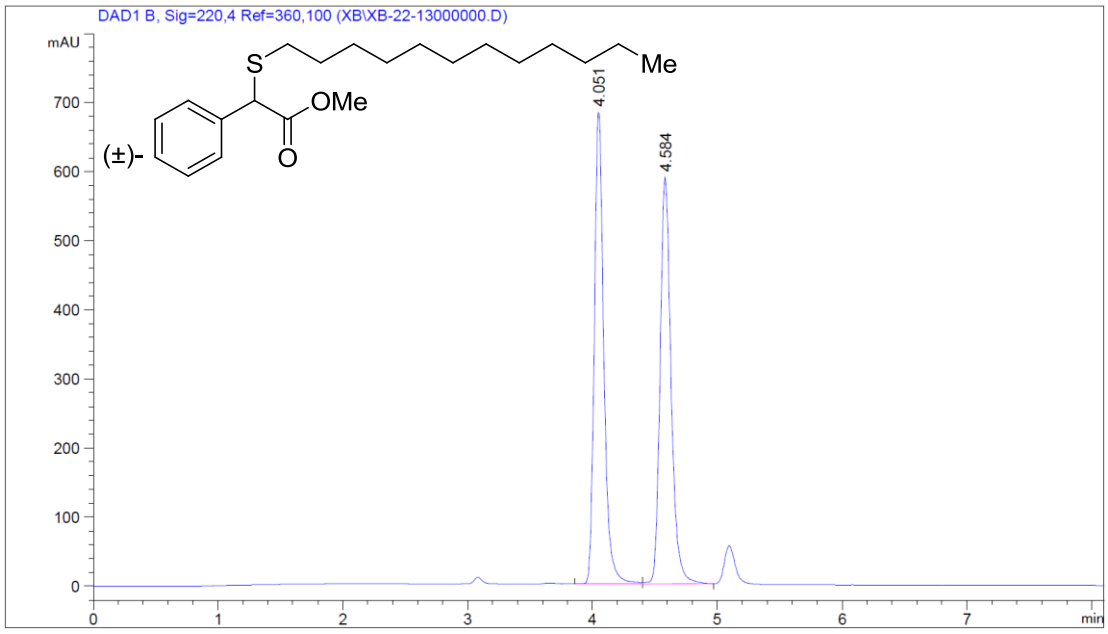


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.024	BV	0.1427	1.39807e4	1528.26758	49.7158
2	8.370	VV	0.1764	1.41406e4	1245.70959	50.2842

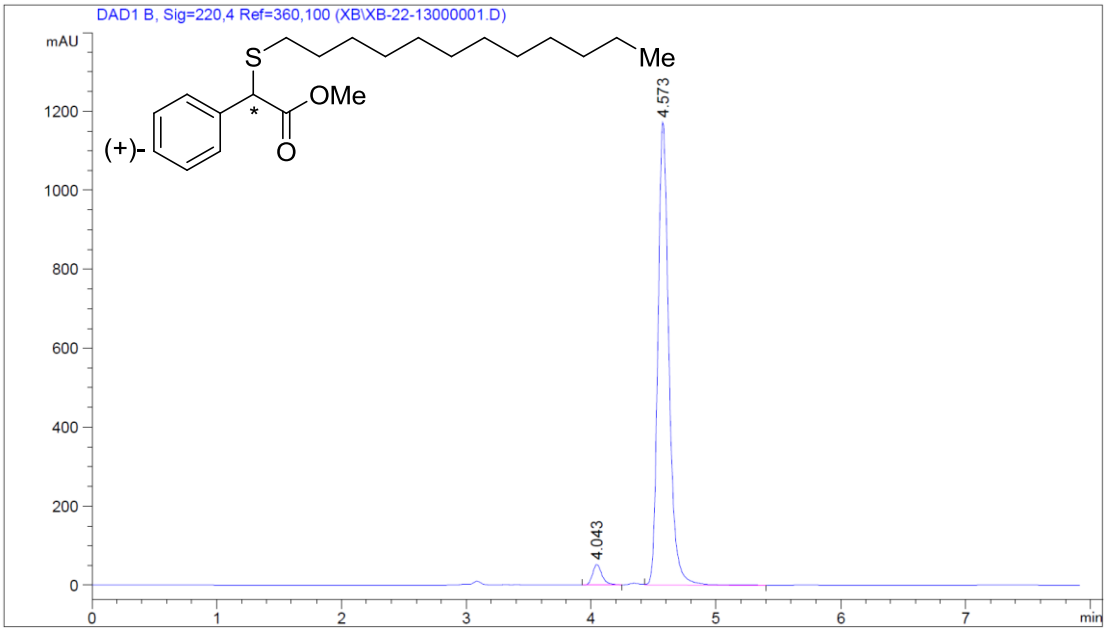


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.017	BB	0.1479	480.89456	50.12620	3.0466
2	8.344	VV	0.1789	1.53039e4	1364.48572	96.9534

Methyl 2-(dodecylthio)-2-phenylacetate (4ad)

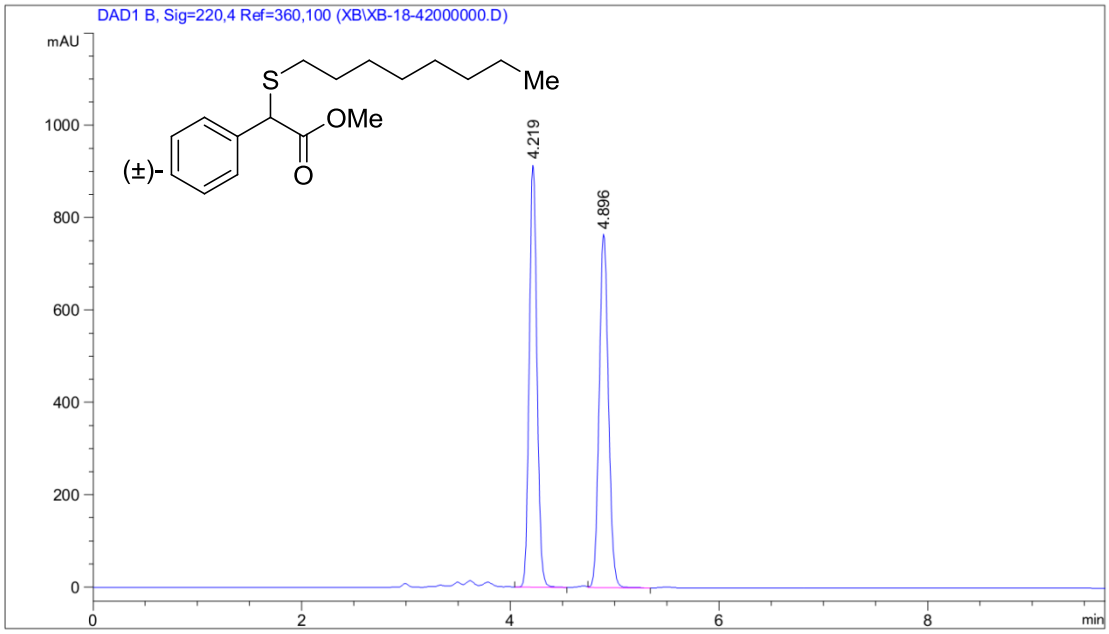


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.051	VV	0.0815	3610.85864	684.60443	50.0802
2	4.584	VB	0.0933	3599.29517	589.27026	49.9198

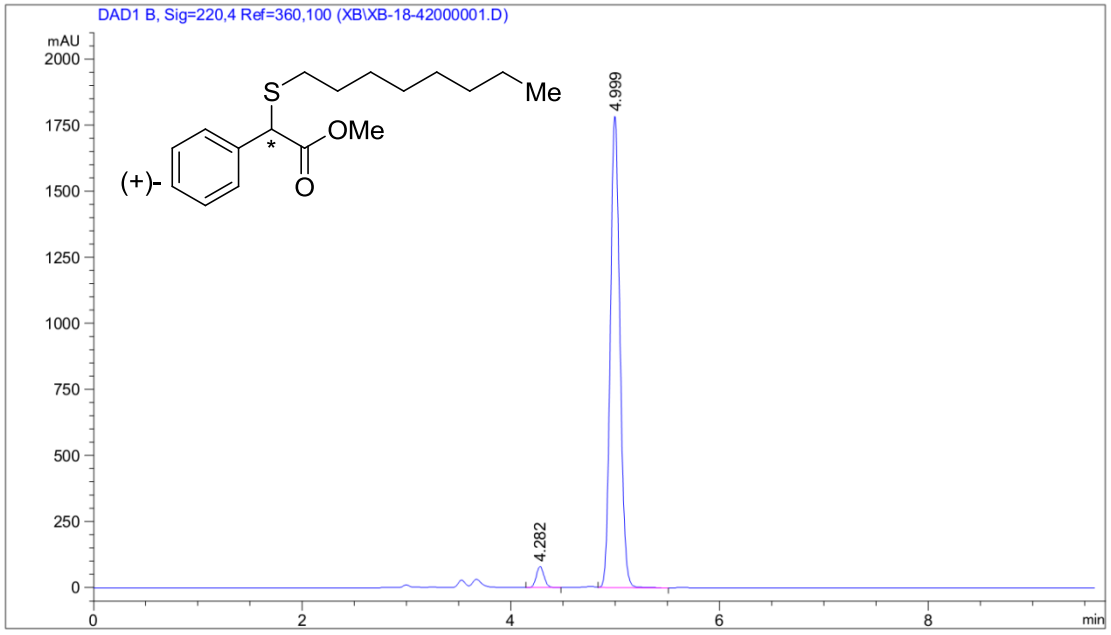


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.043	BB	0.0813	275.20172	52.40919	3.6898
2	4.573	VB	0.0934	7183.17383	1173.07996	96.3102

Methyl 2-(octylthio)-2-phenylacetate (4ae)

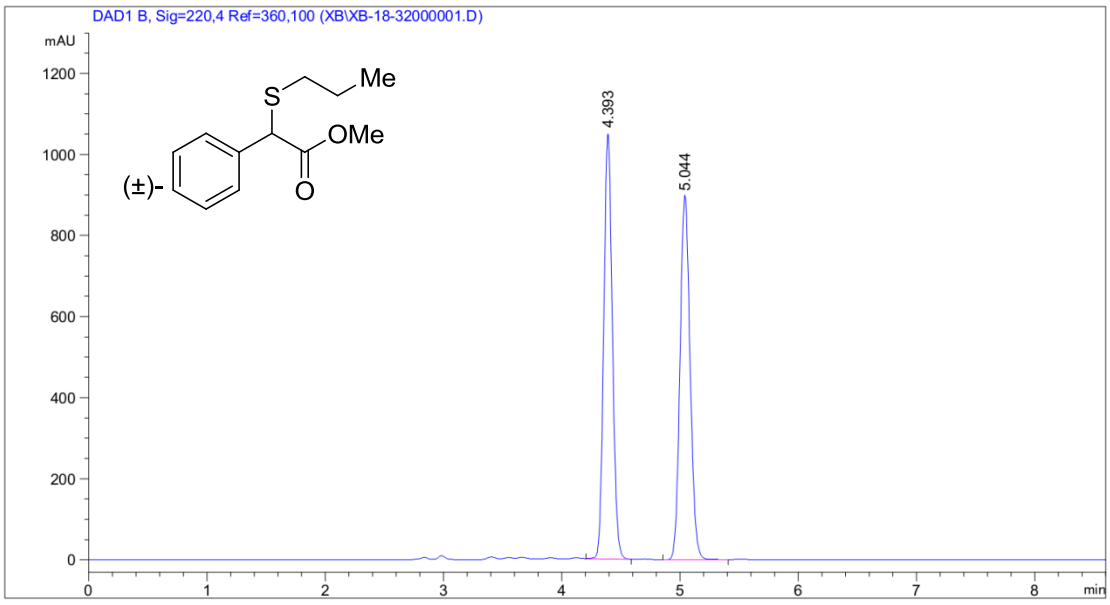


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.219	BB	0.0799	4707.39160	916.58887	49.9556
2	4.896	VB	0.0978	4715.76563	765.95728	50.0444

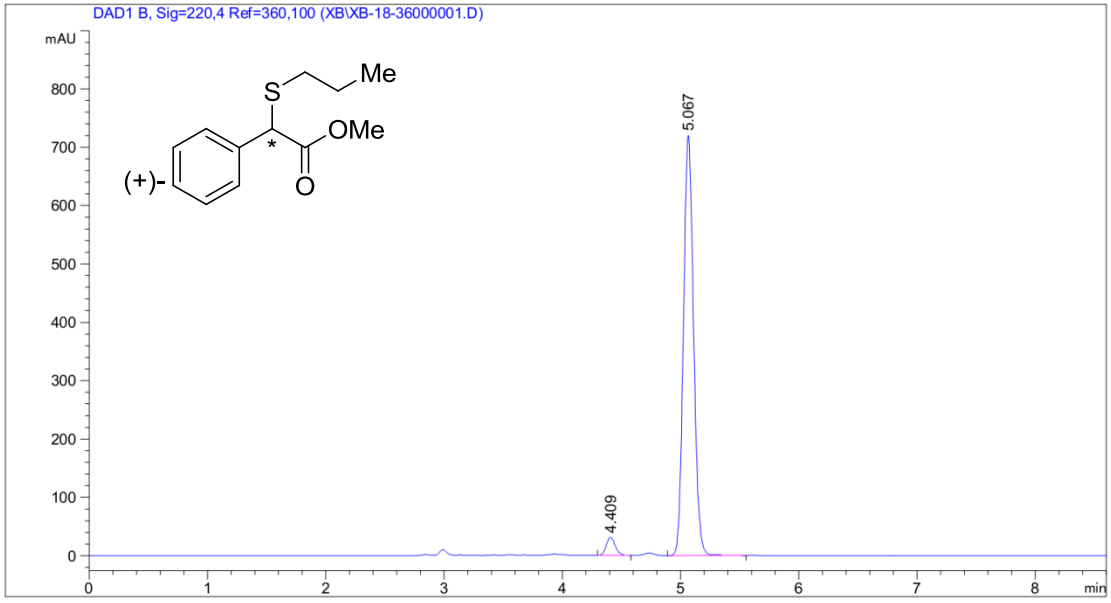


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.282	VB	0.0830	419.31628	80.17834	3.5610
2	4.999	VB	0.0982	1.13559e4	1784.80920	96.4390

Methyl 2-phenyl-2-(propylthio)acetate (4af)

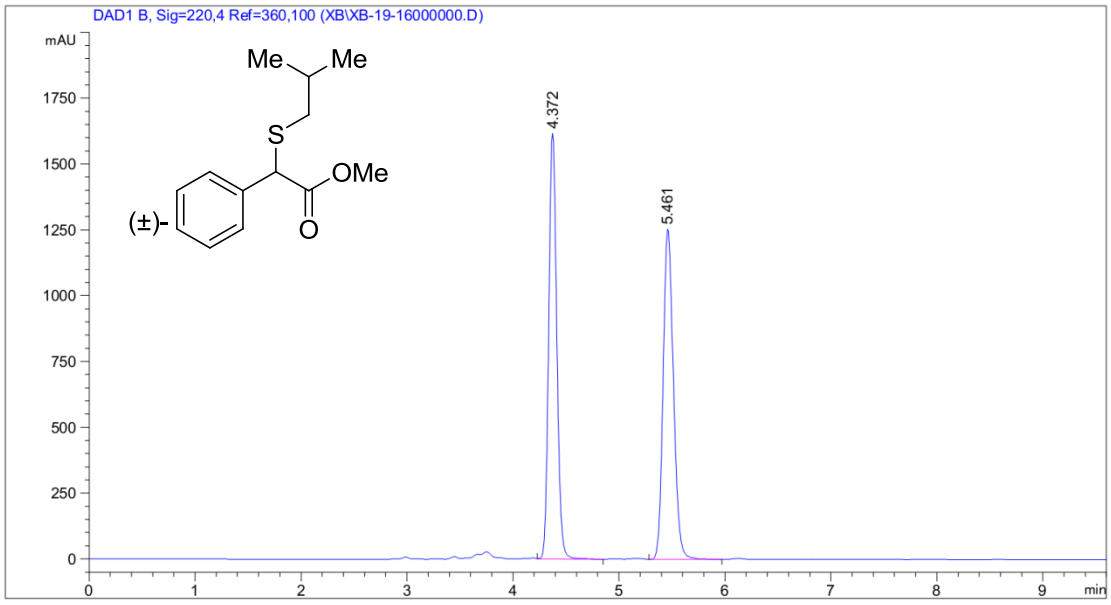


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.393	VV	0.0790	5324.70264	1053.16833	50.0268
2	5.044	BV	0.0909	5318.98730	900.18384	49.9732

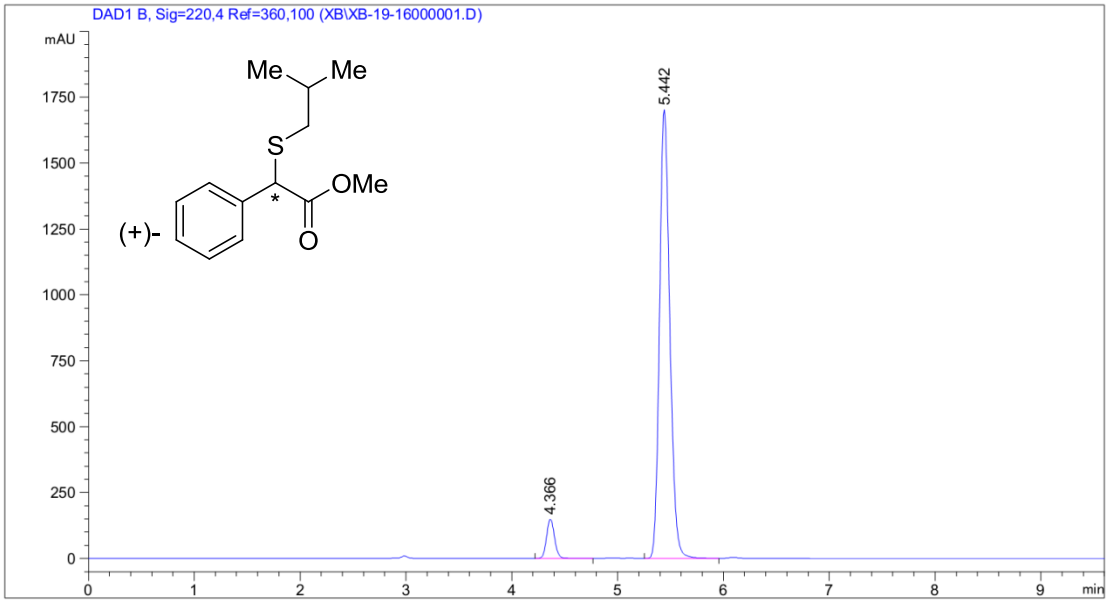


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.409	VB	0.0795	165.33537	31.38791	3.7208
2	5.067	BB	0.0913	4278.17920	720.24194	96.2792

Methyl 2-(isobutylthio)-2-phenylacetate (4ag)

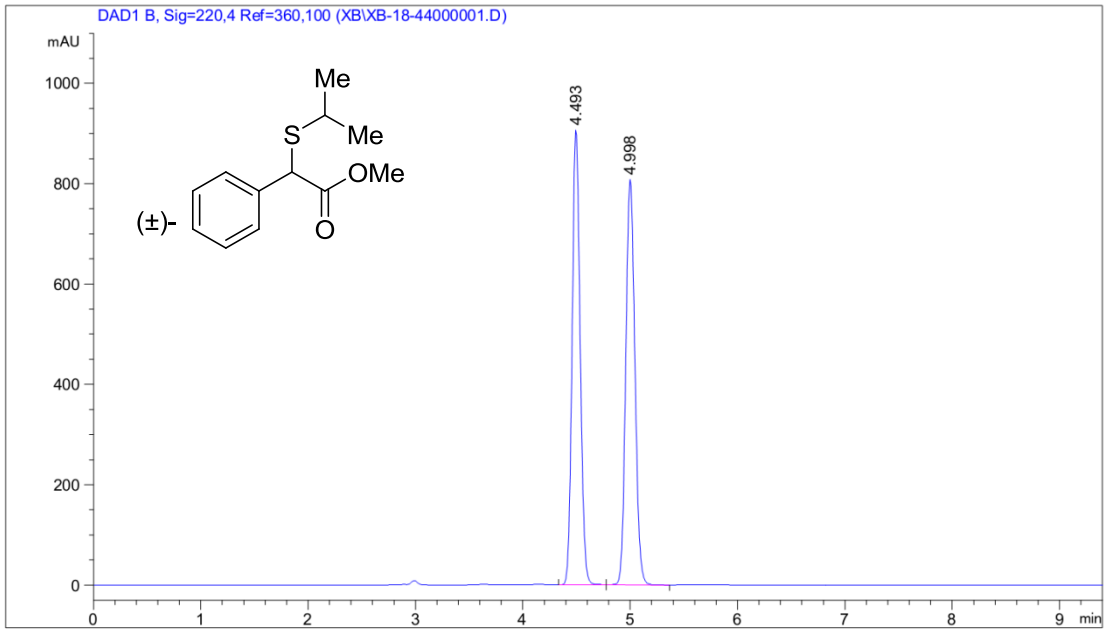


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.372	VB	0.0831	8463.05078	1616.84888	49.8804
2	5.461	BV	0.1050	8503.61914	1255.09863	50.1196

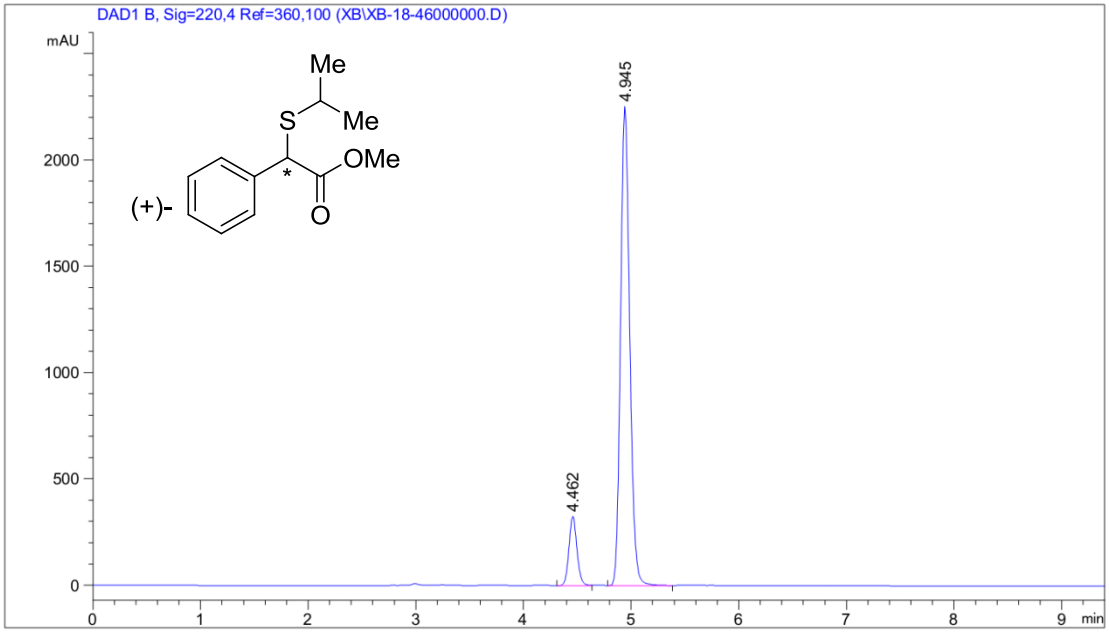


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.366	VB	0.0808	777.76495	149.19547	6.3156
2	5.442	BV	0.1051	1.15373e4	1702.64026	93.6844

Methyl 2-(isopropylthio)-2-phenylacetate (4ah)

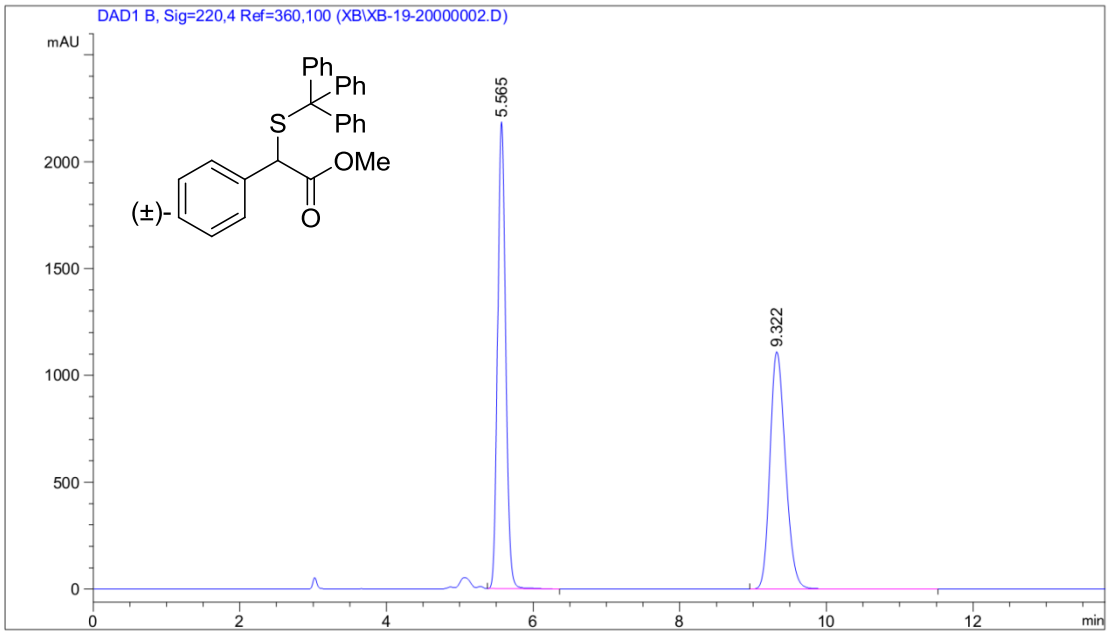


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.493	BB	0.0827	4720.08350	907.22754	49.9341
2	4.998	BB	0.0903	4732.54297	808.31989	50.0659

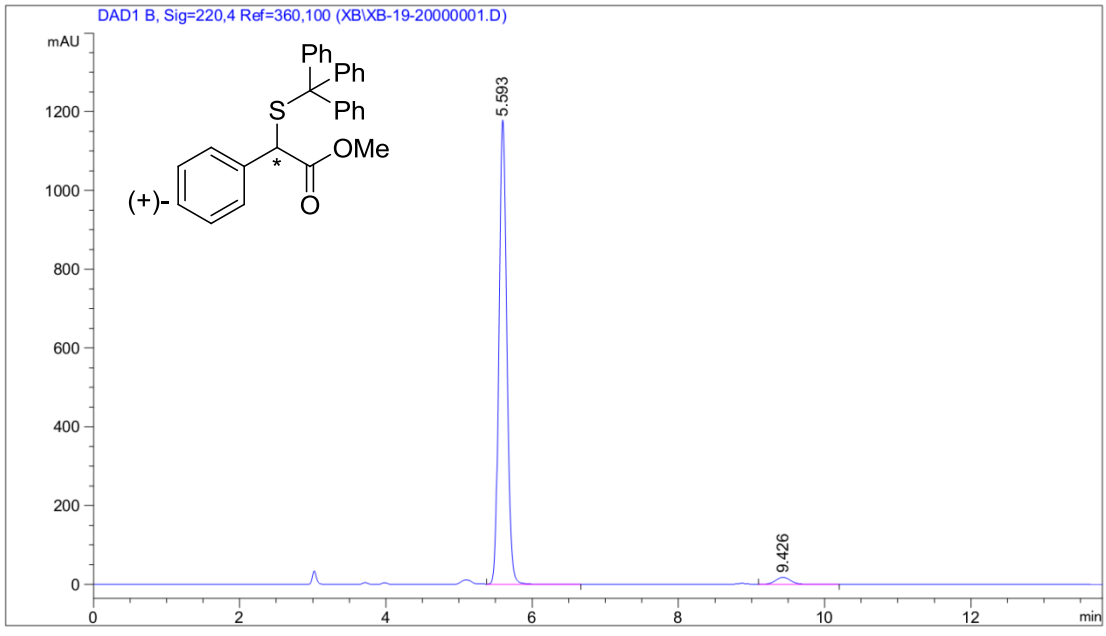


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.462	BV	0.0805	1687.21606	325.18579	11.1818
2	4.945	BB	0.0933	1.34018e4	2256.37036	88.8182

Methyl 2-phenyl-2-(tritylthio)acetate (4ai)

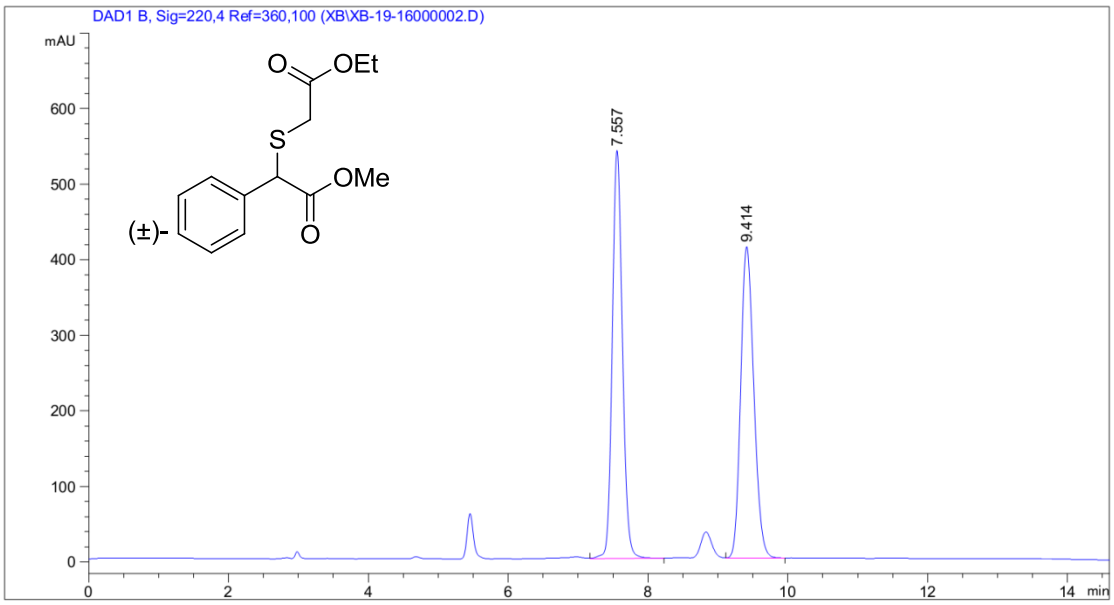


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.565	BB	0.1164	1.61870e4	2185.00049	49.8173
2	9.322	VB	0.2293	1.63057e4	1110.68042	50.1827

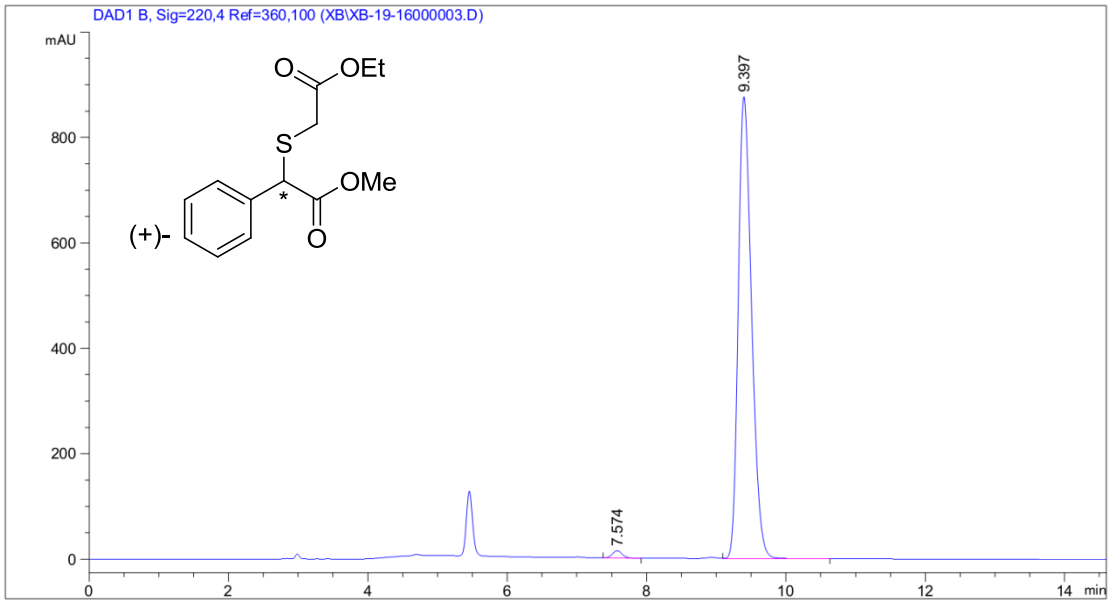


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.593	VB	0.1187	8746.23828	1177.31494	97.0191
2	9.426	VB	0.2303	268.72638	17.98456	2.9809

Methyl 2-(2-ethoxy-2-oxoethylthio)-2-phenylacetate (4aj)

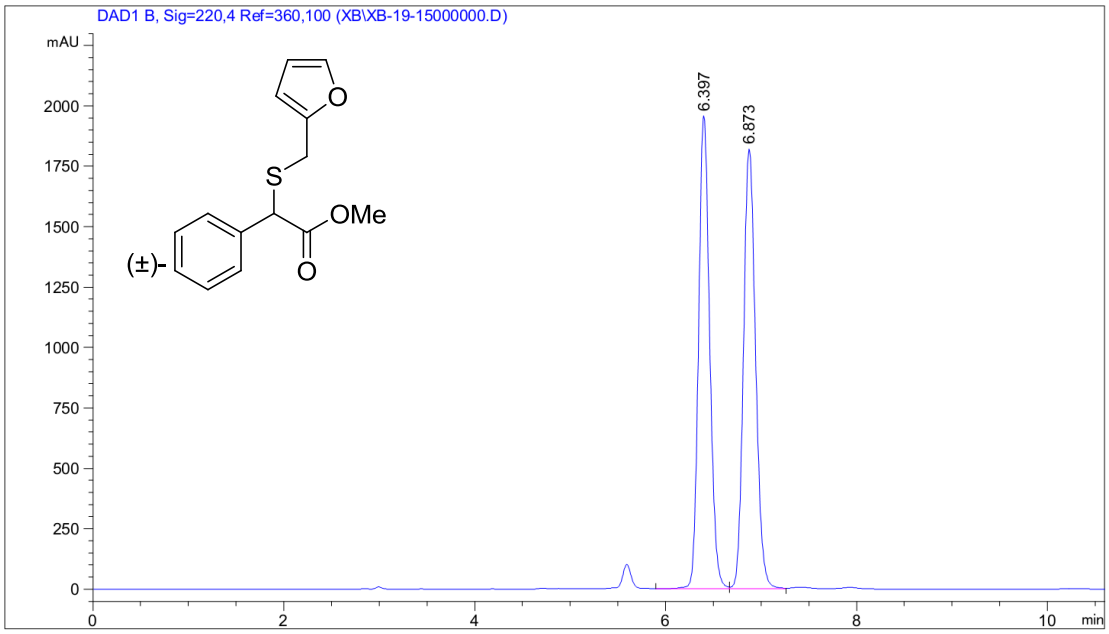


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.557	VB	0.1574	5434.08838	540.17615	50.1828
2	9.414	VV	0.2027	5394.50049	412.18359	49.8172

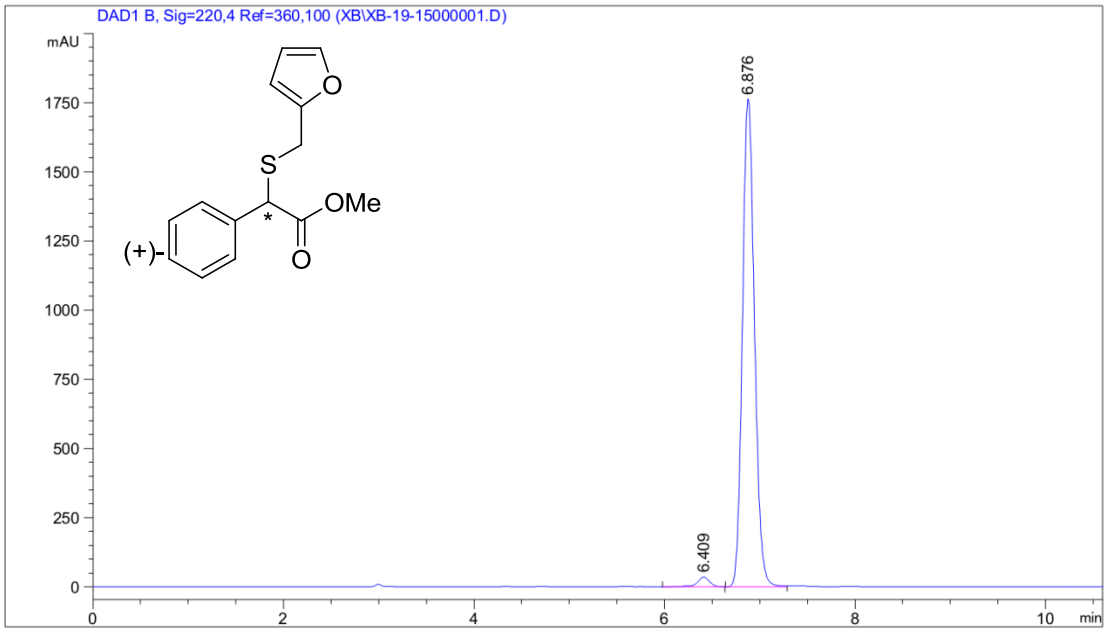


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.574	VB	0.1523	138.45624	14.13406	1.1724
2	9.397	VB	0.2075	1.16708e4	875.86151	98.8276

Methyl 2-(furan-2-ylmethylthio)-2-phenylacetate (4ak)

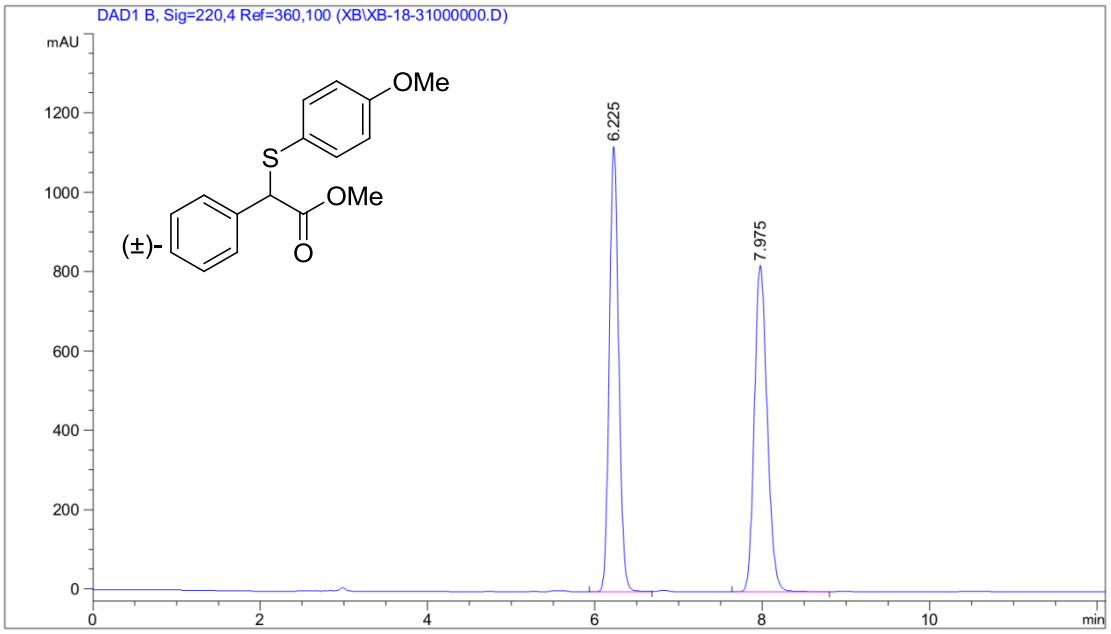


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.397	BV	0.1245	1.58508e4	1957.85510	49.7375
2	6.873	VV	0.1367	1.60181e4	1820.38757	50.2625

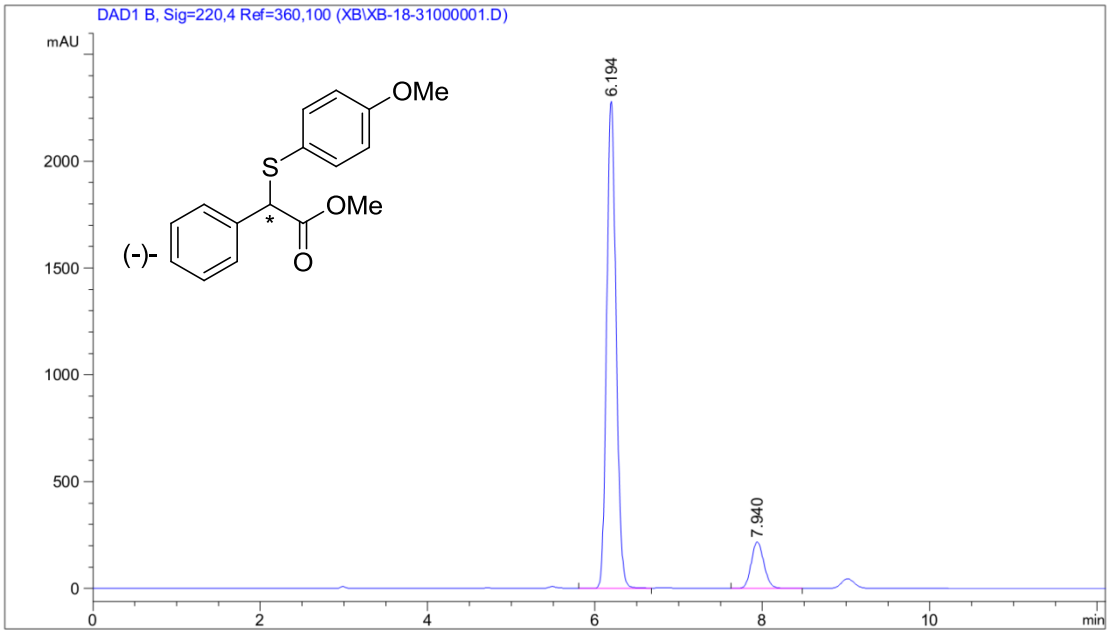


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.409	BB	0.1362	311.97241	34.94438	1.9790
2	6.876	BV	0.1344	1.54518e4	1760.62402	98.0210

(–)-Methyl 2-(4-methoxyphenylthio)-2-phenylacetate (4al)

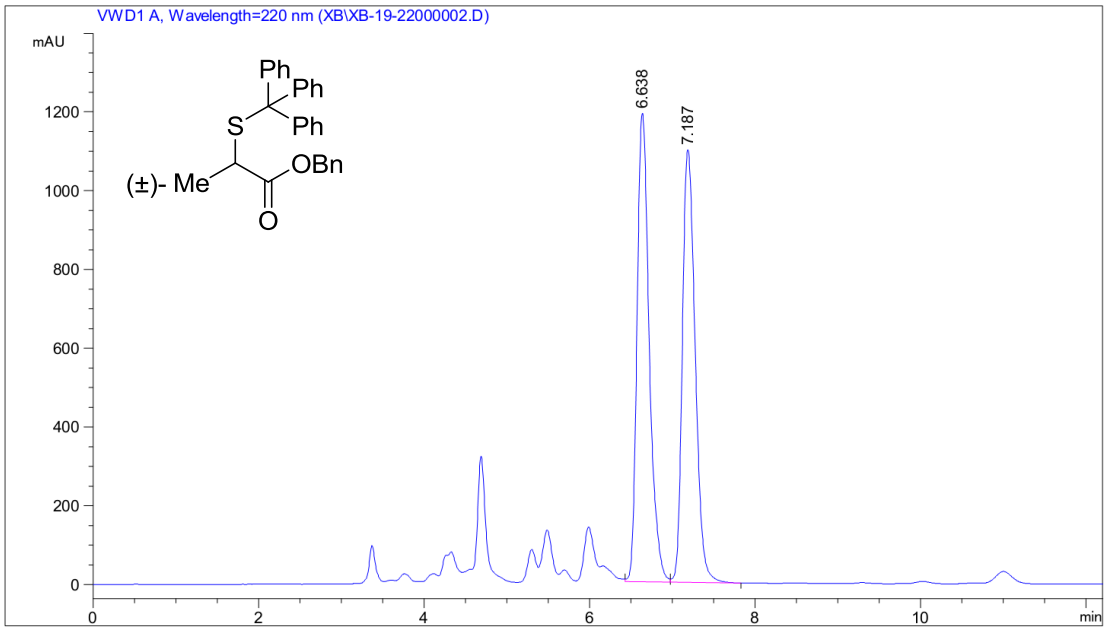


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.225	BV	0.1228	8742.88184	1122.98633	49.9374
2	7.975	BV	0.1662	8764.78516	823.07574	50.0626

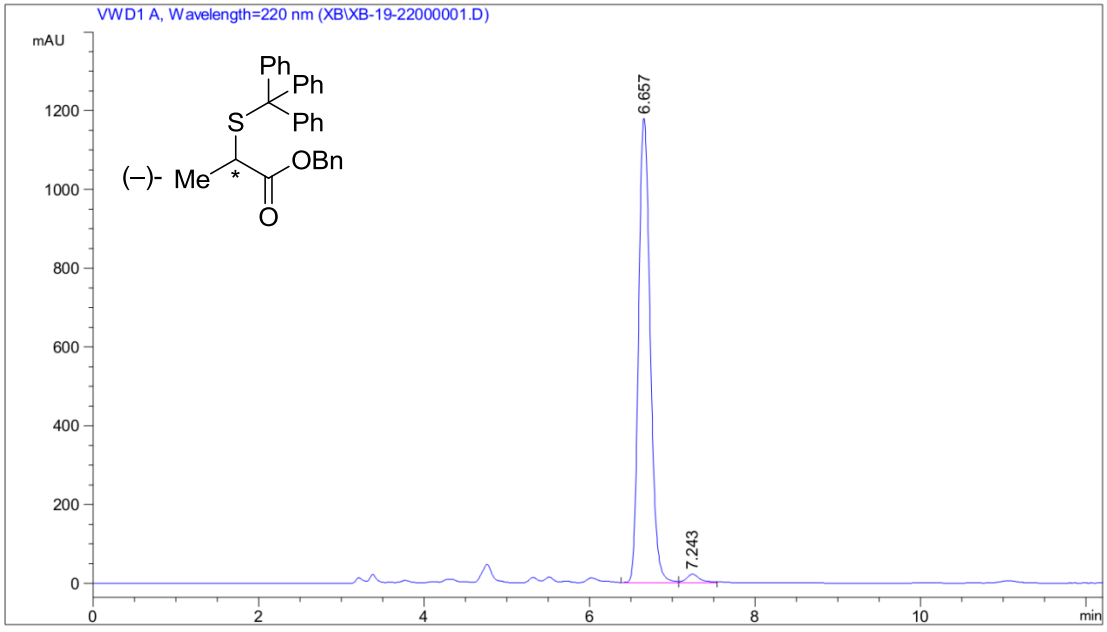


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.194	BV	0.1214	1.78622e4	2279.80835	88.6187
2	7.940	BB	0.1647	2294.03857	218.19154	11.3813

Benzyl 2-(tritylthio)propanoate (6)

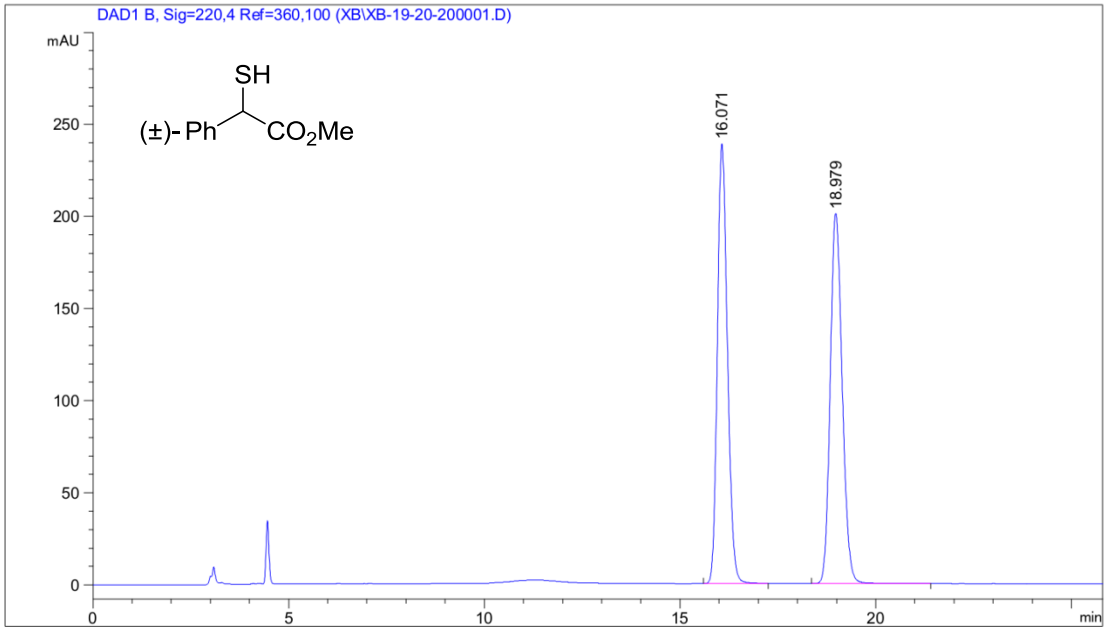


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.638	VV	0.1574	1.21887e4	1189.57971	50.8060
2	7.187	VB	0.1675	1.18020e4	1098.68616	49.1940

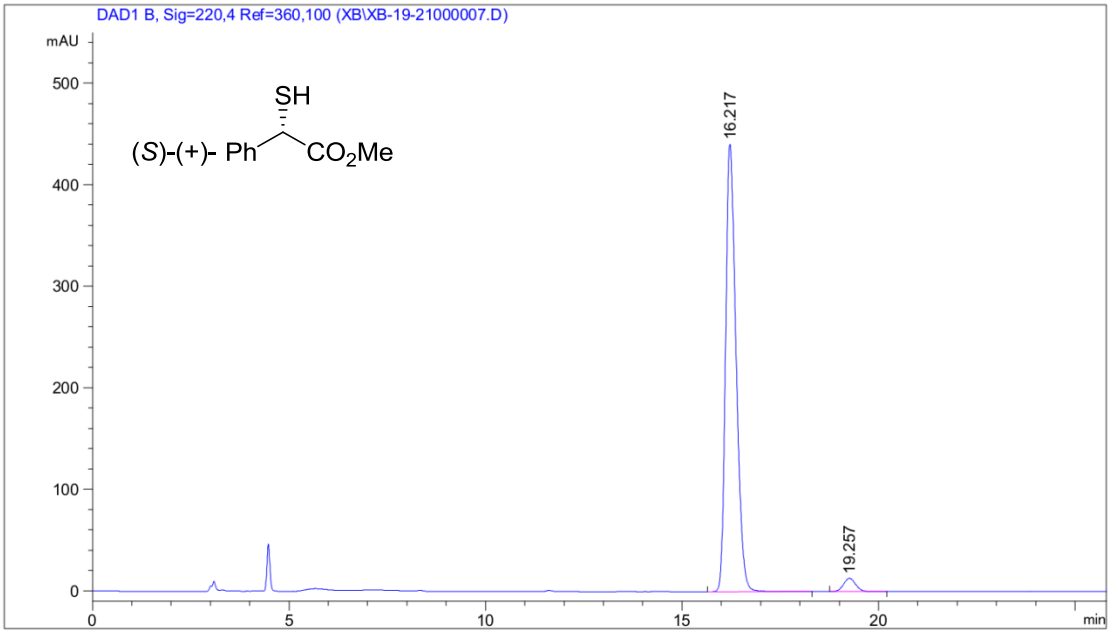


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.657	BV	0.1530	1.14895e4	1179.36584	97.8584
2	7.243	VV	0.1712	251.43896	21.76259	2.1416

Methyl thiomandelate

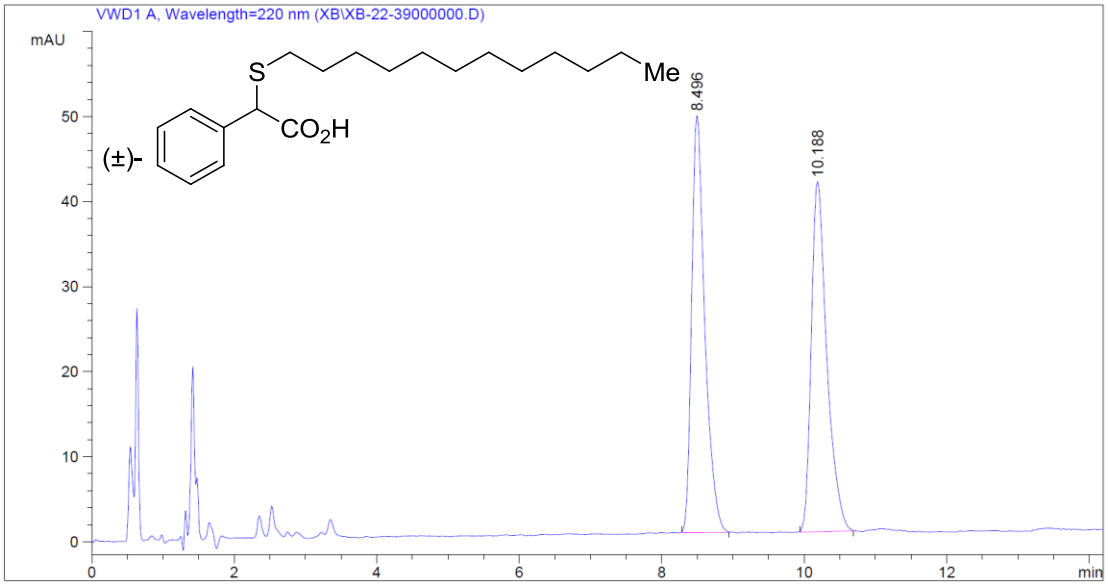


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.071	BB	0.2760	4258.92041	238.88882	49.9116
2	18.979	BB	0.3281	4274.00049	201.01649	50.0884

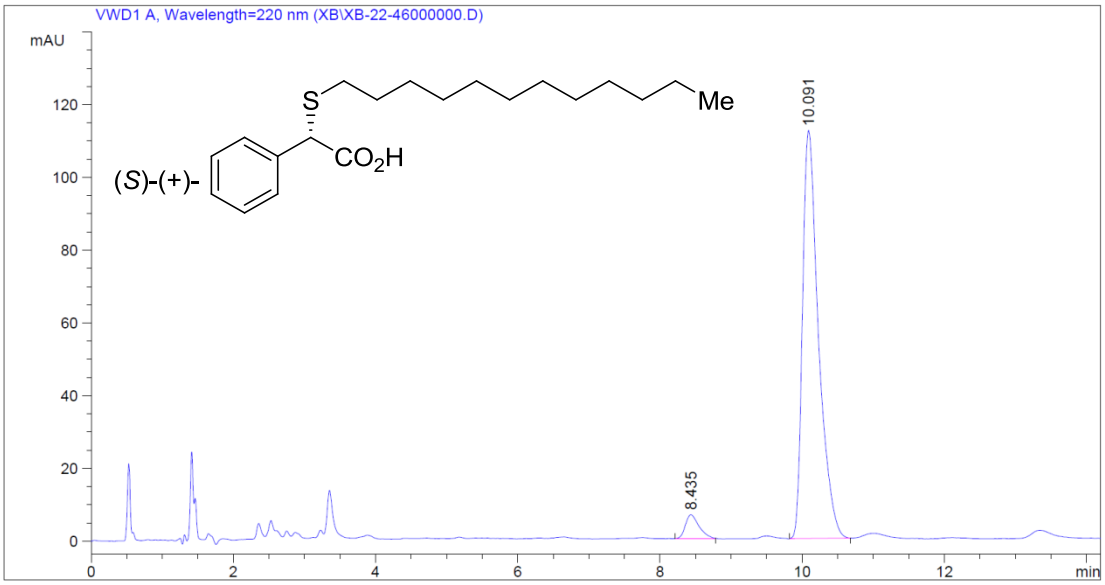


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.217	BB	0.2837	8152.71240	440.87500	96.6940
2	19.257	BB	0.3328	278.74664	13.06981	3.3060

2-(Dodecylthio)-2-phenylacetic acid (7)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	8.496	BB	0.1918	628.67206	50.2026
2	10.188	BB	0.2278	623.59821	49.7974



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Area %
1	8.435	BB	0.2024	88.72300	4.8311
2	10.091	BB	0.2342	1747.77979	95.1689

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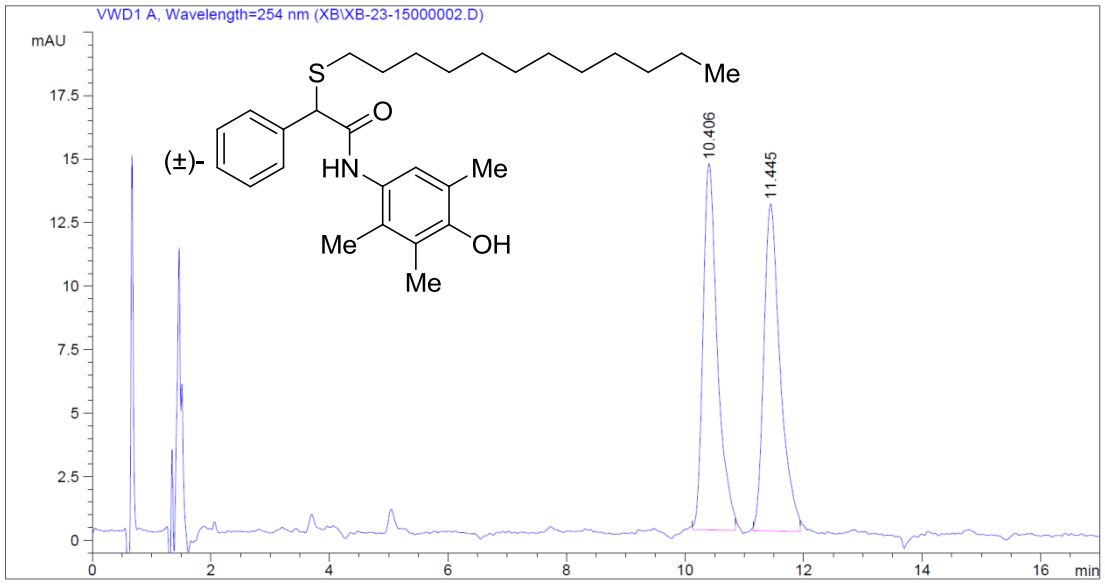
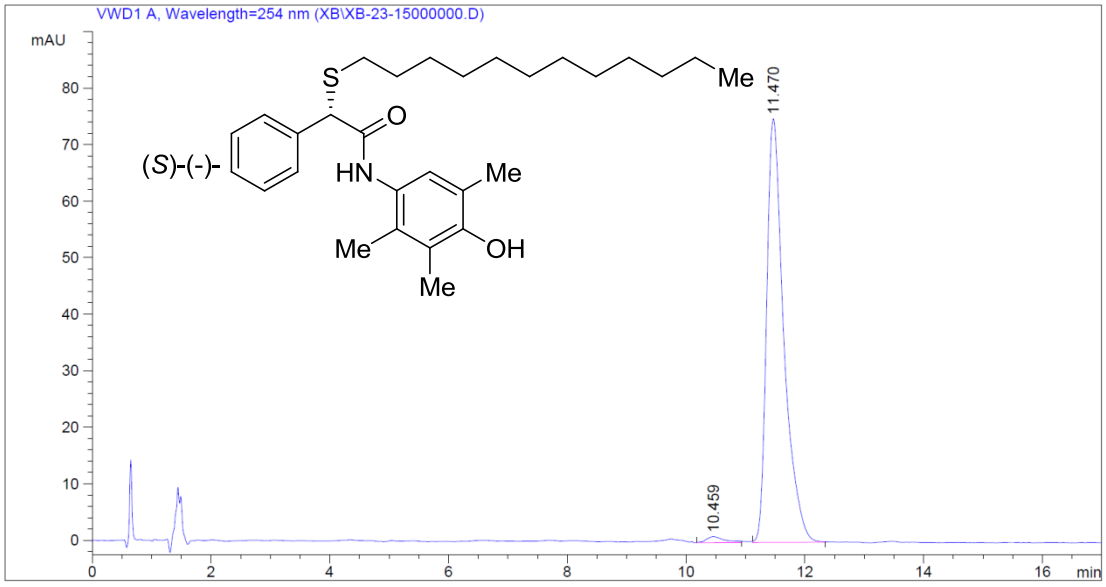


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Area %
1	10.406	BB	0.2531	244.35118		49.6407
2	11.445	BB	0.2871	247.88857		50.3593



Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Area %
1	10.459	BB	0.2916	21.66122		1.4175
2	11.470	BB	0.3001	1506.48755		98.5825