

# Stereoconvergent Arylations and Alkenylations of Unactivated Alkyl Electrophiles: The Catalytic Enantioselective Synthesis of Secondary Sulfonamides and Sulfones

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## Supporting Information

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### I. General Information

The following reagents were purchased and used as received: NiCl<sub>2</sub>·glyme (Strem), ZnI<sub>2</sub> (Strem), and Cp<sub>2</sub>ZrHCl (Strem). Ligands **L1** (available from Aldrich) and **L6** were prepared according to a literature procedure.<sup>1</sup> Grignard reagents were prepared from aryl bromides and magnesium turnings (Strem) or from aryl iodides and *i*-PrMgCl (Aldrich; 2.0 M in THF); on occasion, we have found purchased Grignard reagents to be less suitable. THF was deoxygenated and dried by sparging with argon followed by passage through an activated alumina column (S. G. Water) prior to use. All reactions were carried out in oven-dried glassware under an inert atmosphere.

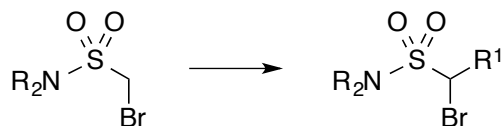
<sup>1</sup>H NMR data and <sup>13</sup>C NMR data were collected on a VARIAN 500 MHz spectrometer at ambient temperature. HPLC analyses were carried out on an Agilent 1100 series system with Daicel CHIRALPAK® columns or Daicel CHIRALCEL® columns (internal diameter 4.6 mm, column length 250 mm, particle size 5 μm or 3 μm). GC analyses were carried out on an Agilent 6890 series system with an HP-5 column (length 30 m, I.D. 0.25 mm).

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(1) Choi, J.; Fu, G. C. *J. Am. Chem. Soc.* **2012**, *134*, 9102–9105.

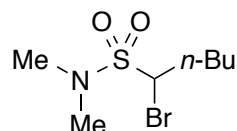
## II. Preparation of Electrophiles

These procedures have not been optimized.



### Representative experimental procedure for the preparation of $\alpha$ -bromosulfonamides.

LDA was prepared by the dropwise addition of *n*-BuLi (1.6 M in hexanes; 13.8 mL, 22 mmol) to a solution of *i*-Pr<sub>2</sub>NH (3.36 mL, 24.0 mmol) in THF (71 mL) in a 500-mL round-bottom flask at  $-78\text{ }^\circ\text{C}$ . The reaction mixture was stirred at  $0\text{ }^\circ\text{C}$  for 15 min, and then it was cooled to  $-78\text{ }^\circ\text{C}$ . A solution of the 1-bromomethanesulfonamide (20.0 mmol; prepared according to a literature procedure from bromomethanesulfonyl chloride<sup>2</sup> and a secondary amine<sup>3</sup>) in THF (40.0 mL) was added over 15 min to the LDA solution at  $-78\text{ }^\circ\text{C}$ . The mixture was stirred for 30 min, and then a solution of the alkyl bromide (26.0 mmol) in THF (43.3 mL) was added over 15 min. The solution was stirred at  $-78\text{ }^\circ\text{C}$  for 2 h, and then it was allowed to slowly warm to r.t. The reaction mixture was stirred at r.t. for 12 h, and then the reaction was quenched by the addition of saturated aqueous NH<sub>4</sub>Cl (100 mL). The mixture was extracted with Et<sub>2</sub>O (3  $\times$  50 mL), and the combined organic layers were rinsed with brine (50 mL), dried over MgSO<sub>4</sub>, and concentrated.



**1-Bromo-*N,N*-dimethylpentane-1-sulfonamide.** The title compound was prepared from 1-bromo-*N,N*-dimethylmethanesulfonamide (5.00 g, 24.7 mmol) and 1-bromobutane (3.45 mL, 32.2 mmol). The product was purified by column chromatography (3%  $\rightarrow$  20% ethyl acetate/hexanes): 3.00 g (47%). Colorless oil.

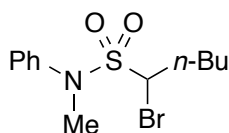
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  4.81 (dd, 1H, *J* = 10.7, 3.1 Hz), 3.03 (s, 6H), 2.34 (dddd, 1H, *J* = 14.4, 10.0, 5.5, 3.1 Hz), 2.10–2.02 (m, 1H), 1.70–1.61 (m, 1H), 1.47–1.30 (m, 3H), 0.94 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  63.3, 38.8, 32.9, 29.2, 21.9, 13.9.

FT-IR (neat) 2958, 2873, 2814, 1483, 1458, 1435, 1414, 1380, 1342, 1287, 1237, 1203, 1171, 1145, 1106, 1064, 973, 930, 782, 750, 734 cm<sup>-1</sup>.

MS (EI) *m/z* (M<sup>+</sup>) calcd for C<sub>7</sub>H<sub>16</sub>BrNO<sub>2</sub>S: 257, found: 257.

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- (2) Gao, F.; Yan, X.; Zahr, O.; Larsen, A.; Vong, K.; Auclair, K. *Bioorg. Med. Chem. Lett.* **2008**, *18*, 5518–5522.
- (3) Brienne, M.-J.; Varech, D.; Leclercq, M.; Jacques, J.; Radembino, N.; Dessalles, M.-C.; Mahuzier, G.; Gueyouche, C.; Bories, C. Loiseau, P.; Gayral, P. *J. Med. Chem.* **1987**, *30*, 2232–2239.



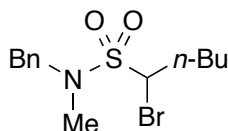
**1-Bromo-N-methyl-N-phenylpentane-1-sulfonamide.** The title compound was prepared from 1-bromo-N-methyl-N-phenylmethanesulfonamide (3.82 g, 14.5 mmol) and 1-bromobutane (2.02 mL, 18.8 mmol). The product was purified by column chromatography on silica gel (2%→15% ethyl acetate/hexanes) and then on C-18 silica gel (10%→100% acetonitrile/water): 3.60 g (78%). Colorless oil.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.50–7.48 (m, 2H), 7.43–7.39 (m, 2H), 7.35–7.31 (m, 1H), 4.74 (dd, 1H, *J* = 10.5, 3.1 Hz), 3.52 (s, 3H), 2.27 (dddd, 1H, *J* = 14.5, 10.2, 5.3, 3.1 Hz), 2.11–2.03 (m, 1H), 1.66–1.58 (m, 1H), 1.40–1.24 (m, 3H), 0.89 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 140.8, 129.7, 128.1, 127.3, 63.3, 42.0, 32.7, 29.1, 21.9, 13.9.

FT-IR (neat) 3062, 3039, 2957, 2931, 2872, 1595, 1493, 1466, 1453, 1436, 1351, 1270, 1237, 1183, 1143, 1106, 1068, 1026, 917, 886, 767, 725 cm<sup>-1</sup>.

MS (ESI) *m/z* (M<sup>+</sup>+H) calcd for C<sub>12</sub>H<sub>19</sub>BrNO<sub>2</sub>S: 320, found: 320.



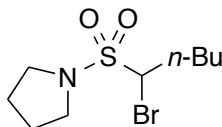
**N-Benzyl-1-bromo-N-methylpentane-1-sulfonamide.** The title compound was prepared from N-benzyl-1-bromo-N-methylmethanesulfonamide (3.75 g, 13.5 mmol) and 1-bromobutane (1.88 mL, 17.5 mmol). The product was purified by column chromatography (2%→15% ethyl acetate/hexanes): 2.04 g (45%). Light-yellow oil.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.39–7.35 (m, 4H), 7.34–7.30 (m, 1H), 4.84 (dd, 1H, *J* = 10.7, 3.1 Hz), 4.61 (d, 1H, *J* = 14.8 Hz), 4.36 (d, 1H, *J* = 14.8 Hz), 2.88 (s, 3H), 2.40 (dddd, 1H, *J* = 14.4, 10.0, 5.6, 3.1 Hz), 2.15–2.07 (m, 1H), 1.72–1.64 (m, 1H), 1.50–1.31 (m, 3H), 0.95 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 135.8, 128.9, 128.3, 128.2, 64.1, 55.5, 35.5, 32.9, 29.3, 21.9, 13.9.

FT-IR (neat) 3088, 3064, 3031, 2958, 2931, 2872, 1605, 1587, 1496, 1467, 1455, 1338, 1278, 1212, 1196, 1151, 1106, 1077, 1029, 994, 944, 910, 858, 787, 733 cm<sup>-1</sup>.

MS (ESI) *m/z* (M<sup>+</sup>+H) calcd for C<sub>13</sub>H<sub>21</sub>BrNO<sub>2</sub>S: 334, found: 334.



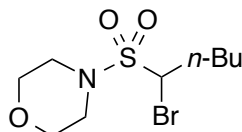
**1-((1-Bromopentyl)sulfonyl)pyrrolidine.** The title compound was prepared from 1-((bromomethyl)sulfonyl)pyrrolidine (3.02 g, 13.2 mmol) and 1-bromobutane (1.85 mL, 17.2 mmol). The product was purified by column chromatography (2%→15% ethyl acetate/hexanes): 1.96 g (52%). Light-yellow oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  4.84 (dd, 1H,  $J = 10.7, 3.1$  Hz), 3.62–3.56 (m, 2H), 3.49–3.43 (m, 2H), 2.36 (dddd, 1H,  $J = 14.4, 10.0, 5.6, 3.1$  Hz), 2.11–2.03 (m, 1H), 1.99–1.94 (m, 4H), 1.70–1.61 (m, 1H), 1.48–1.30 (m, 3H), 0.94 (t, 3H,  $J = 7.2$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  63.7, 49.4, 32.7, 29.3, 26.1, 21.9, 13.9.

FT-IR (neat) 2957, 2872, 1461, 1334, 1238, 1200, 1148, 1076, 1014, 929, 781  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+$ ) calcd for  $\text{C}_9\text{H}_{18}\text{BrNO}_2\text{S}$ : 283, found: 283.



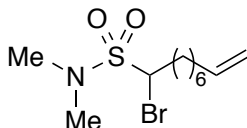
**4-((1-Bromopentyl)sulfonyl)morpholine.** The title compound was prepared from 4-((bromomethyl)sulfonyl)morpholine (3.01 g, 12.3 mmol) and 1-bromobutane (1.72 mL, 16.0 mmol). The product was purified by column chromatography (2%→20% ethyl acetate/hexanes): 1.28 g (35%). White solid.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  4.72 (dd, 1H,  $J = 10.7, 3.1$  Hz), 3.75–3.68 (m, 4H), 3.50–3.42 (m, 4H), 2.32 (dddd, 1H,  $J = 14.3, 9.9, 5.5, 3.0$  Hz), 2.05–1.97 (m, 1H), 1.67–1.58 (m, 1H), 1.45–1.27 (m, 3H), 0.92 (t, 3H,  $J = 7.2$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  67.0, 63.8, 47.3, 32.8, 29.1, 21.8, 13.8.

FT-IR (neat) 2959, 2925, 2860, 1467, 1460, 1450, 1434, 1347, 1328, 1299, 1261, 1237, 1204, 1153, 1114, 1074, 1014, 958, 846, 778, 732  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+$ ) calcd for  $\text{C}_9\text{H}_{18}\text{BrNO}_3\text{S}$ : 299, found: 299.



**1-Bromo-*N,N*-dimethylnon-8-ene-1-sulfonamide.** The title compound was prepared from 1-bromo-*N,N*-dimethylmethanesulfonamide (1.76 g, 8.71 mmol) and 8-bromo-1-octene (1.90 mL, 11.3 mmol). The product was purified by column chromatography (2%→20% ethyl acetate/hexanes): 1.30 g (48%). Colorless oil.

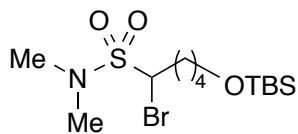
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  5.80 (ddt, 1H,  $J = 16.9, 10.2, 6.7$  Hz), 5.00 (ddt, 1H,  $J = 17.1, 2.2, 1.6$  Hz), 4.94 (ddt, 1H,  $J = 10.2, 2.2, 1.2$  Hz), 4.81 (dd, 1H,  $J = 10.6, 3.1$  Hz), 3.03 (s, 6H), 2.33 (dddd, 1H,  $J = 14.3, 10.0, 5.8, 3.1$  Hz), 2.10–2.02 (m, 3H), 1.71–1.63 (m, 1H), 1.48–1.25 (m, 7H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  139.0, 114.5, 63.3, 38.8, 33.8, 33.1, 28.8, 28.6, 27.1.

FT-IR (neat) 3075, 2923, 2852, 1640, 1479, 1454, 1414, 1340, 1285, 1204, 1143, 1063, 971, 907, 783  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{H}$ ) calcd for  $\text{C}_{11}\text{H}_{23}\text{BrNO}_2\text{S}$ : 312, found: 312.





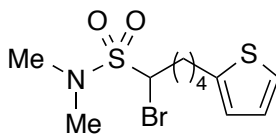
**1-Bromo-5-((*tert*-butyldimethylsilyl)oxy)-*N,N*-dimethylpentane-1-sulfonamide.** A 250-mL round-bottom flask was charged with 1-bromo-*N,N*-dimethylmethanesulfonamide (0.808 g, 4.00 mmol) and toluene (24 mL). *tert*-Butyl(4-iodobutoxy)dimethylsilane (5.03 g, 16.0 mmol), aqueous NaOH (50% w/v; 24 mL), and benzyltriethylammonium chloride (0.911 g, 4.00 mmol) were added to the solution at r.t. The resulting mixture was stirred at r.t. for 24 h, and then water (50 mL) was added. The organic phase was separated, and the aqueous solution was extracted with ethyl acetate (2 × 25 mL). The combined organic layers were dried over MgSO<sub>4</sub> and concentrated. The product was purified by column chromatography (hexanes→30% ethyl acetate/hexanes): 1.21 g (78%). Colorless oil.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.82 (dd, 1H, *J* = 10.7, 3.1 Hz), 3.62 (t, 2H, *J* = 6.1 Hz), 3.02 (s, 6H), 2.38–2.32 (m, 1H), 2.13–2.04 (m, 1H), 1.79–1.70 (m, 1H), 1.67–1.45 (m, 3H), 0.89 (s, 9H), 0.05 (s, 6H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 63.2, 62.6, 38.8, 33.0, 31.8, 26.1, 23.7, 18.5, –5.2.

FT-IR (neat) 2952, 2929, 2885, 2856, 1471, 1462, 1389, 1343, 1287, 1256, 1205, 1146, 1127, 1106, 1006, 973, 939, 836, 812, 776, 740 cm<sup>-1</sup>.

MS (ESI) *m/z* (*M*<sup>+</sup>+H) calcd for C<sub>13</sub>H<sub>31</sub>BrNO<sub>3</sub>SSi: 388, found: 388.



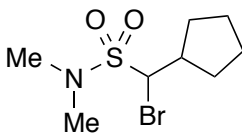
**1-Bromo-*N,N*-dimethyl-5-(thiophen-2-yl)pentane-1-sulfonamide.** The title compound was prepared from 1-bromo-*N,N*-dimethylmethanesulfonamide (3.00 g, 14.8 mmol) and 2-(4-bromobutyl)thiophene (4.23 g, 19.3 mmol). The product was purified by column chromatography (3%→20% ethyl acetate/hexanes): 1.44 g (29%). Light-yellow solid.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.12 (dd, 1H, *J* = 5.1, 1.2 Hz), 6.92 (dd, 1H, *J* = 5.1, 3.4 Hz), 6.79 (dddd, 1H, *J* = 3.3, 1.0, 1.0, 1.0 Hz), 4.80 (dd, 1H, *J* = 10.5, 3.2 Hz), 3.02 (s, 6H), 2.92–2.82 (m, 2H), 2.40–2.34 (m, 1H), 2.14–2.07 (m, 1H), 1.80–1.69 (m, 3H), 1.56–1.47 (m, 1H).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 144.8, 126.9, 124.4, 123.2, 63.0, 38.8, 33.0, 30.9, 29.7, 26.6.

FT-IR (neat) 2935, 2857, 1480, 1454, 1414, 1340, 1286, 1203, 1180, 1145, 1063, 972, 850, 784 cm<sup>-1</sup>.

MS (ESI) *m/z* (*M*<sup>+</sup>+H) calcd for C<sub>11</sub>H<sub>19</sub>BrNO<sub>2</sub>S<sub>2</sub>: 340, found: 340.



**1-Bromo-1-cyclopentyl-*N,N*-dimethylmethanesulfonamide.** The title compound was prepared from 1-bromo-*N,N*-dimethylmethanesulfonamide (3.03 g, 15.0 mmol) and cyclopentyl

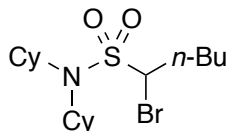
4-methylbenzenesulfonate (4.69 g, 19.5 mmol). The product was purified by column chromatography (10% ethyl acetate/hexanes): 668 mg (16%). Colorless oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  4.99 (d, 1H,  $J = 4.8$  Hz), 3.00 (s, 6H), 2.66–2.59 (m, 1H), 1.99–1.88 (m, 2H), 1.75–1.55 (m, 5H), 1.54–1.45 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  68.5, 41.8, 38.7, 31.8, 30.0, 25.6, 25.5.

FT-IR (neat) 2947, 2869, 2812, 1481, 1452, 1413, 1333, 1284, 1205, 1180, 1142, 1063, 969, 898, 862, 786  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+ - \text{Br}$ ) calcd for  $\text{C}_8\text{H}_{16}\text{NO}_2\text{S}$ : 190, found: 190.



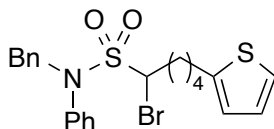
**1-Bromo-*N,N*-dicyclohexylpentane-1-sulfonamide.** The title compound was prepared from 1-bromo-*N,N*-dicyclohexylmethanesulfonamide (2.10 g, 6.21 mmol) and 1-bromobutane (0.867 mL, 8.07 mmol). The product was purified by column chromatography (1%→8% ethyl acetate/hexanes): 2.06 g (84%). Colorless oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  4.57 (dd, 1H,  $J = 10.6, 2.9$  Hz), 3.38–3.33 (br m, 2H), 2.35 (dddd, 1H,  $J = 14.3, 10.1, 5.3, 2.9$  Hz), 2.07–2.00 (m, 1H), 1.95–1.91 (m, 2H), 1.86–1.59 (m, 13H), 1.45–1.23 (m, 7H), 1.09 (qt, 2H,  $J = 13.1, 3.5$  Hz), 0.92 (t, 3H,  $J = 7.2$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  66.6, 59.3, 33.9, 33.3, 32.4, 29.5, 26.6, 25.4, 22.0, 13.9.

FT-IR (neat) 2931, 2855, 1467, 1454, 1401, 1381, 1329, 1275, 1256, 1235, 1188, 1166, 1142, 1101, 1074, 1048, 1027, 997, 982, 929, 917, 895, 856, 847, 824, 801, 774, 760, 749, 733  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+$ ) calcd for  $\text{C}_{17}\text{H}_{32}\text{BrNO}_2\text{S}$ : 393, found: 393.



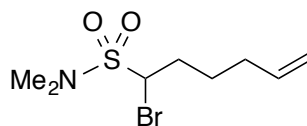
***N*-Benzyl-1-bromo-*N*-phenyl-5-(thiophen-2-yl)pentane-1-sulfonamide.** The title compound was prepared from *N*-benzyl-1-bromo-*N*-phenylmethanesulfonamide (2.70 g, 7.94 mmol) and 2-(4-bromobutyl)thiophene (2.26 g, 10.3 mmol). The product was purified by column chromatography on silica gel (2%→12% ethyl acetate/hexanes) and then preparative HPLC on C-18 silica gel (80%→100% acetonitrile/water; water was doped with 0.1% AcOH): 0.881 g (23%). White solid.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.34–7.27 (m, 5H), 7.26–7.20 (m, 5H), 7.11 (dd, 1H,  $J = 5.1, 1.2$  Hz), 6.90 (dd, 1H,  $J = 5.1, 3.4$  Hz), 6.76 (dddd, 1H,  $J = 3.2, 1.0, 1.0, 1.0$  Hz), 5.34 (d, 1H,  $J = 14.8$  Hz), 4.75 (dd, 1H,  $J = 10.5, 3.1$  Hz), 4.69 (d, 1H,  $J = 14.9$  Hz), 2.88–2.78 (m, 2H), 2.38–2.31 (m, 1H), 2.21–2.13 (m, 1H), 1.79–1.65 (m, 3H), 1.51–1.43 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  144.8, 138.1, 136.3, 129.6, 129.4, 128.7, 128.6, 128.5, 127.9, 126.9, 124.4, 123.2, 63.3, 58.9, 32.7, 30.9, 29.6, 26.6.

FT-IR (neat) 3064, 3031, 2932, 2858, 1594, 1492, 1454, 1439, 1348, 1214, 1178, 1150, 1093, 1066, 1028, 917, 868, 822, 781  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $M^+ + H$ ) calcd for  $\text{C}_{22}\text{H}_{25}\text{BrNO}_2\text{S}_2$ : 478, found: 478.



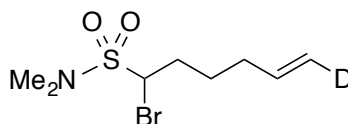
**1-Bromo-*N,N*-dimethylhex-5-ene-1-sulfonamide.** The title compound was prepared from 1-bromo-*N,N*-dimethylmethanesulfonamide (4.00 g, 19.8 mmol) and 5-bromo-1-pentene (3.05 mL, 25.7 mmol). The product was purified by column chromatography (3%  $\rightarrow$  15% ethyl acetate/hexanes): 2.29 g (43%). Colorless oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  5.79 (ddt, 1H,  $J = 16.9, 10.2, 6.7$  Hz), 5.05 (dq, 1H,  $J = 17.1, 1.7$  Hz), 5.01 (ddt, 1H,  $J = 10.2, 1.9, 1.2$  Hz), 4.82 (dd, 1H,  $J = 10.5, 3.2$  Hz), 3.02 (s, 6H), 2.35 (dddd, 1H,  $J = 14.5, 10.2, 6.0, 3.2$  Hz), 2.19–2.04 (m, 3H), 1.84–1.75 (m, 1H), 1.60–1.51 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.5, 115.8, 63.0, 38.8, 32.8, 32.7, 26.4.

FT-IR (neat) 3076, 2918, 1640, 1482, 1454, 1415, 1341, 1285, 1204, 1143, 1063, 970, 912, 856, 786, 738  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $M^+ + H$ ) calcd for  $\text{C}_8\text{H}_{17}\text{BrNO}_2\text{S}$ : 270, found: 270.



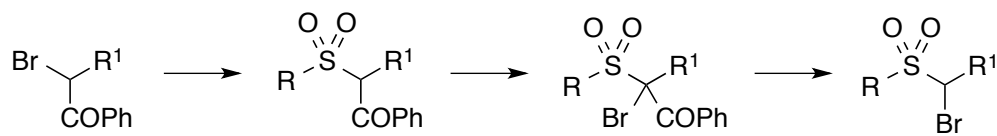
**(*E*)-1-Bromo-*N,N*-dimethylhex-5-ene-1-sulfonamide-6-*d*.** The title compound was prepared from 1-bromo-*N,N*-dimethylmethanesulfonamide (762 mg, 3.77 mmol) and (*E*)-pent-4-en-1-yl-5-*d* 4-methylbenzenesulfonate (1.18 g, 4.90 mmol). The product was purified by column chromatography (2%  $\rightarrow$  20% ethyl acetate/hexanes): 408 mg (40%). Colorless oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  5.78 (dt, 1H,  $J = 16.9, 6.5$  Hz), 5.05–5.00 (m, 1H), 4.82 (dd, 1H,  $J = 10.5, 3.2$  Hz), 3.01 (s, 6H), 2.37–2.30 (m, 1H), 2.18–2.03 (m, 3H), 1.83–1.74 (m, 1H), 1.59–1.50 (m, 1H).

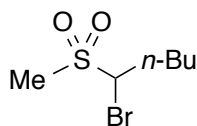
$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.4, 115.5 (t,  $J = 24$  Hz), 63.1, 38.8, 32.8, 32.7, 26.4.

FT-IR (neat) 3028, 2949, 2862, 2264, 1621, 1483, 1455, 1435, 1414, 1342, 1287, 1204, 1183, 1144, 1064, 972, 868, 785, 744  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $M^+ + H$ ) calcd for  $\text{C}_8\text{H}_{16}\text{DBrNO}_2\text{S}$ : 271, found: 271.



**Representative experimental procedure for the preparation of  $\alpha$ -bromosulfones.** The target molecules were prepared according to literature procedures from  $\alpha$ -bromoketones.<sup>4,5</sup> A 100-mL round-bottom flask was charged with the  $\alpha$ -bromo- $\beta$ -keto-sulfone (10.0 mmol) and aqueous KOH (30% w/v; 50 mL), and the mixture was stirred at r.t. for 48 h. When the reaction was complete (monitored by TLC), the reaction mixture was extracted with dichloromethane (3  $\times$  30 mL). The combined organic layers were dried over MgSO<sub>4</sub> and concentrated.



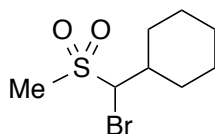
**1-Bromo-1-(methylsulfonyl)pentane.** The title compound was prepared from 2-bromo-2-(methylsulfonyl)-1-phenylhexan-1-one (12.0 g, 36.0 mmol). The product was purified by column chromatography (hexanes  $\rightarrow$  20% ethyl acetate/hexanes): 8.08 g (98%). White solid.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  4.61 (dd, 1H,  $J$  = 11.0, 3.0 Hz), 3.09 (s, 3H), 2.43 (dddd, 1H,  $J$  = 14.4, 9.9, 5.7, 3.0 Hz), 1.96 (dddd, 1H,  $J$  = 14.2, 11.1, 9.5, 4.4 Hz), 1.72–1.64 (m, 1H), 1.50–1.31 (m, 3H), 0.94 (t, 3H,  $J$  = 7.2 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  64.3, 37.6, 30.1, 29.2, 21.8, 13.8.

FT-IR (neat) 3010, 2958, 2932, 2873, 1467, 1454, 1434, 1413, 1381, 1311, 1237, 1208, 1140, 1121, 1106, 956, 928, 815, 771, 748, 735 cm<sup>-1</sup>.

MS (ESI)  $m/z$  ( $M^+$ +H) calcd for C<sub>6</sub>H<sub>14</sub>BrO<sub>2</sub>S: 229, found: 229.



**(Bromo(methylsulfonyl)methyl)cyclohexane.** The bromination of 2-cyclohexyl-2-(methylsulfonyl)-1-phenylethan-1-one was conducted at 60 °C, and extra KBr and H<sub>2</sub>O<sub>2</sub> were added until the reaction was complete. The title compound was prepared from 2-bromo-2-cyclohexyl-2-(methylsulfonyl)-1-phenylethan-1-one (8.13 g, 22.6 mmol). The reaction was run at 40 °C for 96 h. The product was purified by column chromatography on silica gel (5%  $\rightarrow$  30% ethyl acetate/hexanes) and then on C-18 silica gel (10%  $\rightarrow$  100% acetonitrile/water): 1.69 g (29%). White solid.

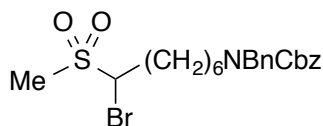
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- (4) Suryakiran, N.; Reddy, T. S.; Ashalatha, K.; Lakshman, M.; Venkateswarlu, Y. *Tetrahedron Lett.* **2006**, *47*, 3853–3856.
- (5) Suryakiran, N.; Prabhakar, P.; Reddy, T. S.; Mahesh, K. C.; Rajesh, K.; Venkateswarlu, Y. *Tetrahedron Lett.* **2007**, *48*, 877–881.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  4.60 (d, 1H,  $J = 2.7$  Hz), 3.10 (s, 3H), 2.41–2.35 (m, 1H), 2.08–2.04 (m, 1H), 1.84–1.76 (m, 2H), 1.72–1.67 (m, 1H), 1.64–1.61 (m, 1H), 1.48–1.30 (m, 4H), 1.21–1.12 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  71.0, 39.9, 37.4, 31.8, 28.5, 26.0, 25.6, 25.3.

FT-IR (neat) 3011, 2930, 2855, 1452, 1411, 1370, 1310, 1240, 1171, 1138, 1090, 1080, 1060, 1032, 968, 922, 896, 885, 848, 792, 774, 728  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+\text{+H}$ ) calcd for  $\text{C}_8\text{H}_{16}\text{BrO}_2\text{S}$ : 255, found: 255.



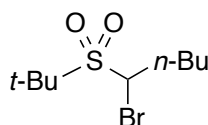
**Benzyl benzyl(7-bromo-7-(methylsulfonyl)heptyl)carbamate.** The title compound was prepared from benzyl benzyl(7-bromo-7-(methylsulfonyl)-8-oxo-8-phenyloctyl)carbamate (3.08 g, 5.13 mmol). The product was purified by column chromatography on silica gel (10%→50% ethyl acetate/hexanes) and then on C-18 silica gel (10%→100% acetonitrile/water): 1.57 g (62%). Viscous colorless oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.39–7.20 (br m, 10H), 5.18–5.14 (m, 2H), 4.68–4.60 (m, 1H), 4.50 (s, 2H), 3.28–3.20 (m, 2H), 3.06 (s, 3H), 2.40–2.30 (br m, 1H), 1.97–1.86 (br m, 1H), 1.70–1.25 (br m, 8H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  156.9, 156.4, 138.6, 137.6, 128.82, 128.78, 128.2, 128.05, 127.98, 127.5, 67.3, 64.7, 50.8, 50.5, 47.4, 46.7, 37.8, 30.7, 28.6, 28.3, 27.9, 27.2, 26.7.

FT-IR (neat) 3087, 3062, 3030, 2930, 2858, 1692, 1605, 1585, 1496, 1467, 1453, 1421, 1365, 1315, 1230, 1140, 1119, 1072, 1028, 955, 915, 819, 768, 733  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+\text{+H}$ ) calcd for  $\text{C}_{23}\text{H}_{31}\text{BrNO}_4\text{S}$ : 496, found: 496.



**1-Bromo-1-(tert-butylsulfonyl)pentane.** A mixture of 2-bromo-1-phenylhexan-1-one (5.10 g, 20.0 mmol), 2-methyl-2-propanethiol (1.80 g, 20.0 mmol), benzyltriethylammonium bromide (0.272 g, 1.00 mmol), and NaOH (3.00 g, 75.0 mmol) in dichloromethane (40 mL) and water (40 mL) in a 250-mL round-bottom flask was stirred at r.t. for 8 h. Then, water (100 mL) was added, and the mixture was extracted with dichloromethane (3 × 50 mL). The combined organic layers were dried over  $\text{MgSO}_4$  and concentrated. The residue was dissolved in MeOH (50 mL) and water (50 mL), and then oxone<sup>®</sup> (30.7 g, 100 mmol) was added. The reaction mixture was stirred at r.t. overnight, and most of the MeOH was removed under reduced pressure. The resulting aqueous mixture was extracted with dichloromethane (3 × 30 mL). The combined organic layers were dried over  $\text{MgSO}_4$  and concentrated. 2-(tert-Butylsulfonyl)-1-phenylhexan-1-one was purified by column chromatography (5%→60% ethyl acetate/hexanes): 5.34 g (90%). White solid.

2-Bromo-2-(*tert*-butylsulfonyl)-1-phenylhexan-1-one was prepared from 2-(*tert*-butylsulfonyl)-1-phenylhexan-1-one following the described procedure.

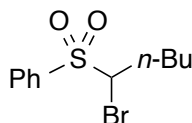
The title compound was prepared from 2-bromo-2-(*tert*-butylsulfonyl)-1-phenylhexan-1-one (2.30 g, 6.13 mmol). The reaction was conducted at 40 °C. The product was purified by column chromatography (hexanes→20% ethyl acetate/hexanes): 1.41 g (85%). White solid.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.84 (dd, 1H, *J* = 10.5, 3.0 Hz), 2.43 (dddd, 1H, *J* = 14.5, 10.2, 5.3, 2.9 Hz), 2.11–2.03 (m, 1H), 1.75–1.66 (m, 1H), 1.55 (s, 9H), 1.48–1.30 (m, 3H), 0.94 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 63.3, 59.2, 30.8, 28.8, 25.2, 22.0, 13.9.

FT-IR (neat) 2959, 2933, 2873, 1479, 1467, 1399, 1366, 1305, 1192, 1167, 1118, 1104, 1020, 986, 964, 929, 801, 733 cm<sup>-1</sup>.

MS (ESI) *m/z* (M<sup>+</sup>+Na) calcd for C<sub>9</sub>H<sub>19</sub>BrNaO<sub>2</sub>S: 293, found: 293.



**((1-Bromopentyl)sulfonyl)benzene.** The title compound was prepared from 2-bromo-1-phenyl-2-(phenylsulfonyl)hexan-1-one (12.0 g, 30.4 mmol). The reaction was conducted at 60 °C. The product was purified by column chromatography (hexanes→20% ethyl acetate/hexanes): 8.50 g (96%). White solid.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.98–7.95 (m, 2H), 7.72–7.68 (m, 1H), 7.61–7.57 (m, 2H), 4.70 (dd, 1H, *J* = 11.1, 2.9 Hz), 2.41 (dddd, 1H, *J* = 14.3, 9.9, 5.8, 2.9 Hz), 1.89 (dddd, 1H, *J* = 14.1, 11.1, 9.4, 4.4 Hz), 1.67–1.58 (m, 1H), 1.45–1.26 (m, 3H), 0.91 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 135.5, 134.6, 130.2, 129.2, 66.0, 31.0, 29.2, 21.8, 13.8.

FT-IR (neat) 3065, 2958, 2932, 2872, 1584, 1478, 1466, 1447, 1381, 1324, 1309, 1236, 1203, 1149, 1133, 1083, 1024, 999, 929, 792, 778, 746 cm<sup>-1</sup>.

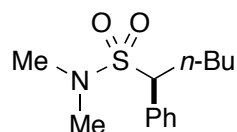
MS (ESI) *m/z* (M<sup>+</sup>+H) calcd for C<sub>11</sub>H<sub>16</sub>BrO<sub>2</sub>S: 291, found: 291.

### III. Enantioselective Arylations

**General Procedure.** An oven-dried 8-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and then filled with nitrogen. ZnI<sub>2</sub> (290 mg, 0.910 mmol) was added to the vial, and the vial was then immediately placed under vacuum and refilled with nitrogen (three cycles). Next, THF (2.73 mL) was added to the vial, followed by a solution of ArMgBr (prepared according to a literature procedure;<sup>1</sup> 1.00 M in THF; 0.910 mL, 0.910 mmol). The mixture was stirred at r.t. for 30 min. An oven-dried 20-mL vial equipped with a magnetic stir bar was charged with NiCl<sub>2</sub>·glyme (15.4 mg, 0.070 mmol), (*R,R*)-L1 (30.4 mg, 0.091 mmol), and the electrophile (0.70 mmol). The vial was sealed with a PTFE-lined septum cap, placed under vacuum, and then filled with nitrogen; this cycle was repeated three times. THF (4.14 mL) was added, and the mixture was stirred at r.t. for 20 min, at which

time it had become homogenous. Both vials were wrapped with electrical tape, attached with nitrogen-filled balloons, and cooled to  $-20\text{ }^{\circ}\text{C}$  for 15 min. The heterogeneous mixture of the nucleophile was then transferred by syringe over 2 min to the vial that contained the electrophile. The nitrogen-filled balloon was removed, and the septum cap was covered with grease. The reaction mixture was stirred at  $-20\text{ }^{\circ}\text{C}$  for 24 h, and then the reaction was quenched by the addition of ethanol (0.70 mL). The solution was allowed to warm to r.t., and then it was filtered through a pad of silica (eluted with  $\text{Et}_2\text{O}$ ). The filtrate was concentrated, and the residue was purified by column chromatography.

A second run was conducted with (*S,S*)-L1.



**(*S*)-*N,N*-Dimethyl-1-phenylpentane-1-sulfonamide (Table 2, Entry 1).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20%  $\rightarrow$  25%  $\text{Et}_2\text{O}$ /hexanes). Light-yellow solid. First run: 159 mg (89%, 96% ee). Second run: 162 mg (91%, 96% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 10.9$  min (major), 13.4 min (minor).

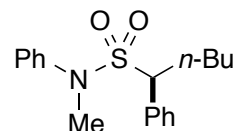
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42–7.34 (m, 5H), 4.08 (dd, 1H,  $J = 11.3, 3.8$  Hz), 2.53 (s, 6H), 2.34 (dddd, 1H,  $J = 13.7, 10.2, 6.5, 3.8$  Hz), 2.15 (dddd, 1H,  $J = 13.6, 11.4, 10.0, 5.1$  Hz), 1.38–1.23 (m, 2H), 1.22–1.09 (m, 2H), 0.84 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  133.9, 129.6, 129.0, 128.9, 67.7, 37.8, 29.6, 28.9, 22.4, 13.9.

FT-IR (neat) 3017, 2952, 2930, 2872, 1497, 1455, 1326, 1305, 1288, 1204, 1137, 1109, 1064, 973, 820, 808  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{13}\text{H}_{21}\text{NNaO}_2\text{S}$ : 278, found: 278.

$[\alpha]_{\text{D}}^{25} = -30^{\circ}$  ( $c = 1.02, \text{CHCl}_3$ ).



**(*S*)-*N*-Methyl-*N*,1-diphenylpentane-1-sulfonamide (Table 2, Entry 2).** 1-Bromo-*N*-methyl-*N*-phenylpentane-1-sulfonamide (224 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (10%  $\text{Et}_2\text{O}$ /hexanes). Light-yellow solid. First run: 211 mg (95%, 93% ee). Second run: 211 mg (95%, 95% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 10.5$  min (major), 11.7 min (minor).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41–7.35 (m, 5H), 7.31–7.27 (m, 2H), 7.21–7.18 (m, 1H), 7.17–7.14 (m, 2H), 4.11 (dd, 1H,  $J = 11.4, 3.7$  Hz), 2.88 (s, 3H), 2.32 (dddd, 1H,  $J = 13.6, 10.1, 6.5, 3.7$

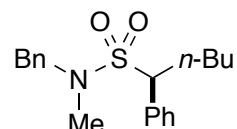
Hz), 2.14 (dddd, 1H,  $J = 13.4, 11.4, 9.9, 5.2$  Hz), 1.34–1.18 (m, 2H), 1.17–1.03 (m, 2H), 0.80 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  141.7, 133.7, 129.9, 129.1, 129.0, 128.8, 126.5, 125.8, 68.2, 39.2, 30.0, 28.9, 22.4, 13.9.

FT-IR (neat) 3063, 3030, 2957, 2932, 2872, 1596, 1493, 1455, 1423, 1380, 1342, 1266, 1179, 1143, 1108, 1067, 1028, 1003, 969, 917, 880, 801, 765  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{18}\text{H}_{23}\text{NNaO}_2\text{S}$ : 340, found: 340.

$[\alpha]_{\text{D}}^{25} = -105^\circ$  ( $c = 1.01$ ,  $\text{CHCl}_3$ ).



**(S)-N-Benzyl-N-methyl-1-phenylpentane-1-sulfonamide (Table 2, Entry 3).** *N*-Benzyl-1-bromo-*N*-methylpentane-1-sulfonamide (234 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (7% ethyl acetate/hexanes). Light-yellow solid. First run: 219 mg (94%, 94% ee). Second run: 221 mg (95%, 93% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 25.8$  min (major), 28.9 min (minor).

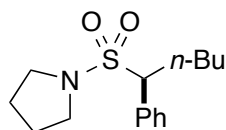
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42–7.36 (m, 5H), 7.31–7.23 (m, 3H), 7.22–7.18 (m, 2H), 4.12 (dd, 1H,  $J = 11.3, 3.8$  Hz), 4.01 (d, 1H,  $J = 14.7$  Hz), 3.68 (br d, 1H,  $J = 11.0$  Hz), 2.42 (s, 3H), 2.38 (dddd, 1H,  $J = 13.7, 10.1, 6.2, 3.8$  Hz), 2.21 (dddd, 1H,  $J = 13.5, 11.3, 9.8, 5.2$  Hz), 1.42–1.26 (m, 2H), 1.26–1.12 (m, 2H), 0.85 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  136.3, 133.9, 129.7, 129.0, 128.9, 128.6, 128.3, 127.9, 68.5, 54.2, 34.6, 29.6, 29.0, 22.4, 13.9.

FT-IR (neat) 3063, 3030, 2954, 2930, 2870, 1495, 1454, 1363, 1327, 1214, 1149, 1133, 1075, 1003, 944, 890, 807, 760  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{19}\text{H}_{25}\text{NNaO}_2\text{S}$ : 354, found: 354.

$[\alpha]_{\text{D}}^{25} = -54^\circ$  ( $c = 1.03$ ,  $\text{CHCl}_3$ ).



**(S)-1-((1-Phenylpentyl)sulfonyl)pyrrolidine (Table 2, Entry 4).** 1-((1-Bromopentyl)sulfonyl)pyrrolidine (199 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (10% ethyl acetate/hexanes). White solid. First run: 166 mg (84%, 96% ee). Second run: 170 mg (86%, 96% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 13.8$  min (minor), 20.2 min (major).



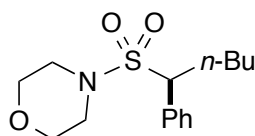
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43–7.39 (m, 2H), 7.39–7.33 (m, 3H), 4.11 (dd, 1H,  $J = 11.3, 3.8$  Hz), 3.21–3.13 (m, 2H), 2.84–2.77 (m, 2H), 2.33 (dddd, 1H,  $J = 13.8, 10.1, 6.4, 3.8$  Hz), 2.17 (dddd, 1H,  $J = 13.5, 11.3, 9.6, 5.2$  Hz), 1.74–1.67 (m, 2H), 1.67–1.58 (m, 2H), 1.39–1.24 (m, 2H), 1.24–1.10 (m, 2H), 0.84 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  134.3, 129.7, 128.8, 128.7, 67.7, 48.2, 29.2, 29.0, 25.9, 22.4, 13.9.

FT-IR (neat) 3436, 2957, 2887, 2872, 2857, 1498, 1467, 1456, 1325, 1294, 1240, 1198, 1143, 1128, 1084, 1015, 829, 806, 728  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{15}\text{H}_{23}\text{NNaO}_2\text{S}$ : 304, found: 304.

$[\alpha]_{\text{D}}^{25} = -51^\circ$  ( $c = 0.97, \text{CHCl}_3$ ).



**(S)-4-((1-Phenylpentyl)sulfonyl)morpholine (Table 2, Entry 5).** 4-((1-

Bromopentyl)sulfonyl)morpholine (210 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20% ethyl acetate/hexanes). White solid. First run: 197 mg (95%, 98% ee). Second run: 186 mg (89%, 95% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (3% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 13.9$  min (major), 16.7 min (minor).

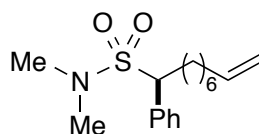
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44–7.35 (m, 5H), 4.02 (dd, 1H,  $J = 11.3, 3.8$  Hz), 3.56–3.52 (m, 2H), 3.48–3.43 (m, 2H), 3.06–3.02 (m, 2H), 2.75 (br s, 2H), 2.34 (dddd, 1H,  $J = 13.8, 10.1, 6.3, 3.8$  Hz), 2.13 (dddd, 1H,  $J = 13.4, 11.3, 9.8, 5.1$  Hz), 1.39–1.23 (m, 2H), 1.23–1.08 (m, 2H), 0.84 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  133.5, 129.7, 129.2, 129.0, 68.5, 67.0, 46.3, 29.7, 28.9, 22.4, 13.9.

FT-IR (neat) 2955, 2923, 2859, 1496, 1455, 1336, 1323, 1257, 1214, 1152, 1128, 1110, 1076, 955, 924, 848, 803  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{15}\text{H}_{23}\text{NNaO}_3\text{S}$ : 320, found: 320.

$[\alpha]_{\text{D}}^{25} = -34^\circ$  ( $c = 1.02, \text{CHCl}_3$ ).



**(S)-*N,N*-Dimethyl-1-phenylnon-8-ene-1-sulfonamide (Table 2, Entry 6).** 1-Bromo-*N,N*-dimethylnon-8-ene-1-sulfonamide (219 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (5%→10% ethyl acetate/hexanes). Light-yellow solid. First run: 192 mg (89%, 95% ee). Second run: 189 mg (87%, 95% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 12.8$  min (major), 20.6 min (minor).

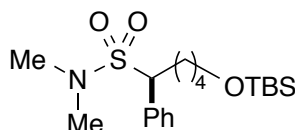
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41–7.34 (m, 5H), 5.76 (dddd, 1H,  $J = 16.9, 10.2, 6.7, 6.7$  Hz), 4.96 (dddd, 1H,  $J = 17.1, 2.2, 1.6, 1.6$  Hz), 4.91 (dddd, 1H,  $J = 10.2, 2.3, 1.2, 1.2$  Hz), 4.08 (dd, 1H,  $J = 11.3, 3.9$  Hz), 2.53 (s, 6H), 2.30 (dddd, 1H,  $J = 13.7, 10.2, 6.5, 3.9$  Hz), 2.19–2.11 (m, 1H), 2.01–1.96 (m, 2H), 1.35–1.11 (m, 8H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  139.1, 133.9, 129.6, 129.0, 128.9, 114.4, 67.7, 37.8, 33.8, 29.8, 29.1, 28.8, 26.7.

FT-IR (neat) 3062, 2924, 2853, 1640, 1497, 1468, 1456, 1414, 1327, 1208, 1137, 1066, 977, 912, 824  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{17}\text{H}_{27}\text{NNaO}_2\text{S}$ : 332, found: 332.

$[\alpha]_{\text{D}}^{25} = -19.2^\circ$  ( $c = 0.98$ ,  $\text{CHCl}_3$ ).



**(S)-5-((*tert*-Butyldimethylsilyloxy)-*N,N*-dimethyl-1-phenylpentane-1-sulfonamide (Table 2, Entry 7).** 1-Bromo-5-((*tert*-butyldimethylsilyloxy)-*N,N*-dimethylpentane-1-sulfonamide (272 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (2%  $\rightarrow$  20% ethyl acetate/hexanes). White solid. First run: 248 mg (92%, >99% ee). Second run: 250 mg (93%, 98% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 8.2$  min (major), 11.0 min (minor).

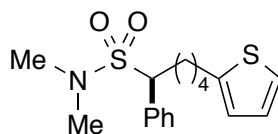
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41–7.33 (m, 5H), 4.09 (dd, 1H,  $J = 11.3, 3.9$  Hz), 3.56–3.49 (m, 2H), 2.53 (s, 6H), 2.35–2.28 (m, 1H), 2.21–2.13 (m, 1H), 1.57–1.42 (m, 2H), 1.27–1.18 (m, 2H), 0.82 (s, 9H),  $-0.02$  (s, 6H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  133.7, 129.6, 129.0, 128.9, 67.6, 62.7, 37.8, 32.4, 29.7, 26.0, 23.1, 18.4,  $-5.2$ .

FT-IR (neat) 3065, 2931, 2897, 2860, 1458, 1385, 1359, 1329, 1280, 1257, 1200, 1143, 1132, 1110, 1092, 966, 900, 872, 833, 808, 779, 736  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{19}\text{H}_{35}\text{NNaO}_3\text{SSi}$ : 408, found: 408.

$[\alpha]_{\text{D}}^{25} = -15.0^\circ$  ( $c = 0.98$ ,  $\text{CHCl}_3$ ).



**(S)-*N,N*-Dimethyl-1-phenyl-5-(thiophen-2-yl)pentane-1-sulfonamide (Table 2, Entry 8).** 1-Bromo-*N,N*-dimethyl-5-(thiophen-2-yl)pentane-1-sulfonamide (238 mg, 0.700 mmol) and phenylzinc iodide (1.05 mmol) were used. The product was purified by column chromatography (10%  $\rightarrow$  15% ethyl acetate/hexanes). Yellow solid. First run: 128 mg (54%, 90% ee). Second run: 131 mg (55%, 91% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r$  = 18.3 min (major), 22.8 min (minor).

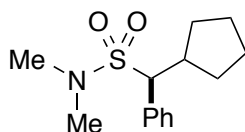
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41–7.34 (m, 5H), 7.08 (dd, 1H,  $J$  = 5.1, 1.2 Hz), 6.88 (dd, 1H,  $J$  = 5.1, 3.4 Hz), 6.71 (dddd, 1H,  $J$  = 3.3, 1.0, 1.0, 1.0 Hz), 4.08 (dd, 1H,  $J$  = 11.2, 3.9 Hz), 2.82–2.70 (m, 2H), 2.52 (s, 6H), 2.39–2.32 (m, 1H), 2.23–2.15 (m, 1H), 1.74–1.61 (m, 2H), 1.35–1.21 (m, 2H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  145.1, 133.8, 129.6, 129.0, 128.9, 126.8, 124.2, 123.0, 67.6, 37.8, 31.4, 29.65, 29.59, 26.2.

FT-IR (neat) 3064, 2932, 2856, 1495, 1480, 1454, 1331, 1282, 1200, 1140, 1062, 1030, 967, 849, 820  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{17}\text{H}_{23}\text{NNaO}_2\text{S}_2$ : 360, found: 360.

$[\alpha]_{\text{D}}^{25} = -9.4^\circ$  ( $c = 0.99$ ,  $\text{CHCl}_3$ ).



**(S)-1-Cyclopentyl-*N,N*-dimethyl-1-phenylmethanesulfonamide (Table 2, Entry 9).** 1-Bromo-1-cyclopentyl-*N,N*-dimethylmethanesulfonamide (189 mg, 0.700 mmol) and phenylzinc iodide (1.05 mmol) were used. The product was purified by column chromatography (first purification: 10% ethyl acetate/hexanes; second purification: 12% → 100% dichloromethane/hexanes). White solid. First run: 86 mg (46%, >99% ee). Second run: 79 mg (42%, >99% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r$  = 12.7 min (major), 14.6 min (minor).

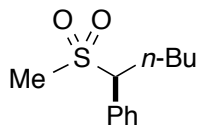
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41–7.38 (m, 2H), 7.37–7.31 (m, 3H), 3.92 (d, 1H,  $J$  = 10.3 Hz), 2.78–2.69 (m, 1H), 2.43 (s, 6H), 2.29–2.22 (m, 1H), 1.75–1.67 (m, 1H), 1.66–1.60 (m, 1H), 1.59–1.41 (m, 4H), 1.03–0.95 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  135.2, 129.7, 128.69, 128.67, 73.2, 41.8, 37.6, 32.3, 32.1, 25.5, 24.1.

FT-IR (neat) 3090, 3064, 3025, 2960, 2871, 2812, 1496, 1479, 1452, 1323, 1293, 1206, 1188, 1131, 1081, 1063, 1030, 1003, 969, 911, 872, 848, 807, 732  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+ - \text{SO}_2\text{NMe}_2$ ) calcd for  $\text{C}_{12}\text{H}_{15}$ : 159, found: 159.

$[\alpha]_{\text{D}}^{25} = -43^\circ$  ( $c = 1.04$ ,  $\text{CHCl}_3$ ).



**(S)-1-(1-(Methylsulfonyl)pentyl)benzene (Table 3, Entry 1).** 1-Bromo-1-(methylsulfonyl)pentane (160 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20% → 30% ethyl acetate/hexanes). White solid. First run: 150 mg (95%, 94% ee). Second run: 153 mg (97%, 94% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r$  = 17.6 min (major), 20.8 min (minor).

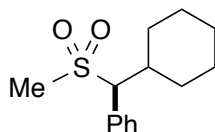
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42–7.37 (m, 5H), 3.99 (dd, 1H,  $J$  = 11.5, 3.7 Hz), 2.59 (s, 3H), 2.45–2.37 (m, 1H), 2.12 (dddd, 1H,  $J$  = 13.6, 11.5, 9.6, 5.3 Hz), 1.41–1.26 (m, 2H), 1.25–1.14 (m, 2H), 0.85 (t, 3H,  $J$  = 7.1 Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  133.4, 129.5, 129.28, 129.27, 70.4, 38.7, 28.9, 26.7, 22.4, 13.9.

FT-IR (neat) 3088, 3065, 3051, 3011, 2931, 2869, 1496, 1468, 1456, 1417, 1379, 1292, 1277, 1263, 1211, 1158, 1130, 1107, 1072, 1036, 966, 936, 904, 805, 722  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+$ +Na) calcd for  $\text{C}_{12}\text{H}_{18}\text{NaO}_2\text{S}$ : 249, found: 249.

$[\alpha]_D^{25} = -6.2^\circ$  ( $c$  = 1.00,  $\text{CHCl}_3$ ).



**(S)-(Cyclohexyl(methylsulfonyl)methyl)benzene (Table 3, Entry 2).**

(Bromo(methylsulfonyl)methyl)cyclohexane (179 mg, 0.700 mmol) and phenylzinc iodide (1.05 mmol) were used. The product was purified by column chromatography (10%→15% ethyl acetate/hexanes). White solid. First run: 145 mg (82%, 99% ee). Second run: 148 mg (84%, 99% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (4% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r$  = 16.7 min (minor), 25.8 min (major).

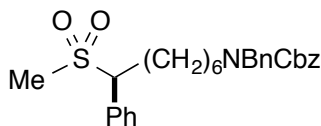
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43–7.36 (m, 5H), 3.87 (d, 1H,  $J$  = 7.9 Hz), 2.53–2.45 (m, 1H), 2.46 (s, 3H), 2.29–2.24 (m, 1H), 1.80–1.74 (m, 1H), 1.67–1.56 (m, 3H), 1.42–1.33 (m, 1H), 1.28–1.18 (m, 2H), 1.14–1.05 (m, 1H), 0.93–0.85 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  133.9, 129.8, 129.2, 129.1, 75.9, 41.4, 38.1, 32.4, 30.6, 26.11, 26.06, 26.0.

FT-IR (neat) 3004, 2930, 2853, 1496, 1454, 1413, 1378, 1348, 1319, 1302, 1292, 1244, 1221, 1170, 1127, 1076, 1036, 970, 896, 854, 804, 742  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+$ +Na) calcd for  $\text{C}_{14}\text{H}_{20}\text{NaO}_2\text{S}$ : 275, found: 275.

$[\alpha]_D^{25} = -40^\circ$  ( $c$  = 1.06,  $\text{CHCl}_3$ ).



**Benzyl (S)-benzyl(7-(methylsulfonyl)-7-phenylheptyl)carbamate (Table 3, Entry 3).** Benzyl benzyl(7-bromo-7-(methylsulfonyl)heptyl)carbamate (199 mg, 0.400 mmol) and phenylzinc iodide (0.520 mmol) were used. The product was purified by column chromatography on silica gel (25% ethyl acetate/hexanes) and then preparative HPLC on C-18 silica gel (80%→100% acetonitrile/water; water was doped with 0.1% AcOH). Viscous colorless oil. First run: 149 mg (75%, 89% ee). Second run: 145 mg (73%, 91% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (20% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 31.5$  min (major), 40.0 min (minor).

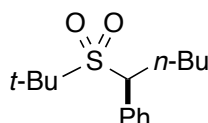
$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.44–7.17 (m, 15H), 5.14–5.12 (m, 2H), 4.45 (s, 2H), 4.01–3.95 (m, 1H), 3.22–3.15 (m, 2H), 2.59 (s, 3H), 2.35–2.23 (br m, 1H), 2.12–1.99 (br m, 1H), 1.48–1.40 (br m, 2H), 1.35–1.09 (br m, 6H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  156.9, 156.3, 138.7, 137.6, 133.6, 129.9, 129.40, 129.36, 128.8, 128.7, 128.2, 128.01, 127.95, 127.5, 70.3, 67.3, 50.8, 50.4, 47.4, 46.7, 38.9, 29.2, 28.4, 27.9, 27.4, 26.9, 26.8.

FT-IR (neat) 3088, 3063, 3031, 3007, 2931, 2858, 1697, 1605, 1586, 1496, 1468, 1454, 1422, 1366, 1305, 1232, 1137, 1086, 1071, 1029, 1002, 954, 916, 801  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+\text{+H}$ ) calcd for  $\text{C}_{29}\text{H}_{36}\text{NO}_4\text{S}$ : 494, found: 494.

$[\alpha]_{\text{D}}^{25} = -0.037^\circ$  ( $c = 4.1$ ,  $\text{CHCl}_3$ ).



**(S)-1-(*tert*-Butylsulfonyl)pentylbenzene (Table 3, Entry 4).** 1-Bromo-1-(*tert*-butylsulfonyl)pentane (190 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (15% ethyl acetate/hexanes). White solid. First run: 179 mg (95%, 99% ee). Second run: 182 mg (97%, 98% ee).

The ee was determined by HPLC on a CHIRALPAK IB-3 column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 8.4$  min (major), 9.9 min (minor).

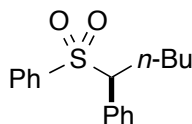
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47–7.45 (m, 2H), 7.39–7.32 (m, 3H), 4.14 (dd, 1H,  $J = 11.6, 3.3$  Hz), 2.47 (dddd, 1H,  $J = 13.6, 10.6, 6.2, 3.3$  Hz), 2.06 (dddd, 1H,  $J = 13.4, 11.6, 10.2, 4.9$  Hz), 1.40–1.30 (m, 1H), 1.29–1.21 (m, 1H), 1.16 (s, 9H), 1.15–1.01 (m, 2H), 0.82 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  134.9, 129.6, 129.0, 128.9, 65.3, 62.1, 28.9, 28.7, 24.4, 22.4, 13.9.

FT-IR (neat) 3032, 2986, 2954, 2872, 1497, 1466, 1455, 1366, 1279, 1190, 1115, 1100, 782  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+\text{+Na}$ ) calcd for  $\text{C}_{15}\text{H}_{24}\text{NaO}_2\text{S}$ : 291, found: 291.

$[\alpha]_{\text{D}}^{25} = -20.3^\circ$  ( $c = 1.01$ ,  $\text{CHCl}_3$ ).



**(S)-1-(1-Phenylpentyl)sulfonylbenzene (Table 3, Entry 5).** ((1-Bromopentyl)sulfonyl)benzene (204 mg, 0.700 mmol) and phenylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (10% → 20%  $\text{Et}_2\text{O}$ /hexanes). White solid. First run: 195 mg (97%, 86% ee). Second run: 193 mg (96%, 83% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 13.6$  min (major), 18.7 min (minor).

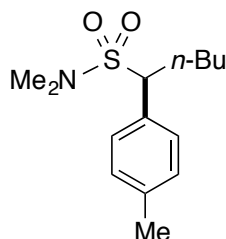
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.54–7.49 (m, 3H), 7.38–7.34 (m, 2H), 7.29–7.26 (m, 1H), 7.24–7.20 (m, 2H), 7.10–7.07 (m, 2H), 4.01 (dd, 1H,  $J = 11.6, 3.6$  Hz), 2.46–2.39 (m, 1H), 2.20–2.10 (m, 1H), 1.38–1.23 (m, 2H), 1.22–1.13 (m, 2H), 0.83 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.6, 133.5, 132.6, 130.0, 129.2, 128.8, 128.7, 128.6, 71.8, 29.0, 27.1, 22.4, 13.9.

FT-IR (neat) 2952, 2926, 2857, 1584, 1496, 1467, 1455, 1447, 1379, 1316, 1304, 1294, 1214, 1147, 1084, 1070, 1037, 1024, 998, 968, 800, 758, 713  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{17}\text{H}_{20}\text{NaO}_2\text{S}$ : 311, found: 311.

$[\alpha]_{\text{D}}^{25} = -78^\circ$  ( $c = 1.08$ ,  $\text{CHCl}_3$ ).



**(S)-N,N-Dimethyl-1-(*p*-tolyl)pentane-1-sulfonamide (Table 4, Entry 1).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and *p*-tolylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20%  $\text{Et}_2\text{O}$ /hexanes). Light-yellow oil. First run: 172 mg (91%, 96% ee). Second run: 165 mg (87%, 95% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 8.1$  min (major), 10.1 min (minor).

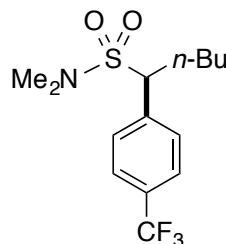
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30–7.27 (m, 2H), 7.19–7.17 (m, 2H), 4.05 (dd, 1H,  $J = 11.3, 3.8$  Hz), 2.54 (s, 6H), 2.36 (s, 3H), 2.29 (dddd, 1H,  $J = 13.7, 10.1, 6.4, 3.8$  Hz), 2.12 (dddd, 1H,  $J = 13.5, 11.4, 9.7, 5.3$  Hz), 1.38–1.22 (m, 2H), 1.22–1.09 (m, 2H), 0.83 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  138.8, 130.8, 129.6, 129.5, 67.4, 37.8, 29.6, 28.9, 22.4, 21.3, 13.9.

FT-IR (neat) 3025, 2956, 2932, 2872, 2811, 1515, 1479, 1457, 1413, 1380, 1331, 1283, 1204, 1141, 1107, 1062, 1022, 968, 843, 832, 716  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{14}\text{H}_{23}\text{NNaO}_2\text{S}$ : 292, found: 292.

$[\alpha]_{\text{D}}^{25} = -30^\circ$  ( $c = 0.99$ ,  $\text{CHCl}_3$ ).



**(S)-N,N-Dimethyl-1-(4-(trifluoromethyl)phenyl)pentane-1-sulfonamide (Table 4, Entry 2).** An oven-dried 8-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and filled with nitrogen. 4-Iodobenzotrifluoride (248 mg,

0.910 mmol) and THF (1.35 mL) were added to the vial, followed by the dropwise addition over 1 min of *i*-PrMgCl (1.92 M in THF; 0.474 mL, 0.910 mmol), and the resulting mixture was stirred at r.t. for 1 h. An oven-dried 4-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and filled with nitrogen. ZnI<sub>2</sub> (290 mg, 0.910 mmol) was added into the vial. The vial was immediately evacuated and refilled with nitrogen (three cycles), and then THF (1.82 mL) was added to the vial. The solution of ZnI<sub>2</sub> was transferred by syringe to the Grignard reagent, and then the reaction mixture was stirred at r.t. for 30 min.

1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and (4-(trifluoromethyl)phenyl)zinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20% Et<sub>2</sub>O/hexanes). Light-yellow solid. First run: 209 mg (92%, 98% ee). Second run: 216 mg (95%, 98% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (3% *i*-PrOH/hexanes, 1.0 mL/min) with *t*<sub>r</sub> = 8.8 min (major), 12.0 min (minor).

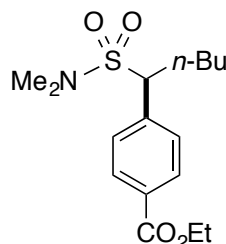
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.65 (d, 2H, *J* = 8.2 Hz), 7.55 (d, 2H, *J* = 8.2 Hz), 4.14 (dd, 1H, *J* = 11.4, 3.8 Hz), 2.58 (s, 6H), 2.32 (dddd, 1H, *J* = 13.9, 10.3, 6.3, 3.9 Hz), 2.14 (dddd, 1H, *J* = 13.7, 11.4, 10.1, 4.9 Hz), 1.38–1.24 (m, 2H), 1.22–1.06 (m, 2H), 0.84 (t, 3H, *J* = 7.3 Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 138.2 (d, *J*<sub>CF</sub> = 1.3 Hz), 131.1 (q, *J*<sub>CF</sub> = 32.7 Hz), 130.0, 125.8 (q, *J*<sub>CF</sub> = 3.7 Hz), 123.6 (q, *J*<sub>CF</sub> = 272.2 Hz), 67.3, 37.8, 29.6, 28.8, 22.3, 13.8.

FT-IR (neat) 2958, 2875, 1325, 1167, 1122, 1069, 1019, 968, 856, 727 cm<sup>-1</sup>.

MS (ESI) *m/z* (M<sup>+</sup>+Na) calcd for C<sub>14</sub>H<sub>20</sub>F<sub>3</sub>NNaO<sub>2</sub>S: 346, found: 346.

[α]<sub>D</sub><sup>25</sup> = -23.3° (c = 1.02, CHCl<sub>3</sub>).



**Ethyl (S)-4-(1-(*N,N*-dimethylsulfamoyl)pentyl)benzoate (Table 4, Entry 3).** An oven-dried 8-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and then filled with nitrogen. Ethyl 4-iodobenzoate (251 mg, 0.910 mmol) was added to the vial, and then the vial was evacuated and refilled with nitrogen (three cycles). Next, THF (1.31 mL) was added to the vial, and the vial was wrapped with electrical tape and fitted with a nitrogen-filled balloon. Then, the reaction mixture was cooled to -20 °C. *i*-PrMgCl (1.78 M in THF; 0.511 mL, 0.910 mmol) was added over 1 min, and the mixture was stirred at -20 °C for 2 h. An oven-dried 4-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and filled with nitrogen. ZnI<sub>2</sub> (291 mg, 0.910 mmol) was added to the vial. The vial was immediately placed under vacuum and then filled with nitrogen. This evacuation-refill cycle was repeated three times, and then THF (1.82 mL) was added to the vial. The solution of ZnI<sub>2</sub> was transferred by syringe to the Grignard reagent,

and then the reaction mixture was stirred at  $-20\text{ }^{\circ}\text{C}$  for 30 min. The reaction mixture was allowed to warm to r.t. and stirred for an additional 30 min.

1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and (4-(ethoxycarbonyl)phenyl)zinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20% ethyl acetate/hexanes). Colorless oil. First run: 229 mg (>99%, 97% ee). Second run: 229 mg (>99%, 97% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 8.7$  min (major), 11.4 min (minor).

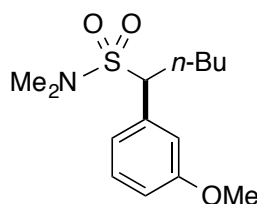
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07–8.05 (m, 2H), 7.50–7.48 (m, 2H), 4.38 (q, 2H,  $J = 7.1$  Hz), 4.14 (dd, 1H,  $J = 11.3, 3.8$  Hz), 2.55 (s, 6H), 2.32 (dddd, 1H,  $J = 14.0, 10.2, 6.2, 3.8$  Hz), 2.16 (dddd, 1H,  $J = 13.6, 11.3, 10.0, 4.8$  Hz), 1.40 (t, 3H,  $J = 7.1$  Hz), 1.37–1.21 (m, 2H), 1.21–1.05 (m, 2H), 0.82 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.2, 139.0, 131.1, 130.0, 129.6, 67.5, 61.4, 37.9, 29.6, 28.9, 22.4, 14.5, 13.9.

FT-IR (neat) 2956, 2934, 2872, 2813, 1718, 1611, 1576, 1507, 1477, 1457, 1417, 1367, 1334, 1278, 1182, 1143, 1110, 1063, 1021, 968, 867, 799, 776, 753, 712  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ - \text{SO}_2\text{NMe}_2$ ) calcd for  $\text{C}_{14}\text{H}_{19}\text{O}_2$ : 219, found: 219.

$[\alpha]_{\text{D}}^{25} = -36^{\circ}$  ( $c = 1.00, \text{CHCl}_3$ ).



**(S)-1-(3-Methoxyphenyl)-*N,N*-dimethylpentane-1-sulfonamide (Table 4, Entry 4).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and (3-methoxyphenyl)zinc iodide (0.910 mmol) were used. The product was purified by column chromatography (15% ethyl acetate/hexanes). White solid. First run: 175 mg (88%, 95% ee). Second run: 174 mg (87%, 96% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (3% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 10.5$  min (major), 12.9 min (minor).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30–7.27 (m, 1H), 6.99–6.97 (m, 2H), 6.90–6.88 (m, 1H), 4.05 (dd, 1H,  $J = 11.3, 3.8$  Hz), 3.82 (s, 3H), 2.56 (s, 6H), 2.29 (dddd, 1H,  $J = 13.6, 10.2, 6.6, 3.8$  Hz), 2.12 (dddd, 1H,  $J = 13.5, 11.3, 9.8, 5.2$  Hz), 1.38–1.23 (m, 2H), 1.23–1.10 (m, 2H), 0.84 (t, 3H,  $J = 7.3$  Hz).

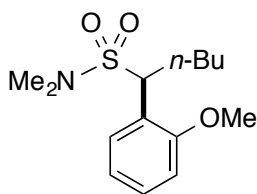
$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  159.9, 135.4, 129.8, 122.0, 115.2, 114.2, 67.6, 55.5, 37.8, 29.7, 28.9, 22.4, 13.9.

FT-IR (neat) 3002, 2956, 2873, 2839, 1601, 1585, 1489, 1456, 1438, 1380, 1330, 1262, 1204, 1142, 1111, 1049, 968, 888, 806  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{14}\text{H}_{23}\text{NNaO}_3\text{S}$ : 308, found: 308.

$[\alpha]_{\text{D}}^{25} = -28^{\circ}$  ( $c = 1.00, \text{CHCl}_3$ ).





**(S)-1-(2-Methoxyphenyl)-N,N-dimethylpentane-1-sulfonamide (Table 4, Entry 5).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and (2-methoxyphenyl)zinc iodide (1.05 mmol) were used. The product was purified by column chromatography on silica gel (10% → 15% ethyl acetate/hexanes) and then on C-18 silica gel (10% → 100% acetonitrile/water). Light-yellow oil. First run: 125 mg (63%, 96% ee). Second run: 128 mg (64%, 96% ee).

The ee was determined by HPLC on a CHIRALPAK AS-H column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r$  = 16.6 min (major), 19.3 min (minor).

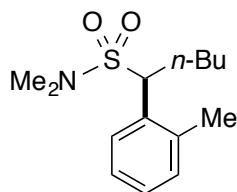
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (dd, 1H,  $J$  = 7.8, 1.7 Hz), 7.30 (ddd, 1H,  $J$  = 8.2, 7.4, 1.7 Hz), 7.00 (ddd, 1H,  $J$  = 7.6, 7.6, 1.1 Hz), 6.91 (dd, 1H,  $J$  = 8.3, 1.1 Hz), 4.87 (dd, 1H,  $J$  = 11.4, 3.9 Hz), 3.87 (s, 3H), 2.51 (s, 6H), 2.32 (dddd, 1H,  $J$  = 13.7, 10.2, 6.4, 3.9 Hz), 2.13–2.05 (m, 1H), 1.36–1.22 (m, 2H), 1.22–1.07 (m, 2H), 0.83 (t, 3H,  $J$  = 7.3 Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  157.7, 129.7, 129.6, 122.2, 121.1, 110.5, 57.3, 55.8, 37.6, 29.7, 28.6, 22.4, 13.9.

FT-IR (neat) 3070, 3005, 2957, 2873, 1601, 1587, 1494, 1463, 1442, 1380, 1330, 1290, 1247, 1202, 1142, 1124, 1090, 1052, 1026, 967, 796, 756, 726  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{14}\text{H}_{23}\text{NNaO}_3\text{S}$ : 308, found: 308.

$[\alpha]_D^{25} = +40^\circ$  ( $c$  = 1.03,  $\text{CHCl}_3$ ).



**(S)-N,N-Dimethyl-1-(*o*-tolyl)pentane-1-sulfonamide (Table 4, Entry 6).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and *o*-tolylzinc iodide (1.05 mmol) were used. The product was purified by column chromatography (5% → 10% ethyl acetate/hexanes). Light-yellow oil. First run: 148 mg (78%, 97% ee). Second run: 149 mg (79%, 97% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r$  = 9.8 min (major), 11.9 min (minor).

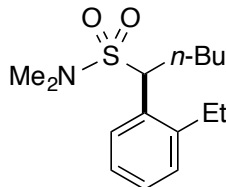
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62–7.58 (m, 1H), 7.25–7.19 (m, 3H), 4.43 (dd, 1H,  $J$  = 11.3, 3.8 Hz), 2.60 (s, 6H), 2.39 (s, 3H), 2.33 (dddd, 1H,  $J$  = 13.6, 10.1, 6.1, 3.8 Hz), 2.16–2.08 (m, 1H), 1.37–1.22 (m, 2H), 1.21–1.06 (m, 2H), 0.83 (t, 3H,  $J$  = 7.3 Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.4, 132.3, 130.7, 128.4, 128.3, 126.6, 63.2, 38.0, 30.7, 28.7, 22.6, 20.1, 13.9.

FT-IR (neat) 3064, 3023, 2957, 2872, 2813, 1604, 1493, 1461, 1380, 1329, 1283, 1203, 1178, 1141, 1119, 1063, 967, 834, 802  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $M^+ + \text{Na}$ ) calcd for  $\text{C}_{14}\text{H}_{23}\text{NNaO}_2\text{S}$ : 292, found: 292.

$[\alpha]_{\text{D}}^{25} = +7.9^\circ$  ( $c = 1.05$ ,  $\text{CHCl}_3$ ).



**(S)-1-(2-Ethylphenyl)-*N,N*-dimethylpentane-1-sulfonamide (Table 4, Entry 7).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol), (2-ethylphenyl)zinc iodide (1.40 mmol),  $\text{NiCl}_2 \cdot \text{glyme}$  (30.8 mg, 0.140 mmol), and (*R,R*)-L1 (60.9 mg, 0.182 mmol) were used. The product was purified by column chromatography (first purification: 10% ethyl acetate/hexanes; second purification: 15%  $\rightarrow$  90% dichloromethane/hexanes). Light-yellow oil. First run: 178 mg (90%, 97% ee). Second run: 165 mg (83%, 97% ee).

The ee was determined by HPLC on a CHIRALPAK IC column (15% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 16.9$  min (minor), 22.7 min (major).

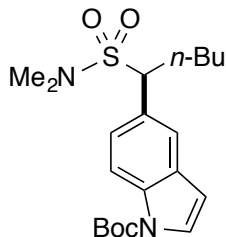
$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.57–7.54 (m, 1H), 7.30–7.22 (m, 3H), 4.46 (dd, 1H,  $J = 11.1, 4.0$  Hz), 2.79 (dq, 1H,  $J = 14.9, 7.5$  Hz), 2.68 (dq, 1H,  $J = 15.2, 7.6$  Hz), 2.62 (s, 6H), 2.29–2.22 (m, 1H), 2.15–2.07 (m, 1H), 1.39–1.24 (m, 2H), 1.22 (t, 3H,  $J = 7.6$  Hz), 1.24–1.15 (m, 1H), 1.13–1.04 (m, 1H), 0.84 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  144.1, 131.9, 129.2, 128.7, 128.5, 126.5, 62.8, 38.0, 30.8, 29.3, 26.0, 23.0, 15.7, 13.9.

FT-IR (neat) 3063, 3021, 2959, 2933, 2873, 2813, 1490, 1455, 1378, 1330, 1282, 1201, 1177, 1141, 1120, 1062, 968, 803, 760  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $M^+ + \text{Na}$ ) calcd for  $\text{C}_{15}\text{H}_{25}\text{NNaO}_2\text{S}$ : 306, found: 306.

$[\alpha]_{\text{D}}^{25} = +8.9^\circ$  ( $c = 1.03$ ,  $\text{CHCl}_3$ ).



***tert*-Butyl (S)-5-(1-(*N,N*-dimethylsulfamoyl)pentyl)-1*H*-indole-1-carboxylate (Table 4, Entry 8).** An oven-dried 8-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and filled with nitrogen. *tert*-Butyl 5-iodo-1*H*-indole-1-carboxylate (360 mg, 1.05 mmol) was added to the vial, and then the vial was evacuated and refilled with nitrogen (three cycles). THF (1.56 mL) was added to the vial, and the vial was

wrapped with electrical tape and fitted with a nitrogen-filled balloon. Then, the reaction mixture was cooled to  $-20\text{ }^{\circ}\text{C}$ . *i*-PrMgCl (1.93 M in THF; 0.544 mL, 1.05 mmol) was added over 1 min, and the mixture was stirred at  $-20\text{ }^{\circ}\text{C}$  for 2 h. An oven-dried 4-mL vial equipped with a magnetic stir bar was capped with a PTFE-lined septum cap, cooled under vacuum, and filled with nitrogen.  $\text{ZnI}_2$  (338 mg, 1.06 mmol) was added to the vial. The vial was immediately placed under vacuum and then filled with nitrogen. This evacuation-refill cycle was repeated three times, and then THF (2.10 mL) was added to the vial. The solution of  $\text{ZnI}_2$  was transferred by syringe to the Grignard reagent, and then the reaction mixture was stirred at  $-20\text{ }^{\circ}\text{C}$  for 30 min. The reaction mixture was allowed to warm to r.t. and stirred for an additional 30 min.

1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (181 mg, 0.700 mmol) and (1-(*tert*-butoxycarbonyl)-1*H*-indol-5-yl)zinc iodide (1.05 mmol) were used. The product was purified by column chromatography on silica gel (10%→15% ethyl acetate/hexanes) and then on C-18 silica gel (10%→100% acetonitrile/water). Yellow solid. First run: 180 mg (65%, 88% ee). Second run: 200 mg (72%, 90% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 11.7$  min (major), 15.4 min (minor).

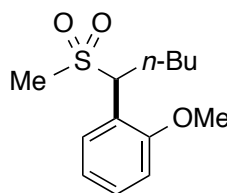
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.14 (d, 1H,  $J = 8.5$  Hz), 7.63–7.62 (m, 2H), 7.33 (dd, 1H,  $J = 8.6, 1.8$  Hz), 6.58 (dd, 1H,  $J = 3.7, 0.8$  Hz), 4.18 (dd, 1H,  $J = 11.4, 3.8$  Hz), 2.51 (s, 6H), 2.36 (dddd, 1H,  $J = 13.7, 10.2, 6.4, 3.8$  Hz), 2.20 (dddd, 1H,  $J = 13.6, 11.4, 10.0, 5.0$  Hz), 1.68 (s, 9H), 1.38–1.23 (m, 2H), 1.22–1.08 (m, 2H), 0.82 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 135.4, 130.9, 128.0, 126.9, 125.7, 121.9, 115.4, 107.4, 84.2, 67.6, 37.9, 29.9, 28.9, 28.3, 22.4, 13.9.

FT-IR (neat) 3152, 3120, 2956, 2934, 2873, 1736, 1536, 1470, 1445, 1374, 1351, 1329, 1256, 1218, 1193, 1164, 1138, 1107, 1084, 1042, 1024, 968, 841, 768, 729  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{20}\text{H}_{30}\text{N}_2\text{NaO}_4\text{S}$ : 417, found: 417.

$[\alpha]_D^{25} = -23.7^{\circ}$  ( $c = 1.04, \text{CHCl}_3$ ).



**(S)-1-Methoxy-2-(1-(methylsulfonyl)pentyl)benzene (Table 4, Entry 9).** 1-Bromo-1-(methylsulfonyl)pentane (160 mg, 0.700 mmol) and (2-methoxyphenyl)zinc iodide (0.910 mmol) were used. The product was purified by column chromatography (20%→25% ethyl acetate/hexanes). Colorless oil. First run: 148 mg (82%, 96% ee). Second run: 154 mg (86%, 96% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 17.6$  min (minor), 18.9 min (major).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.52 (dd, 1H,  $J = 7.8, 1.7$  Hz), 7.34 (ddd, 1H,  $J = 8.3, 7.4, 1.7$  Hz), 7.04 (ddd, 1H,  $J = 7.6, 7.6, 1.1$  Hz), 6.93 (dd, 1H,  $J = 8.3, 1.1$  Hz), 4.81 (dd, 1H,  $J = 11.5, 3.9$  Hz),

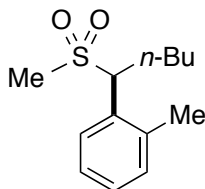
3.87 (s, 3H), 2.58 (s, 3H), 2.40 (dddd, 1H,  $J = 13.5, 9.6, 6.9, 3.9$  Hz), 2.05 (dddd, 1H,  $J = 13.5, 11.5, 9.4, 5.3$  Hz), 1.38–1.24 (m, 2H), 1.23–1.12 (m, 2H), 0.84 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  157.6, 130.1, 129.2, 121.7, 121.6, 110.9, 60.4, 55.9, 38.6, 28.7, 25.9, 22.4, 13.9.

FT-IR (neat) 3009, 2957, 2872, 1601, 1587, 1494, 1464, 1440, 1412, 1380, 1296, 1247, 1192, 1164, 1137, 1090, 1051, 1025, 956, 792, 755  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{13}\text{H}_{20}\text{NaO}_3\text{S}$ : 279, found: 279.

$[\alpha]_{\text{D}}^{25} = +61^\circ$  ( $c = 1.00$ ,  $\text{CHCl}_3$ ).



**(S)-1-Methyl-2-(1-(methylsulfonyl)pentyl)benzene (Table 4, Entry 10).** 1-Bromo-1-(methylsulfonyl)pentane (160 mg, 0.700 mmol) and *o*-tolylzinc iodide (0.910 mmol) were used. The product was purified by column chromatography (15% → 20% ethyl acetate/hexanes). Colorless oil. First run: 137 mg (81%, 97% ee). Second run: 134 mg (80%, 97% ee).

The ee was determined by HPLC on a CHIRALPAK AS-H column (10% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 18.4$  min (minor), 28.0 min (major).

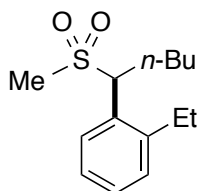
$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.52–7.50 (m, 1H), 7.30–7.23 (m, 3H), 4.37 (dd, 1H,  $J = 11.4, 3.7$  Hz), 2.61 (s, 3H), 2.40 (s, 3H), 2.37–2.31 (m, 1H), 2.12–2.04 (m, 1H), 1.40–1.24 (m, 2H), 1.24–1.10 (m, 2H), 0.84 (t, 3H,  $J = 7.3$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  138.4, 132.0, 131.2, 129.0, 127.9, 127.1, 65.0, 38.7, 29.1, 28.5, 22.8, 20.3, 13.9.

FT-IR (neat) 3025, 2957, 2931, 2872, 1493, 1464, 1411, 1380, 1294, 1224, 1208, 1177, 1138, 1113, 1051, 958, 825, 796, 771, 736  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{13}\text{H}_{20}\text{NaO}_2\text{S}$ : 263, found: 263.

$[\alpha]_{\text{D}}^{25} = +24.2^\circ$  ( $c = 0.99$ ,  $\text{CHCl}_3$ ).



**(S)-1-Ethyl-2-(1-(methylsulfonyl)pentyl)benzene (Table 4, Entry 11).** 1-Bromo-1-(methylsulfonyl)pentane (160 mg, 0.700 mmol), (2-ethylphenyl)zinc iodide (1.40 mmol),  $\text{NiCl}_2 \cdot \text{glyme}$  (30.8 mg, 0.140 mmol), and (*R,R*)-L1 (60.9 mg, 0.182 mmol) were used. The product was purified by column chromatography (15% ethyl acetate/hexanes). Light-yellow oil. First run: 145 mg (81%, 98% ee). Second run: 146 mg (82%, 98% ee).

The ee was determined by HPLC on a CHIRALPAK AS-H column (10% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 13.1$  min (minor), 22.1 min (major).

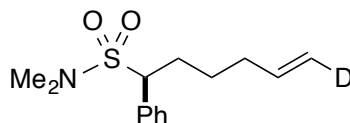
$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.52–7.51 (m, 1H), 7.34–7.26 (m, 3H), 4.41 (dd, 1H,  $J = 11.2, 3.9$  Hz), 2.82–2.75 (m, 1H), 2.73–2.66 (m, 1H), 2.62 (s, 3H), 2.35 (dddd, 1H,  $J = 13.5, 11.0, 5.7, 3.8$  Hz), 2.12–2.04 (m, 1H), 1.41–1.20 (m, 3H), 1.23 (t, 3H,  $J = 7.6$  Hz), 1.19–1.09 (m, 1H), 0.85 (t, 3H,  $J = 7.2$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  144.4, 131.2, 129.6, 129.1, 127.9, 126.9, 64.5, 38.8, 29.3, 28.7, 26.2, 23.0, 15.7, 13.9.

FT-IR (neat) 3063, 3026, 2960, 2932, 2873, 1491, 1453, 1411, 1379, 1294, 1218, 1176, 1138, 1113, 1061, 958, 831, 797, 757  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{14}\text{H}_{22}\text{NaO}_2\text{S}$ : 277, found: 277.

$[\alpha]_{\text{D}}^{25} = +24.1^\circ$  ( $c = 1.01$ ,  $\text{CHCl}_3$ ).



**(*S,E*)-*N,N*-Dimethyl-1-phenylhex-5-ene-1-sulfonamide-6-*d* (eq 3).** White solid.

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 13.9$  min (major), 17.4 min (minor).

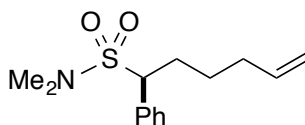
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42–7.34 (m, 5H), 5.70 (dt, 1H,  $J = 17.0, 6.5$  Hz), 4.95 (dt, 1H,  $J = 17.1, 1.6$  Hz), 4.09 (dd, 1H,  $J = 11.2, 3.9$  Hz), 2.53 (s, 6H), 2.32 (dddd, 1H,  $J = 13.9, 10.3, 6.4, 3.9$  Hz), 2.20–2.12 (m, 1H), 2.10–1.98 (m, 2H), 1.36–1.22 (m, 2H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.8, 134.0, 129.6, 129.0, 128.9, 115.0 (t,  $J = 24$  Hz), 67.8, 37.8, 33.3, 29.5, 26.2.

FT-IR (neat) 3088, 3065, 3024, 2926, 2860, 2822, 2261, 1623, 1496, 1480, 1456, 1436, 1326, 1292, 1256, 1200, 1140, 1064, 1043, 984, 970, 917, 906, 822, 799, 778, 745  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+ - \text{SO}_2\text{NMe}_2$ ) calcd for  $\text{C}_{12}\text{H}_{14}\text{D}$ : 160, found: 160.

$[\alpha]_{\text{D}}^{25} = -34^\circ$  ( $c = 0.99$ ,  $\text{CHCl}_3$ ); 96% ee.



**(*S*)-*N,N*-Dimethyl-1-phenylhex-5-ene-1-sulfonamide (Figure 1).** White solid.

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 14.1$  min (major), 17.8 min (minor).

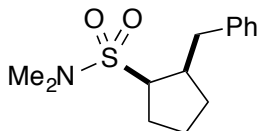
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42–7.34 (m, 5H), 5.70 (ddt, 1H,  $J = 17.0, 10.3, 6.7$  Hz), 4.98–4.92 (m, 2H), 4.09 (dd, 1H,  $J = 11.2, 3.9$  Hz), 2.53 (s, 6H), 2.32 (dddd, 1H,  $J = 14.1, 10.3, 6.3, 3.9$  Hz), 2.20–2.12 (m, 1H), 2.10–1.98 (m, 2H), 1.36–1.22 (m, 2H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  138.0, 134.0, 129.6, 129.0, 128.9, 115.3, 67.8, 37.8, 33.4, 29.5, 26.2.

FT-IR (neat) 3067, 3033, 2934, 2908, 2868, 2821, 1640, 1497, 1480, 1455, 1417, 1329, 1282, 1199, 1141, 1063, 1043, 993, 966, 916, 906, 870, 814, 781, 746, 735  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+ - \text{SO}_2\text{NMe}_2$ ) calcd for  $\text{C}_{12}\text{H}_{15}$ : 159, found: 159.

$[\alpha]_{\text{D}}^{25} = -33^\circ$  ( $c = 0.82$ ,  $\text{CHCl}_3$ ); 97% ee.



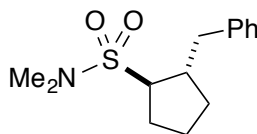
***syn*-2-Benzyl-*N,N*-dimethylcyclopentane-1-sulfonamide (Figure 1).** White solid.

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.30–7.26 (m, 2H), 7.20–7.16 (m, 3H), 3.54 (ddd, 1H,  $J = 8.7, 8.7, 6.3$  Hz), 3.31–3.25 (m, 1H), 2.89 (s, 6H), 2.60–2.52 (m, 2H), 2.15–2.07 (m, 1H), 2.04–1.97 (m, 1H), 1.95–1.87 (m, 1H), 1.66–1.44 (m, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  141.8, 129.4, 128.6, 126.2, 62.8, 44.7, 37.8, 35.7, 29.7, 26.8, 22.7.

FT-IR (neat) 3084, 3060, 3024, 2922, 2874, 2850, 2806, 1602, 1583, 1495, 1473, 1452, 1332, 1273, 1195, 1136, 1073, 1058, 1029, 958, 845, 822, 727  $\text{cm}^{-1}$ .

MS (EI)  $m/z$  ( $\text{M}^+$ ) calcd for  $\text{C}_{14}\text{H}_{21}\text{NO}_2\text{S}$ : 267, found: 267.



***anti*-2-Benzyl-*N,N*-dimethylcyclopentane-1-sulfonamide (Figure 1).** Colorless oil.

$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.32–7.28 (m, 2H), 7.22–7.19 (m, 3H), 3.20 (ddd, 1H,  $J = 8.9, 6.1, 6.1$  Hz), 2.97 (dd, 1H,  $J = 12.6, 4.9$  Hz), 2.78 (s, 6H), 2.65–2.53 (m, 2H), 2.08–1.95 (m, 2H), 1.82–1.74 (m, 1H), 1.73–1.61 (m, 2H), 1.42–1.35 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  140.7, 129.6, 128.7, 126.5, 64.5, 43.6, 41.3, 37.8, 32.1, 28.5, 24.9.

FT-IR (neat) 3084, 3060, 3025, 2917, 2849, 1602, 1583, 1494, 1461, 1453, 1435, 1315, 1199, 1136, 1082, 1059, 1029, 960, 882, 849, 733  $\text{cm}^{-1}$ .

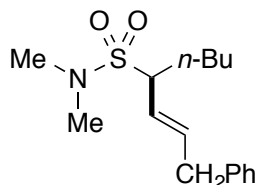
MS (EI)  $m/z$  ( $\text{M}^+$ ) calcd for  $\text{C}_{14}\text{H}_{21}\text{NO}_2\text{S}$ : 267, found: 267.

#### IV. Enantioselective Alkenylations

**General Procedure.**  $\text{Cp}_2\text{ZrHCl}$  (Schwartz's reagent; 258 mg, 1.00 mmol) was added to an oven-dried 4-mL vial equipped with a magnetic stir bar, and then the vial was capped with a PTFE-lined septum cap. The vial was evacuated and refilled with nitrogen (three cycles). 1,2-Dimethoxyethane (1.00 ml) was added to the vial, followed by the alkyne (1.00 mmol). The reaction mixture was stirred at r.t. for 1.5 h, at which time it had become homogenous. An oven-dried 20-mL vial equipped with a magnetic stir bar was charged with  $\text{NiCl}_2 \cdot \text{glyme}$  (11.0 mg, 0.050 mmol), (3*R*,8*S*)-L6 (23.3 mg, 0.065 mmol), and the electrophile (0.500 mmol). The vial

was sealed with a PTFE-lined septum cap, placed under vacuum, and then filled with nitrogen. This evacuation-refill cycle was repeated three times. 1,2-Dimethoxyethane (2.57 mL) was added, and the mixture was stirred at r.t. for 1 h. The solution of the nucleophile was transferred by syringe over 2 min to the vial that contained the electrophile. The reaction mixture was stirred at r.t. for 24 h, and then the reaction was quenched by the addition of ethanol (0.50 mL). The solution was filtered through a pad of silica (eluted with Et<sub>2</sub>O). The filtrate was concentrated, and the resulting residue was purified by column chromatography.

A second run was conducted with (3*S*,8*R*)-L6.



**(*S,E*)-*N,N*-Dimethyl-1-phenyloct-2-ene-4-sulfonamide (Table 5, Entry 1).** 1-Bromo-*N,N*-dimethylpentane-1-sulfonamide (129 mg, 0.500 mmol) and (*E*)-(3-phenylprop-1-en-1-yl)zirconium reagent (1.00 mmol) were used. The product was purified by column chromatography on silica gel (15% ethyl acetate/hexanes). Colorless oil. First run: 116 mg (79%, 91% ee). Second run: 122 mg (83%, 90% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 18.2$  min (major), 20.9 min (minor).

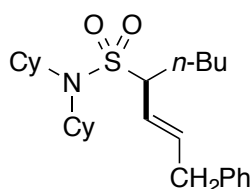
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.32–7.28 (m, 2H), 7.24–7.20 (m, 1H), 7.18–7.15 (m, 2H), 5.87 (dddd, 1H,  $J = 15.3, 6.9, 6.9, 0.4$  Hz), 5.44 (dddd, 1H,  $J = 15.3, 9.7, 1.5, 1.5$  Hz), 3.57 (ddd, 1H,  $J = 10.5, 10.5, 3.5$  Hz), 3.49–3.39 (m, 2H), 2.82 (s, 6H), 2.04–1.97 (m, 1H), 1.75–1.68 (m, 1H), 1.41–1.18 (m, 4H), 0.89 (t, 3H,  $J = 7.1$  Hz).

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  139.3, 136.9, 128.7, 128.6, 126.5, 125.1, 65.8, 39.1, 38.3, 28.8, 28.7, 22.4, 14.0.

FT-IR (neat) 3061, 3027, 2954, 2930, 2871, 1663, 1603, 1494, 1453, 1379, 1329, 1281, 1198, 1139, 1076, 1062, 1029, 966, 804, 747, 730 cm<sup>-1</sup>.

MS (EI)  $m/z$  ( $M^+ - \text{SO}_2\text{NMe}_2$ ) calcd for C<sub>14</sub>H<sub>19</sub>: 187, found: 187.

$[\alpha]_D^{25} = +22.9^\circ$  ( $c = 1.01$ , CHCl<sub>3</sub>).



**(*S,E*)-*N,N*-Dicyclohexyl-1-phenyloct-2-ene-4-sulfonamide (Table 5, Entry 2).** 1-Bromo-*N,N*-dicyclohexylpentane-1-sulfonamide (197 mg, 0.500 mmol) and (*E*)-(3-phenylprop-1-en-1-yl)zirconium reagent (1.00 mmol) were used. The product was purified by column chromatography on silica gel (5% Et<sub>2</sub>O/hexanes) and then on C-18 silica gel (10%→100%

acetonitrile/water). Viscous light-yellow oil. First run: 179 mg (83%, 95% ee). Second run: 180 mg (83%, 94% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (1% *i*-PrOH/hexanes, 0.6 mL/min) with  $t_r$  = 16.6 min (major), 17.7 min (minor).

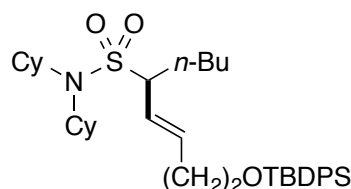
$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.31–7.28 (m, 2H), 7.22–7.17 (m, 3H), 5.80 (dddd, 1H,  $J$  = 15.3, 7.4, 6.0, 0.4 Hz), 5.42 (dddd, 1H,  $J$  = 15.4, 9.8, 1.5, 1.5 Hz), 3.48–3.38 (m, 2H), 3.33 (ddd, 1H,  $J$  = 10.8, 10.0, 3.2 Hz), 3.17–3.10 (m, 2H), 2.04–1.97 (m, 1H), 1.79–1.56 (m, 15H), 1.41–1.16 (m, 8H), 1.08 (qt, 2H,  $J$  = 13.1, 3.4 Hz), 0.89 (t, 3H,  $J$  = 7.2 Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  140.1, 136.6, 128.9, 128.8, 126.6, 126.0, 69.0, 58.4, 39.2, 34.0, 33.1, 29.5, 29.3, 26.99, 26.97, 25.8, 22.7, 14.1.

FT-IR (neat) 3084, 3062, 3027, 2931, 2855, 1603, 1495, 1466, 1453, 1401, 1381, 1322, 1274, 1256, 1188, 1164, 1139, 1108, 1074, 1047, 1028, 981, 895, 854, 823, 750  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{26}\text{H}_{41}\text{NNaO}_2\text{S}$ : 454, found: 454.

$[\alpha]_{\text{D}}^{25} = -6.9^\circ$  ( $c$  = 1.02,  $\text{CHCl}_3$ ).



**(*S,E*)-1-((*tert*-Butyldiphenylsilyl)oxy)-*N,N*-dicyclohexylnon-3-ene-5-sulfonamide (Table 5, Entry 3).** 1-Bromo-*N,N*-dicyclohexylpentane-1-sulfonamide (197 mg, 0.500 mmol) and (*E*)-(4-((*tert*-butyldiphenylsilyl)oxy)but-1-en-1-yl)zirconium reagent (1.00 mmol) were used. The product was purified by column chromatography on silica gel (3% ethyl acetate/hexanes) and then on C-18 silica gel (10%→100% acetonitrile/water). Viscous light-yellow oil. First run: 254 mg (81%, 95% ee). Second run: 259 mg (83%, 94% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (0.5% *i*-PrOH/hexanes, 0.8 mL/min) with  $t_r$  = 14.6 min (minor), 17.9 min (major).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67–7.64 (m, 4H), 7.45–7.41 (m, 2H), 7.40–7.36 (m, 4H), 5.69 (ddd, 1H,  $J$  = 15.5, 6.4, 6.4 Hz), 5.42 (dddd, 1H,  $J$  = 15.5, 9.7, 1.4, 1.4 Hz), 3.75–3.68 (m, 2H), 3.26 (ddd, 1H,  $J$  = 10.6, 9.5, 3.2 Hz), 3.15–3.09 (m, 2H), 2.39–2.29 (m, 2H), 2.08–2.01 (m, 1H), 1.76–1.57 (m, 14H), 1.39–1.14 (m, 9H), 1.12–1.02 (m, 2H), 1.05 (s, 9H), 0.86 (t, 3H,  $J$  = 7.2 Hz).

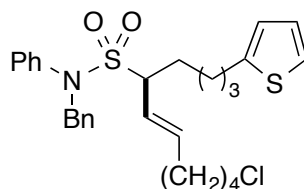
$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  135.7, 135.6, 134.3, 133.9, 133.8, 129.79, 129.78, 127.79, 127.78, 126.10, 69.5, 63.2, 58.2, 36.0, 33.9, 32.8, 29.3, 29.0, 26.9, 26.7, 25.5, 22.5, 19.3, 14.0.

FT-IR (neat) 3071, 3048, 2931, 2856, 1590, 1471, 1453, 1428, 1389, 1323, 1257, 1221, 1188, 1164, 1138, 1110, 1048, 1028, 998, 980, 939, 895, 854, 822, 764, 738  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{37}\text{H}_{57}\text{NNaO}_3\text{SSi}$ : 646, found: 646.

$[\alpha]_{\text{D}}^{25} = +1.7^\circ$  ( $c$  = 0.99,  $\text{CHCl}_3$ ).





**(*S,E*)-*N*-Benzyl-11-chloro-*N*-phenyl-1-(thiophen-2-yl)undec-6-ene-5-sulfonamide (Table 5, Entry 4).** *N*-Benzyl-1-bromo-*N*-phenyl-5-(thiophen-2-yl)pentane-1-sulfonamide (239 mg, 0.500 mmol) and (*E*)-(6-chlorohex-1-en-1-yl)zirconium reagent (1.00 mmol) were used. The product was purified by column chromatography (first purification: 5% ethyl acetate/hexanes; second purification: 15% cyclopentyl methyl ether/hexanes). Viscous light-yellow oil. First run: 165 mg (64%, 80% ee). Second run: 156 mg (60%, 81% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (10% *i*-PrOH/hexanes, 0.8 mL/min) with  $t_r = 17.5$  min (major), 23.8 min (minor).

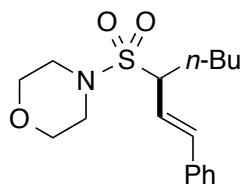
$^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  7.32–7.28 (m, 2H), 7.27–7.19 (m, 8H), 7.12 (dd, 1H,  $J = 5.1, 1.2$  Hz), 6.91 (dd, 1H,  $J = 5.1, 3.4$  Hz), 6.77 (dddd, 1H,  $J = 3.3, 1.0, 1.0, 1.0$  Hz), 5.80 (ddd, 1H,  $J = 15.3, 6.8, 6.8$  Hz), 5.46 (dddd, 1H,  $J = 15.4, 9.7, 1.5, 1.5$  Hz), 4.99 (d, 1H,  $J = 15.1$  Hz), 4.67 (d, 1H,  $J = 15.1$  Hz), 3.60–3.55 (m, 1H), 3.58 (t, 2H,  $J = 6.6$  Hz), 2.87–2.76 (m, 2H), 2.26–2.13 (m, 2H), 2.04 (dddd, 1H,  $J = 13.6, 9.9, 6.3, 3.4$  Hz), 1.86–1.72 (m, 3H), 1.72–1.56 (m, 4H), 1.50–1.41 (m, 1H), 1.32–1.22 (m, 1H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  145.6, 139.7, 139.0, 137.3, 129.4, 129.3, 128.7, 128.6, 127.9, 127.8, 127.0, 124.5, 124.2, 123.2, 66.7, 56.7, 45.4, 32.5, 32.2, 31.6, 29.9, 29.2, 26.5, 26.2.

FT-IR (neat) 3064, 3032, 2933, 2860, 1595, 1493, 1454, 1337, 1216, 1145, 1093, 1065, 1028, 976, 916, 862, 775  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{28}\text{H}_{34}\text{ClNNaO}_2\text{S}_2$ : 538, found: 538.

$[\alpha]_D^{25} = -23.0^\circ$  ( $c = 1.03, \text{CHCl}_3$ ).



**(*S,E*)-4-((1-Phenylhept-1-en-3-yl)sulfonyl)morpholine (Table 5, Entry 5).** 4-((1-Bromopentyl)sulfonyl)morpholine (150 mg, 0.500 mmol), and (*E*)-styrylzirconium reagent (1.00 mmol) were used. The product was purified by column chromatography (15% ethyl acetate/hexanes). White solid. First run: 110 mg (68%, 97% ee). Second run: 110 mg (68%, 95% ee).

The ee was determined by HPLC on a CHIRALPAK AS-H column (10% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 18.7$  min (minor), 30.1 min (major).

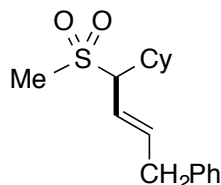
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42–7.39 (m, 2H), 7.38–7.34 (m, 2H), 7.32–7.29 (m, 1H), 6.62 (d, 1H,  $J = 15.9$  Hz), 6.06 (dd, 1H,  $J = 15.9, 9.8$  Hz), 3.70–3.62 (m, 5H), 3.38–3.30 (m, 4H), 2.17–2.10 (m, 1H), 1.87–1.79 (m, 1H), 1.45–1.22 (m, 4H), 0.90 (t, 3H,  $J = 7.0$  Hz).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.0, 135.7, 129.0, 128.7, 126.7, 122.7, 67.1, 67.0, 46.8, 29.0, 28.8, 22.4, 14.0.

FT-IR (neat) 2958, 2923, 2859, 1450, 1339, 1324, 1260, 1148, 1114, 1073, 955, 743  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{17}\text{H}_{25}\text{NNaO}_3\text{S}$ : 346, found: 346.

$[\alpha]_{\text{D}}^{25} = -82^\circ$  ( $c = 0.98$ ,  $\text{CHCl}_3$ ).



**(S,E)-(4-Cyclohexyl-4-(methylsulfonyl)but-2-en-1-yl)benzene (Table 5, Entry 6).**

(Bromo(methylsulfonyl)methyl)cyclohexane (179 mg, 0.700 mmol), (E)-(3-phenylprop-1-en-1-yl)zirconium reagent (1.40 mmol), and (R,R)-L1 (30.4 mg, 0.091 mmol) were used. The product was purified by column chromatography (15% ethyl acetate/hexanes). Light-yellow oil. First run: 109 mg (53%, 93% ee). Second run: 98 mg (48%, 93% ee).

The ee was determined by HPLC on a CHIRALPAK IB-3 column (5% *i*-PrOH/hexanes, 1.0 mL/min) with  $t_r = 13.0$  min (minor), 22.9 min (major).

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.33–7.30 (m, 2H), 7.25–7.21 (m, 1H), 7.18–7.16 (m, 2H), 5.89 (ddd, 1H,  $J = 15.2, 6.9, 6.9$  Hz), 5.71 (dddd, 1H,  $J = 15.3, 10.4, 1.4, 1.4$  Hz), 3.48 (d, 2H,  $J = 6.9$  Hz), 3.29 (dd, 1H,  $J = 10.4, 3.8$  Hz), 2.76 (s, 3H), 2.32 (tq, 1H,  $J = 11.9, 3.5$  Hz), 2.08–2.02 (m, 1H), 1.78–1.72 (m, 2H), 1.70–1.61 (m, 2H), 1.40–1.26 (m, 2H), 1.23–1.07 (m, 3H).

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  139.2, 139.0, 128.8, 128.6, 126.6, 122.6, 73.2, 39.8, 39.3, 36.0, 32.2, 28.9, 26.4, 26.1, 26.0.

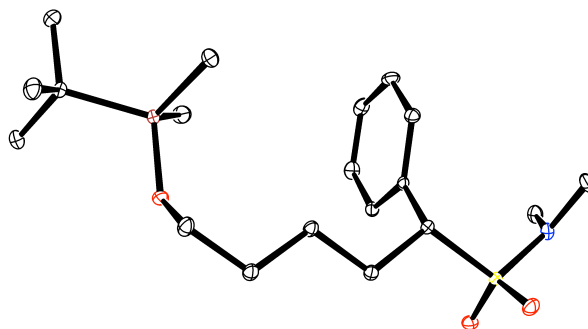
FT-IR (neat) 3083, 3060, 3026, 2927, 2852, 1660, 1602, 1494, 1452, 1411, 1351, 1295, 1240, 1173, 1133, 1077, 1029, 978, 894, 852, 784, 751, 700  $\text{cm}^{-1}$ .

MS (ESI)  $m/z$  ( $\text{M}^+ + \text{Na}$ ) calcd for  $\text{C}_{17}\text{H}_{24}\text{NaO}_2\text{S}$ : 315, found: 315.

$[\alpha]_{\text{D}}^{25} = +60.8^\circ$  ( $c = 1.00$ ,  $\text{CHCl}_3$ ).

## V. Determination of Absolute Stereochemistry

Product from entry 7 of Table 2 (run with (S,S)-L1). (*R*)-5-((*tert*-Butyldimethylsilyl)oxy)-*N,N*-dimethyl-1-phenylpentane-1-sulfonamide. A crystal suitable for X-ray crystallography was grown by vapor diffusion with dichloromethane and pentane.



A suitable crystal of C<sub>19</sub>H<sub>35</sub>NO<sub>3</sub>Si was selected for analysis. All measurements were made on a Bruker SMART 1000 CCD with filtered Mo-K $\alpha$  radiation at a temperature of 100 K. Using Olex2,<sup>6</sup> the structure was solved with the ShelXS<sup>7</sup> structure solution program using Direct Methods and refined with the ShelXL<sup>7</sup> refinement package using Least Squares minimization. The absolute stereochemistry was determined on the basis of the absolute structure parameter.

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- (6) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. J. *Appl. Crystallogr.* **2009**, *42*, 339–341.  
(7) Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112–122.

Table S-1. Crystal data and structure refinement for crystal01.

Identification code	crystal01	
Empirical formula	$C_{19}H_{35}INO_3SSi$	
Formula weight	385.63	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	$a = 5.9209(6)$ Å	$\alpha = 90^\circ$ .
	$b = 10.6607(12)$ Å	$\beta = 99.2230(10)^\circ$ .
	$c = 17.0647(19)$ Å	$\gamma = 90^\circ$ .
Volume	$1063.2(2)$ Å <sup>3</sup>	
Z	2	
Density (calculated)	1.205 Mg/m <sup>3</sup>	
Absorption coefficient	0.226 mm <sup>-1</sup>	
F(000)	420	
Crystal size	0.4 x 0.4 x 0.1 mm <sup>3</sup>	
Theta range for data collection	1.209 to 29.107°.	
Index ranges	-7 ≤ h ≤ 8, -13 ≤ k ≤ 14, -22 ≤ l ≤ 23	
Reflections collected	16770	
Independent reflections	5160 [R(int) = 0.0236]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9257	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5160 / 1 / 233	
Goodness-of-fit on F <sup>2</sup>	1.098	
Final R indices [I > 2σ(I)]	R1 = 0.0279, wR2 = 0.0669	
R indices (all data)	R1 = 0.0308, wR2 = 0.0690	
Absolute structure parameter	0.02(2)	
Largest diff. peak and hole	0.325 and -0.163 e/Å <sup>-3</sup>	

Table S-2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )

for crystal01.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
S(1)	-4031(1)	5489(1)	517(1)	14(1)
Si(1)	2618(1)	1014(1)	3465(1)	14(1)
O(1)	-3746(3)	5244(1)	-291(1)	20(1)
O(2)	-6212(2)	5232(1)	755(1)	19(1)
O(3)	648(2)	432(2)	2769(1)	19(1)
N(1)	-3503(3)	6967(2)	689(1)	16(1)
C(1)	-4272(4)	7610(2)	1361(1)	20(1)
C(2)	-1459(4)	7506(2)	435(1)	22(1)
C(3)	-1857(3)	4582(2)	1132(1)	12(1)
C(4)	-2416(3)	3172(2)	1032(1)	15(1)
C(5)	-552(3)	2381(2)	1521(1)	16(1)
C(6)	-952(4)	967(2)	1416(1)	18(1)
C(7)	820(4)	204(2)	1957(1)	21(1)
C(8)	-1531(3)	5030(2)	1983(1)	12(1)
C(9)	508(3)	5621(2)	2311(1)	17(1)
C(10)	842(3)	6027(2)	3095(1)	21(1)
C(11)	-835(4)	5849(2)	3558(1)	21(1)
C(12)	-2858(4)	5251(2)	3243(1)	20(1)
C(13)	-3211(3)	4849(2)	2456(1)	16(1)
C(14)	1116(4)	2120(2)	4054(1)	24(1)
C(15)	4837(4)	1893(2)	3029(1)	27(1)
C(16)	3960(3)	-312(2)	4110(1)	15(1)
C(17)	5647(4)	216(2)	4811(1)	23(1)
C(18)	2103(4)	-1074(2)	4431(1)	22(1)
C(19)	5248(4)	-1178(2)	3614(1)	24(1)

Table S-3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for crystal01.

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S(1)-O(1)	1.4394(15)
S(1)-O(2)	1.4405(15)
S(1)-N(1)	1.6247(18)
S(1)-C(3)	1.8048(19)
Si(1)-O(3)	1.6471(14)
Si(1)-C(14)	1.865(2)
Si(1)-C(15)	1.863(2)
Si(1)-C(16)	1.886(2)
O(3)-C(7)	1.426(2)
N(1)-C(1)	1.469(3)
N(1)-C(2)	1.466(3)
C(3)-C(4)	1.543(3)
C(3)-C(8)	1.512(3)
C(4)-C(5)	1.526(3)
C(5)-C(6)	1.532(3)
C(6)-C(7)	1.517(3)
C(8)-C(9)	1.396(3)
C(8)-C(13)	1.391(3)
C(9)-C(10)	1.390(3)
C(10)-C(11)	1.378(3)
C(11)-C(12)	1.387(3)
C(12)-C(13)	1.393(3)
C(16)-C(17)	1.537(3)
C(16)-C(18)	1.537(3)
C(16)-C(19)	1.535(3)
O(1)-S(1)-O(2)	118.93(9)
O(1)-S(1)-N(1)	107.45(9)
O(1)-S(1)-C(3)	106.10(9)
O(2)-S(1)-N(1)	106.79(9)
O(2)-S(1)-C(3)	108.81(9)
N(1)-S(1)-C(3)	108.40(9)
O(3)-Si(1)-C(14)	106.44(9)
O(3)-Si(1)-C(15)	111.35(9)
O(3)-Si(1)-C(16)	108.79(9)

C(14)-Si(1)-C(16)	110.66(10)
C(15)-Si(1)-C(14)	108.96(11)
C(15)-Si(1)-C(16)	110.57(10)
C(7)-O(3)-Si(1)	127.79(13)
C(1)-N(1)-S(1)	121.23(14)
C(2)-N(1)-S(1)	118.06(14)
C(2)-N(1)-C(1)	114.98(17)
C(4)-C(3)-S(1)	109.70(13)
C(8)-C(3)-S(1)	111.03(13)
C(8)-C(3)-C(4)	113.95(16)
C(5)-C(4)-C(3)	110.75(15)
C(4)-C(5)-C(6)	113.27(16)
C(7)-C(6)-C(5)	112.19(16)
O(3)-C(7)-C(6)	110.46(17)
C(9)-C(8)-C(3)	119.76(17)
C(13)-C(8)-C(3)	121.38(17)
C(13)-C(8)-C(9)	118.86(18)
C(10)-C(9)-C(8)	120.46(18)
C(11)-C(10)-C(9)	120.29(19)
C(10)-C(11)-C(12)	119.91(19)
C(11)-C(12)-C(13)	120.06(19)
C(8)-C(13)-C(12)	120.41(19)
C(17)-C(16)-Si(1)	109.87(14)
C(17)-C(16)-C(18)	109.15(17)
C(18)-C(16)-Si(1)	110.21(14)
C(19)-C(16)-Si(1)	109.22(14)
C(19)-C(16)-C(17)	109.34(17)
C(19)-C(16)-C(18)	109.03(17)

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Table S-4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal01. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
S(1)	14(1)	14(1)	12(1)	1(1)	-1(1)	0(1)
Si(1)	14(1)	12(1)	15(1)	2(1)	1(1)	-1(1)
O(1)	26(1)	21(1)	13(1)	0(1)	-2(1)	0(1)
O(2)	14(1)	19(1)	23(1)	1(1)	-1(1)	-1(1)
O(3)	21(1)	20(1)	14(1)	2(1)	-2(1)	-6(1)
N(1)	20(1)	13(1)	16(1)	2(1)	4(1)	1(1)
C(1)	24(1)	14(1)	22(1)	0(1)	5(1)	3(1)
C(2)	27(1)	17(1)	24(1)	2(1)	8(1)	-6(1)
C(3)	12(1)	13(1)	11(1)	1(1)	1(1)	2(1)
C(4)	18(1)	13(1)	12(1)	-2(1)	1(1)	0(1)
C(5)	19(1)	14(1)	13(1)	-1(1)	-1(1)	2(1)
C(6)	24(1)	15(1)	14(1)	-1(1)	-2(1)	0(1)
C(7)	27(1)	15(1)	18(1)	-1(1)	-1(1)	4(1)
C(8)	15(1)	10(1)	12(1)	1(1)	1(1)	1(1)
C(9)	14(1)	20(1)	18(1)	1(1)	3(1)	0(1)
C(10)	18(1)	20(1)	22(1)	-5(1)	-5(1)	-1(1)
C(11)	30(1)	19(1)	14(1)	-3(1)	0(1)	5(1)
C(12)	24(1)	21(1)	16(1)	0(1)	8(1)	2(1)
C(13)	18(1)	14(1)	15(1)	1(1)	2(1)	0(1)
C(14)	23(1)	20(1)	29(1)	-5(1)	0(1)	4(1)
C(15)	23(1)	28(1)	29(1)	12(1)	2(1)	-8(1)
C(16)	16(1)	14(1)	15(1)	2(1)	1(1)	1(1)
C(17)	23(1)	25(1)	20(1)	5(1)	-4(1)	-2(1)
C(18)	24(1)	17(1)	24(1)	5(1)	4(1)	-2(1)
C(19)	24(1)	21(1)	29(1)	1(1)	5(1)	6(1)



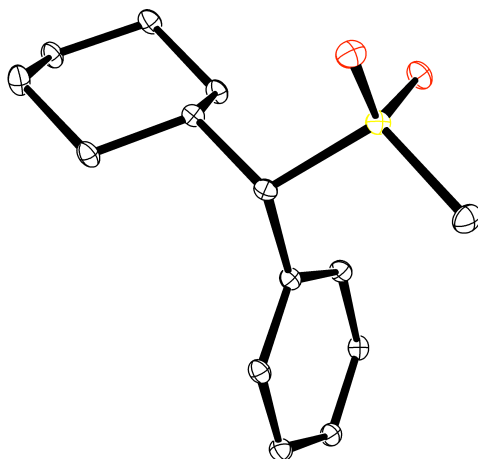
Table S-5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal01.

	x	y	z	U(eq)
H(1A)	-5587	7185	1497	30
H(1B)	-4669	8461	1216	30
H(1C)	-3064	7603	1809	30
H(2A)	-208	7483	869	33
H(2B)	-1761	8359	270	33
H(2C)	-1070	7027	-1	33
H(3)	-413	4726	934	15
H(4A)	-3873	3002	1201	18
H(4B)	-2546	2944	476	18
H(5A)	-473	2592	2077	19
H(5B)	911	2591	1368	19
H(6A)	-2463	763	1529	22
H(6B)	-902	741	869	22
H(7A)	586	-681	1840	25
H(7B)	2340	428	1861	25
H(9)	1649	5743	2003	20
H(10)	2205	6421	3308	25
H(11)	-611	6130	4081	26
H(12)	-3980	5118	3558	24
H(13)	-4578	4458	2246	19
H(14A)	483	2801	3721	36
H(14B)	2183	2444	4490	36
H(14C)	-93	1686	4254	36
H(15A)	5788	1311	2802	40
H(15B)	5761	2371	3437	40
H(15C)	4107	2449	2624	40
H(17A)	6824	681	4613	35
H(17B)	6325	-463	5136	35
H(17C)	4846	759	5121	35
H(18A)	1374	-556	4777	32
H(18B)	2791	-1786	4721	32

H(18C)	986	-1356	3996	32
H(19A)	4214	-1474	3160	37
H(19B)	5860	-1880	3931	37
H(19C)	6475	-722	3439	37

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**Product from entry 2 of Table 3: (S)-(Cyclohexyl(methylsulfonyl)methyl)benzene (from a reaction using (R,R)-L1).** A crystal suitable for X-ray crystallography was grown by vapor diffusion with dichloromethane and pentane.



A suitable crystal of  $C_{14}H_{20}O_2S$  was selected for analysis. All measurements were made on a Bruker APEX-II CCD with filtered Mo- $K\alpha$  radiation at a temperature of 100 K. Using Olex2,<sup>6</sup> the structure was solved with the ShelXS<sup>7</sup> structure solution program using Direct Methods and refined with the ShelXL<sup>7</sup> refinement package using Least Squares minimization. The absolute stereochemistry was determined on the basis of the absolute structure parameter.

Table S-6. Crystal data and structure refinement for crystal03.

Identification code	crystal03	
Empirical formula	$C_{14}H_{20}O_2S$	
Formula weight	252.36	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	
Unit cell dimensions	a = 6.2283(3) Å	$\alpha = 90^\circ$ .
	b = 13.7866(7) Å	$\beta = 90^\circ$ .
	c = 15.3937(8) Å	$\gamma = 90^\circ$ .
Volume	1321.81(12) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.268 Mg/m <sup>3</sup>	
Absorption coefficient	0.233 mm <sup>-1</sup>	
F(000)	544	
Crystal size	0.62 x 0.16 x 0.09 mm <sup>3</sup>	
Theta range for data collection	1.983 to 33.731°.	
Index ranges	-9 ≤ h ≤ 9, -21 ≤ k ≤ 20, -23 ≤ l ≤ 23	
Reflections collected	39471	
Independent reflections	4910 [R(int) = 0.0621]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8575	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	4910 / 0 / 155	
Goodness-of-fit on F <sup>2</sup>	1.141	
Final R indices [I > 2σ(I)]	R1 = 0.0540, wR2 = 0.1115	
R indices (all data)	R1 = 0.0741, wR2 = 0.1179	
Absolute structure parameter	0.01(3)	
Largest diff. peak and hole	0.692 and -0.385 e/Å <sup>-3</sup>	

Table S-7. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal03.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
S(1)	7502(1)	3757(1)	4892(1)	17(1)
O(1)	6971(3)	3206(1)	5662(1)	21(1)
O(2)	9662(3)	4136(1)	4836(1)	21(1)
C(1)	5566(4)	4731(2)	4817(2)	14(1)
C(2)	5963(4)	5465(2)	5570(2)	14(1)
C(3)	7759(4)	6208(2)	5418(2)	17(1)
C(4)	8064(4)	6849(2)	6224(2)	20(1)
C(5)	5993(4)	7371(2)	6464(2)	21(1)
C(6)	4161(4)	6651(2)	6587(2)	23(1)
C(7)	3868(4)	5994(2)	5790(2)	19(1)
C(8)	5392(4)	5139(2)	3904(2)	15(1)
C(9)	7131(4)	5552(2)	3461(2)	17(1)
C(10)	6869(4)	5905(2)	2620(2)	18(1)
C(11)	4895(4)	5840(2)	2207(2)	18(1)
C(12)	3168(4)	5434(2)	2644(2)	19(1)
C(13)	3419(4)	5081(2)	3483(2)	17(1)
C(14)	7027(5)	3018(2)	3977(2)	23(1)

Table S-8. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for crystal03.

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S(1)-O(1)	1.4458(19)
S(1)-O(2)	1.4461(19)
S(1)-C(1)	1.809(2)
S(1)-C(14)	1.763(3)
C(1)-H(1)	1.0000
C(1)-C(2)	1.557(3)
C(1)-C(8)	1.518(3)
C(2)-H(2)	1.0000
C(2)-C(3)	1.535(3)
C(2)-C(7)	1.533(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.536(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(4)-C(5)	1.523(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(5)-C(6)	1.524(4)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(6)-C(7)	1.536(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.401(3)
C(8)-C(13)	1.391(4)
C(9)-H(9)	0.9500
C(9)-C(10)	1.393(3)
C(10)-H(10)	0.9500
C(10)-C(11)	1.387(4)
C(11)-H(11)	0.9500
C(11)-C(12)	1.386(4)
C(12)-H(12)	0.9500
C(12)-C(13)	1.390(4)
C(13)-H(13)	0.9500

C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
O(1)-S(1)-O(2)	116.89(12)
O(1)-S(1)-C(1)	106.82(11)
O(1)-S(1)-C(14)	108.23(11)
O(2)-S(1)-C(1)	110.34(10)
O(2)-S(1)-C(14)	108.51(13)
C(14)-S(1)-C(1)	105.43(13)
S(1)-C(1)-H(1)	105.6
C(2)-C(1)-S(1)	109.22(16)
C(2)-C(1)-H(1)	105.6
C(8)-C(1)-S(1)	112.41(17)
C(8)-C(1)-H(1)	105.6
C(8)-C(1)-C(2)	117.36(18)
C(1)-C(2)-H(2)	107.1
C(3)-C(2)-C(1)	115.9(2)
C(3)-C(2)-H(2)	107.1
C(7)-C(2)-C(1)	109.8(2)
C(7)-C(2)-H(2)	107.1
C(7)-C(2)-C(3)	109.60(18)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
C(2)-C(3)-C(4)	110.6(2)
H(3A)-C(3)-H(3B)	108.1
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
C(3)-C(4)-H(4A)	109.4
C(3)-C(4)-H(4B)	109.4
H(4A)-C(4)-H(4B)	108.0
C(5)-C(4)-C(3)	111.3(2)
C(5)-C(4)-H(4A)	109.4
C(5)-C(4)-H(4B)	109.4
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
C(4)-C(5)-C(6)	110.9(2)

H(5A)-C(5)-H(5B)	108.1
C(6)-C(5)-H(5A)	109.5
C(6)-C(5)-H(5B)	109.5
C(5)-C(6)-H(6A)	109.2
C(5)-C(6)-H(6B)	109.2
C(5)-C(6)-C(7)	111.9(2)
H(6A)-C(6)-H(6B)	107.9
C(7)-C(6)-H(6A)	109.2
C(7)-C(6)-H(6B)	109.2
C(2)-C(7)-C(6)	110.9(2)
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(9)-C(8)-C(1)	123.1(2)
C(13)-C(8)-C(1)	118.2(2)
C(13)-C(8)-C(9)	118.7(2)
C(8)-C(9)-H(9)	119.9
C(10)-C(9)-C(8)	120.2(2)
C(10)-C(9)-H(9)	119.9
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-C(9)	120.5(2)
C(11)-C(10)-H(10)	119.7
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-C(10)	119.4(2)
C(12)-C(11)-H(11)	120.3
C(11)-C(12)-H(12)	119.8
C(11)-C(12)-C(13)	120.4(2)
C(13)-C(12)-H(12)	119.8
C(8)-C(13)-H(13)	119.6
C(12)-C(13)-C(8)	120.8(2)
C(12)-C(13)-H(13)	119.6
S(1)-C(14)-H(14A)	109.5
S(1)-C(14)-H(14B)	109.5
S(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14B)	109.5



H(14A)-C(14)-H(14C) 109.5

H(14B)-C(14)-H(14C) 109.5

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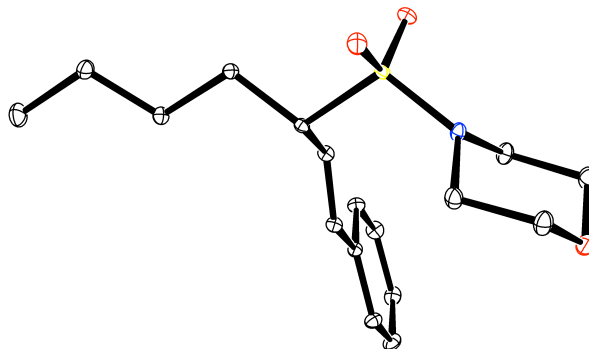
Table S-9. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal03. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
S(1)	19(1)	13(1)	18(1)	1(1)	-1(1)	-1(1)
O(1)	26(1)	17(1)	20(1)	2(1)	-1(1)	-2(1)
O(2)	17(1)	16(1)	29(1)	2(1)	0(1)	0(1)
C(1)	11(1)	15(1)	17(1)	1(1)	-1(1)	-3(1)
C(2)	14(1)	11(1)	18(1)	2(1)	-1(1)	-2(1)
C(3)	11(1)	17(1)	24(1)	-2(1)	0(1)	-3(1)
C(4)	15(1)	16(1)	28(1)	-2(1)	-3(1)	-2(1)
C(5)	18(1)	15(1)	29(1)	-4(1)	-1(1)	2(1)
C(6)	17(1)	22(1)	31(2)	-6(1)	4(1)	0(1)
C(7)	12(1)	18(1)	26(1)	-2(1)	0(1)	0(1)
C(8)	15(1)	12(1)	18(1)	1(1)	0(1)	0(1)
C(9)	14(1)	17(1)	20(1)	0(1)	-1(1)	-3(1)
C(10)	19(1)	14(1)	20(1)	1(1)	4(1)	-1(1)
C(11)	22(1)	14(1)	18(1)	0(1)	-1(1)	3(1)
C(12)	18(1)	18(1)	21(1)	-2(1)	-3(1)	2(1)
C(13)	12(1)	17(1)	21(1)	0(1)	1(1)	-2(1)
C(14)	32(2)	14(1)	22(1)	-3(1)	-2(1)	-1(1)

Table S-10. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal03.

	x	y	z	U(eq)
H(1)	4140	4428	4942	17
H(2)	6373	5077	6093	17
H(3A)	7392	6620	4912	21
H(3B)	9117	5865	5286	21
H(4A)	8533	6442	6719	23
H(4B)	9203	7333	6109	23
H(5A)	5613	7837	6000	25
H(5B)	6210	7741	7009	25
H(6A)	2812	7011	6695	28
H(6B)	4457	6244	7103	28
H(7A)	2725	5513	5908	22
H(7B)	3415	6392	5286	22
H(9)	8494	5592	3736	20
H(10)	8051	6192	2327	21
H(11)	4728	6071	1629	22
H(12)	1806	5398	2368	23
H(13)	2229	4797	3773	20
H(14A)	7233	3400	3447	34
H(14B)	5551	2773	3996	34
H(14C)	8032	2471	3980	34

**Product from entry 5 of Table 5 (run with (3*R*,8*S*)-L6). (*S,E*)-4-((1-Phenylhept-1-en-3-yl)sulfonyl)morpholine.** A crystal suitable for X-ray crystallography was grown by vapor diffusion with Et<sub>2</sub>O and pentane.



A suitable crystal of C<sub>17</sub>H<sub>25</sub>NO<sub>3</sub>S was selected for analysis. All measurements were made on a Bruker APEX-II CCD with filtered Mo-K $\alpha$  radiation at a temperature of 100 K. Using Olex2,<sup>6</sup> the structure was solved with the ShelXS<sup>7</sup> structure solution program using Direct Methods and refined with the ShelXL<sup>7</sup> refinement package using Least Squares minimization. The absolute stereochemistry was determined on the basis of the absolute structure parameter.

Table S-11. Crystal data and structure refinement for crystal02.

Identification code	crystal02	
Empirical formula	$C_{17}H_{25}I\text{NO}_3S$	
Formula weight	323.44	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	$a = 12.8350(6)$ Å	$\alpha = 90^\circ$ .
	$b = 5.6272(3)$ Å	$\beta = 113.133(2)^\circ$ .
	$c = 12.9187(6)$ Å	$\gamma = 90^\circ$ .
Volume	$858.03(7)$ Å <sup>3</sup>	
Z	2	
Density (calculated)	1.252 Mg/m <sup>3</sup>	
Absorption coefficient	0.201 mm <sup>-1</sup>	
F(000)	348	
Crystal size	0.5 x 0.12 x 0.12 mm <sup>3</sup>	
Theta range for data collection	1.714 to 31.552°.	
Index ranges	-18 ≤ h ≤ 18, -8 ≤ k ≤ 8, -19 ≤ l ≤ 19	
Reflections collected	57330	
Independent reflections	5731 [R(int) = 0.0344]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8839	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5731 / 1 / 200	
Goodness-of-fit on F <sup>2</sup>	1.073	
Final R indices [I > 2σ(I)]	R1 = 0.0258, wR2 = 0.0683	
R indices (all data)	R1 = 0.0273, wR2 = 0.0695	
Absolute structure parameter	0.019(11)	
Largest diff. peak and hole	0.444 and -0.190 e/Å <sup>-3</sup>	

Table S-12. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal02.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
S(1)	4726(1)	7787(1)	3347(1)	12(1)
O(1)	4294(1)	10123(2)	2942(1)	19(1)
O(2)	5535(1)	7480(2)	4482(1)	18(1)
O(3)	6358(1)	4985(2)	1135(1)	21(1)
N(1)	5344(1)	6838(2)	2534(1)	14(1)
C(1)	3537(1)	5903(2)	3176(1)	11(1)
C(2)	3067(1)	6643(2)	4055(1)	13(1)
C(3)	2154(1)	4910(2)	4061(1)	14(1)
C(4)	1833(1)	5268(3)	5067(1)	18(1)
C(5)	944(1)	3484(3)	5081(1)	25(1)
C(6)	2671(1)	6069(2)	1991(1)	13(1)
C(7)	2415(1)	4264(2)	1261(1)	13(1)
C(8)	1574(1)	4329(2)	93(1)	12(1)
C(9)	797(1)	6196(2)	-325(1)	16(1)
C(10)	21(1)	6194(3)	-1441(1)	19(1)
C(11)	9(1)	4336(3)	-2156(1)	20(1)
C(12)	764(1)	2453(3)	-1748(1)	20(1)
C(13)	1539(1)	2453(2)	-630(1)	16(1)
C(14)	4862(1)	7376(2)	1320(1)	18(1)
C(15)	5820(1)	7255(3)	909(1)	21(1)
C(16)	6847(1)	4566(3)	2317(1)	21(1)
C(17)	5947(1)	4555(3)	2806(1)	19(1)

Table S-13. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for crystal02.

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S(1)-O(1)	1.4424(10)
S(1)-O(2)	1.4360(9)
S(1)-N(1)	1.6356(11)
S(1)-C(1)	1.7985(12)
O(3)-C(15)	1.4267(18)
O(3)-C(16)	1.4241(17)
N(1)-C(14)	1.4733(16)
N(1)-C(17)	1.4694(17)
C(1)-C(2)	1.5379(17)
C(1)-C(6)	1.5001(15)
C(2)-C(3)	1.5265(17)
C(3)-C(4)	1.5241(18)
C(4)-C(5)	1.525(2)
C(6)-C(7)	1.3364(17)
C(7)-C(8)	1.4711(16)
C(8)-C(9)	1.4021(17)
C(8)-C(13)	1.3993(17)
C(9)-C(10)	1.3937(16)
C(10)-C(11)	1.391(2)
C(11)-C(12)	1.393(2)
C(12)-C(13)	1.3954(17)
C(14)-C(15)	1.5194(19)
C(16)-C(17)	1.5189(19)
O(1)-S(1)-N(1)	106.16(6)
O(1)-S(1)-C(1)	107.85(6)
O(2)-S(1)-O(1)	120.05(6)
O(2)-S(1)-N(1)	106.10(6)
O(2)-S(1)-C(1)	107.05(6)
N(1)-S(1)-C(1)	109.34(6)
C(16)-O(3)-C(15)	109.98(11)
C(14)-N(1)-S(1)	120.64(9)
C(17)-N(1)-S(1)	118.32(9)
C(17)-N(1)-C(14)	113.32(11)
C(2)-C(1)-S(1)	108.03(8)

C(6)-C(1)-S(1)	109.94(8)
C(6)-C(1)-C(2)	112.83(10)
C(3)-C(2)-C(1)	110.77(10)
C(4)-C(3)-C(2)	112.63(10)
C(3)-C(4)-C(5)	112.19(12)
C(7)-C(6)-C(1)	123.45(11)
C(6)-C(7)-C(8)	125.69(11)
C(9)-C(8)-C(7)	122.55(11)
C(13)-C(8)-C(7)	118.95(11)
C(13)-C(8)-C(9)	118.50(11)
C(10)-C(9)-C(8)	120.60(12)
C(11)-C(10)-C(9)	120.30(13)
C(10)-C(11)-C(12)	119.73(12)
C(11)-C(12)-C(13)	119.96(12)
C(12)-C(13)-C(8)	120.90(12)
N(1)-C(14)-C(15)	107.67(11)
O(3)-C(15)-C(14)	111.21(11)
O(3)-C(16)-C(17)	111.08(11)
N(1)-C(17)-C(16)	108.16(11)

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Table S-14. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal02. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
S(1)	12(1)	11(1)	11(1)	-1(1)	4(1)	-3(1)
O(1)	24(1)	11(1)	23(1)	0(1)	11(1)	-2(1)
O(2)	15(1)	26(1)	12(1)	-3(1)	2(1)	-7(1)
O(3)	22(1)	22(1)	21(1)	0(1)	12(1)	1(1)
N(1)	16(1)	16(1)	13(1)	3(1)	7(1)	2(1)
C(1)	10(1)	10(1)	11(1)	0(1)	3(1)	-1(1)
C(2)	12(1)	12(1)	13(1)	-1(1)	5(1)	0(1)
C(3)	11(1)	16(1)	14(1)	1(1)	4(1)	0(1)
C(4)	18(1)	20(1)	19(1)	-2(1)	10(1)	-1(1)
C(5)	22(1)	29(1)	28(1)	2(1)	15(1)	-4(1)
C(6)	11(1)	13(1)	12(1)	1(1)	2(1)	0(1)
C(7)	11(1)	14(1)	12(1)	0(1)	2(1)	0(1)
C(8)	11(1)	14(1)	11(1)	-2(1)	3(1)	-2(1)
C(9)	15(1)	16(1)	14(1)	-1(1)	3(1)	1(1)
C(10)	15(1)	21(1)	16(1)	2(1)	2(1)	2(1)
C(11)	16(1)	29(1)	12(1)	-2(1)	2(1)	-4(1)
C(12)	18(1)	26(1)	15(1)	-7(1)	6(1)	-3(1)
C(13)	13(1)	18(1)	17(1)	-4(1)	5(1)	0(1)
C(14)	18(1)	23(1)	13(1)	4(1)	7(1)	3(1)
C(15)	24(1)	23(1)	19(1)	4(1)	12(1)	1(1)
C(16)	18(1)	24(1)	23(1)	4(1)	10(1)	4(1)
C(17)	21(1)	16(1)	22(1)	7(1)	12(1)	4(1)

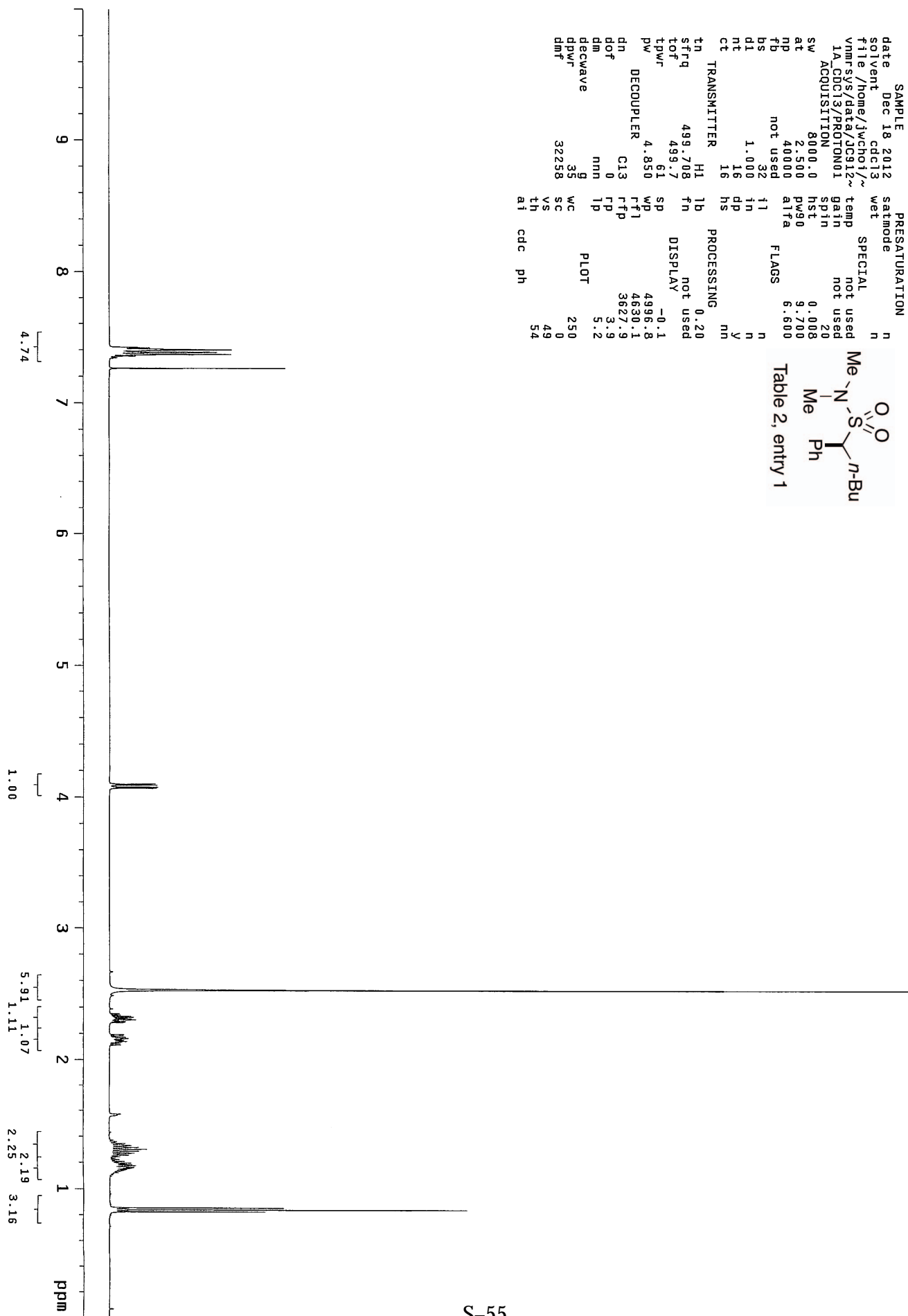
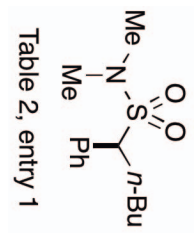
Table S-15. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for crystal02.

	x	y	z	U(eq)
H(1)	3809	4223	3327	13
H(2A)	3691	6680	4811	15
H(2B)	2742	8262	3881	15
H(3A)	1471	5115	3359	16
H(3B)	2431	3264	4072	16
H(4A)	1536	6898	5045	22
H(4B)	2520	5104	5770	22
H(5A)	764	3776	5741	37
H(5B)	1241	1868	5118	37
H(5C)	257	3664	4395	37
H(6)	2285	7535	1747	16
H(7)	2810	2813	1519	15
H(9)	800	7474	156	19
H(10)	-503	7467	-1715	23
H(11)	-513	4352	-2920	24
H(12)	752	1170	-2231	24
H(13)	2051	1161	-356	19
H(14A)	4520	8982	1187	22
H(14B)	4266	6206	911	22
H(15A)	5514	7563	89	25
H(15B)	6385	8503	1288	25
H(16A)	7412	5819	2689	25
H(16B)	7245	3017	2467	25
H(17A)	5409	3231	2480	23
H(17B)	6304	4338	3632	23

# VI. <sup>1</sup>H NMR Spectra

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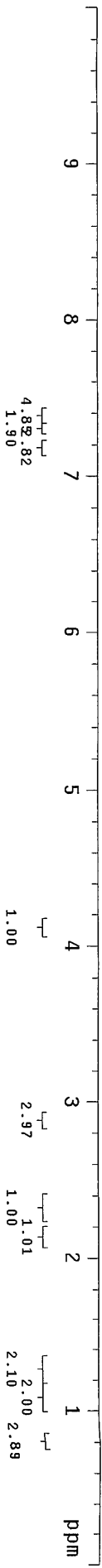
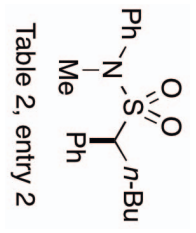
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			ph



JC9153A CDC13

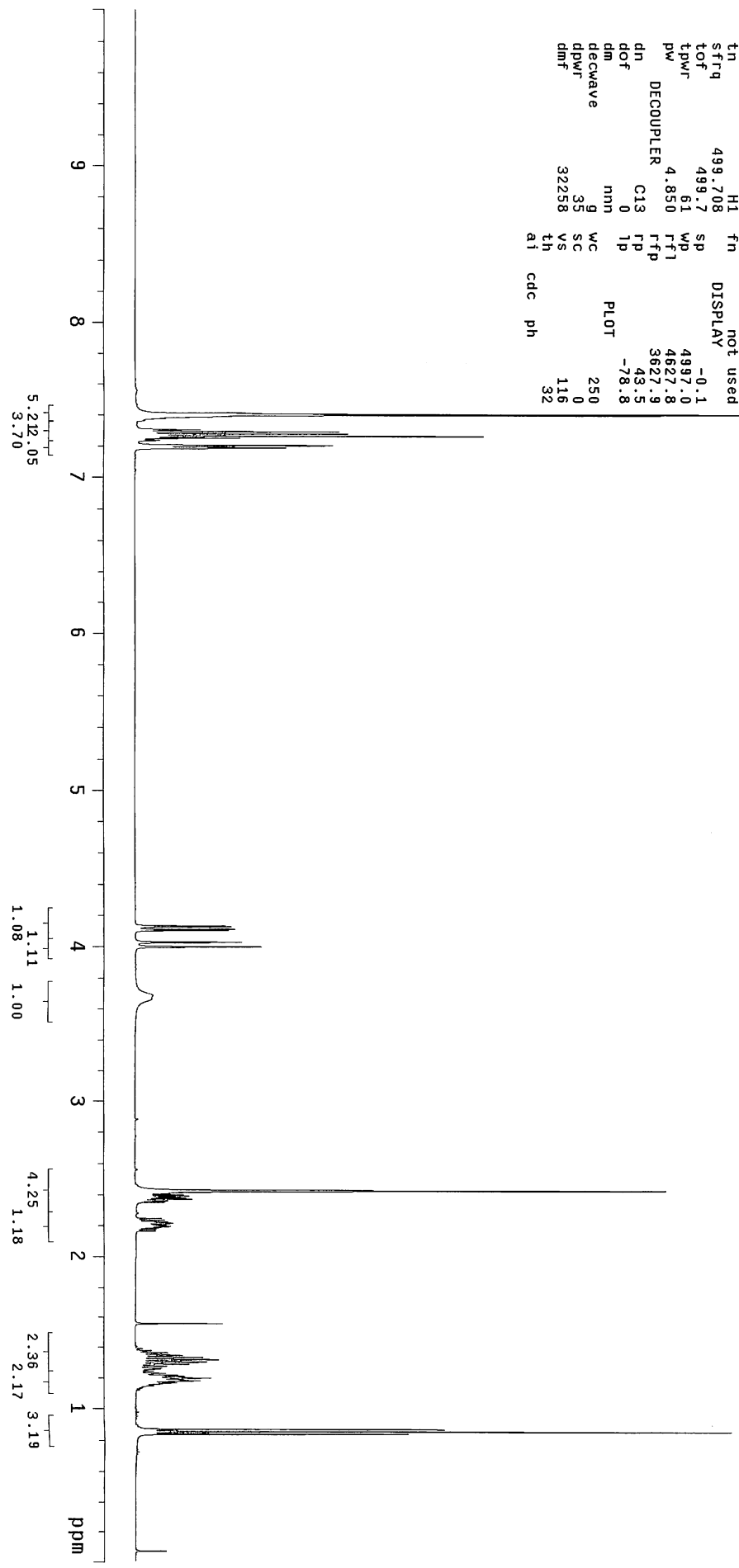
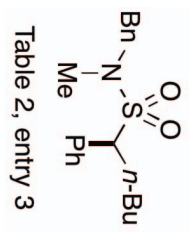
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 AT cdc ph



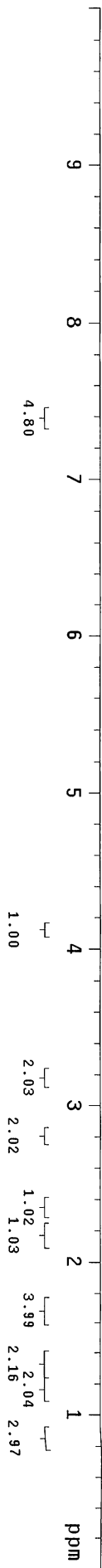
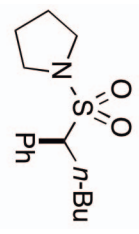
JC9149B 1H CDC13  
exp23 PROTON

SAMPLE PRESATURATION  
 date Jan 13 2013 satmode n  
 solvent cdc13 wet n  
 file /data/indy/jw~ SPECIAL not used  
 Choi/vnmr/sys/data/~ temp 30  
 JC9149B\_1H\_CDC13/P~ gain 20  
 ROTOM04.fid spin 20  
 ACQUISITION hst 0.008  
 SW 7995.2 pw90 9.700  
 at 3.000 alfa 10.000  
 np 47972  
 fb 4000 i1 n  
 bs 32 in n  
 dl 1.000 dp nm  
 nt 16 hs y  
 ct 16  
 TRANSMITTER H1 fb not used  
 tn 499.708 H1 fn not used  
 sfrq 499.708 SP DISPLAY  
 tof 499.7 WP 4997.0  
 tpwr 61 rff1 4627.8  
 pw 4.850 rffp 3627.9  
 DECOUPLER C13 rfp 43.5  
 dn 0 tp -78.8  
 dof 0  
 dm nmh PLOT  
 decwave 9 WC 250  
 dpwr 35 SC 0  
 dmf 32258 VS 116  
 at1 cdc ph 32



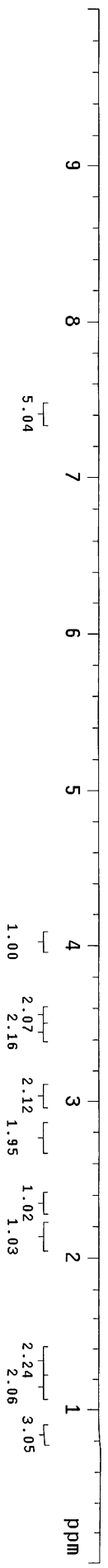
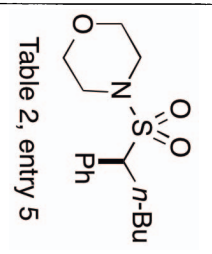
JC9147A 1H CDC13  
exp23 PROTON

SAMPLE PRESATURATION  
 date Jan 3 2013 satmode n  
 solvent cdc13 wet n  
 file /data/inhy/jw SPECIAL not used  
 ch01/vmr/sys/data/~ gain 46  
 JC9147A\_1H.CDC13/P~ ROTON01.fid spin 20  
 ACQUISITION hst 0.008  
 7995.2 PW90 9.700  
 SW 3.000 alfa 10.000  
 NP 47972  
 FB 4000 I1 n  
 BS 32 IN n  
 D1 1.000 DP nm  
 NT 16 HS y  
 CT 16  
 TRANSMITTER H1  
 TN 499.708 1b 0.20  
 SFRq 499.7 fn not used  
 TOF 61 SP DISPLAY  
 TPWR 4.850 WP 4997.0  
 PW DECOUPLER rffl 4627.6  
 C13 rfp 3627.9  
 0 1p 47.0  
 dn dof 0 PLOT -86.6  
 dm mn 250  
 decwave g WC 0  
 dpwr 35 SC 0  
 dmf 32258 VS 24  
 th 35



JC9155 1H CDC13  
 exp23 PROTON

SAMPLE PRESATURATION  
 date Jan 17 2013 satmode n  
 solvent cdc13 wet SPECIAL n  
 f1le /data/indy/Jw~ temp not used  
 Choi/vnmr/sys/data/~ gain 44  
 JC9155\_1H.CDC13/PR~ spin 20  
 OTOM01.fid hst 0.008  
 ACQUISITION pw90 9.700  
 7995.2 pw90 10.000  
 at 3.000 alfa  
 np 47972  
 fb 4000 i1  
 bs 32 in n  
 d1 1.000 dp n  
 nt 16 hs y  
 ct 16  
 TRANSMITTER 1b  
 tn H1 fn not used  
 sfrq 499.708 DISPLAY  
 tof 499.7 SP -0.1  
 tpwr 61 WP 4997.0  
 pw 4.850 rff1 4627.8  
 DECOUPLER rfp 3627.9  
 dn C13 fp 47.0  
 dof 0 1p -86.3  
 dm mnm PLOT  
 decwve 250  
 dpwr 9 WC 0  
 35 SC 50  
 32258 th 50  
 dmf ai cdc ph



JC10093B 1H CDC13  
 exp24 PROTON

SAMPLE		PRESATURATION	
date	May 14 2013	satmode	n
solvent	cdcl3	SPECIAL	n
file	/indy/jwcho1/~	not used	
nmrSYS	/data/JC100~	gain	32
93B_1H_CDC13/PROT0~		spin	20
		hst	0.008
ACQUISITION	N01.fid	pw90	9.900
		aiFa	10.000
SW	8000.0	FLAGS	
at	3.000		
np	48000		
fb	not used		
bs	not used		
d1	2.000		
nt	16		
ct	16		
TRANSMITTER	H1	PROCESSING	0.20
tn	499.708	fn	not used
sfrq	499.7	DISPLAY	
tof	61	wp	-0.1
tpwr	4.950	rf1	4996.8
pw	DECOUPLER	rfp	4630.1
dn	C13	rp	3627.9
dof	0	lp	6.8
dm	nm		-79.6
dm	nm	PLOT	250
decwave	w40_autox7~	WC	0
dpwr	41	VS	65
dmf	32258	th	13
	ai	cdc	ph

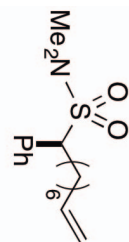
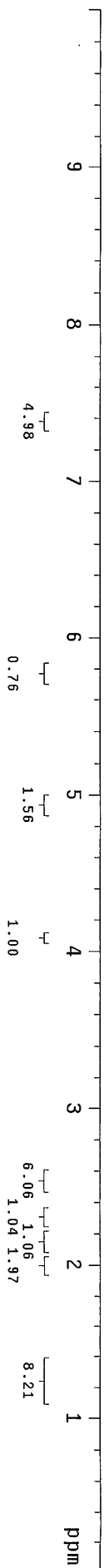


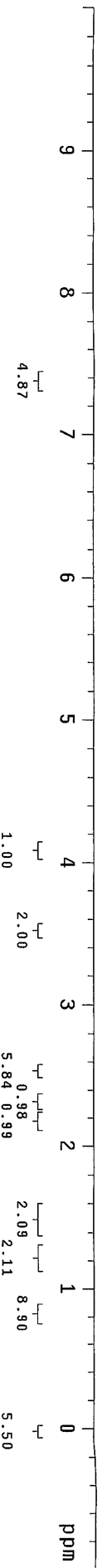
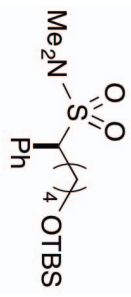
Table 2, entry 6





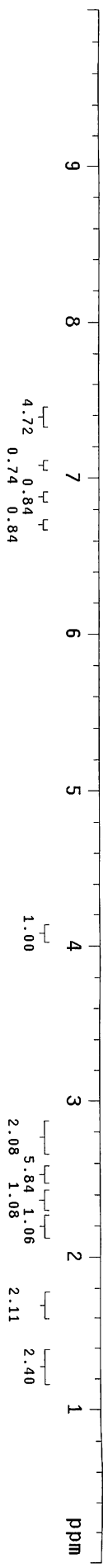
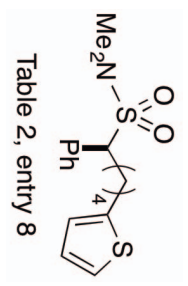
PM2-21A 1H CDC13  
 exp30 PROTON

SAMPLE date Oct 21 2013 satmode n  
 solvent cdc13 wet SPECIAL n  
 file /indy/jwchoi/~ vnmr/svs/data/PM2-2~ gain temp not used 26  
 1A\_1H\_CDC13/PROTON~ 01.fid hst 0.008 20  
 ACQUISITION 8000.0 pw90 9.900  
 SW 3.000 a1fa 10.000  
 AT 48000  
 NP not used  
 FB 32 in  
 BS 2.000 dp  
 D1 16 hs  
 NT 16  
 CT 16  
 TRANSMITTER 1b  
 TN H1 fn 0.20  
 SFrq 499.698 DISPLAY not used  
 TOF 499.7 SP -499.9  
 TPWR 61 WP 5496.6  
 PW 4.950 rfp 4632.1  
 DECOUPLER C13 rfp 3627.8  
 DN 0 1p -87.1  
 DOF 0 1p -73.6  
 DM nnn PLOT 250  
 decwave w40\_autoxr~ wc 0  
 991 sc 16  
 41 vs 25  
 dpwr 32258  
 dmf at cdc ph



JG9221B 1H CDC13  
 exp23 PROTON

SAMPLE date Feb 22 2013  
 solvent cdc13  
 file /data/indy/Jw~  
 Choi/vmr/sys/data/~  
 JG9221B\_1H\_CDC13/P~  
 ROTOM01.fid  
 ACQUISITION  
 SW 8000.0  
 at 3.000  
 np 48000  
 fb not used  
 bs 32  
 d1 1.000  
 nt 32  
 ct 32  
 TRANSMITTER H1  
 tn 499.708  
 sfrq 499.7  
 tof 61  
 tpwr 4.850  
 pw 4.850  
 DECOUPLER C13  
 dn 0  
 dof 0  
 dm nmh  
 decwve 9  
 dpwr 35  
 dmf 32258  
 PRESATURATION satmode n  
 wet cdc13  
 SPECIAL not used  
 temp 30  
 gain 20  
 sp in  
 hst 0.008  
 pw90 9.700  
 alfa 10.000  
 FLAGS n  
 in n  
 dp n  
 hs y  
 nm  
 PROCESSING 0.20  
 lb not used  
 fn not used  
 DISPLAY -0.1  
 sp 4996.8  
 wp 4630.1  
 tffl 3627.9  
 tffp 46.0  
 fp -72.7  
 lp PLOT  
 wc 250  
 sc 0  
 vs 111  
 th 13  
 ai cdc ph



JC12043A CDC13  
exp57 PROTON

SAMPLE	Jun 18 2014	satmode	n
solvent	CDCl3	wet	n
file	/indy/heini/sc	SPECIAL	not used
h/vnmr	sys/data/JC13	temp	26
2043A_CDC13/PROTON	01.fid	gain	20
ACQUISITION	8000.0	spin	9.900
at	3.000	hst	10.000
np	48000	pw90	9.900
fb	not used	alpha	10.000
bs	not used	flags	n
d1	2.000	il	n
d2	16	in	n
nt	16	dp	Y
ct	16	hs	nn
TRANSMITTER	H1	tb	0.20
fn	fn	PROCESSING	not used
sfrq	499.689	sp	-0.2
tof	499.7	wp	4996.8
tpwr	61	rf1	4635.7
pw	4.950	rfp	3627.7
DECOUPLER	C13	rfp	-166.7
dn	0	tp	-78.7
dof	0	PLOT	250
dm	nmn	WC	0
decwv	W40_autox7~	SC	64
dpwr	91	VS	25
dmf	32258	th	25
	ai	cdc	ph

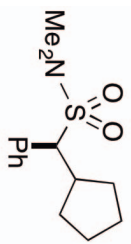
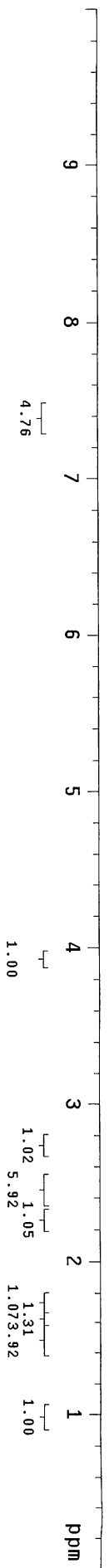
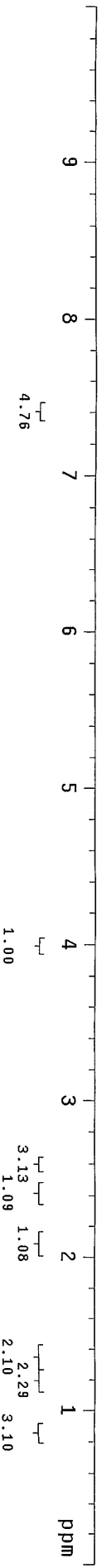
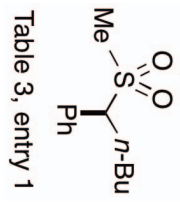


Table 2, entry 9



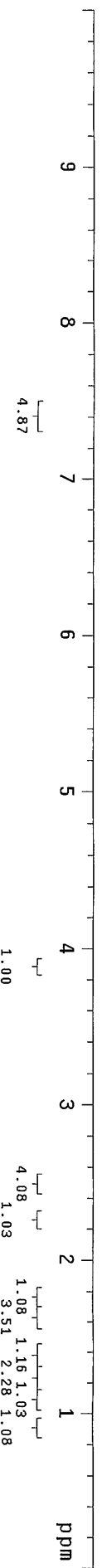
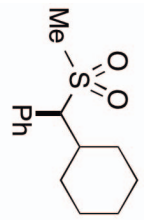
JC9111B 1H CDC13  
 exp23 PROTON

SAMPLE Dec 9 2012 satmode n  
 date Dec 9 2012 satmode n  
 solvent cdcl3  
 file /data/indy/jw~  
 JC9111B\_1H\_CDC13/P~  
 ROTON03.fid  
 ACQUISITION  
 sw 8000.0 pw90 9.700  
 at 2.500 aifa 6.600  
 np 40000  
 fb not used  
 bs 32 in n  
 d1 1.000 dp hs n  
 nt 16  
 ct 16  
 TRANSMITTER H1  
 tn 499.708 1b 0.20  
 sfrq 499.708 fn not used  
 tof 499.708 sp DISPLAY  
 tpwr 61 wp -0.1  
 pw 4.850 rft 4996.8  
 dn C13 rfp 4630.1  
 dof 0 1p 3627.9  
 dm mnn 5.2  
 decwve g 5.6  
 dpwr 33 WC 250  
 dmf 3258 VS 0  
 ai cdc ph th 37  
 54



JC10185 CDC13  
 exp23 PROTON

SAMPLE date Jul 19 2013 PRESATURATION satmode n  
 solvent cdc13 wet SPECIAL n  
 file /Indy/jwchoi/ vnmr/sys/data/JC10185\_CDC13/PROTON01.~ temp gain not used  
 85\_CDC13/PROTON01.~ fid hst spin 32 20  
 ACQUISITION sw 8000.0 pw90 0.008  
 at 3.000 alfa 10.000  
 np 48000  
 fb not used  
 bs 32 in  
 d1 2.000 dp  
 nt 16 hs  
 ct 16  
 TRANSMITTER tn 1b PROCESSING 0.20  
 tn H1 fn not used  
 sfrq 499.698 DISPLAY  
 tof 499.7 sp -0.1  
 tpwr 61 wp 4996.8  
 pw 4.950 rffl 1001.8  
 DECOUPLER dn C13 rfp 0  
 dn 0 tp -76.4  
 dof 0  
 dm mn PLOT -76.7  
 decwave W40\_autox7~ wc 250  
 991 vs 0  
 41 vt 59  
 32258 th 13  
 dmf at cdc ph



JC10181 CD2C12  
 exp2 PROTON

SAMPLE 7 2013 PRESATURATION  
 date Aug cd2c12 satmode n  
 solvent cd2c12 wet n  
 file /Indy/jwchoi/~ SPECIAL  
 vnmr sys/data/JC101~ not used  
 81\_CD2C12/PROTON02~ gain 20  
 .fid spin 20  
 ACQUISITION hst 0.008  
 SW 8000.0 pw90 9.900  
 at 3.000 aifa 10.000  
 np 48000 FLAGS  
 fb not used 11 n  
 bs 32 in 32 n  
 d1 5.000 dp 16 y  
 nt 16 hs 16 nm  
 ct 16  
 TRANSMITTER 1b 1b PROCESSING 0.20  
 tn H1 fn not used  
 sfreq 499.699 DISPLAY  
 tof 499.7 SP -0.1  
 tpwr 61 WP 4998.8  
 pw 4.950 rftl 3669.9  
 DECOUPLER C13 rfp 2658.4  
 dn C13 tp -67.4  
 dof 0 1p -76.2  
 dm nnn WC 250  
 decouple w40\_autok7~ 991 SC 0  
 dpwr 41 VS 284  
 dmf 32258 th 41  
 ai cdc ph

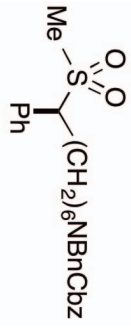
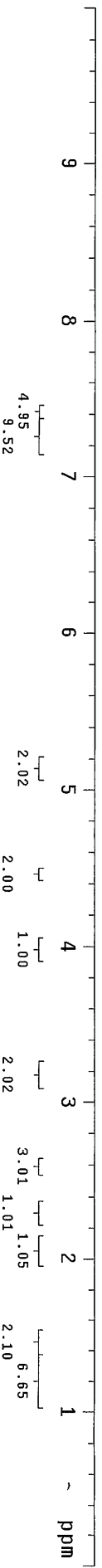


Table 3, entry 3



PM 2-20A CDC13  
exp27 PROTON

SAMPLE 1 2013  
date Aug 1 2013  
solvent cdcl3  
file /indy/jwchoi/~  
vnmr/sv/data/PM\_2-~  
20A\_CDC13/PROTON01~  
ACQUISITION  
sw 8000.0  
at 3.000  
np 48000  
fb not used  
bs 32  
d1 2.000  
nt 16  
ct 16  
tn H1  
sfreq 499.698  
tof 499.7  
tpwr 4.950  
pw 4.950  
dn C13  
dof 0  
dm nm  
decwave w40\_autox7~  
dpmr 41  
dmf 32258

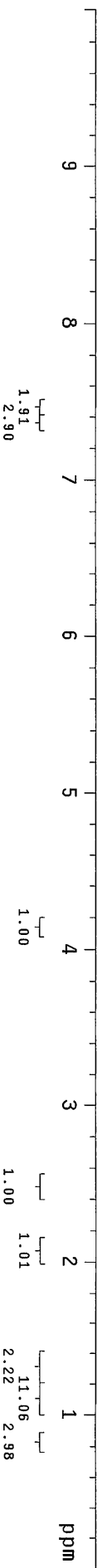
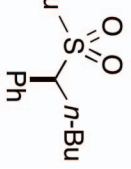
PRESATURATION  
satmode n  
wet SPECIAL  
temp not used  
gain 32  
spin 20  
hst 0.008  
pw90 9.900  
atfa 10.000

PROCESsing  
0.20  
not used  
DISPLAY  
-0.1  
4996.8  
4632.1  
3627.8  
-85.4  
-74.5

PLOT  
250  
0  
63  
13

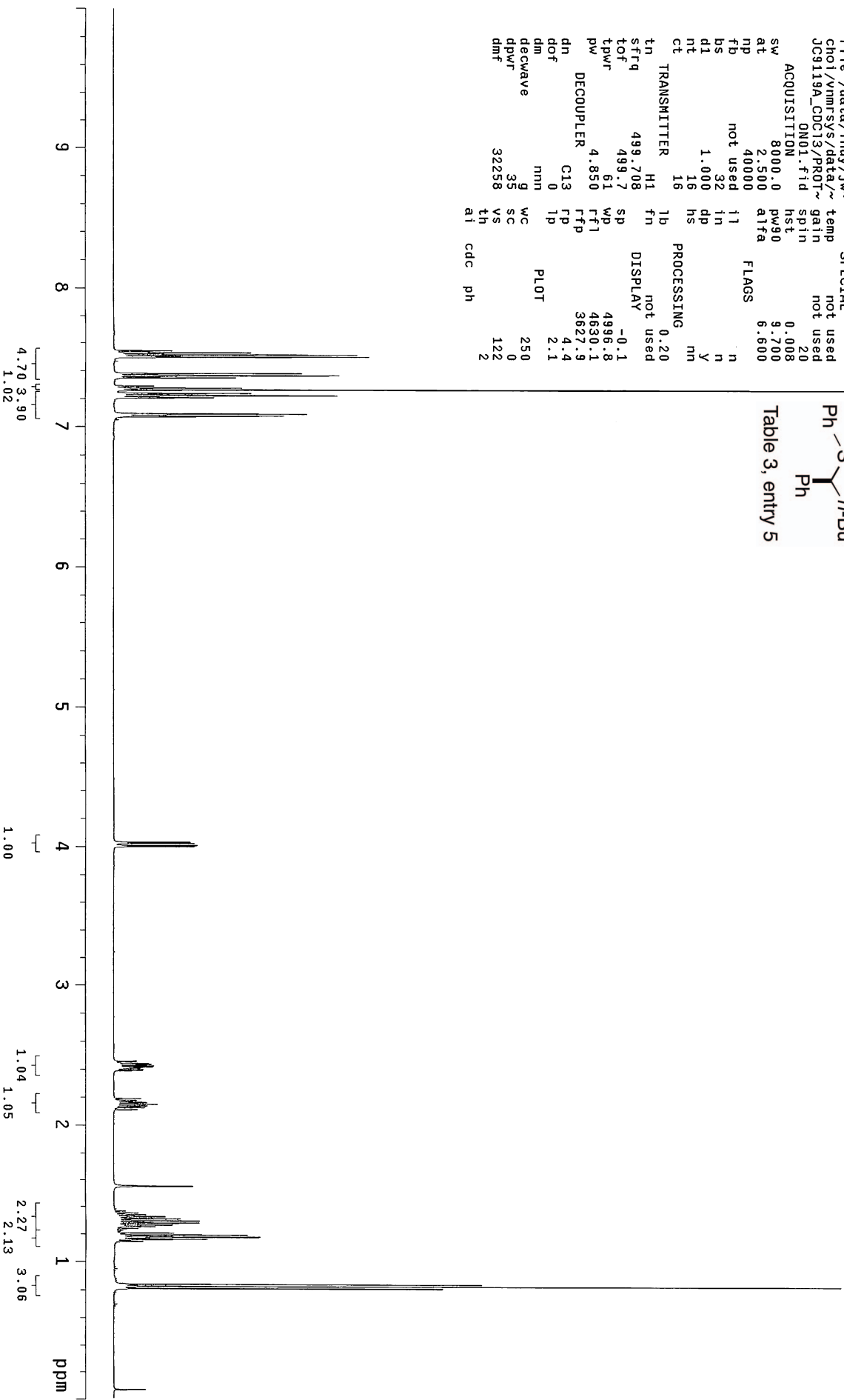
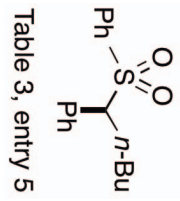
ai cdc ph

Table 3, entry 4



JC9119A CDC13  
exp30 PROTON

date	Dec 14 2012	SAMPLE	Dec 14 2012	satmode	n
solvent	cdc13	solvent	cdc13	wet	n
file	/data/jindy/jw~	file	/data/jindy/jw~	SPECIAL	n
ChOI/VmtrSYs/data/~		ChOI/VmtrSYs/data/~		temp	not used
JC9119A_CDC13/PROT~		JC9119A_CDC13/PROT~		gain	not used
ON01.fid		ON01.fid		spin	20
ACQUISITION		ACQUISITION		hst	0.008
sw	8000.0	sw	8000.0	pw90	9.700
at	2.500	at	2.500	alfa	6.600
np	40000	np	40000	FLAGS	
fb	not used	fb	not used	11	n
bs	32	bs	32	in	n
d1	1.000	d1	1.000	dp	y
nt	16	nt	16	hs	nm
ct	16	ct	16	PROCESSING	0.20
TRANSMITTER		TRANSMITTER		1b	fn
tn	H1	tn	H1	not used	DISPLAY
sfrq	499.708	sfrq	499.708	SP	-0.1
tof	499.7	tof	499.7	WP	4996.8
tpwr	61	tpwr	61	FT1	4630.1
pw	4.850	pw	4.850	FFP	3627.9
DECOUPLER	C13	DECOUPLER	C13	FP	4.4
dn	0	dn	0	1p	2.1
dof	nmn	dof	nmn	WC	250
decwve	g	decwve	g	SC	0
dpwr	35	dpwr	35	VS	122
dmf	32258	dmf	32258	th	2
				ai	cdc ph

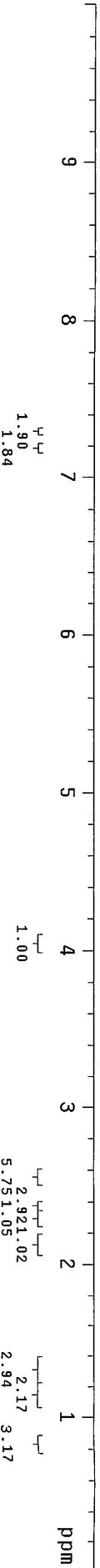
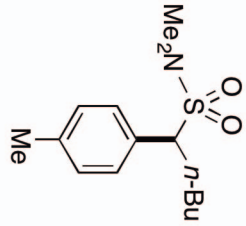




JC9229 CDC13  
 exp23 PROTON

SAMPLE PRESATURATION  
 date Feb 16 2013 satmode n  
 solvent cdc13 wet n  
 file /data/indy/jw~ SPECIAL not used  
 Choi/vmr/sys/data/~ temp 30  
 JC9229\_1H\_13C\_CDC1~ gain 20  
 3/PROTON02.fid spin 0.008  
 ACQUISITION hst 9.700  
 SW 8000.0 aifa 10.000  
 at 3.000  
 np 48000  
 fb not used  
 bs 32 in n  
 d1 1.000 dp n  
 nt 16 hs y  
 ct 16  
 TRANSMITTER 1b  
 tn H1 fn  
 sfra 499.708 . DISPLAY not used  
 tof 499.7 SP -0.1  
 tpwr 61 WP 4996.8  
 pw 4.850 rffl 4630.1  
 DECOUPLER C13 rfp 3627.9  
 dn 0 tp 43.7  
 dof 0 1p -71.3  
 dm mn 250  
 decwve g WC  
 dpwr 35 SC 0  
 dmf 32258 VS 45  
 ai cdc ph 50

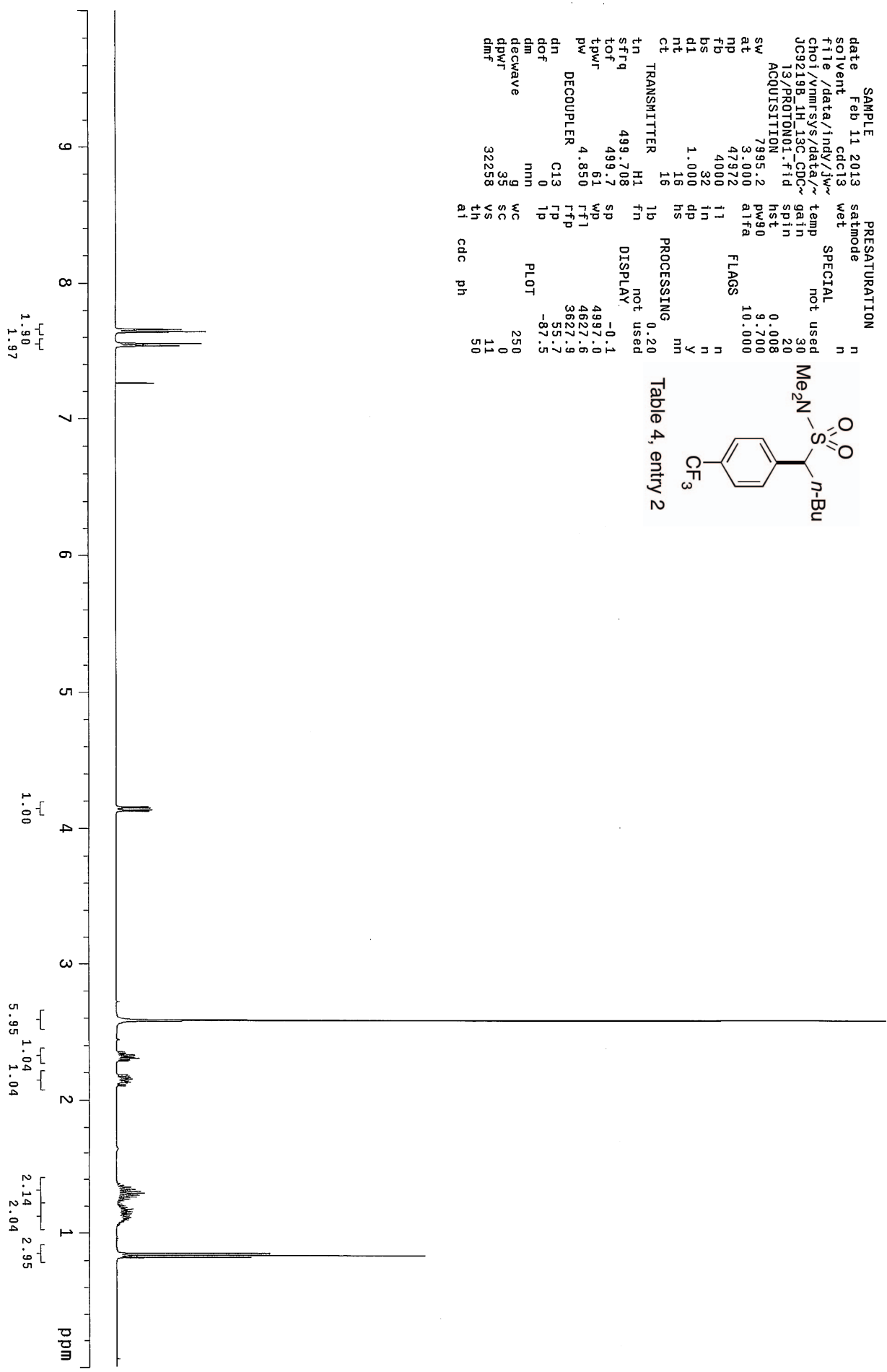
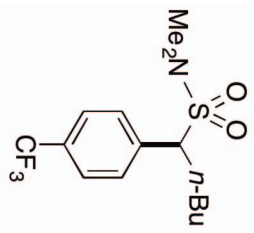
Table 4, entry 1



JC92198 CDC13  
 exp23 PROTON

SAMPLE date Feb 11 2013  
 solvent cdc13  
 F1 file /data/indy/jw~  
 ChOI/vmr/sys/data/~  
 JC92198\_1H\_13C.CDC~  
 13/PROTON01.Fid  
 ACQUISITION  
 SW 7995.2  
 at 3.000  
 np 47972  
 fb 4000  
 bs 32  
 dl 1.000  
 nt 16  
 ct 16  
 TRANSMITTER H1  
 tn 499.708  
 sfrq 499.7  
 tpwr 61  
 pw 4.850  
 DECOUPLER C13  
 dn 0  
 dof 0  
 dm 0  
 decwave 35  
 dpwr 32258  
 dmf 32258  
 PRESATURATION satmode n  
 wet not used  
 SPECIAL not used  
 temp 30  
 gain 20  
 spin 0.008  
 hst 9.700  
 pw90 10.000  
 a1fa 10.000  
 FLAGS n  
 i1 n  
 in n  
 dp n  
 hs y  
 PROCESSING 0.20  
 fn not used  
 DISPLAY -0.1  
 sp 4997.0  
 wd 4627.6  
 rffl 3627.9  
 tffp 55.7  
 tp -87.5  
 PLOT 250  
 wc 0  
 sc 11  
 vs 11  
 th 50  
 at cdc ph

Table 4, entry 2

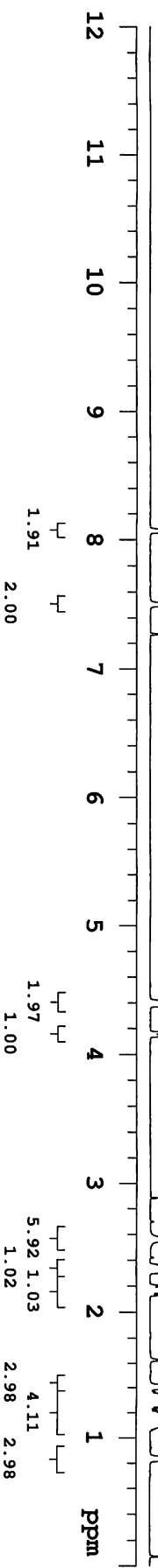
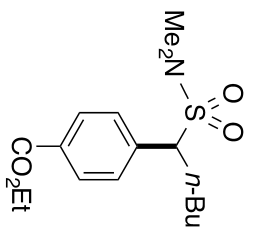


JC12077B 1H CDC13

exp64 PROTON

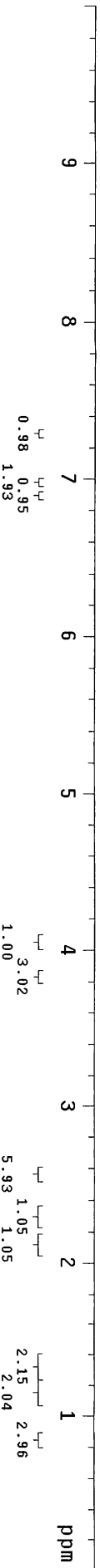
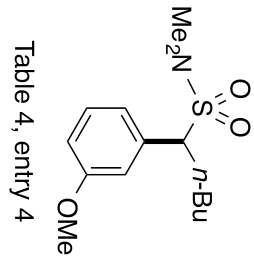
SAMPLE		PRESATURATION	
date	Aug 3 2014	satmode	n
solvent	cdcl3	wet	n
file	/indy/jwchoi/~	SPECIAL	
nmrsys	/data/JC1207	temp	25.0
77B_CDC13	/PROTON02~	gain	26
	.fid	spin	0
ACQUISITION		hst	0.008
sw	8000.0	pw90	9.900
at	3.000	alfa	10.000
np	48000	FLAGS	
fb	not used	il	n
bs	32	in	n
d1	2.000	dp	Y
nt	16	hs	nn
ct	16	PROCESSING	
tn	TRANSMITTER	lb	0.20
fn	H1	fn	not used
strq	499.689	DISPLAY	
tof	499.7	sp	-0.2
tpwr	61	wp	5996.1
pw	4.950	rfl	1001.9
DECOUPLER		rfp	0
dn	C13	ip	-172.0
dof	0	lp	-73.1
dm	nmn	PILOT	
decwave	W40_autok7~	wc	234
dpwr	991	sc	8
dmf	41	vs	55
	32258	th	22
		ai	cdc
			ph

Table 4, entry 3



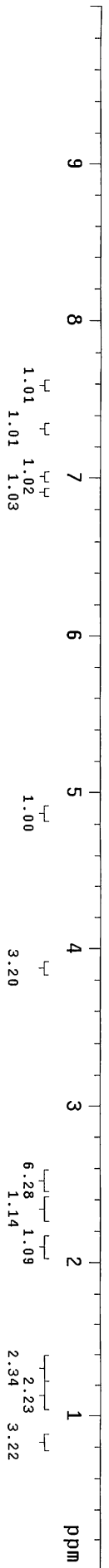
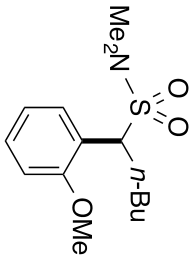
JC9159B CDC13  
 exp23 PROTON

SAMPLE PRESATURATION  
 date Jan 17 2013 satmode n  
 solvent cdc13 wet n  
 file /data/indy/jw~ SPECIAL not used  
 Choi/Vmmr/sys/data/~ gain 30  
 JC9159B\_CDC13/PROT~ spin 20  
 0N01.fid hst 0.008  
 ACQUISITION pw90 9.700  
 SW 7995.2 atfa 10.000  
 at 3.000  
 np 47972  
 fb 4000  
 bs 32  
 di 1.000  
 nt 16  
 ct 16  
 TRANSMITTER lb  
 tn H1 0.20  
 sfreq 499.708 fn not used  
 tof 499.7 sp DISPLAY  
 tpwr 61 wp 4997.0  
 pw 4.850 rft 4627.6  
 DECOUPLER C13 rfp 3627.9  
 dn 0 lp -86.6  
 dof 0  
 dm nmm  
 decwve g WC 250  
 dpwr 35 SC 0  
 dmf 32258 th VS 36  
 ai cdc ph 50



JC10223B CDC13  
 exp28 PROTON

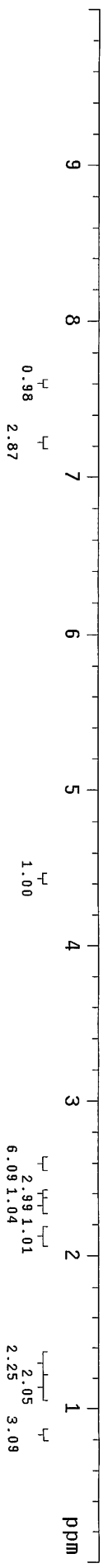
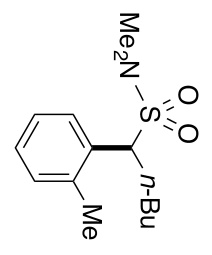
SAMPLE PRESATURATION  
 date Aug 6 2013 satmode n  
 solvent cdc13 wet n  
 file /Indy/jwchoi/~ SPECIAL  
 Vnmr/sys/data/JC10223B\_CDC13/PROTON01~ gain temp not used  
 32  
 20  
 0.008  
 9.900  
 10.000  
 ACQUISITION  
 .fid hst  
 8000.0 pw90  
 3.000 atfa  
 48000  
 not used  
 32  
 2.000 dp  
 16 hs  
 16  
 16  
 TRANSMITTER  
 tn 1b  
 sfreq 499.698 fn  
 499.7 SP  
 tof 61 WP  
 4.950 rfp  
 3627.8  
 -84.4  
 -75.3  
 DECOUPLER C13 rf1  
 0 1p  
 dn dof 0 WC PLOT  
 dm dm nm  
 decouple w40\_autox?~ wc 250  
 991 sc 0  
 41 vs 24  
 32258 th 50  
 ai cdc ph



JC102098 CDC13  
 exp28 PROTON

SAMPLE date Aug 9 2013 satmode n  
 solvent cdc13 wet SPECIAL n  
 file /Indy/jwchoi/~ temp not used 20  
 vnmr/sys/data/JC102~ gain 20  
 09B\_CDC13/PROTON01~ .fid hst 0.008  
 ACQUISITION .fid hst 20  
 sw 8000.0 pw90 9.900  
 at 3.000 alfa 10.000  
 np 48000  
 fb not used  
 bs 32 in  
 d1 2.000 dp  
 nt 16 hs  
 ct 16  
 TRANSMITTER H1 lb  
 tn H1 fn 0.20  
 sfrq 499.698 not used  
 tof 499.7 DISPLAY  
 tpwr 61 wp 4996.8  
 pw 4.950 tffl 4632.1  
 DECOUPLER C13 rfp 3627.8  
 dn 0 lp -81.2  
 dof 0  
 dm nmh -72.5  
 decwave W40\_autox7~ WC PLOT 250  
 931 SC 0  
 41 VS 72  
 32258 th 50  
 ai cdc ph

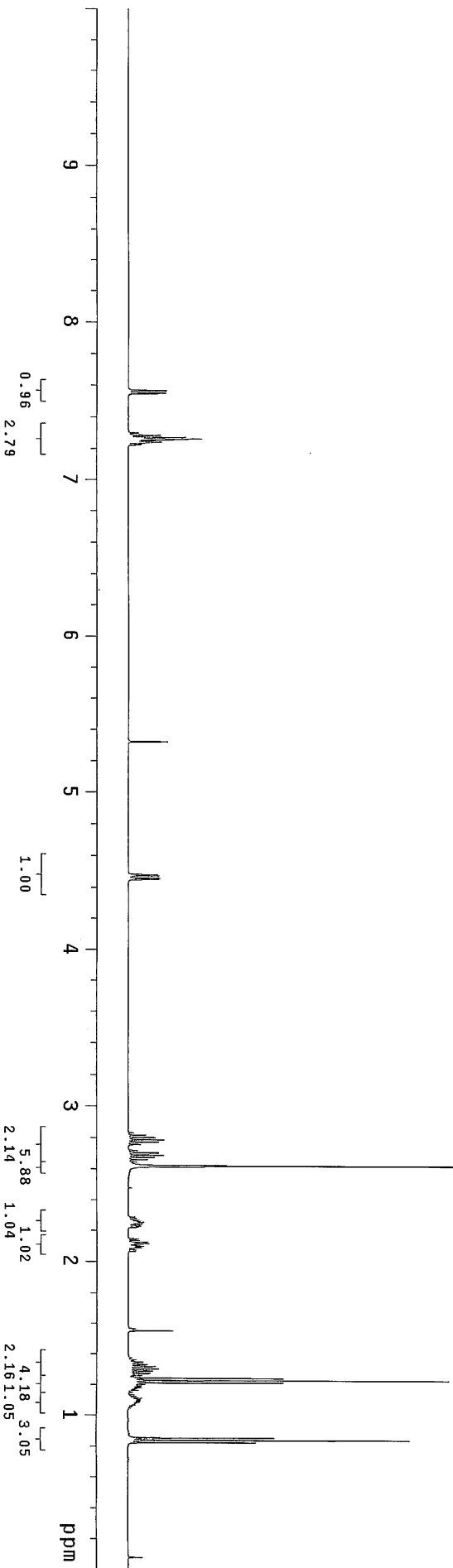
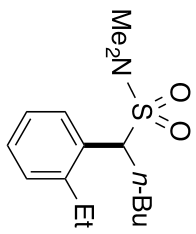
Table 4, entry 6



JC11021 CD2C12  
 exp30 PROTON

SAMPLE	date	Oct 16 2013	PRESATURATION	satmode	n
SOIvent	cd2c12		wet		n
file	/indy/jwchoi/~		SPECIAL		
nmrsvs	/data/JC110~		temp	not used	28
21_CD2C12/PROTON01~	gain		sb1n	20	
	.fid		hst	0.008	
ACQUISITION	sw	8000.0	ai	9.900	
	at	3.000	alpha	10.000	
	np	48000	FLAGS		
	fb	not used	i1	n	
	bs	32	in	n	
	d1	2.000	dp	y	
	nt	16	hs	nn	
ct	16		PROCESSING		
TRANSMITTER	H1		lb	0.20	
tn	499.699		fn	not used	
sfrq	499.7		sp	-0.1	
tof	61		wp	4996.8	
tpwr	4.950		rfl	3669.9	
pw	0		TFP	2658.4	
DECOUPLER	C13		TP	-85.2	
dn	0		TP	-72.4	
dof	0				
dm	nmn		WC	250	
decwave	W40_autox7~		SC	0	
dpwr	931		VS	27	
dmf	41		th	50	
	32258		ai	cdc	ph

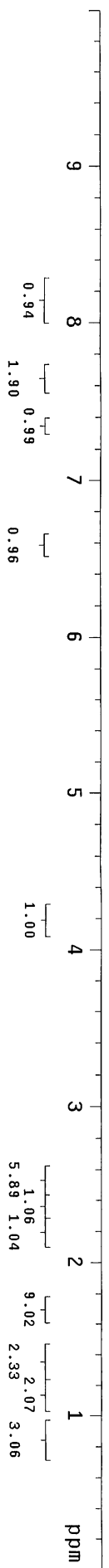
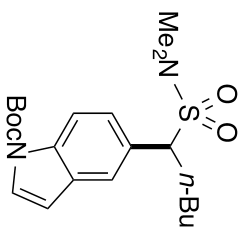
Table 4, entry 7



JC101438 CDC13  
 exp23 PROTON

SAMPLE PRESATURATION  
 date Jul 20 2013 satmode n  
 solvent cdcl3 wet n  
 file /indy/jwcho1/~ SPECIAL  
 vnmr\_sys/data/JC101~ temp not used  
 438\_CDC13/PROTON01~ gain 32  
 .fid hst 20  
 ACQUISITION spin 0.008  
 SW 8000.0 pw90 9.900  
 at 3.000 a1fa 10.000  
 np 48000  
 fb not used  
 bs 32 in n  
 d1 2.000 dp n  
 nt 16 hs y  
 ct 16  
 TRANSMITTER H1  
 tn 1b  
 sfra 499.698 fn not used  
 tof 499.7 SP DISPLAY  
 tpwr 61 wp 4996.8  
 pw 4.950 rfp 4632.1  
 DECOUPLER C13 rfp 3627.8  
 dn 0 tp -83.7  
 dof 1p -75.2  
 dm nm  
 dm decouple w40\_autox7~ WC PLOT 250  
 dpwr 41 vs 0  
 dmf 32258 th 60  
 ai cdc ph 50

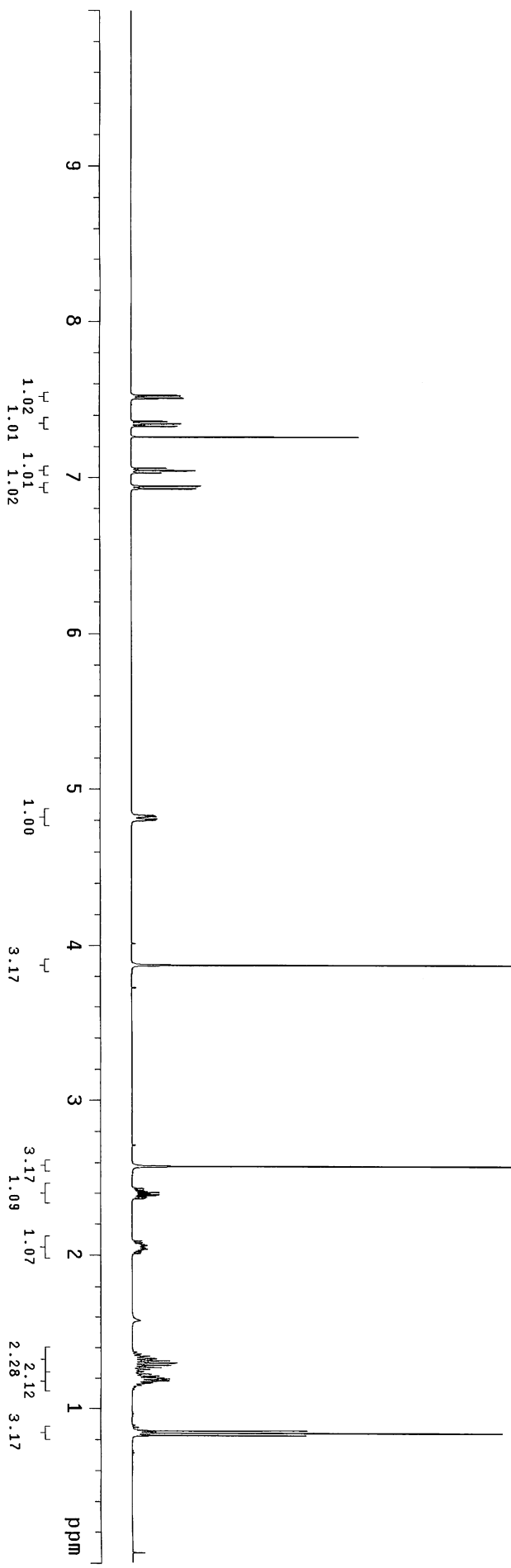
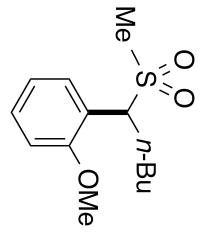
Table 4, entry 8





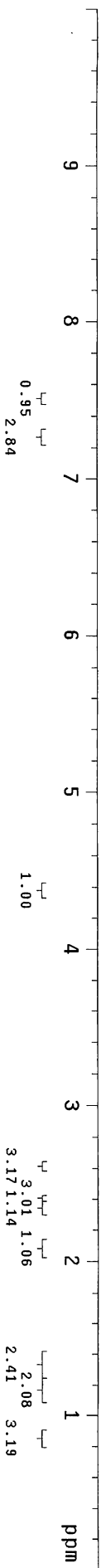
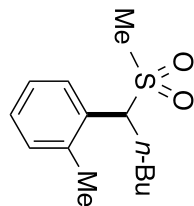
JC10219B CDC13  
 exp26 PROTON

SAMPLE PRESATURATION  
 date Aug 1 2013 satmode n  
 solvent cdc13 wet n  
 file /Indy/jwchoi/~ SPECIAL not used  
 vnmr/sys/data/JC102~ temp gain 32  
 19B\_CDC13/PROTON01~ spn 20  
 .fid hst 0.008  
 ACQUISITION pw90 9.900  
 SW 8000.0 alfa 10.000  
 AT 3.000  
 NP 48000  
 FB not used  
 BS 32  
 DI 2.000  
 NT 16  
 CT 16  
 TRANSMITTER H1  
 TN 499.698  
 SFRQ 499.7  
 TOF 61  
 TPWR 4.950  
 PW DECOUPLER C13  
 DN 0  
 DOF 0  
 DM mn  
 decwave W40\_autox7~ WC  
 dpwr 991  
 dmf 41  
 32258 th  
 at cdc ph  
 50



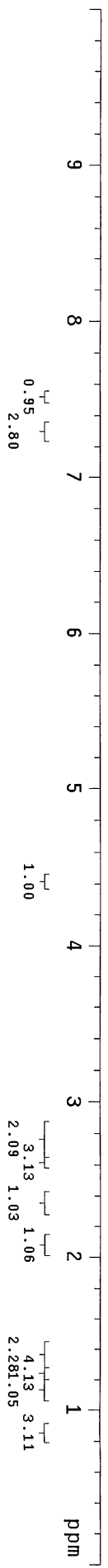
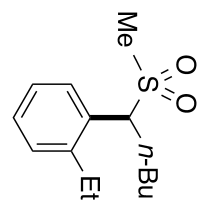
JC10215A CD2C12  
 exp34 PROTON

SAMPLE date Jul 30 2013 PRESATURATION satmode n  
 solvent CD2Cl2 wet SPECIAL n  
 file /indy/jwchoi/~ vnmr/sys/data/JC102~ temp not used 32  
 15A\_CD2C12/PROTON0~ gain 0.008 20  
 ACQUISITION 1.fid hst 9.900  
 SW 8000.0 pwr90 10.000  
 at 3.000 alfa  
 np 48000  
 fb not used  
 bs 32 in n  
 d1 2.000 dp n  
 nt 16 hs y  
 ct 16  
 TRANSMITTER H1 1b PROCESSING 0.20  
 tn H1 1b not used  
 sfrq 499.699 fn DISPLAY  
 tof 499.7 sp -0.1  
 tpwr 61 wp 4995.8  
 pw 4.950 rfp 3669.9  
 DECOUPLER C13 rfp 2658.4  
 dn 0 1p -74.6  
 dof 0 1p -73.4  
 dm nmh PLOT 250  
 decwave w40\_autox7~ wc 0  
 991 sc 0  
 41 vs 37  
 dmf 32258 th 50  
 ai cdc ph



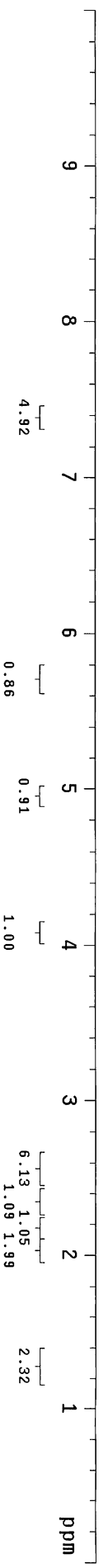
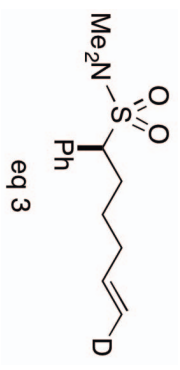
JC11023A 1H CD2C12  
exp30 PROTON

SAMPLE Oct 17 2013 PRESATURATION n  
 date Oct 17 2013 satmode n  
 solvent c6d6 wet n  
 file /indy/jwchoi/~ SPECIAL not used  
 vnmr/sys/data/JC11023A\_1H\_CD2C12/PROT1~ gain 32  
 23A\_1H\_CD2C12/PROT1~ spm 20  
 ON01.fid hst 0.008  
 ACQUISITION pw90 9.900  
 SW 8000.0 a1fa 10.000  
 at 3.000  
 np 48000  
 fb not used  
 bs 32 in  
 d1 2.000 dp  
 nt 16 hs  
 ct 16  
 TRANSMITTER 1b  
 tn H1 fn  
 sfreq 499.698 not used  
 tof 499.7 DISPLAY  
 tpwr 61 sp -0.1  
 pw 4.950 wfp 4996.8  
 dn C13 rfp 4584.5  
 dof 0 ffp 2658.4  
 dm 0 tp -86.5  
 decouple W40\_autox7~ PLOT -76.6  
 decwave W40\_autox7~ WC 250  
 931 SC 0  
 vs th 24  
 dmf 32258 50  
 at cdc ph



JC11079 CDC13  
 exp51 PROTON

SAMPLE Jun 5 2014 PRESATURATION n  
 solvent cdc13 satmode n  
 file /indy/jwchoi/~ cdc13 SPECIAL n  
 ynmrSYS/data/JC11079\_79\_CDC13/PROTON02.~ gain 28 not used 20  
 f1d hst 0.008  
 sp in 9.900  
 atfa 10.000  
 ACQUISITION  
 sw 8000.0 atfa 10.000  
 at 3.000  
 np 48000  
 fb not used i1 n  
 bs 32 in n  
 d1 2.000 dp y  
 nt 16 hs  
 ct 16 hs  
 TRANSMITTER 1b 0.20  
 tn H1 fn not used  
 sfrq 499.689 SP DISPLAY -0.2  
 tof 499.7 WP 4996.8  
 tpwr 61 rfp 4635.7  
 pw 4.950 rfp 3627.7  
 dn C13 TP -169.3  
 dof 0 TP -79.4  
 dm nm  
 decwave W40\_autox7~ WC PLOT 250  
 931 SC 0  
 vs VS 42  
 th th 13  
 dmf 32258  
 at cdc ph



JC10045B1 CDC13

exp51 PROTON

SAMPLE		PRESATURATION	
date	Jun 3 2014	satmode	n
solvent	cdcl3	wet	n
file	/indy/jwchoi/~	SPECIAL	not used
nmrSYS/data/JC1004		temp	28
45B1_CDC13/PROTON0~		gain	20
	1.fid	spIn	0.008
		hst	9.900
ACQUISITION		pw90	10.000
sw	8000.0	at1fa	10.000
at	3.000	al1fa	
np	46000	FLAGS	
fb	not used	i1	n
bs	32	in	n
d1	2.000	dp	Y
nt	16	hs	nh
ct	16	PROCESSING	0.20
		fn	not used
tn	H1	lb	0.20
sfrq	499.689	fn	not used
tof	499.7	sp	-0.2
tpwr	61	wp	4996.8
pw	4.950	rft1	4635.3
		rffp	3627.7
dn	C13	fp	-167.5
dof	0	lp	-79.6
dm	nmr		
decwave	w40_autox7~	WC	250
dpwr	41	SC	0
dmf	32258	VS	47
		th	25
		al	cdc ph

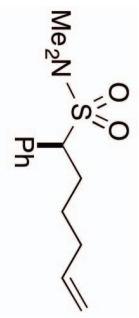
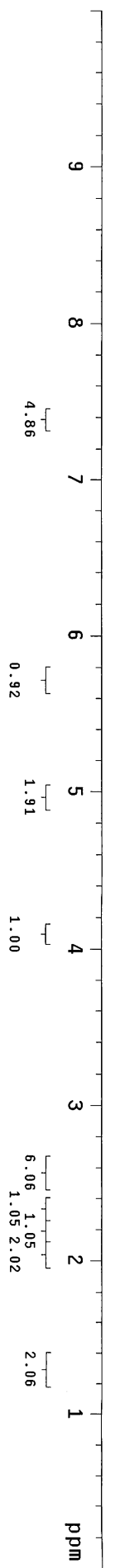


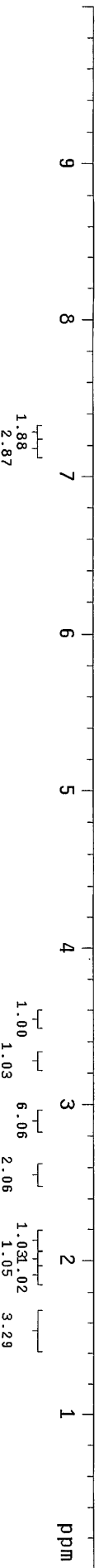
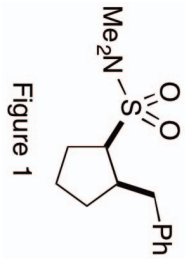
Figure 1



JC10187A IC-1 CD2C12

exp1 PROTON

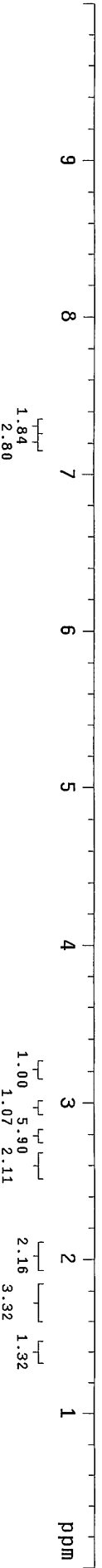
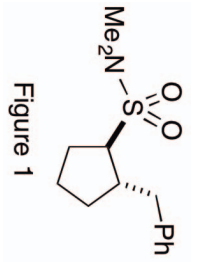
SAMPLE PRESATURATION  
date Nov 9 2013 satmode n  
solvent cd2c12 wet n  
file /indy/jvchoi/~ SPECIAL not used  
vnmr sys/data/JC10187A\_IC-1\_CD2C12/PR~ gain 24  
OTON01.fid spin 20  
ACQUISITION hst 0.008  
pw 9.900  
sw 8000.0 a1fa 10.000  
at 3.000  
np 48000  
fb not used i1 n  
bs 32 in n  
d1 2.000 dp n  
nt 16 hs y  
ct 16 hs mn  
tn TRANSMITTER 1b 0.20  
fn not used  
sfrq 499.699 DISPLAY  
tof 499.7 sp -0.1  
tpwr 61 wd 4996.8  
pw 4.950 rfp 3669.7  
dn DECOUPLER C13 rfp 2658.4  
dof 0 rfp -70.6  
dm 0 1p -73.6  
decwave w40\_autox7~ PLOT 250  
vs 991 wc 0  
th 41 vs 19  
dmf 32258 th 6  
at cdic ph



JC10187A IA-1 CD2C12

exp1 PROTON

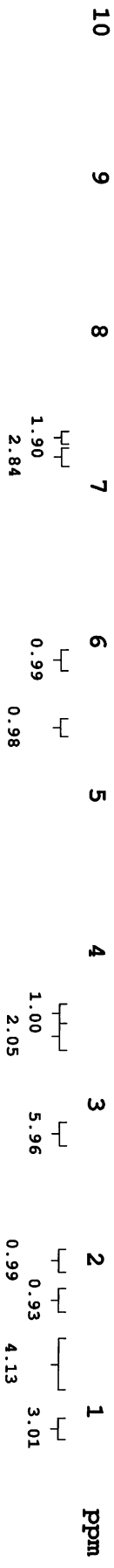
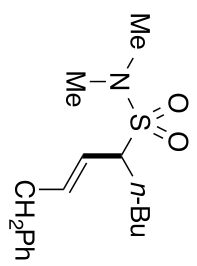
SAMPLE PRESATURATION  
 date Nov 10 2013 satmode n  
 solvent cd2c12 wet n  
 file /indy/jwchoi/~ SPECIAL not used  
 vnmr sys/data/JC10187A IA-1\_CD2C12/PR~ ga1n 24  
 87A IA-1\_CD2C12/PR~ sp1n 20  
 OTON01.fid hst 0.008  
 ACQUISITION pw90 9.900  
 SW 8000.0 atfa 10.000  
 at 3.000  
 np 48000  
 fb not used  
 bs 32 in n  
 d1 2.000 dp n  
 nt 16 hs Y  
 ct 16  
 PROCESSING  
 tn 1b 0.20  
 TRANSMITTER H1 fn not used  
 sfreq 499.699 DISPLAY -0.1  
 tof 499.7 sp 4996.8  
 tpwr 61 wp 3670.2  
 pw 4.950 ffp 2658.4  
 DECOUPLER C13 ffp -66.3  
 dn 0 1p -80.4  
 dof 0  
 dm nm  
 decouple w40\_autox7~ WC PLOT 250  
 991 SC 0  
 41 VS 26  
 32258 th 6  
 at cdc ph



JC12075B CDCl3

exp64 PROTON

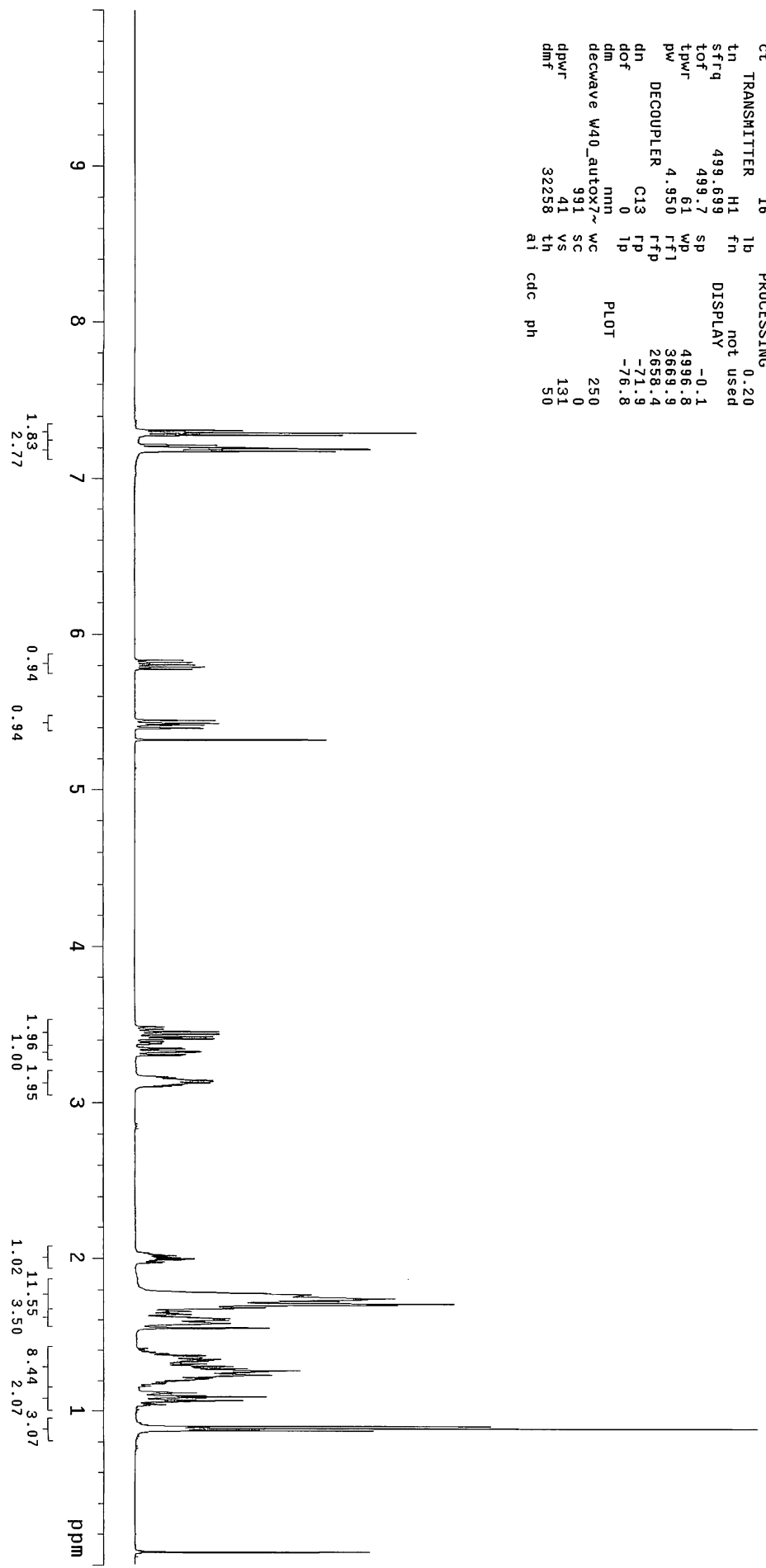
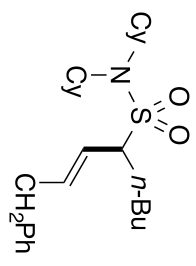
SAMPLE PRESATURATION  
date Aug 1 2014 satmode n  
solvent cdcl3 wet n  
file /indy/jwchoi/~ SPECIAL  
vnmrsvs/data/JC120~ temp 25.0  
75B\_CDCl3/PROTON01~ gain 28  
.fid spin 20  
ACQUISITION hst 0.008  
sw 8000.0 pw90 9.900  
at 3.000 alfa 10.000  
np 48000 FLAGS  
fb not used i1 n  
bs 32 in n  
d1 2.000 dp y  
nt 16 hs nm  
ct 16 PROCESSING  
TRANSMITTER lb 0.20  
tn H1 fn not used  
sfrq 499.689 DISPLAY  
tof 499.7 sp -0.2  
tpwr 61 wp 4996.8  
pw 4.950 rfl 4635.7  
DECOUPLER rfp 3627.7  
dn C13 ip -173.5  
dof 0 lp -68.6  
dm nnn PLOT  
decwawe W40\_autocx7~ wc 234  
991 sc 8  
dpwr 41 vs 35  
dmtf 32258 th 11  
ai cdc ph





JC10275 CD2C12  
exp30 PROTON

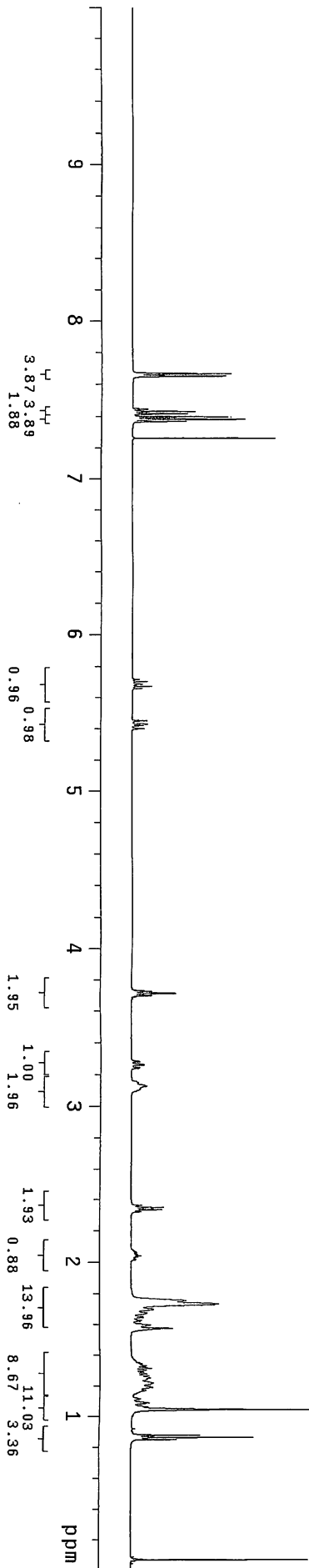
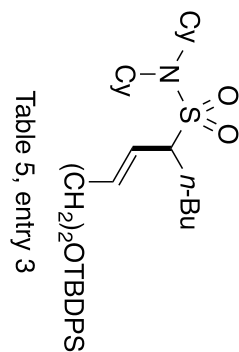
date	Sep 5 2013	SAMPLE	CD2C12	satmode	n
solvent	/indy/jwcho1/~	file	cd2c12	wet	n
nmr/sys	/data/JC10275	temp	28	SPECIAL	not used
75_CD2C12/PROTON01		gain	20		
		spin	20		
ACQUISITION	.fid	hst	0.008		
sw	8000.0	pw90	9.900		
at	3.000	alfta	10.000	FLAGS	
np	48000				
fb	not used	fl			
bs	32	in			
d1	2.000	dp			
nt	16	hs			
ct	16	hs			
TRANSMITTER	H1	tb	0.20	PROCESSING	
tn	499.699	fn	not used		
sfrq	499.7	sp	-0.1	DISPLAY	
tof	61	wp	4996.8		
tpwr	4.950	fft	3669.9		
pw	4.950	ffp	2658.4		
DECOUPLER	C13	rfp	-71.9		
dn	0	tp	-76.8	PLOT	
dof	0				
dm	nmn				
decwave	W40_autox7~	wc	250		
dpwr	41	vs	131		
dmf	32258	th	50		
		at	cdc	ph	



JC11025A 1H CDC13

expt1 PROTON

date	Oct 23 2013	PRESATURATION	
solvent	cdcl3	satmode	n
file	/indy/jwcho1/~	wet	n
nmr	sys/data/JC110~	SPECIAL	not used
25A_1H_CDC13/PROT0~		gain	26
		spn	20
		hst	0.008
		pw30	9.900
ACQUISITION		atfta	10.000
sw	8000.0	flags	
at	3.000		
np	48000		
fb	not used		
bs	32		
d1	2.000		
nt	16		
ct	16		
TRANSMITTER		PROCESSING	
tn	H1	fb	0.20
sftq	499.698	fn	not used
tof	499.7	sp	-0.1
tpwr	61	wp	4996.8
pw	4.950	rf1	4632.1
DECOUPLER		rfp	3627.8
dn	C13	fp	-87.5
dof	0	tp	-72.5
dm	nmn		
decwave	w40_autox7~	WC	250
dpwr	991	SC	0
dmf	41	VS	37
	32258	th	13
		ai	cdc ph



JC10279A CD2C12

exp30 PROTON

SAMPLE	date	Sep 16 2013	PRESATURATION	satmode	n
SOVENT	solvent	cd2c12	satmode	not used	n
FILE	file	/indy/jwchoi/~	SPECIAL	not used	n
VMR	vmr	sys/data/JC102~	temp	24	24
79A	79A_CD2C12/PROTON0~	1.fid	gain	20	20
ACQUISITION	sw	8000.0	hst	0.008	0.008
at	at	3.000	pw90	9.900	9.900
np	np	48000	ai	10.000	10.000
fb	fb	not used	alpha		
bs	bs	not used	flags		
d1	d1	2.000	i1	n	n
nt	nt	16	in	n	n
ct	ct	16	dp	y	y
TRANSMITTER	td	hs	hs	nn	nn
tn	tn	1d	PROCESSING	0.20	0.20
sfrq	sfrq	499.699	fn	not used	not used
tof	tof	499.7	DISPLAY		
tpwr	tpwr	61	WD	-0.1	4996.8
pw	pw	4.950	TF1	3669.9	3669.9
DECOUPLER	C13	0	TFP	2658.4	2658.4
dn	dn	0	TP	-68.2	-68.2
dof	dof	0	TP	-78.6	-78.6
dm	dm	nm	WC		
deccave	deccave	w40_autox7~	WC		
dpr	dpr	931	SC		
dmf	dmf	41	VS		
		32258	TH		
			AI		
			cdc		
			ph		

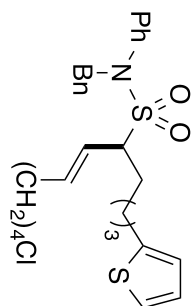
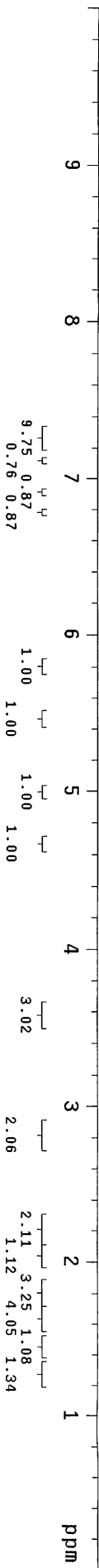
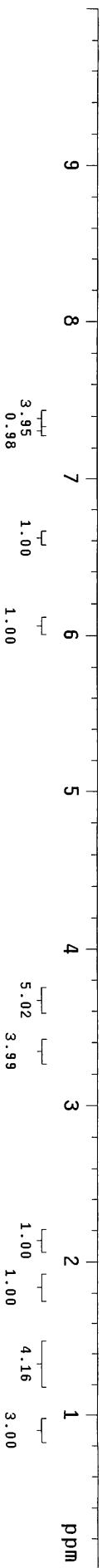
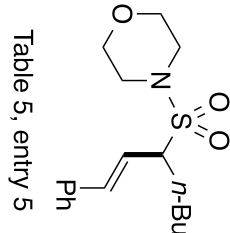


Table 5, entry 4



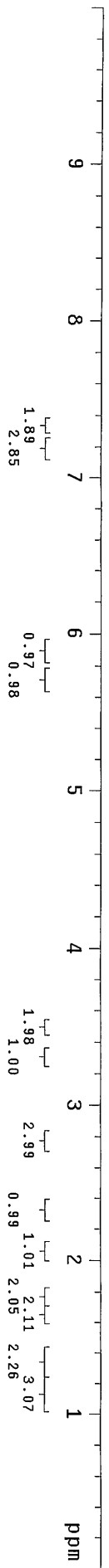
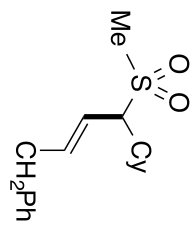
JC10281A 1H CDC13  
exp2 PROTON

SAMPLE Nov 2 2013 PRESATURATION  
 solvent cdc13 satmode n  
 file /indy/jwchoi/~ cdc13 wet n  
 vnmr sys/data/JC102~ temp SPECIAL not used  
 81A\_1H\_CDC13/PRO10~ gain 24  
 N01.fid spm 20  
 hst 0.008  
 pw90 9.900  
 ACQUISITION 8000.0 atfa 10.000  
 sw 3.000  
 at 46000  
 np 46000  
 fb not used  
 bs 32  
 di 2.000  
 nt 16  
 ct 16  
 TRANSMITTER H1  
 tn H1  
 sfrq 499.698  
 tof 499.7  
 tpwr 61  
 pw 4.950  
 DECOUPLER C13  
 dn C13  
 dof 0  
 dm nnn  
 decouple w40\_autocx7~ WC  
 dpwr 41  
 dmf 32258  
 th 50  
 at cdc ph  
 PLOT 250  
 103  
 50  
 PROCESSING 0.20  
 fn not used  
 DISPLAY  
 -0.1  
 4996.8  
 4632.1  
 3627.8  
 -79.0  
 -77.6



JC11123 CDC13  
exp37 PROTON

date	Feb 5 2014	SAMPLE	satmode	n
solvent	cdc13	PROTON	satmode	n
file	/indy/jwchoi/~		SPECIAL	not used
nmr	23_CDC13/PROTON02.~		temp	26
fid			gain	20
sw	8000.0	ACQUISITION	hst	0.008
at	3.000		spn	9.900
np	48000		atfa	10.000
fb	not used		FLAGS	
bs	32		i1	n
d1	2.000		in	n
nt	16		dp	y
ct	16		hs	mn
tn	TRANSMITTER		PROCESSING	0.20
sfrq	499.698		fn	not used
tof	499.7		DISPLAY	
tpwr	4.950		wp	-0.1
pw	4.950		ftf1	4996.8
dn	0		ftf2	4632.1
dof	0		ftf3	3627.8
dm	nmr		tp	-77.7
decouple	W40_autox7~		WC	250
dmf	32258		SC	0
			VS	41
			TH	13
			AI	cdc ph



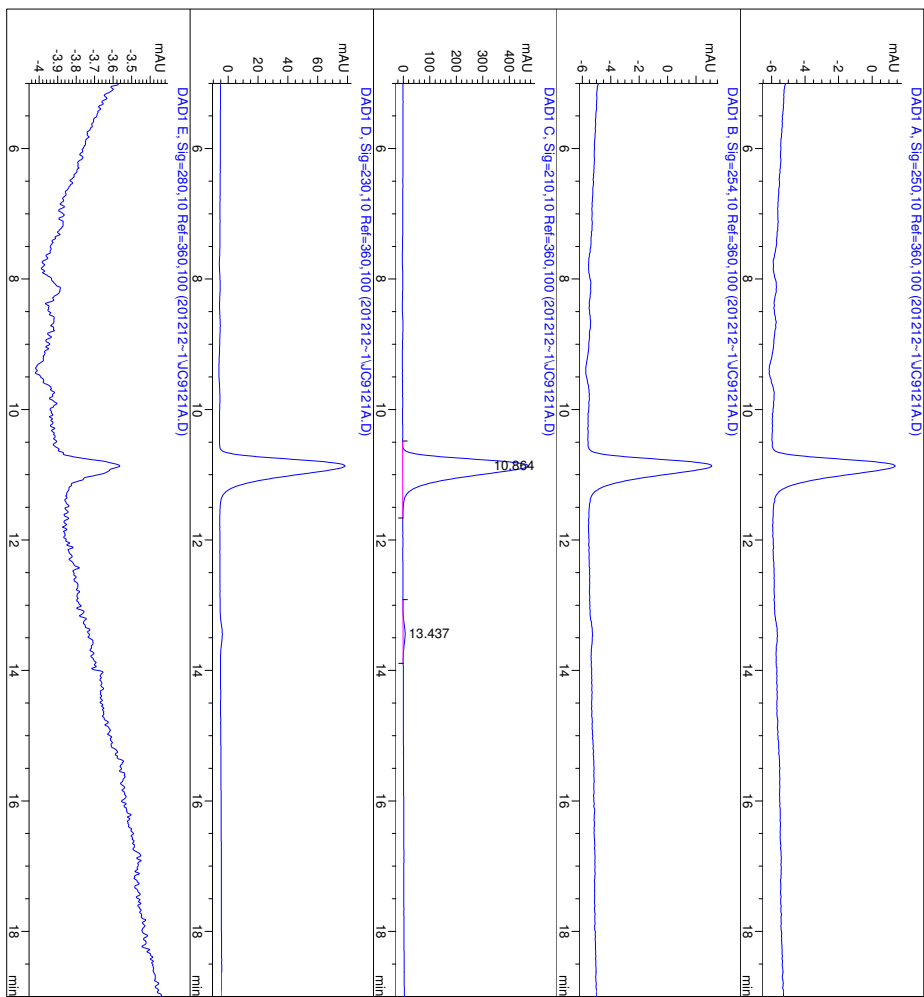
# VII. HPLC Data

Data File C:\HPCHEM\1\DATA\201212-1\JC9121A.D

Sample Name: JC9121A

```

=====
Injection Date : 12/18/2012 2:33:11 PM      Seq. Line : 1
Sample Name    : JC9121A                    Location  : Vial 4
Acq. Operator  : CE                          Inj       : 1
Acq. Instrument : Instrument 1                Inj Volume: 15 µl
Different Inj Volume from Sequence 1         Actual Inj Volume : 5 µl
Acq. Method    : C:\HPCHEM\1\METHODS\VD-01-40.M
Last changed   : 12/18/2012 2:48:17 PM by CE
                (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\VD-02-20.M
Last changed   : 7/30/2014 4:56:50 PM by MK
                (modified after loading)
=====
    
```



Data File C:\HPCHEM\1\DATA\201212-1\JC9121A.D

Sample Name: JC9121A

```

=====
Area Percent Report
=====
Sorted By      : Signal
Multiplier    : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

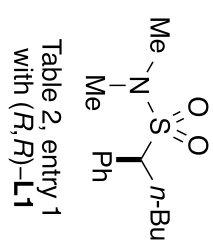


Table 2, entry 1  
with (R,R)-L1

Signal	Retention Time (min)	Type	Width (min)	Area (mAU*s)	Height (mAU)	Area %
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	10.864	BB	0.2815	8588.73828	473.84717	98.0169
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	13.437	PV	0.2756	173.77281	7.93276	1.9831

Totals : 8762.51109 481.77993

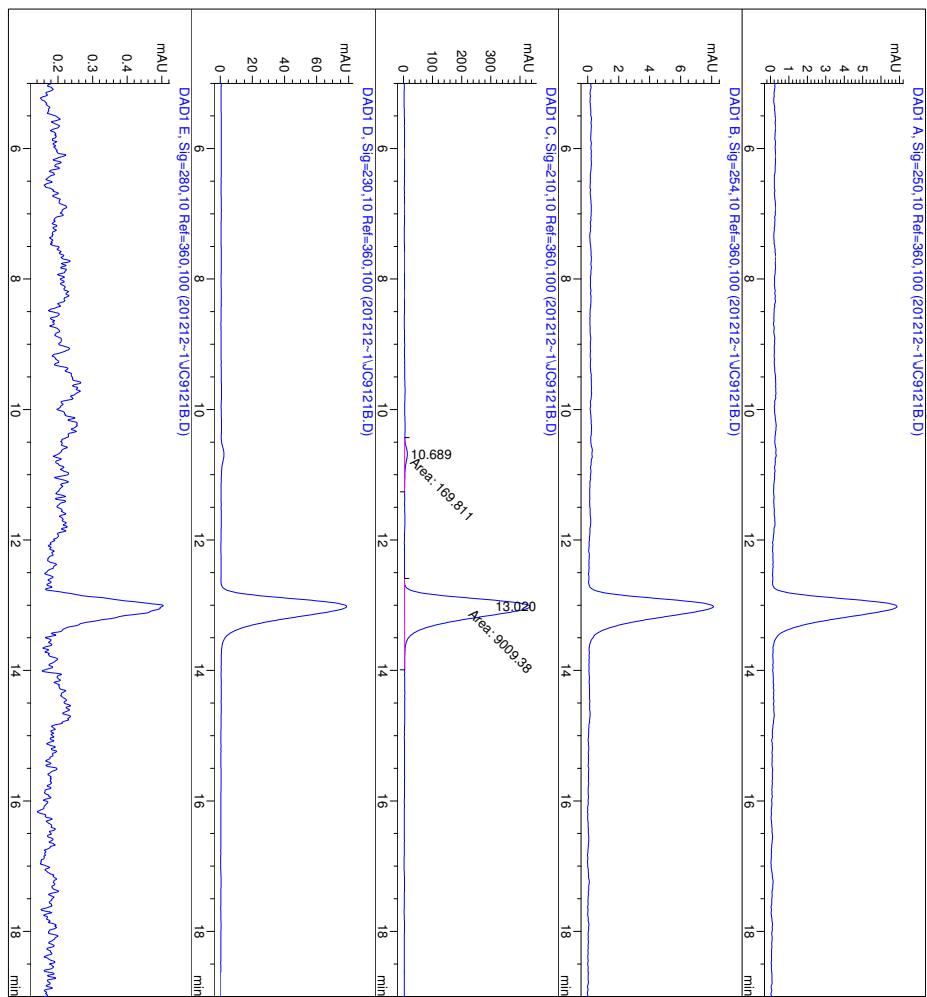
Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

Injection Date : 12/18/2012 3:04:38 PM  
 Sample Name : JC9121B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl  
 Last changed : 4/7/2011 2:40:51 AM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 8:33:12 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.689	FM	0.2978	169.81142	9.50396	1.8500
2	13.020	MM	0.3481	9009.37891	431.37000	98.1500

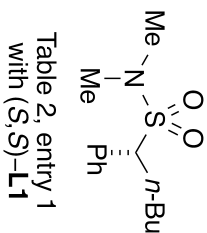
Totals : 9179.19032 440.87395

Results obtained with enhanced integrator!

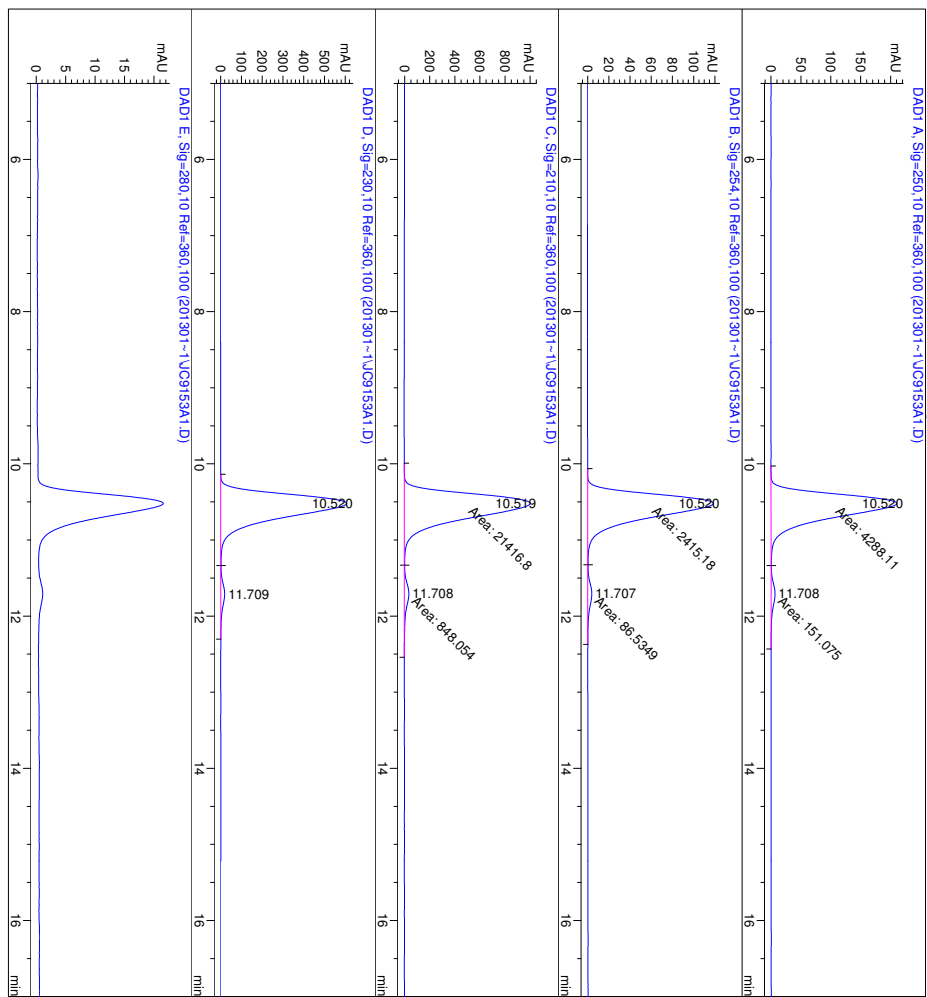
Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*



=====  
 Injection Date : 1/13/2013 11:37:20 PM      Seq. Line : 2  
 Sample Name : JC9153A                            Location : Vial 3  
 Acq. Operator : CE                                Inj : 1  
 Acq. Instrument : Instrument 1                    Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1            Actual Inj Volume : 3 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-02-40.M  
 Last changed : 8/9/2012 4:54:01 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 4:55:19 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.520	MF	0.3390	4288.11475	210.79234	96.5968
2	11.708	FM	0.3773	151.07475	6.67396	3.4032
Totals :				4439.18950	217.46631	

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.520	MF	0.3389	2415.18042	118.77131	96.5410
2	11.707	FM	0.3774	86.53488	3.82184	3.4590
Totals :				2501.71530	122.59315	

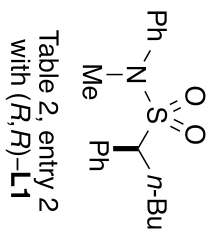
Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.519	MF	0.3557	21416.8e4	1003.47882	96.1911
2	11.708	FM	0.3883	848.05426	36.40364	3.8089
Totals :				2.22649e4	1039.88247	

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

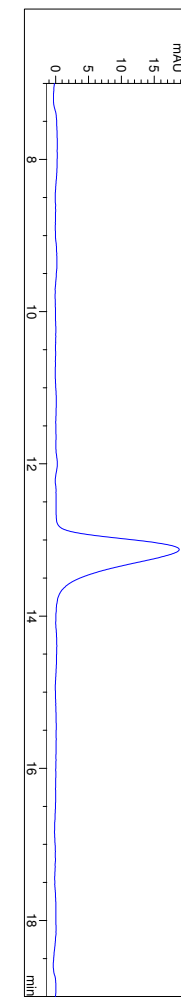
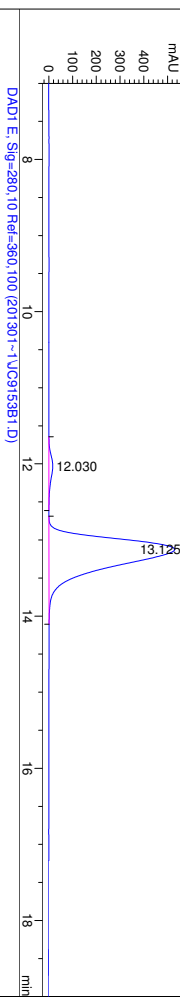
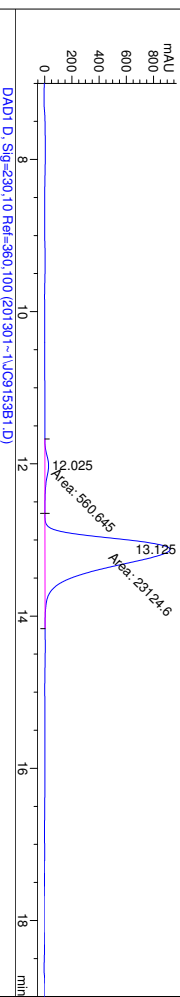
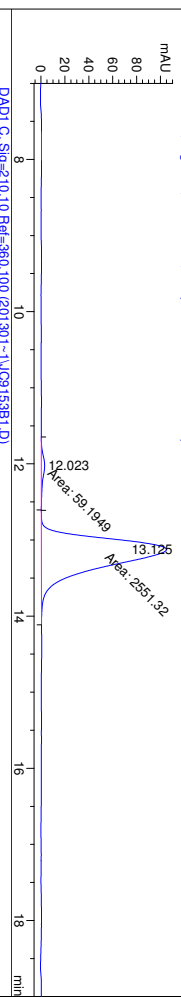
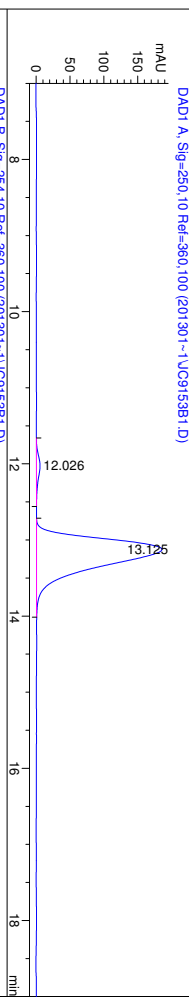
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.520	BB	0.3125	1.22823e4	606.00146	96.7746
2	11.709	BB	0.3369	409.36346	18.58926	3.2254
Totals :				1.26917e4	624.59073	

Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100  
 Results obtained with enhanced integrator!  
 \*\*\* End of Report \*\*\*





=====  
Injection Date : 1/13/2013 9:26:32 PM      Seq. Line : 3  
Sample Name : JC9153B                              Location : Vial 4  
Acq. Operator : CE                                    Inj : 1  
Acq. Instrument : Instrument 1                    Inj Volume : 15 µl  
Diluent Inj Volume from Sequence 1            Actual Inj Volume : 3 µl  
Acq. Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
Last changed : 4/19/2010 4:08:56 PM by sz  
Analysis Method : C:\HPCHEM\1\METHODS\AD003-40.M  
Last changed : 8/1/2014 11:08:32 PM by MK  
(modified after loading)



=====  
Area Percent Report  
=====

Sorted By	Signal
Multiplier	1.0000
Dilution	1.0000
Use Multiplier & Dilution Factor with ISTDs	

Signal 1: DADI A, Sig=250,10 Ref=360,100  
Results obtained with enhanced integrator!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.026	BP	0.3146	113.62238	5.33121	2.4632
2	13.125	BB	0.3752	4499.24658	185.38203	97.5368

Totals : 4612.86896 190.71324

Signal 2: DADI B, Sig=254,10 Ref=360,100  
Results obtained with enhanced integrator!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.023	MM	0.3532	59.19486	2.79296	2.2676
2	13.125	MM	0.4060	2551.31982	104.72879	97.7324

Totals : 2610.51468 107.52175

Signal 3: DADI C, Sig=210,10 Ref=360,100  
Results obtained with enhanced integrator!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.025	MM	0.3401	560.64459	27.47764	2.3671
2	13.125	MM	0.4189	23124.6	919.98969	97.6329

Totals : 2.36852e4 947.46732

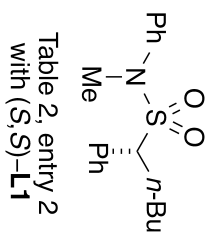
Signal 4: DADI D, Sig=230,10 Ref=360,100  
Results obtained with enhanced integrator!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.030	BP	0.3344	358.89542	16.20137	2.7223
2	13.125	BB	0.3746	12824.7	529.39978	97.2777

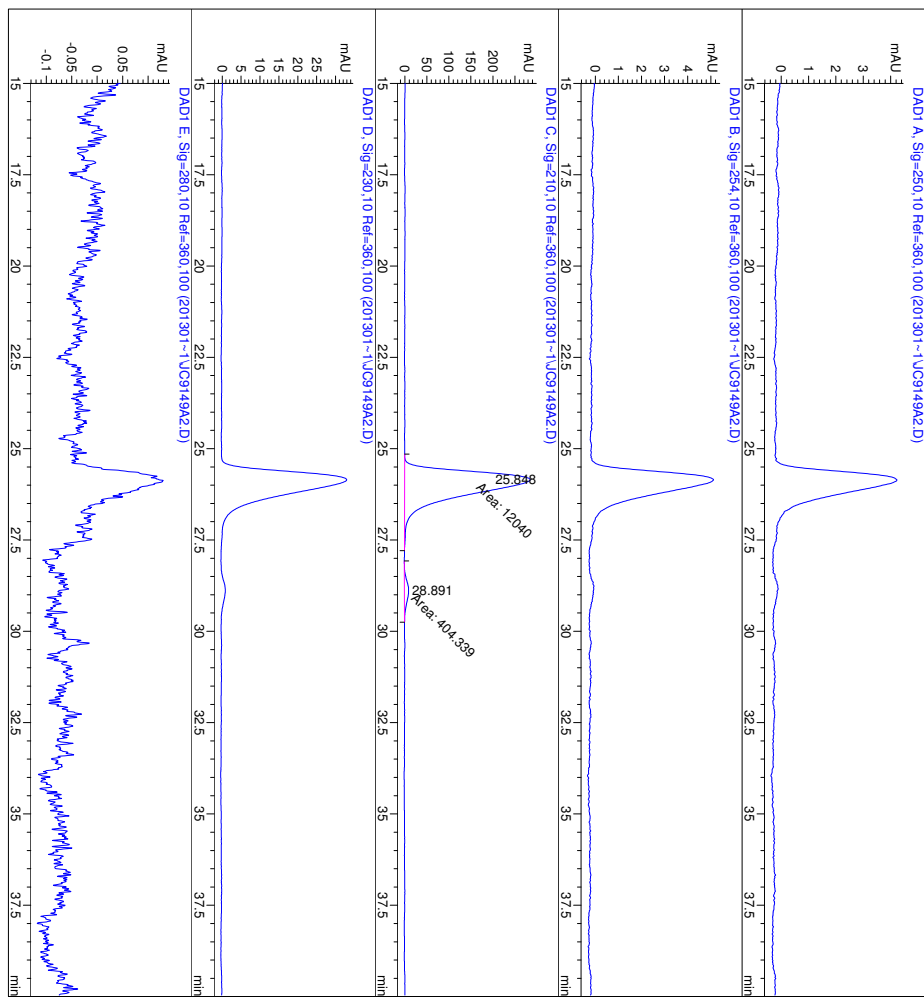
Totals : 1.31836e4 545.60115

Signal 5: DADI E, Sig=280,10 Ref=360,100  
Results obtained with enhanced integrator!

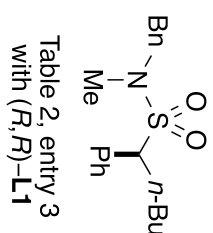
\*\*\* End of Report \*\*\*



=====  
 Injection Date : 1/5/2013 12:33:05 AM      Seq. Line : 6  
 Sample Name : JC9149A                              Location : Vial 6  
 Acq. Operator : CE                                    Inj : 1  
 Acq. Instrument : Instrument 1                    Inj Volume : 15 µl  
 Different Inj Volume from Sequence !          Actual Inj Volume : 5 µl  
 Last changed : 1/4/2013 10:05:27 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD-02-40.M  
 Last changed : 7/30/2014 4:58:11 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

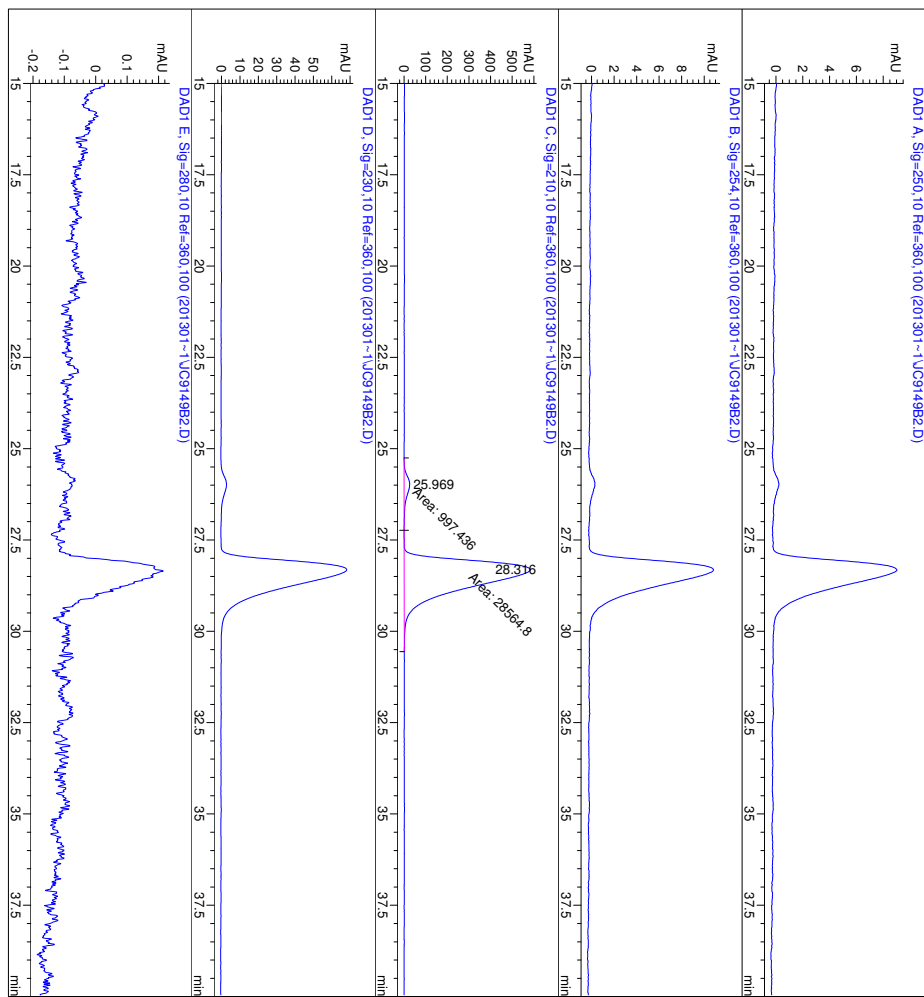


Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	25.848	MM	0.7041	1.20400e4	285.00970	96.7508
Signal 4: DAD1 D, Sig=230,10 Ref=360,100	28.891	MM	0.7018	404.33865	9.60306	3.2492

Totals : 1.24443e4 294.61277  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

=====  
 Injection Date : 1/5/2013 1:14:21 AM      Seq. Line : 7  
 Sample Name : JC9149B                      Location : Vial 7  
 Acq. Operator : CE                            Inj : 1  
 Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
 Different Inj Volume from Sequence !      Actual Inj Volume : 5 µl  
 Last changed : 1/4/2013 10:05:27 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD-02-40.M  
 Last changed : 8/1/2014 11:12:30 PM by MK  
 Last changed : 8/1/2014 11:12:30 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====

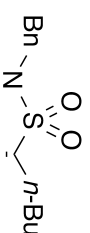


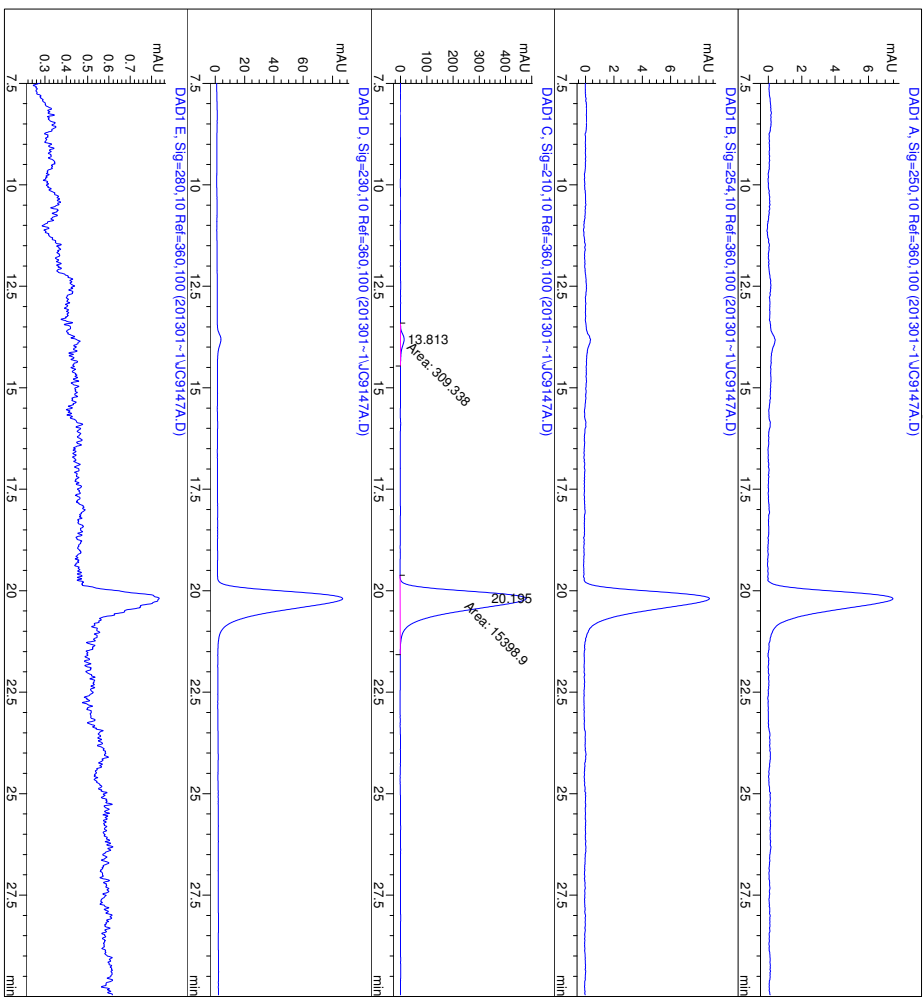
Table 2, entry 3  
 with (S,S)-L1

Sorted By	Signal					
Multiplier	: 1.0000					
Dilution	: 1.0000					
Use Multiplier & Dilution Factor with ISTDs						
Signal 1:	DAD1 A, Sig=250,10 Ref=360,100					
Signal 2:	DAD1 B, Sig=254,10 Ref=360,100					
Signal 3:	DAD1 C, Sig=210,10 Ref=360,100					
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.969	MM	0.6423	997.43585	25.88220	3.3740
2	28.316	MM	0.8177	2.85648e4	582.20422	96.6260

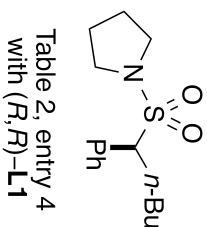
Totals : 2.95622e4 608.08643  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

=====  
 \*\*\* End of Report \*\*\*  
 =====

=====  
 Injection Date : 1/3/2013 5:51:12 PM      Seq. Line : 2  
 Sample Name : JC9147A                      Location : Vial 4  
 Acq. Operator : CE                            Inj : 1  
 Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1      Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AD-02-30.M  
 Last changed : 1/3/2013 5:29:04 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 5:00:07 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs



Signal 1: DADI A, Sig=250,10 Ref=360,100

Signal 2: DADI B, Sig=254,10 Ref=360,100

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.813	MM	0.3644	309.33765	14.14928	1.9693
2	20.195	MM	0.5342	1.53989e4	480.47076	98.0307

Totals : 1.57082e4 494.62004

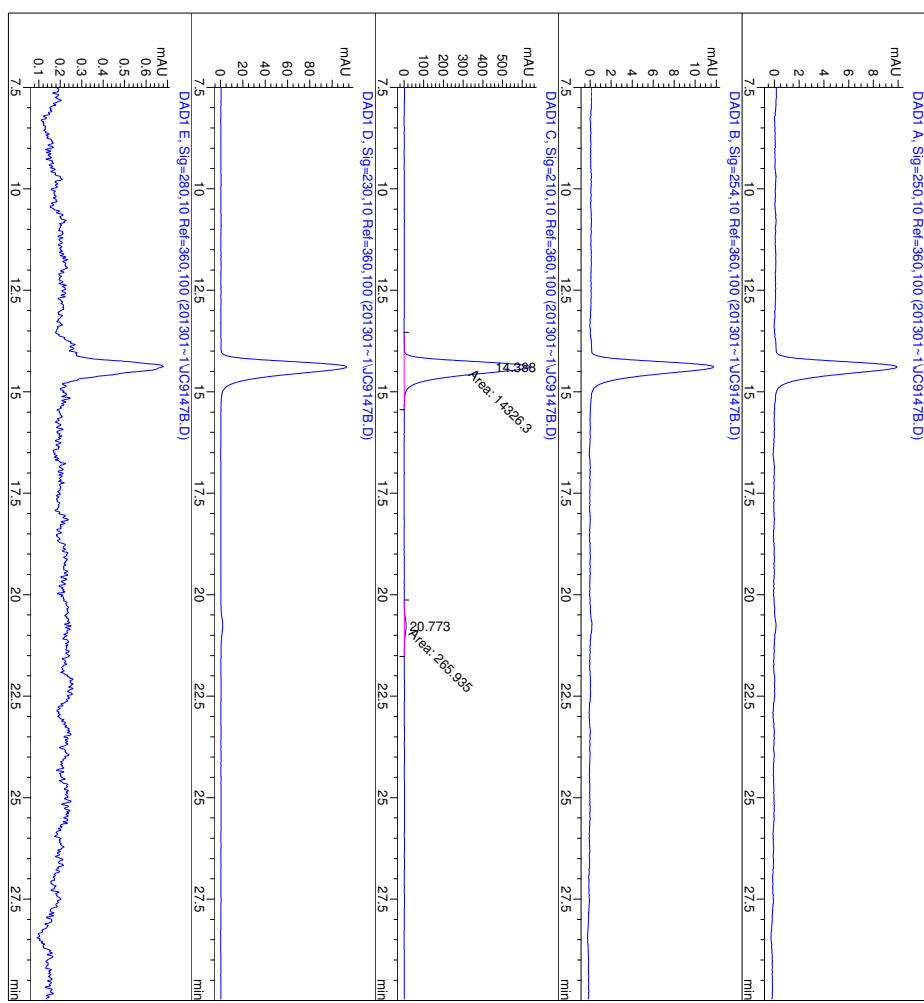
Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

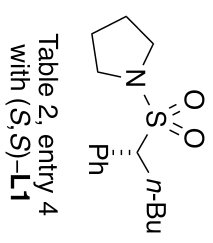
Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

=====  
Injection Date : 1/3/2013 6:22:31 PM      Seq. Line : 3  
Sample Name : JC9147B                      Location : Vial 5  
Acq. Operator : CE                            Inj : 1  
Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
Different Inj Volume from Sequence 1      Actual Inj Volume : 5 µl  
Acq. Method : C:\HPCHEM\1\METHODS\AD-02-30.M  
Last changed : 1/3/2013 5:29:04 PM by CE  
Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 8/1/2014 11:14:55 PM by MK  
(modified after loading)



=====  
Area Percent Report  
=====  
Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs



Signal 1: DAD1 A, Sig=250,10 Ref=360,100  
Signal 2: DAD1 B, Sig=254,10 Ref=360,100  
Signal 3: DAD1 C, Sig=210,10 Ref=360,100

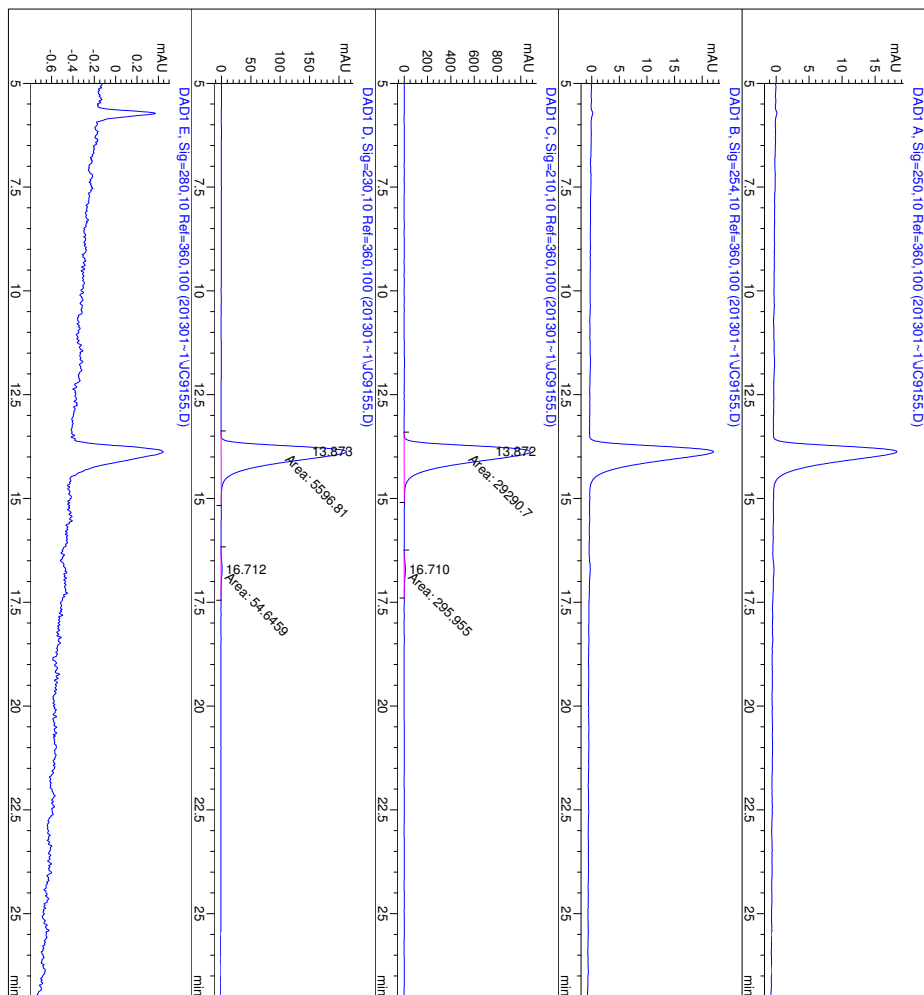
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.388	MM	0.3734	1.43263e4	639.37732	98.1776
2	20.773	MM	0.4779	265.93488	9.27401	1.8224

Totals : 1.45922e4 648.65133

Results obtained with enhanced integrator!  
Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

Injection Date : 1/17/2013 6:42:19 PM  
 Sample Name : JC9155  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 5 µl  
 Inj Volume : 15 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-03-30.M  
 Last changed : 12/31/2012 2:58:25 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 5:02:27 PM by MK  
 (modified after loading)



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

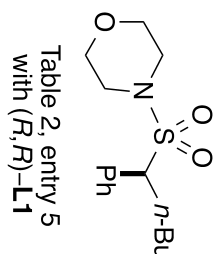
Signal	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	13.872	0.4517	2.92907e4	1080.68958	98.9997
Signal 2: DADI B, Sig=254,10 Ref=360,100	16.710	0.4686	295.95520	10.52571	1.0003
Signal 3: DADI C, Sig=210,10 Ref=360,100	13.872	0.4517	2.92907e4	1080.68958	98.9997
Signal 4: DADI D, Sig=230,10 Ref=360,100	16.710	0.4778	54.64594	1.90619	0.9669
Signal 5: DADI E, Sig=280,10 Ref=360,100	13.872	0.4361	5596.80615	213.91138	99.0331
Signal 5: DADI E, Sig=280,10 Ref=360,100	16.712	0.4778	54.64594	1.90619	0.9669

Totals : 2.95866e4 1091.21529

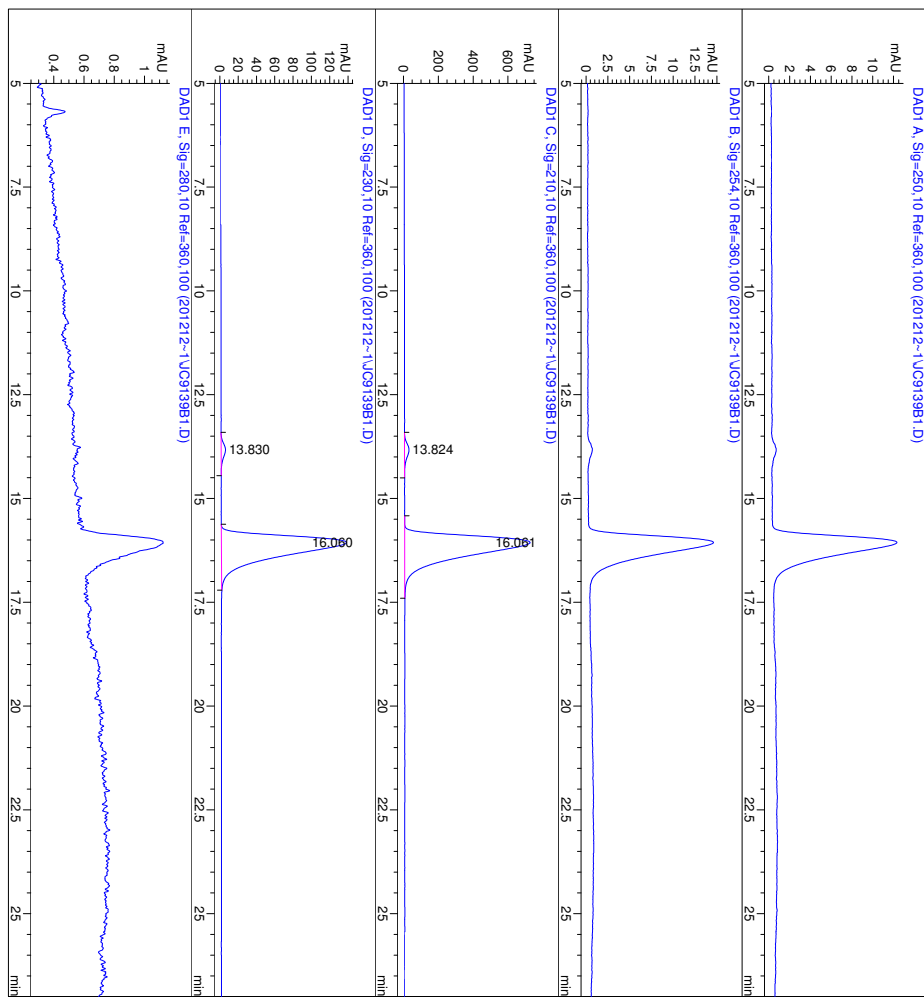
Results obtained with enhanced integrator!

Results obtained with enhanced integrator!  
 Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*



=====  
Injection Date : 12/31/2012 3:20:37 PM      Seq. Line : 2  
Sample Name : JC9139B                            Location : Vial 3  
Acq. Operator : CE                                Inj : 1  
Acq. Instrument : Instrument 1                   Inj Volume : 15 µl  
Different Inj Volume from Sequence 1  
Acq. Method : C:\HPCHEM\1\METHODS\VD-03-30.M  
Last changed : 12/31/2012 2:58:25 PM by CE  
Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 8/1/2014 11:17:34 PM by MK  
(modified after loading)



=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.824	PB	0.3375	612.77722	25.76346	2.5717
2	16.061	PB	0.4739	2.32153e4	720.54395	97.4283

Totals : 2.38281e4 746.30741

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.830	BP	0.3511	110.67741	4.72843	2.4877
2	16.060	BB	0.4794	4338.34521	137.02046	97.5123

Totals : 4449.02262 141.74889

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

=====  
\*\*\* End of Report \*\*\*  
=====

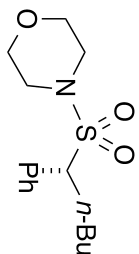
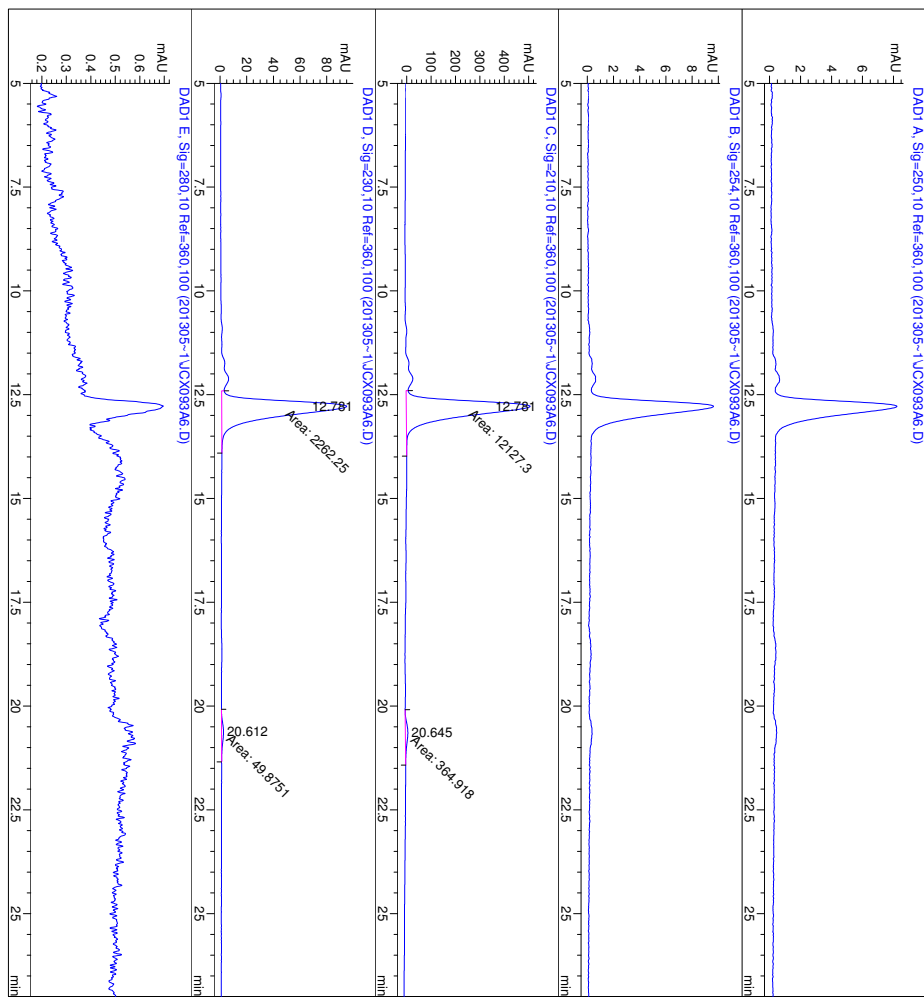
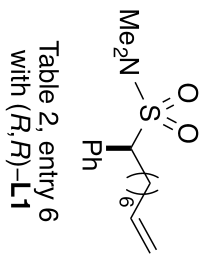


Table 2, entry 5  
with (S,S)-L1

Injection Date : 5/19/2013 5:16:09 PM  
 Sample Name : JCI10093A  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-01-40.M  
 Last changed : 12/18/2012 2:31:36 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 5:05:01 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.781	FM	0.3974	1.21273e4	508.56665	97.0788
2	20.645	MM	0.5908	364.91779	10.29492	2.9212

Totals : 1.24922e4 518.86157  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.781	FM	0.4017	2262.25317	93.85459	97.8429
2	20.612	MM	0.5479	49.87514	1.51723	2.1571

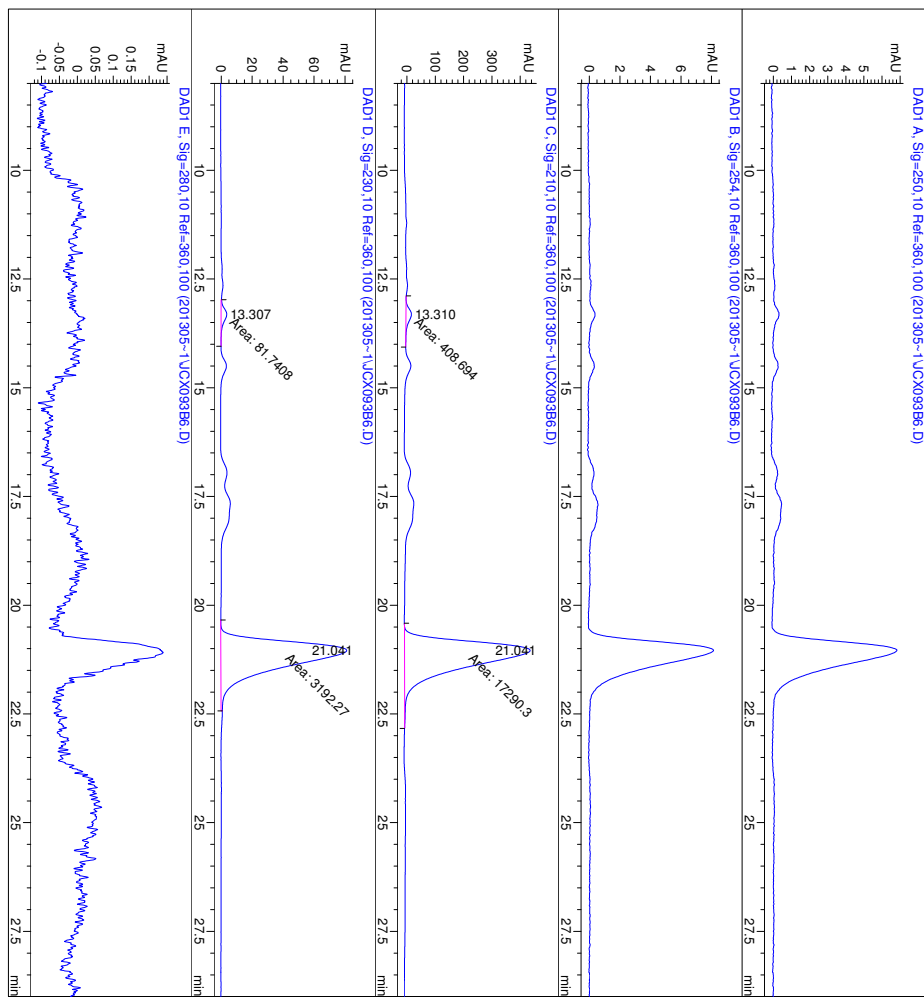
Totals : 2312.12832 95.37182  
 Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*



Injection Date : 5/19/2013 5:57:27 PM  
 Sample Name : JCI10093B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 1  
 Last changed : 12/18/2012 2:31:36 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\A0005-40.M  
 Last changed : 8/2/2014 9:01:58 PM by MK  
 (modified after loading)

Seq. Line : 3  
 Location : Vial 42  
 Inj : 1  
 Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl



Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

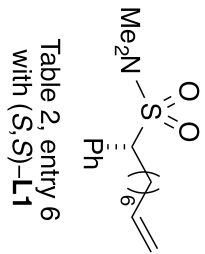
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.310	MM	0.3540	408.69366	19.24129	2.3091
2	21.041	MM	0.6492	1.72903e4	443.91245	97.6909

Totals : 1.76990e4 463.15373  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100

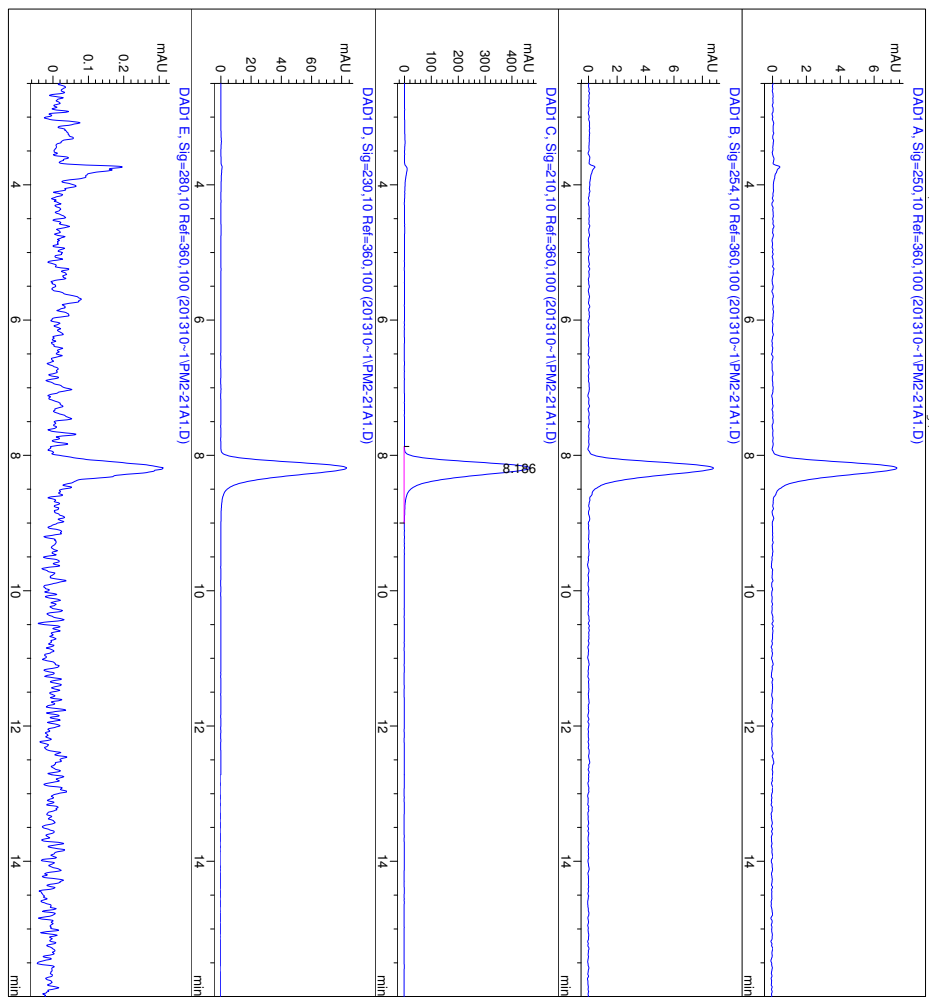
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.307	FM	0.3703	81.74083	3.67898	2.4967
2	21.041	MF	0.6541	3192.27197	81.33752	97.5033

Totals : 3274.01280 85.01650  
 Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*



=====  
 Injection Date : 10/23/2013 1:57:18 PM      Seq. Line : 2  
 Sample Name : PM2-21A                              Location : Vial 13  
 Acq. Operator : MK                                    Inj : 1  
 Acq. Instrument : Instrument 1                    Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1          Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
 Last changed : 9/13/2013 12:42:31 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 5:07:11 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Signal 2: DADI B, Sig=254,10 Ref=360,100

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.186	VB	0.2249	6870.03662	468.96442	100.0000

Totals : 6870.03662 468.96442

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

Signal 5: DADI E, Sig=280,10 Ref=360,100

=====  
 \*\*\* End of Report \*\*\*  
 =====

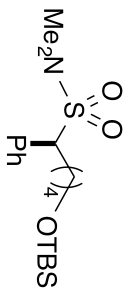
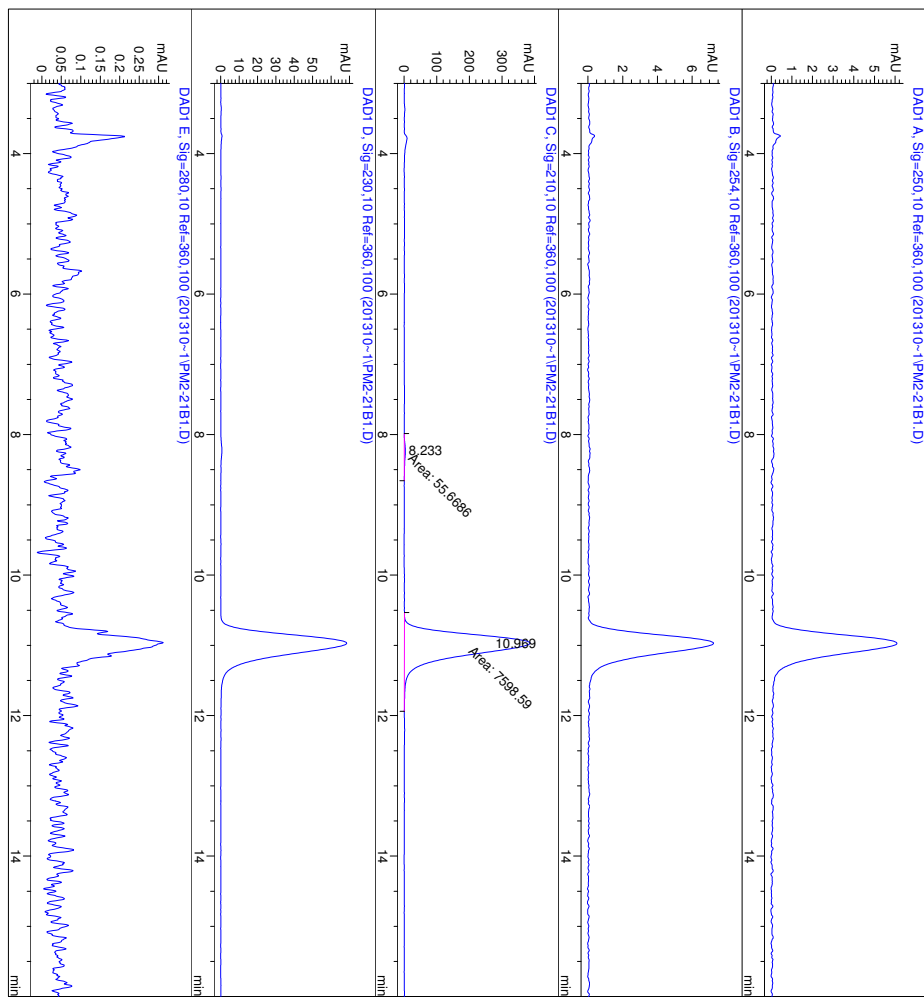


Table 2, entry 7  
 with (R,R)-L1

=====  
 Injection Date : 10/23/2013 2:28:36 PM      Seq. Line : 3  
 Sample Name : PM2-21B                            Location : Vial 14  
 Acq. Operator : MK                                Inj : 1  
 Acq. Instrument : Instrument 1                   Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1          Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
 Last changed : 9/13/2013 12:42:31 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:25:57 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.233	MM	0.2711	55.66857	3.42192	0.7273
2	10.969	MM	0.3284	7598.58594	385.60574	99.2727

Totals : 7654.25451 389.02767

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

=====  
 \*\*\* End of Report \*\*\*  
 =====

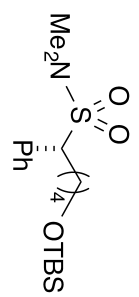
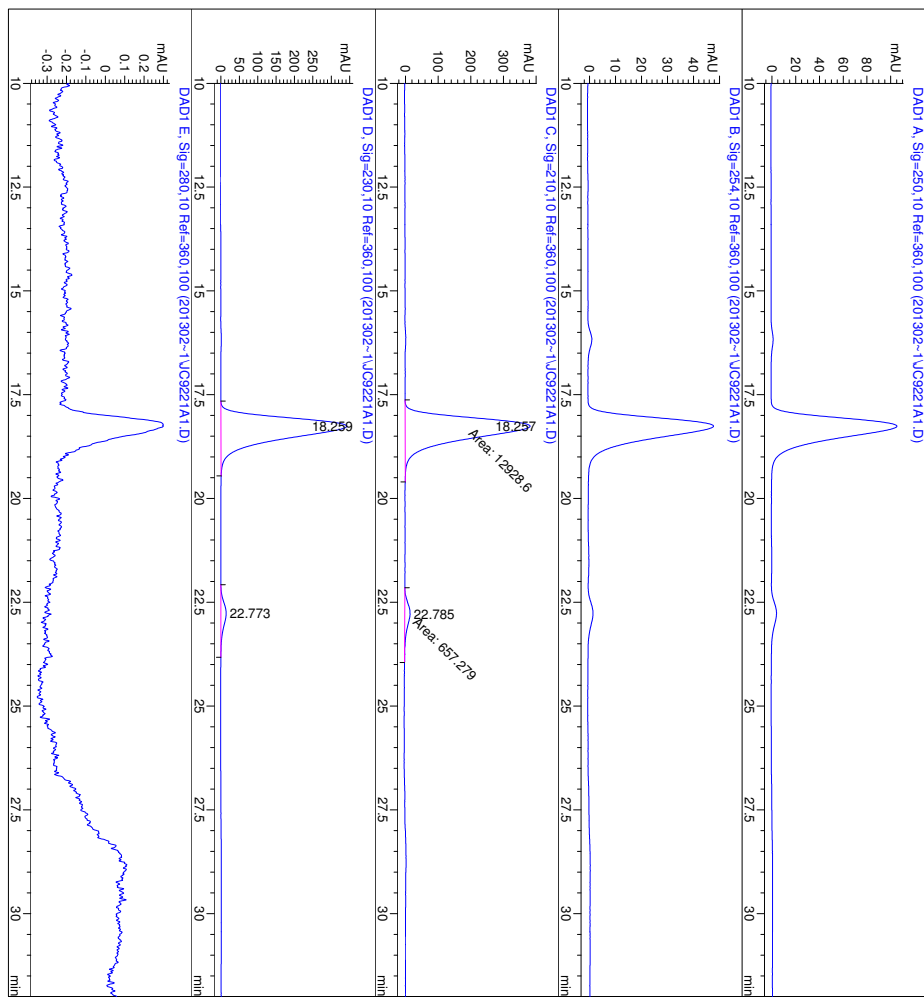


Table 2, entry 7  
 with (S,S)-L1

Injection Date : 2/22/2013 11:28:27 AM  
 Sample Name : JC9221A  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 15 µl  
 Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-05-40.M  
 Last changed : 4/7/2011 5:39:35 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 5:09:46 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.257	MM	0.5628	1.29286e4	382.84482	95.1621
2	22.785	MM	0.6684	657.27887	16.39051	4.8379

Totals : 1.35859e4 399.23533

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

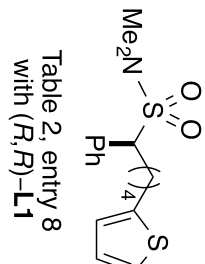
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.259	BB	0.5223	1.15049e4	342.18851	95.1596
2	22.773	BB	0.5728	585.20709	14.37923	4.8404

Totals : 1.20901e4 356.56774

Results obtained with enhanced integrator!

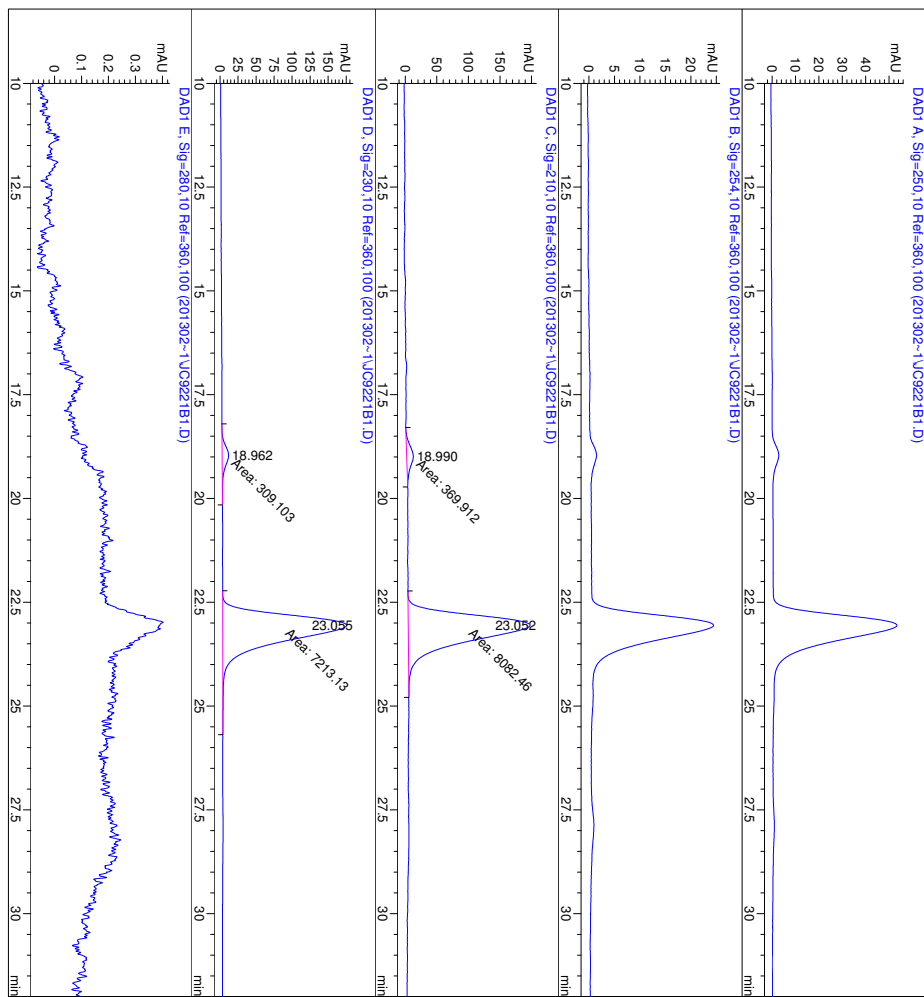
Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*



Injection Date : 2/22/2013 12:09:44 PM  
 Sample Name : JC9221B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 4/7/2011 5:39:35 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 9:04:09 PM by MK  
 (modified after loading)

Seq. Line : 3  
 Location : Vial 10  
 Inj : 1  
 Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.990	MM	0.5818	369.91183	10.59696	4.3764
2	23.052	MM	0.6975	8082.46289	193.11874	95.6236

Totals : 8452.37473 203.71571

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.962	MM	0.5785	309.10349	8.90468	4.1092
2	23.055	MM	0.6991	7213.12598	171.96364	95.8908

Totals : 7522.22946 180.86832

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

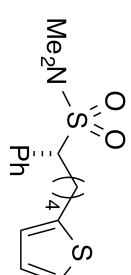
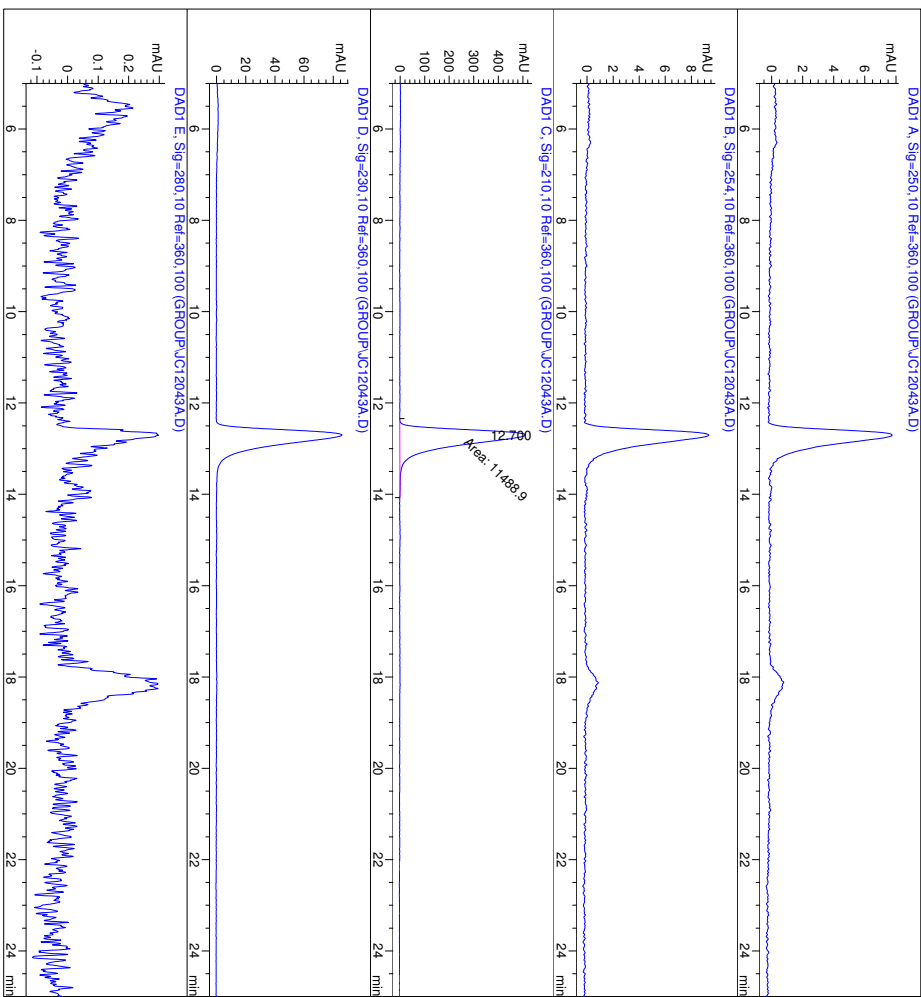


Table 2, entry 8 with (S,S)-L1

```

=====
Injection Date : 6/16/2014 7:47:41 PM      Seq. Line : 4
Sample Name    : JC12043A                  Location  : Vial 11
Acq. Operator  : MK                        Inj       : 1
Acq. Instrument : Instrument 1              Inj Volume: 15 µl
Different Inj Volume from Sequence 1       Actual Inj Volume : 6 µl
Acq. Method    : C:\HPCHEM\1\METHODS\OD-01-30.M
Last changed   : 6/16/2014 7:51:29 PM by MK
              (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M
Last changed   : 7/30/2014 6:54:33 PM by MK
              (modified after loading)
=====
    
```



```

=====
Area Percent Report
=====
Sorted By      : Signal
Multiplier    : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
Signal 1: DADI A, Sig=250,10 Ref=360,100
Signal 2: DADI B, Sig=254,10 Ref=360,100
Signal 3: DADI C, Sig=210,10 Ref=360,100
Signal 4: DADI D, Sig=230,10 Ref=360,100
Signal 5: DADI E, Sig=280,10 Ref=360,100
=====
    
```

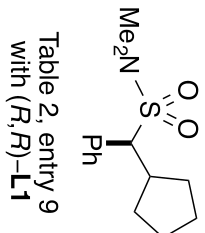
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.700	MM	0.3740	1.14889e4	512.01752	100.0000
Totals :				1.14889e4	512.01752	

Results obtained with enhanced integrator!

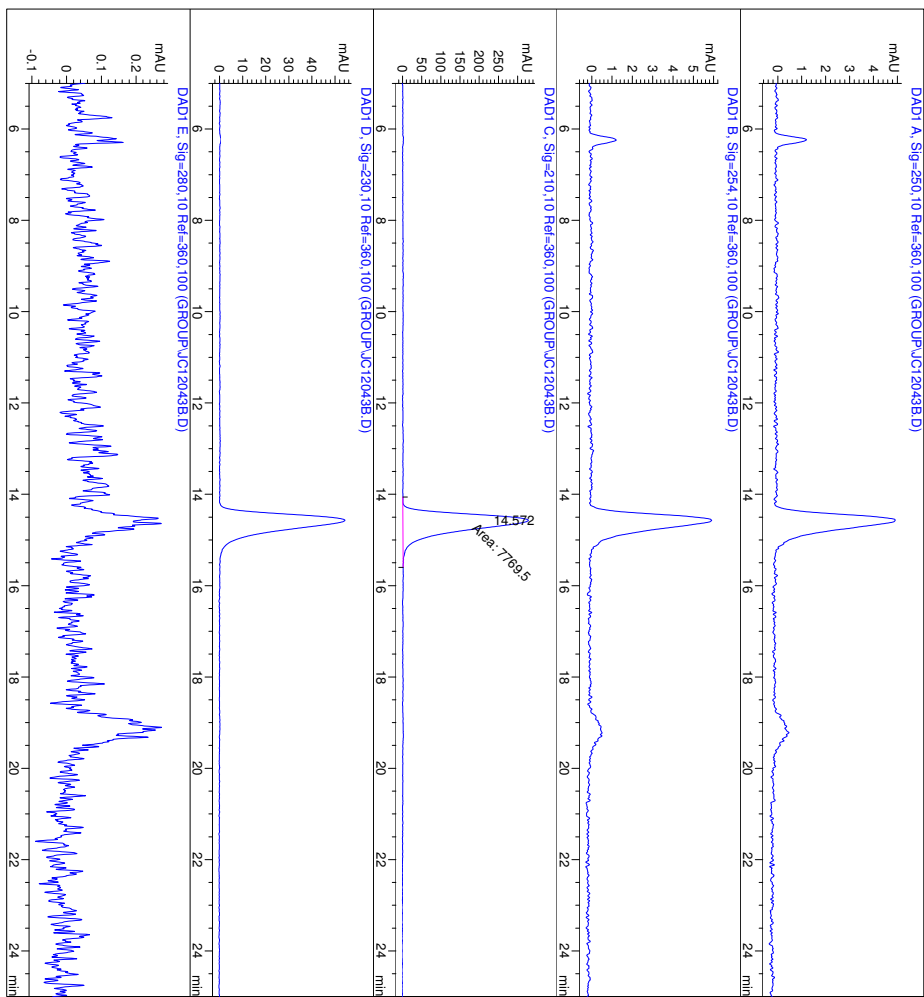
Signal 4: DADI D, Sig=230,10 Ref=360,100

Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*



=====  
 Injection Date : 6/16/2014 8:19:00 PM      Seq. Line : 5  
 Sample Name : JC12043B                      Location : Vial 12  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1                Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1        Actual Inj Volume : 6 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 6/16/2014 7:51:29 PM by MK  
 (modified after loading)  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:32:53 PM by MK  
 (modified after loading)



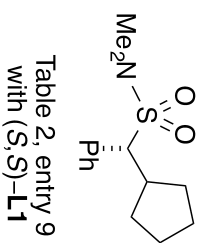
=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

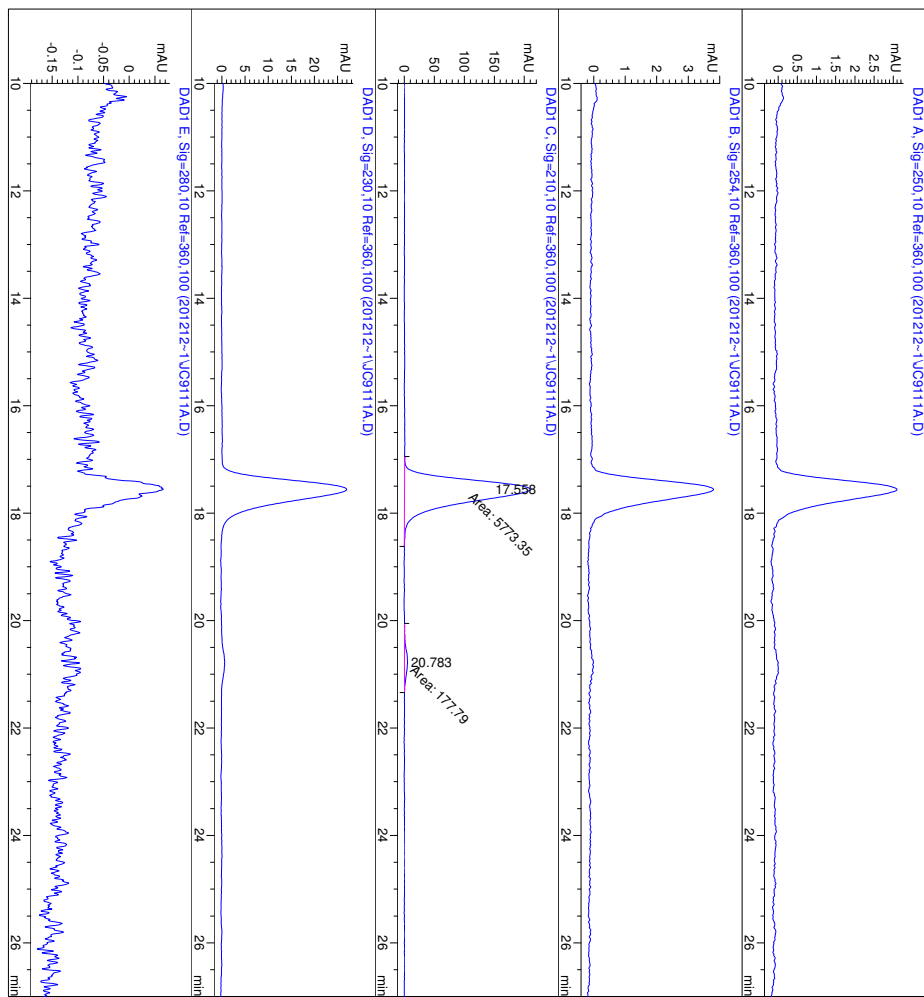
Signal 1: DADI A, Sig=250,10 Ref=360,100  
 Signal 2: DADI B, Sig=254,10 Ref=360,100  
 Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.572	MM	0.3958	7769.50049	327.13113	100.0000

Totals :                      7769.50049    327.13113  
 Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Signal 5: DADI E, Sig=280,10 Ref=360,100  
 \*\*\* End of Report \*\*\*



=====  
Injection Date : 12/7/2012 3:31:19 PM      Seq. Line : 3  
Sample Name : JC9111A                            Location : Vial 35  
Acq. Operator : CE                                Inj : 1  
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl  
Diluent Inj Volume from Sequence 1  
Actual Inj Volume : 5 µl  
Acq. Method : C:\HPCHEM\1\METHODS\OD-05-40.M  
Last changed : 4/7/2011 5:39:35 PM by CC  
Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
Last changed : 7/30/2014 6:56:15 PM by MK  
(modified after loading)



Area Percent Report

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Signal 2: DADI B, Sig=254,10 Ref=360,100

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.558	MM	0.4595	5773.34912	209.42706	97.0125
2	20.783	MM	0.5738	177.79001	5.16444	2.9875

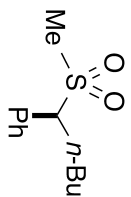
Totals : 5951.13913 214.59150

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

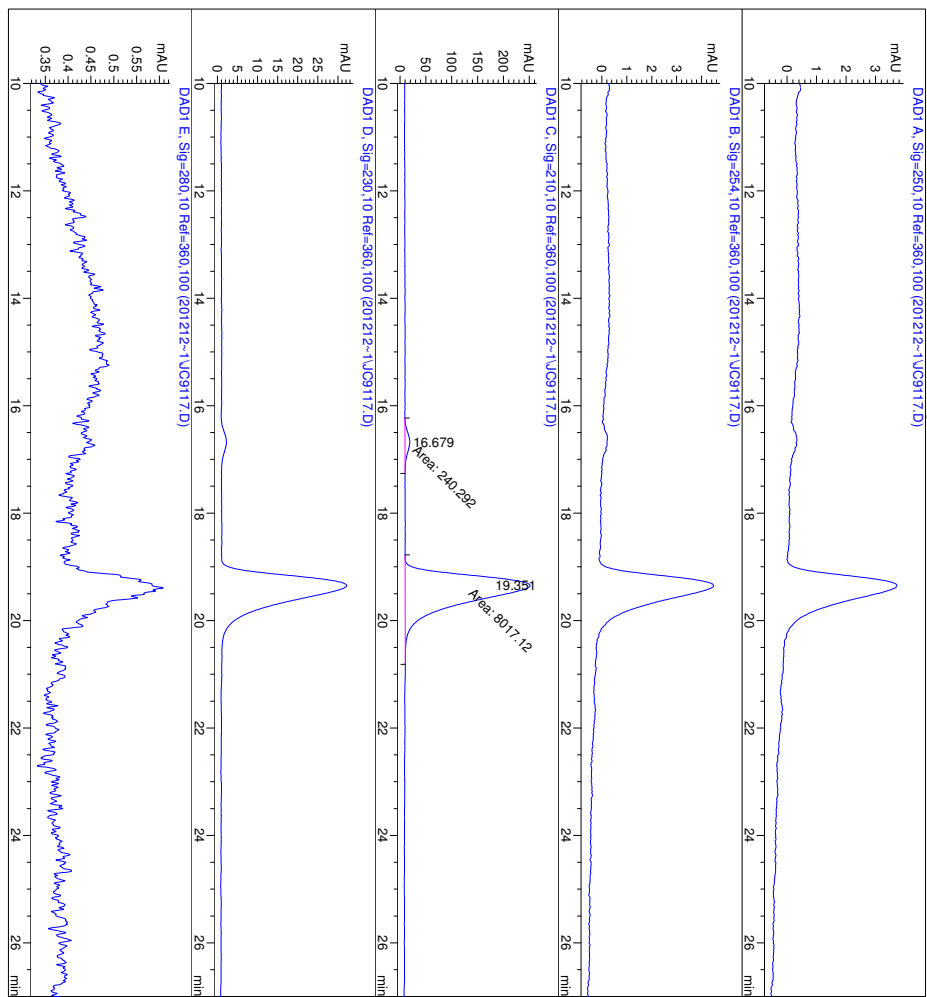
Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*



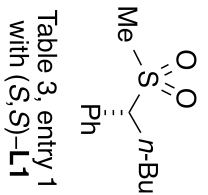


Injection Date : 12/14/2012 4:31:29 PM  
 Sample Name : JC9117  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 4/7/2011 5:39:35 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\A0005-40.M  
 Last changed : 8/1/2014 11:34:56 PM by MK  
 (modified after loading)



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs



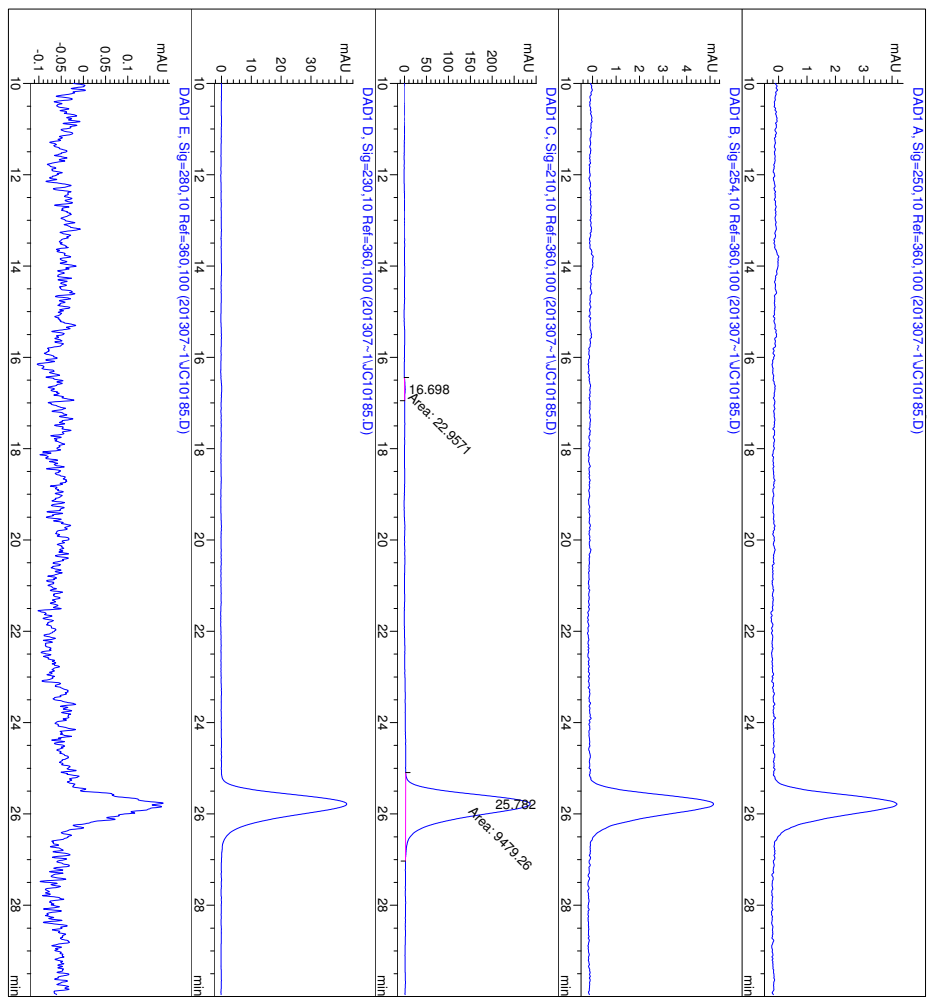
Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	19.351	MM	0.5532	8257.41116	241.52242	97.0900
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	19.351	MM	0.5532	240.29202	9.33470	2.9100
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	16.679	MM	0.4290	240.29202	9.33470	2.9100
Signal 4: DAD1 D, Sig=230,10 Ref=360,100	16.679	MM	0.4290	240.29202	9.33470	2.9100
Signal 5: DAD1 E, Sig=280,10 Ref=360,100	16.679	MM	0.4290	240.29202	9.33470	2.9100

Totals : 8257.41116 250.85712

Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

=====  
 Injection Date : 7/20/2013 9:37:03 AM      Seq. Line : 34  
 Sample Name : JC10185                              Location : Vial 82  
 Acq. Operator : CE                                      Inj : 1  
 Acq. Instrument : Instrument 1                      Inj Volume : 15 µl  
 Different Inj Volume from Sequence !              Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AD-04-30.M  
 Last changed : 11/29/2010 7:04:08 PM by JTM  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 6:59:32 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.698	MM	0.2409	22.95708	1.58850	0.2416
2	25.782	MM	0.5562	9479.26074	284.07181	99.7584

Totals : 9502.21782 285.66031

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

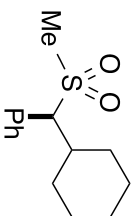
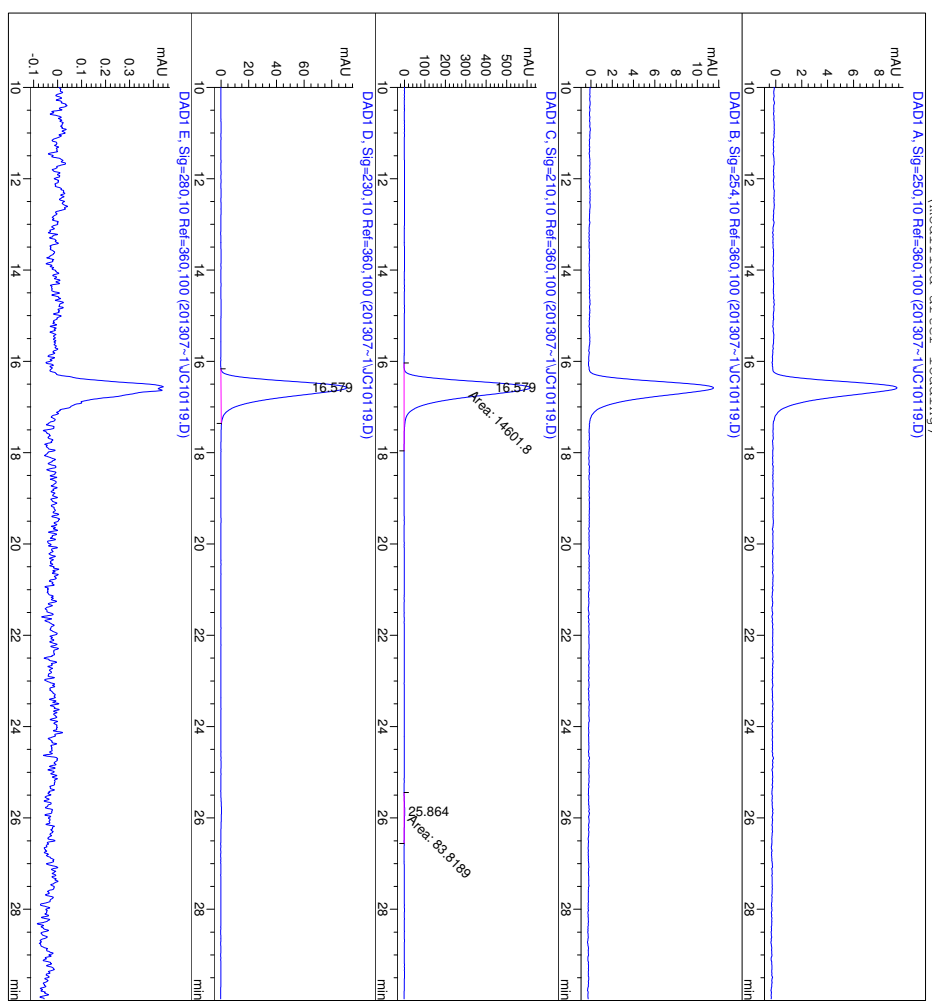


Table 3, entry 2  
 with (R,R)-L1

Injection Date : 7/20/2013 9:05:45 AM  
 Sample Name : JCI0119B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 11/29/2010 7:04:08 PM by JTM  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:37:12 PM by MK  
 (modified after loading)

Seq. Line : 33  
 Location : Vial 81  
 Inj : 1  
 Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl



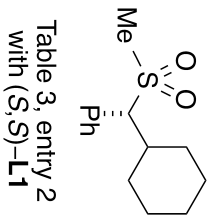
Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Area Percent Report
Signal 1: DADI A, Sig=250,10 Ref=360,100
Signal 2: DADI B, Sig=254,10 Ref=360,100
Signal 3: DADI C, Sig=210,10 Ref=360,100
Signal 4: DADI D, Sig=230,10 Ref=360,100
Signal 5: DADI E, Sig=280,10 Ref=360,100

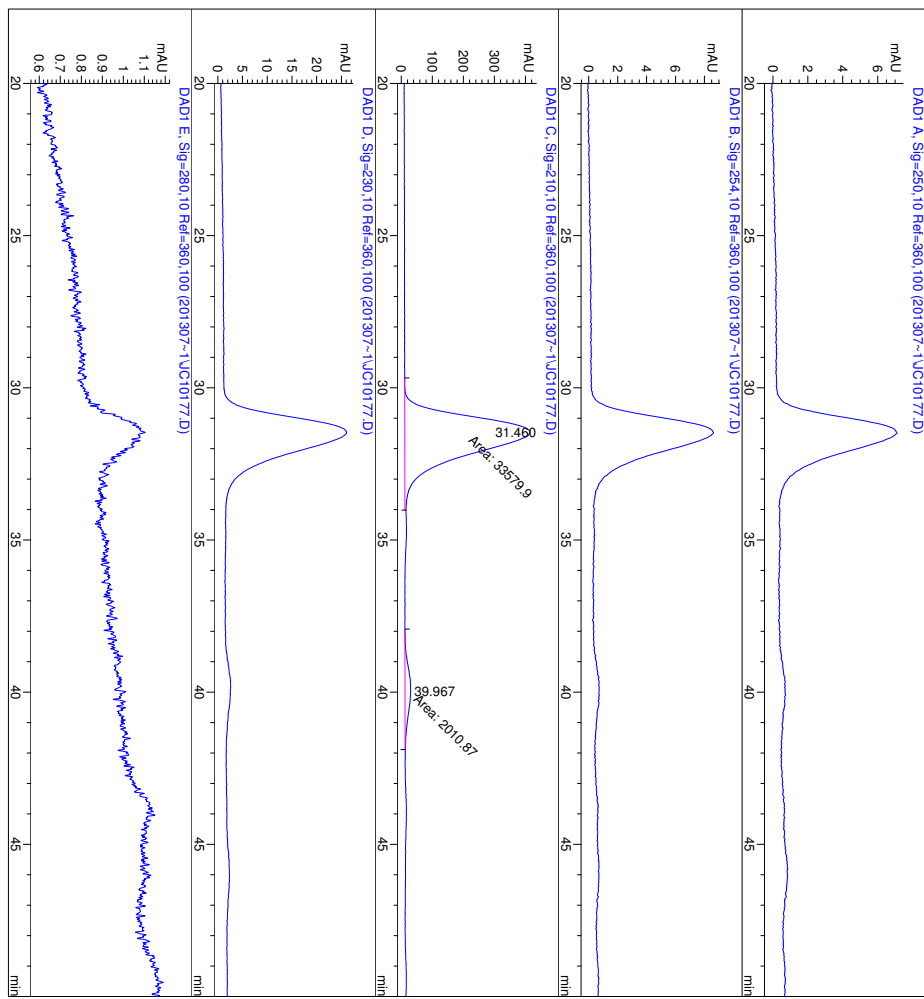
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.579	MM	0.3945	1.46018e4	616.82446	99.4292
2	25.864	MM	0.5283	83.81888	2.64443	0.5708

Totals : 1.46856e4 619.46889

Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Results obtained with enhanced integrator!  
 Signal 5: DADI E, Sig=280,10 Ref=360,100  
 \*\*\* End of Report \*\*\*



=====  
Injection Date : 7/11/2013 9:50:27 AM      Seq. Line : 2  
Sample Name : JC10177                            Location : Vial 1  
Acq. Operator : CE                                Inj : 1  
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl  
Different Inj Volume from Sequence !  
Last changed : 6/28/2013 4:31:36 PM by CE      Actual Inj Volume : 5 µl  
Analysis Method : C:\HPCHEM\1\METHODS\OD-20-60.M  
                  : C:\HPCHEM\1\METHODS\OD-02-20.M  
Last changed : 7/30/2014 7:02:19 PM by MK  
                  (modified after loading)  
=====

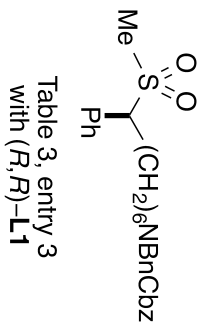


=====  
Area Percent Report  
=====

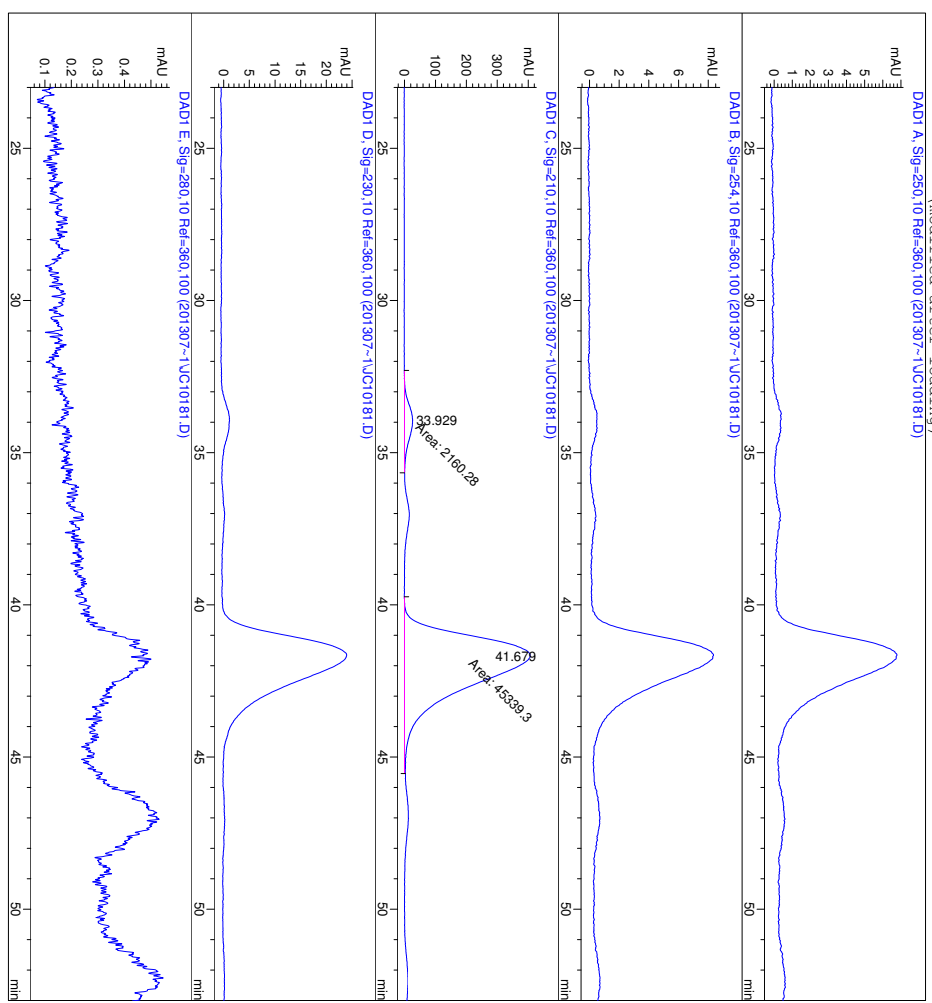
Sorted By	Signal
Multiplier	1.0000
Dilution	1.0000
Use Multiplier & Dilution Factor with ISTDs	

Signal	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	31.460	1.3866	3.35799e4	403.62396	94.3500
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	39.967	1.8199	2010.86841	18.41513	5.6500
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	31.460	1.3866	3.35799e4	403.62396	94.3500
Signal 4: DAD1 D, Sig=230,10 Ref=360,100	31.460	1.3866	3.35799e4	403.62396	94.3500
Signal 5: DAD1 E, Sig=280,10 Ref=360,100	31.460	1.3866	3.35799e4	403.62396	94.3500

Totals : 3.55907e4 422.03910  
Results obtained with enhanced integrator!  
Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
Signal 5: DAD1 E, Sig=280,10 Ref=360,100  
=====



=====  
Injection Date : 7/20/2013 7:21:29 AM      Seq. Line : 30  
Sample Name : JC10181                            Location : Vial 10  
Acq. Operator : CE                                Inj : 1  
Acq. Instrument : Instrument 1                   Inj Volume : 15 µl  
Different Inj Volume from Sequence !  
Accr. Method : C:\HPCHEM\1\METHODS\OD-20-60.M  
Last changed : 6/28/2013 4:31:36 PM by CE  
Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 8/1/2014 11:39:47 PM by MK  
(modified after loading)



=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Signal 2: DADI B, Sig=254,10 Ref=360,100

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.929	MF	1.3461	2160.27637	26.74717	4.5480
2	41.679	MF	1.8592	4.53393e4	406.43207	95.4520

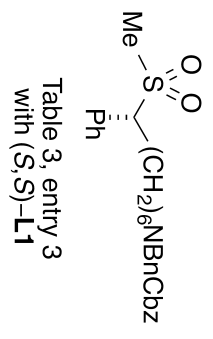
Totals : 4.74996e4 433.17924

Results obtained with enhanced integrator!

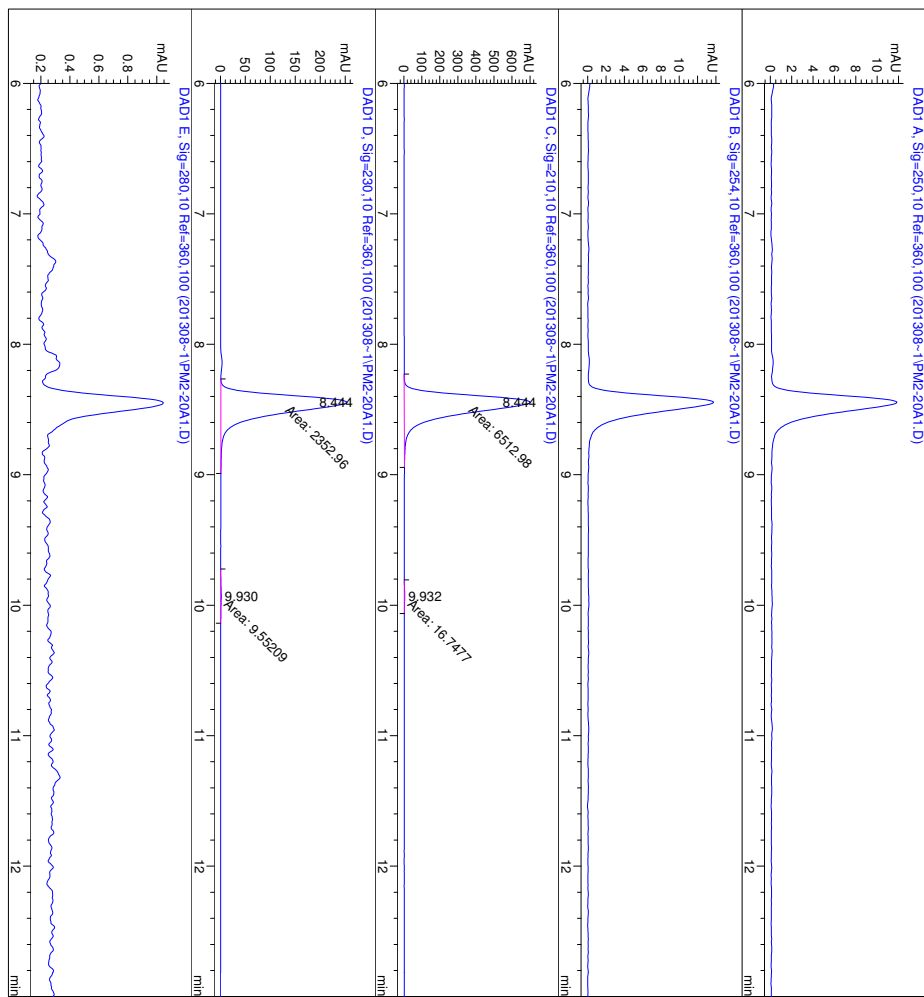
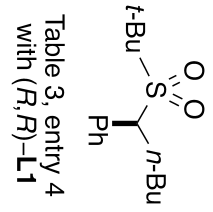
Signal 4: DADI D, Sig=230,10 Ref=360,100

Signal 5: DADI E, Sig=280,10 Ref=360,100

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\*\*\* End of Report \*\*\*  
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Injection Date : 8/2/2013 10:41:10 AM  
 Sample Name : PM2-20A  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 3/19/2012 12:43:39 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\IB-01-20.M  
 Last changed : 7/30/2014 7:04:50 PM by MK  
 (modified after loading)



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1	8.444	FM	0.1553	6512.97803	698.96423	99.7435
Signal 2	9.932	MM	0.1343	16.74774	2.07831	0.2565

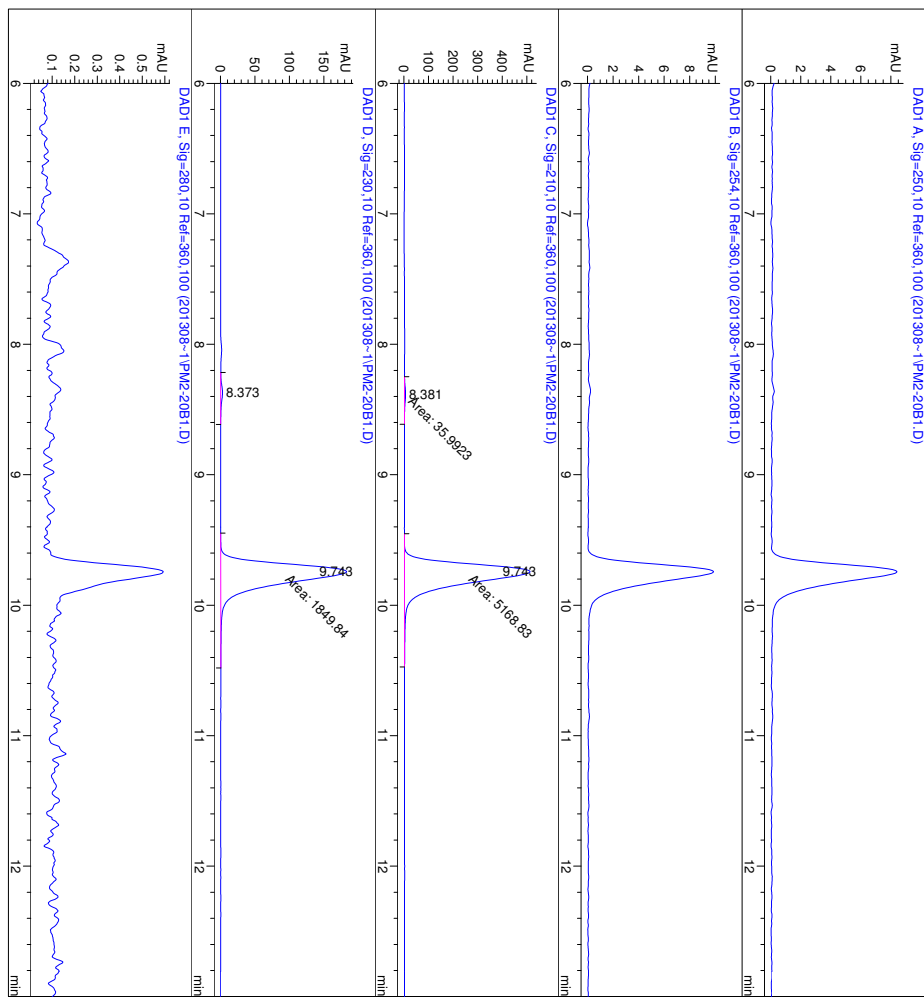
Totals : 6529.72577 701.04255  
 Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.444	FM	0.1553	2352.96094	252.45752	99.5957
2	9.930	MM	0.1630	9.55209	9.76556e-1	0.4043

Totals : 2362.51303 253.43408  
 Results obtained with enhanced integrator!  
 Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

Injection Date : 8/2/2013 11:02:26 AM  
 Sample Name : PM2-20B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 15 µl  
 Inj Volume : 3 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\IB-01-20.M  
 Last changed : 3/19/2012 12:43:39 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:41:35 PM by MK  
 (modified after loading)



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Signal 2: DADI B, Sig=254,10 Ref=360,100

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.381	MM	0.1398	35.99226	4.28965	0.6915
2	9.743	MM	0.1683	5168.82764	511.87228	99.3085

Totals : 5204.81990 516.16193

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.373	VB	0.1312	22.56680	2.60208	1.2052
2	9.743	MM	0.1686	1849.83777	182.89543	98.7948

Totals : 1872.40457 185.49751

Results obtained with enhanced integrator!

Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

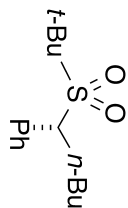
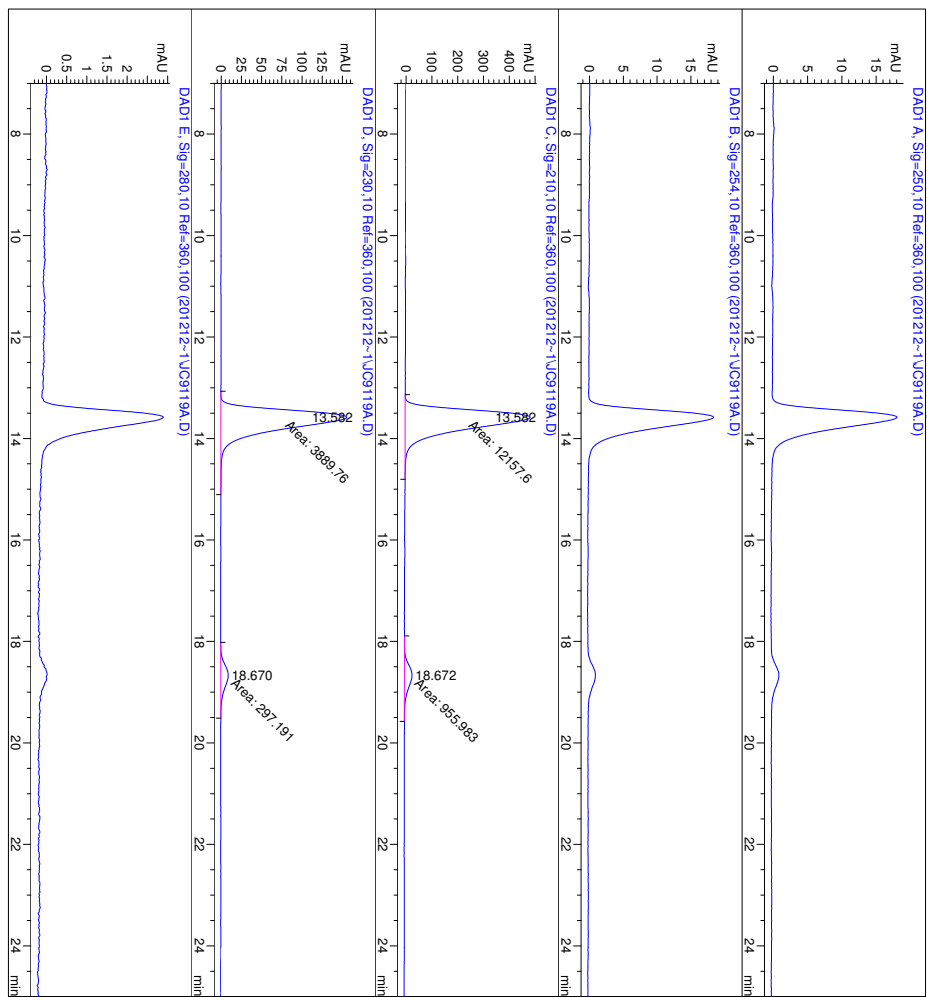
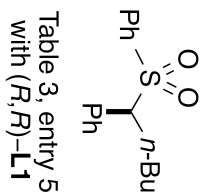


Table 3, entry 4 with (S,S)-L1

Injection Date : 12/14/2012 5:34:16 PM  
 Sample Name : JC9119A  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 3 µl  
 Location : Vial 22  
 Inj : 1  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-01-40.M  
 Last changed : 8/17/2010 4:39:48 PM by JTM  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 7:15:04 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs



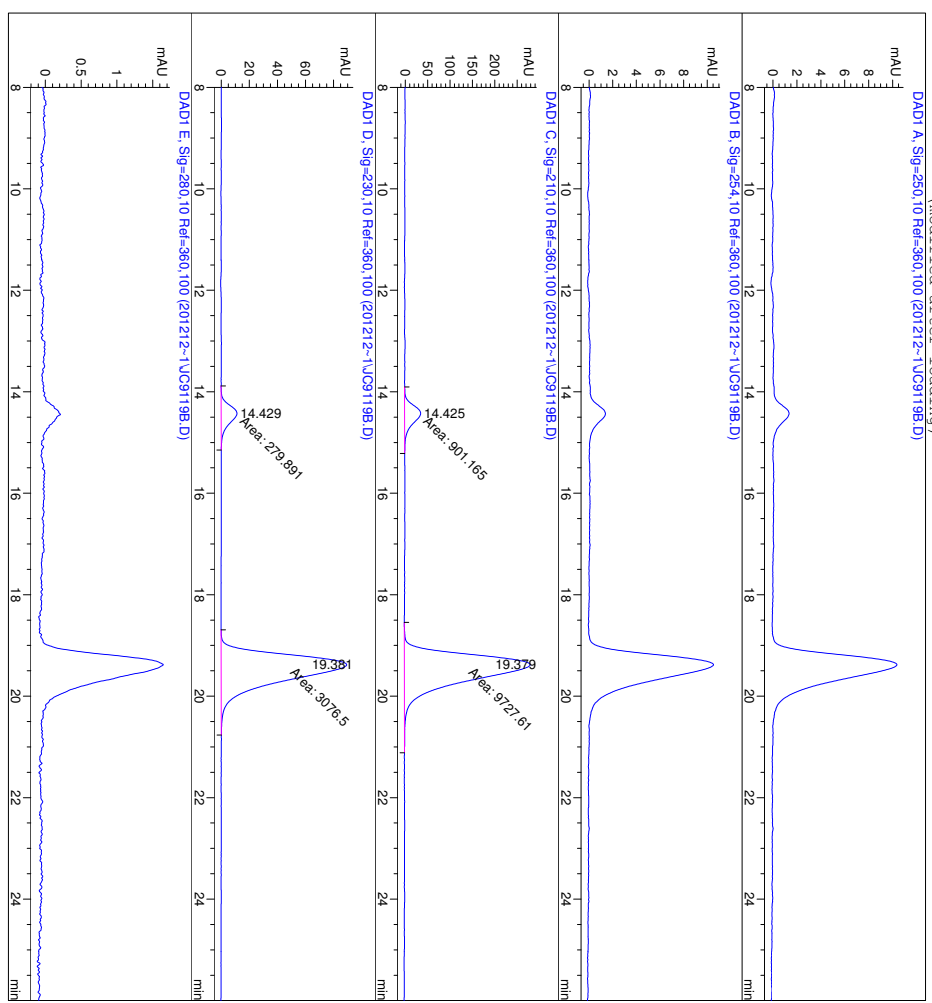
Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	13.582	MM	0.4179	12157.6	484.81223	92.7100
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	18.672	MM	0.5410	955.98328	29.44996	7.2900
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	13.582	MM	0.4179	3689.76	155.62090	92.9020
Signal 4: DAD1 D, Sig=230,10 Ref=360,100	18.670	MM	0.5358	297.19092	9.24424	7.0980

Totals : 1.31136e4 514.26218  
 Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100  
 Results obtained with enhanced integrator!  
 Totals : 4186.94995 164.86513

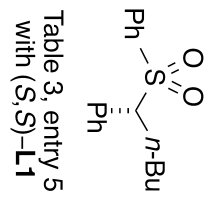
\*\*\* End of Report \*\*\*



=====  
 Injection Date : 12/14/2012 6:15:28 PM      Seq. Line : 5  
 Sample Name : JC9119B                            Location : Vial 23  
 Acq. Operator : CE                                Inj : 1  
 Acq. Instrument : Instrument 1                    Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1            Actual Inj Volume : 3 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-01-40.M  
 Last changed : 8/17/2010 4:39:48 PM by JTM  
 Analysis Method : C:\HPCHEM\1\METHODS\AD003-40.M  
 Last changed : 8/2/2014 10:20:42 PM by MK  
 (modified after loading)  
 =====



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs



Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.425	MM	0.4183	901.16510	35.90579	8.4785
2	19.379	MM	0.5770	9727.60840	280.98239	91.5215

Totals : 1.06288e4 316.88818

Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.429	MM	0.4146	279.89063	11.25042	8.3390
2	19.381	MM	0.5735	3076.50317	89.40532	91.6610

Totals : 3356.39380 100.65574

Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.429	MM	0.4146	279.89063	11.25042	8.3390
2	19.381	MM	0.5735	3076.50317	89.40532	91.6610

Totals : 3356.39380 100.65574

\*\*\* End of Report \*\*\*

Injection Date : 2/16/2013 5:08:58 PM  
 Sample Name : JC9225  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Last changed : 2/16/2013 4:45:43 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
 Last changed : 7/30/2014 7:16:00 PM by MK  
 Last changed : 7/30/2014 7:16:00 PM by MK  
 (modified after loading)

Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.120	MM	0.2662	1.62037e4	1014.59381	97.9659
2	10.117	MM	0.2798	336.43698	20.03921	2.0341

Totals : 1.65402e4 1034.63302

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.119	MM	0.2655	1.16168e4	729.36182	97.8639
2	10.121	MM	0.2835	253.56413	14.90512	2.1361

Totals : 1.18703e4 744.26694

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.119	MM	0.2655	1.16168e4	729.36182	97.8639
2	10.121	MM	0.2835	253.56413	14.90512	2.1361

Totals : 1.18703e4 744.26694

Results obtained with enhanced integrator!

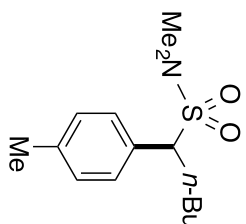
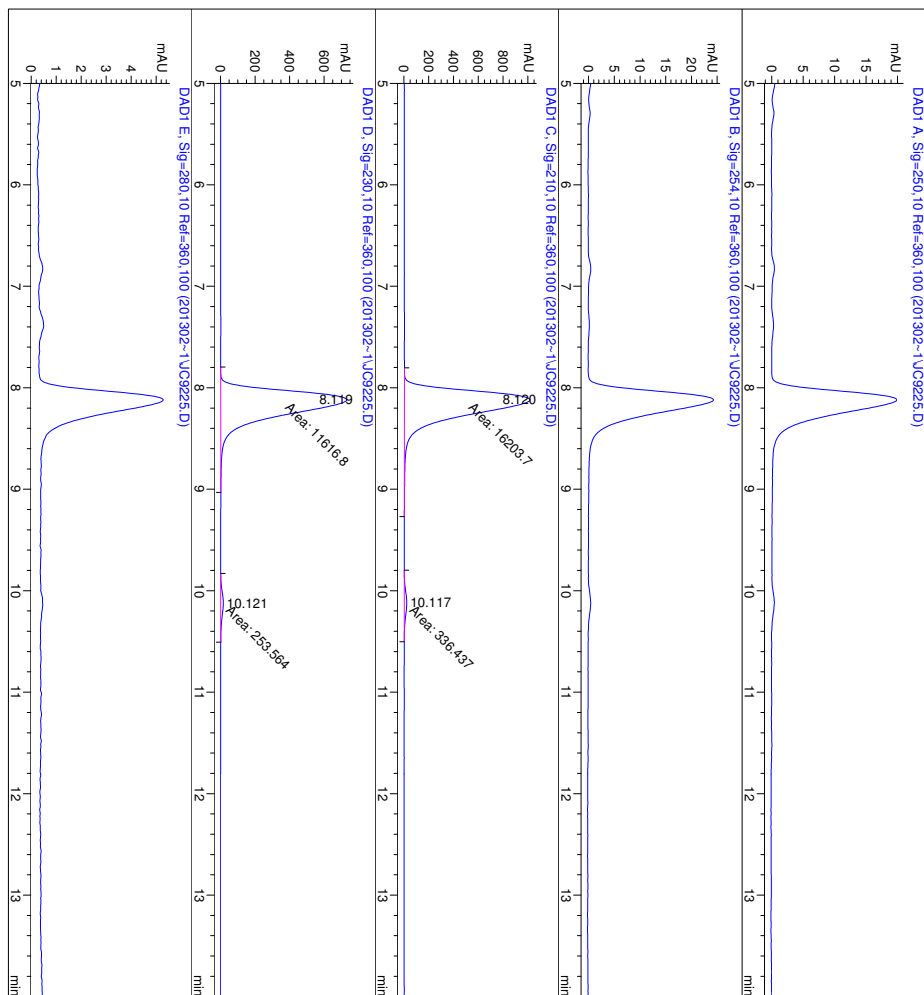
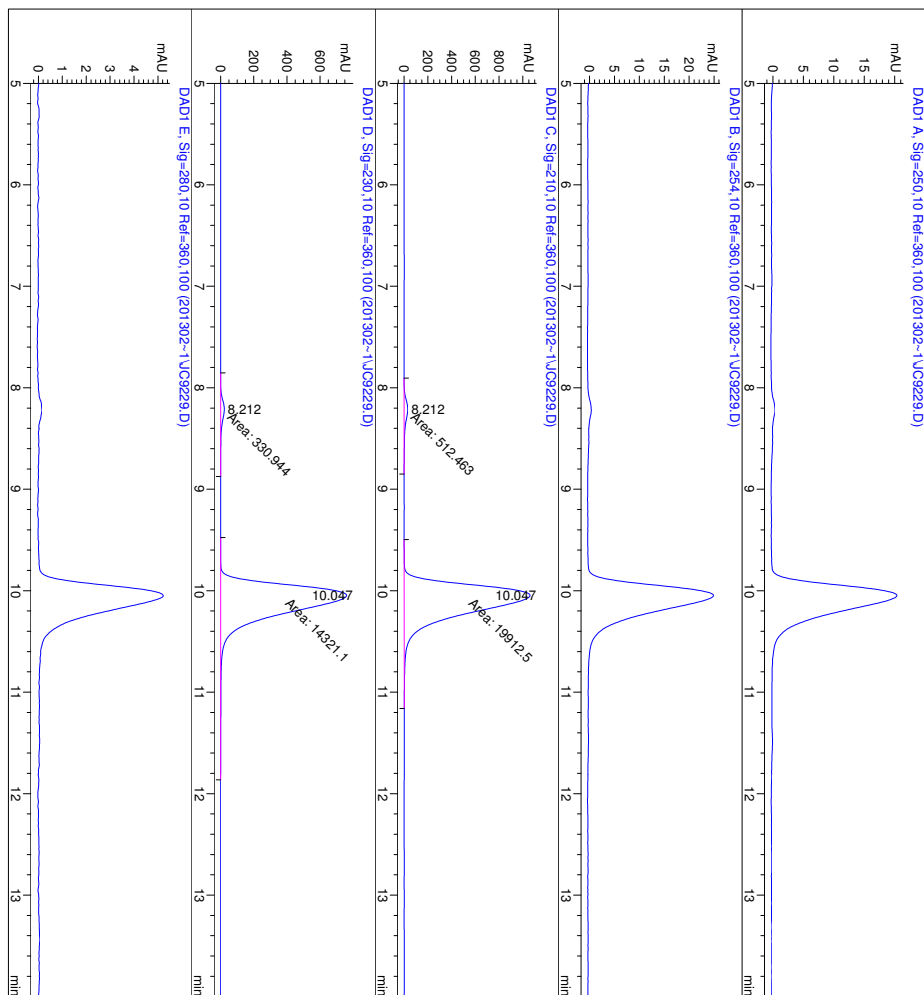


Table 4, entry 1  
 with (R,R)-L1

Injection Date : 2/16/2013 5:40:14 PM  
 Sample Name : JC9229  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
 Last changed : 2/16/2013 4:45:43 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:49:11 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	1	8.212	MM	0.2747	512.46289	31.09460	2.5090
Signal 2: DADI B, Sig=254,10 Ref=360,100	2	10.047	MM	0.3127	1.99125e4	1061.17505	97.4910
Signal 3: DADI C, Sig=210,10 Ref=360,100	1	8.212	MM	0.2747	512.46289	31.09460	2.5090
Signal 4: DADI D, Sig=230,10 Ref=360,100	2	10.047	MM	0.3127	1.99125e4	1061.17505	97.4910

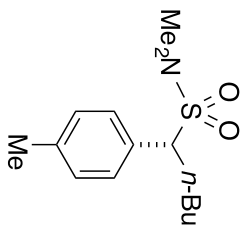
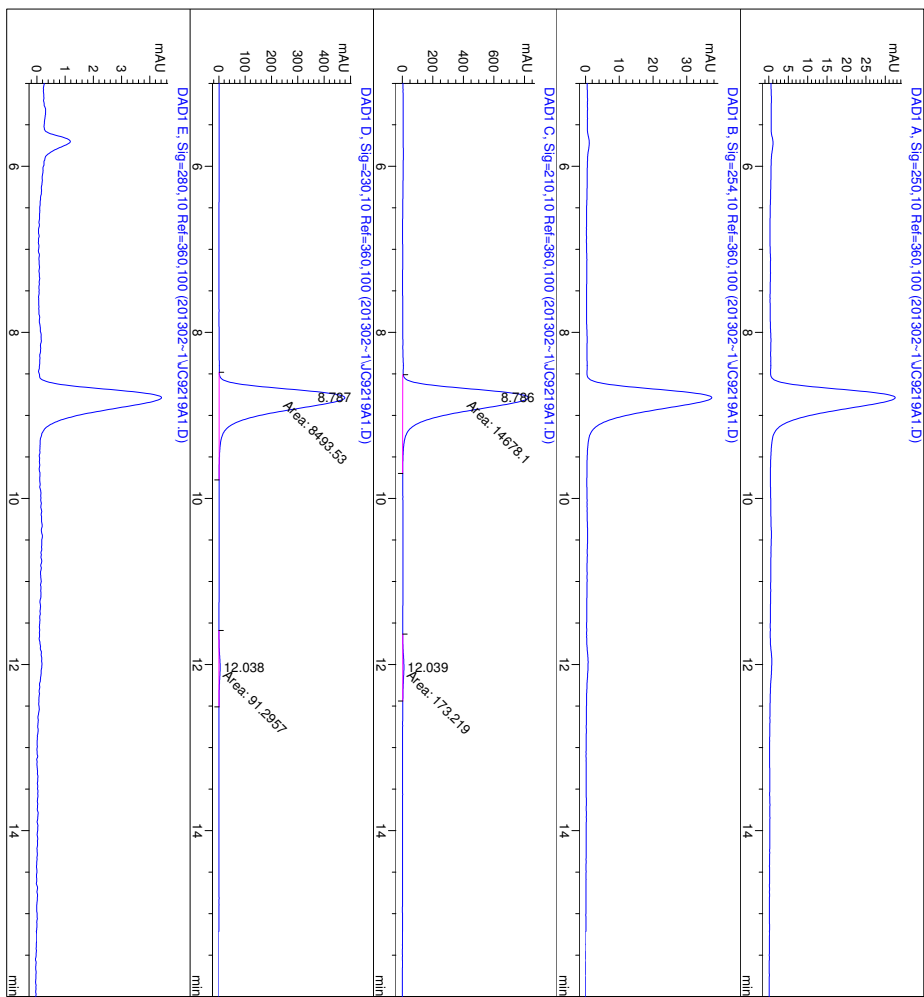


Table 4, entry 1  
 with (S,S)-L1

Injection Date : 2/11/2013 7:19:54 PM  
 Sample Name : JC9219A  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-03-40.M  
 Last changed : 2/11/2013 7:37:52 PM by CE  
 (modified after loading)  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 7:18:31 PM by MK  
 (modified after loading)

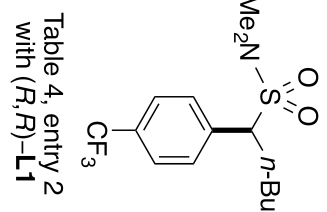


Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

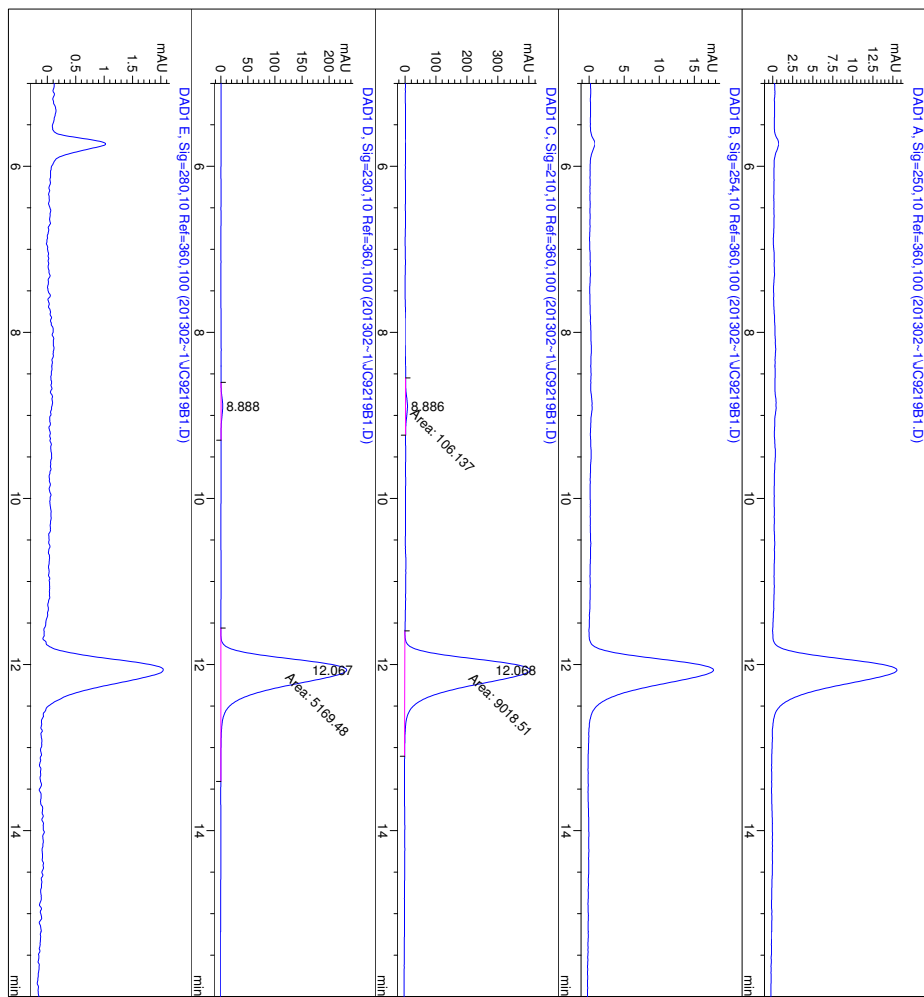
Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	8.786	FM	0.2972	1.46781e4	823.10712	98.8336
Signal 2: DADI B, Sig=254,10 Ref=360,100	12.039	MM	0.3704	173.21939	7.79425	1.1664
Signal 3: DADI C, Sig=210,10 Ref=360,100	12.038	MM	0.3593	91.29572	4.23473	1.0635

Totals : 1.48513e4 830.90137  
 Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Results obtained with enhanced integrator!  
 Signal 5: DADI E, Sig=280,10 Ref=360,100  
 Results obtained with enhanced integrator!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.787	FM	0.2959	8493.53320	478.45062	98.9365
2	12.038	MM	0.3593	91.29572	4.23473	1.0635



Injection Date : 2/11/2013 7:51:20 PM  
 Sample Name : JC9219B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\NOD-03-30.M  
 Last changed : 12/31/2012 2:58:25 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:50:49 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	8.886	PP	0.2387	46.58376	2.97409	0.1831
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	12.068	MM	0.3708	5169.47754	232.32732	98.1069
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	12.067	MM	0.3709	9018.51172	405.22449	98.8368
Totals :				9124.64835	411.41491	

Results obtained with enhanced integrator!

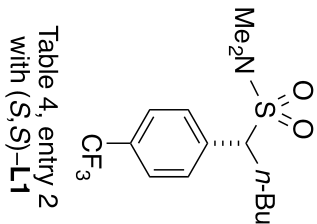
Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.888	PP	0.2387	46.58376	2.97409	0.1831
2	12.067	MM	0.3708	5169.47754	232.32732	98.1069
Totals :				5216.06130	235.30141	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*



Injection Date : 8/2/2014 11:04:39 AM  
 Sample Name : JC12077A  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 5 µl  
 Last changed : 12/28/2013 3:19:26 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\A0005-40.M  
 Last changed : 8/2/2014 12:57:50 PM by MK  
 (modified after loading)

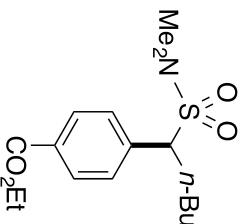
Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.670	MM	0.2815	1.39820e4	827.70404	98.6305
2	11.410	MM	0.3566	194.14923	9.07509	1.3695

Totals : 1.41762e4 836.77913

Table 4, entry 3  
 with (R,R)-L1



Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.670	MM	0.2817	8988.77344	531.88464	98.6412
2	11.407	MM	0.3539	123.82027	5.83146	1.3588

Totals : 9112.59371 537.71610

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.669	MM	0.2922	7836.80811	447.05707	98.6123
2	11.389	MM	0.3057	110.27897	6.01225	1.3877

Totals : 7947.08707 453.06932

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.671	MM	0.2825	1.62668e4	959.65015	98.6183
2	11.422	MM	0.3601	227.91589	10.54932	1.3817

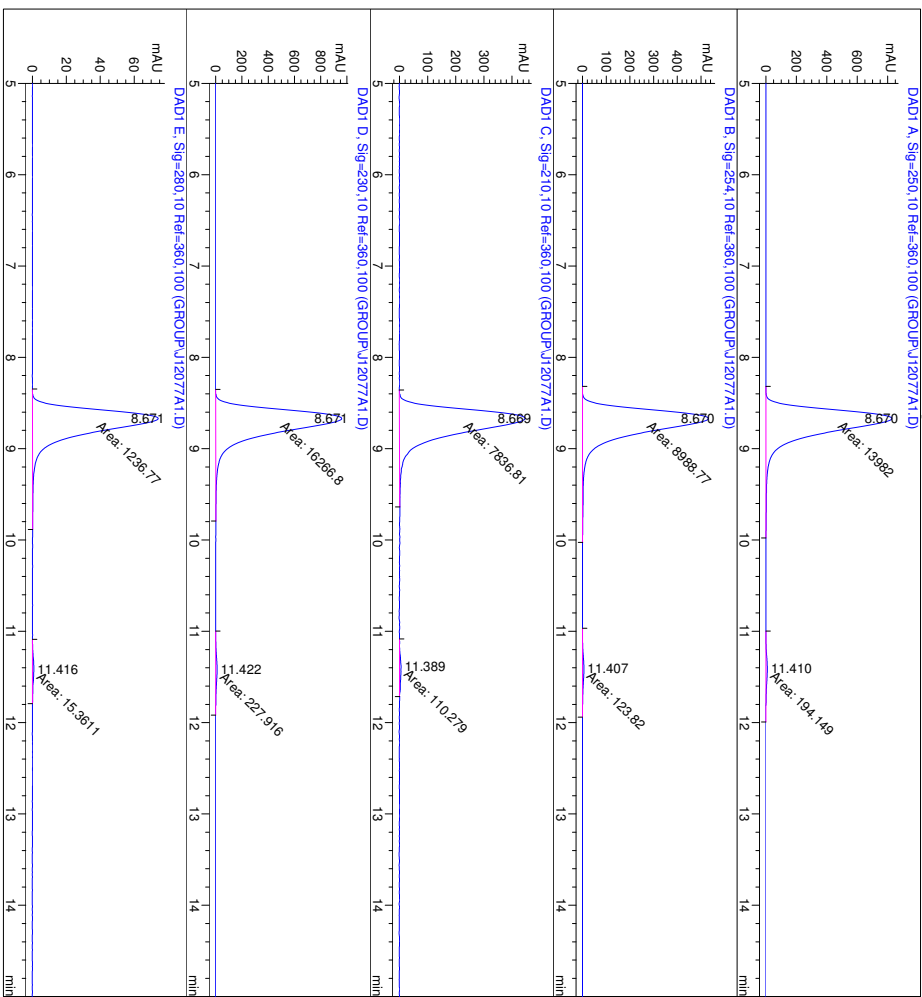
Totals : 1.64948e4 970.19947

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

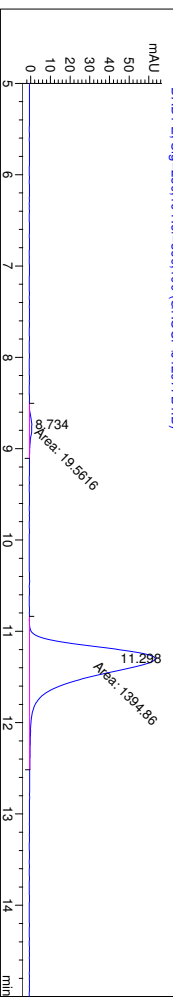
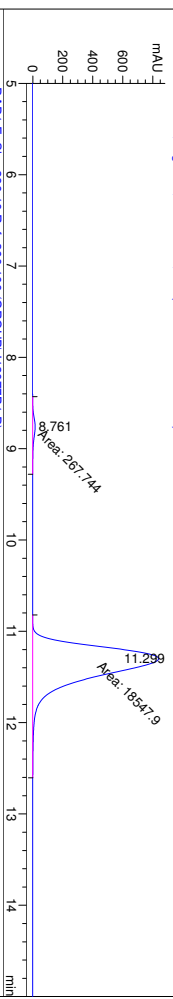
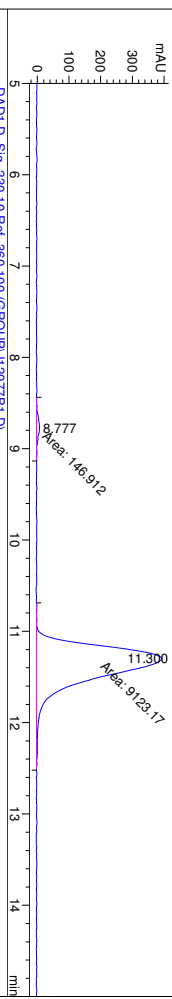
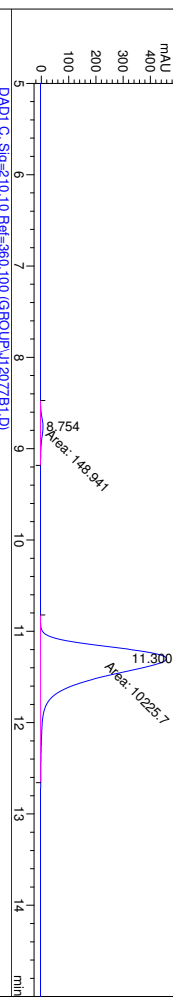
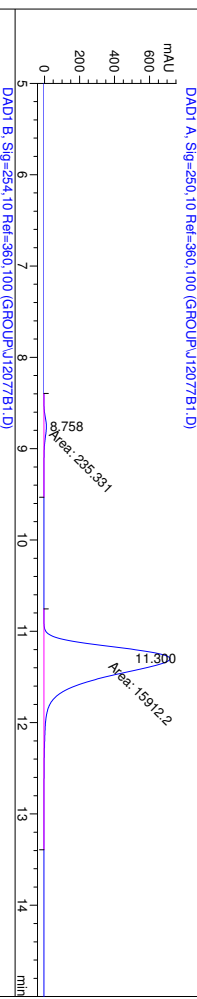
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.671	MM	0.2779	1236.76501	74.16629	98.7732
2	11.416	MM	0.3130	15.36111	8.18057e-1	1.2268

Totals : 1252.12613 74.98435

Results obtained with enhanced integrator!  
 \*\*\* End of Report \*\*\*



Injection Date : 8/2/2014 11:46:00 AM  
 Sample Name : JCI2077B  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 5 µl  
 Last changed : C:\HPCHEM\1\METHODS\NOD-05-40.M  
 Analysis Method : C:\HPCHEM\1\METHODS\NOD05-40.M  
 Last changed : 8/2/2014 12:57:50 PM by MK  
 (modified after loading)

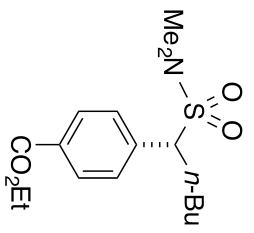


Area Percent Report

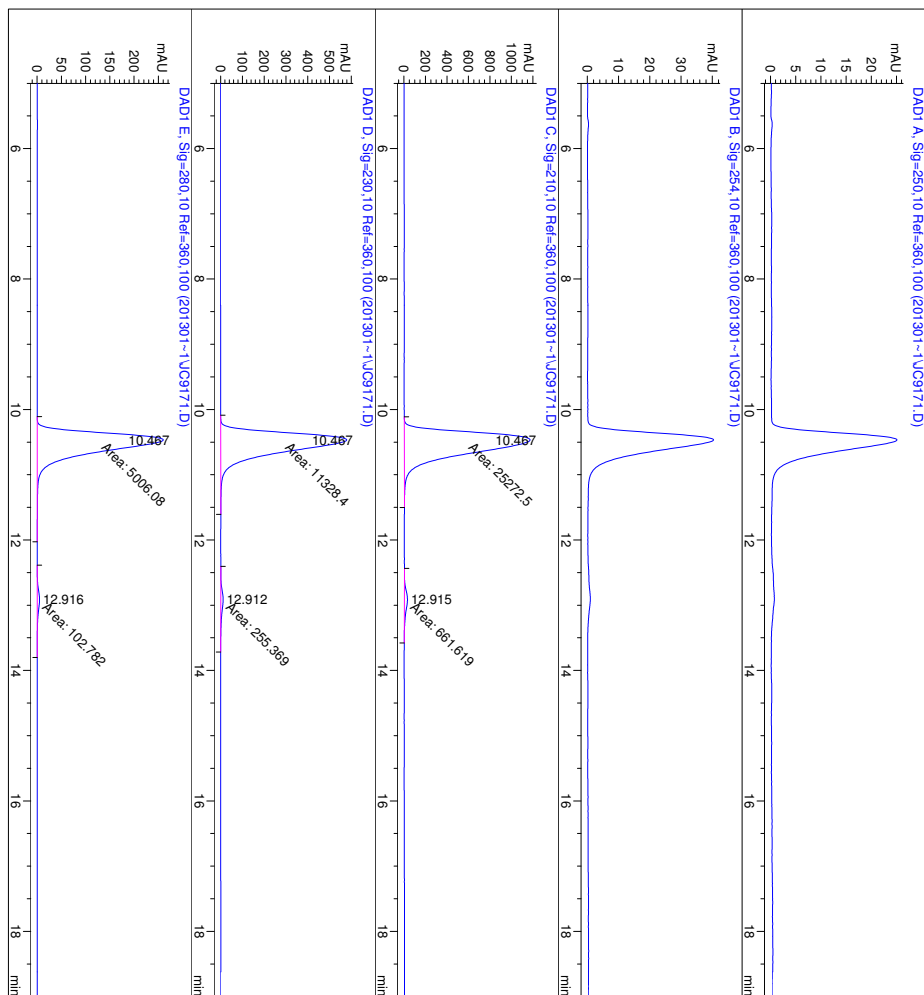
Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	Peak RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250.10 Ref=360.100	1	8.758	235.33102	14.16449	1.4574
	2	11.300	1.59122e4	719.25024	98.5426
Totals :			1.61475e4	733.41473	
Signal 2: DADI B, Sig=254.10 Ref=360.100	1	8.754	148.94130	9.09059	1.4356
	2	11.300	1.02257e4	462.43088	98.5644
Totals :			1.03746e4	471.52147	
Signal 3: DADI C, Sig=210.10 Ref=360.100	1	8.777	146.91231	9.21852	1.5848
	2	11.300	0.38311923	396.85388	98.4152
Totals :			9270.08516	406.07240	
Signal 4: DADI D, Sig=230.10 Ref=360.100	1	8.761	267.74371	16.69801	1.4230
	2	11.299	1.85479e4	840.07916	98.5770
Totals :			1.88156e4	856.77717	
Signal 5: DADI E, Sig=280.10 Ref=360.100	1	8.734	19.56164	1.24219	1.3830
	2	11.298	0.363561394	63.93124	98.6170
Totals :			1414.41723	65.17344	

Table 4, entry 3  
 with (S,S)-L1



Injection Date : 1/24/2013 2:01:50 PM  
 Sample Name : JC9171  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 15 µl  
 Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\NOD-03-30.M  
 Last changed : 12/31/2012 2:58:25 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 10:57:44 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	1	10.467	MM	0.3264	1.13284e4	578.50757	97.7955
	2	12.916	MM	0.3720	255.36906	10.87842	2.2045
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	1	10.467	MM	0.3598	2.52725e4	1170.62231	97.4488
	2	12.916	MM	0.3802	661.61938	29.00374	2.5512
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	1	10.467	MM	0.3209	5006.08350	260.03439	97.9882
	2	12.916	MM	0.3720	102.78178	4.60473	2.0118

Totals : 2.59342e4 1199.62605  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Peak RetTime Type Width Area Height Area %  
 # [min] [min] [mAU\*s] [mAU] %  
 1 10.467 MM 0.3264 1.13284e4 578.50757 97.7955  
 2 12.916 MM 0.3912 255.36906 10.87842 2.2045  
 Totals : 1.15838e4 589.38598  
 Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100  
 Peak RetTime Type Width Area Height Area %  
 # [min] [min] [mAU\*s] [mAU] %  
 1 10.467 MM 0.3209 5006.08350 260.03439 97.9882  
 2 12.916 MM 0.3720 102.78178 4.60473 2.0118  
 Totals : 5108.86527 264.63913  
 Results obtained with enhanced integrator!  
 \*\*\* End of Report \*\*\*

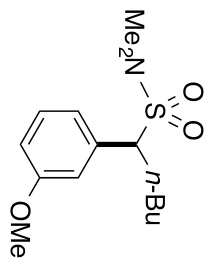
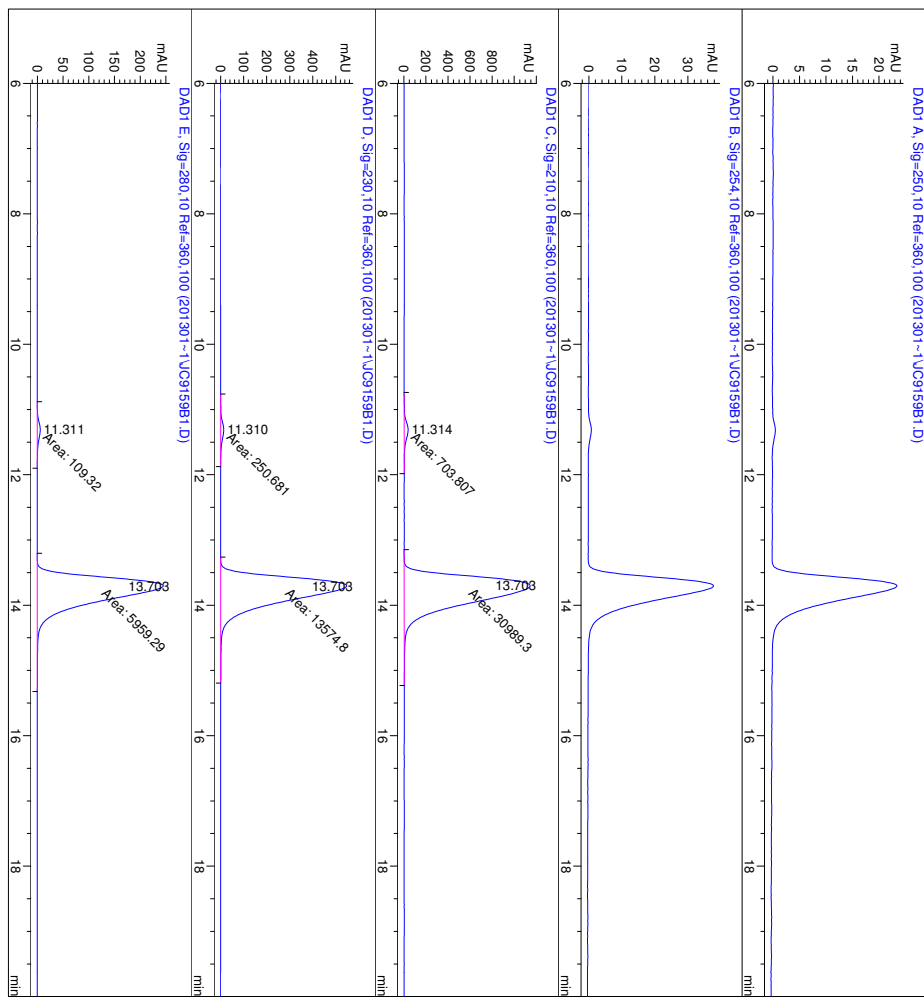


Table 4, entry 4 with (R,R)-L1



Injection Date : 1/17/2013 6:11:02 PM  
 Sample Name : JC9159B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 5 µl  
 Last changed : 12/31/2012 2:58:25 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\A0005-40.M  
 Last changed : 8/1/2014 11:54:28 PM by MK  
 (modified after loading)



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.314	MM	0.3282	703.80688	35.73879	2.2207
2	13.703	MM	0.4525	3.09893e4	1141.28613	97.7793

Totals : 3.16931e4 1177.02492

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.310	MM	0.3180	250.68091	13.13707	1.8132
2	13.703	MM	0.4130	1.35748e4	547.84503	98.1868

Totals : 1.38255e4 560.98210

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.311	MM	0.3191	109.32001	5.70986	1.8014
2	13.703	MM	0.4053	5959.28662	245.05873	98.1986

Totals : 6068.60663 250.76859

Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

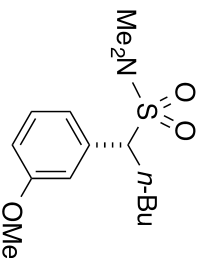


Table 4, entry 4  
 with (S,S)-L1

Injection Date : 8/5/2013 11:54:59 PM  
 Sample Name : JCI0223A  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 5 µl  
 Last changed : 4/7/2011 5:40:42 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\AS-05-40.M  
 Last changed : 7/30/2014 7:21:45 PM by MK  
 (modified after loading)

=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

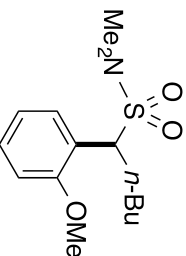
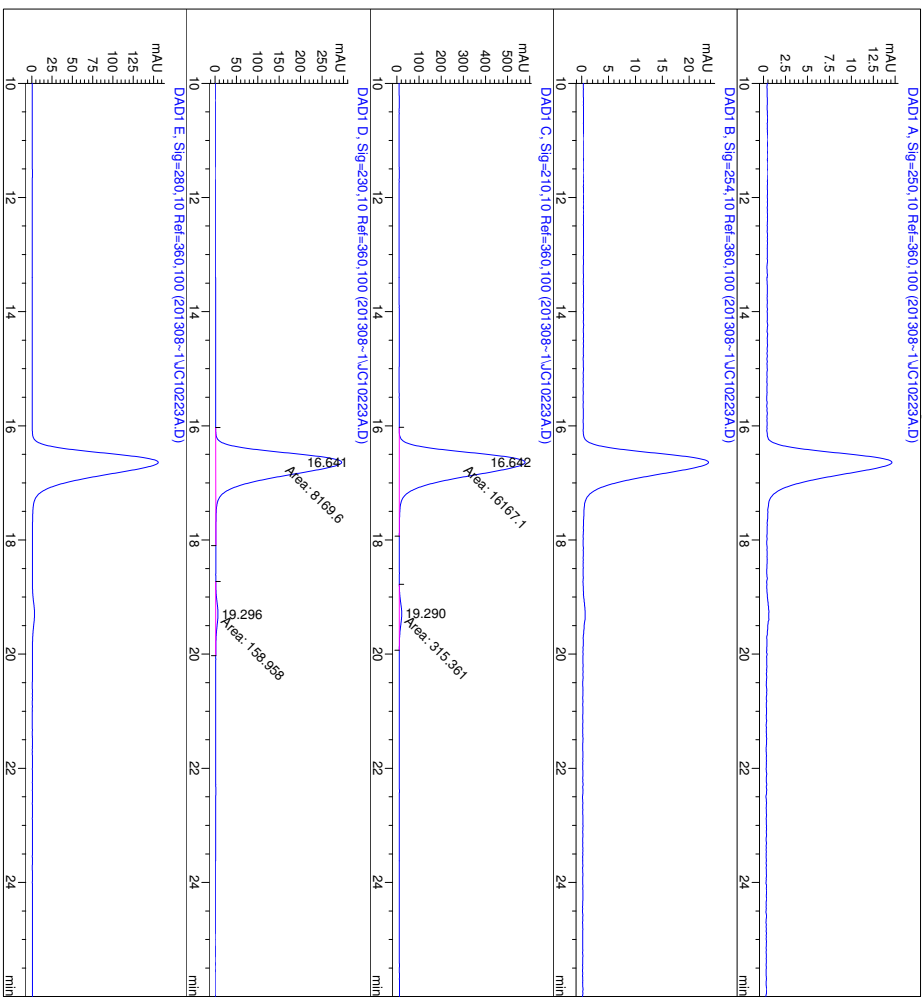


Table 4, entry 5  
 with (R,R)-L1



Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	1	16.642	MM	0.4739	1.61671e4	568.63507	98.0867
	2	19.290	MM	0.4751	315.36053	11.06335	1.9133
Totals : 1.64825e4 579.69842							
Results obtained with enhanced integrator!							
Signal 4: DADI D, Sig=230,10 Ref=360,100							
Signal 3: DADI C, Sig=210,10 Ref=360,100	1	16.641	MM	0.4629	8169.60059	294.14471	98.0914
	2	19.296	MM	0.5049	158.95808	5.24689	1.9086
Totals : 8328.55867 299.39160							
Results obtained with enhanced integrator!							
Signal 5: DADI E, Sig=280,10 Ref=360,100							

\*\*\* End of Report \*\*\*

Injection Date : 8/6/2013 12:36:17 AM  
 Sample Name : JCI0223B  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 4/7/2011 5:40:42 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\AS-05-40.M  
 Last changed : 8/1/2014 11:56:57 PM by MK  
 (modified after loading)

Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.717	MM	0.4488	433.83279	16.11137	2.1630
2	19.053	MM	0.5754	1.96231e4	568.36749	97.8370

Totals : 2.00569e4 584.47886

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.722	MM	0.4358	196.73267	7.52359	1.9765
2	19.050	MM	0.5650	9756.66211	287.81458	98.0235

Totals : 9953.39478 295.33817

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.730	BP	0.3569	92.86021	3.75030	1.8070
2	19.050	BB	0.5188	5045.99463	150.64299	98.1930

Totals : 5138.85484 154.39329

Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

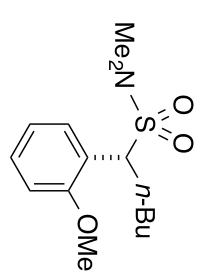
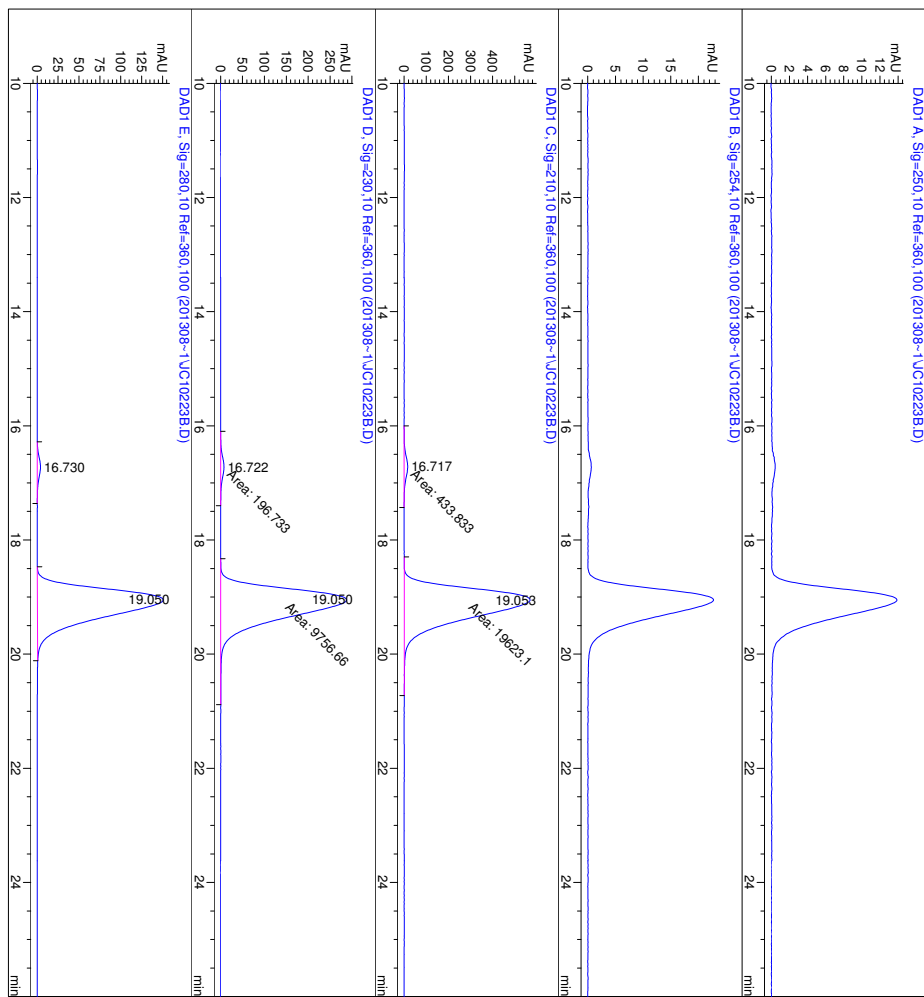
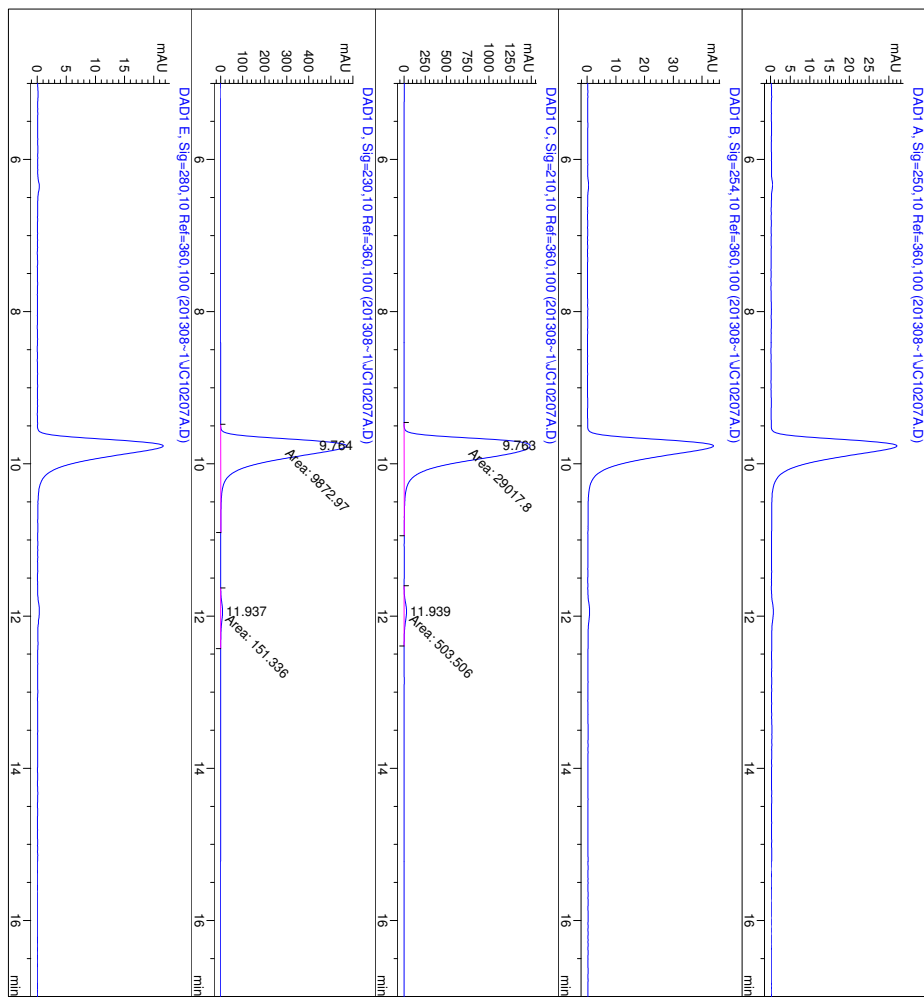


Table 4, entry 5  
with (S,S)-L1



=====  
 Injection Date : 8/9/2013 1:39:02 AM      Seq. Line : 6  
 Sample Name : JC10207A                      Location : Vial 42  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1              Inj Volume : 5 µl  
 Different Inj Volume from Sequence !  
 Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
 Last changed : 2/16/2013 4:45:43 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 11:04:53 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

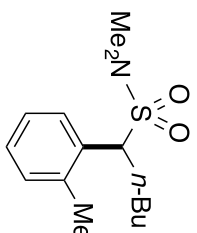
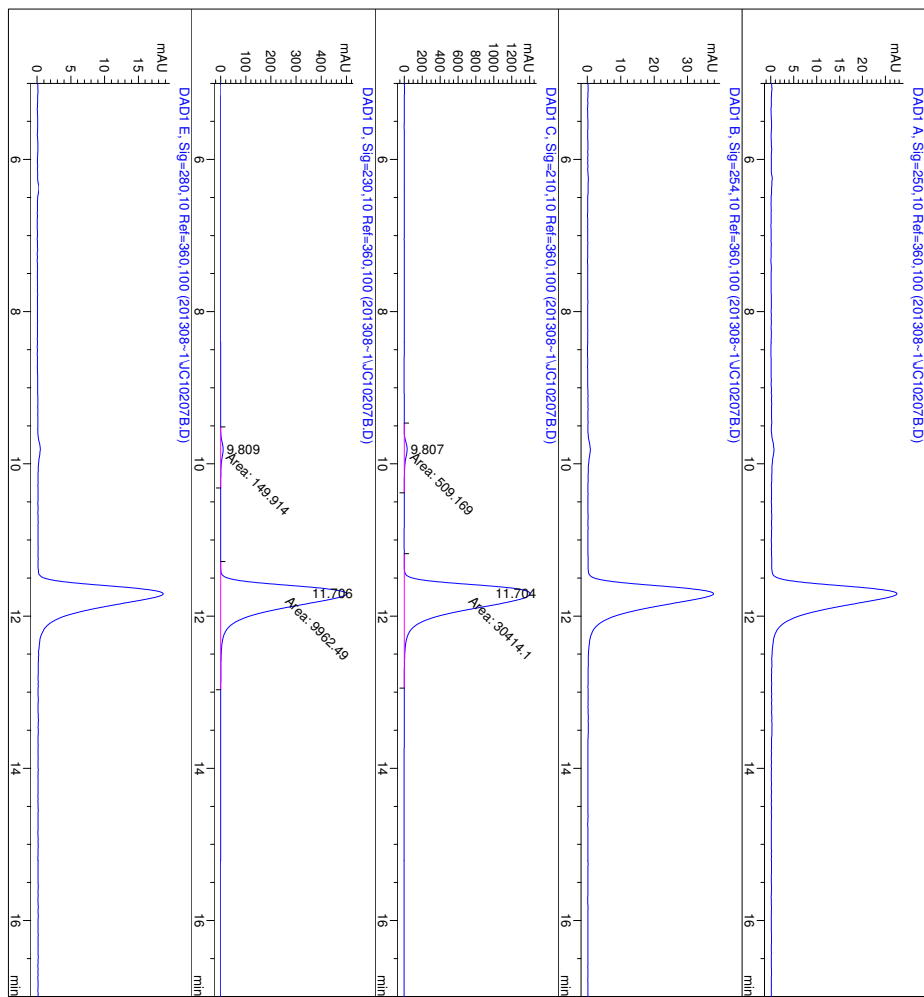


Table 4, entry 6  
 with (R,R)-L1

Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	1	9.763	MM	0.3255	2.90178e4	1485.83618	98.2944
	2	11.939	MM	0.2984	503.50601	28.12491	1.7056
Totals :					2.95213e4	1513.96109	
Results obtained with enhanced integrator!							
Signal 4: DADI D, Sig=230,10 Ref=360,100							
Signal 5: DADI E, Sig=280,10 Ref=360,100	1	9.764	MM	0.2880	9872.96777	571.38434	98.4903
	2	11.937	MM	0.2972	151.33591	8.48584	1.5097
Totals :					1.00243e4	579.87018	
Results obtained with enhanced integrator!							
Signal 5: DADI E, Sig=280,10 Ref=360,100							

\*\*\* End of Report \*\*\*

=====  
 Injection Date : 8/9/2013 2:10:20 AM      Seq. Line : 7  
 Sample Name : JCI10207B                      Location : Vial 43  
 Acq. Operator : MK                              Inj : 1  
 Acq. Instrument : Instrument 1                Inj Volume : 15 µl  
 Different Inj Volume from Sequence !        Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OD-02-30.M  
 Last changed : 2/16/2013 4:45:43 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/1/2014 11:59:09 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100  
 Signal 2: DADI B, Sig=254,10 Ref=360,100  
 Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.807	MM	0.2614	509.16885	32.46480	1.6466
2	11.704	MM	0.3607	3.04141e4	1405.28198	98.3534

Totals : 3.09233e4 1437.74678  
 Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Signal 5: DADI E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.809	MM	0.2538	149.91431	9.84457	1.4825
2	11.706	MM	0.3315	9962.49023	500.87515	98.5175

Totals : 1.01124e4 510.71973  
 Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

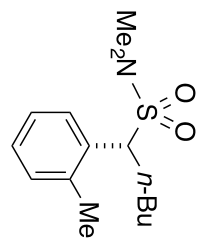
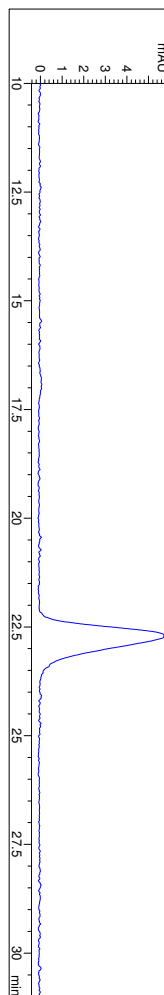
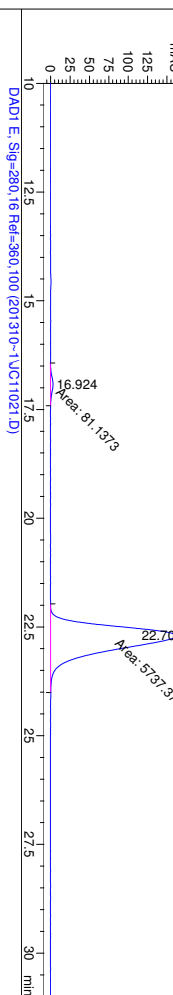
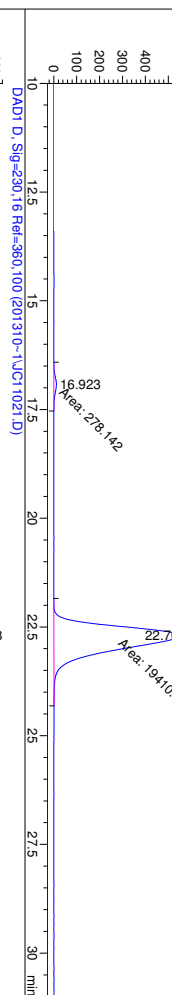
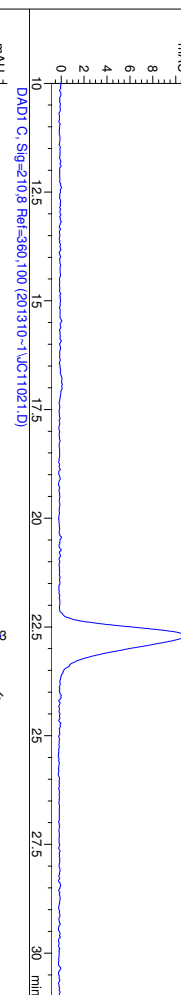
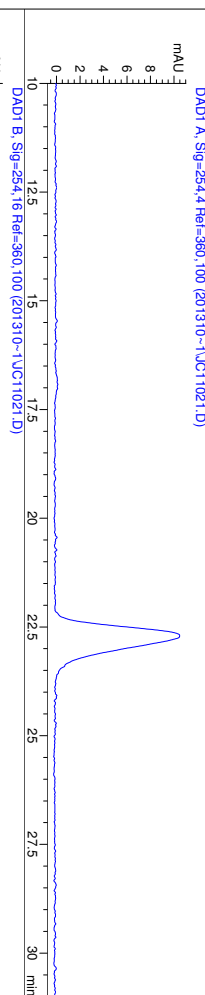


Table 4: entry 6  
 with (S,S)-L1

```

Injection Date : 10/16/2013 10:17:19 PM      Seq. Line : 3
Sample Name    : JC11021                    Location  : Vial 12
Acq. Operator  : TMB                        Inj       : 1
Acq. Instrument : Instrument 1              Inj Volume: 5 µl
Acq. Method    : C:\HPCHEM\1\METHODS\IC-1540.M
Last changed   : 5/17/2012 7:45:15 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-0440.M
Last changed    : 7/30/2014 7:44:57 PM by TMB
                (modified after loading)
    
```



Area Percent Report

Sorted By	Signal
Multiplier	1.0000
Dilution	1.0000
Use Multiplier & Dilution Factor with ISTDs	

Signal 1: DADI A, Sig=254,4 Ref=360,100

Signal 2: DADI B, Sig=254,16 Ref=360,100

Signal 3: DADI C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.923	MM	0.4228	278.14233	10.96450	1.4127
2	22.703	MM	0.5880	1.94105e4	550.20209	98.5873

Totals : 1.96886e4 561.16659

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.924	MM	0.4149	81.13730	3.25970	1.3945
2	22.703	MM	0.5891	5737.36523	162.31212	98.6055

Totals : 5818.50253 165.57181

Results obtained with enhanced integrator!

Signal 5: DADI E, Sig=280,16 Ref=360,100

\*\*\* End of Report \*\*\*

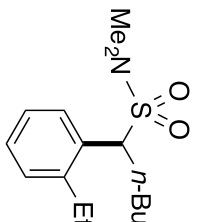
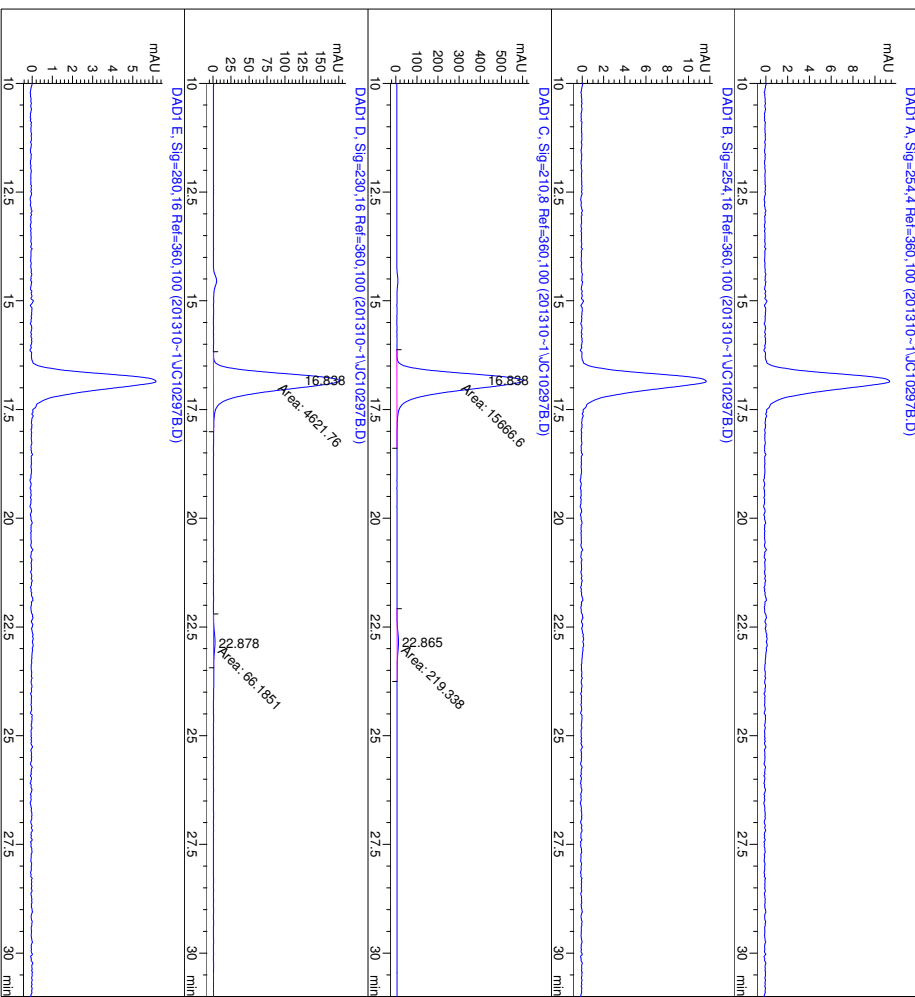


Table 4, entry 7  
with (R,R)-L1

Injection Date : 10/16/2013 9:36:03 PM  
 Sample Name : JCI0297B  
 Acq. Operator : TMB  
 Acq. Instrument : Instrument 1  
 Acq. Method : C:\HPCHEM\1\METHODS\IC-1540.M  
 Last changed : 5/17/2012 7:45:15 PM by JTM  
 Analysis Method : C:\HPCHEM\1\METHODS\ODH-0440.M  
 Last changed : 8/2/2014 12:24:05 AM by TMB



=====  
 Area Percent Report  
 =====

Sorted By :  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.838	MM	0.4381	1.56666e4	596.02325	98.6193
2	22.865	MM	0.5524	219.33803	6.61832	1.3807

Totals : 1.58860e4 602.64157

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.838	MM	0.4396	4621.76465	175.22726	98.5682
2	22.878	MM	0.5719	66.18513	1.92889	1.4118

Totals : 4687.94978 177.15616

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

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 \*\*\* End of Report \*\*\*  
 =====

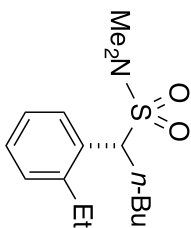
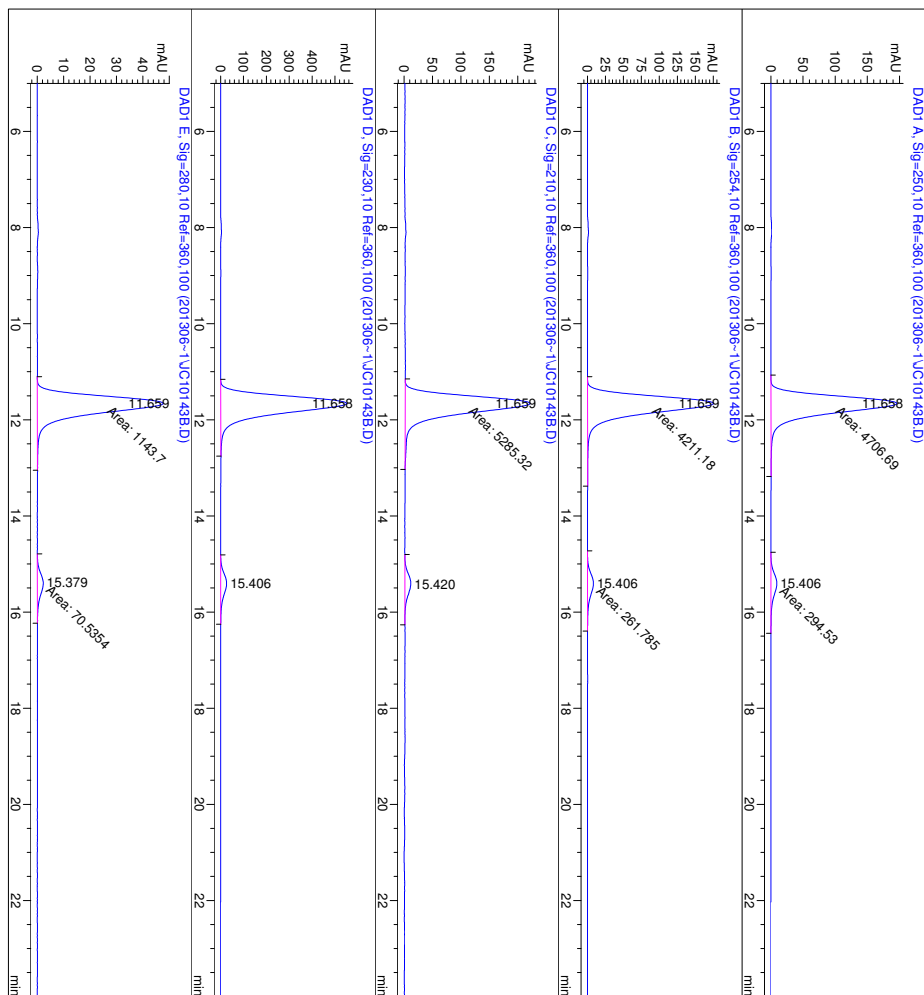


Table 4, entry 7  
 with (S,S)-L1

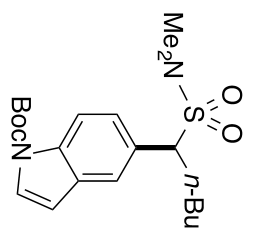
Injection Date : 6/15/2013 12:06:30 AM  
 Sample Name : JC10143B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 15 µl  
 Last changed : 2/22/2013 10:06:44 AM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 7:30:18 PM by MK  
 (modified after loading)



Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.658	MM	0.4004	4706.68896	195.89636	94.1108
2	15.406	MM	0.5371	294.53040	9.13878	5.8892
Totals : 5001.21936 205.03514						

Table 4, entry 8 with (R,R)-L1

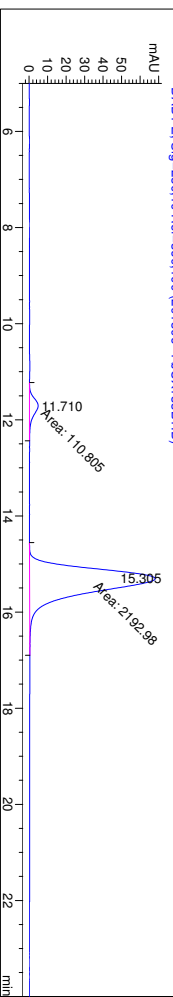
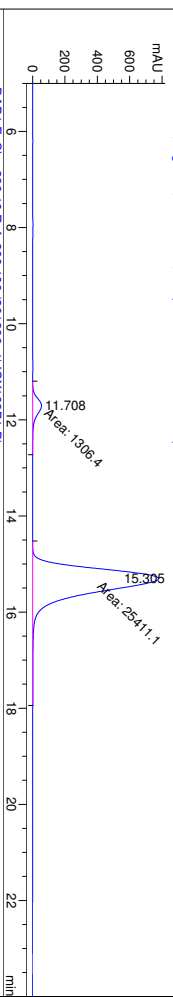
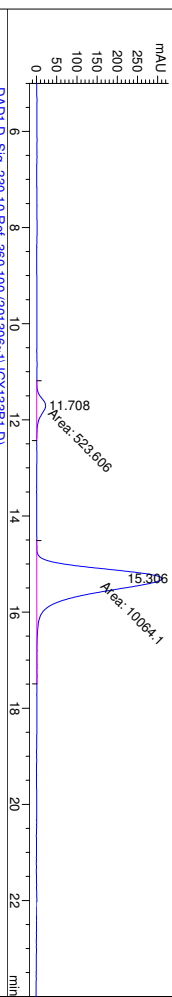
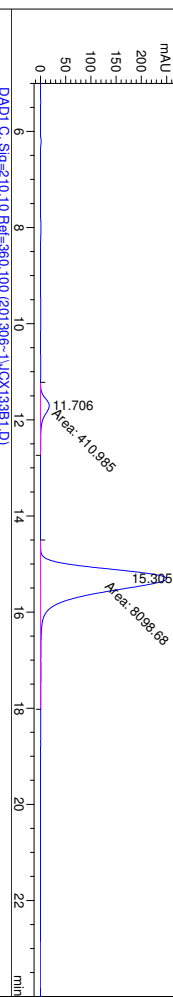
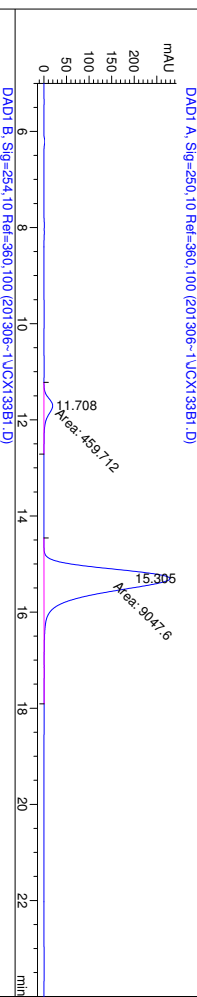


Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	11.658	MM	0.4004	4706.68896	195.89636	94.1108
	15.406	MM	0.5371	294.53040	9.13878	5.8892
Totals : 5001.21936 205.03514						
Signal 2: DADI B, Sig=254,10 Ref=360,100	11.659	MM	0.4006	4211.17676	175.21336	94.1474
	15.406	MM	0.5364	261.78525	8.13331	5.8526
Totals : 4472.96201 183.34668						
Signal 3: DADI C, Sig=210,10 Ref=360,100	11.659	MM	0.4013	5285.31982	219.49617	94.0588
	15.420	PV	0.3792	333.84775	10.60698	5.9412
Totals : 5619.16757 230.10315						
Signal 4: DADI D, Sig=230,10 Ref=360,100	11.658	BB	0.3701	1.32119e4	550.22070	94.1265
	15.406	BB	0.4979	824.42981	25.86081	5.8735
Totals : 1.40364e4 576.08152						
Signal 5: DADI E, Sig=280,10 Ref=360,100	11.659	MM	0.4000	1143.70020	47.65256	94.1910
	15.379	MM	0.5311	70.53535	2.21351	5.8090
Totals : 1214.23555 49.86587						

Results obtained with enhanced integrator!  
 Results obtained with enhanced integrator!  
 Results obtained with enhanced integrator!  
 \*\*\* End of Report \*\*\*



=====  
Injection Date : 6/14/2013 11:25:16 PM      Seq. Line : 3  
Sample Name : JCI10133B                      Location : Vial 31  
Acq. Operator : CE                              Inj : 1  
Acq. Instrument : Instrument 1                Inj Volume : 15 µl  
Dilution : 1.0000  
Different Inj Volume from Sequence !        Actual Inj Volume : 2 µl  
Acq. Method : C:\HPCHEM\1\METHODS\VD-02-40.M  
Last changed : 2/22/2013 10:06:44 AM by CE  
Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 8/2/2014 12:07:02 AM by MK  
(modified after loading)  
=====



=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.708	0.4004	459.71191	19.13779	4.8354
2	15.305	0.5404	9047.59863	279.01901	95.1646

Totals : 9507.31055 298.15680

Signal 2: DADI B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.706	0.4003	410.98477	17.11033	4.8296
2	15.305	0.5407	8098.67578	249.64102	95.1704

Totals : 8509.66055 266.75135

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.708	0.4001	523.60632	21.81178	4.9454
2	15.306	0.5401	1.00641e4	310.58426	95.0546

Totals : 1.05877e4 332.39604

Signal 4: DADI D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.708	0.4006	1306.40112	54.35100	4.8897
2	15.305	0.5438	2.54111e4	778.85779	95.1103

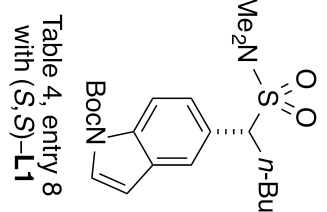
Totals : 2.67175e4 833.20879

Signal 5: DADI E, Sig=280,10 Ref=360,100

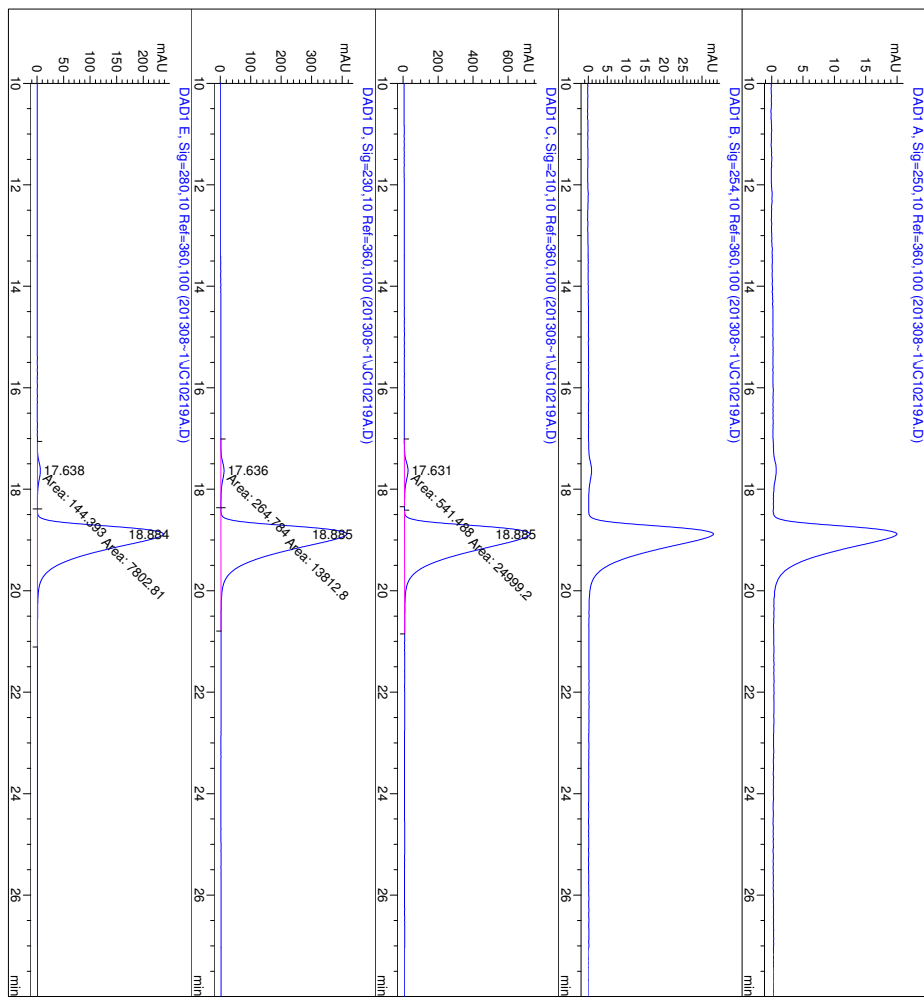
Peak #	RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.710	0.3975	110.80473	4.64648	4.8097
2	15.305	0.5379	2192.98193	67.95478	95.1903

Totals : 2303.78667 72.60126

Results obtained with enhanced integrator!  
=====



Injection Date : 8/1/2013 10:52:58 AM  
 Sample Name : JCI0219A  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl  
 Accr. Method : C:\HPCHEM\1\METHODS\OD-05-40.M  
 Last changed : 4/7/2011 5:39:35 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 7:32:55 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.631	MM	0.4328	541.48834	20.85328	2.1201
2	18.885	MM	0.5805	2.49992e4	717.76105	97.8799

Totals : 2.55407e4 738.61432

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.636	MM	0.4283	264.78415	10.30480	1.8809
2	18.885	MM	0.5576	1.38128e4	412.84863	98.1191

Totals : 1.40776e4 423.15343

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.638	MM	0.4283	144.39316	5.61829	1.8169
2	18.884	MM	0.5489	7802.81396	236.90977	98.1831

Totals : 7947.20712 242.52807

Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

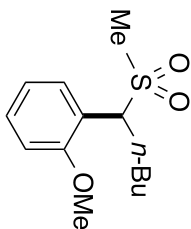
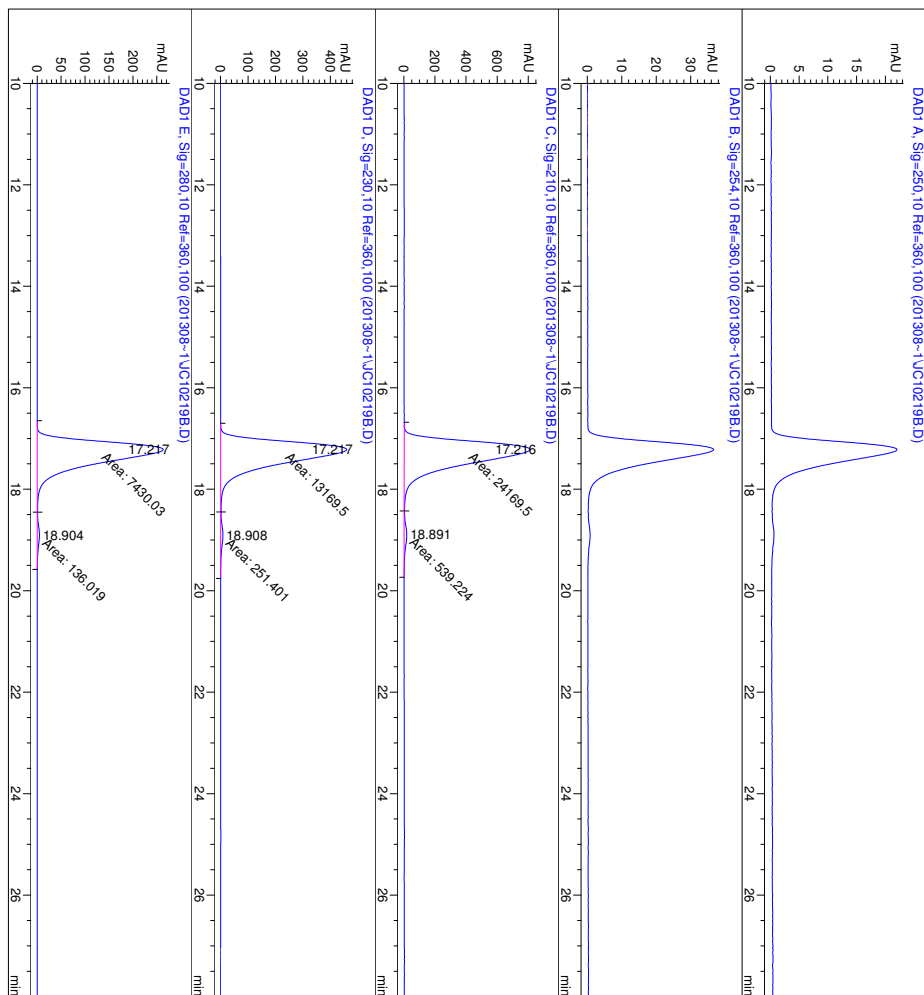


Table 4, entry 9 with (R,R)-Li

Injection Date : 8/1/2013 11:34:20 AM  
 Sample Name : JC10219B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 15 µl  
 Inj Volume : 5 µl  
 Accr. Method : C:\HPCHEM\1\METHODS\OD-05-40.M  
 Last changed : 4/7/2011 5:39:35 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 12:10:26 AM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	1	17.216	MF	0.4968	2.41695e4	810.78070	97.8177
Signal 2: DADI B, Sig=254,10 Ref=360,100	2	18.891	FM	0.5248	539.22418	17.12366	2.1823
Signal 3: DADI C, Sig=210,10 Ref=360,100	1	17.217	MF	0.4700	7430.02881	263.47412	98.2022
Signal 4: DADI D, Sig=230,10 Ref=360,100	2	18.904	FM	0.5030	136.01933	4.50659	1.7978

Totals : 2.47087e4 827.90436  
 Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Peak RetTime Type Width Area Height Area %  
 # [min] [min] [mAU\*s] [mAU] %  
 1 17.217 MF 0.4777 1.31695e4 459.48663 98.1268  
 2 18.908 FM 0.5063 251.40105 8.27497 1.8732  
 Totals : 1.34209e4 467.76160  
 Results obtained with enhanced integrator!  
 Signal 5: DADI E, Sig=280,10 Ref=360,100  
 Peak RetTime Type Width Area Height Area %  
 # [min] [min] [mAU\*s] [mAU] %  
 1 17.217 MF 0.4700 7430.02881 263.47412 98.2022  
 2 18.904 FM 0.5030 136.01933 4.50659 1.7978  
 Totals : 7566.04814 267.98071  
 Results obtained with enhanced integrator!  
 \*\*\* End of Report \*\*\*

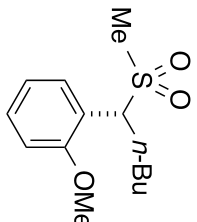
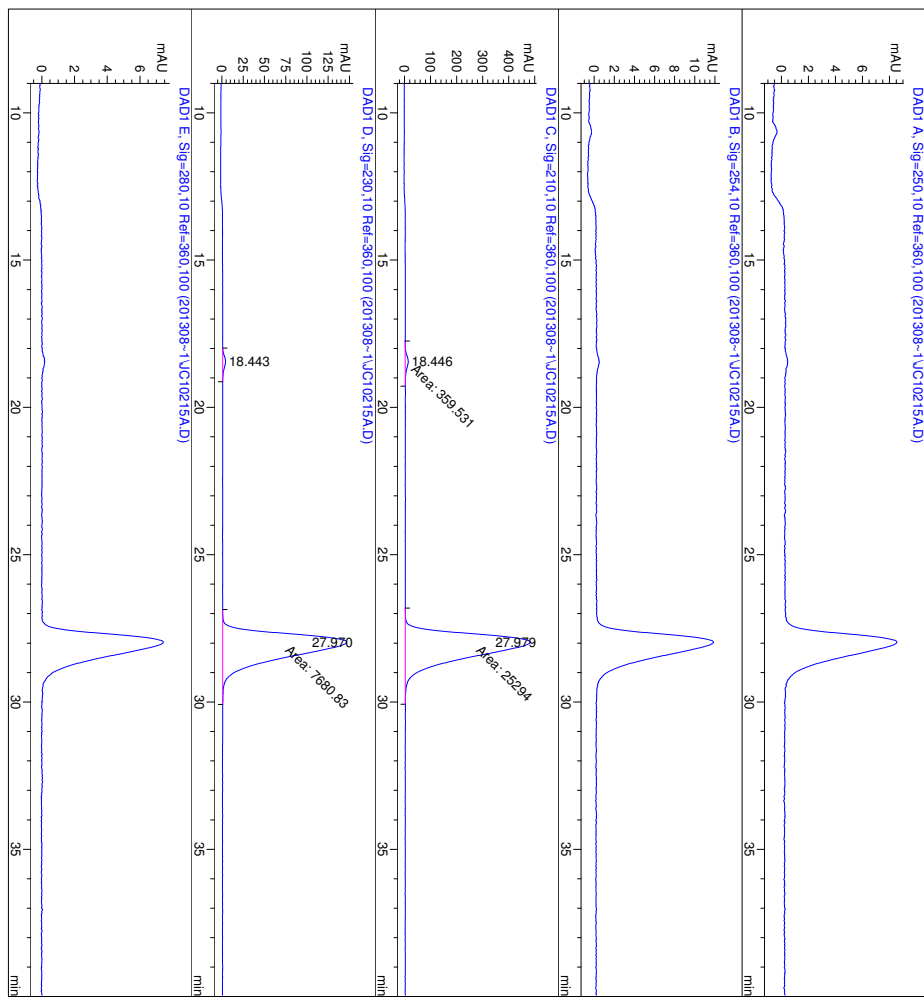


Table 4, entry 9  
 with (S,S)-L1

=====  
 Injection Date : 8/1/2013 2:28:49 AM      Seq. Line : 18  
 Sample Name : JC10215A                      Location : Vial 79  
 Acq. Operator : CE                            Inj : 1  
 Acq. Instrument : Instrument 1                Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1        Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AS-10-40.M  
 Last changed : 4/6/2011 9:32:30 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 7:34:25 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

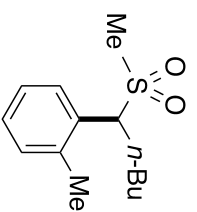


Table 4, entry 10  
 with (R<sub>1</sub>R)-L1

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.446	MM	0.5153	359.53079	11.62884	1.4015
2	27.979	MM	0.8786	2.52940e4	479.81430	98.5985
Totals :				2.56535e4	491.44314	

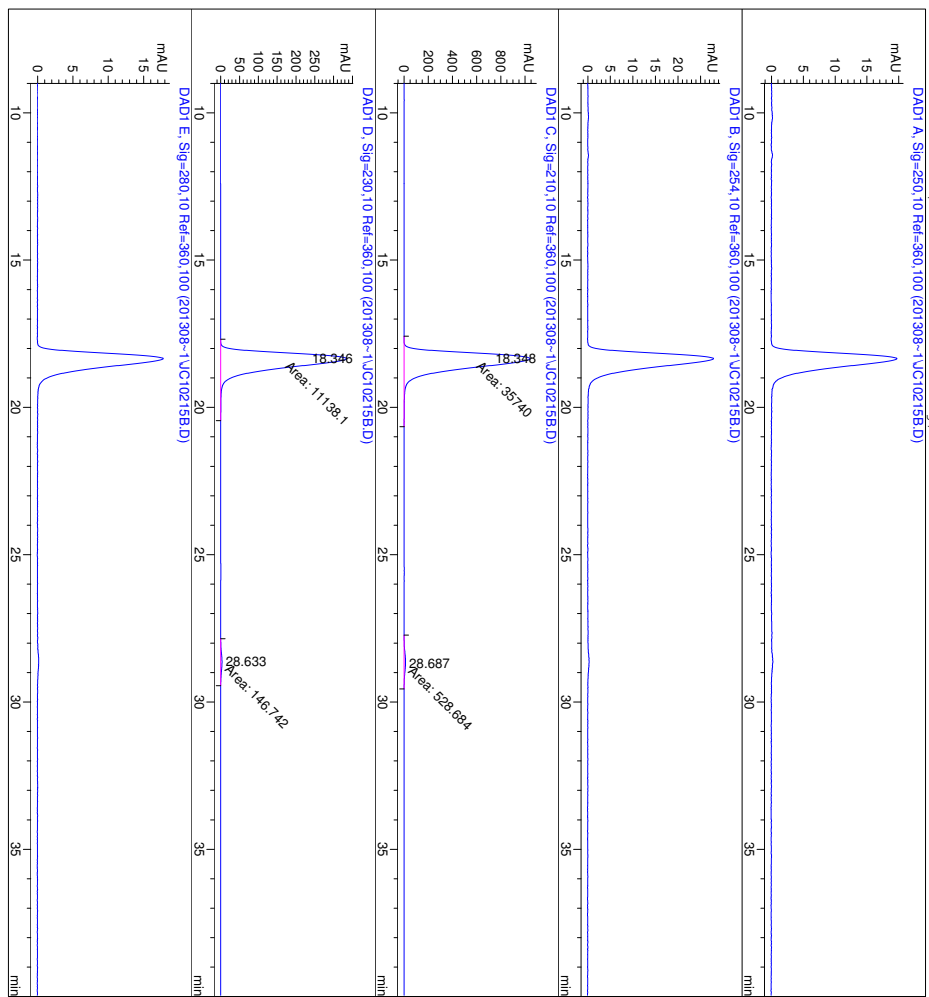
Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.443	BB	0.3614	96.55293	3.35807	1.2415
2	27.970	MM	0.8773	7680.83154	145.92509	98.7585
Totals :				7777.38447	149.28317	

Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

=====  
 \*\*\* End of Report \*\*\*  
 =====

Injection Date : 8/1/2013 3:10:07 AM  
 Sample Name : JC10215B  
 Acq. Operator : CE  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Last changed : 4/6/2011 9:32:30 PM by CC  
 Analysis Method : C:\HPCHEM\1\METHODS\AS-10-40.M  
 Last changed : 8/2/2014 12:12:31 AM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.348	MM	0.5711	3.57400e4	1042.94275	98.5423
2	28.687	MM	0.7471	528.68359	11.79463	1.4577

Totals : 3.62687e4 1054.73737

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.346	MM	0.5543	1.11381e4	334.92871	98.6997
2	28.633	MM	0.6968	146.74203	3.50967	1.3003

Totals : 1.12849e4 338.43838

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

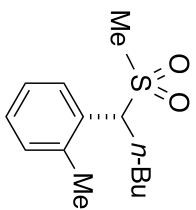
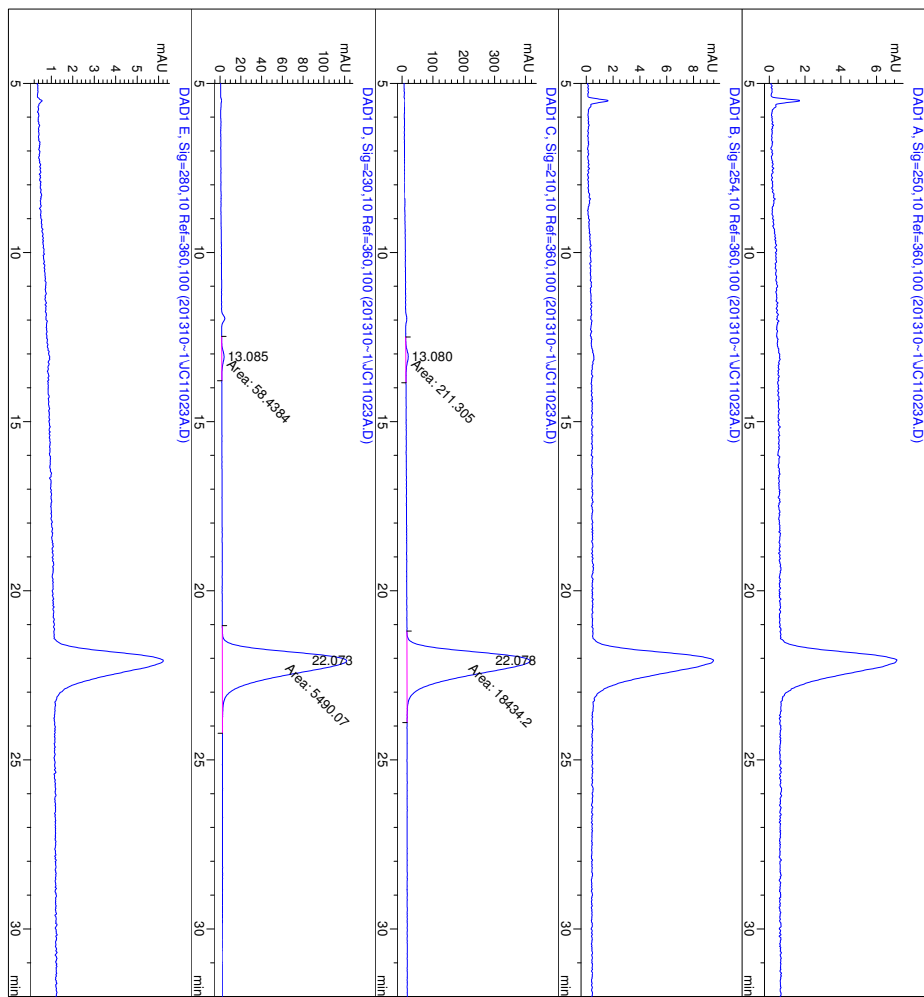


Table 4, entry 10  
with (S,S)-L1

=====  
 Injection Date : 10/16/2013 10:37:14 PM      Seq. Line : 2  
 Sample Name : JC11023A                              Location : Vial 91  
 Acq. Operator : MK                                    Inj : 1  
 Acq. Instrument : Instrument 1                      Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1              Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AS-10-40.M  
 Last changed : 9/3/2013 3:07:57 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\AD003-40.M  
 Last changed : 8/2/2014 12:15:46 AM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

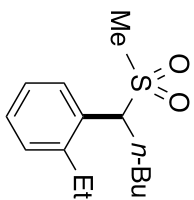


Table 4, entry 11  
 with (R,R)-L1

Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 3: DAD1 C, Sig=210,10 Ref=360,100	1	13.080	MM	0.4495	211.30522	7.83469	1.1333
	2	22.078	MM	0.7688	1.84342e4	399.62811	98.8667

Totals : 1.86455e4 407.46281

Results obtained with enhanced integrator!

Signal	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 4: DAD1 D, Sig=230,10 Ref=360,100	1	13.085	MM	0.4251	58.43836	2.29142	1.0532
	2	22.073	MM	0.7638	5430.07422	119.79153	98.9468

Totals : 5548.51258 122.08295

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

=====  
 \*\*\* End of Report \*\*\*

Injection Date : 10/16/2013 11:18:31 PM  
 Sample Name : JC11023B  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Last changed : 9/3/2013 3:07:57 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\AS-10-40.M  
 Last changed : 8/2/2014 12:15:46 AM by MK  
 (modified after loading)

=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

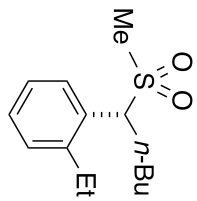
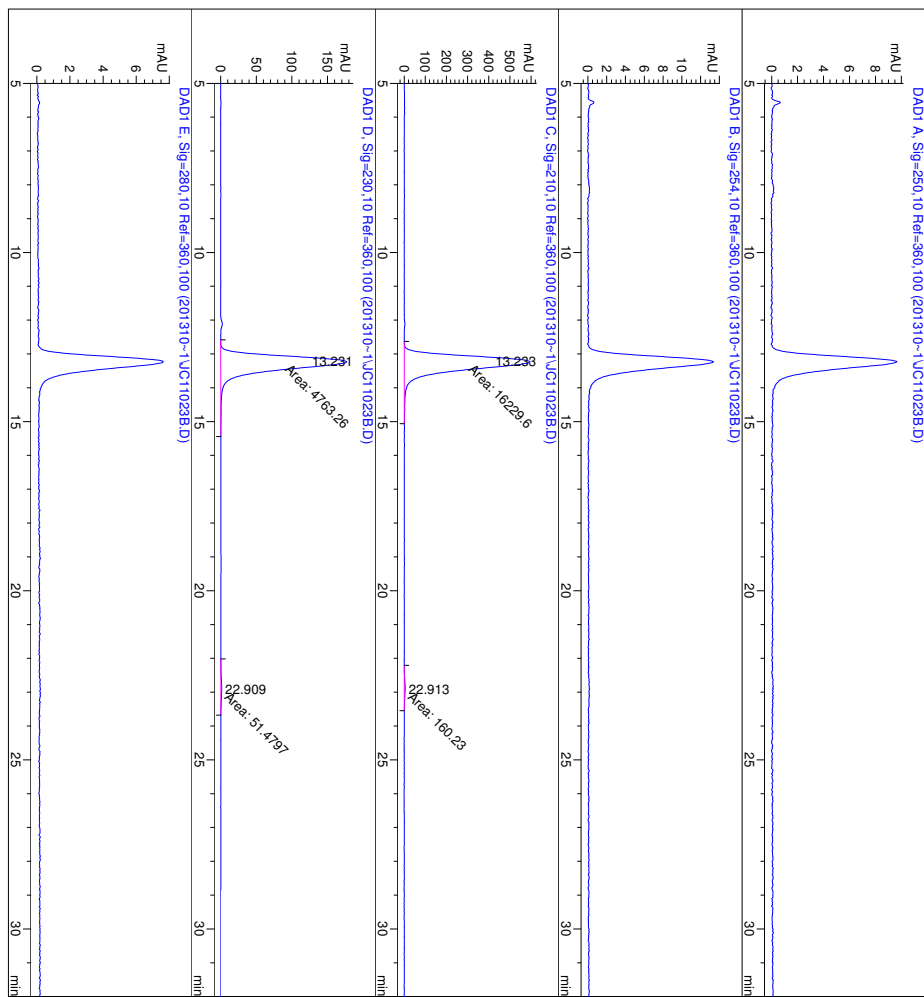


Table 4, entry 11  
 with (S,S)-L1



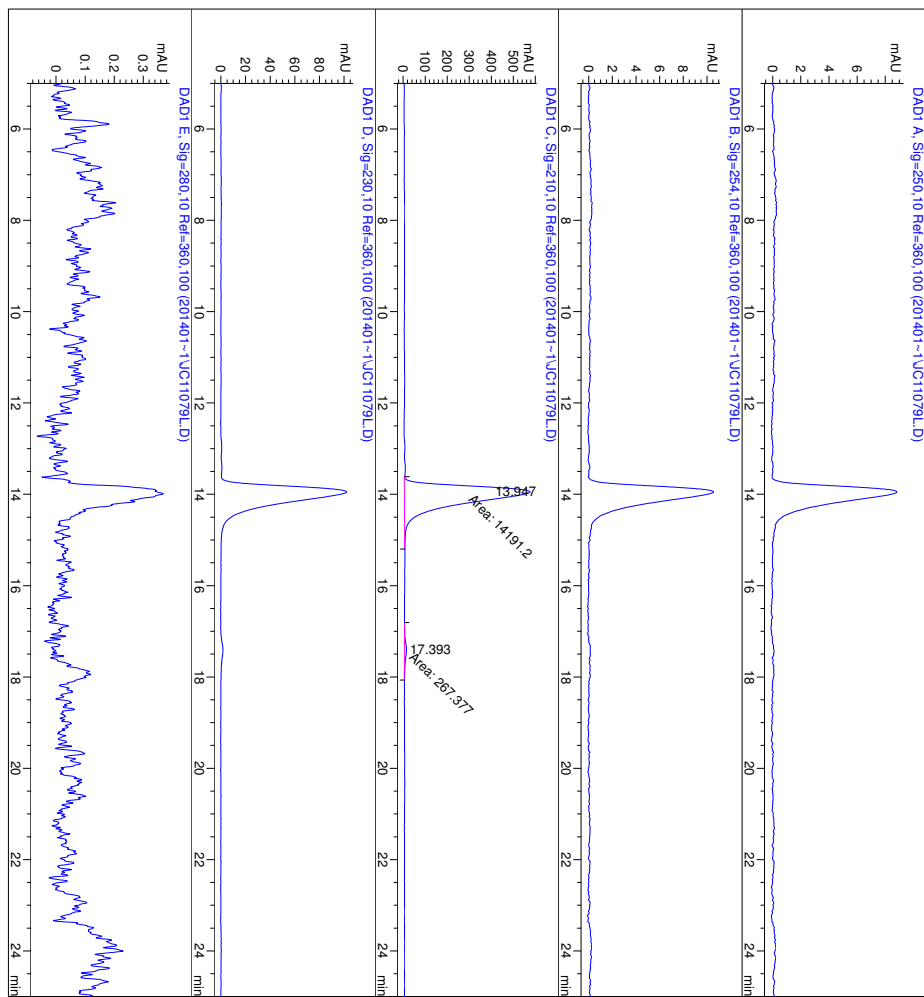
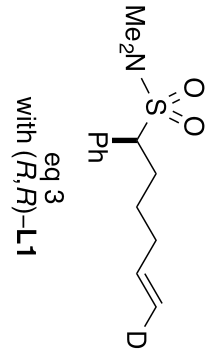
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.233	MM	0.4545	1.62296e4	595.18054	99.0224
2	22.913	MM	0.6434	160.23030	4.15061	0.9776

Totals : 1.63899e4 599.33115  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Peak RetTime Type Width Area Height Area  
 # [min] [min] [mAU\*s] [mAU] %  
 1 13.231 MM 0.4491 4763.26123 176.78093 98.9308  
 2 22.909 MM 0.6799 51.47974 1.26191 1.0692  
 Totals : 4814.74097 178.04284  
 Results obtained with enhanced integrator!  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

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 \*\*\* End of Report \*\*\*  
 =====

Injection Date : 1/31/2014 1:15:03 PM  
 Sample Name : JC11079 LINEAR  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Inj Volume : 15 µl  
 Last changed : 12/28/2013 4:11:34 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\A0005-40.M  
 Last changed : 8/2/2014 11:58:47 PM by MK  
 (modified after loading)

=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

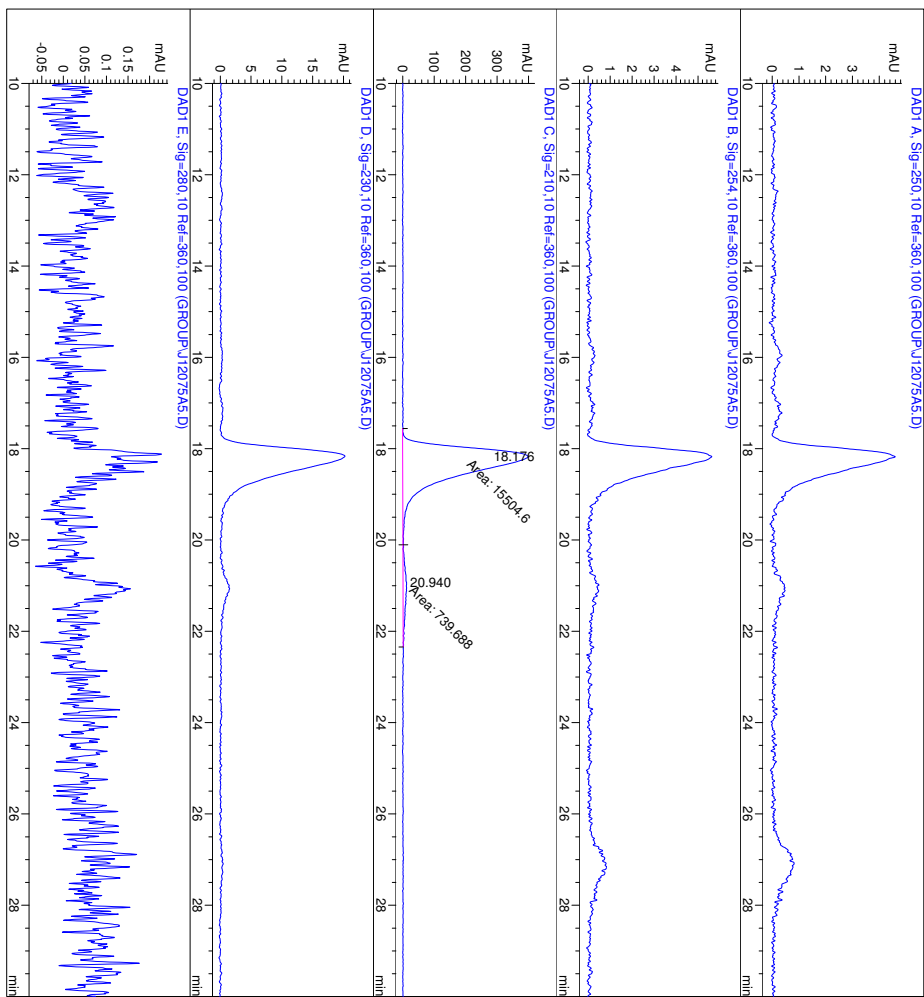


Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1	13.947	FM	0.4147	14,912e4	570.28912	98.1507
Signal 2	17.393	MM	0.4723	267.37726	9.43601	1.8493

Totals : 1.44586e4 579.72513  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100



=====  
 Injection Date : 8/1/2014 10:06:30 PM      Seq. Line : 2  
 Sample Name : JCI12075A                      Location : Vial 19  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1                Inj Volume : 15 µl  
 Different Inj Volume from Sequence !        Actual Inj Volume : 4 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\07-05-30.M  
 Last changed : 8/1/2014 10:12:37 PM by MK  
 (modified after loading)  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 12:51:14 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====

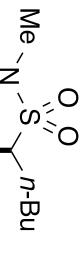


Table 5, entry 1  
 with (3R,8S)-L6

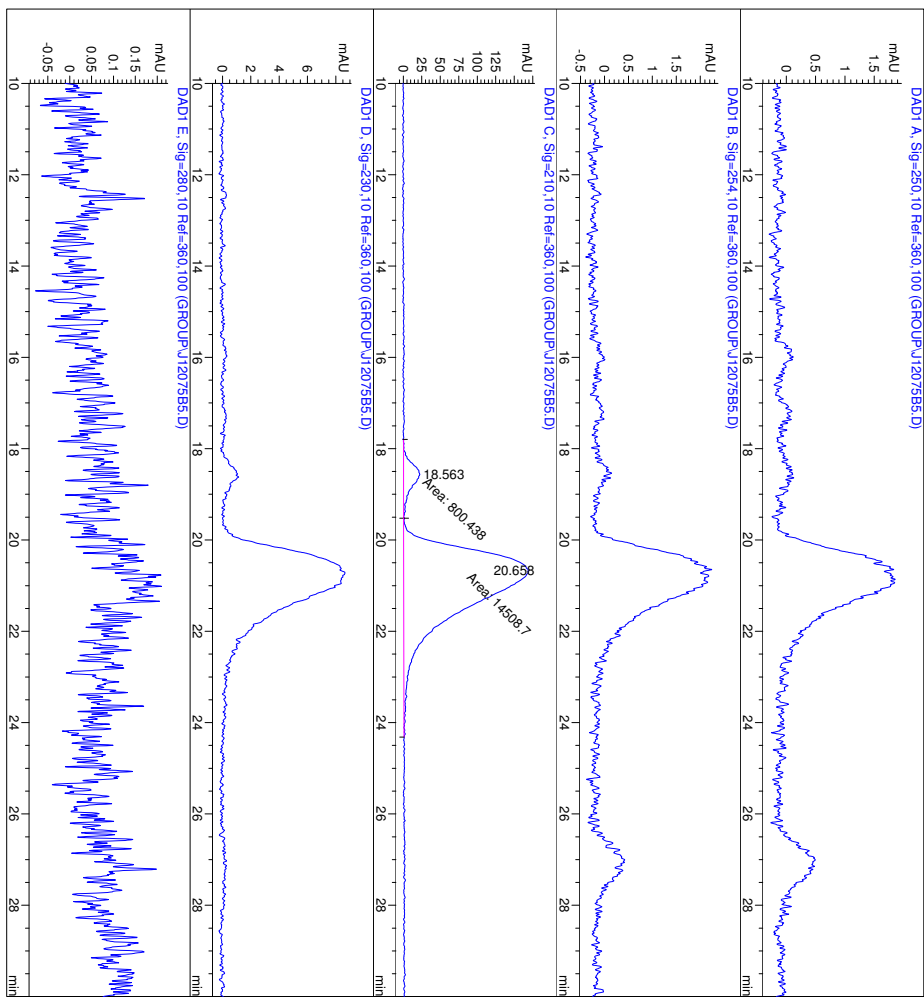
Sorted By	Signal					
Multiplier	: 1.0000					
Dilution	: 1.0000					
Use Multiplier & Dilution Factor with ISTDs						
Signal 1: DADI A, Sig=250,10 Ref=360,100						
Signal 2: DADI B, Sig=254,10 Ref=360,100						
Signal 3: DADI C, Sig=210,10 Ref=360,100						
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.176	MF	0.6470	1.55046e4	399.41086	95.4465
2	20.940	FM	1.0783	739.68774	11.43283	4.5335
Totals :				1.62443e4	410.84368	

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

=====  
 Injection Date : 8/1/2014 10:47:48 PM      Seq. Line : 3  
 Sample Name : JCI12075B                      Location : Vial 20  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1                Inj Volume : 15 µl  
 Different Inj Volume from Sequence !        Actual Inj Volume : 4 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\OJ-05-30.M  
 Last changed : 8/1/2014 10:12:37 PM by MK  
 (modified after Loading)  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 12:51:14 PM by MK  
 (modified after Loading)



=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100  
 Signal 2: DADI B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.563	MF	0.6055	800.43811	22.03275	5.2285
2	20.658	FM	1.4329	14508.764	168.75829	94.7715

Totals : 1.53092e4 190.79103  
 Results obtained with enhanced integrator!  
 Signal 4: DADI D, Sig=230,10 Ref=360,100  
 Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

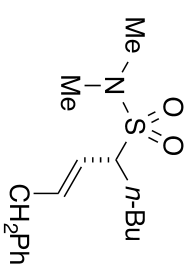
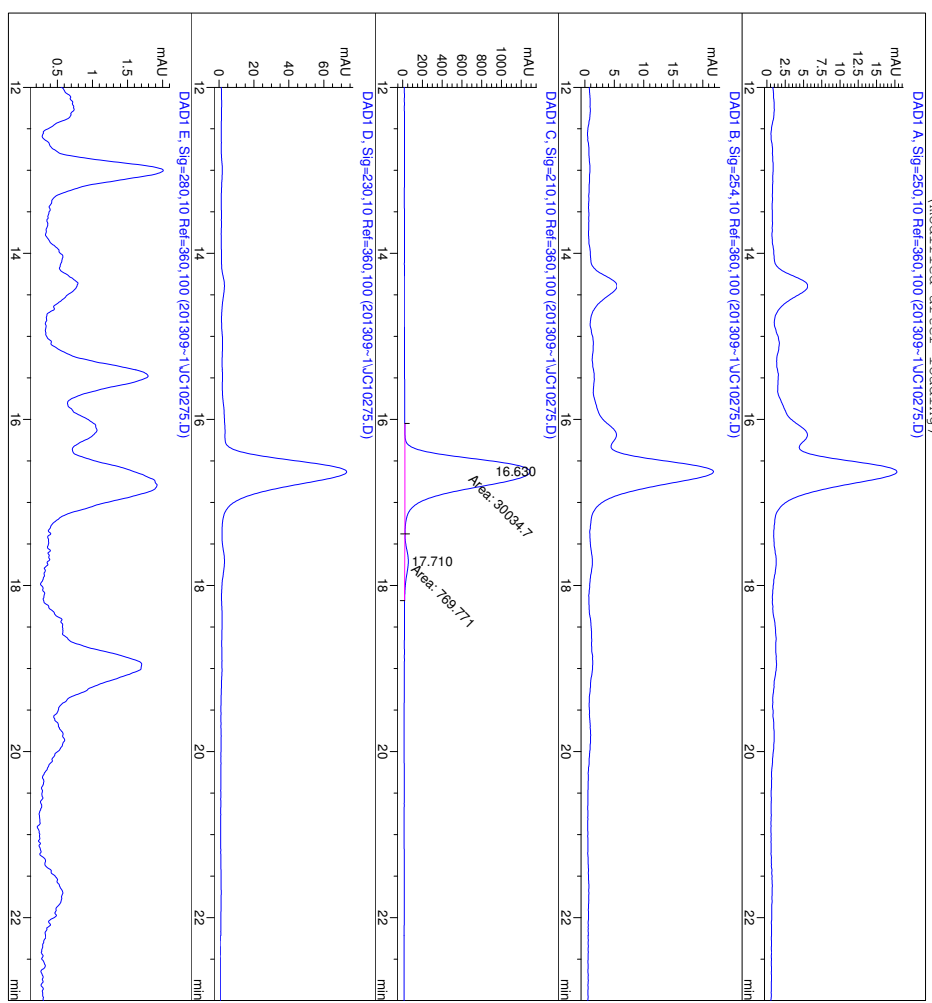


Table 5, entry 1  
 with (3S,8R)-L6

=====  
 Injection Date : 9/4/2013 1:38:06 PM      Seq. Line : 11  
 Sample Name : JC10275                      Location : Vial 9  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
 Different Inj Volume from Sequence !  
 Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\JC-ADD01A.M  
 Last changed : 11/14/2012 10:39:31 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\ADD005-40.M  
 Last changed : 8/3/2014 12:34:42 AM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100  
 Signal 2: DAD1 B, Sig=254,10 Ref=360,100  
 Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.630	MM	0.3948	3.00347e4	1267.95288	97.5011
2	17.710	MM	0.3597	769.77083	35.66695	2.4989

Totals : 3.08045e4 1303.61983  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

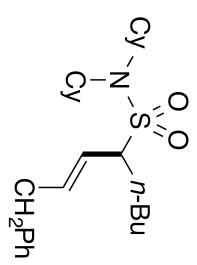
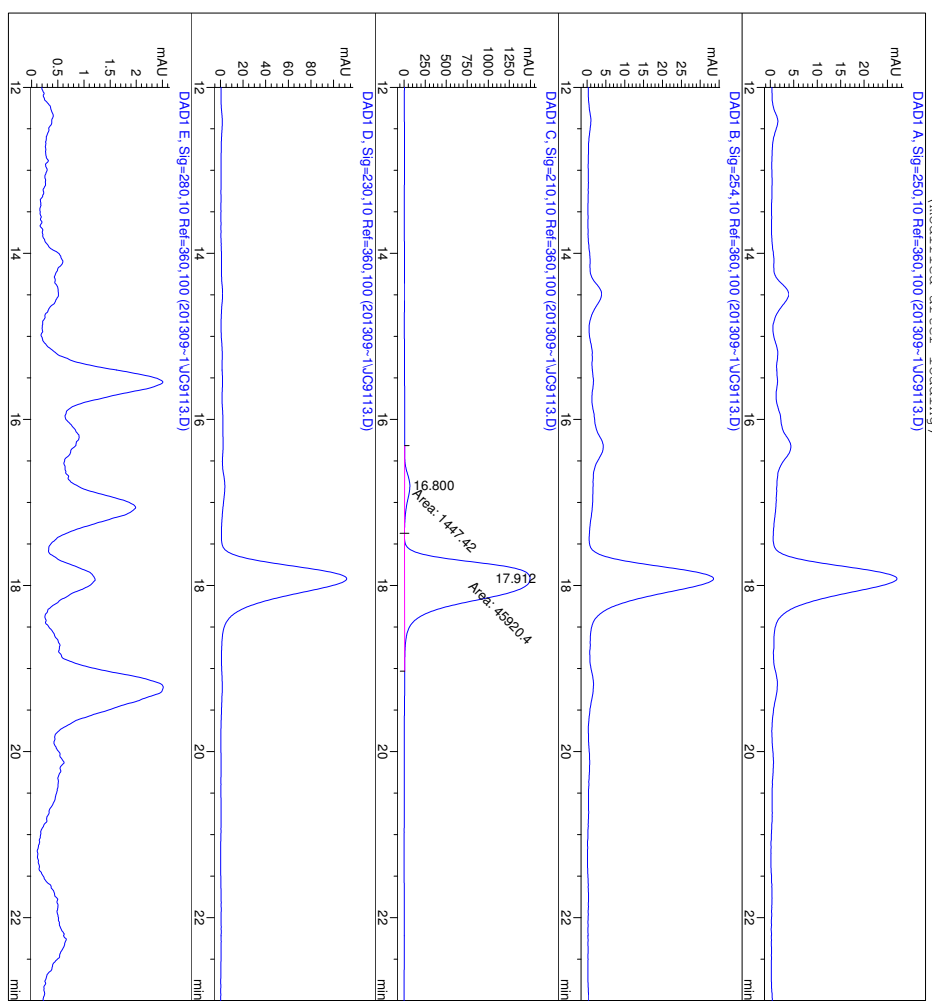


Table 5, entry 2  
 with (3*R*,8*S*)-L6

=====  
 Injection Date : 9/4/2013 2:19:25 PM      Seq. Line : 12  
 Sample Name : JC9113                              Location : Vial 10  
 Acq. Operator : MK                                Inj : 1  
 Acq. Instrument : Instrument 1                    Inj Volume : 15 µl  
 Different Inj Volume from Sequence 1          Actual Inj Volume : 5 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\JC-AD01A.M  
 Last changed : 11/14/2012 10:39:31 PM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 12:18:32 AM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	16.800	MM	0.3820	1447.42444	63.15571	3.0557
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	17.912	MM	0.5129	4.59204e4	1492.23425	96.9443

Totals : 4.73678e4 1555.38996  
 Results obtained with enhanced integrator!  
 Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100  
 \*\*\*\*\*  
 \*\*\* End of Report \*\*\*  
 \*\*\*\*\*

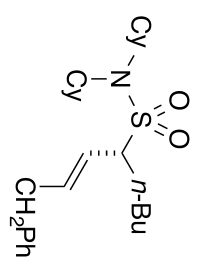
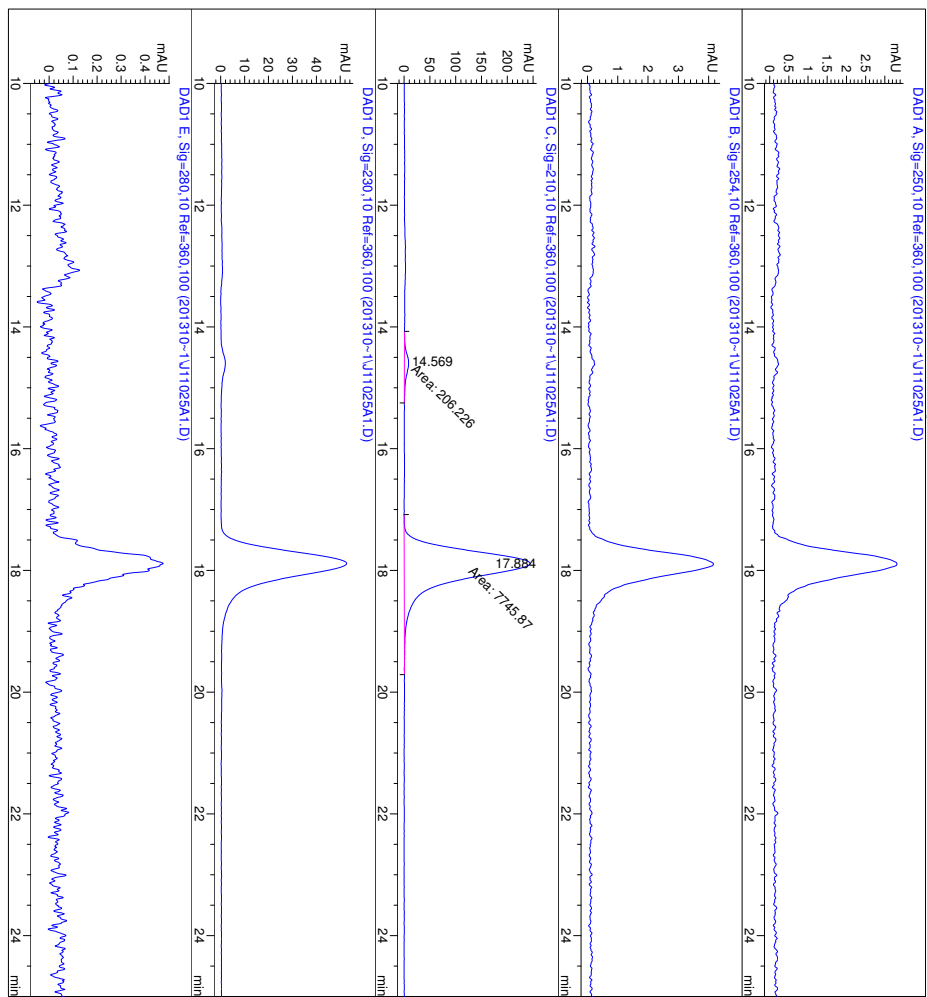


Table 5, entry 2  
 with (3S,8R)-L6

Injection Date : 10/22/2013 5:01:30 PM  
 Sample Name : JCI1025A  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence : Actual Inj Volume : 15 µl  
 Inj Volume : 3 µl  
 Last changed : 10/22/2013 9:47:57 AM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 7/30/2014 10:35:34 PM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DAD1 A, Sig=250,10 Ref=360,100	14.569	MM	0.4233	206.22578	8.11952	2.5934
Signal 2: DAD1 B, Sig=254,10 Ref=360,100	17.884	MM	0.5286	7745.87012	244.24510	97.4066
Totals :				7952.09590	252.36462	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100  
 Signal 5: DAD1 E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

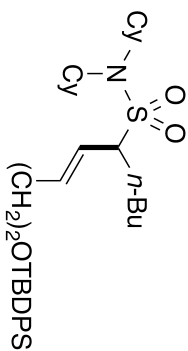
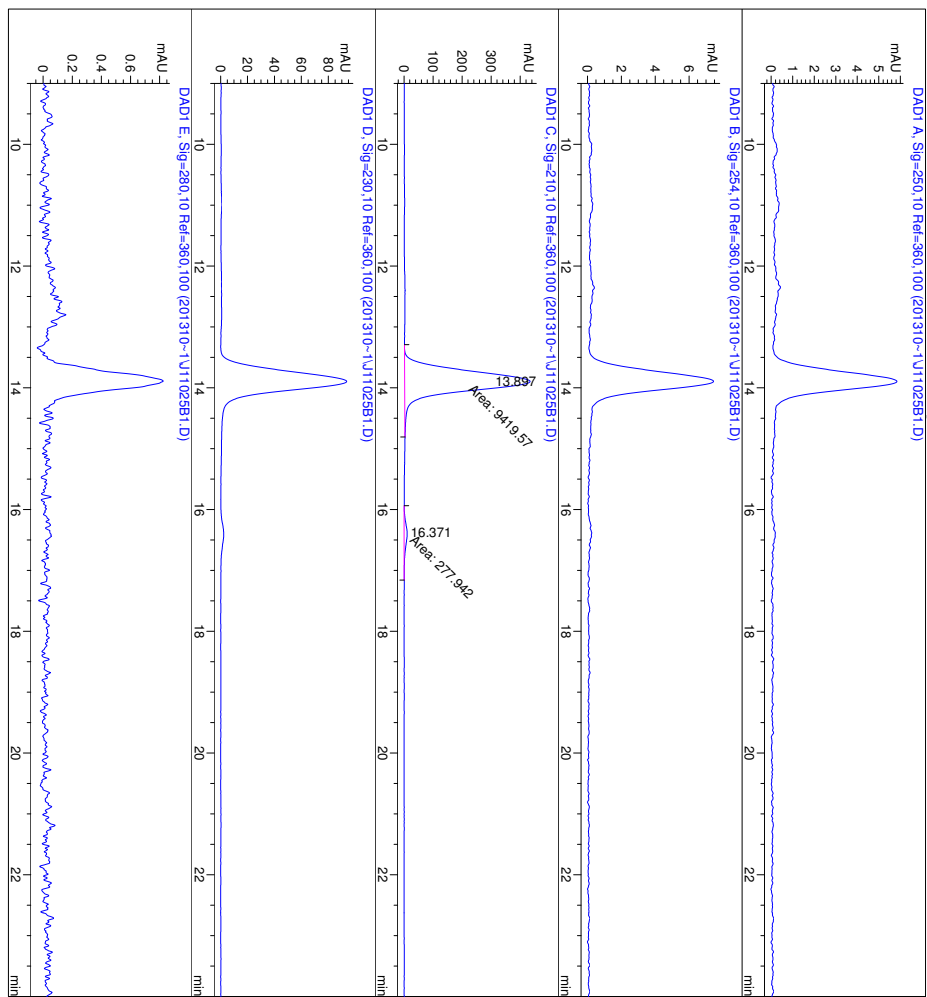


Table 5, entry 3  
 with (3R,8S)-L6

=====  
Injection Date : 10/22/2013 5:42:45 PM      Seq. Line : 9  
Sample Name : JC11025B                            Location : Vial 10  
Acq. Operator : MK                                Inj : 1  
Acq. Instrument : Instrument 1                   Inj Volume : 15 µl  
Different Inj Volume from Sequence 1          Actual Inj Volume : 3 µl  
Acq. Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 10/22/2013 9:47:57 AM by MK  
Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 8/2/2014 12:21:07 AM by MK  
    (modified after loading)



=====  
Area Percent Report  
=====  
Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100  
Signal 2: DADI B, Sig=254,10 Ref=360,100  
Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.897	MM	0.3634	9419.56641	432.00473	97.1339
2	16.371	MM	0.4602	277.94183	10.06597	2.8861

Totals : 9697.50824 442.07070

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

Signal 5: DADI E, Sig=280,10 Ref=360,100

=====  
\*\*\* End of Report \*\*\*  
=====

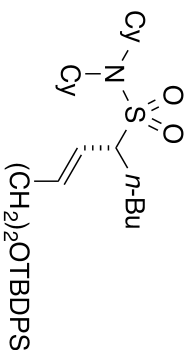
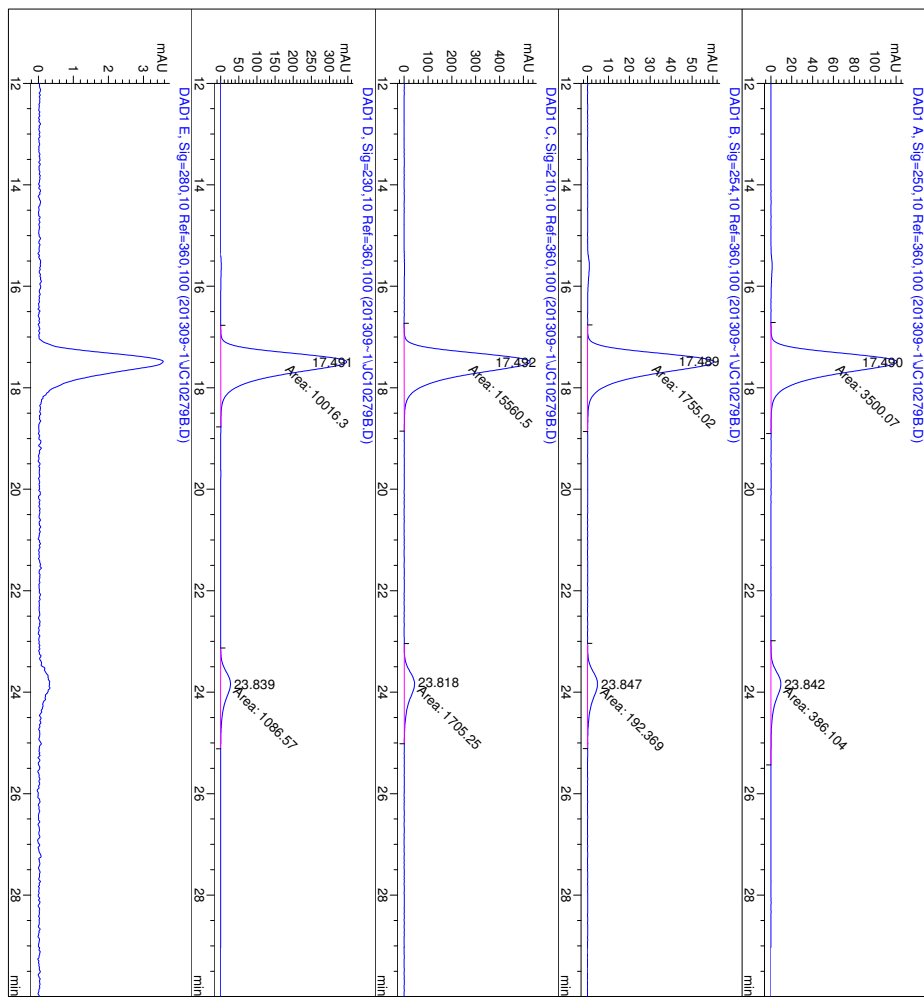


Table 5, entry 3  
with (3S,8R)-L6

=====  
Injection Date : 9/16/2013 1:56:44 PM      Seq. Line : 9  
Sample Name : JCI0279B                      Location : Vial 95  
Acq. Operator : MK                            Inj : 1  
Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
Different Inj Volume from Sequence !  
Accr. Method : C:\HPCHEM\1\METHODS\AD-10-40.M      Actual Inj Volume : 1 µl  
Last changed : 7/12/2012 11:12:25 AM by CE  
Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
Last changed : 8/3/2014 12:46:07 AM by MK  
(modified after loading)



=====  
Area Percent Report  
Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

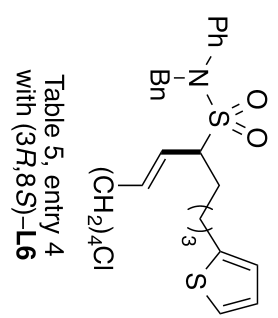
Signal	Peak RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	17.490	0.4828	3500.07324	120.82352	90.0647
	23.842	0.6752	386.10425	9.53050	9.9353
Totals :			3886.17749	130.35402	

Signal	Peak RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 2: DADI B, Sig=254,10 Ref=360,100	17.489	0.4850	1755.02209	60.31308	90.1217
	23.847	0.6731	192.36926	4.76325	9.8783
Totals :			1947.39136	65.07632	

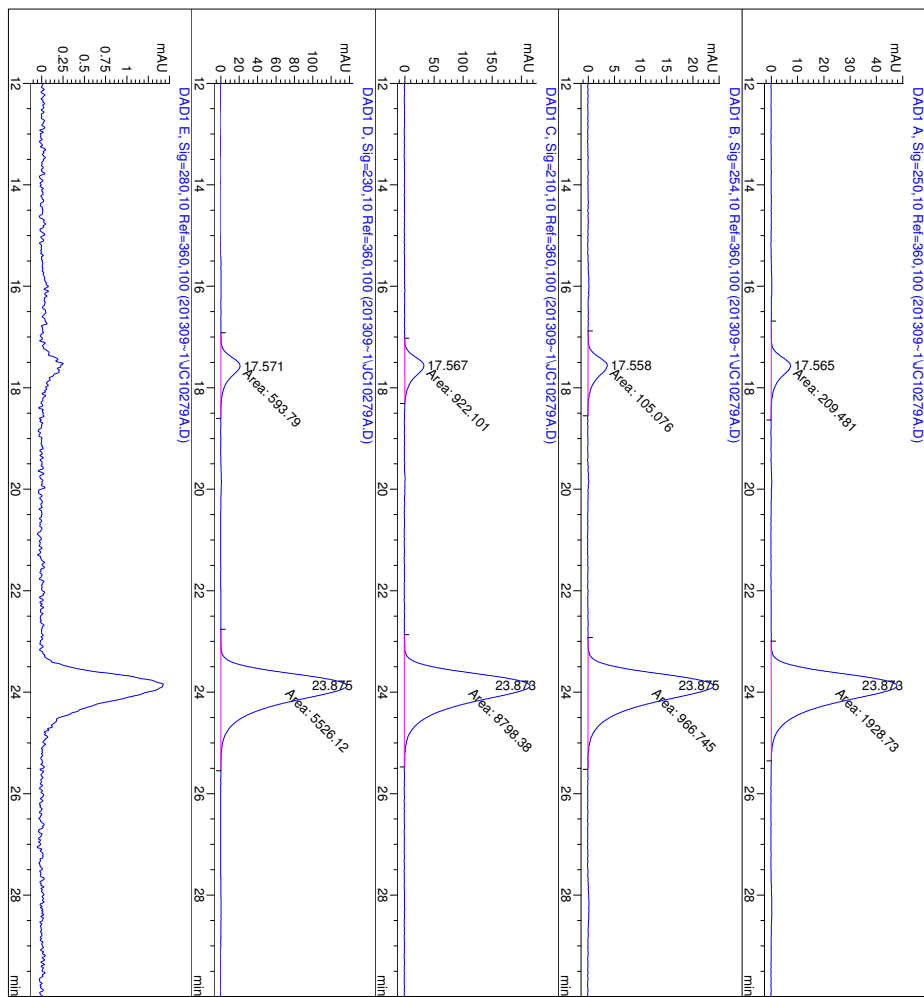
Signal	Peak RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 3: DADI C, Sig=210,10 Ref=360,100	17.492	0.4910	1.55605e4	528.16541	90.1235
	23.818	0.6559	1705.25134	43.32966	9.8765
Totals :			1.72657e4	571.49507	

Signal	Peak RetTime [min]	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 4: DADI D, Sig=230,10 Ref=360,100	17.491	0.4814	1.00163e4	346.80835	90.2137
	23.839	0.6694	1086.56787	27.05270	9.7863
Totals :			1.11029e4	373.86105	

Results obtained with enhanced integrator!  
Signal 5: DADI E, Sig=280,10 Ref=360,100  
\*\*\* End of Report \*\*\*



=====  
 Injection Date : 9/16/2013 1:15:30 PM      Seq. Line : 8  
 Sample Name : JCI0279A                      Location : Vial 94  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
 Different Inj Volume from Sequence !  
 Actual Inj Volume : 1 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AD-10-40.M  
 Last changed : 7/12/2012 11:12:25 AM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\AD005-40.M  
 Last changed : 8/2/2014 12:24:51 AM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.565	MM	0.4749	209.48149	7.35103	9.7971
2	23.873	MM	0.6716	1928.72815	47.86718	90.2029
Totals :				2138.20964	55.21821	

Results obtained with enhanced integrator!

Signal 2: DADI B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.558	MM	0.4747	105.07636	3.68929	9.8035
2	23.875	MM	0.6715	966.74506	23.99374	90.1965
Totals :				1071.82142	27.68303	

Results obtained with enhanced integrator!

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.567	MM	0.4652	922.10120	33.03711	9.4862
2	23.873	MM	0.6781	8798.38086	216.24049	90.5138
Totals :				9720.48206	249.27760	

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.571	MM	0.4736	593.79047	20.89495	9.7026
2	23.875	MM	0.6721	5526.11816	137.03973	90.2974
Totals :				6119.90863	157.93469	

Results obtained with enhanced integrator!

Signal 5: DADI E, Sig=280,10 Ref=360,100

=====  
 \*\*\* End of Report \*\*\*

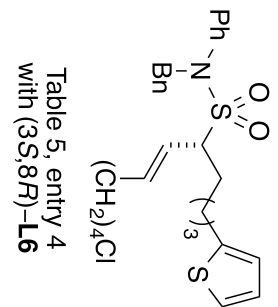
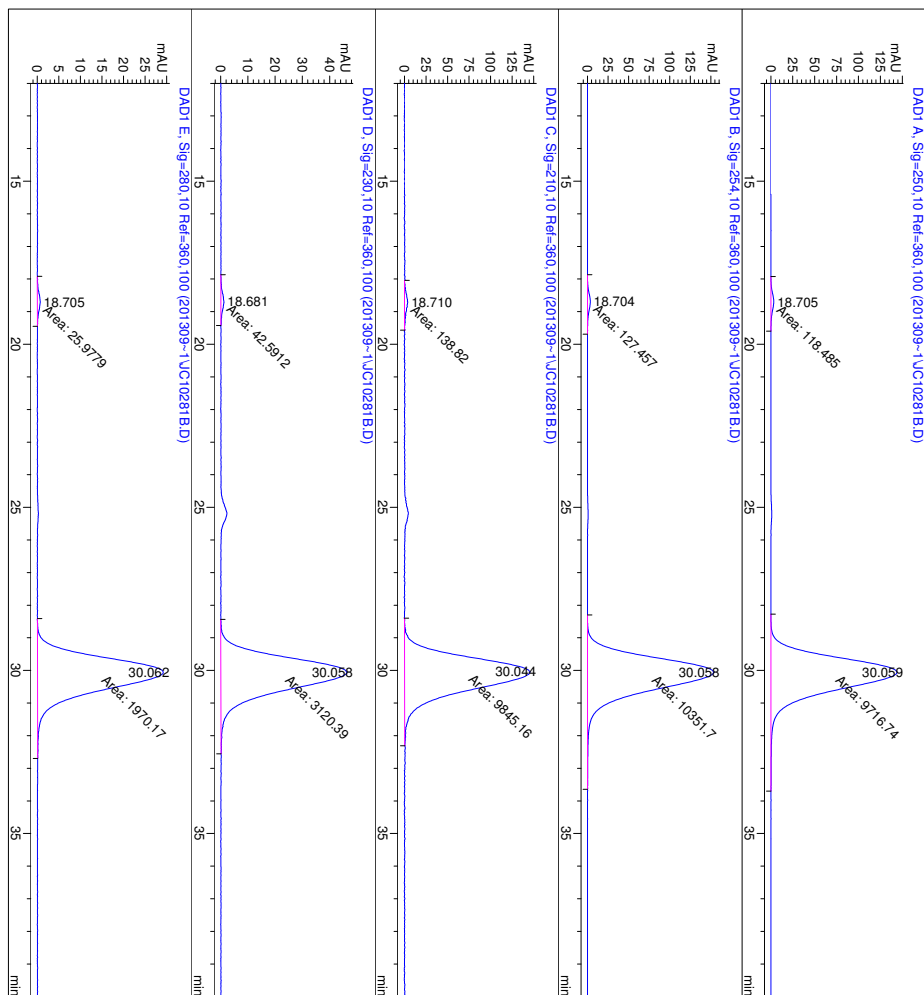


Table 5, entry 4  
 with (3S,8R)-L6



=====  
 Injection Date : 9/17/2013 5:04:56 AM      Seq. Line : 24  
 Sample Name : JCI0281B                      Location : Vial 97  
 Acq. Operator : MK                            Inj : 1  
 Acq. Instrument : Instrument 1              Inj Volume : 15 µl  
 Different Inj Volume from Sequence !  
 Actual Inj Volume : 6 µl  
 Acq. Method : C:\HPCHEM\1\METHODS\AS-10-40.M  
 Last changed : 9/3/2013 3:07:57 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\OD-02-20.M  
 Last changed : 7/30/2014 10:40:14 PM by MK  
 (modified after loading)



=====  
 Area Percent Report  
 =====  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.705	MM	0.6218	118.48459	3.17571	1.2047
2	30.059	MM	1.1259	9716.74219	143.83633	98.7953
Totals :				9835.22678	147.01204	

Results obtained with enhanced integrator!

Signal 2: DADI B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.704	MM	0.6262	127.45731	3.39228	1.2163
2	30.058	MM	1.1261	1.03517e4	153.21146	98.7837
Totals :				1.04792e4	156.60374	

Results obtained with enhanced integrator!

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.710	MM	0.6299	138.81970	3.67318	1.3904
2	30.044	MM	1.1245	9845.16113	145.92497	98.6096
Totals :				9983.98083	149.59815	

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.681	MM	0.6396	42.59124	1.10979	1.3466
2	30.058	MM	1.1261	3120.39331	46.18145	98.6534
Totals :				3162.98455	47.29125	

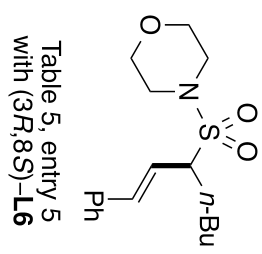
Results obtained with enhanced integrator!

Signal 5: DADI E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.705	MM	0.6513	25.97787	6.64763e-1	1.3014
2	30.062	MM	1.1250	1970.16589	29.18823	98.6986
Totals :				1996.14376	29.85299	

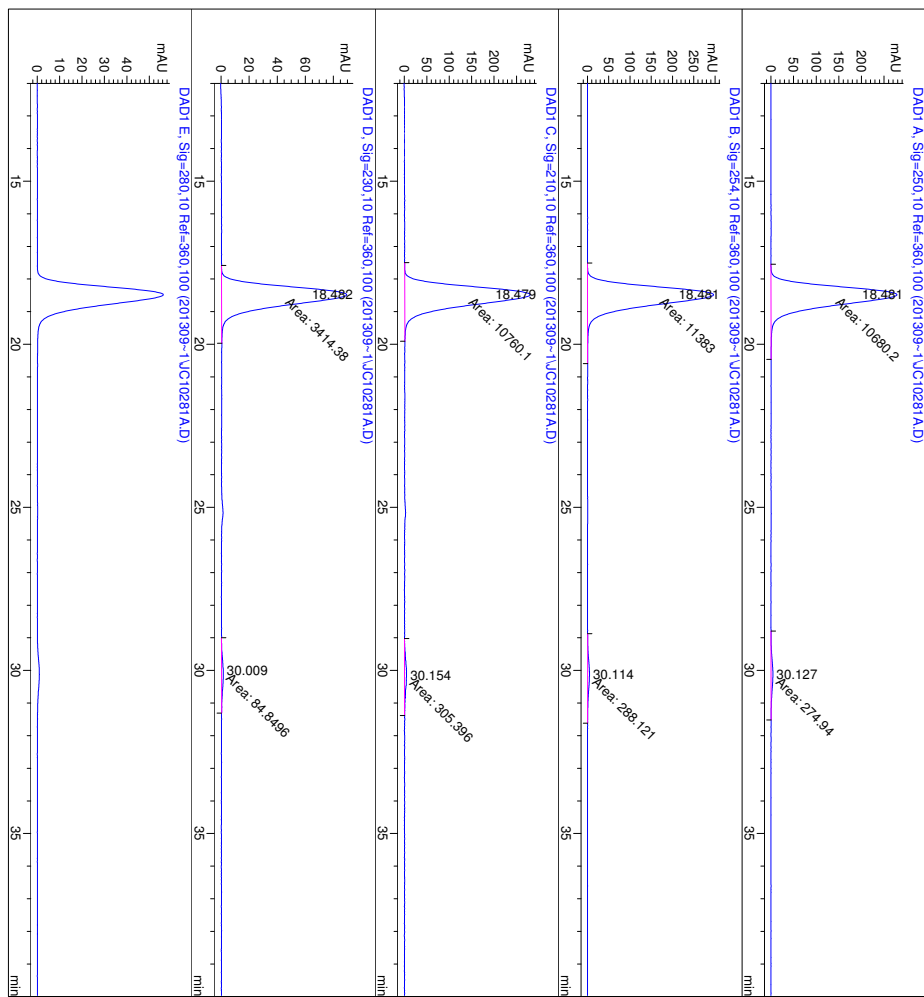
Results obtained with enhanced integrator!

=====  
 \*\*\* End of Report \*\*\*



Injection Date : 9/17/2013 4:23:37 AM  
 Sample Name : JCI0281A  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 9/3/2013 3:07:57 PM by MK  
 Analysis Method : C:\HPCHEM\1\METHODS\AS-10-40.M  
 Last changed : 8/2/2014 12:27:30 AM by MK  
 (modified after loading)

Seq. Line : 23  
 Location : Vial 96  
 Inj : 1  
 Inj Volume : 15 µl  
 Actual Inj Volume : 3 µl



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	Peak RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.481	MM	0.6395	1.06802e4	278.33743	97.4903
2	30.127	MM	1.1077	274.94009	4.13675	2.5097
Totals :				1.09552e4	282.47418	

Results obtained with enhanced integrator!

Signal	Peak RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.481	MM	0.6401	1.13830e4	296.37387	97.5313
2	30.114	MM	1.0968	288.12051	4.37829	2.4687
Totals :				1.16711e4	300.75216	

Results obtained with enhanced integrator!

Signal	Peak RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.479	MM	0.6415	1.07601e4	279.53766	97.2401
2	30.154	MM	1.0830	305.39581	4.69971	2.7599
Totals :				1.10655e4	284.23737	

Results obtained with enhanced integrator!

Signal	Peak RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.482	MM	0.6382	3414.37500	89.16418	97.5752
2	30.009	MM	1.0444	84.84958	1.35400	2.4248
Totals :				3499.22458	90.51818	

Results obtained with enhanced integrator!

Signal 5: DADI E, Sig=280,10 Ref=360,100  
 \*\*\* End of Report \*\*\*

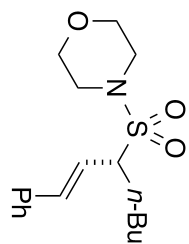
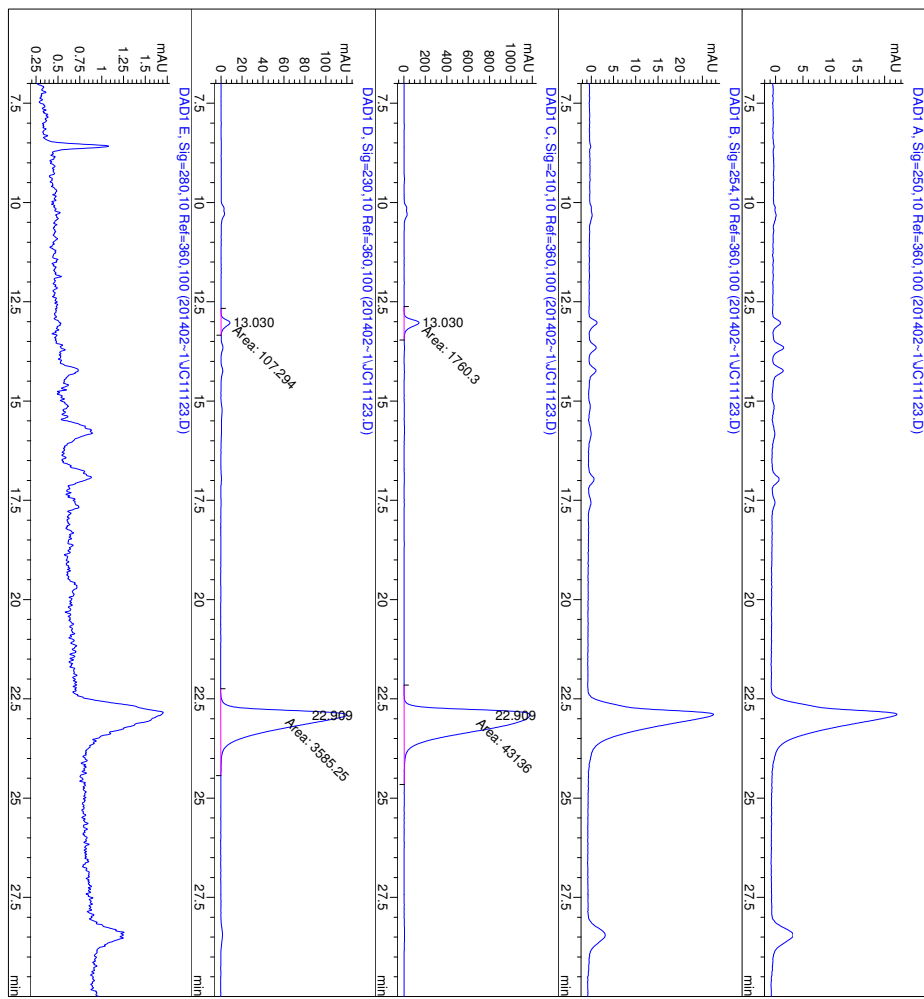


Table 5, entry 5 with (S,S)-L6

Injection Date : 2/5/2014 11:58:40 PM  
 Sample Name : JC11123  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Last changed : 7/6/2013 9:54:10 AM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\IB-05-40.M  
 Last changed : 7/30/2014 10:42:05 PM by MK  
 (modified after loading)

Seq. Line : 2  
 Location : Vial 31  
 Inj : 1  
 Inj Volume : 15 µl  
 Actual Inj Volume : 5 µl



Area Percent Report

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DADI A, Sig=250,10 Ref=360,100

Signal 2: DADI B, Sig=254,10 Ref=360,100

Signal 3: DADI C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.030	MF	0.2116	1760.29651	138.68036	3.9208
2	22.909	MM	0.6103	4.31360e4	1177.93591	96.0792

Totals : 4.48962e4 1316.61627

Results obtained with enhanced integrator!

Signal 4: DADI D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.030	MF	0.2092	107.29430	8.54649	2.9057
2	22.909	MM	0.4974	3585.25415	120.13020	97.0943

Totals : 3692.54845 128.67670

Results obtained with enhanced integrator!

Signal 5: DADI E, Sig=280,10 Ref=360,100

\*\*\* End of Report \*\*\*

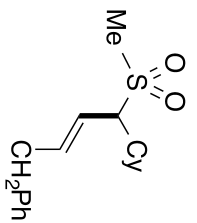
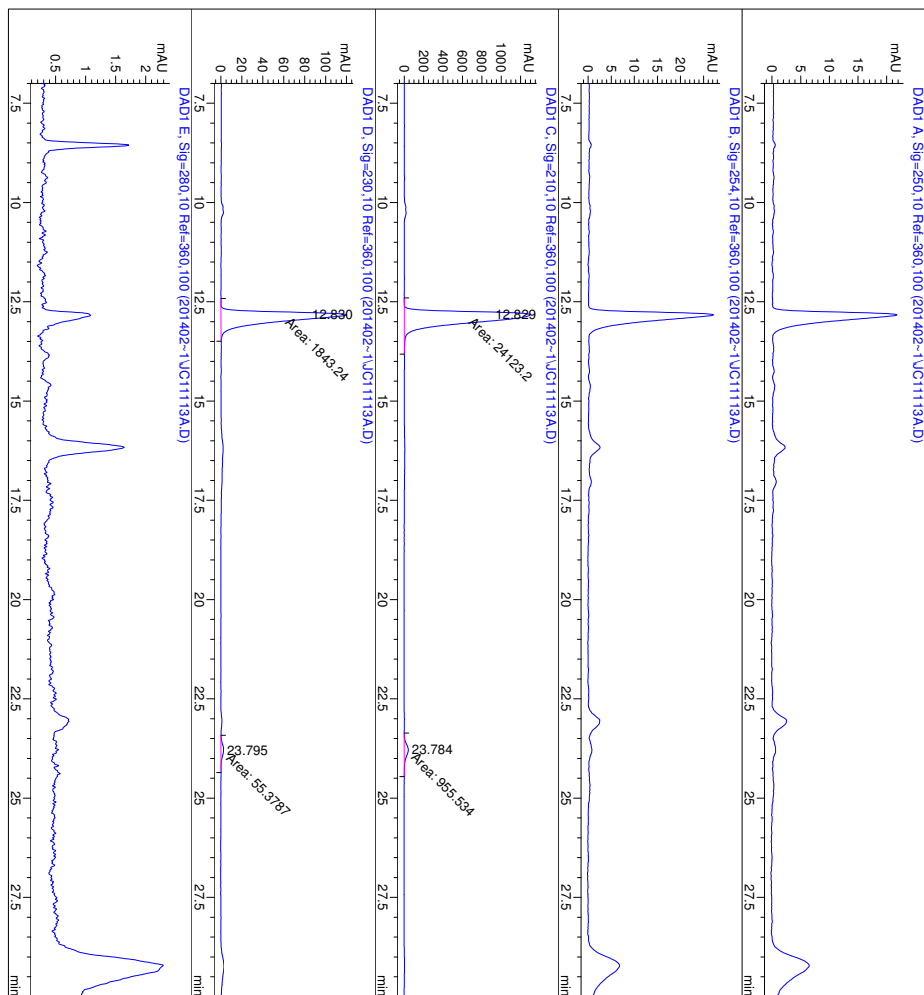


Table 5, entry 6  
 with (R,R)-L1

Injection Date : 2/6/2014 12:39:55 AM  
 Sample Name : JC11113  
 Acq. Operator : MK  
 Acq. Instrument : Instrument 1  
 Different Inj Volume from Sequence :  
 Actual Inj Volume : 15 µl  
 Inj Volume : 5 µl  
 Location : Vial 32  
 Seq. Line : 3  
 Last changed : 7/6/2013 9:54:10 AM by CE  
 Analysis Method : C:\HPCHEM\1\METHODS\IB-05-40.M  
 Last changed : 8/2/2014 12:33:23 AM by MK  
 (modified after loading)



Area Percent Report  
 Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 1: DADI A, Sig=250,10 Ref=360,100	12.829	MF	0.3098	24123.2e4	1297.61914	96.1899
Signal 2: DADI B, Sig=254,10 Ref=360,100	23.784	FM	0.3747	955.53381	42.49660	3.8101
Totals :				2.50787e4	1340.11574	

Results obtained with enhanced integrator!

Signal	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Signal 4: DADI D, Sig=230,10 Ref=360,100	12.830	MF	0.2556	1843.23779	120.16679	97.0832
	23.795	FM	0.3695	55.37868	2.49811	2.9168
Totals :				1898.61647	122.66490	

Results obtained with enhanced integrator!  
 Signal 5: DADI E, Sig=280,10 Ref=360,100  
 \*\*\* End of Report \*\*\*

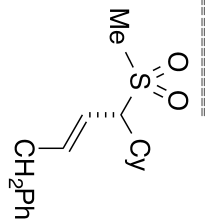


Table 5, entry 6 with (S,S)-L1