

# Lithium Enolates in the Enantioselective Construction of Tetrasubstituted Carbon Centers with Chiral Lithium Amides as Non-Covalent Stereodirecting Auxiliaries

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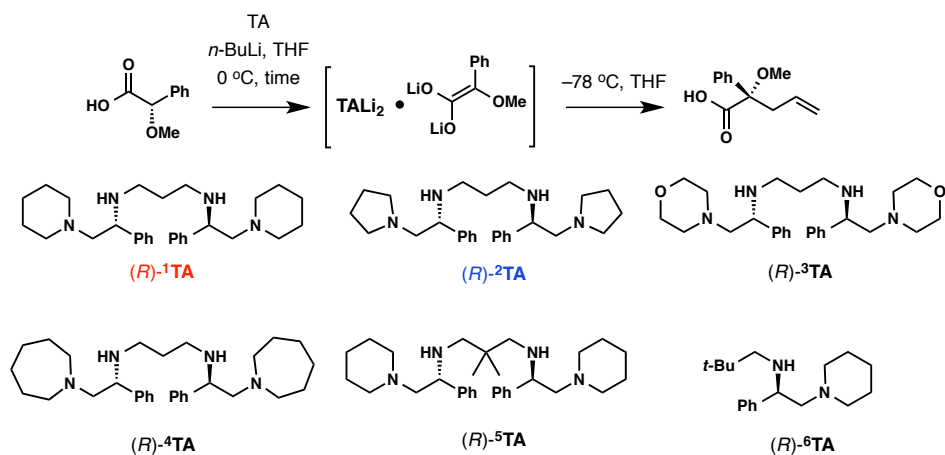
## Supplementary Information

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## I. Optimization of enantioselective allylation of 2-methoxy-2-phenylacetic acid

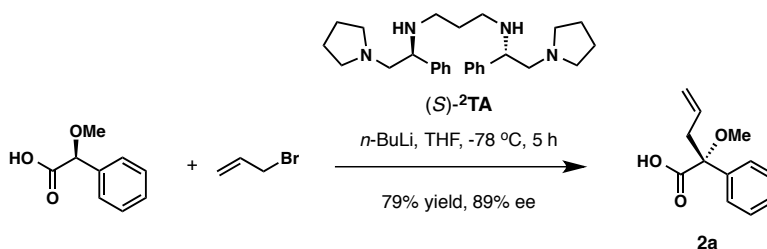
**Table S1.** Identification of optimal chiral lithium amides for the enantioselective allylation of (*S*)-2-methoxy-2-phenylacetic acid.<sup>a</sup>



entry	aggregation time at 0 °C (h)	( <i>R</i> )-TA	yield (%)	ee (%)
1 <sup>b</sup>	0.5	<sup>1</sup> TA	79	77
2	0.5	<sup>1</sup> TA	76	81
3 <sup>c</sup>	0.5	<sup>1</sup> TA	79	65
4	0.25	<sup>1</sup> TA	77	78
5	2	<sup>1</sup> TA	78	83
6	0.5	<sup>2</sup> TA	74	84
7	0.5	<sup>3</sup> TA	77	84
8	0.5	<sup>4</sup> TA	73	77
9	0.5	<sup>5</sup> TA	60	10
10	0.5	<sup>6</sup> TA	66	53
11	2	<sup>2</sup> TA	79	89
12	2	<sup>3</sup> TA	76	86
13 <sup>d</sup>	2	<sup>2</sup> TA	76	89

**a.** *n*-BuLi, (*S*)-2-methoxy-2-phenylacetic acid (0.50 mmol), and (*R*)-TA were combined at 0 °C in THF. After the indicated aggregate formation time, allyl bromide was added at -78 °C over 10 min. Enantiomeric excesses were measured using chiral HPLC analysis; all results in the Table are corrected to bases with the *R* configuration shown. **b.** *i*-Pr<sub>2</sub>NH (2 equiv) was used together with tetramine. **c.** The mixed aggregate was formed at -20 °C. **d.** (±)-2-Methoxy-2-phenylacetic acid was used.

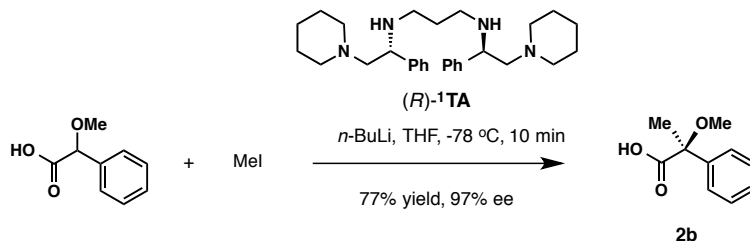
**II. General Information.** All reactions were carried out under an inert atmosphere of dry argon in oven or flame-dried glassware, unless the reaction procedure states otherwise. Tetrahydrofuran (THF) and ether (diethyl ether) were distilled from sodium-benzophenone in a continuous still under an atmosphere of argon. Dichloromethane, di-*iso*-propylamine and triethylamine were distilled from calcium hydride in a continuous still under an atmosphere of argon. Reaction temperatures were controlled by IKA ETS-D4 fuzzy thermo couples. Analytical thin-layer chromatography (TLC) was performed using pre-coated TLC plates with Silica Gel 60 F<sub>254</sub> (EMD no. 5715-7) and visualized using combinations of UV, anisaldehyde, ceric ammonium molybdate (CAM), potassium permanganate, and iodine staining. Flash column chromatography was performed using 40–63  $\mu\text{m}$  silica gel (EMD, Geduran, no. 1.11567.9026) as the stationary phase. Proton nuclear magnetic resonance spectra were recorded at 400, 500, and 600 MHz on Varian Unity Inova. Carbon nuclear magnetic resonance spectra were recorded at 100 MHz, 125 MHz, and 150 MHz on Varian Unity Inova, and Varian Unity Inova spectrometers. All chemical shifts were reported in  $\delta$  units relative to tetramethylsilane. Optical Rotations were measured on a Rudolph Autopol III polarimeter. High resolution mass spectral data were obtained by the Mass Spectrometry laboratory at the University of California, Santa Barbara.



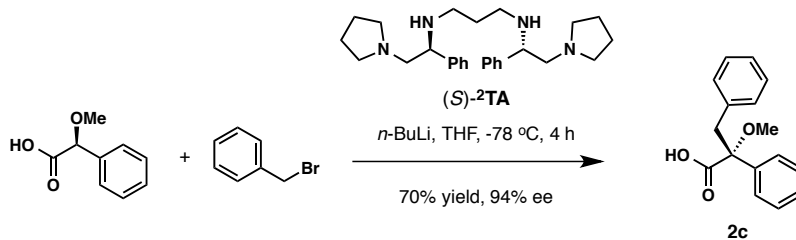
### General Procedure I:

**(R)-2-methoxy-2-phenylpent-4-enoic acid (2a).** A solution of *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol) and (*S*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv) in THF (3.5 mL) at 0 °C and the resulting mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to –78 °C and stirred for an additional 5 min. Allyl bromide (0.17 mL, 0.238 g, 1.96 mmol, 3.9 equiv) was added to the above reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 5 h before a quench with a mixture of THF–MeOH (3:1, 0.64 mL) at –78 °C. After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford product **2a** (81.9 mg, 0.397 mmol, 79% yield). Ee: 89% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA;

flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=30.1$  min (major);  $t_2=38.1$  min).  $[\alpha]_D^{27} -10.8$  ( $c$  1.67, MeOH).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.50–7.45 (m, 2H), 7.40–7.35 (m, 2H), 7.34–7.30 (m, 1H), 7.18 (brs, 1H), 5.77–5.67 (m, 1H), 5.23–5.12 (m, 2H), 3.25 (s, 3H), 3.18 (ddt,  $J$  = 14.9, 7.3, 1.3 Hz, 1H), 2.96 (ddt,  $J$  = 14.9, 6.6, 1.4 Hz, 1H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 175.1, 137.8, 131.2, 128.5, 128.4, 126.4, 119.3, 83.7, 51.4, 37.3. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{12}\text{H}_{14}\text{O}_3\text{Na}$ , 229.0841; found, 229.0831.

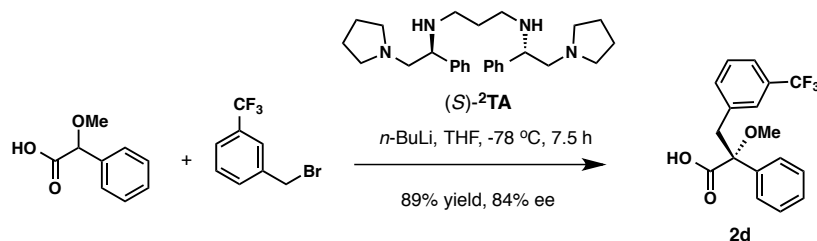


**(S)-2-Methoxy-2-phenylpropanoic acid (2b).** The title compound was prepared according to **general procedure I** using (+)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.81 mL, 2.47 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of iodomethane (0.12 mL, 0.274 g, 1.93 mmol, 3.9 equiv) at  $-78$  °C over 10 min. The reaction was quenched immediately, and product **2b** (69.2 mg, 0.384 mmol, 77% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane). Ee: 97% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_2=47.0$  min (major);  $t_1=40.7$  min).  $[\alpha]_D^{25} +32.1$  ( $c$  2.61, MeOH); *lit.*<sup>1</sup>  $[\alpha]_D^{23} +38$  ( $c$  1.0, MeOH).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.50–7.46 (m, 2H), 7.40–7.36 (m, 2H), 7.35–7.31 (m, 1H), 3.27 (s, 3H), 1.84 (s, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 175.8, 138.9, 128.6, 128.4, 126.2, 81.3, 51.7, 20.7. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{10}\text{H}_{12}\text{O}_3\text{Na}$ , 203.0684; found, 203.0664.

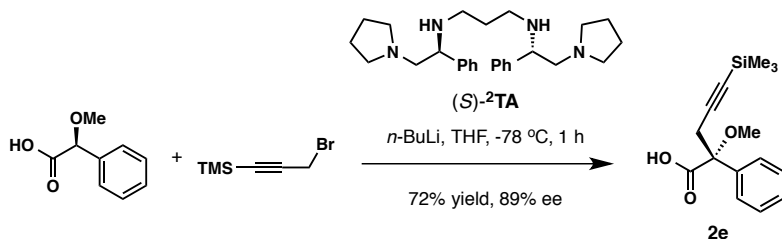


**(R)-2-Methoxy-2,3-diphenylpropanoic acid (2c).** The title compound was prepared according to **general procedure I** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)-**2TA** (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of benzyl bromide (0.23 mL, 0.331 g, 1.93 mmol, 4.0 equiv) at  $-78$  °C. The reaction was quenched after 4 h and product **2c** (89.2 mg,

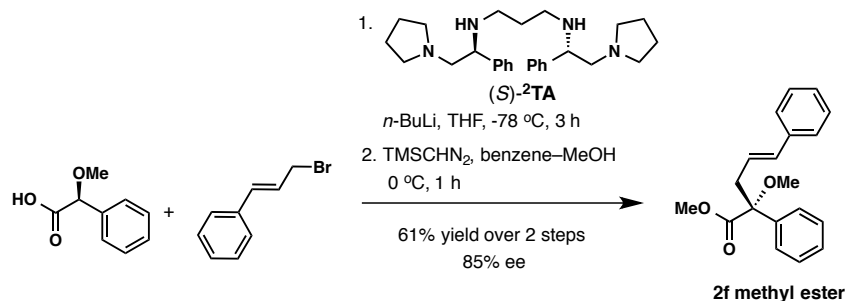
0.348 mmol, 70% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane). Ee: 94% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=43.9$  min (major);  $t_2=53.0$  min).  $[\alpha]_D^{22} -12.7$  (*c* 1.75, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 9.10 (brs, 1H), 7.52–7.47 (m, 2H), 7.43–7.34 (m, 3H), 7.27–7.23 (m, 3H), 7.22–7.17 (m, 2H), 3.71 (d, *J* = 14.4 Hz, 1H), 3.50 (d, *J* = 14.4 Hz, 1H), 3.32 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 175.0, 137.8, 135.0, 130.1, 128.6, 128.5, 128.1, 126.8, 126.7, 84.9, 52.0, 38.8. HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>16</sub>H<sub>16</sub>O<sub>3</sub>Na, 279.0997; found, 279.0984.



**(R)-2-Methoxy-2-phenyl-3-(3'-(trifluoromethyl)phenyl)propanoic acid (2d).** The title compound was prepared according to **general procedure I** using (±)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.81 mL, 2.47 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of 3-(trifluoromethyl)benzyl bromide (0.30 mL, 0.470 g, 1.96 mmol, 3.9 equiv) at  $-78$  °C. The reaction was quenched immediately, and product **2d** (0.145 g, 0.447 mmol, 89% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane). Ee: 84% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=30.3$  min (major);  $t_2=40.6$  min).  $[\alpha]_D^{22} +6.53$  (*c* 1.99, MeOH). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 9.43 (brs, 1 H), 7.51–7.46 (m, 1H), 7.45–7.42 (m, 2H), 7.42–7.34 (m, 4H), 7.34–7.31 (m, 2H), 3.70 (d, *J* = 14.4 Hz, 1H), 3.52 (d, *J* = 14.4 Hz, 1H), 3.34 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 175.3, 137.3, 136.1, 133.6 (q, *J* = 1.4 Hz), 130.3 (q, *J* = 32.1 Hz), 128.69, 128.65, 128.5, 126.98 (q, *J* = 3.9 Hz), 126.5, 124.1 (q, *J* = 272 Hz), 123.7 (q, *J* = 3.9 Hz), 84.9, 52.4, 39.4. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm):  $-62.8$ . HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>17</sub>H<sub>15</sub>O<sub>3</sub>F<sub>3</sub>Na, 347.0871; found, 347.0854.



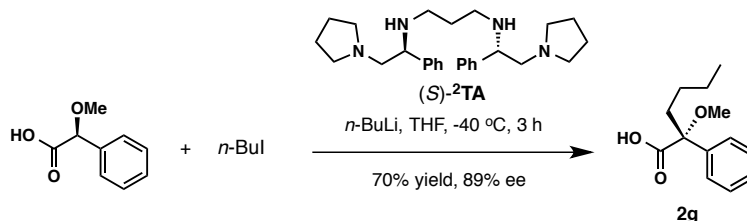
**(R)-2-Methoxy-2-phenyl-5-(trimethylsilyl)pent-4-ynoic acid (2e).** The title compound was prepared according to **general procedure I** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.81 mL, 2.47 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of 3-bromo-1-(trimethylsilyl)-1-propyne (0.191 g, 1.00 mmol, 2.0 equiv) at -78 °C. The reaction was quenched after 1 h, and product **2e** (99.5 mg, 0.360 mmol, 72% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane). Ee: 89% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 0.5 mL/min; detection at 215 nm;  $t_1=23.2$  min (major);  $t_2=26.8$  min).  $[\alpha]_D^{24} +5.6$  ( $c$  0.77, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 9.53 (brs, 1H), 7.47–7.43 (m, 2H), 7.39–7.31 (m, 3H), 3.37 (s, 3H), 3.33 (d,  $J$  = 17.2 Hz, 1H), 3.07 (d,  $J$  = 17.2 Hz, 1H), 0.10 (s, 9H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 174.6, 137.1, 128.6, 128.5, 126.2, 100.0, 88.9, 83.1, 52.2, 26.2, -0.2. HRMS-ESI ( $m/z$ ): [M+Na]<sup>+</sup> calcd for C<sub>15</sub>H<sub>20</sub>O<sub>3</sub>NaSi, 299.1079; found, 299.1090.



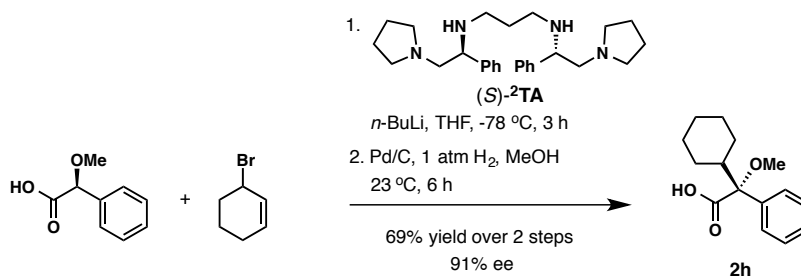
**(2R,4E)-2-Methoxy-2,5-diphenylpent-4-enoic acid (2f).** The alkylation product was prepared according to **general procedure I** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of 3-bromo-1-phenyl-1-propene (0.191 g, 1.00 mmol, 2.0 equiv) in THF (0.5 mL) at -78 °C. The reaction was quenched after 3 h, and product **2f** (0.117 g) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane) contaminated with inseparable mixture.

**(2S,4E)-Methyl 2-methoxy-2,5-diphenylpent-4-enoate (2f methyl ester).** A solution of TMSCHN<sub>2</sub> in hexanes (1.2 mL, 0.65 M, 0.780 mmol) was added dropwise to a solution of above product **2f** (0.117 g) in a mixture of benzene-MeOH (4:1, 5.0 mL) at 0 °C. The resultant mixture was stirred at the same temperature for 1 h. The solvent was removed on a rotary evaporator and the residue was purified by column chromatography on silica gel (9% ethyl acetate in hexanes) to afford the product **2f methyl ester** (90.9 mg, 0.307 mmol, 61% yield over 2 steps). Ee: 85% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=12.6$  min (major);  $t_2=14.2$  min).  $[\alpha]_D^{19} +37.1$  ( $c$  2.00, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.52–7.48 (m, 2H), 7.40–7.36 (m, 2H), 7.34–7.24 (m, 5H), 7.21–

7.17 (m, 1H), 6.45 (virt. dt,  $J = 15.9, 1.4$  Hz, 1H), 6.06 (ddd,  $J = 15.9, 7.8, 6.3$  Hz, 1H), 3.73 (s, 3H), 3.31 (s, 3H), 3.24 (ddd,  $J = 15.1, 7.9, 1.3$  Hz, 1H), 3.11 (ddd,  $J = 15.1, 6.3, 1.7$  Hz, 1H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 172.7, 139.0, 137.3, 133.5, 128.4, 128.0, 127.2, 126.24, 126.15, 123.6, 84.4, 52.4, 52.0, 38.2. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{19}\text{H}_{20}\text{O}_3\text{Na}$ , 319.1310; found, 319.1309.



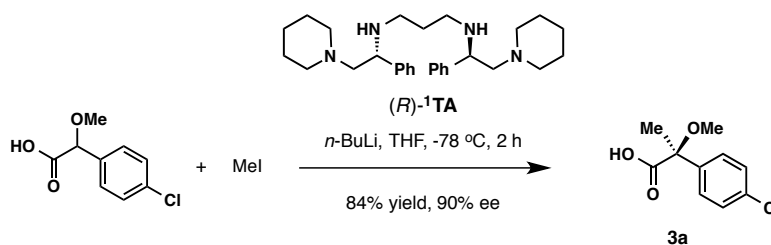
**(R)-2-Methoxy-2-phenylhexanoic acid (2g).** The title compound was prepared according to **general procedure I** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)- $^2\text{TA}$  (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.79 mL, 2.52 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of iodobutane (0.23 mL, 0.317 g, 2.00 mmol, 4.0 equiv) at  $-78$  °C. The reaction was quenched after stirring at  $-40$  °C for 3 h, and product **2g** (77.6 mg, 0.349 mmol, 70% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane). Ee: 89% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1 mL/min; detection at 215 nm;  $t_1=22.1$  min (major);  $t_2=29.9$  min).  $[\alpha]_{\text{D}}^{20} -42.3$  ( $c$  1.89,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 9.22 (brs, 1H), 7.50–7.46 (m, 2H), 7.40–7.35 (m, 2H), 7.34–7.29 (m, 1H), 3.20 (s, 3H), 2.41 (ddd,  $J = 14.1, 11.4, 4.6$  Hz, 1H), 2.13 (ddd,  $J = 14.1, 11.9, 4.2$  Hz, 1H), 1.44–1.18 (m, 4H), 0.92 (t,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 175.7, 138.2, 128.5, 128.3, 126.4, 83.9, 51.1, 32.1, 25.1, 22.7, 13.9. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{13}\text{H}_{17}\text{O}_3$ , 221.1178; found, 221.1181.



**(R)-2-Cyclohexyl-2-methoxy-2-phenylacetic acid (2h).** A solution of *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol) and (*S*)- $^2\text{TA}$  (0.217 g, 0.515 mmol, 1.03 equiv) in THF (3.5 mL) at 0 °C and the reaction mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to  $-78$  °C and stirred for an additional 5 min. 3-

bromocyclohexene (0.17 mL, 0.238 g, 1.48 mmol, 3.0 equiv) was added to the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 3 h before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at  $-78\text{ }^{\circ}\text{C}$ . After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford the diastereomeric product **S-1** (0.106 g, 0.430 mmol, 86% yield). The product was directly submitted to the next step without further characterization.

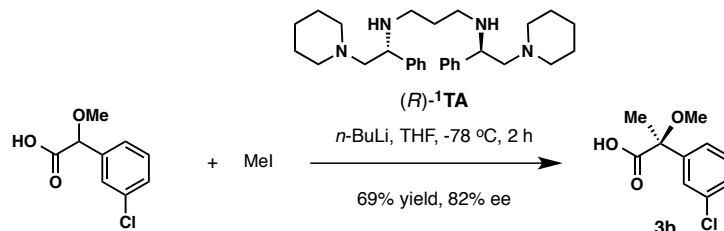
A solution of above compound **S-1** (0.106 g, 0.430 mmol) and 10% Pd/C (27.2 mg, 25.7  $\mu\text{mol}$ ) in methanol (5 mL) was stirred at  $23\text{ }^{\circ}\text{C}$  under 1 atm of hydrogen atmosphere for 6 h. The mixture was then filtered through a pad of celite and rinsed with ethyl acetate. The combined filtrate was concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford the product **2h** (85.7 mg, 0.345 mmol, 69% yield over two steps). Ee: 91% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=16.5$  min (major);  $t_2=20.2$  min).  $[\alpha]_{\text{D}}^{20} +8.3$  (*c* 1.99,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  (ppm): 7.47 (d, *J* = 7.1 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.28 (t, *J* = 7.3 Hz, 1H), 3.17 (s, 3H), 2.09 (*virt. tt*, *J* = 12.0, 2.9 Hz, 1H), 1.93 (d, *J* = 12.5 Hz, 1H), 1.73 (d, *J* = 13.2 Hz, 1H), 1.70–1.57 (m, 2H), 1.54 (d, *J* = 12.9 Hz, 1H), 1.30–1.14 (m, 2H), 1.07–0.88 (m, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  (ppm): 174.8, 138.5, 129.3, 128.6, 128.6, 89.6, 53.9, 48.3, 29.3, 28.7, 27.73, 27.70, 27.6. HRMS-ESI (*m/z*):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{15}\text{H}_{19}\text{O}_3$ , 247.1334; found, 247.1328.



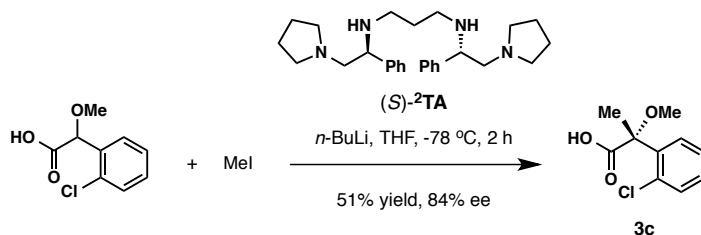
**(S)-2-(4-chlorophenyl)-2-methoxypropanoic acid (3a)**. The title compound was prepared according to **general procedure I** using 2-(4-chlorophenyl)-2-methoxyacetic acid (0.101 g, 0.500 mmol), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of iodomethane (0.12 mL, 0.331 g, 1.93 mmol, 3.9 equiv) at  $-78\text{ }^{\circ}\text{C}$ . The reaction was quenched after 2 h, and product **3a** (90.1 mg, 0.419 mmol, 84% yield) was obtained after purification by column chromatography on silica gel (3% methanol in dichloromethane). Ee: 90% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=34.6$  min (major);  $t_2=30.1$  min).  $[\alpha]_{\text{D}}^{23} +39.9$  (*c* 1.0,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 9.50



(brs, 1H), 7.43 (d,  $J = 8.6$  Hz, 2H), 7.34 (d,  $J = 8.6$  Hz, 2H), 3.28 (s, 3H), 1.81 (s, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 176.1, 137.7, 134.5, 128.7, 127.6, 80.9, 51.8, 20.9. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{10}\text{H}_{10}\text{ClO}_3$ , 213.0318; found, 213.0314.

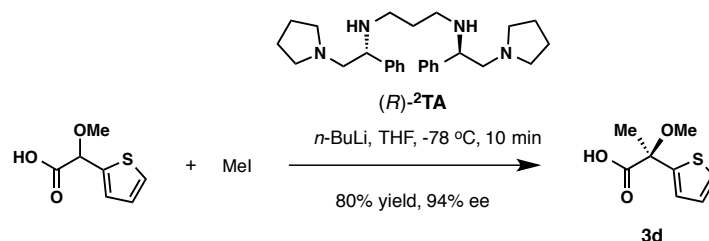


**(S)-2-(3-chlorophenyl)-2-methoxypropanoic acid (3b).** The title compound was prepared according to **general procedure I** using (2-(3-chlorophenyl)-2-methoxyacetic acid (0.101 g, 0.500 mmol), (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of iodomethane (0.12 mL, 0.331 g, 1.93 mmol, 3.9 equiv) at  $-78$  °C. The reaction was quenched after 2 h, and product **3b** (74.1 mg, 0.344 mmol, 69% yield) was obtained after purification by column chromatography on silica gel (40% diethyl ether in hexanes with 0.5% acetic acid). Ee: 82% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=34.8$  min (major);  $t_2=29.1$  min).  $[\alpha]_{\text{D}}^{23} +38.5$  ( $c$  1.0,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.48 (s, 1H), 7.38–7.34 (m, 1H), 7.33–7.29 (m, 2 H), 3.30 (s, 3H), 1.83 (s, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 175.5, 141.3, 134.7, 129.6, 128.6, 126.5, 124.4, 80.9, 51.9, 20.9. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{10}\text{H}_{10}\text{ClO}_3$ , 213.0318; found, 213.0320.

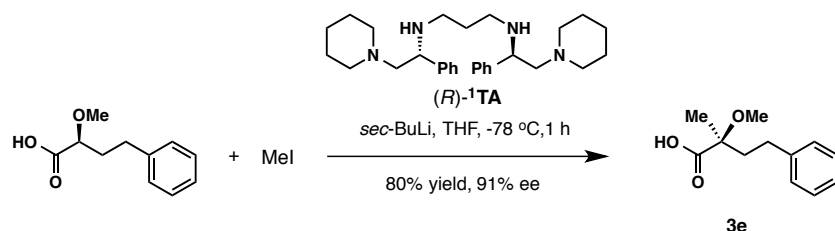


**(R)-2-(2-chlorophenyl)-2-methoxypropanoic acid (3c).** The title compound was prepared according to **general procedure I** using (2-(2-chlorophenyl)-2-methoxyacetic acid (0.101 g, 0.500 mmol), (*S*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of iodomethane (0.12 mL, 0.331 g, 1.93 mmol, 3.9 equiv) at  $-78$  °C. The reaction was quenched after 2 h, and product **3c** (55.1 mg, 0.256 mmol, 51% yield) was obtained after purification by column chromatography on silica gel (40% diethyl ether in hexanes with 0.5% acetic acid). Ee: 84% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=60.7$  min (major);  $t_2=49.1$  min).  $[\alpha]_{\text{D}}^{25} -22.3$  ( $c$  0.33,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR

(600 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.84 (brs, 1 H), 7.57 (d,  $J$  = 7.2 Hz, 1H), 7.39 (d,  $J$  = 7.8 Hz, 1H), 7.33–7.27 (m, 2H), 3.19 (s, 3H), 1.83 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 174.8, 136.0, 133.3, 130.9, 129.9, 128.9, 126.7, 80.6, 51.3, 20.9. HRMS-ESI ( $m/z$ ): [M-H]<sup>-</sup> calcd for C<sub>10</sub>H<sub>10</sub>ClO<sub>3</sub>, 213.0318; found, 213.0318.

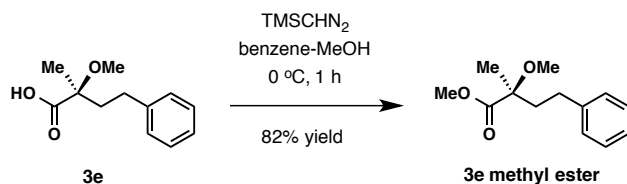


**(R)-2-methoxy-2-(thiophen-2-yl)propanoic acid (3d).** The title compound was prepared according to **general procedure I** using 2-methoxy-2-(thiophen-2-yl)acetic acid (83.1 mg, 0.500 mmol), (*R*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of iodomethane (0.12 mL, 0.331 g, 1.93 mmol, 3.9 equiv) at -78 °C. The reaction was quenched after 10 min and product **3d** (89.2 mg, 0.348 mmol, 80% yield) was obtained after purification by column chromatography on silica gel (3% methanol in dichloromethane). Ee: 94% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1$ =53.9 min (major);  $t_2$ =50.4 min).  $[\alpha]_D^{24}$  -15.1 ( $c$  = 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.33 (d,  $J$  = 5.1 Hz, 1H), 7.11 (d,  $J$  = 3.6 Hz, 1H), 7.00 (t,  $J$  = 4.3 Hz, 1H), 3.33 (s, 3H), 1.90 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 174.5, 142.7, 126.9, 126.43, 126.37, 79.6, 52.0, 22.2. HRMS-ESI ( $m/z$ ): [M-H]<sup>-</sup> calcd for C<sub>8</sub>H<sub>9</sub>O<sub>3</sub>S, 185.0272; found, 185.0271.

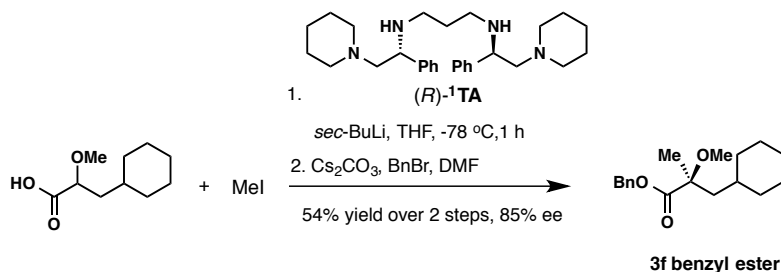


**(S)-2-methoxy-2-methyl-4-phenylbutanoic acid (3e).** A solution of *sec*-BuLi (1.38 mL, 1.45 M in cyclohexane, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (*S*)-2-methoxy-4-phenylbutyric acid (97.1 mg, 0.500 mmol) and (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv) in THF (4 mL) at 0 °C and the reaction mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to -78 °C and stirred for an additional 5 min. Iodomethane (0.12 mL, 0.274 g, 1.93 mmol, 3.9 equiv) was added to the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 50 min before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at -78 °C. After 5 min, the reaction

mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with a mixture of 1 M aqueous solution of HCl and drops of saturated aqueous solution of sodium sulfite, brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford the pure product **3e** (83.1 mg, 0.400 mmol, 80% yield).  $[\alpha]_D^{23}$  -2.0 (*c* 1.47, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 9.08 (brs, 1H), 7.31–7.25 (m, 2H), 7.21–7.16 (m, 3H), 3.39 (s, 3H), 2.71 (ddd, *J* = 13.8, 12.2, 5.1 Hz, 1H), 2.60 (ddd, *J* = 13.8, 12.2, 5.0 Hz, 1H), 2.15 (ddd, *J* = 14.2, 12.2, 5.0 Hz, 1H), 2.05 (ddd, *J* = 14.2, 12.2, 5.1 Hz, 1H), 1.51 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 178.1, 141.2, 128.4, 128.3, 126.0, 79.9, 51.3, 38.6, 29.8, 20.9. HRMS-ESI (*m/z*): [M-H]<sup>-</sup> calcd for C<sub>12</sub>H<sub>15</sub>O<sub>3</sub>, 207.1021; found, 207.1019.

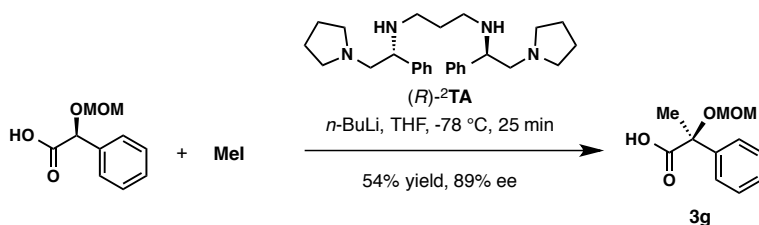


**(S)-Methyl 2-methoxy-2-methyl-4-phenylbutanoate (3e methyl ester).** A solution of TMSCHN<sub>2</sub> (0.16 mL, 1.1 M in hexanes, 0.176 mmol) was added dropwise to a solution of carboxylic acid **3e** (18.7 mg, 89.9 μmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at 0 °C. The resultant mixture was stirred at the same temperature for 1 h. The solvent was removed on a rotary evaporator and the residue was purified by column chromatography on silica gel (10% ethyl acetate in hexanes) to afford the product **3e methyl ester** (16.4 mg, 73.9 μmol, 82% yield). Ee: 83% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm; *t*<sub>1</sub>=7.8 min (major); *t*<sub>2</sub>=10.5 min).  $[\alpha]_D^{24}$  -13.3 (*c* 0.49, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 7.29–7.25 (m, 2H), 7.20–7.15 (m, 3H), 3.74 (s, 3H), 3.33 (s, 3H), 2.70 (ddd, *J* = 13.7, 11.8, 5.5 Hz, 1H), 2.57 (ddd, *J* = 13.7, 11.8, 5.3 Hz, 1H), 2.12–1.99 (m, 2H), 1.47 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 174.5, 141.6, 128.4, 128.3, 125.9, 80.0, 52.1, 51.9, 39.8, 29.8, 20.9. LRMS-CI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>13</sub>H<sub>19</sub>O<sub>3</sub>, 223; found 223.

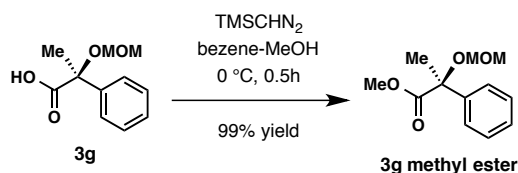


**(S)-3-Cyclohexyl-2-methoxy-2-methylpropanoic acid (3f)**. A solution of *sec*-BuLi (1.4 mL, 1.43 M in cyclohexane, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of 3-cyclohexyl-2-methoxypropionic acid (93.2 mg, 0.500 mmol) and (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv) in THF (4 mL) at 0 °C and the reaction mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to -78 °C and stirred for an additional 5 min. Iodomethane (0.16 mL, 0.365 g, 2.57 mmol, 5.1 equiv) was added to the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 50 min before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at -78 °C. After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with a mixture of 1 M aqueous solution of HCl and drops of saturated aqueous solution of sodium sulfite, brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford the product **3f** (65.9 mg, 0.329 mmol, 66% yield) together with inseparable starting material 3-cyclohexyl-2-methoxypropionic acid (8.2 mg, 43.9 μmol, 9% yield).

**(S)-Benzyl 3-cyclohexyl-2-methoxy-2-methylpropanoate (3f benzyl ester)**. Cesium carbonate (0.240 g, 0.737 mmol) and benzyl bromide (90 μL, 0.129 g, 0.757 mmol) were added sequentially to a solution of the above mixture (74.1 mg) in DMF (4 mL). The resultant mixture was stirred at 23 °C for 16 h before a quench with water. Then the reaction mixture was extracted with 10% ethyl acetate in hexanes. The combined organic phase was sequentially washed with water (three times), brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (8% ethyl acetate in hexanes) to afford the product **3f benzyl ester** (78.0 mg, 0.269 mmol, 82% yield) together with benzyl 3-cyclohexyl-2-methoxypropionate (10.3 mg, 37.3 μmol, 85% yield). The analytically pure product **3f benzyl ester** was obtained using preparative HPLC (YMC-Pack-SIL 250x30 mm; 10% MTBE in hexanes; flow rate = 20 mL/min; detection at 215 nm, t = 15 min). Ee: 85% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm; t<sub>1</sub>=6.1 min (major); t<sub>2</sub>=5.7 min). [α]<sub>D</sub><sup>23</sup> -35.3 (c 1.12, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 7.40–7.29 (m, 5H), 5.17 (s, 2H), 3.25 (s, 3H), 1.70–1.53 (m, 7H), 1.41 (s, 3H), 1.43–1.34 (m, 1 H), 1.21–1.02 (m, 3H), 0.94–0.80 (m, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 174.4, 135.8, 128.5, 128.4, 128.2, 80.2, 66.6, 51.7, 45.8, 34.6, 34.2, 33.2, 26.30, 26.27, 26.2, 21.2. HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>18</sub>H<sub>26</sub>O<sub>3</sub>Na, 313.1780; found 313.1771.

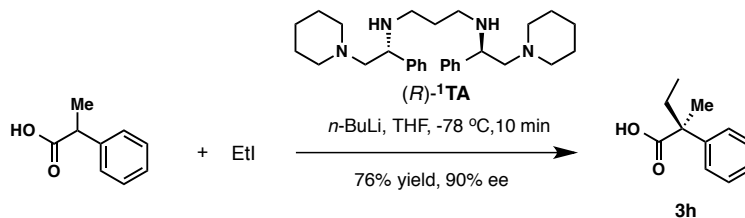


**(S)-2-(methoxymethoxy)-2-phenylpropanoic acid (3g).** A solution of *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (S)-2-(methoxymethoxy)-2-phenylacetic acid (98.1 mg, 0.500 mmol) and (R)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv) in THF (4.0 mL) at 0 °C and the reaction mixture was stirred at this temperature for 2 hours. The reaction mixture was then cooled to -78 °C and stirred for an additional 5 min. Methyl iodide (0.284 g, 2.00 mmol, 4.0 equiv) was then added to the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 15 min before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at -78 °C. After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford the pure product **3g** (56.5 mg, 0.269 mmol, 54% yield).  $[\alpha]_{\text{D}}^{26} +28.9$  (*c* 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.55–7.48 (m, 2H), 7.43–7.36 (m, 2 H), 7.35–7.29 (m, 1H), 4.76 (d, *J* = 7.2 Hz, 1H), 4.74 (d, *J* = 7.2 Hz, 1H), 3.42 (s, 3H), 1.91 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 176.1, 139.5, 128.6, 128.5, 126.0, 92.8, 81.6, 56.2, 23.1. HRMS-CI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>11</sub>H<sub>15</sub>O<sub>4</sub>, 211.0970; found, 211.0979.

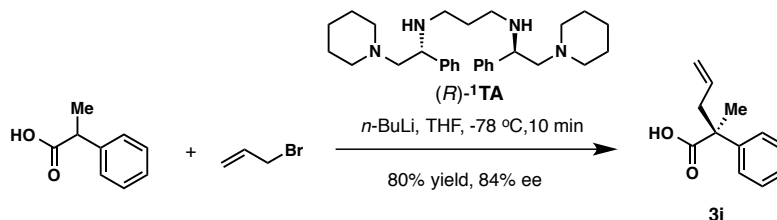


**(S)-Methyl 2-(methoxymethoxy)-2-phenylpropanoate (3g methyl ester).** A solution of TMSCHN<sub>2</sub> in hexane (0.31 mL, 1.03 M, 0.308 mmol) was added dropwise to a solution of carboxylic acid **3g** (32.4 mg, 0.154 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at 0 °C. The resultant mixture was stirred at the same temperature for 0.5 h. The solvent was removed on a rotary evaporator and the residue was purified by column chromatography on silica gel (20% ethyl acetate in hexanes) to afford the product **3g methyl ester** (34.3 mg, 0.153 mmol, 99% yield). Ee: 89% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1$ =10.8 min (major);  $t_2$ =8.4 min).  $[\alpha]_{\text{D}}^{25} +4.6$  (*c* 1.0, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.51–7.45 (m, 2H), 7.38–7.33 (m, 2H), 7.32–7.27 (m, 1H), 4.81 (d, *J* = 7.3 Hz, 1H), 4.79 (d, *J* = 7.3 Hz, 1H), 3.72 (s, 3H), 3.42 (s, 3H), 1.86 (s, 3H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.6, 141.3, 128.3, 127.9, 125.5, 92.8, 81.2, 56.0, 52.5, 23.8. LRMS-FD ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{12}\text{H}_{16}\text{O}_4$ , 224; found 224.

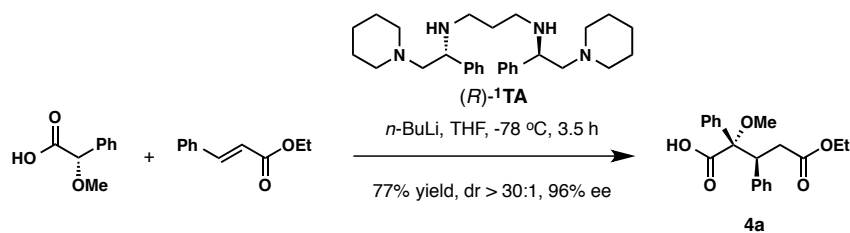


**(S)-2-Methyl-2-phenylbutanoic acid (3h).** A solution of *n*-BuLi (0.55 mL, 2.46 M in hexanes, 1.35 mmol, 4.0 equiv) was added dropwise to a solution of 2-phenylpropanoic acid (51.0 mg, 0.338 mmol) and (*R*)- $^1\text{TA}$  (0.155 g, 0.346 mmol, 1.03 equiv) in THF (2.3 mL) at 0  $^\circ\text{C}$ . The reaction mixture was warmed to room temperature and stirred for 1 h. The reaction mixture was then cooled to  $-78$   $^\circ\text{C}$  and stirred for an additional 10 min. Iodoethane (0.11 mL, 1.35 mmol, 4.0 equiv) was added to the reaction mixture dropwise over 10 min. The resultant mixture was immediately quenched with a mixture of THF-MeOH (3:1, 1.0 mL) at  $-78$   $^\circ\text{C}$ . After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was purified by column chromatography on silica gel (40% diethyl ether in hexanes with 0.5% acetic acid) to afford the pure product as a white crystalline solid **3h** (46.1 mg, 0.257 mmol, 76% yield). Ee: 90% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=22.6$  min (major);  $t_2=19.9$  min).  $[\alpha]_{\text{D}}^{20} +24.2$  (*c* 1.0, PhH); *lit*<sup>2</sup>:  $[\alpha]_{\text{D}}^{20} +30.2$  (*c* 4.5, PhH).  $^1\text{H}$  NMR (500 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  (ppm): 7.23–7.20 (m, 2H), 7.05–7.01 (m, 2H), 6.98–6.94 (m, 1H), 2.00–1.92 (m, 1H), 1.83–1.75 (m, 1H), 1.36 (s, 3H), 0.64 (t, *J* = 7.4 Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  (ppm): 183.4, 143.3, 128.7, 127.0, 126.6, 50.8, 32.0, 21.8, 9.2. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{11}\text{H}_{13}\text{O}_2\text{Na}$ , 177.0916; found, 177.0911.



**(S)-2-Methyl-2-phenylpent-4-enoic acid (3i).** A solution of *n*-BuLi (0.55 mL, 2.46 M in hexanes, 1.35 mmol, 4.0 equiv) was added dropwise to a solution of 2-phenylpropanoic acid (51 mg, 0.338 mmol) and (*R*)- $^1\text{TA}$  (0.155 g, 0.346 mmol, 1.03 equiv) in THF (2.3 mL) at 0  $^\circ\text{C}$ .

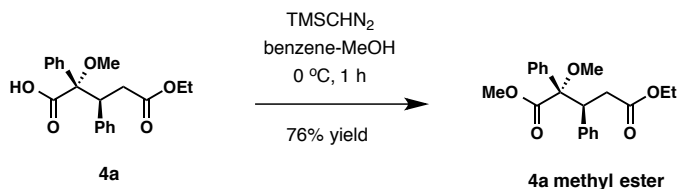
The reaction mixture was warmed to room temperature and stirred for 1 hour. The reaction mixture was then cooled to  $-78\text{ }^{\circ}\text{C}$  and stirred for an additional 10 min. Allylbromide (0.12 mL, 1.35 mmol, 4.0 equiv) was added to the reaction mixture dropwise over 10 min. The resultant mixture was immediately quenched with a mixture of THF-MeOH (3:1, 1.0 mL) at  $-78\text{ }^{\circ}\text{C}$ . After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was purified by column chromatography on silica gel (40% diethyl ether in hexanes with 0.5% acetic acid) to afford the pure product and a colorless film (51 mg, 0.270 mmol, 80% yield). Ee: 84% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=34.1$  min (major);  $t_2=32.4$  min).  $[\alpha]_{\text{D}}^{20} +50.5$  (*c* 1.0, EtOH).  $^1\text{H}$  NMR (500 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  (ppm): 7.23–7.18 (m, 2H), 7.05–7.00 (m, 2H), 6.98–6.93 (m, 1H), 5.52 (ddt,  $J = 17.2, 10.1, 7.2$  Hz, 1H), 5.09 (m, 2H), 2.73 (ddt,  $J = 13.8, 7.4, 1.2$  Hz, 1H), 2.52 (ddt,  $J = 13.8, 17.1, 1.2$ , 1H), 1.40 (s, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  (ppm): 182.8, 142.8, 134.1, 128.7, 127.2, 126.5, 118.6, 50.0, 43.8, 22.2. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{12}\text{H}_{13}\text{O}_2$ , 189.0916; found, 189.0913.



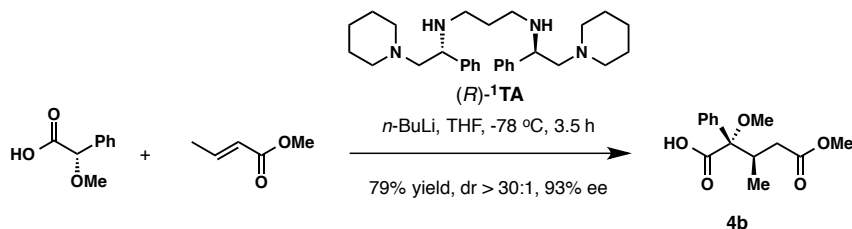
## General Procedure II:

**(2*S*,3*S*)-5-Ethoxy-2-methoxy-5-oxo-2,3-diphenylpentanoic acid (4a).** A solution of *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), and (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv) in THF (3.5 mL) at 0  $^{\circ}\text{C}$  and the reaction mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to  $-78\text{ }^{\circ}\text{C}$  and stirred for an additional 5 min. A solution of (*E*)-ethyl cinnamate (85.0  $\mu\text{L}$ , 88.9 mg, 0.505 mmol, 1.01 equiv) in THF (0.30 mL, plus 2  $\times$  0.10 mL) was added to the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 3.5 h before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at  $-78\text{ }^{\circ}\text{C}$ . After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried

over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (2–4% methanol in dichloromethane) to afford product **4a** (0.132 g, 0.384 mmol, 77% yield). [ $\alpha$ ]<sub>D</sub><sup>25</sup> –53.5 (*c* 0.57, MeOH). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.97 (brs, 1H), 7.39–7.30 (m, 5H), 7.23–7.17 (m, 3H), 7.16–7.11 (m, 2H), 4.11 (dd, *J* = 11.3, 3.7 Hz, 1H), 3.99–3.84 (m, 2H), 3.22 (s, 3H), 2.99 (dd, *J* = 16.3, 11.3 Hz, 1H), 2.80 (dd, *J* = 16.3, 3.7 Hz, 1H), 1.02 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 175.2, 172.1, 137.6, 135.0, 129.8, 128.4, 128.2, 128.0, 127.7, 127.3, 87.9, 60.3, 53.9, 49.7, 36.1, 13.9. HRMS–ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>20</sub>H<sub>22</sub>O<sub>5</sub>Na, 365.1365; found, 365.1352.



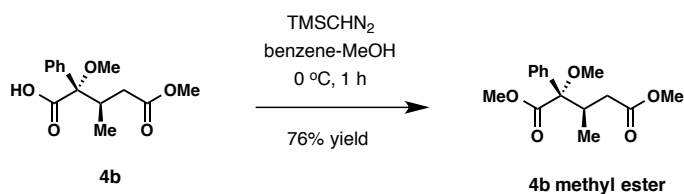
**(2*S*,3*S*)-5-Ethyl 1-methyl 2-methoxy-2,3-diphenylpentanedioate (4a methyl ester).** A solution of TMSCHN<sub>2</sub> (0.13 mL, 0.57 M in hexanes, 74.1  $\mu$ mol) was added dropwise to a solution of carboxylic acid **4a** (12.1 mg, 35.4  $\mu$ mol) in a mixture of benzene–MeOH (4:1, 1.0 mL) at 0 °C. The resultant mixture was stirred at the same temperature for 1 h. The solvent was removed on a rotary evaporator and the residue was purified by column chromatography on silica gel (9% ethyl acetate in hexanes) to afford the product **4a methyl ester** (12.2 mg, 34.2  $\mu$ mol, 97% yield). Ee: 96% (Chiralcel® OD–H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm; *t*<sub>1</sub>=14.5 min; *t*<sub>2</sub>=16.8 min). [ $\alpha$ ]<sub>D</sub><sup>26</sup> –42.2 (*c* 0.60, CHCl<sub>3</sub>). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.28–7.24 (m, 3H), 7.23–7.19 (m, 2H), 7.17–7.14 (m, 3H), 7.00–6.96 (m, 2H), 4.02 (dd, *J* = 11.0, 4.3 Hz, 1H), 3.95–3.83 (m, 2H), 3.80 (s, 3H), 3.22 (s, 3H), 2.81 (dd, *J* = 16.0, 11.0 Hz, 1H), 2.73 (dd, *J* = 16.0, 4.3 Hz, 1H), 1.00 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 172.0, 171.7, 137.9, 135.7, 129.9, 128.3, 128.0, 127.6, 127.5, 127.1, 88.5, 60.2, 54.4, 51.9, 51.2, 35.7, 13.9. LRMS–ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>19</sub>H<sub>20</sub>O<sub>4</sub>Na, 379, found 379.



**(2*S*,3*R*)-2,5-Dimethoxy-3-methyl-5-oxo-2-phenylpentanoic acid (4b).** The title compound was prepared according to **general procedure II** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in

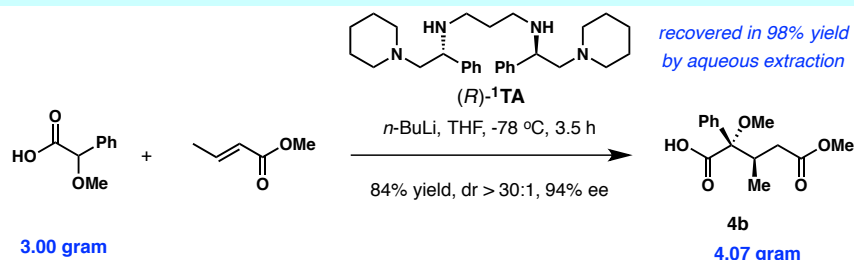


hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-methyl crotonate (50.1 mg, 0.500 mmol, 1.0 equiv) in THF (0.50 mL) at  $-78\text{ }^{\circ}\text{C}$ . The reaction was quenched after 3.5 h, and product **4b** (0.105 g, 0.394 mmol, 79% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_{\text{D}}^{26} -42.4$  (*c* 0.92,  $\text{CHCl}_3$ ).  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.47–7.42 (m, 2H), 7.41–7.37 (m, 2H), 7.36–7.32 (m, 1H), 3.64 (s, 3H), 3.19 (s, 3H), 3.10–2.99 (m, 1H), 2.52 (dd, *J* = 16.4, 2.7 Hz, 1H), 2.16 (dd, *J* = 16.4, 10.7 Hz, 1H), 1.07 (d, *J* = 6.7 Hz, 3H).  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 174.6, 173.5, 135.1, 128.6, 128.4, 128.1, 87.6, 53.0, 51.7, 37.1, 36.2, 15.2. HRMS-ESI (*m/z*):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{14}\text{H}_{18}\text{O}_5\text{Na}$ , 289.1052; found, 289.1039.

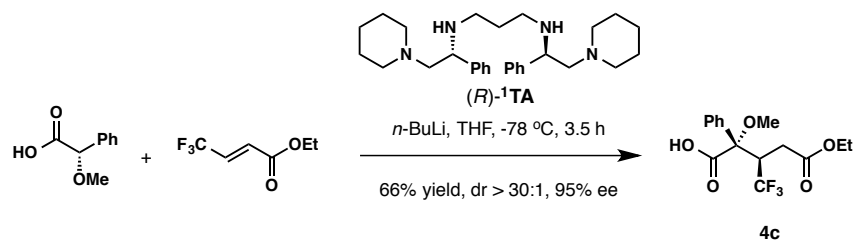


**(2*S*,3*R*)-Dimethyl 2-methoxy-3-methyl-2-phenylpentanedioate (4b methyl ester)**. The title compound was prepared using carboxylic acid **4b** (22.3 mg, 83.7  $\mu\text{mol}$ ),  $\text{TMSCHN}_2$  (0.30 mL, 0.57 M in hexanes, 0.171 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at  $0\text{ }^{\circ}\text{C}$  for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **4b methyl ester** (19.5 mg, 69.6  $\mu\text{mol}$ , 83% yield). Ee: 93% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=9.9$  min (major);  $t_2=11.8$  min).  $[\alpha]_{\text{D}}^{25} -28.9$  (*c* 0.96,  $\text{CHCl}_3$ ).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.41–7.28 (m, 5H), 3.84 (s, 3H), 3.62 (s, 3H), 3.20 (s, 3H), 2.92 (dq, *J* = 10.7, 6.7, 3.0 Hz, 1H), 2.47 (dd, *J* = 15.8, 3.0 Hz, 1H), 1.91 (dd, *J* = 15.8, 10.7 Hz, 1H), 0.96 (d, *J* = 6.7 Hz, 3H).  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.4, 171.8, 136.1, 128.0, 128.0, 127.9, 88.1, 53.8, 52.0, 51.5, 38.4, 36.8, 15.5. LRMS-ESI (*m/z*):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{15}\text{H}_{20}\text{O}_5\text{Na}$ , 303; found, 303.

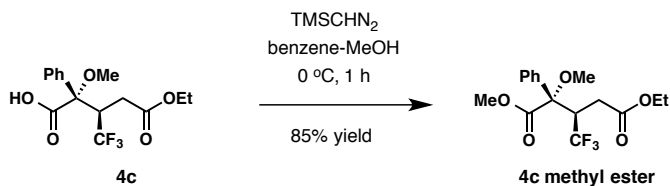
#### 4-Gram scale procedure for conjugate addition with the recovery of chiral tetramine:



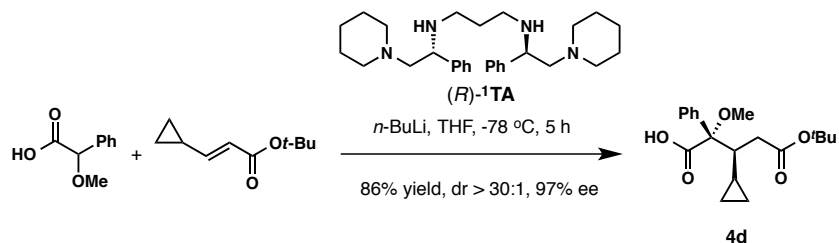
A three-neck round-bottom flask was equipped with a gas-inlet adapter, glass-stopper, and thermometer adapter fitted with a low-temperature thermometer. After flame drying under vacuum and back filling with argon, the flask was charged with ( $\pm$ )-2-methoxy-2-phenylacetic acid (3.00 g, 18.1 mmol), and (*R*)-<sup>1</sup>TA (8.35 g, 18.6 mmol, 1.03 equiv) and THF (126 mL) under a positive pressure of argon gas. The reaction mixture was cooled in an ice-water bath to 0 °C, and a solution of *n*-BuLi (29.0 mL, 2.50 M in hexanes, 72.2 mmol, 4.0 equiv) over 30 min, keeping the internal reaction temperature below 15 °C. After stirring in an ice-water bath for 2 h, the reaction mixture was then cooled to -78 °C and stirred for an additional 5 min. A solution of (*E*)-methyl crotonate (1.93 mL, 1.82 g, 18.2 mmol, 1.01 equiv) in THF (16 mL, plus 2 × 1 mL rinses) was added to the reaction mixture dropwise over 30 min. The resultant mixture was stirred for additional 3 h before a quench with a mixture of THF-MeOH (3:1, 23.4 mL) at -78 °C. After 5 min, the reaction mixture was acidified with 6 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (2% methanol in dichloromethane) to afford product **4b** (4.07 g, 15.3 mmol, 84% yield). Ee: 94% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm; *t*<sub>1</sub>=9.9 min (major); *t*<sub>2</sub>=11.8 min).



**(2*S*,3*R*)-5-Ethoxy-2-methoxy-5-oxo-2-phenyl-3-(trifluoromethyl)pentanoic acid (4c).** The title compound was prepared according to **general procedure II** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-ethyl-3-trifluoromethylacrylate (84.1 mg, 0.500 mmol, 1.0 equiv) in THF (0.50 mL) at -78 °C. The reaction was quenched after 3 h, and product **4c** (0.110 g, 0.330 mmol, 66% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane). [ $\alpha$ ]<sub>D</sub><sup>21</sup> -58.3 (*c* 0.50, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.78 (brs, 1H), 7.48–7.37 (m, 5H), 4.21–4.06 (m, 3H), 3.15 (s, 3H), 2.75–2.61 (m, 2H), 1.23 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 173.4, 171.4, 133.7, 129.0, 128.9, 127.9, 126.2 (q, *J* = 281 Hz), 83.8, 61.3, 53.0, 45.5, 31.7, 14.0. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): -65.5 (d, *J* = 8.6 Hz). HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>15</sub>H<sub>17</sub>O<sub>5</sub>F<sub>3</sub>Na, 357.0926; found, 357.0915.

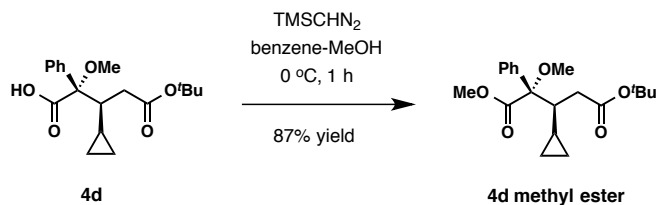


**(2*S*,3*R*)-5-Ethyl 1-methyl 2-methoxy-2-phenyl-3-(trifluoromethyl)pentanedioate (4c methyl ester)**. The title compound was prepared using carboxylic acid **4c** (27.1 mg, 81.1  $\mu\text{mol}$ ),  $\text{TMSCHN}_2$  (0.29 mL, 0.57 M in hexanes, 0.165 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **4c methyl ester** (24.0 mg, 68.9  $\mu\text{mol}$ , 85% yield). Ee: 95% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=6.7$  min (major);  $t_2=7.6$  min).  $[\alpha]_D^{21} -39.0$  (*c* 0.63,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.44–7.33 (m, 5H), 4.18–4.04 (m, 2H), 4.05–3.92 (m, 1H), 3.89 (s, 3H), 3.15 (s, 3H), 2.56 (dd,  $J = 17.3, 3.3$  Hz, 1H), 2.48 (dd,  $J = 17.3, 7.8$  Hz, 1H), 1.22 (t,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 171.1, 170.4, 134.2, 128.9, 128.4, 128.2, 126.1 (q,  $J = 282$  Hz), 84.4 (q,  $J = 1.6$  Hz), 61.0, 53.8, 52.5, 48.7 (q,  $J = 25.3$  Hz), 31.2 (q,  $J = 2.5$  Hz), 14.1.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): -64.8 (d,  $J = 8.8$  Hz). LRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{16}\text{H}_{19}\text{O}_5\text{F}_3\text{Na}$ , 371; found, 371.

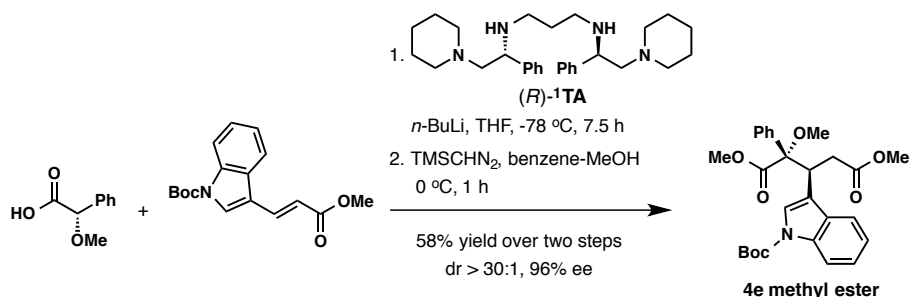


**(2*S*,3*S*)-5-(*tert*-Butoxy)-3-cyclopropyl-2-methoxy-5-oxo-2-phenylpentanoic acid (4d)**. The title compound was prepared according to **general procedure II** using ( $\pm$ )-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv),  $n\text{-BuLi}$  (0.81 mL, 2.47 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-*tert*-butyl-3-cyclopropylacrylate (88.2 mg, 0.525 mmol, 1.05 equiv) in THF (0.5 mL) at -78 °C. The reaction was quenched after 5 h, and product **4d** (0.143 g, 0.427 mmol, 86% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_D^{24} +3.2$  (*c* 0.92,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.52–7.49 (m, 2H), 7.41–7.36 (m, 2H), 7.36–7.32 (m, 1H), 3.14 (s, 3H), 2.53–2.44 (m, 2H), 2.14–2.05 (m, 1H), 1.43 (s, 9H), 0.66–0.58 (m, 1H), 0.55–0.48 (m, 1H), 0.45–0.37 (m, 2H), 0.30–0.23 (m, 1H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 175.7, 172.7, 135.0, 128.6,

128.1, 127.8, 88.0, 80.3, 53.2, 46.3, 37.4, 28.0, 12.6, 4.4, 2.8. HRMS-ESI ( $m/z$ ):  $[M+Na]^+$  calcd for  $C_{19}H_{26}O_5Na$ , 357.1678; found, 357.1683.

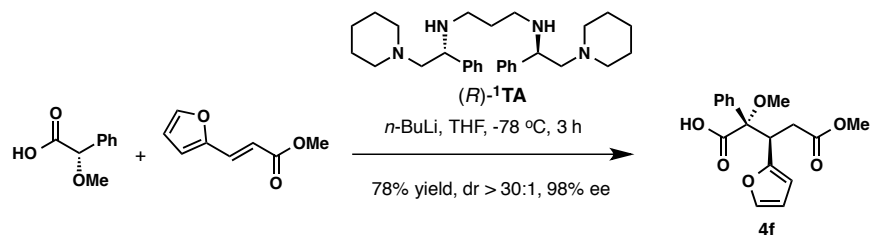


**(2*S*,3*S*)-5-(*tert*-Butyl) 1-methyl 3-cyclopropyl-2-methoxy-2-phenylpentanedioate (4d methyl ester).** The title compound was prepared using carboxylic acid **4d** (40.1 mg, 0.120 mmol), TMSCHN<sub>2</sub> (0.42 mL, 0.57 M in hexanes, 0.239 mmol) in a mixture of benzene-MeOH (4:1, 2.0 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **4d methyl ester** (36.2 mg, 0.104 mol, 87% yield). Ee: 97% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 0.5 mL/min; detection at 215 nm;  $t_1=11.5$  min (major);  $t_2=12.1$  min).  $[\alpha]_D^{24} +43.8$  ( $c$  1.5, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.54–7.48 (m, 2H), 7.39–7.32 (m, 2H), 7.34–7.27 (m, 1H), 3.83 (s, 3H), 3.19 (s, 3H), 2.50 (dd,  $J = 15.1, 4.0$  Hz, 1H), 2.31 (virt. td,  $J = 9.1, 3.9$  Hz, 1H), 1.81 (dd,  $J = 15.1, 9.0$  Hz, 1H), 1.42 (s, 9H), 0.47–0.29 (m, 3H), 0.26–0.15 (m, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 172.6, 172.1, 135.5, 128.7, 127.7, 127.5, 88.0, 80.0, 53.5, 51.8, 47.8, 37.3, 28.0, 12.8, 4.3, 3.3. LRMS-ESI ( $m/z$ ):  $[M+Na]^+$  calcd for  $C_{20}H_{28}O_5Na$ , 371; found, 371.

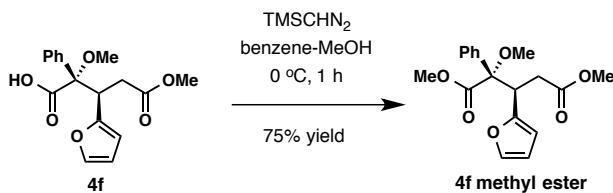


**(2*S*,3*S*)-3-(1-(*tert*-Butoxycarbonyl)-1*H*-indol-3-yl)-2,5-dimethoxy-5-oxo-2-phenylpentanoic acid (4e).** The title compound was prepared according to **general procedure II** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-*tert*-butyl 3-(3-methoxy-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (0.151 g, 0.501 mmol, 1.0 equiv) in THF (0.5 mL) at –78 °C. The reaction was quenched after 7.5 h and the product **4e** (0.160 g), contaminated with inseparable impurity, was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).

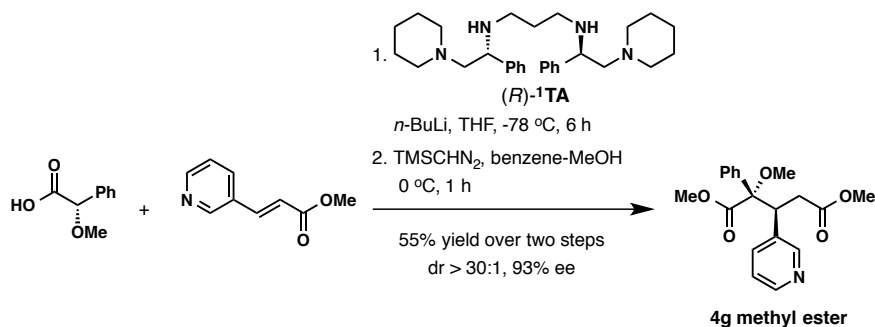
**(2*S*,3*S*)- Dimethyl 3-(1-(*tert*-butoxycarbonyl)-1*H*-indol-3-yl)-2-methoxy-2-phenyl pentane-dioate (4e methyl ester).** The title compound was prepared using above crude acid **4e** (0.160 g), TMSCHN<sub>2</sub> (1.3 mL, 0.57 M in hexanes, 0.741 mmol) in a mixture of benzene-MeOH (4:1, 5 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **4e methyl ester** (0.139 g, 0.288 mmol, 58% yield over 2 steps). Ee: 96% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1$ =13.4 min (major);  $t_2$ =15.1 min).  $[\alpha]_D^{23}$  -62.4 (*c* 0.72, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.14–7.97 (m, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.40–7.34 (m, 2H), 7.33–7.27 (m, 3H), 7.28–7.20 (m, 1H), 7.19–7.12 (m, 1H), 7.08 (s, 1H), 4.37 (dd, *J* = 10.9, 3.9 Hz, 1H), 3.77 (s, 3H), 3.43 (s, 3H), 3.23 (s, 3H), 2.84 (dd, *J* = 16.3, 3.9 Hz, 1H), 2.75 (dd, *J* = 16.3, 10.9 Hz, 1H), 1.64 (s, 9H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 172.3, 171.6, 149.6, 135.7, 134.8, 131.1, 128.3, 128.2, 127.7, 124.5, 124.0, 122.2, 120.0, 118.6, 114.7, 88.5, 83.4, 54.3, 51.9, 51.5, 42.2, 36.6, 28.2. HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>27</sub>H<sub>31</sub>NO<sub>7</sub>Na, 504.1998; found, 504.1975.



**(2*S*,3*S*)-3-(Furan-2-yl)-2,5-dimethoxy-5-oxo-2-phenylpentanoic acid (4f).** The title compound was prepared according to **general procedure II** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.79 mL, 2.52 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of (*E*)-methyl 3-(2'-furyl)acrylate (78.3 mg, 0.515 mmol, 1.03 equiv) at -78 °C. The reaction was quenched after 3 h, and product **4f** (0.125 g, 0.392 mmol, 78% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_D^{23}$  -20.3 (*c* 2.13, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 9.91 (s, 1H), 7.39–7.31 (m, 3H), 7.33–7.26 (m, 3H), 6.28 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.14 (d, *J* = 3.2 Hz, 1H), 4.38 (dd, *J* = 10.7, 3.7 Hz, 1H), 3.57 (s, 3H), 3.25 (s, 3H), 2.82 (dd, *J* = 16.7, 10.7 Hz, 1H), 2.75 (dd, *J* = 16.7, 3.7 Hz, 1H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 174.9, 172.4, 151.7, 141.8, 134.5, 128.6, 128.1, 127.8, 110.3, 108.6, 87.0, 53.6, 51.8, 42.8, 34.0. HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>17</sub>H<sub>18</sub>O<sub>6</sub>Na, 341.1001; found, 341.1001.

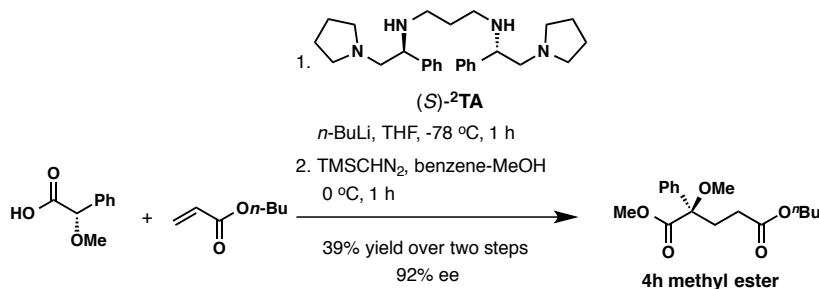


**(2*S*,3*S*)-Dimethyl 3-(furan-2-yl)-2-methoxy-2-phenylpentanedioate (4f methyl ester).** The title compound was prepared using carboxylic acid **4f** (21.1 mg, 66.4  $\mu\text{mol}$ ),  $\text{TMSCHN}_2$  (0.12 mL, 1.1 M in hexanes, 0.132 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **4f methyl ester** (16.6 mg, 50.0  $\mu\text{mol}$ , 75% yield). Ee: 98% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=20.6$  min (major);  $t_2=23.4$  min).  $[\alpha]_{\text{D}}^{23} +16.0$  (*c* 0.56,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.32–7.25 (m, 3H), 7.26 (dd,  $J = 1.9, 0.8$  Hz, 1H), 7.15–7.07 (m, 2H), 6.25 (dd,  $J = 3.2, 1.8$  Hz, 1H), 5.99 (dt,  $J = 3.2, 0.8$  Hz, 1H), 4.29 (dd,  $J = 11.2, 3.5$  Hz, 1H), 3.87 (s, 3H), 3.55 (s, 3H), 3.24 (s, 3H), 2.73 (dd,  $J = 16.4, 3.5$  Hz, 1H), 2.55 (dd,  $J = 16.4, 11.2$  Hz, 1H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 172.4, 171.2, 152.1, 141.5, 135.0, 128.1, 127.8, 127.7, 110.3, 108.6, 87.4, 54.2, 52.2, 51.7, 44.5, 33.2. LRMS-CI ( $m/z$ ):  $[\text{M}+\text{C}_2\text{H}_5]^+$  calcd for  $\text{C}_{20}\text{H}_{25}\text{O}_6$ , 361; found, 361.



**(2*S*,3*S*)-2,5-Dimethoxy-5-oxo-2-phenyl-3-(pyridin-3-yl)pentanoic acid (4g).** The title compound was prepared according to **general procedure II** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv),  $n\text{-BuLi}$  (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-methyl 3-(pyridin-3-yl)acrylate (82.1 mg, 0.503 mmol, 1.0 equiv) in THF (0.5 mL) at -78 °C. The resultant mixture was stirred for additional 6 h before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at -78 °C. After 5 min, the reaction mixture was acidified to pH value around 4–5 using 1 M aqueous solution of HCl (4 mL) and drops of 1 M aqueous solution of NaOH. The reaction mixture was then extracted with ethyl acetate, and the combined organic phase was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the crude product **4g** (0.154 g) was directly used for the next step.

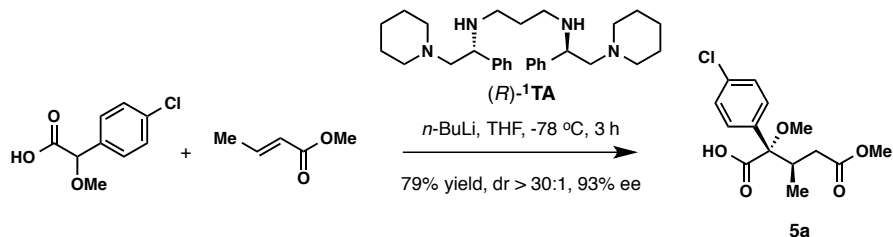
**(2*S*,3*S*)-Dimethyl 2-methoxy-2-phenyl-3-(pyridin-3-yl)pentanedioate (4g methyl ester).** The title compound was prepared using above crude acid **4g** (0.154 g), TMSCHN<sub>2</sub> (2.2 mL, 0.65 M in hexanes, 1.43 mmol) in a mixture of benzene-MeOH (4:1, 7.5 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (33-50% ethyl acetate in hexanes) to afford product **4g methyl ester** (94.8 mg, 0.276 mmol, 55% yield over 2 steps). Ee: 93% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=10.0$  min (major);  $t_2=12.7$  min).  $[\alpha]_D^{23} -60.6$  (*c* 1.2, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.40 (d, *J* = 4.2 Hz, 1H), 8.24 (s, 1H), 7.31–7.23 (m, 4H), 7.18–7.14 (m, 2H), 7.09 (dd, *J* = 7.9, 4.8 Hz, 1H), 3.98 (dd, *J* = 11.2, 3.9 Hz, 1H), 3.81 (s, 3H), 3.45 (s, 3H), 3.27 (s, 3H), 2.90 (dd, *J* = 16.4, 11.2 Hz, 1H), 2.77 (dd, *J* = 16.4, 3.9 Hz, 1H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 172.0, 171.5, 151.2, 148.3, 137.1, 135.6, 133.8, 128.3, 128.0, 127.7, 122.5, 88.0, 54.7, 52.1, 51.6, 49.2, 35.2. HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>19</sub>H<sub>21</sub>NO<sub>5</sub>Na, 366.1317; found, 366.1313.



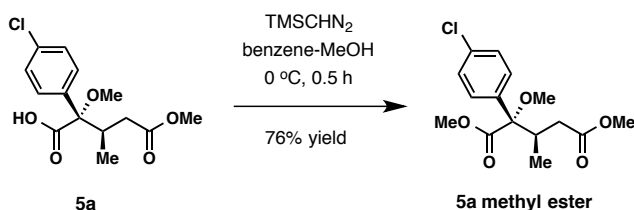
**(R)-5-butoxy-2-methoxy-5-oxo-2-phenylpentanoic acid (4h).** The title compound was prepared according to general procedure II using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)-**2TA** (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of *n*-butyl acrylate (75  $\mu$ L, 67.1 mg, 0.523 mmol, 1.05 equiv) in THF (0.5 mL) at -78 °C. The reaction was quenched after 1 h and the product **4h** (0.116 g), contaminated with inseparable impurity, was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).

**(R)-5-Butyl 1-methyl 2-methoxy-2-phenylpentanedioate (4h methyl ester).** The title compound was prepared using above crude acid **4h** (0.116 g), TMSCHN<sub>2</sub> (1.3 mL, 0.57 M in hexanes, 0.741 mmol) in a mixture of benzene-MeOH (4:1, 5 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **4h methyl ester** (60.0 mg, 0.195 mmol, 39% yield over 2 steps). Ee: 92% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=15.3$  min (major);  $t_2=16.0$  min).  $[\alpha]_D^{23} +18.9$  (*c* 1.04, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.47–7.43 (m, 2H), 7.38–7.30 (m, 2H), 7.32–7.25 (m, 1H), 4.02 (t, *J* = 6.5 Hz, 2H), 3.71 (s, 3H), 3.24 (s, 3H), 2.64 (ddd, *J* = 15.5, 9.8, 6.6 Hz, 1H), 2.51

(ddd,  $J = 15.0, 9.7, 6.7$  Hz, 1H), 2.18 (ddd,  $J = 9.7, 6.1, 3.1$  Hz, 2H), 1.61–1.52 (m, 2H), 1.40–1.29 (m, 2H), 0.91 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.1, 172.5, 138.7, 128.4, 128.0, 125.9, 83.4, 64.4, 52.5, 51.8, 30.6, 28.8, 28.1, 19.0, 13.6. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{17}\text{H}_{24}\text{O}_5\text{Na}$ , 331.1521; found, 331.1505.



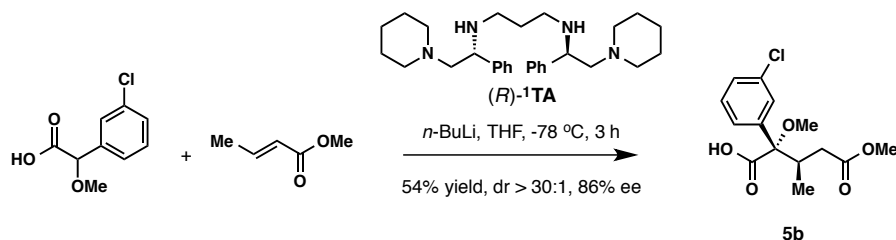
**(2S,3R)-2-(4-Chlorophenyl)-2,5-dimethoxy-3-methyl-5-oxopentanoic acid (5a).** The title compound was prepared according to **general procedure II** using 2-(4-chlorophenyl)-2-methoxyacetic acid (0.100 g, 0.500 mmol), (R)- $^1\text{TA}$  (0.231 g, 0.515 mmol, 1.03 equiv),  $n\text{-BuLi}$  (0.80 mL, 2.51 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (E)-methyl crotonate (50.6 mg, 0.505 mmol, 1.01 equiv) in THF (0.5 mL) at  $-78$  °C. The reaction was quenched after 3 h and the product **5a** (0.118 g, 0.393 mmol, 79% yield) was obtained after purification by column chromatography on silica gel (2–4% methanol in dichloromethane).  $[\alpha]_{\text{D}}^{25} -36.2$  ( $c$  1.03,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.41 (d,  $J = 8.8$  Hz, 2H), 7.36 (d,  $J = 8.8$  Hz, 2H), 3.64 (s, 3H), 3.21 (s, 3H), 2.96 (dq,  $J = 10.5, 6.7, 2.9$  Hz, 1H), 2.47 (dd,  $J = 16.1, 2.9$  Hz, 1H), 2.07 (dd,  $J = 16.1, 10.5$  Hz, 1H), 1.02 (d,  $J = 6.7$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 174.7, 173.3, 134.5, 133.8, 129.5, 128.5, 87.3, 53.4, 51.8, 37.3, 36.9, 15.2. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{14}\text{H}_{16}\text{ClO}_5$ , 299.0686; found, 299.0686.



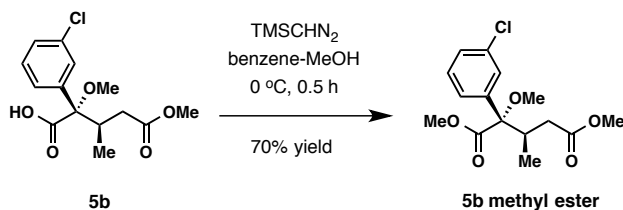
**(2S,3R)-Dimethyl 2-(4-chlorophenyl)-2-methoxy-3-methylpentanedioate (5a methyl ester).** The title compound was prepared using above acid **5a** (54.1 mg, 0.180 mmol),  $\text{TMSCHN}_2$  (0.33 mL, 1.13 M in hexanes, 0.373 mmol) in a mixture of benzene–MeOH (4:1, 2.0 mL) at  $0$  °C for 0.5 h. The solvent was removed and the residue was purified by column chromatography on silica gel (20% ethyl acetate in hexanes) to afford product **5a methyl ester** (43.3 mg, 0.138 mmol, 76% yield). Ee: 93% (Chiralcel® OD-H; 1%  $i\text{-PrOH}$  in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=10.3$  min (major);  $t_2=13.3$  min).  $[\alpha]_{\text{D}}^{25} -20.8$  ( $c$  1.06,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.38–7.31 (m, 4H), 3.83 (s, 3H), 3.62 (s, 3H),



3.19 (s, 3H), 2.89 (dq,  $J = 10.6, 6.8, 3.2$  Hz, 1H), 2.44 (dd,  $J = 15.8, 3.2$  Hz, 1H), 1.85 (dd,  $J = 15.8, 10.6$  Hz, 1H), 0.92 (d,  $J = 6.8, 3H$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 173.1, 171.4, 134.5, 134.0, 129.4, 128.1, 87.6, 53.8, 52.1, 51.6, 38.5, 36.5, 15.5. LRMS-FD ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{15}\text{H}_{19}\text{ClO}_5$ , 314; found, 314.

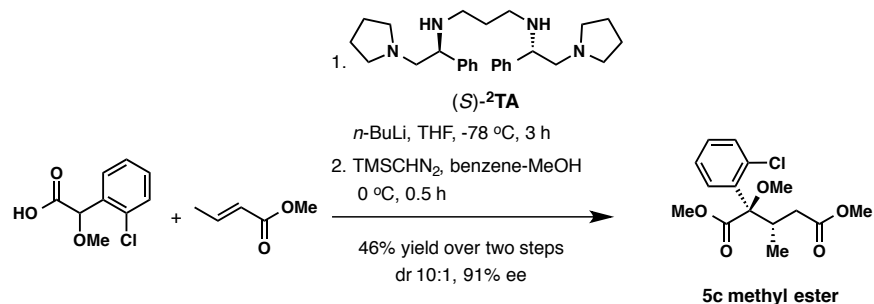


**(2*S*,3*R*)-2-(3-Chlorophenyl)-2,5-dimethoxy-3-methyl-5-oxopentanoic acid (5b).** The title compound was prepared according to general procedure II using 2-(3'-chlorophenyl)-2-methoxyacetic acid (100.3 mg, 0.500 mmol), (*R*)- $^1\text{TA}$  (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.51 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-methyl crotonate (50.6 mg, 0.505 mmol, 1.01 equiv) in THF (0.5 mL) at  $-78$   $^\circ\text{C}$ . The reaction was quenched after 3 h and the product **5b** (81.9 mg, 0.272 mmol, 54% yield) was obtained after purification by column chromatography on silica gel (2-4% methanol in dichloromethane).  $[\alpha]_{\text{D}}^{25} -28.8$  ( $c$  1.00,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.49–7.45 (m, 1H), 7.39–7.31 (m, 3H), 3.65 (s, 3H), 3.23 (s, 3H), 3.08–2.86 (m, 1H), 2.51 (dd,  $J = 16.2, 2.8$  Hz, 1H), 2.10 (dd,  $J = 16.2, 10.6$  Hz, 1H), 1.04 (d,  $J = 6.7$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 174.0, 173.2, 137.4, 134.5, 129.5, 128.8, 128.2, 126.2, 87.2, 53.4, 51.8, 36.8, 15.2. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{14}\text{H}_{16}\text{ClO}_5$ , 299.0686; found, 299.0676.



**(2*S*,3*R*)-Dimethyl 2-(3'-chlorophenyl)-2-methoxy-3-methylpentanedioate (5b methyl ester).** The title compound was prepared using above acid **5b** (26.5 mg, 88.1  $\mu\text{mol}$ ),  $\text{TMSCHN}_2$  (0.16 mL, 1.13 M in hexanes, 0.181 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at  $0$   $^\circ\text{C}$  for 0.5 h. The solvent was removed and the residue was purified by column chromatography on silica gel (20% ethyl acetate in hexanes) to afford product **5b methyl ester** (19.2 mg, 61.0  $\mu\text{mol}$ , 70% yield). Ee: 86% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 0.5 mL/min; detection at 215 nm;  $t_1=26.8$  min (major);  $t_2=28.3$  min).  $[\alpha]_{\text{D}}^{25} -18.4$  ( $c$  0.96,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.43–7.41 (m, 1H), 7.33–7.29 (m, 3H), 3.85 (s,

3H), 3.63 (s, 3H), 3.22 (s, 3H), 2.94–2.84 (m, 1H), 2.47 (dd,  $J = 15.7, 3.2$  Hz, 1H), 1.86 (dd,  $J = 15.7, 10.7$  Hz, 1H), 0.93 (d,  $J = 6.7$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.1, 171.3, 138.3, 134.1, 129.2, 128.2, 128.1, 126.1, 87.6, 54.0, 52.2, 51.6, 38.5, 36.5, 15.5. LRMS-FD ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{15}\text{H}_{19}\text{ClO}_5$ , 314; found, 314.



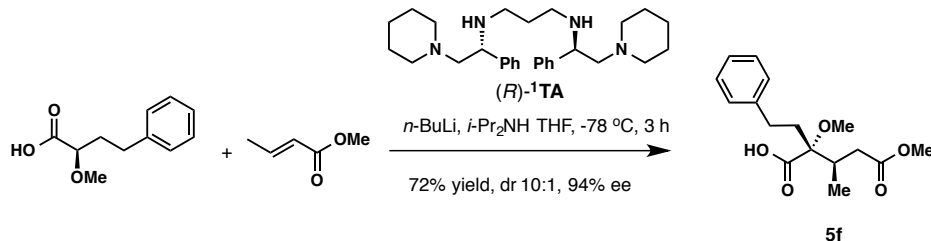
**(2*R*,3*S*)-2-(2-Chlorophenyl)-2,5-dimethoxy-3-methyl-5-oxopentanoic acid (5c).** The title compound was prepared according to **general procedure II** using 2-(2'-chlorophenyl)-2-methoxyacetic acid (100.3 mg, 0.500 mmol), (*S*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.51 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of (*E*)-methyl crotonate (50.6 mg, 0.505 mmol, 1.01 equiv) in THF (0.50 mL) at  $-78$  °C. The resultant mixture was stirred for additional 3 h before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at  $-78$  °C. After 5 min, the reaction mixture was acidified using 1 M aqueous solution of HCl (4 mL). The reaction mixture was then extracted with ethyl acetate, and the combined organic phase was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the crude product **5c** (85.3 mg) was directly used for the next step.

**(2*R*,3*S*)-Dimethyl 2-(2-chlorophenyl)-2-methoxy-3-methylpentanedioate (5c methyl ester).** The title compound was prepared using above crude acid **5c** (36.3 mg),  $\text{TMSCHN}_2$  (0.22 mL, 1.13 M in hexanes, 0.249 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at  $0$  °C for 0.5 h. The solvent was removed and the residue was purified by column chromatography on silica gel (20% ethyl acetate in hexanes) to afford product **5c methyl ester** (28.9 mg, 91.8  $\mu\text{mol}$ , 46% yield over steps). Ee: 91% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=13.7$  min (major),  $t_2=11.6$  min).  $[\alpha]_{\text{D}}^{25} +37.1$  ( $c$  0.69,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.53 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.39 (dd,  $J = 7.7, 1.6$  Hz, 1H), 7.34–7.26 (m, 2H), 3.79 (s, 3H), 3.70 (s, 3H), 3.32–3.24 (m, 1H), 3.18 (s, 3H), 2.80 (d,  $J = 15.9$  Hz, 1H), 1.98 (dd,  $J = 16.1, 10.5$  Hz, 1H), 0.97 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 173.6, 170.6, 135.2, 133.8, 131.2, 129.5, 129.3, 126.4, 85.3, 52.24, 52.21, 51.7, 37.2, 33.7, 15.7. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{15}\text{H}_{19}\text{ClO}_5\text{Na}$ , 337.0819; found, 337.0806.

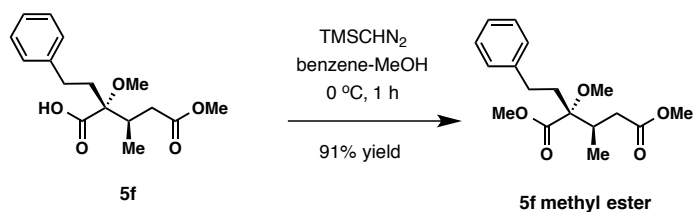




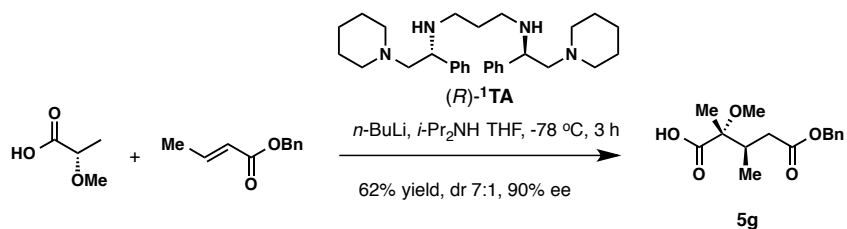
$\mu\text{L}$ , 2.0 M in hexanes, 0.160 mmol) in a mixture of benzene-MeOH (4:1, 1 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (11% ethyl acetate in hexanes) to afford product **5e methyl ester** (25.5 mg, 67.7  $\mu\text{mol}$ , 86% yield). Ee: 98% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=8.0$  min (major);  $t_2=9.9$  min).  $[\alpha]_D^{23} +8.5$  ( $c$  1.38,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.38–7.29 (m, 5H), 5.12 (s, 2H), 3.71 (s, 3H), 3.27 (s, 3H), 2.61 (dd,  $J = 15.7, 3.0$  Hz, 1H), 2.54 (dq,  $J = 9.9, 6.8, 3.1$  Hz, 1H), 2.22 (dd,  $J = 15.7, 10.6$  Hz, 1H), 1.77 (dd,  $J = 14.9, 7.6$  Hz, 1H), 1.72–1.55 (m, 6H), 1.48–1.38 (m, 1H), 1.29–1.05 (m, 3H), 1.01–0.81 (m, 2H), 0.92 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.3, 172.9, 135.9, 128.5, 128.21, 128.17, 84.0, 66.3, 51.8, 50.7, 38.9, 37.3, 34.9, 34.7, 33.3, 33.0, 26.4, 26.3, 26.2, 14.6. LRMS-CI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{22}\text{H}_{33}\text{O}_5$ , 377; found, 377.



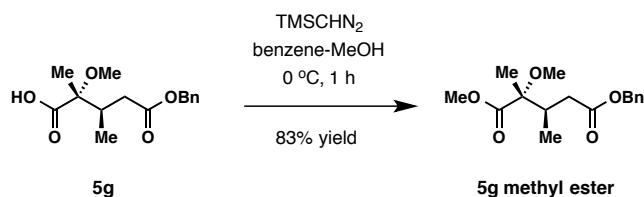
**(2R,3R)-2,5-Dimethoxy-3-methyl-5-oxo-2-phenethylpentanoic acid (5f)**. The title compound was prepared according to **general procedure III** using isopropylamine (0.14 mL, 0.101 g, 1.00 mmol, 2 eq), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3 mL), followed by addition of a solution of (*R*)-2-methoxy-4-phenylbutyric acid (97.2 mg, 0.500 mmol) in THF (1 mL). After stirring at 0 °C for 1 h, a solution of (*E*)-methyl crotonate (55  $\mu\text{L}$ , 51.9 mg, 0.519 mmol, 1.04 equiv) in THF (0.5 mL) was added at  $-78$  °C. The reaction was quenched after 3 h, and product **5f** (0.106 g, 0.360 mmol, 72% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_D^{23} +15.0$  ( $c$  0.50,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.31–7.24 (m, 2H), 7.23–7.13 (m, 3H), 3.65 (s, 3H), 3.42 (s, 3H), 2.68–2.44 (m, 4H), 2.38 (dd,  $J = 16.0, 10.0$  Hz, 1H), 2.27 (ddd,  $J = 14.5, 12.2, 4.8$  Hz, 1H), 2.00 (ddd,  $J = 14.5, 12.3, 4.7$  Hz, 1H), 0.98 (d,  $J = 6.7$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.3, 140.8, 128.5, 128.2, 126.2, 84.8, 51.7, 49.9, 36.6, 33.7, 33.4, 29.9, 14.6. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{16}\text{H}_{21}\text{O}_5$ , 293.1389; found, 293.1376.



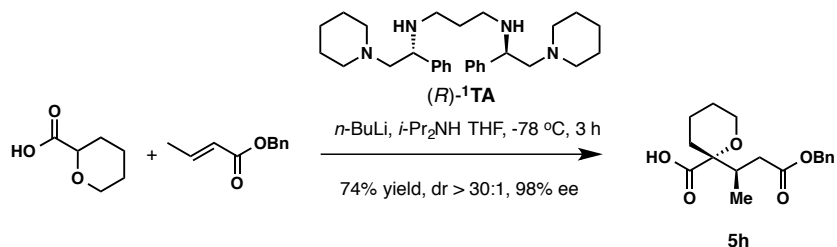
**(2R,3R)-Dimethyl 2-methoxy-3-methyl-2-phenethylpentanedioate (5f methyl ester).** The title compound was prepared using acid **5f** (31.2 mg, 0.106 mmol), TMSCHN<sub>2</sub> (0.19 mL, 1.1 M in hexanes, 0.209 mmol) in a mixture of benzene-MeOH (4:1, 1 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (11% ethyl acetate in hexanes) to afford product **5f methyl ester** (29.6 mg, 96.0 μmol, 91% yield). Ee: 94% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=15.6$  min (major);  $t_2=20.4$  min).  $[\alpha]_D^{23} +14.0$  ( $c$  0.86, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.32–7.25 (m, 2H), 7.22–7.17 (m, 3H), 3.75 (s, 3H), 3.68 (s, 3H), 3.38 (s, 3H), 2.79–2.69 (m, 1H), 2.64–2.48 (m, 3H), 2.24–2.03 (m, 3H), 1.00 (d,  $J$  = 6.8 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 173.3, 172.9, 141.6, 128.4, 128.2, 126.0, 84.2, 51.8, 51.7, 51.3, 37.0, 34.9, 33.5, 29.8, 14.6. LRMS–CI ( $m/z$ ):  $[M+H]^+$  calcd for C<sub>17</sub>H<sub>25</sub>O<sub>5</sub>, 309; found, 309.



**(2R,3R)-5-(Benzyloxy)-2-methoxy-2,3-dimethyl-5-oxopentanoic acid (5g).** The title compound was prepared according to **general procedure III** using isopropylamine (0.14 mL, 0.101 g, 1.00 mmol, 2.0 equiv), (*R*)-<sup>1</sup>TA (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.50 M in hexanes, 2.00 mmol, 4.0 equiv) in THF (3 mL), followed by addition of a solution of (*S*)-2-methoxypropionic acid (52.3 mg, 0.500 mmol) in THF (1 mL). After stirring at 0 °C for 1 h, a solution of (*E*)-benzyl crotonate (90.6 mg, 0.515 mmol, 1.03 equiv) in THF (0.5 mL) was added at –78 °C. The reaction was quenched after 3 h, and product **5g** (87.2 mg, 0.311 mmol, 62% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_D^{22} +25.2$  ( $c$  0.94, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.75 (brs, 1H), 7.39–7.27 (m, 5H), 5.12 (s, 2H), 3.28 (s, 3H), 2.67 (dd,  $J$  = 15.6, 3.9 Hz, 1H), 2.54 (dq,  $J$  = 9.9, 6.8, 3.3 Hz, 1H), 2.24 (dd,  $J$  = 15.6, 10.0 Hz, 1H), 1.35 (s, 3H), 0.96 (d,  $J$  = 6.8 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 177.7, 172.9, 135.8, 128.5, 128.1, 82.3, 66.3, 51.9, 37.1, 36.3, 15.9, 14.6. HRMS–ESI ( $m/z$ ):  $[M-H]^-$  calcd for C<sub>15</sub>H<sub>19</sub>O<sub>5</sub>, 279.1233; found, 279.1227.

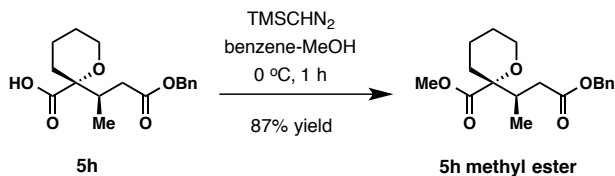


**(2*R*,3*R*)-5-Benzyl 1-methyl 2-methoxy-2,3-dimethylpentanedioate (5g methyl ester).** The title compound was prepared using acid **5g** (21.9 mg, 78.1  $\mu\text{mol}$ ),  $\text{TMSCHN}_2$  (80  $\mu\text{L}$ , 2.0 M in hexanes, 0.160 mmol) in a mixture of benzene-MeOH (4:1, 1 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (11% ethyl acetate in hexanes) to afford product **5g methyl ester** (19.1 mg, 64.9  $\mu\text{mol}$ , 83% yield). Ee: 90% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=12.2$  min (major);  $t_2=19.7$  min).  $[\alpha]_{\text{D}}^{23} +29.6$  ( $c$  0.56,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.40–7.27 (m, 5H), 5.11 (d,  $J$  = 12.0 Hz, 1H), 5.09 (d,  $J$  = 12.0 Hz, 1H), 3.73 (s, 3H), 3.21 (s, 3H), 2.65 (dd,  $J$  = 15.6, 3.7 Hz, 1H), 2.53 (dq,  $J$  = 10.5, 6.9, 3.7 Hz, 1H), 2.14 (dd,  $J$  = 15.6, 10.2 Hz, 1H), 1.30 (s, 3H), 0.89 (d,  $J$  = 6.8 Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 174.0, 172.8, 136.0, 128.5, 128.2, 128.1, 82.6, 66.2, 52.2, 52.0, 37.5, 36.2, 15.5, 14.9. LRMS-CI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{16}\text{H}_{23}\text{O}_5$ , 295; found, 295.

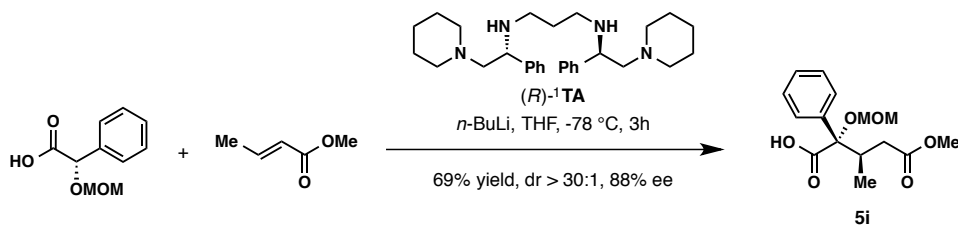


**(*R*)-2-((*R*)-4-methoxy-4-oxobutan-2-yl)tetrahydro-2*H*-pyran-2-carboxylic acid (5h).** The title compound was prepared according to **general procedure III** using isopropylamine (0.14 mL, 0.101 g, 1.00 mmol, 2.0 eq), (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv),  $n\text{-BuLi}$  (0.80 mL, 2.49 M in hexanes, 1.99 mmol, 4.0 equiv) in THF (3 mL), followed by addition of a solution of tetrahydro-2*H*-pyran-2-carboxylic acid (65.1 mg, 0.500 mmol) in THF (1 mL). After stirring at 0 °C for 1 h, a solution of (*E*)-benzyl crotonate (90.6 mg, 0.515 mmol, 1.03 equiv) in THF (0.5 mL) was added at -78 °C. The reaction was quenched after 3 h, and product **5h** (0.113 g, 0.369 mmol, 74% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_{\text{D}}^{23} +44.4$  ( $c$  1.9,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 8.00 (brs, 1 H), 7.39–7.29 (m, 5H), 5.13 (d,  $J$  = 13.0 Hz, 1H), 5.10 (d,  $J$  = 13.0 Hz, 1H), 3.87–3.80 (m, 1H), 3.63 (ddd,  $J$  = 11.6, 8.9, 4.4 Hz, 1H), 2.74 (dd,  $J$  = 15.6, 4.0 Hz, 1H), 2.45 (dq,  $J$  = 10.7, 6.9, 3.9 Hz, 1H), 2.22 (dd,  $J$  = 15.6, 9.8 Hz, 1H), 2.10–2.03 (m, 1H), 1.78–1.70 (m, 1H), 1.56–1.42 (m, 4H), 0.97 (d,  $J$  =

6.9 Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 176.9, 172.9, 135.9, 128.5, 128.20, 128.17, 81.8, 66.3, 65.1, 37.5, 36.4, 27.5, 25.0, 20.1, 14.4. HRMS-ESI ( $m/z$ ):  $[\text{M}-\text{H}]^-$  calcd for  $\text{C}_{17}\text{H}_{21}\text{O}_5$ , 305.1389; found, 305.1380.



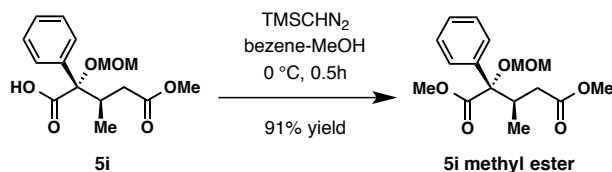
**(R)-Methyl 2-((R)-4-(benzyloxy)-4-oxobutan-2-yl)tetrahydro-2H-pyran-2-carboxylate (5h methyl ester).** The title compound was prepared using acid **5h** (41.6 mg, 0.136 mmol),  $\text{TMSCHN}_2$  (0.13 mL, 2.0 M in hexanes, 0.260 mmol) in a mixture of benzene-MeOH (4:1, 2 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (11% ethyl acetate in hexanes) to afford product **5h methyl ester** (37.9 mg, 0.118 mmol, 87% yield). Ee: 98% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=14.3$  min(major);  $t_2=13.6$  min).  $[\alpha]_{\text{D}}^{23} +49.2$  ( $c$  1.83,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.39–7.27 (m, 5H), 5.11 (d,  $J$  = 12.5 Hz, 1H), 5.10 (d,  $J$  = 12.5 Hz, 1H), 3.88–3.80 (m, 1H), 3.75 (s, 3H), 3.53 (td,  $J$  = 11.7, 3.1 Hz, 1H), 2.71 (dd,  $J$  = 15.6, 3.7 Hz, 1H), 2.38 (dq,  $J$  = 10.5, 6.9, 3.7 Hz, 1H), 2.14 (dd,  $J$  = 15.6, 10.2 Hz, 1H), 2.11–2.05 (m, 1H), 1.79–1.68 (m, 1H), 1.55–1.33 (m, 4H), 0.91 (d,  $J$  = 6.9 Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.6, 172.8, 136.0, 128.5, 128.2, 128.1, 82.2, 66.2, 65.2, 51.9, 38.2, 36.3, 27.8, 25.2, 20.5, 14.4. LRMS-CI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{25}\text{O}_5$ , 321; found, 321.



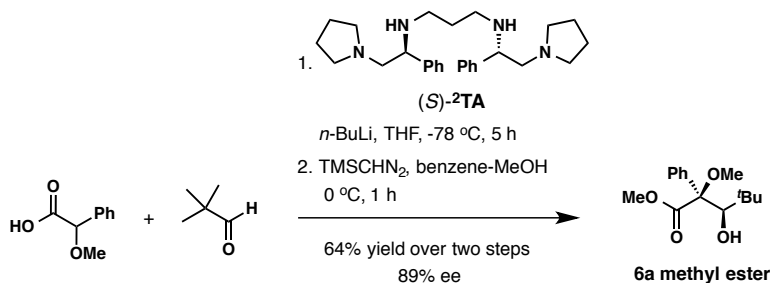
**(2S,3R)-5-Methoxy-2-(methoxymethoxy)-3-methyl-5-oxo-2-phenylpentanoic acid (5i).** The title compound was prepared according to **general procedure II** using (*S*)-2-(methoxymethoxy)-2-phenylacetic acid (98.1 mg, 0.500 mmol), (*R*)- $^1\text{TA}$  (0.231 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.80 mL, 2.49 M in hexanes, 1.99 mmol, 4.0 equiv) in THF (7 mL). After stirring at 0 °C for 2 h, a solution of (*E*)-benzyl crotonate (90.6 mg, 0.515 mmol, 1.03 equiv) in THF (1.0 mL) was added at  $-78$  °C. The reaction was quenched after 3 h, and product **5i** (0.102 g, 0.345 mmol, 69% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_{\text{D}}^{23} -34.4$  ( $c$  1.00,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.47–7.42 (m, 2H), 7.41–7.31 (m, 3H), 4.66 (d,  $J$  =



6.7 Hz, 1H), 4.63 (d,  $J = 6.7$  Hz, 1H), 3.61 (s, 3H), 3.43 (s, 3H), 3.02–2.94 (m, 1 H), 2.38 (dd,  $J = 16.3, 2.9$  Hz, 1H), 2.27 (dd,  $J = 16.3, 10.5$  Hz, 1H), 1.09 (dd,  $J = 6.7, 0.7$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.3, 135.4, 128.8, 128.5, 127.9, 93.6, 89.26, 56.5, 51.6, 39.4, 37.1, 15.1. HRMS–CI ( $m/z$ ):  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{15}\text{H}_{21}\text{O}_6$ , 297.1338; found, 297.1329.



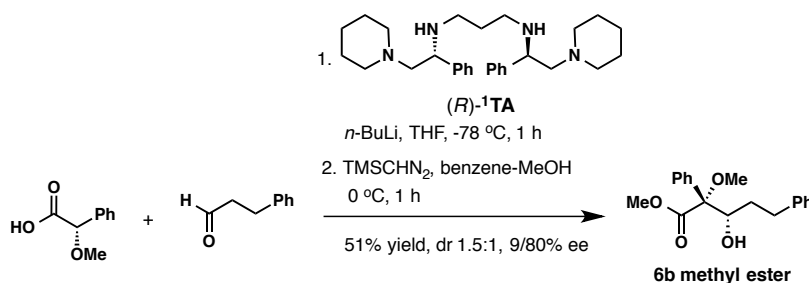
**(2*S*,3*R*)-Dimethyl 2-(methoxymethoxy)-3-methyl-2-phenylpentanedioate (5i methyl ester).** A solution of  $\text{TMSCHN}_2$  in hexane (0.26 mL, 1.03 M, 0.262 mmol) was added dropwise to a solution of carboxylic acid **5i** (25.1 mg, 84.7  $\mu\text{mol}$ ) in a mixture of benzene–MeOH (4:1, 1.0 mL) at 0 °C. The resultant mixture was stirred at the same temperature for 0.5 h. The solvent was removed on a rotary evaporator and the residue was purified by column chromatography on silica gel (20% ethyl acetate in hexanes) to afford the product **5i methyl ester** (24.0 mg, 77.3  $\mu\text{mol}$ , 91% yield). Ee: 88% (Chiralcel® AD–H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=21.4$  min (major),  $t_2=16.6$  min).  $[\alpha]_{\text{D}}^{26} -77.5$  ( $c$  1.00,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.38–7.35 (m, 4H), 7.34–7.28 (m, 1H), 4.80 (d,  $J = 6.5$  Hz, 1H), 4.64 (d,  $J = 6.5$  Hz, 1H), 3.80 (s, 3H), 3.64 (s, 3H), 3.38 (s, 3H), 3.04 (dq,  $J = 10.3, 6.8, 3.4$  Hz, 1H), 2.52 (dd,  $J = 15.7, 3.4$  Hz, 1H), 1.91 (dd,  $J = 15.7, 10.3$  Hz, 1H), 0.92 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.4, 172.0, 136.1, 128.1, 127.9, 127.8, 93.5, 86.9, 56.1, 52.3, 51.5, 38.4, 36.7, 15.4. LRMS–FD ( $m/z$ ):  $[\text{M}]^+$  calcd for  $\text{C}_{16}\text{H}_{22}\text{O}_6$ , 310; found, 310.



**(2*S*,3*R*)-3-Hydroxy-2-methoxy-4,4-dimethyl-2-phenylpentanoic acid (6a).** A solution of *n*-BuLi (0.81 mL, 2.47 M in hexanes, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (±)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), and (*R*)-<sup>2</sup>TA (0.217 g, 0.515 mmol, 1.03 equiv) in THF (3.5 mL) at 0 °C and the reaction mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to –78 °C and stirred for an additional 5 min. Then pivaldehyde (0.11 mL, 87.2 mg, 1.01 mmol, 2.03 equiv) was added to

the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 5 h before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at  $-78\text{ }^{\circ}\text{C}$ . After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was directly used for the next step without further purification.

**(2*S*,3*R*)-Methyl 3-hydroxy-2-methoxy-4,4-dimethyl-2-phenylpentanoate (6a methyl ester).** The title compound was prepared using above crude acid **6a**,  $\text{TMSCHN}_2$  in hexane (1.75 mL, 0.57 M, 1.00 mmol) in a mixture of benzene-MeOH (4:1, 5 mL) at  $0\text{ }^{\circ}\text{C}$  for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **6a methyl ester** (84.9 mg, 0.319 mmol, 64% yield over steps). Ee: 89% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=7.1$  min (major);  $t_2=7.6$  min).  $[\alpha]_{\text{D}}^{23} +21.2$  ( $c$  1.6,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.54–7.48 (m, 2H), 7.39–7.31 (m, 2H), 7.34–7.26 (m, 1H), 4.03 (d,  $J = 8.2$  Hz, 1H), 3.83 (s, 3H), 3.30 (s, 3H), 3.18 (d,  $J = 8.2$  Hz, 1H), 0.92 (s, 9H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 173.8, 138.3, 128.2, 128.0, 127.2, 87.2, 83.0, 54.6, 52.2, 36.5, 27.7. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{15}\text{H}_{22}\text{O}_4\text{Na}$ , 289.1416; found, 289.1403.

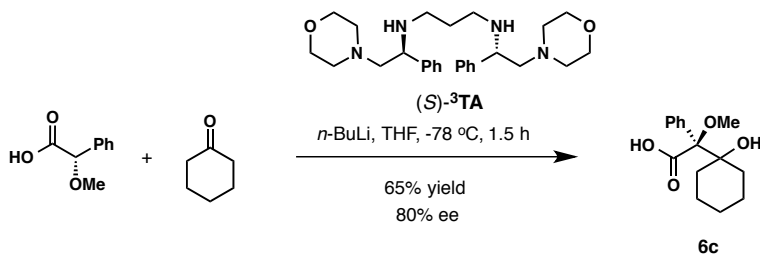


**(2*R*,3*S*)-3-Hydroxy-2-methoxy-2,5-diphenylpentanoic acid (6b).** A solution of  $n\text{-BuLi}$  (0.79 mL, 2.53 M in hexanes, 2.00 mmol, 4.0 equiv) was added dropwise to a solution of (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), and (*R*)-**1TA** (0.231 g, 0.515 mmol, 1.03 equiv) in THF (3.5 mL) at  $0\text{ }^{\circ}\text{C}$  and the reaction mixture was stirred at this temperature for 2 h. The reaction mixture was then cooled to  $-78\text{ }^{\circ}\text{C}$  and stirred for an additional 5 min. Then a solution of hydrocinnamaldehyde (70  $\mu\text{L}$ , 71.3 mg, 0.531 mmol, 1.06 equiv) in THF (0.5 mL) was added to the reaction mixture dropwise over 10 min. The resultant mixture was stirred for additional 50 min before a quench with a mixture of THF-MeOH (3:1, 0.64 mL) at  $-78\text{ }^{\circ}\text{C}$ . After 5 min, the reaction mixture was acidified with 1 M aqueous solution of HCl and extracted with ethyl acetate. The combined organic phase was sequentially washed with 1 M aqueous solution of HCl and brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was directly used for the next step without further purification.

**(2R,3S)-Methyl 3-hydroxy-2-methoxy-2,5-diphenylpentanoate (6b methyl ester).** The title compound was prepared using above crude acid **6b**, TMSCHN<sub>2</sub> in hexane (0.9 mL, 1.1 M, 0.99 mmol) in a mixture of benzene-MeOH (4:1, 5 mL) at 0 °C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford products diastereomeric mixtures **6b methyl ester-1** and **6b methyl ester-2** (79.7 mg, 0.254 mmol, 51% yield). The analytically pure products was obtained using preparative HPLC (YMC-Pack-SIL 250x30 mm; 1% *i*-PrOH in hexanes; flow rate = 5 mL/min; detection at 215 nm,  $t_1=6.5$  min (major),  $t_2=7.2$  min (minor)).

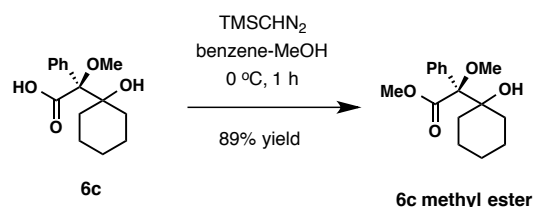
Major diastereomer **6b methyl ester-1**: Ee: 9% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=24.6$  min;  $t_2=33.8$  min). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.45–7.38 (m, 2H), 7.38–7.30 (m, 3H), 7.23 (t,  $J = 7.4$  Hz, 2H), 7.19–7.13 (m, 1H), 7.09 (d,  $J = 6.8$  Hz, 2H), 4.19 (ddd,  $J = 10.4, 6.5, 2.1$  Hz, 1H), 3.81 (s, 3H), 3.46 (s, 3H), 2.94–2.84 (m, 2H), 2.58 (ddd,  $J = 13.9, 9.5, 7.3$  Hz, 1H), 1.85–1.76 (m, 1H), 1.68–1.57 (m, 1H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 173.1, 141.9, 136.6, 128.4, 128.3, 128.2, 128.1, 126.7, 125.7, 87.1, 55.0, 52.4, 32.3, 32.0.  $[\alpha]_D^{25} -14.4$  (c 1.0, CHCl<sub>3</sub>). HRMS-ESI ( $m/z$ ): [M+Na]<sup>+</sup> calcd for C<sub>19</sub>H<sub>22</sub>O<sub>4</sub>Na, 337.1416; found, 337.1410.

Minor diastereomer **6b methyl ester-2**: Ee: 80% (Chiralcel® AD-H; 1% *i*-PrOH in hexanes; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=31.4$  min;  $t_2=38.8$  min). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.43–7.28 (m, 5H), 7.24 (t,  $J = 7.2$  Hz, 2H), 7.19–7.12 (m, 1H), 7.14–7.08 (m, 2H), 4.16 (ddd,  $J = 10.5, 3.6, 1.8$  Hz, 1H), 3.84 (s, 3H), 3.21 (s, 3H), 2.90 (d,  $J = 2.4$  Hz, 1H), 2.83 (ddd,  $J = 13.9, 9.3, 4.8$  Hz, 1H), 2.57 (dt,  $J = 13.8, 8.4$  Hz, 1H), 1.69 (dt,  $J = 15.5, 8.3$  Hz, 1H), 1.53 (dddd,  $J = 14.0, 10.5, 8.8, 4.8$  Hz, 1H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 172.1, 141.8, 135.4, 128.6, 128.23, 128.19, 128.1, 127.5, 125.7, 87.6, 75.2, 53.8, 52.2, 32.3, 32.1.  $[\alpha]_D^{25} -31.7$  (c 1.0, CHCl<sub>3</sub>). HRMS-ESI ( $m/z$ ): [M+Na]<sup>+</sup> calcd for C<sub>19</sub>H<sub>22</sub>O<sub>4</sub>Na, 337.1416; found, 337.1415.



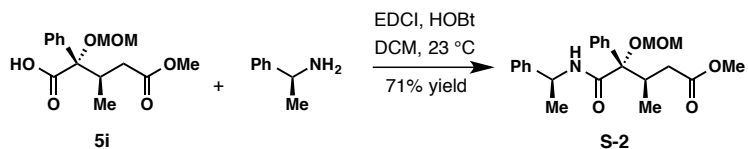
**(S)-2-(1-Hydroxycyclohexyl)-2-methoxy-2-phenylacetic acid (6c).** The title compound was prepared according to **general procedure II** using (*S*)-2-methoxy-2-phenylacetic acid (83.1 mg, 0.500 mmol), (*S*)-<sup>3</sup>TA (0.233 g, 0.515 mmol, 1.03 equiv), *n*-BuLi (0.81 mL, 2.47 M in

hexanes, 2.00 mmol, 4.0 equiv) in THF (3.5 mL) followed by addition of a solution of cyclohexanone (65  $\mu$ L, 61.6 mg, 0.628 mmol, 1.26 equiv) in THF (0.5 mL) at  $-78$   $^{\circ}$ C. The reaction was quenched after 1.5 h, and product **6c** (90.3 mg, 0.324 mmol, 65% yield) was obtained after purification by column chromatography on silica gel (2% methanol in dichloromethane).  $[\alpha]_{\text{D}}^{23} -50.4$  (*c* 1.5,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.47–7.41 (m, 2H), 7.40–7.32 (m, 3H), 3.35 (s, 3H), 3.17 (brs, 1H), 1.82–1.75 (m, 2H), 1.71–1.41 (m, 6H), 0.96–0.83 (m, 2H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 170.6, 133.5, 129.2, 128.1, 127.4, 89.9, 77.9, 54.4, 31.4, 30.4, 25.2, 20.9, 20.8. HRMS-ESI (*m/z*):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{15}\text{H}_{20}\text{O}_4\text{Na}$ , 287.1259; found, 287.1251.

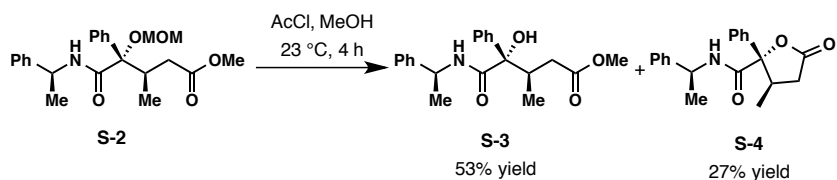


**(S)-Methyl 2-(1-hydroxycyclohexyl)-2-methoxy-2-phenylacetate (6c methyl ester).** The title compound was prepared using carboxylic acid **6c** (24.5 mg, 92.7  $\mu$ mol),  $\text{TMSCHN}_2$  (0.33 mL, 0.57 M in hexanes, 0.188 mmol) in a mixture of benzene-MeOH (4:1, 1.0 mL) at  $0$   $^{\circ}$ C for 1 h. The solvent was removed and the residue was purified by column chromatography on silica gel (6% ethyl acetate in hexanes) to afford product **6c methyl ester** (22.9 mg, 82.3  $\mu$ mol, 89% yield). Ee: 80% (Chiralcel® OJ-H; 1% *i*-PrOH in hexanes; flow rate = 0.5 mL/min; detection at 215 nm;  $t_1=17.6$  min (major);  $t_2=20.5$  min).  $[\alpha]_{\text{D}}^{23} +6.90$  (*c* 1.23,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.66–7.60 (m, 2H), 7.38–7.29 (m, 3H), 3.85 (s, 3H), 3.33 (s, 3H), 2.81 (s, 1H), 1.77–1.69 (m, 1H), 1.63–1.36 (m, 7H), 1.32–1.22 (m, 1H), 1.05–0.93 (m, 1H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm):  $\delta$  172.5, 134.6, 128.9, 127.9, 127.5, 91.0, 76.7, 55.4, 51.9, 32.3, 31.6, 25.6, 21.7, 21.6. LRMS-ESI (*m/z*):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{16}\text{H}_{22}\text{O}_4\text{Na}$ , 301; found, 301.

### III. Determination of absolute configuration



**(3*R*,4*S*)-Methyl 4-(methoxymethoxy)-3-methyl-5-oxo-4-phenyl-5-(((*S*)-1-phenylethyl)amino)pentanoate (S-2).** Hydroxybenzotriazole monohydrate (HOBt•H<sub>2</sub>O, 28.3 mg, 0.185 mmol, 1.5 equiv), *N*-(3-Dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride (EDCI•HCl, 35.4 mg, 0.185 mmol, 1.5 equiv) and (*S*)-(-)- $\alpha$ -methylbenzylamine (29.9 mg, 0.246 mmol, 2.0 equiv) were added sequentially to a solution of acid **5i** (36.5 mg, 0.123 mmol, 1.0 equiv) in CH<sub>2</sub>Cl<sub>2</sub> (2 mL). The solution was stirred at room temperature for 24 h. The reaction mixture was then diluted with hexanes/ethyl acetate (10 mL, 5:1) and quenched with 0.5 M aqueous solution of HCl. The aqueous solution was extracted with ethyl acetate and the combination of the organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated. The residue was purified by column chromatography on silica gel (20% ethyl acetate with hexanes) to afford the pure amide product (34.7 mg, 86.9  $\mu$ mol, 71% yield).  $[\alpha]_{\text{D}}^{26} -72.1$  (*c* 1.04, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.86 (d, *J* = 7.9 Hz, 1H), 7.55–7.44 (m, 2H), 7.42–7.26 (m, 8H), 5.18 (*virt. p*, *J* = 7.0 Hz, 1H), 4.50 (d, *J* = 6.5 Hz, 1H), 4.44 (d, *J* = 6.5 Hz, 1H), 3.59 (s, 3H), 3.33 (s, 3H), 3.00–2.94 (m, 1H), 2.41 (dd, *J* = 16.6, 2.8 Hz, 1H), 2.33 (dd, *J* = 16.6, 10.4 Hz, 1H), 1.53 (d, *J* = 6.9 Hz, 3H), 1.00 (d, *J* = 6.6 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 173.8, 170.2, 143.3, 137.4, 128.6, 128.5, 128.4, 128.2, 127.3, 126.2, 93.5, 88.6, 56.2, 51.4, 48.8, 38.3, 37.5, 22.0, 15.0. HRMS-ESI (*m/z*): [M+Na]<sup>+</sup> calcd for C<sub>23</sub>H<sub>29</sub>NO<sub>5</sub>Na, 422.1943; found, 422.1935.



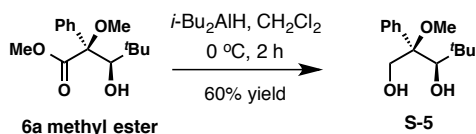
**(3*R*,4*S*)-Methyl 4-hydroxy-3-methyl-5-oxo-4-phenyl-5-(((*S*)-1-phenylethyl)amino)pentanoate (S-3)** Acetyl chloride (3.6 mg, 45.3  $\mu$ mol, 1.0 equiv) was added to a solution of amide **S-2** (18.1 mg, 45.3  $\mu$ mol) in methanol (0.5 mL) at 0 °C. After 5 min, the reaction mixture was warmed up to 23 °C and stirred for further 4 h. The reaction mixture was then concentrated and the residue was purified by column chromatography on silica gel (10% ethyl acetate with hexanes) to afford **S-3** (8.6 mg, 24.2  $\mu$ mol, 53% yield) and **S-4** (4.0 mg, 12.4  $\mu$ mol, 27% yield).

**S-3:**  $[\alpha]_{\text{D}}^{25} -29.2$  (*c* 0.53, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.76–7.70 (m, 2H), 7.41–7.32 (m, 3H), 7.31–7.25 (m, 3H), 7.25–7.21 (m, 3H), 5.71 (*brs*, 1H), 4.96 (*virt. p*, *J* =

7.1 Hz, 1H), 3.68 (s, 3H), 2.95 (virt. qt,  $J = 7.1, 4.8$  Hz, 1H), 2.55 (dd,  $J = 17.2, 4.6$  Hz, 1H), 2.48 (dd,  $J = 17.2, 5.1$  Hz, 1H), 1.36 (d,  $J = 7.0$  Hz, 3H), 0.77 (d,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 176.1, 173.8, 143.9, 141.4, 128.5, 128.1, 127.3, 127.1, 125.8, 125.4, 80.8, 52.2, 48.8, 37.3, 37.0, 22.0, 12.3. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{21}\text{H}_{25}\text{NO}_4\text{Na}$ , 378.1681; found, 378.1681.

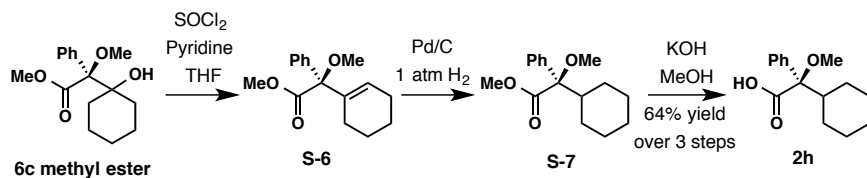
The structure of S-3 was unambiguously determined by X-ray Crystallography, and crystallographic data are deposited with the Cambridge Crystallographic Data Centre under the accession number CCDC 1489339.

(2*R*,3*R*)-3-methyl-5-oxo-2-phenyl-*N*-((*S*)-1-phenylethyl)tetrahydrofuran-2-carboxamide (S-4).  $[\alpha]_{\text{D}}^{25} -78.7$  ( $c$  0.27,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.61–7.52 (m, 2H), 7.43–7.30 (m, 5H), 7.30–7.22 (m, 3H), 6.60 (d,  $J = 7.8$  Hz, 1H), 5.00 (virt. p,  $J = 7.1$  Hz, 1H), 3.35 (virt. pd,  $J = 7.2, 3.9$  Hz, 1H), 2.62 (dd,  $J = 17.5, 7.6$  Hz, 1H), 2.22 (dd,  $J = 17.5, 4.0$  Hz, 1H), 1.36 (d,  $J = 7.0$  Hz, 3H), 0.76 (d,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 174.9, 169.9, 142.9, 135.0, 128.8, 128.51, 128.47, 127.5, 125.7, 124.9, 90.8, 49.5, 37.4, 36.6, 21.8, 16.4. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{20}\text{H}_{21}\text{NO}_3\text{Na}$ , 346.1419; found, 346.1423.



(2*R*,3*R*)-2-Methoxy-4,4-dimethyl-2-phenylpentane-1,3-diol (S-5). To a solution of ester 6a (66.1 mg, 0.248 mmol) in  $\text{CH}_2\text{Cl}_2$  (4 mL) was added  $i\text{-Bu}_2\text{AlH}$  (1 mL, 1.0 M in toluene, 1.00 mmol) at 0 °C. After stirring at the same temperature for 2 h, the reaction mixture was quenched with a saturated solution of sodium potassium tartrate. The reaction mixture was stirred at 23 °C for 0.5 h, and extracted with  $\text{CH}_2\text{Cl}_2$ . The combined organic phase was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was purified by column chromatography on silica gel (25% ethyl acetate in hexanes) to afford product S-5 (35.4 mg, 0.149 mmol, 60% yield).  $[\alpha]_{\text{D}}^{23} +53.8$  ( $c$  0.92,  $\text{CHCl}_3$ ).  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  (ppm): 7.45–7.42 (m, 2H), 7.34–7.30 (m, 2H), 7.25–7.21 (m, 1H), 4.39 (d,  $J = 12.2$  Hz, 1H), 4.01 (d,  $J = 12.2$  Hz, 1H), 3.71 (s, 1H), 3.41 (s, 3H), 0.72 (s, 9H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  (ppm): 142.5, 128.9, 128.5, 128.0, 85.1, 84.9, 66.4, 52.1, 37.6, 28.6. HRMS-ESI ( $m/z$ ):  $[\text{M}+\text{Na}]^+$  calcd for  $\text{C}_{14}\text{H}_{22}\text{O}_3\text{Na}$ , 261.1467; found, 261.1473.

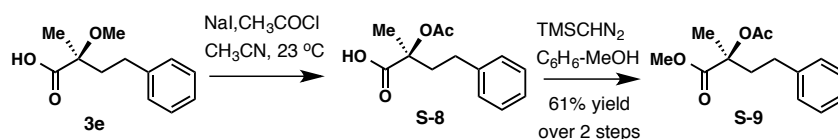
The structure of S-5 was unambiguously determined by X-ray Crystallography, and crystallographic data are deposited with the Cambridge Crystallographic Data Centre under the accession number CCDC 1489338.



**(R)-2-Cyclohexyl-2-methoxy-2-phenylacetic acid (2h).** Thionyl chloride (20  $\mu\text{L}$ , 32.8 mg, 0.276 mmol) and pyridine (30  $\mu\text{L}$ , 29.4 mg, 0.372 mmol) were added sequentially to a solution of **6a methyl ester** (22.9 mg, 82.3  $\mu\text{mol}$ ) in THF (1 mL) at 0  $^\circ\text{C}$ . The resultant mixture was stirred at the same temperature for 2 h and quenched with water, and extracted with ethyl acetate. The combined organic phase was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , concentrated, and the residue was concentrated to afford crude alkene product **S-6** (21.1 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.56–7.50 (m, 2H), 7.36–7.29 (m, 2H), 7.31–7.25 (m, 1H), 5.99 (*virt. tt*,  $J = 3.8, 1.6$  Hz, 1H), 3.72 (s, 3H), 3.31 (s, 3H), 2.21–2.15 (m, 2H), 1.81–1.75 (m, 2H), 1.63–1.56 (m, 4H). The product was directly used to the next step without further characterization.

A solution of crude product **S-6** (21.1 mg), 10% Pd/C (8.8 mg, 8.30  $\mu\text{mol}$ ) in MeOH (1 mL) was stirred at 23  $^\circ\text{C}$  under 1 atm of hydrogen atmosphere for 18 h. The mixture was then filtered through a pad of celite and rinsed with ethyl acetate. The combined filtrate was concentrated to afford the crude product **S-7** (19.0 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.46–7.40 (m, 2H), 7.37–7.32 (m, 2H), 7.31–7.27 (m, 1H), 3.82 (s, 3H), 3.19 (s, 3H), 2.10 (*tt*,  $J = 12.0, 2.9$  Hz, 1H), 1.89–1.81 (m, 1H), 1.75–1.52 (m, 4H), 1.30–1.11 (m, 2H), 1.06–0.94 (m, 1H), 0.96–0.77 (m, 2H). The product was directly used to the next step without further characterization.

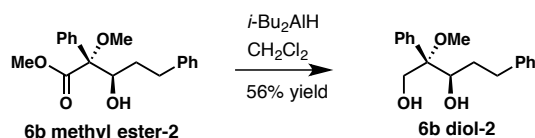
A solution of crude product **S-7** (19.0 mg) and KOH (56.0 mg, 1.00 mmol) in a mixture of MeOH– $\text{H}_2\text{O}$  (3:1, 1.0 mL) was heated for 40 h at 80  $^\circ\text{C}$ . After cooling, the reaction mixture was extracted with ether. Then the aqueous phase was acidified, and extracted with ethyl acetate. The combined organic phase was washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , and concentrated to product **2h** (13.1 mg, 52.8  $\mu\text{mol}$ , 64% combined yield over 3 steps).  $[\alpha]_{\text{D}}^{23} +4.2$  ( $c$  0.62,  $\text{CHCl}_3$ ). Ee: 83% (Chiralcel® OD-H; 1% *i*-PrOH in hexanes with 0.1% TFA; flow rate = 1.0 mL/min; detection at 215 nm;  $t_1=16.5$  min (major);  $t_2=20.2$  min).



**(2S)-Methyl 2-hydroxy-2-methyl-4-phenylbutanoate (S-8).** The following procedure was slightly modified from original literature.<sup>3</sup> A 10-mL round flask was charged with sodium iodide (87.0 mg, 0.580 mmol) under an argon atmosphere through a gas inlet. Then the flask was flame-dried under vacuum and back filled with argon. After cooling to 23  $^\circ\text{C}$ , a

solution of **3e** (29.2 mg, 0.132 mmol) in CH<sub>3</sub>CN (2 mL) was added and followed by acetyl chloride (40 μL, 44.0 mg, 0.561 mmol). The flask was wrapped with aluminium foil and the resultant mixture was stirred for 24 h at 23 °C before quenched with a mixture of 1 M aqueous solution of HCl and saturated aqueous solution of NaHSO<sub>3</sub>. The aqueous solution was extracted with ethyl acetate and the combination of the organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated to afford crude product **S-8**. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 7.32–7.27 (m, 2H), 7.23–7.16 (m, 3H), 2.76 (ddd, *J* = 13.7, 11.8, 5.3 Hz, 1H), 2.68 (ddd, *J* = 13.7, 11.8, 5.3 Hz, 1H), 2.32–2.26 (m, 1H), 2.18–2.10 (m, 1H), 2.07 (s, 3H), 1.67 (s, 3H). **S-8** was directly used to the next step without further characterization.

**(2S)-Methyl 2-acetoxy-2-methyl-4-phenylbutanoate (S-9)**. A solution of TMSCHN<sub>2</sub> (0.25 mL, 1.03 M in hexanes, 0.258 mmol) was added dropwise to a solution of above crude acid **S-8** in a mixture of benzene–MeOH (4:1, 2.0 mL) at 0 °C. The resultant mixture was stirred at the same temperature for 1 h. The solvent was removed on a rotary evaporator and the residue was purified by column chromatography on silica gel (9% ethyl acetate in hexanes) to afford the product **S-9** (20.2 mg, 80.7 μmol, 61% yield over 2 steps). [α]<sub>D</sub><sup>22</sup> –6.7 (*c* 1.0, CHCl<sub>3</sub>); *lit*<sup>4</sup> [α]<sub>D</sub><sup>20</sup> –5.3 (*c* 2.4, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 7.32–7.25 (m, 2H), 7.23–7.15 (m, 3H), 3.72 (s, 3H), 2.70 (ddd, *J* = 13.8, 11.6, 5.5 Hz, 1H), 2.63 (ddd, *J* = 13.8, 11.6, 5.5 Hz, 1H), 2.23 (ddd, *J* = 14.0, 11.6, 5.5 Hz, 1H), 2.11 (ddd, *J* = 14.0, 11.6, 5.5 Hz, 1H), 2.06 (s, 3H), 1.65 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 172.5, 170.0, 141.0, 128.4, 128.3, 126.1, 80.4, 52.3, 39.8, 29.6, 21.5, 21.1. LRMS-FD (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>16</sub>H<sub>23</sub>O<sub>4</sub>, 251; found, 251.

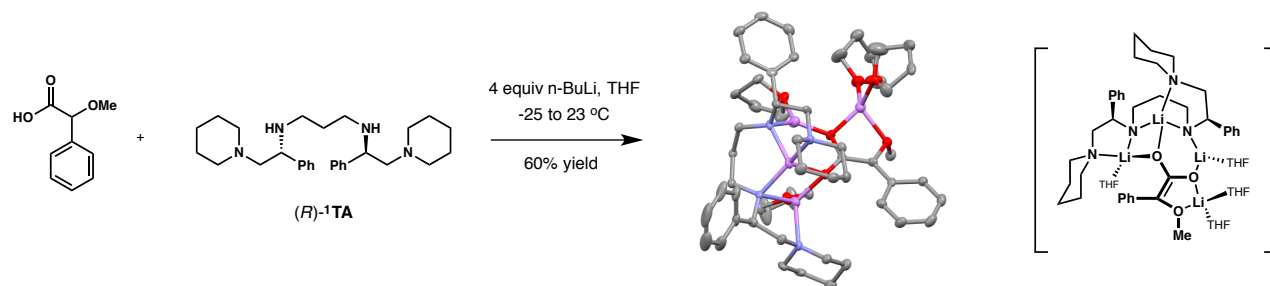


**(2S,3R)-2-Methoxy-2-phenyl-5-phenylpentane-1,3-diol (6b diol-2)**. To a solution of ester **6b-methyl ester-2** (14.2 mg, 45.2 μmol) in CH<sub>2</sub>Cl<sub>2</sub> (2 mL) was added *i*-Bu<sub>2</sub>AlH (0.26 mL, 1.0 M in toluene, 0.260 mmol) at 0 °C. After stirring at the same temperature for 2 h, the reaction mixture was quenched with a saturated solution of sodium potassium tartrate. The reaction mixture was stirred at 23 °C for 0.5 h, and extracted with CH<sub>2</sub>Cl<sub>2</sub>. The combined organic phase was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated, and the residue was purified by column chromatography on silica gel (40% ethyl acetate in hexanes) to afford product **6b-diol-2** (7.2 mg, 25.1 μmol, 56% yield). [α]<sub>D</sub><sup>22</sup> +1.88 (*c* 0.35, CHCl<sub>3</sub>). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ (ppm): 7.36–7.27 (m, 3H), 7.23–7.18 (m, 4H), 7.16–7.12 (m, 1H), 7.03–7.00 (m, 2H), 4.51 (d, *J* = 12.2 Hz, 1H), 4.12 (dd, *J* = 12.2, 1.6 Hz, 1H), 3.85 (virt. dt, *J* = 10.2, 1.9 Hz, 1H), 3.21 (s, 3H), 2.87 (ddd, *J* = 14.4, 9.9, 5.0 Hz, 1H), 2.49 (ddd, *J* =



13.8, 9.4, 7.3 Hz, 1H), 1.75–1.57 (m, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ (ppm): 141.6, 138.4, 128.5, 128.34, 128.27, 127.9, 126.7, 125.8, 81.3, 78.8, 61.3, 50.6, 32.7, 32.4. LRMS-FD (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>18</sub>H<sub>23</sub>O<sub>3</sub>, 287; found, 287.

**The structure of 6b diol-2 was unambiguously determined by X-ray Crystallography, and crystallographic data are deposited with the Cambridge Crystallographic Data Centre under the accession number CCDC 1489340.**



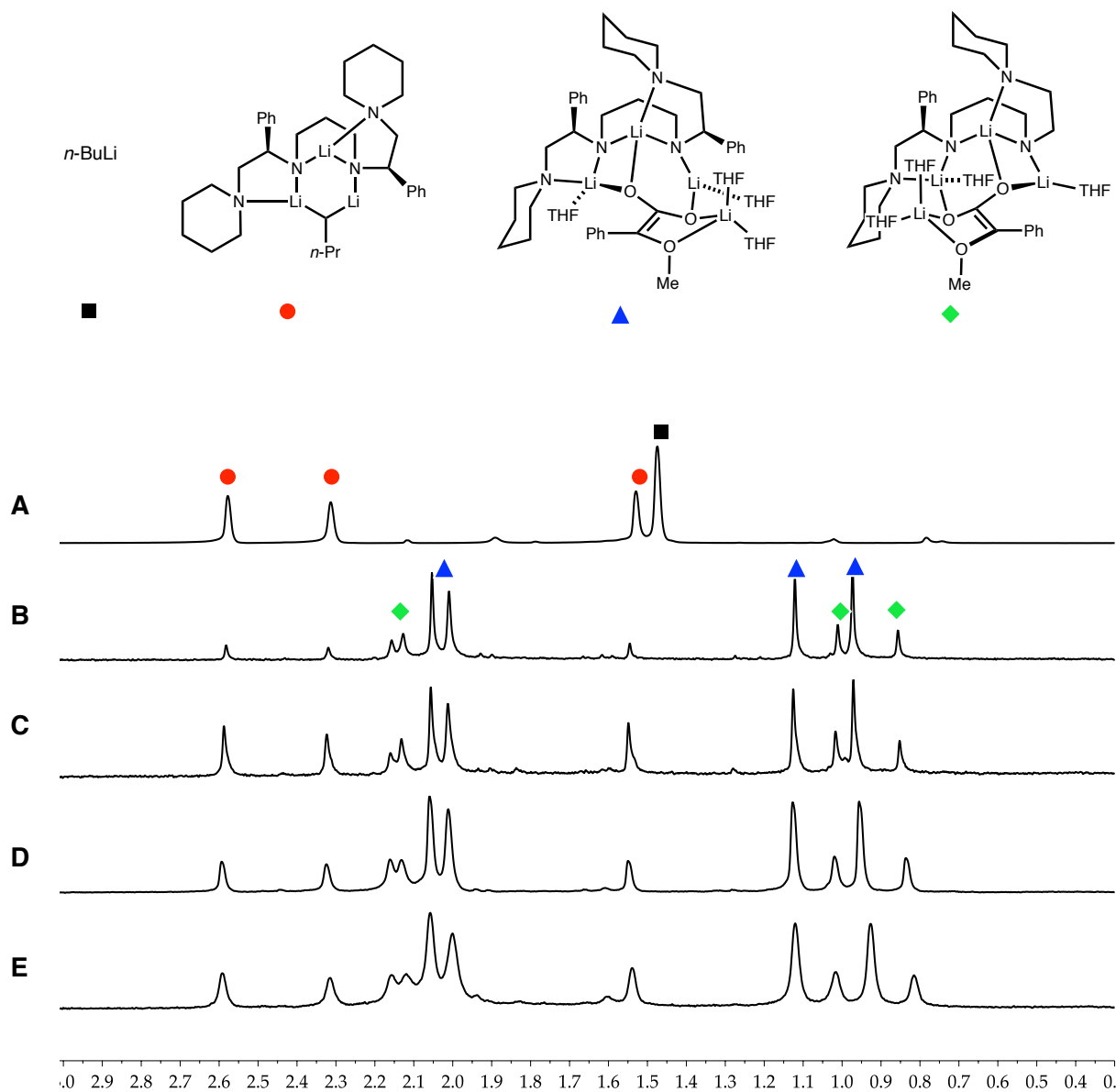
**Preparation of  $[\text{Li}_4((R)\text{-}^1\text{TA})(\text{PhC}(\text{OMe})(\text{CO}_2))(\text{THF})_4]$  (**S-10**).** A THF solution (3 mL) of ( $\pm$ )-2-methoxy-2-phenylacetic acid (36.1 mg, 0.217 mmol) and ( $R$ )- $^1\text{TA}$  (0.101 g, 0.224 mmol) were stirred at room temperature for 10 min. The slightly cloudy, colorless solution was then cooled to  $-25\text{ }^\circ\text{C}$  and  $n\text{-BuLi}$  in hexanes (0.35 mL, 0.869 mmol, 2.5 M) was added dropwise. During the course of the addition of  $n\text{-BuLi}$ , the reaction mixture formed a thick yellow gel, but with further addition of  $n\text{-BuLi}$ , the reaction mixture became a clear yellow solution. The reaction mixture was then stirred for 15 min, while warming to room temperature. The solution was filtered through a Celite column (1.5 cm  $\times$  0.5 cm) supported on glass wool. The yellow filtrate was then concentrated *in vacuo* to ca. 2 mL and then layered with hexanes (7 mL). Subsequent storage of this solution at  $-25\text{ }^\circ\text{C}$  resulted in the deposition of pale yellow crystalline material (0.114 g, 0.130 mmol, 60% yield). A single crystal suitable for X-ray diffraction was grown from a THF solution (3 mL) layered with hexanes (4 mL).

**X-ray Crystallography.** Data for **S-10**·THF were collected on a Bruker KAPPA APEX II diffractometer equipped with an APEX II CCD detector using a TRIUMPH monochromator with a MoK $\alpha$  X-ray source ( $\alpha = 0.71073\text{ \AA}$ ). Crystals were mounted on a cryoloop under Paratone-N oil, and all data were collected at 100(2) K using an Oxford nitrogen gas cryostream system. X-ray data for **S-10**·THF were collected utilizing frame exposures of 50 s. Data collection and cell parameter determination were conducted using the SMART program.<sup>5</sup> Integration of the data frames and final cell parameter refinement were performed using SAINT software.<sup>6</sup> Absorption correction of the data were carried out using the multi-scan method SADABS.<sup>7</sup> Subsequent calculations were carried out using SHELXTL.<sup>8</sup> Structure determination was done using direct methods and difference Fourier techniques. All hydrogen atom positions were idealized, and rode on the atom of attachment. The final refinement included anisotropic temperature factors on all non H atoms. Structure solution, refinement, graphics, and creation of publication materials were performed using SHELXTL.<sup>8</sup> Further crystallographic details can be found in **Table S2**. Crystallographic data are also deposited with the Cambridge Crystallographic Data Centre under accession number CCDC 1489341.

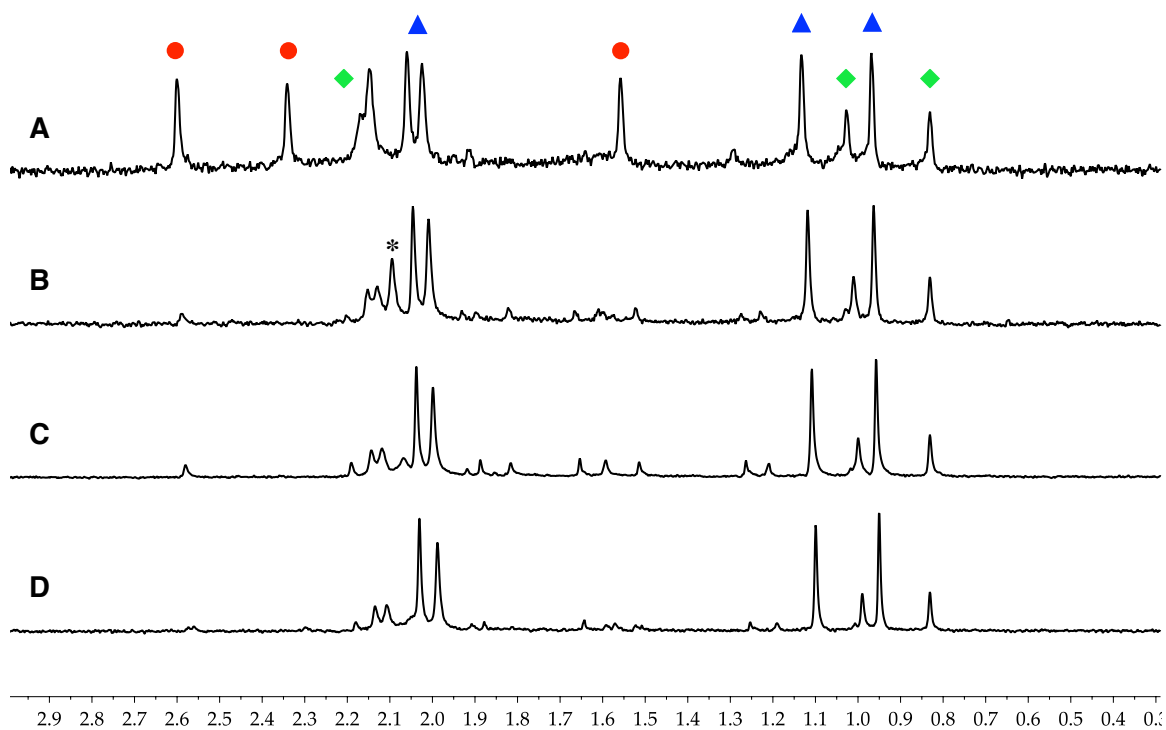
**Table S2.** X-ray Crystallographic Data for **S-10**·THF.

	<b>S-10</b> ·THF
empirical formula	C <sub>58</sub> H <sub>88</sub> Li <sub>4</sub> N <sub>4</sub> O <sub>8</sub>
crystal habit, color	block, pale yellow
crystal size (mm)	0.15 × 0.1 × 0.1
crystal system	monoclinic
space group	<i>P</i> 2 <sub>1</sub>
volume (Å <sup>3</sup> )	2834.3(3)
<i>a</i> (Å)	12.3684(7)
<i>b</i> (Å)	18.2504(9)
<i>c</i> (Å)	13.2045(8)
<i>α</i> (deg)	90
<i>β</i> (deg)	108.027(3)
<i>γ</i> (deg)	90
<i>Z</i>	2
formula weight (g/mol)	997.08
density (calculated) (Mg/m <sup>3</sup> )	1.168
absorption coefficient (mm <sup>-1</sup> )	0.075
<i>F</i> <sub>000</sub>	1080
total no. reflections	16174
unique reflections	8252
final R indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0624 <i>wR</i> <sub>2</sub> = 0.1385
largest diff. peak and hole (e <sup>-</sup> Å <sup>-3</sup> )	0.630 and -0.336
GOF	1.019

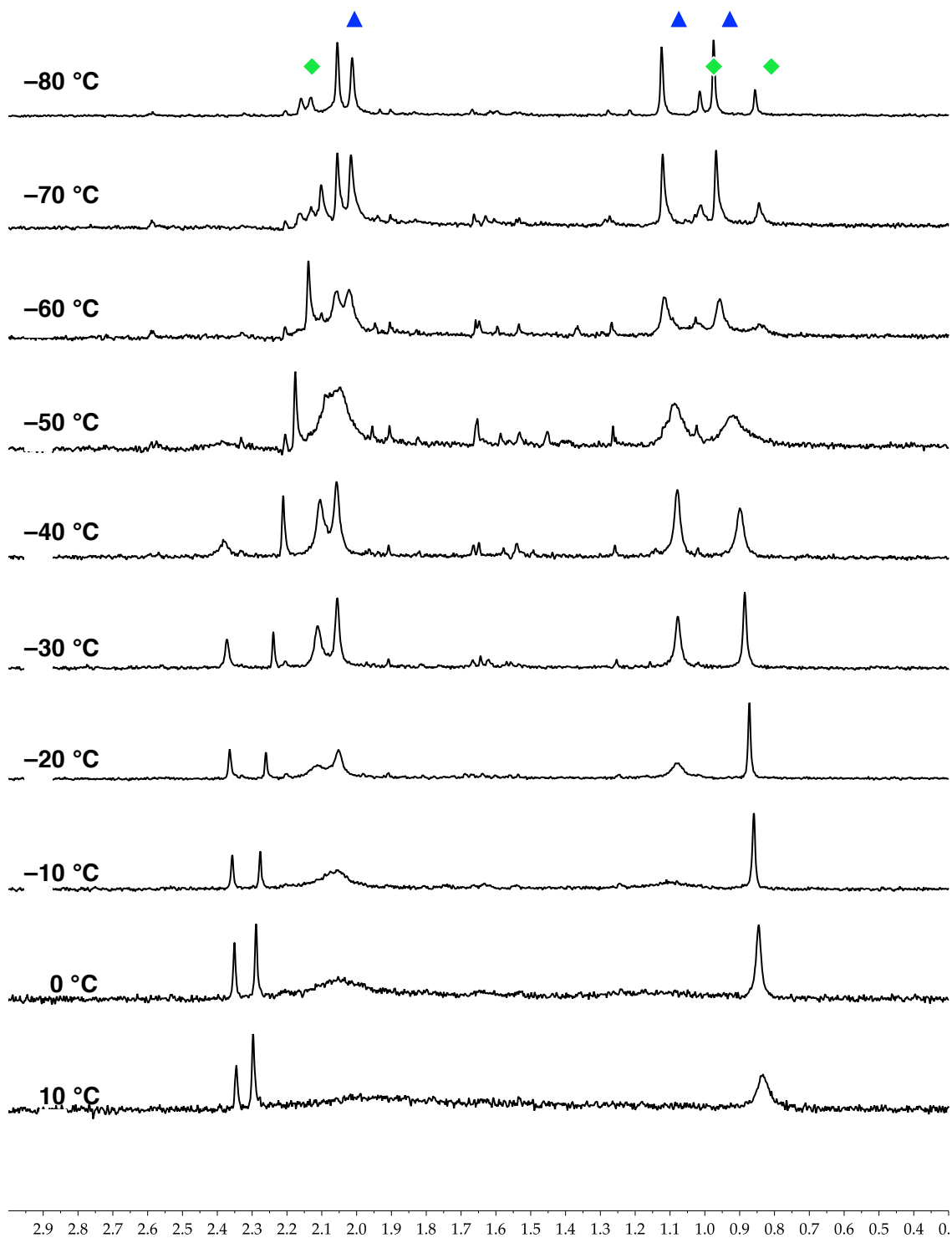
## NMR Spectroscopic Studies



**Figure S1.**  ${}^6\text{Li}$  NMR spectra of the isomers of  $[\text{}^6\text{Li}]\text{-7}$  prepared from a 1:4:1 ratio of (*R*)- ${}^1\text{TA}$ , *n*-BuLi, and ( $\pm$ )- $\alpha$ -methoxyphenylacetic acid in 10.0 M THF–hexane. The spectra were recorded at  $-80\text{ }^\circ\text{C}$  after aging at  $0\text{ }^\circ\text{C}$  for 2 hr: (A) spectrum showing *n*-BuLi-derived mixed aggregate in the absence of acid; (B) 0.025 M acid; (C) 0.050 M acid; (D) 0.10 M acid; (E) 0.20 M acid.



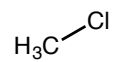
**Figure S2.**  $^6\text{Li}$  NMR spectra of the isomers of  $[\text{}^6\text{Li}]\text{-7}$  prepared from 0.025 M (*R*)- $^1\text{TA}$ , 0.10 M *n*-BuLi, and 0.025 M ( $\pm$ )- $\alpha$ -methoxyphenylacetic acid at varying THF concentrations. The spectra were recorded at  $-80\text{ }^\circ\text{C}$  after aging at  $0\text{ }^\circ\text{C}$  for 2 hr: (A) 4.0 M THF; (B) 6.0 M THF; (C) 8.0 M THF; (D) 10.0 M THF. (The \* indicates an unknown species.)



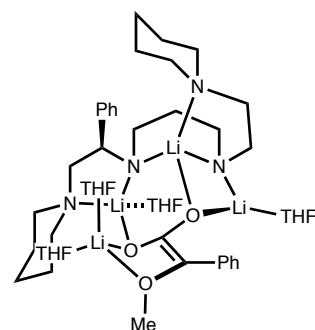
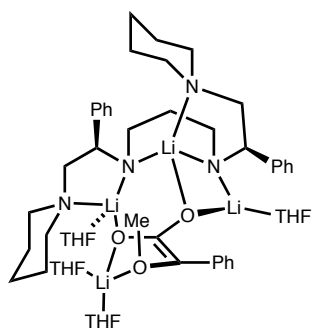
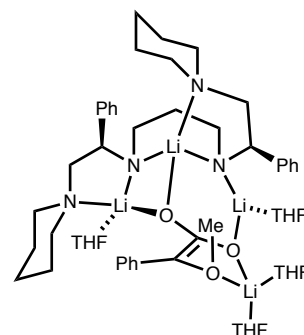
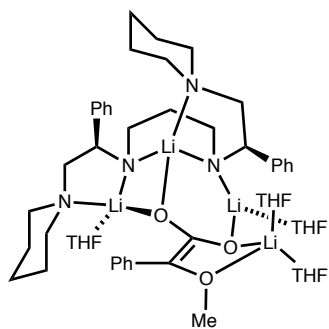
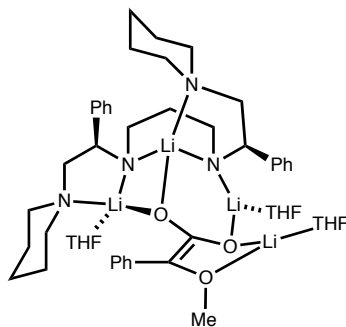
**Figure S3.** Variable temperature  ${}^6\text{Li}$  NMR spectra of the isomers of  $[\text{}^6\text{Li}]\text{-7}$  prepared from 0.025 M (*R*)- ${}^1\text{TA}$ , 0.10 M *n*-BuLi, and 0.025 M ( $\pm$ )- $\alpha$ -methoxyphenylacetic acid in 10.0 M THF-hexane. The spectra were recorded after aging at 0 °C for 2 hr.

#### **DFT Computational Studies**

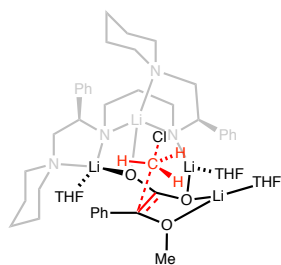
# Chart 1



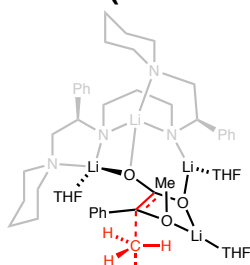
CH<sub>3</sub>Cl



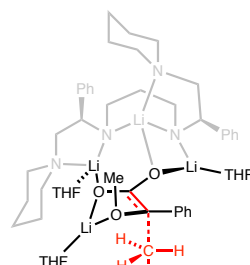
### Chart 1 (continued)



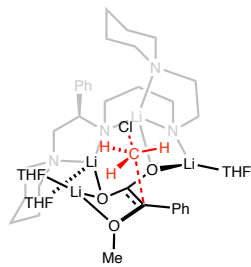
TS I



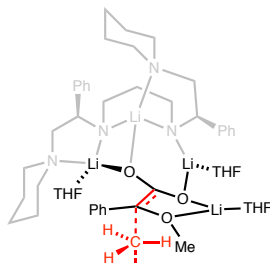
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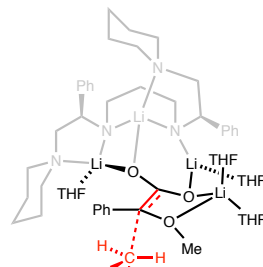
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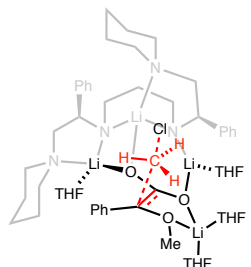
TS IV



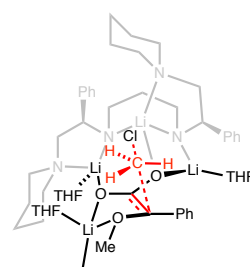
TS V



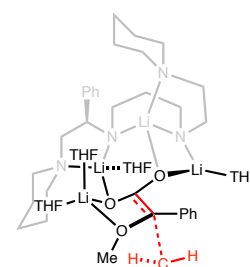
TS VI



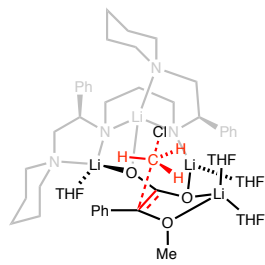
TS VII



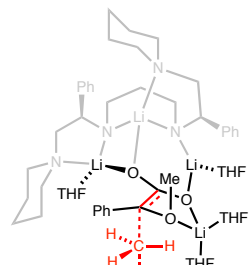
TS VIII



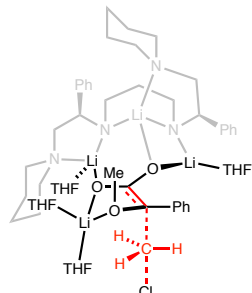
TS IX



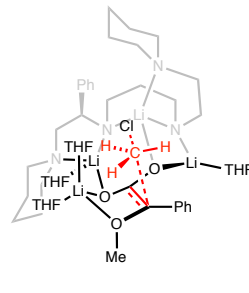
TS X



TS XI



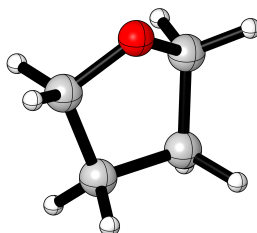
TS XII



TS XIII



**Table S1.** Optimized geometries at the B3LYP level of theory with 6-31G(d) basis set for the ground states at  $-78\text{ }^{\circ}\text{C}$  with free energies (Hartrees) and cartesian coordinates (X, Y, Z). (Note:  $G_{\text{MP2}}$  includes single-point MP2 corrections to B3LYP/6-31G(d) optimized structures.)

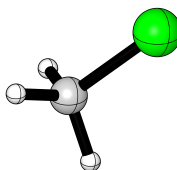
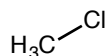


**THF**

$G = -232.34927$

$G_{\text{MP2}} = -231.569420$

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	2.35957000	2.11540200	0.56207900
O	1.13072500	-0.73921500	-0.44609100	H	2.29989300	1.81771600	-1.17778200
C	2.26413700	-0.01293100	0.01309700	H	2.43971000	-0.21425900	1.08390100
C	1.92140000	1.47528500	-0.20996300	H	3.13466300	-0.36010700	-0.55024500
C	0.36725000	1.48895700	-0.19255200	H	-0.86394200	-0.32564100	-0.58587700
H	-0.03986900	2.11280100	0.60919800	H	-0.20057200	-0.21479800	1.06351600
H	-0.02796900	1.86922100	-1.13920400				

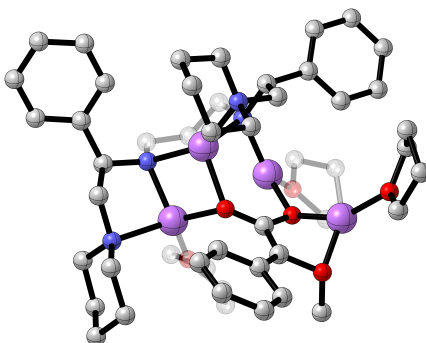
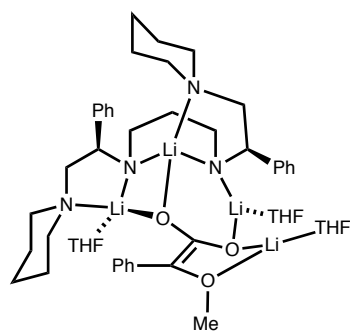


**CH<sub>3</sub>Cl**

$G = -500.084149$

$G_{\text{MP2}} = -499.329931$

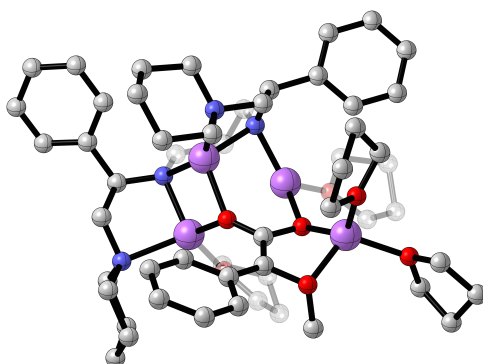
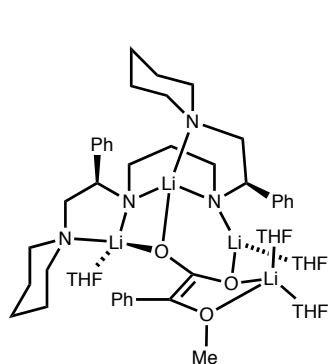
Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	H	0.89529400	-0.51689800	-0.34631800
H	0.00000000	1.03379600	-0.34631800	Cl	0.00000000	0.00000000	1.80340400
H	-0.89529400	-0.51689800	-0.34631800				



I  
 $G = -2649.505424$   
 $G_{MP2} = -2640.707212$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	2.46126200	-3.56470600	-0.60186500
N	-0.31511700	-1.87003000	-0.74008400	N	2.89303800	-2.33751800	-1.24819400
C	-1.71565700	-1.89309300	-1.10908900	Li	1.31903400	-1.23296400	-1.81792400
C	-2.20342100	-0.49307400	-1.53748100	Li	3.32138700	-0.93120500	0.05021100
N	-2.07739700	0.54864700	-0.48911300	O	3.57961600	0.90948800	-0.19579300
C	-2.42872600	1.85785900	-1.07727900	Li	4.83809800	1.95875600	-1.04811900
H	-1.77308400	2.03318400	-1.93173600	O	6.22510400	2.22599900	-2.33163900
H	-3.46835400	1.82845600	-1.46085800	C	7.03724200	1.26639100	-3.05182100
C	-2.29482300	3.00250900	-0.07357200	C	6.85820000	1.63667400	-4.51958300
H	-2.56145200	3.94414000	-0.56847700	C	6.81244300	3.17242800	-4.45242600
H	-1.24311000	3.09098300	0.22897700	C	6.08505500	3.44542600	-3.12766100
C	-3.18091000	2.75261300	1.15195300	H	5.01541900	3.62914500	-3.25829700
C	-2.88142000	1.36465600	1.73019500	H	6.51859500	4.27633300	-2.56347100
C	-2.96704100	0.27250200	0.65781600	H	6.29192200	3.62226600	-5.30230800
H	-2.68803900	-0.69121300	1.09143500	H	7.82876500	3.58135100	-4.42563300
H	-4.01479100	0.18021700	0.30782100	H	5.91124700	1.23379300	-4.89603000
H	-3.57958300	1.11962500	2.54137800	H	7.66834100	1.25732100	-5.14901100
H	-1.87013100	1.35661600	2.15389900	H	8.08322100	1.37312900	-2.73323000
H	-4.23823200	2.80395500	0.85266800	H	6.68636300	0.26567200	-2.79100000
H	-3.03020800	3.53001300	1.91188300	O	3.78269600	3.48985400	-0.71234000
H	-3.25043400	-0.54841800	-1.88434200	C	2.60067500	2.80520400	-1.18146300
H	-1.59884800	-0.16379200	-2.39263800	C	2.51881100	1.44661200	-0.80986500
H	-2.34240800	-2.19636800	-0.23973600	O	1.49309800	0.68609300	-1.04866900
C	-2.13476000	-2.89629900	-2.21276900	C	1.74274800	3.61587600	-2.02268300
C	-3.48300300	-3.24964100	-2.37136500	C	2.05355300	4.97766900	-2.27412800
C	-3.88767000	-4.14316900	-3.36302700	C	1.25893100	5.76851300	-3.10096800
C	-2.94055400	-4.71882500	-4.21365900	C	0.12397100	5.24494900	-3.72246100
C	-1.59361300	-4.39081300	-4.05639300	C	-0.19363500	3.90220700	-3.49613200
C	-1.19823900	-3.48754600	-3.06559200	C	0.58843500	3.10391300	-2.66620900
H	-0.14965100	-3.24143800	-2.92333300	H	0.33429800	2.06473000	-2.50488200
H	-0.84517500	-4.84495500	-4.70222200	H	-1.06637100	3.46509400	-3.97811200
H	-3.24932900	-5.42228800	-4.98305800	H	-0.49401700	5.86274100	-4.36830000
H	-4.94026400	-4.39694300	-3.46758000	H	1.53594100	6.80874500	-3.26198600
H	-4.22730500	-2.82317600	-1.69975200	H	2.93749800	5.41133200	-1.81921800
C	-0.03749000	-3.09643900	0.00165000	C	3.61787400	4.08743400	0.57591900
C	1.40572400	-3.30331000	0.48729300	H	4.53451500	4.64641300	0.79670300

H	2.76606400	4.77580100	0.56621100	H	4.47207500	-1.50680700	-4.14126500
H	3.45997800	3.31901700	1.34200700	H	3.99103000	-0.50571700	-2.75562200
O	4.28083400	-1.31501200	1.78796000	H	3.34062300	-3.47781700	-2.97026500
C	5.12443800	-0.31571100	2.39873600	C	5.18821000	-2.97237000	-2.07139600
C	5.90521900	-1.04794700	3.49044000	C	5.73863400	-4.19762900	-2.46578000
C	6.07287800	-2.44484600	2.87282000	C	7.05979400	-4.53742000	-2.15851200
C	4.73826900	-2.64580100	2.15171200	C	7.86790700	-3.64542000	-1.45424500
H	3.98208400	-3.09792200	2.80459800	C	7.33729500	-2.41530600	-1.05240300
H	4.81964500	-3.23759000	1.23861800	C	6.01236300	-2.09196800	-1.35141400
H	6.26761900	-3.22664600	3.61292800	H	5.60313500	-1.14185400	-1.01232200
H	6.89644000	-2.44763300	2.14981200	H	7.95926700	-1.70788000	-0.50674100
H	5.31492800	-1.10337400	4.41313900	H	8.89684400	-3.90369700	-1.21707800
H	6.85544800	-0.55810300	3.72441500	H	7.45598500	-5.50124200	-2.46970800
H	5.79617300	0.10074200	1.63588200	H	5.11853900	-4.89915400	-3.02078000
H	4.48541800	0.49041200	2.76749600	H	2.02210500	-4.28292600	-1.33001400
C	3.72586800	-2.60813500	-2.39827400	H	3.30089300	-4.13131500	-0.13849500
C	3.71126700	-1.38702500	-3.34565600	H	1.72278700	-2.44364100	1.10150400
N	2.39096300	-1.10496100	-3.94724200	H	1.39023800	-4.16892500	1.16711800
C	2.38810900	0.26451000	-4.50194400	H	-0.69646700	-3.16604900	0.90161200
C	1.06951600	0.61266300	-5.19482800	H	-0.29556500	-4.00586100	-0.57881800
C	0.75310200	-0.38338800	-6.31390700	O	0.40518300	0.24980900	1.98102200
H	1.50302400	-0.28917900	-7.11380100	C	1.23476800	1.30813600	2.52254600
H	-0.22245900	-0.16589400	-6.76605000	C	1.44010100	0.96998600	4.00738300
C	0.78089600	-1.80431100	-5.74361600	C	1.21454500	-0.55060600	4.03949100
C	2.09777100	-2.08506500	-5.01529600	C	0.09911300	-0.71293000	3.00998500
H	2.06799300	-3.08368600	-4.57057700	H	-0.88290900	-0.48094500	3.44729400
H	2.92640800	-2.08428500	-5.75292900	H	0.05505500	-1.69664200	2.54003600
H	-0.05586200	-1.93891300	-5.04871800	H	0.93650900	-0.92766800	5.02849100
H	0.65598000	-2.55043000	-6.53901800	H	2.11362900	-1.07796300	3.70101500
H	1.12718800	1.63950800	-5.57395200	H	0.69203400	1.47739300	4.62775700
H	0.26269600	0.59532600	-4.45122400	H	2.42972700	1.26889200	4.36723000
H	2.57146100	0.96331800	-3.68012700	H	2.17192600	1.30996800	1.95837000
H	3.21817900	0.37979500	-5.23114000	H	0.72592400	2.26551500	2.36857100



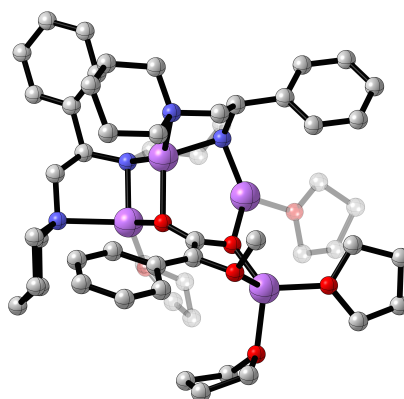
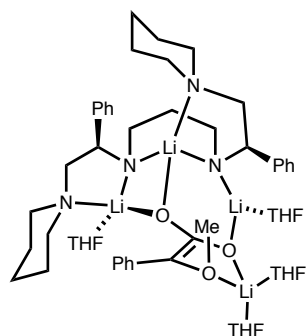
**II (6c)**

G = -2881.856196

G<sub>MP2</sub> = -2872.294063

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	10.1002050	1.93756100	2.33668200
O	1.60322300	0.90060300	0.40380600	C	5.75598500	3.15032500	2.64068800
Li	5.03158300	0.36551300	1.60125800	C	4.32596900	3.71069300	2.66560200
N	6.03237600	2.13844100	1.63015300	C	3.94388300	4.60358000	1.46826300
C	7.43253800	1.78603400	1.72277400	N	3.51737600	3.82536800	0.31653100
C	7.72758300	0.50418700	0.91614300	Li	4.80003700	2.31785600	-0.01211700
N	6.99712100	-0.69780800	1.38591900	N	4.83647600	3.01901000	-2.25871100
C	7.17555700	-1.78178600	0.39783700	C	4.68618100	1.90451600	-3.22100000
H	6.81686600	-1.41859600	-0.56844000	C	5.99796200	1.15345400	-3.45366200
H	8.25414700	-2.00815800	0.27840100	C	7.09776300	2.09904800	-3.94451100
C	6.43413500	-3.05821800	0.79680100	H	6.83554700	2.48167500	-4.94238900
H	6.59356800	-3.82233100	0.02652300	H	8.05237200	1.56820000	-4.04962700
H	5.35638300	-2.85228200	0.81844600	C	7.23285100	3.26648600	-2.96291800
C	6.90812700	-3.55188300	2.16798300	C	5.88467000	3.95144000	-2.72527300
C	6.79913000	-2.41570500	3.19091000	H	6.00061800	4.74428100	-1.98112900
C	7.50407400	-1.14668800	2.69930400	H	5.55415800	4.43726700	-3.66603200
H	7.36088300	-0.33962300	3.42238200	H	7.62763900	2.90235500	-2.00752500
H	8.59512500	-1.33269600	2.63578800	H	7.94546200	4.01463500	-3.33326200
H	7.23575600	-2.71270000	4.15363200	H	5.81933100	0.33993900	-4.16615800
H	5.74250200	-2.18142600	3.36717100	H	6.31068600	0.68396400	-2.51212000
H	7.95555300	-3.88005500	2.09532400	H	3.92745000	1.22101900	-2.82901300
H	6.32648100	-4.42400200	2.49309600	H	4.31659200	2.29240600	-4.19232600
H	8.81318300	0.30110100	0.90619000	C	3.54339300	3.72595600	-2.12849300
H	7.42408000	0.68304300	-0.12305400	H	3.33229100	4.30568500	-3.04699900
H	7.71632400	1.57624100	2.78096100	H	2.76973300	2.95370300	-2.04926400
C	8.45954400	2.86153200	1.28778300	C	3.45281600	4.63521800	-0.88664000
C	9.79773000	2.76571200	1.69645800	H	4.30864600	5.34081500	-0.92553700
C	10.7450760	3.71274200	1.30737700	C	2.20426900	5.53112600	-0.95138300
C	10.3648400	4.79327500	0.50740800	C	2.28629100	6.88370900	-0.59120000
C	9.03317900	4.91139300	0.10781200	C	1.15351900	7.70251700	-0.56198500
C	8.09249400	3.95311500	0.49521800	C	-0.09415700	7.18589700	-0.91217300
H	7.05037100	4.04571800	0.20305000	C	-0.19493800	5.84136500	-1.28420400
H	8.72234200	5.75685100	-0.50231000	C	0.93799500	5.02638900	-1.29229400
H	11.0974440	5.53875500	0.20772200	H	0.83813200	3.98118700	-1.57663700
H	11.7779210	3.61275600	1.63393000	H	-1.15908100	5.43249800	-1.58122500

H	-0.97562800	7.82228000	-0.90544600	H	1.18758500	-0.41289600	4.73506900
H	1.24916300	8.74684500	-0.27349700	H	2.24498700	-0.29170100	2.55111400
H	3.25803400	7.29986700	-0.33337500	H	2.90800400	-1.87672600	3.02515400
Li	2.06096800	2.64154200	0.88284100	O	-1.71284300	1.01073300	-0.02696600
O	3.80507300	0.43262300	0.11482200	C	-3.03249600	0.46364800	0.15051100
C	2.57344800	0.27412000	-0.26925800	C	-3.87318400	1.65084700	0.61009400
C	2.19412900	-0.52734800	-1.36584900	C	-3.30275100	2.79045000	-0.25422200
C	2.94410200	-1.50103300	-2.12781900	C	-1.82017100	2.40207300	-0.42950700
C	2.29343300	-2.35384800	-3.06119800	H	-1.14386800	2.97350900	0.20976700
C	2.99478600	-3.30536000	-3.79890500	H	-1.48534200	2.49838800	-1.46773800
C	4.37418100	-3.45828200	-3.64974900	H	-3.41811300	3.77502300	0.20802900
C	5.03452600	-2.62872000	-2.73719000	H	-3.81046400	2.81890500	-1.22442200
C	4.34612600	-1.67490800	-1.99445300	H	-3.69860100	1.84334400	1.67514500
H	4.86949200	-1.03254200	-1.29959400	H	-4.94582600	1.49510200	0.46158800
H	6.11165700	-2.72081400	-2.60806800	H	-3.40135500	0.06107400	-0.80472600
H	4.92047100	-4.19715100	-4.22969800	H	-2.95007500	-0.35356300	0.86899100
H	2.45122100	-3.93404900	-4.50217100	O	-0.68043600	-1.81194100	0.65058400
H	1.22100300	-2.26508300	-3.19943900	C	-0.07002100	-2.52520100	1.73991800
O	0.62601500	3.30469500	2.12948000	C	0.90479900	-3.48614100	1.06248900
C	-0.11999200	2.44421700	3.02039800	C	0.14004200	-3.89929600	-0.21742700
C	-0.86938600	3.37094300	3.99470300	C	-0.91462600	-2.78302600	-0.40241000
C	-0.88125200	4.71702800	3.25043000	H	-1.93815600	-3.16717200	-0.30121200
C	0.46456200	4.68484800	2.53287700	H	-0.81130000	-2.24764800	-1.34635200
H	1.28485900	4.96511000	3.20583100	H	-0.34685300	-4.87204100	-0.09407200
H	0.51952100	5.29652900	1.63168500	H	0.81276800	-3.96009600	-1.07619300
H	-0.98229700	5.57717000	3.91886500	H	1.16556300	-4.33875600	1.69699900
H	-1.70013600	4.75312100	2.52165300	H	1.82323600	-2.95436300	0.79649900
H	-0.31662500	3.46662600	4.93610600	H	0.39488900	-1.78471100	2.39340900
H	-1.87037200	2.99855100	4.23368800	H	-0.84600300	-3.06373800	2.30571000
H	-0.79805600	1.84341200	2.40544100	C	0.54938800	0.43232200	-2.80290500
H	0.57566700	1.76917000	3.53027800	O	0.79648600	-0.45435500	-1.70967400
O	4.14329000	-0.23643400	3.32904200	H	4.82807600	5.23582600	1.23032200
C	2.82136000	-0.82306800	3.31476300	H	3.17719200	5.33421500	1.81121200
C	2.25659100	-0.65003400	4.73756600	H	3.60286700	2.88201000	2.75781700
C	3.12344600	0.47970700	5.31976800	H	4.22884000	4.30427200	3.58777100
C	4.47155800	0.20414000	4.65873700	H	5.97936200	2.76322200	3.66622900
H	5.01779600	-0.59162400	5.18697100	H	6.42458600	4.03037900	2.55033300
H	5.11514500	1.08044100	4.56547300	H	1.13334100	0.13195800	-3.67939600
H	3.17507800	0.46422800	6.41278100	H	-0.51935100	0.37013300	-3.04120800
H	2.74949800	1.46096700	5.00537700	H	0.80971800	1.46402600	-2.53449300
H	2.39090800	-1.56724000	5.32252700				



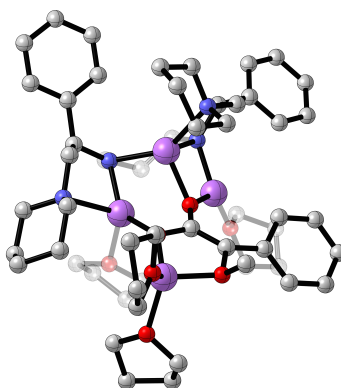
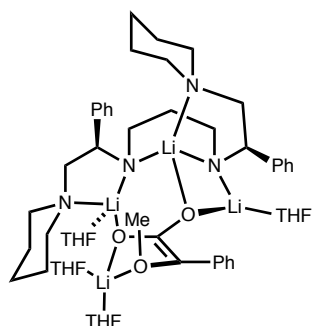
### III (6a)

G = -2881.857725

G<sub>MP2</sub> = -2872.292524

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	10.1010450	1.93578000	2.33689500
O	1.60335200	0.89986600	0.40461900	C	5.75672500	3.14881100	2.64214700
Li	5.03211700	0.36420200	1.60223100	C	4.32680600	3.70942200	2.66707200
N	6.03301000	2.13720100	1.63131700	C	3.94491500	4.60251800	1.46982300
C	7.43313800	1.78465800	1.72375700	N	3.51832400	3.82452300	0.31797000
C	7.72795100	0.50277200	0.91713000	Li	4.80072200	2.31689800	-0.01066200
N	6.99730500	-0.69912000	1.38694000	N	4.83716700	3.01812300	-2.25737900
C	7.17614300	-1.78329900	0.39915300	C	4.68652500	1.90363300	-3.21961200
H	6.81777200	-1.42032100	-0.56733200	C	5.99814000	1.15233900	-3.45245600
H	8.25478900	-2.00961900	0.28013300	C	7.09804600	2.09772600	-3.94346200
C	6.43469000	-3.05971500	0.79812400	H	6.83575900	2.48040100	-4.94130400
H	6.59446000	-3.82397300	0.02806000	H	8.05254100	1.56670000	-4.04871400
H	5.35691200	-2.85388300	0.81936400	C	7.23348700	3.26514700	-2.96189400
C	6.90827500	-3.55305700	2.16956200	C	5.88546400	3.95035000	-2.72409600
C	6.79879800	-2.41668200	3.19221500	H	6.00162700	4.74318900	-1.97998400
C	7.50378300	-1.14768200	2.70062800	H	5.55491800	4.43621300	-3.66482500
H	7.36018200	-0.34049800	3.42348900	H	7.62832200	2.90095800	-2.00654100
H	8.59488500	-1.33355300	2.63759900	H	7.94619500	4.01315500	-3.33233100
H	7.23511300	-2.71342900	4.15515400	H	5.81927000	0.33884400	-4.16491600
H	5.74208300	-2.18248000	3.36805900	H	6.31090900	0.68281500	-2.51094900
H	7.95576100	-3.88113000	2.09732200	H	3.92774800	1.22026600	-2.82748000
H	6.32661400	-4.42517200	2.49466000	H	4.31685000	2.29155400	-4.19089400
H	8.81351500	0.29949400	0.90716800	C	3.54426800	3.72534300	-2.12702400
H	7.42445500	0.68163200	-0.12207100	H	3.33323000	4.30520300	-3.04546100
H	7.71706300	1.57487000	2.78190100	H	2.77042300	2.95327200	-2.04780100
C	8.46016900	2.86009100	1.28861800	C	3.45394100	4.63451600	-0.88507700
C	9.79846300	2.76406200	1.69688900	H	4.30992900	5.33993200	-0.92392300
C	10.7457940	3.71105800	1.30768800	C	2.20558700	5.53070500	-0.94981100
C	10.3654390	4.79176400	0.50800900	C	2.28799300	6.88340700	-0.59018900
C	9.03367300	4.91008800	0.10882200	C	1.15541700	7.70249400	-0.56108500
C	8.09300100	3.95184300	0.49634300	C	-0.09244500	7.18601700	-0.91080800
H	7.05080600	4.04458900	0.20448100	C	-0.19361500	5.84134800	-1.28224000
H	8.72274600	5.75568000	-0.50106800	C	0.93912700	5.02610800	-1.29022800
H	11.0980350	5.53721500	0.20822900	H	0.83897300	3.98079600	-1.57406600
H	11.7787240	3.61090600	1.63392100	H	-1.15792100	5.43257400	-1.57886200

H	-0.97377200	7.82260200	-0.90416500	H	1.18654300	-0.41554800	4.73402600
H	1.25136200	8.74691300	-0.27303000	H	2.24521800	-0.29338400	2.55075100
H	3.25987800	7.29943900	-0.33269300	H	2.90870000	-1.87823100	3.02476600
Li	2.06196500	2.64050200	0.88426200	O	-1.71258800	1.01106700	-0.02717800
O	3.80518900	0.43163200	0.11612300	C	-3.03215400	0.46402900	0.15141900
C	2.57362900	0.27326700	-0.26822100	C	-3.87255800	1.65132000	0.61127200
C	2.19445000	-0.52815100	-1.36491100	C	-3.30266300	2.79066500	-0.25369700
C	2.94433200	-1.50212300	-2.12656500	C	-1.82005100	2.40261200	-0.42898100
C	2.29369600	-2.35464800	-3.06023500	H	-1.14396800	2.97384400	0.21072700
C	2.99494900	-3.30647400	-3.79762700	H	-1.48501000	2.49952700	-1.46708200
C	4.37421200	-3.46001000	-3.64785800	H	-3.41824400	3.77547000	0.20800300
C	5.03451700	-2.63075600	-2.73499300	H	-3.81054300	2.81838900	-1.22383900
C	4.34621800	-1.67664100	-1.99255300	H	-3.69729800	1.84410300	1.67616500
H	4.86955400	-1.03452200	-1.29744300	H	-4.94529200	1.49552400	0.46349000
H	6.11154600	-2.72334800	-2.60538000	H	-3.40166400	0.06120600	-0.80345300
H	4.92042800	-4.19912200	-4.22756700	H	-2.94921200	-0.35300500	0.87004100
H	2.45141500	-3.93491400	-4.50114100	O	-0.68082800	-1.81209500	0.65078300
H	1.22136600	-2.26539000	-3.19893100	C	-0.07081400	-2.52580200	1.74004200
O	0.62735700	3.30370200	2.13099100	C	0.90357500	-3.48708600	1.06250800
C	-0.11978600	2.44311400	3.02083000	C	0.13846900	-3.89991700	-0.21728500
C	-0.86923900	3.36966500	3.99524000	C	-0.91533600	-2.78285500	-0.40244500
C	-0.88009700	4.71612800	3.25165700	H	-1.93918000	-3.16629100	-0.30170900
C	0.46610300	4.68376100	2.53483700	H	-0.81126800	-2.24739500	-1.34626200
H	1.28613500	4.96348300	3.20833200	H	-0.34919300	-4.87224500	-0.09363700
H	0.52172800	5.29576300	1.63390400	H	0.81108300	-3.96148300	-1.07608400
H	-0.98114400	5.57597700	3.92046900	H	1.16411600	-4.33981300	1.69695600
H	-1.69855900	4.75295400	2.52244300	H	1.82215600	-2.95561500	0.79640100
H	-0.31691400	3.46458100	4.93698000	H	0.39439000	-1.78562700	2.39368200
H	-1.87052100	2.99761000	4.23351900	H	-0.84707500	-3.06408300	2.30570500
H	-0.79783300	1.84312300	2.40505500	C	0.55046300	0.43191900	-2.80261700
H	0.57509600	1.76727300	3.53071700	O	0.79691400	-0.45468400	-1.70917800
O	4.14300700	-0.23740200	3.32988900	H	0.81160600	1.46347900	-2.53446000
C	2.82135400	-0.82469500	3.31460700	H	1.13414700	0.13087700	-3.67905000
C	2.25562600	-0.65234300	4.73712300	H	-0.51833400	0.37048400	-3.04085700
C	3.12172600	0.47747900	5.32030100	H	4.82923600	5.23462800	1.23199900
C	4.47032500	0.20265200	4.65995100	H	3.17834700	5.33325400	1.81283100
H	5.01650300	-0.59316000	5.18819300	H	3.60356500	2.88085300	2.75919200
H	5.11370800	1.07919100	4.56746800	H	4.22974700	4.30290800	3.58931300
H	3.17271200	0.46157500	6.41333800	H	5.97991500	2.76134600	3.66759100
H	2.74761300	1.45873400	5.00608500	H	6.42550000	4.02877000	2.55211600
H	2.38985300	-1.56971000	5.32185000				



**IV (6d)**

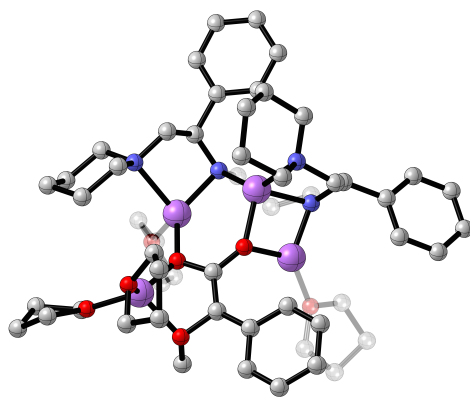
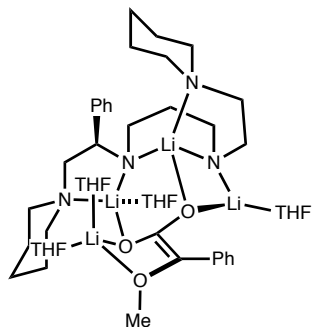
G = -2881.852893

G<sub>MP2</sub> = -2872.292097

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.08484100	7.42064100	2.45888800
O	-1.57071600	0.89036900	0.44331900	C	-4.93338100	3.32488300	3.27837700
Li	-2.42346300	2.05109100	1.89848400	C	-5.84967400	2.09330600	3.38402200
N	-4.02429900	3.39247700	2.13366600	C	-6.99668400	2.01744700	2.35507500
C	-3.45658700	4.72271300	2.11701400	N	-6.54823500	1.50718900	1.07057000
C	-2.20192600	4.76992500	1.22060100	Li	-4.76600200	2.27004200	0.59227600
N	-1.05353200	3.98809100	1.73379400	N	-5.56903100	2.41446900	-1.57729200
C	-0.03305300	3.89643400	0.67506000	C	-4.67264700	1.75161200	-2.54639000
H	-0.48931000	3.37947200	-0.17457900	C	-3.39478000	2.56020000	-2.78377200
H	0.25775600	4.91158300	0.33396500	C	-3.71739800	3.98005200	-3.26540900
C	1.22042900	3.14469300	1.12956800	H	-4.15859200	3.92933000	-4.27207900
H	1.94705200	3.13078200	0.30730900	H	-2.80308900	4.58136900	-3.35258300
H	0.94755600	2.10418900	1.34008700	C	-4.71193600	4.64478200	-2.30623100
C	1.82814700	3.77813700	2.38452300	C	-5.93561500	3.75560100	-2.07488000
C	0.74825900	3.88932000	3.46402300	H	-6.60475600	4.22389000	-1.34841700
C	-0.48227100	4.62876100	2.93291500	H	-6.50279600	3.65853200	-3.02291600
H	-1.25234900	4.66768500	3.70639300	H	-4.22868400	4.84564900	-1.34310700
H	-0.20282900	5.67814700	2.70508900	H	-5.04496500	5.61381300	-2.69860400
H	1.12814500	4.41718800	4.34811300	H	-2.77249100	2.03109000	-3.51819400
H	0.45021900	2.88381400	3.78669800	H	-2.82257300	2.59786900	-1.84677600
H	2.21081300	4.78078300	2.14366500	H	-4.41249000	0.76532100	-2.15324000
H	2.68398000	3.19158300	2.74397300	H	-5.19496700	1.60032200	-3.51257200
H	-1.88888800	5.81489400	1.04551200	C	-6.78738100	1.59844500	-1.35946000
H	-2.47212200	4.34941700	0.24359500	H	-7.50756200	1.76256600	-2.18054500
H	-3.13238900	5.02450600	3.13960100	H	-6.49225500	0.54557000	-1.40966900
C	-4.39280700	5.88639300	1.69347900	C	-7.46745300	1.83827200	0.00734800
C	-4.02482400	7.21650500	1.94700100	H	-7.75216400	2.91407500	0.05241600
C	-4.84023700	8.28210700	1.56579100	C	-8.80832400	1.07783700	0.03249600
C	-6.06087200	8.03596000	0.93215300	C	-10.0273060	1.76152800	0.10635500
C	-6.45094200	6.71785800	0.69335600	C	-11.2453910	1.07684400	0.13925100
C	-5.62335600	5.65688400	1.07160400	C	-11.2661320	-0.31675200	0.09068100
H	-5.93129000	4.62886400	0.90660800	C	-10.0579300	-1.01631400	0.01642900
H	-7.40921800	6.51200000	0.22096600	C	-8.84688600	-0.32440100	-0.00417300
H	-6.70423400	8.86227300	0.63966900	H	-7.91166200	-0.87873300	-0.04409900
H	-4.52783900	9.30404400	1.76970900	H	-10.0623800	-2.10362400	-0.02825200



H	-12.2110150	-0.85411700	0.11294300	H	-3.44077600	-1.25610000	5.56754600
H	-12.1773920	1.63383000	0.20473600	H	-3.41753100	-0.37349900	3.30542100
H	-10.0201630	2.84954800	0.14400800	H	-1.77202000	-1.03251700	3.36225000
Li	-5.42689900	-0.09316500	1.25999600	O	1.33195500	0.68236200	-1.34877400
O	-3.75877700	0.49080600	0.68345600	C	2.76007600	0.45641900	-1.30978400
C	-2.60279800	0.10661000	0.20786200	C	3.31557300	1.06675900	-2.60059900
C	-2.43905200	-1.11083300	-0.47789100	C	2.31127500	2.19441400	-2.88534300
C	-3.38501400	-2.18865200	-0.66501700	C	0.99280400	1.55512200	-2.45187200
C	-2.94377000	-3.53759100	-0.76010100	H	0.55599500	0.95219400	-3.25789200
C	-3.83212700	-4.59144400	-0.95397300	H	0.24202100	2.26569700	-2.09954600
C	-5.20717200	-4.36400300	-1.07323700	H	2.29804300	2.50815300	-3.93320900
C	-5.66614800	-3.04458700	-1.00426800	H	2.53420300	3.07321700	-2.26927700
C	-4.78367100	-1.98564100	-0.80647400	H	3.29943500	0.32979600	-3.41200500
H	-5.16133200	-0.97014600	-0.82274800	H	4.34440600	1.41979900	-2.48428500
H	-6.72554700	-2.83100100	-1.13370400	H	3.16381900	0.95093600	-0.41833800
H	-5.89674200	-5.18665600	-1.24118500	H	2.93956900	-0.61907200	-1.22237000
H	-3.44432900	-5.60695500	-1.01133700	O	1.19443200	-0.92161700	1.33198400
H	-1.88250000	-3.74640000	-0.66250700	C	1.27145400	-2.36320600	1.24956300
O	-5.87142400	-1.56992400	2.49847600	C	0.86403800	-2.86118300	2.63326200
C	-5.22900300	-2.84543900	2.69502200	C	1.46809900	-1.78183000	3.54666200
C	-6.36407700	-3.89047500	2.80664800	C	1.30338000	-0.49823200	2.71769900
C	-7.65970800	-3.04184400	2.85070000	H	2.16164100	0.17623900	2.80930100
C	-7.15084100	-1.63232500	3.15600400	H	0.39196300	0.05227100	2.97110700
H	-7.01294700	-1.47438900	4.23640600	H	2.52850000	-1.99072900	3.72940900
H	-7.76548300	-0.82863400	2.74953500	H	0.96967400	-1.71084900	4.51807000
H	-8.37653500	-3.39486500	3.59829700	H	1.23961800	-3.86636300	2.84704900
H	-8.15852200	-3.04782700	1.87679400	H	-0.22840000	-2.87746700	2.71782100
H	-6.24695200	-4.49417900	3.71239900	H	0.60098900	-2.67431600	0.44606500
H	-6.35840000	-4.56837500	1.94975000	H	2.30314800	-2.65658800	1.00662700
H	-4.56463600	-3.00701900	1.84567400	C	-0.90866300	-1.53304900	-2.26056500
H	-4.63436300	-2.80274600	3.61899200	O	-1.08129400	-1.41416800	-0.84513700
O	-1.91825600	1.00649900	3.69145000	H	-1.46655100	-2.39234100	-2.64851400
C	-2.46261700	-0.32893400	3.83686600	H	-1.25837700	-0.62553600	-2.76811800
C	-2.63351600	-0.55244200	5.34180700	H	0.16035600	-1.67913700	-2.44724500
C	-2.91044700	0.87157000	5.84721900	H	-7.42480400	3.03938000	2.26156900
C	-1.99109400	1.70625500	4.95537600	H	-7.82338200	1.42060500	2.80267300
H	-0.97918200	1.77570200	5.37816800	H	-4.36742200	3.39541100	4.23971500
H	-2.36796800	2.71264700	4.76157800	H	-5.61067300	4.20113900	3.31484100
H	-2.69422000	1.00542500	6.91168600	H	-6.29361800	2.11456300	4.39161600
H	-3.95630000	1.14416700	5.67089300	H	-5.25053600	1.16957800	3.33952600
H	-1.70956900	-0.94415800	5.78613600				



**V (6b)**

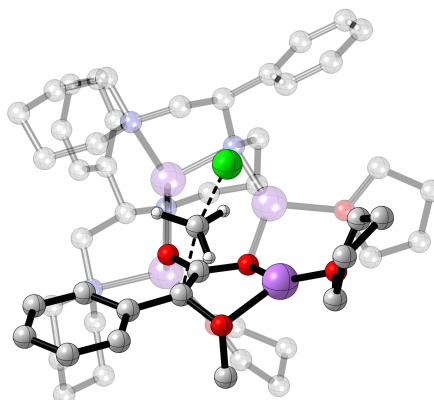
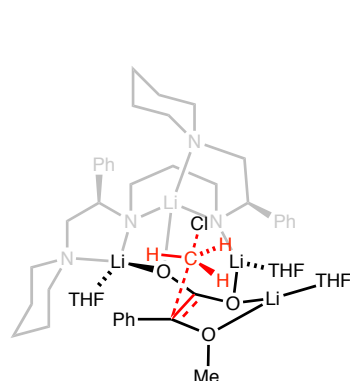
G = -2881.858128

G<sub>MP2</sub> = -2872.293179

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.13371800	7.85218400	0.53518600
O	-1.53472600	0.93036200	0.58893100	C	-4.49485200	3.95050900	2.40232000
Li	-2.04242300	2.73081600	1.13906300	C	-5.32190400	2.73768200	2.86713200
N	-3.80323800	3.81724800	1.12124800	C	-6.61651400	2.46004900	2.07339200
C	-3.35557200	5.12727200	0.70052200	N	-6.35656100	1.72472300	0.84842700
C	-2.38812300	4.98953900	-0.49496200	Li	-4.67230200	2.36633500	-0.02890000
N	-1.08181200	4.37785800	-0.15136200	N	-5.92122300	2.14252600	-2.07416100
C	-0.43317300	3.89466200	-1.38691100	C	-5.18729700	1.35978900	-3.08770400
H	-1.08863400	3.13949300	-1.83278600	C	-4.06584100	2.17595700	-3.73404400
H	-0.34234500	4.72307400	-2.11767700	C	-4.61201000	3.45731400	-4.37498100
C	0.95292700	3.29793000	-1.13075600	H	-5.24409900	3.18901300	-5.23437800
H	1.38947300	2.98649700	-2.08860000	H	-3.79571400	4.07841600	-4.76549100
H	0.84753100	2.39748500	-0.51519700	C	-5.44596200	4.23762600	-3.35232300
C	1.86723500	4.29806900	-0.41401000	C	-6.50514300	3.34406900	-2.70275200
C	1.16755600	4.81419000	0.84808400	H	-7.04781400	3.90687600	-1.93959400
C	-0.21472500	5.37503000	0.50727200	H	-7.24645200	3.03946700	-3.46951900
H	-0.71549400	5.72577100	1.41300200	H	-4.79604200	4.64739000	-2.57058200
H	-0.09156100	6.25780400	-0.15207400	H	-5.94429200	5.09253000	-3.82637700
H	1.76220700	5.59878400	1.33358200	H	-3.55280000	1.55406300	-4.47981700
H	1.05417600	3.99477100	1.56990500	H	-3.32630700	2.43164200	-2.96251200
H	2.08551100	5.14426600	-1.08158900	H	-4.77006200	0.47656600	-2.59680500
H	2.83265100	3.83631700	-0.16772200	H	-5.87952000	1.00542200	-3.87840600
H	-2.22276700	5.96472600	-0.98480100	C	-6.98771000	1.30989000	-1.47175100
H	-2.87414600	4.33796500	-1.23035200	H	-7.84612100	1.23191000	-2.16352000
H	-2.79354700	5.64448800	1.51599800	H	-6.58013700	0.29914200	-1.36008500
C	-4.44597900	6.15715600	0.30891300	C	-7.45986400	1.79188200	-0.08288500
C	-4.13770300	7.52466100	0.26597600	H	-7.81958800	2.83932900	-0.19463400
C	-5.08991900	8.47274100	-0.10867100	C	-8.70826800	0.99411000	0.34218400
C	-6.38628000	8.06789100	-0.43636900	C	-9.87010700	1.65487200	0.75952700
C	-6.71236100	6.71226700	-0.38132700	C	-10.9966970	0.94865100	1.19066900
C	-5.74965300	5.76825600	-0.01343100	C	-10.9863100	-0.44569500	1.20214700
H	-6.00296900	4.71418200	0.04802900	C	-9.83650200	-1.12376600	0.78586600
H	-7.72361000	6.38680400	-0.61599300	C	-8.71141700	-0.41022300	0.37109100
H	-7.13533500	8.80288500	-0.72074800	H	-7.82230500	-0.95608100	0.06230200
H	-4.82387100	9.52714500	-0.13757300	H	-9.81946500	-2.21170500	0.77854300

H	-11.8622330	-1.00019000	1.52979400	H	-1.85257500	1.52934800	6.08663300
H	-11.8823990	1.48999800	1.51569100	H	-2.65701800	1.51430700	3.78339100
H	-9.88847100	2.74316800	0.74797600	H	-1.06879600	0.74768100	3.56025100
Li	-5.21057600	0.16940100	1.11390300	O	0.40505500	-0.34019100	-1.93407200
O	-3.70654500	0.58414700	0.07393400	C	0.84001500	-1.68958700	-2.24919200
C	-2.51287700	0.10637300	0.26525300	C	-0.10253000	-2.19252300	-3.34425100
C	-2.23514700	-1.27499800	0.12524100	C	-0.48446200	-0.89180600	-4.06681600
C	-3.03462400	-2.32941800	-0.44926200	C	-0.58273000	0.09826000	-2.90721700
C	-2.52650400	-3.65699400	-0.54155500	H	-1.56958100	0.07033200	-2.43331400
C	-3.27488500	-4.69816100	-1.08550100	H	-0.34218700	1.12805600	-3.18505900
C	-4.56508200	-4.48443500	-1.57652200	H	-1.42326800	-0.96977500	-4.62274400
C	-5.07953500	-3.18500400	-1.52047300	H	0.30489300	-0.59058900	-4.76630300
C	-4.34424900	-2.13558700	-0.97636900	H	-0.98664200	-2.65741900	-2.89568800
H	-4.76070500	-1.13693000	-0.97252000	H	0.37898800	-2.92499700	-3.99940700
H	-6.07229000	-2.97780800	-1.91664700	H	1.88098500	-1.64038800	-2.59545400
H	-5.14655800	-5.29943500	-1.99824500	H	0.78471500	-2.28193300	-1.33241100
H	-2.83704600	-5.69416100	-1.12644100	O	1.73561900	0.28175100	0.91046000
H	-1.52210900	-3.86187500	-0.18660500	C	1.82562600	0.78017600	2.26721300
O	-5.49251000	-1.16469200	2.51913600	C	3.22825500	1.37538300	2.38538900
C	-4.89350800	-2.48025900	2.66731200	C	4.04137700	0.45941600	1.45690300
C	-5.73566500	-3.21372900	3.72059100	C	3.05255500	0.19264000	0.31801700
C	-7.08510800	-2.48099900	3.64977000	H	3.16361800	-0.79774500	-0.13329800
C	-6.64745500	-1.04428600	3.38391000	H	3.12681700	0.94856000	-0.47266200
H	-6.34977300	-0.53492100	4.31107000	H	4.29744400	-0.47436000	1.97104200
H	-7.38745200	-0.43666900	2.86156000	H	4.97010100	0.91528900	1.10154700
H	-7.67818000	-2.57714400	4.56429300	H	3.59471700	1.38125000	3.41625500
H	-7.68561600	-2.85083700	2.81082800	H	3.23777600	2.40614000	2.01295600
H	-5.29538100	-3.09832000	4.71843400	H	1.01547900	1.49806100	2.41585300
H	-5.81335600	-4.28448800	3.51003200	H	1.69033500	-0.06204500	2.95942400
H	-4.92062800	-2.96898000	1.69014500	C	-0.80571900	-2.11347300	1.84782200
H	-3.84787200	-2.35328400	2.96232400	O	-0.89951000	-1.65943200	0.49878100
O	-1.13380800	2.75134200	3.09079400	H	-1.09526600	-1.32018100	2.54857800
C	-1.57642800	1.64740000	3.91402200	H	-1.45117400	-2.98522000	2.00564500
C	-1.23242400	2.04620300	5.34800800	H	0.23741600	-2.40006000	2.02629100
C	-1.46891600	3.56380800	5.31183700	H	-7.09871500	3.44148800	1.87038000
C	-0.98528200	3.93917600	3.90663800	H	-7.33173200	1.94434500	2.75304500
H	0.07469500	4.22413100	3.90303000	H	-3.77781400	4.19362000	3.22439000
H	-1.57219000	4.74400300	3.45677100	H	-5.19532400	4.80763000	2.40434800
H	-0.93271100	4.10761900	6.09552900	H	-5.59197200	2.91914200	3.91887500
H	-2.53757100	3.78257500	5.41400100	H	-4.69410100	1.83023600	2.86977200
H	-0.18083700	1.82375900	5.56869900				

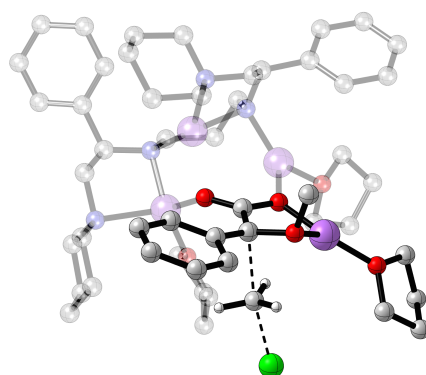
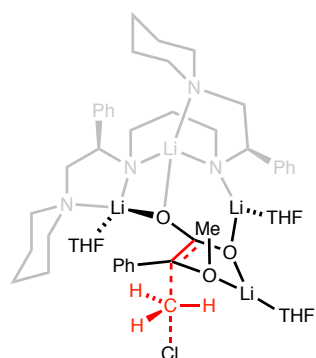
**Table S2.** Optimized geometries at the B3LYP level of theory with 6-31G(d) basis set for transition states of the alkylation of the isomers of **6** with methyl chloride at  $-78\text{ }^{\circ}\text{C}$  with free energies (Hartrees) and cartesian coordinates (X, Y, Z). (Note:  $G_{\text{MP2}}$  includes single-point MP2 corrections to B3LYP/6-31G(d) optimized structures.)



**TS I**  
 $G = -3149.549423$   
 $G_{\text{MP2}} = -3139.996188$

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-2.43967600	-5.82998700	-2.72195000
N	-0.65839300	-1.90306000	-0.19343500	H	-4.89636400	-5.98450900	-2.35749600
C	-2.09430500	-1.76345500	-0.32866400	H	-6.05323300	-4.21663300	-1.03778600
C	-2.43221700	-0.53102700	-1.19432700	H	-4.76350200	-2.32719700	-0.09907500
N	-1.97954500	0.76009300	-0.61895500	C	-0.38834500	-2.90607800	0.82912200
C	-2.05528300	1.80828500	-1.65906800	C	1.09306300	-3.20414500	1.10830700
H	-1.42566800	1.49636900	-2.49688900	C	1.83930400	-3.97041100	-0.00306100
H	-3.09229300	1.88426800	-2.04184700	N	2.28032600	-3.09694900	-1.07918000
C	-1.60634800	3.17507000	-1.14074300	Li	0.79918900	-1.88611700	-1.62175900
H	-1.67990400	3.90782500	-1.95297300	Li	3.37863500	-1.75795200	-0.18885800
H	-0.54583800	3.12138800	-0.86289400	O	3.47805900	0.13466800	-0.28916100
C	-2.44733000	3.60376800	0.06662000	Li	5.17985200	0.84184300	-0.51727200
C	-2.43063700	2.49627900	1.12634700	O	7.06000300	0.62790900	-0.48504700
C	-2.83076200	1.14403300	0.52742200	C	7.66870100	-0.65376200	-0.85424000
H	-2.76030600	0.36272000	1.28897200	C	9.06226800	-0.31040200	-1.37776800
H	-3.89040900	1.18491400	0.20608300	C	8.85469000	1.09391800	-1.96604900
H	-3.11403500	2.73396000	1.95200100	C	7.89664300	1.72314800	-0.95850100
H	-1.42276700	2.40907000	1.55037900	H	7.23786500	2.48383800	-1.38778300
H	-3.48308500	3.78588800	-0.25544700	H	8.42405300	2.14861200	-0.09509500
H	-2.07697800	4.54787800	0.48558000	H	8.37651000	1.01650400	-2.94773400
H	-3.51582200	-0.48945600	-1.39963200	H	9.78379800	1.66374100	-2.06191500
H	-1.92641700	-0.65462300	-2.15978100	H	9.39823700	-1.03296700	-2.12610800
H	-2.56924100	-1.60482600	0.66790200	H	9.79388800	-0.28927600	-0.56083600
C	-2.87123400	-2.97174600	-0.90514900	H	7.66908000	-1.28702600	0.03660000
C	-4.25252000	-3.08572200	-0.69128300	H	7.05323500	-1.10712900	-1.63640000
C	-4.98177600	-4.15365400	-1.21405300	O	4.35322600	2.44263600	-1.20910400
C	-4.33418200	-5.14573200	-1.95458800	C	3.21848200	1.84316700	-1.88026000
C	-2.95720000	-5.05515800	-2.16060600	C	2.65535000	0.72798400	-1.12981100
C	-2.23597600	-3.97722600	-1.64005200	O	1.48265700	0.26671400	-1.32334100
H	-1.16140100	-3.90879700	-1.78200300	C	2.52687500	2.74437200	-2.81010200

C	3.17796800	3.90744400	-3.28297700	H	0.31705200	-4.29790600	-3.74484300
C	2.57978500	4.74529300	-4.22201100	H	0.94821000	-3.84072400	-5.33260800
C	1.31552400	4.45276200	-4.73498200	H	-1.55847000	-2.71948500	-3.96591600
C	0.66480900	3.29892300	-4.29242500	H	-1.50334000	-3.79634800	-5.35497600
C	1.25256000	2.45895500	-3.34833000	H	0.13316400	0.18371400	-5.77183100
H	0.73972100	1.56805600	-3.01334300	H	-0.53952600	-0.29754200	-4.21345200
H	-0.31676200	3.04493400	-4.68690600	H	1.91560900	-0.46826200	-4.18024400
H	0.85136600	5.10403900	-5.47043600	H	1.90329400	-1.51586700	-5.60964600
H	3.11392600	5.63024700	-4.56032300	H	3.00103100	-3.42066100	-4.39219700
H	4.17386800	4.14279100	-2.92165100	H	3.21948400	-2.04161400	-3.31487400
C	4.59389800	0.65534700	-3.25122000	H	1.94528100	-4.67606100	-2.43915500
H	5.23258900	1.50406300	-3.07825000	C	4.03782600	-4.51863600	-2.17456800
H	4.54634300	-0.17057500	-2.56262200	C	4.13196200	-5.81215800	-1.63717800
H	3.91827700	0.67277300	-4.09045100	C	5.36628500	-6.44258700	-1.46273400
Cl	6.25926100	-0.41570500	-4.37052600	C	6.54313000	-5.79595500	-1.84437100
C	4.00252300	3.41761300	-0.21498400	C	6.46763900	-4.51573700	-2.40040500
H	4.93943700	3.84116700	0.16193100	C	5.23194700	-3.88199700	-2.55597500
H	3.39792300	4.21432300	-0.65728800	H	5.21621500	-2.89609000	-3.01432200
H	3.44790300	2.95273700	0.60816000	H	7.37000100	-4.01089400	-2.73796600
O	4.88514400	-2.12573300	1.06722500	H	7.50476900	-6.29025600	-1.72897100
C	5.08312900	-1.35777700	2.27602200	H	5.40590000	-7.44585500	-1.04419300
C	5.56916100	-2.35406000	3.33093300	H	3.21836500	-6.33584800	-1.36397500
C	6.32811500	-3.37966700	2.47456400	H	1.15494700	-4.76467800	-0.37450400
C	5.45736600	-3.45829600	1.22165600	H	2.67194600	-4.53653300	0.47432700
H	4.63601600	-4.17219900	1.34034200	H	1.62299400	-2.26251600	1.33960400
H	6.00042500	-3.69927500	0.30658400	H	1.13395300	-3.80679000	2.02832800
H	6.43961000	-4.35218600	2.96256900	H	-0.86013300	-2.62110900	1.80108100
H	7.33041500	-3.00687600	2.22960900	H	-0.85680600	-3.88313100	0.59731800
H	4.71660200	-2.83062600	3.82876900	O	0.43325500	0.66614100	1.88848300
H	6.18967100	-1.87976400	4.09727400	C	1.48682900	1.58823500	2.25495900
H	5.83757700	-0.58296200	2.07994800	C	1.53819900	1.59843200	3.79064700
H	4.13868100	-0.86830100	2.53139900	C	0.90783600	0.24555700	4.15783800
C	2.65958200	-3.84266000	-2.27430300	C	-0.16027100	0.10066500	3.07707000
C	2.58775300	-2.91576400	-3.50168100	H	-1.06573400	0.66787500	3.33565700
N	1.22563400	-2.40421000	-3.79447100	H	-0.43678500	-0.92967100	2.84984700
C	1.33809100	-1.23746800	-4.69947800	H	0.49043500	0.22344400	5.16897000
C	-0.02397600	-0.67477200	-5.10746100	H	1.64347100	-0.56312600	4.07278300
C	-0.88528400	-1.74876900	-5.77845800	H	0.93221700	2.41865100	4.19233700
H	-0.42801800	-2.03715400	-6.73628700	H	2.55747800	1.71986300	4.17017900
H	-1.88559100	-1.36121100	-6.00848600	H	2.41257100	1.21782400	1.80412400
C	-0.97641400	-2.97096000	-4.85981400	H	1.25459400	2.57245800	1.83284000
C	0.41281000	-3.45955800	-4.44082200				



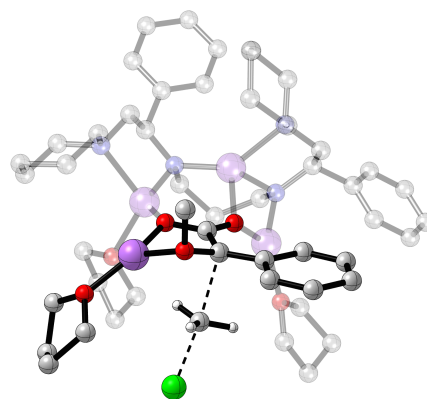
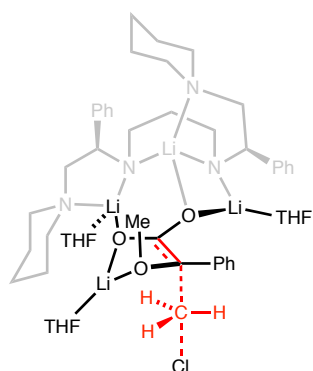
### TS II

G = -3149.554909

G<sub>MP2</sub> = -3139.999057

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	0.38370700	4.35301800	-0.25492000
N	-1.27306100	1.56192500	-0.30698900	N	0.74161900	3.76824600	1.02650800
C	-2.56632900	0.93995000	-0.50823400	Li	-0.38393800	2.16861100	1.41795600
C	-2.71846900	-0.30010500	0.39766900	O	0.90965500	0.37037300	1.74124800
N	-1.74906000	-1.38580300	0.11060700	C	2.06392600	0.45526700	2.28407800
C	-1.82824900	-2.39517900	1.18781200	O	2.95430700	1.31344200	1.83117700
H	-1.62217700	-1.89380900	2.13538900	Li	4.62299000	0.86108700	2.47049800
H	-2.85901100	-2.79762900	1.24929700	O	6.47064800	0.90160500	2.09220500
C	-0.84862500	-3.54982400	0.97737000	C	7.14626300	1.89277800	1.28299200
H	-0.94428400	-4.25754400	1.80946200	C	8.11076700	1.09154800	0.41405100
H	0.17752200	-3.16007400	1.01183600	C	8.56380700	-0.01374500	1.38308800
C	-1.10482000	-4.24037100	-0.36663800	C	7.29241000	-0.31147400	2.18680200
C	-1.10820300	-3.19795600	-1.49085900	H	7.48676100	-0.50541500	3.24560700
C	-2.05620100	-2.03515600	-1.18226700	H	6.71678500	-1.13811000	1.75862300
H	-1.99178100	-1.28468600	-1.97438300	H	9.36183300	0.35793000	2.03595000
H	-3.10072000	-2.40521000	-1.17305300	H	8.93175700	-0.90569900	0.86950100
H	-1.40561300	-3.65290100	-2.44455200	H	8.93865100	1.69929800	0.03695000
H	-0.09552900	-2.79994000	-1.62298300	H	7.58075800	0.65719700	-0.44137500
H	-2.08071500	-4.74674500	-0.33463000	H	6.38108900	2.44447200	0.72984300
H	-0.35249700	-5.01520400	-0.55838500	H	7.68203600	2.58929100	1.94228800
H	-3.74792500	-0.69427200	0.33953300	O	3.75943300	-0.00518100	3.94125000
H	-2.55448000	0.01749900	1.43554100	C	2.52907000	-0.44544900	3.32130600
H	-2.66892200	0.58686300	-1.55969500	C	1.73596200	-1.34688500	4.16612200
C	-3.81655500	1.83273200	-0.31268500	C	2.38305300	-2.13598900	5.14554400
C	-5.05833600	1.42643300	-0.82356500	C	1.67104700	-3.02199500	5.95030600
C	-6.20185400	2.20753900	-0.65852700	C	0.28847400	-3.15765300	5.81007700
C	-6.12176700	3.43054700	0.01247800	C	-0.36673000	-2.38656400	4.84813800
C	-4.89022600	3.85636400	0.51044400	C	0.33946300	-1.49616100	4.04032000
C	-3.75118900	3.06232500	0.34880600	H	-0.17481600	-0.89415400	3.30394200
H	-2.78556600	3.39395300	0.71952900	H	-1.44493600	-2.46956200	4.72901100
H	-4.81260900	4.81395300	1.02083600	H	-0.26638600	-3.84928200	6.43808900
H	-7.00824700	4.04768300	0.13615500	H	2.20407100	-3.61407800	6.69068600
H	-7.15364300	1.86710800	-1.06011800	H	3.45875700	-2.05348100	5.26654200
H	-5.12828400	0.48490000	-1.36720100	C	3.66456800	-1.83208700	1.89081600
C	-1.04934900	2.49933900	-1.40310000	Cl	5.06330600	-2.99609200	0.56038200
C	0.26770900	3.28876200	-1.36303300	H	4.31261200	-1.93440700	2.74486600

H	3.74136400	-0.98999400	1.22637100	H	0.28685000	1.56189800	4.50618300
H	2.83085900	-2.50752900	1.78604500	H	-0.40298400	2.76555400	5.61213800
C	3.57168000	0.88634700	5.05329800	H	0.49601100	4.66682300	4.29977500
H	2.97693400	0.40205200	5.83289100	H	1.32913300	3.28930400	3.56022400
H	4.56636900	1.11782400	5.44787500	H	-0.29338200	5.34464000	1.98512300
H	3.07243200	1.80916400	4.73230100	C	1.78069500	5.71863000	2.18775800
Li	2.40708700	2.78150500	0.82477000	C	1.64014200	7.00654500	1.65215400
O	3.93429400	3.25449600	-0.41209600	C	2.70987500	7.90586000	1.62261300
C	4.28258900	2.37173900	-1.49740000	C	3.94974800	7.53893900	2.14668100
C	5.37211500	3.10506100	-2.31598800	C	4.10786400	6.26197400	2.69483000
C	5.37455400	4.54410500	-1.73719400	C	3.03884300	5.36422500	2.70509700
C	4.08186800	4.59859500	-0.92085500	H	3.18673200	4.37451400	3.13266400
H	3.21446200	4.84453300	-1.54765100	H	5.06355600	5.96966800	3.12529800
H	4.10583500	5.27234800	-0.06390100	H	4.78068300	8.23975800	2.13757400
H	5.40484000	5.31320000	-2.51427700	H	2.57048100	8.89673100	1.19662500
H	6.23866000	4.69715700	-1.08211100	H	0.67267800	7.30799900	1.25584300
H	5.12273200	3.09822600	-3.38114300	H	-0.58831900	4.89191600	-0.20515100
H	6.35057800	2.62770400	-2.20818900	H	1.10549600	5.12968300	-0.59620200
H	4.61099300	1.42832300	-1.05509100	H	1.11701400	2.58692600	-1.28921800
H	3.38831400	2.18095400	-2.10478900	H	0.37130800	3.79147700	-2.33683900
C	0.61310800	4.71878900	2.11715000	H	-1.08883200	1.97180900	-2.38592200
C	0.46834800	3.95902000	3.45042900	H	-1.85569600	3.25595900	-1.48287600
N	-0.74040700	3.10806500	3.53707900	O	1.26157600	-0.55660500	-1.52361400
C	-0.59314200	2.18723000	4.68549400	C	2.42759400	-1.41481200	-1.41639900
C	-1.82446500	1.30489000	4.89630100	C	2.73392700	-1.88394100	-2.83776500
C	-3.08092200	2.15672100	5.09731200	C	2.24717000	-0.69485100	-3.67959000
H	-2.99558100	2.72067500	6.03808700	C	0.99894400	-0.25076600	-2.91371000
H	-3.97229700	1.52360600	5.18663300	H	0.11263200	-0.81185600	-3.23690400
C	-3.22254100	3.12715400	3.92178500	H	0.78216700	0.81639200	-2.99388200
C	-1.94608700	3.94769900	3.71735000	H	2.02592000	-0.95640600	-4.71876500
H	-2.05594000	4.58799600	2.83790900	H	2.99894800	0.10415700	-3.68492800
H	-1.80123700	4.61702300	4.58916100	H	2.15576800	-2.78344000	-3.07943900
H	-3.44578300	2.56790300	3.00630700	H	3.79340900	-2.11829700	-2.96913800
H	-4.06019000	3.81826300	4.07960500	H	3.25520700	-0.83045700	-1.00065300
H	-1.64494600	0.64437900	5.75281400	H	2.20232800	-2.23011000	-0.72640100
H	-1.95706000	0.65849400	4.01868400				



### TS III

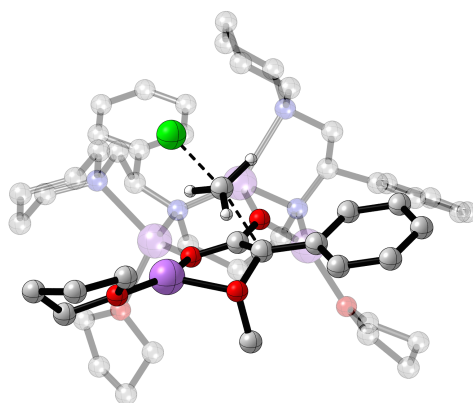
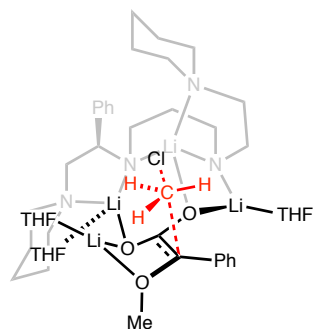
G = -3149.554797

G<sub>MP2</sub> = -3140.000798

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-5.39349700	1.33950000	1.09946000
Li	-2.69482000	0.78532900	-0.80822500	C	-6.01044200	3.37556000	0.76419200
O	-3.31372100	-0.54777100	0.48946500	C	-5.38782700	3.52172000	-0.62853300
Li	-5.07080300	-1.00380500	0.87382600	C	-3.88640400	3.80211400	-0.52773000
O	-6.83746000	-1.01848900	0.17439200	H	-3.44998800	3.87932400	-1.52694000
C	-7.19670400	-0.36079200	-1.07388700	H	-3.73430600	4.78369100	-0.03645500
C	-8.07577300	-1.36691700	-1.81040500	H	-5.86590800	4.33627000	-1.18700600
C	-8.83482500	-2.02878400	-0.65001400	H	-5.54633200	2.59907200	-1.20213800
C	-7.75456600	-2.13007800	0.42771000	H	-5.96160200	4.34032600	1.28896400
H	-7.18959400	-3.06117500	0.33196500	H	-7.07185700	3.10614800	0.69497700
H	-8.13490500	-2.02657600	1.44794300	H	-1.62300600	4.14608300	0.67221900
H	-9.23608300	-3.01153400	-0.91093700	H	-1.29220800	2.46627100	1.11629600
H	-9.66329800	-1.39353400	-0.31468900	H	-1.46600900	3.36402300	-1.78494600
H	-7.45534800	-2.11047900	-2.32173300	C	0.40091000	3.67589800	-0.85513300
H	-8.73504400	-0.88600800	-2.53934200	C	0.36951200	5.07380500	-0.96728600
H	-7.74392300	0.56033900	-0.83361200	C	1.53213700	5.83688500	-0.86076800
H	-6.27004500	-0.10152400	-1.59238600	C	2.76281200	5.20932400	-0.65245000
O	-4.40288800	-2.16217900	2.26220900	C	2.81193200	3.81827000	-0.55632400
C	-3.18051000	-2.60074500	1.63258900	C	1.64076500	3.06217800	-0.65676400
C	-2.56659900	-1.56852900	0.82156800	H	1.67545700	1.97840500	-0.60260600
O	-1.38575100	-1.68184800	0.34426700	H	3.76677800	3.31696800	-0.41362700
Li	-0.23363300	-2.40008100	-0.93548500	H	3.67334600	5.79847200	-0.57683600
N	1.25893000	-1.15189200	-1.01795000	H	1.47989800	6.91982300	-0.94774500
C	1.47645500	-0.62674600	-2.35546700	H	-0.58225700	5.57309600	-1.14694000
C	0.16285400	-0.13446900	-2.99842700	H	-1.08103800	1.58937800	-3.32279200
C	-0.30464900	1.27221100	-2.58616700	H	0.54813400	1.94372800	-2.80027700
N	-0.79088500	1.43762500	-1.21408900	H	0.29659000	-0.11756200	-4.09074000
C	-0.91306700	2.86001500	-0.95696100	H	-0.63664000	-0.87083800	-2.80856500
C	-1.72443300	3.10109000	0.33353100	H	2.18712800	0.22836800	-2.34972000
N	-3.16316600	2.75212700	0.22021700	H	1.94421400	-1.36266600	-3.04628000
C	-3.73279800	2.62513600	1.57742200	C	2.48660600	-1.25910900	-0.25895300
H	-3.19429800	1.82249100	2.09052700	C	2.14877800	-1.44152800	1.23669600
H	-3.56064600	3.55765100	2.15001600	N	1.39917600	-0.30904800	1.83135100
C	-5.23256700	2.32273300	1.56101800	C	0.69268500	-0.76424200	3.04739600
H	-5.59890400	2.26060100	2.59375500	C	-0.10122800	0.36639000	3.70546500



C	0.80956700	1.54825000	4.05835400	H	-0.96185200	-7.12247400	-2.71131300
H	1.50390800	1.24221200	4.85461700	H	-1.31494700	-5.45978100	-1.00689000
H	0.22519900	2.38805600	4.45511000	H	-2.41516700	-4.76989800	-2.22936700
C	1.60679000	1.97873500	2.82173100	C	-2.53990800	-3.74569000	2.28918000
C	2.32525500	0.78894200	2.18121100	C	-3.30693700	-4.58080400	3.13611200
H	2.84138800	1.11096500	1.27355600	C	-2.75832500	-5.70979900	3.73966800
H	3.09960500	0.41030700	2.87812900	C	-1.42467300	-6.05993500	3.52154000
H	0.93786800	2.43446200	2.08234200	C	-0.65193500	-5.25407700	2.68360400
H	2.35007600	2.74216800	3.08289900	C	-1.19286700	-4.12068600	2.07767500
H	-0.60322900	-0.02298700	4.60057000	H	-0.57190700	-3.50090000	1.44576700
H	-0.88826000	0.69858900	3.01339500	H	0.39248800	-5.50039900	2.50443500
H	0.02231900	-1.57921800	2.76371600	H	-0.99784300	-6.94070900	3.99304300
H	1.41693300	-1.17206500	3.78043500	H	-3.38419000	-6.32383600	4.38326100
H	3.06825900	-1.63532300	1.81738900	H	-4.35133100	-4.34155100	3.30887600
H	1.51818300	-2.33139000	1.33818400	C	-4.19497300	-1.48350700	3.51396800
H	3.08999800	-0.32965100	-0.35627200	H	-3.69463900	-2.14601800	4.22592900
C	3.43045000	-2.38833200	-0.71366900	H	-3.59092300	-0.58006800	3.36723200
C	4.64484200	-2.09429600	-1.34535100	H	-5.18350100	-1.21534200	3.90066000
C	5.49640100	-3.10705600	-1.79559700	O	-3.89513300	0.36069000	-2.49532000
C	5.15135100	-4.44535800	-1.61032600	C	-3.83335400	-0.97338400	-3.07668800
C	3.94421900	-4.75904300	-0.97852800	C	-4.15084300	-0.80066300	-4.56331300
C	3.09347900	-3.74126100	-0.54593900	C	-3.64060900	0.61982500	-4.84568800
H	2.15350900	-4.00464700	-0.06467400	C	-3.99678500	1.34832400	-3.55050500
H	3.66931600	-5.79931700	-0.81728700	H	-5.02563600	1.73312300	-3.57434500
H	5.81349000	-5.23686900	-1.95209600	H	-3.31512600	2.16872000	-3.31238900
H	6.43037000	-2.84827200	-2.28909000	H	-4.10238200	1.08205000	-5.72355100
H	4.92516600	-1.05225500	-1.48767800	H	-2.55453200	0.61755400	-4.98861300
O	-0.51017300	-3.91916900	-2.12713700	H	-5.23189300	-0.86454400	-4.73486900
C	-1.38526400	-5.08006200	-2.03201300	H	-3.66852400	-1.56637500	-5.17724500
C	-0.86580900	-6.09176400	-3.06424800	H	-2.82394200	-1.36867400	-2.91916700
C	0.59204600	-5.65406200	-3.27755900	H	-4.54859300	-1.61934000	-2.56195500
C	0.48473800	-4.13823000	-3.15942900	C	-4.25441800	-3.59201600	-0.13821500
H	0.13421300	-3.68388200	-4.09619300	H	-4.21315100	-2.64142700	-0.63894600
H	1.40250500	-3.64350300	-2.83896700	H	-3.43852300	-4.28323300	-0.25710000
H	1.00099500	-5.97039800	-4.24182800	H	-5.00297400	-3.79839500	0.60879600
H	1.24037200	-6.04634400	-2.48557300	Cl	-5.48122300	-4.43091000	-1.81572200
H	-1.42987600	-6.00461700	-3.99958500				



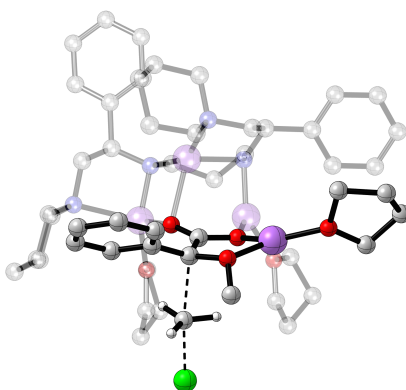
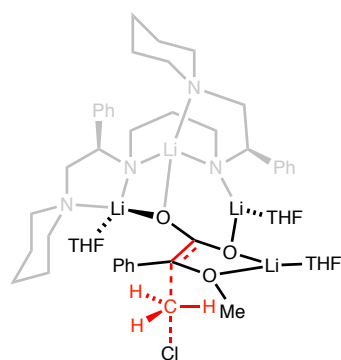
#### TS IV

G = -3149.549335

G<sub>MP2</sub> = -3139.993367

Atom	X	Y	Z	Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000	C	2.04042100	5.17030800	2.95102400
C	-1.23177300	-0.65864700	1.76128300	C	0.68795400	5.79516600	2.60136200
C	-1.66669000	0.66127500	2.19812000	H	0.20190300	6.18033000	3.50185300
O	-0.77845200	1.41169600	2.79137400	H	0.85642100	6.66339900	1.93407200
Li	0.87628600	0.55424000	2.65570700	H	2.67239000	5.93120800	3.42685000
O	2.76472400	0.38027800	2.72340400	H	1.88606200	4.36841800	3.68645300
C	3.76588800	1.15678500	3.42243600	H	2.97179600	5.42414100	1.01475700
C	4.98914000	1.14780000	2.50937600	H	3.65595400	4.09963700	1.94987000
C	4.90737000	-0.25270300	1.88146200	H	-1.28222400	6.50522100	1.15195900
C	3.40216200	-0.45001800	1.69094300	H	-1.99483600	4.92080100	0.82516000
H	3.07379300	-1.48126800	1.84566800	H	-1.91697300	6.10215200	3.62762000
H	3.05419400	-0.09810100	0.71401800	C	-3.52763100	6.73195700	2.41940600
H	5.31711800	-1.00276800	2.56805900	C	-3.17451500	8.08818400	2.47151500
H	5.44666200	-0.32751600	0.93348000	C	-4.08223700	9.08859400	2.12379600
H	5.91922800	1.32260700	3.05815300	C	-5.37759800	8.74845100	1.72646400
H	4.89250600	1.91967500	1.73799600	C	-5.74832900	7.40389600	1.68521700
H	3.35360100	2.15298900	3.60544300	C	-4.83012200	6.40778700	2.02828000
H	3.97798300	0.67585200	4.38687200	H	-5.11960200	5.36151400	2.01484000
O	-0.07308100	-1.11806300	2.49138300	H	-6.75945000	7.12784800	1.39392300
C	-0.36730500	-1.64243600	3.79543500	H	-6.09170400	9.52420100	1.46155300
H	-0.81910500	-0.87047500	4.43150800	H	-3.78200100	10.13304200	2.16882200
H	-1.04606700	-2.49672700	3.72031000	H	-2.17066800	8.36458700	2.79292300
H	0.58268100	-1.97235700	4.22839500	C	-3.72372400	4.41630900	4.38697300
Li	-1.22944800	3.28608100	3.25633800	C	-4.57178000	3.18497700	4.75450500
N	-2.98549600	4.33264700	3.12852300	C	-5.83127800	2.95444300	3.89050300
C	-2.48424600	5.64667900	2.77958200	N	-5.52597500	2.27164500	2.64373600
C	-1.49858700	5.51954600	1.59700500	Li	-3.83274000	2.99614100	1.86826500
N	-0.22852300	4.83734600	1.94697800	Li	-4.44671100	0.67576000	2.85167300
C	0.40427600	4.30836000	0.71710400	O	-2.83518700	1.10744500	1.93736800
H	-0.28450200	3.58993500	0.26135700	O	-4.84690300	-0.76610900	4.11108400
H	0.55084700	5.12452400	-0.01620000	C	-4.35545100	-2.12970700	4.20389400
C	1.75021500	3.63820400	0.99355400	C	-5.36948700	-2.89794700	5.06902100
H	2.16107400	3.25575200	0.05297100	C	-6.62827700	-2.01727600	4.99975700
H	1.58207100	2.76617800	1.64042500	C	-6.03045500	-0.61724200	4.93494400
C	2.71290900	4.60115100	1.69632200	H	-5.73328400	-0.25655200	5.92958300

H	-6.66903100	0.12495100	4.45550600	H	-11.0069870	2.05456200	3.23934700
H	-7.29342000	-2.15052200	5.85815400	H	-8.97454400	3.32240400	2.61380500
H	-7.20079500	-2.21849500	4.08782900	H	-6.29551700	3.94783100	3.70917500
H	-5.01597300	-2.97151600	6.10397200	H	-6.58136800	2.41732600	4.51285200
H	-5.53475100	-3.91421600	4.69980800	H	-4.88769400	3.31234600	5.80100900
H	-4.28021900	-2.52260400	3.18695800	H	-3.94308200	2.27726500	4.73726900
H	-3.35452300	-2.11239600	4.64771400	H	-3.03704800	4.61072200	5.24674400
C	-6.58513600	2.40244400	1.66372400	H	-4.41762600	5.27797500	4.40316000
C	-6.04439400	2.00009300	0.27534200	O	-0.36090600	3.27254200	5.17429300
N	-4.95672600	2.87009900	-0.22719500	C	-0.72082000	2.14861400	6.01083400
C	-4.18748200	2.15368900	-1.26732700	C	-0.41741000	2.58409700	7.44477400
C	-3.05207600	3.00765000	-1.83343700	C	-0.71841300	4.08895000	7.38466400
C	-3.58668500	4.32148700	-2.41487900	C	-0.21622200	4.46344100	5.98870600
H	-4.19199200	4.10229900	-3.30686200	H	0.84422500	4.74595900	5.99978400
H	-2.76156500	4.96472200	-2.74464800	H	-0.79548700	5.26619500	5.52608500
C	-4.45295200	5.03979200	-1.37341300	H	-0.22393900	4.66395500	8.17326100
C	-5.52502900	4.10825900	-0.80404100	H	-1.79758300	4.26377400	7.45745200
H	-6.09269100	4.62510600	-0.02646100	H	0.63883900	2.41124000	7.68490000
H	-6.24177800	3.84383800	-1.60729900	H	-1.02576700	2.04970500	8.18060600
H	-3.82707600	5.41141000	-0.55391100	H	-1.78732900	1.93149000	5.87240500
H	-4.94536600	5.91660800	-1.81228500	H	-0.14242600	1.28188500	5.67958800
H	-2.51146800	2.43146300	-2.59410300	C	-2.07223300	-1.73299700	1.22071200
H	-2.33428000	3.22302600	-1.03029700	C	-1.58748800	-3.06195000	1.18291300
H	-3.78100900	1.24199300	-0.82033000	C	-2.34164100	-4.10011000	0.63927200
H	-4.85789700	1.84460800	-2.09406700	C	-3.60510000	-3.85907900	0.09722900
H	-6.86725100	1.95496000	-0.46058600	C	-4.08836800	-2.54854600	0.09211200
H	-5.63314100	0.98647300	0.34937800	C	-3.34213900	-1.50479900	0.63756800
H	-6.92895300	3.45783800	1.59798600	H	-3.72759700	-0.49499800	0.59890100
C	-7.85643900	1.59647400	1.98898300	H	-5.05667800	-2.32812600	-0.35213800
C	-8.99300300	2.24075700	2.49440600	H	-4.19036300	-4.66867300	-0.32957800
C	-10.1422060	1.52653400	2.84416900	H	-1.92991800	-5.10678800	0.63348000
C	-10.1830000	0.14214600	2.68089000	H	-0.59633900	-3.27584600	1.56864400
C	-9.06067300	-0.51869400	2.17275200	H	0.15563500	0.95183000	0.47849000
C	-7.91135700	0.20064700	1.84187400	H	0.57711600	-0.87071700	0.25852400
H	-7.04735600	-0.33487600	1.45364500	H	-0.80029800	-0.09145500	-0.71723500
H	-9.08505400	-1.59633700	2.02455800	Cl	1.57466900	0.58970500	-1.54507200
H	-11.0780170	-0.41701100	2.94172700				



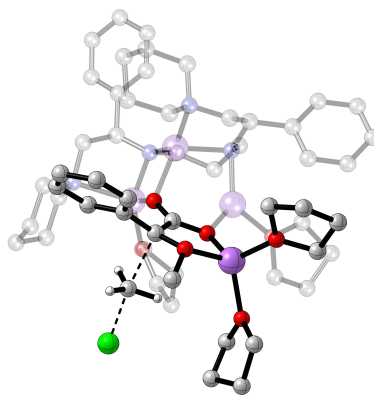
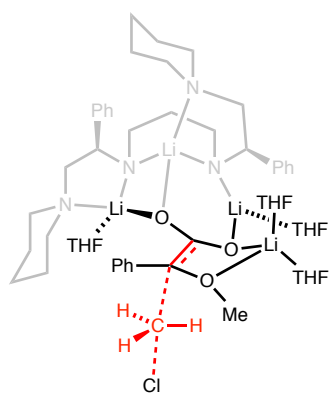
**TS V**

G = -3149.549555

G<sub>MP2</sub> = -3139.995241

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	C	1.75591700	1.91565400	-2.44521900
N	0.03994000	1.97358300	-0.57005600	C	2.93670500	2.70578700	-1.85131600
C	-1.28267500	2.48556800	-0.27425300	N	3.27931000	2.25244700	-0.51107500
C	-1.86399700	1.78815400	0.97299500	Li	1.64846500	2.01352300	0.62264500
N	-2.09219000	0.33189500	0.79821100	Li	3.51239100	0.31765800	-0.50998900
C	-2.47454200	-0.24571300	2.10394300	O	3.71275800	-0.63855400	1.07635600
H	-1.65559300	-0.06242300	2.80538100	Li	5.18142300	-0.86395600	2.11982900
H	-3.36752200	0.27795400	2.49993400	O	7.02548000	-0.42492300	2.26802600
C	-2.77834200	-1.74379900	2.01827800	C	8.07479600	-0.77687100	1.32178700
H	-3.06415300	-2.10890200	3.01249400	C	9.20690100	0.22549200	1.56252600
H	-1.86802300	-2.28579200	1.72902200	C	9.00557500	0.61273400	3.03622800
C	-3.88530700	-2.02743100	0.99801200	C	7.48444700	0.63954900	3.14782000
C	-3.51100700	-1.39241800	-0.34405300	H	7.06860600	1.59046800	2.79474700
C	-3.17176000	0.09151400	-0.18486400	H	7.10405600	0.42640300	4.15043200
H	-2.86301400	0.50129900	-1.14907100	H	9.45504700	1.57665600	3.29038200
H	-4.08335500	0.64162000	0.12323300	H	9.42540700	-0.15018100	3.70209700
H	-4.33130300	-1.49051000	-1.06671900	H	9.07850000	1.10117400	0.91811200
H	-2.64285200	-1.91200300	-0.76661300	H	10.1898890	-0.21053500	1.36269300
H	-4.83211100	-1.59763000	1.35656200	H	8.38070800	-1.80842800	1.53119400
H	-4.04772600	-3.10668200	0.88857600	H	7.65997100	-0.72116000	0.31107500
H	-2.80418800	2.27534500	1.28485200	O	4.07983300	-1.70820300	3.39335400
H	-1.15047500	1.90930900	1.79876400	C	2.69545300	-1.59253300	2.96617400
H	-1.97721800	2.27106600	-1.11576500	C	2.59872400	-0.79926100	1.75298000
C	-1.41952000	4.01943200	-0.09618800	O	1.49912600	-0.32621100	1.30528000
C	-2.68873700	4.61818400	-0.07182900	C	1.76276000	-1.47742900	4.10284900
C	-2.83926100	5.99626400	0.08049000	C	2.22861800	-1.21864400	5.41137700
C	-1.71256200	6.81499600	0.19272500	C	1.35586500	-1.15697000	6.49765100
C	-0.44362600	6.23768000	0.14799800	C	-0.01387700	-1.34935600	6.31831300
C	-0.30290400	4.85415500	0.00627800	C	-0.49322200	-1.60342700	5.03077300
H	0.68304300	4.40138800	-0.04289100	C	0.37589200	-1.67137700	3.94414500
H	0.44186600	6.86639200	0.21407500	H	-0.01424100	-1.88631900	2.95721700
H	-1.82449100	7.89085300	0.30223400	H	-1.55617700	-1.76793000	4.87339500
H	-3.83510500	6.43310200	0.10310700	H	-0.69507400	-1.30875600	7.16380900
H	-3.57512000	3.99499700	-0.18276400	H	1.75314200	-0.95374400	7.48972600
C	0.35946600	2.32154000	-1.95298400	H	3.28792700	-1.04695100	5.57259600

C	2.30735300	-3.51766500	1.73861000	H	0.68126800	1.86029800	3.74185400
H	2.20138100	-4.08340900	2.64883500	H	3.03952600	1.24068100	3.43361200
H	1.44058300	-3.03476800	1.32414700	H	3.57858600	2.70672600	4.27637600
H	3.28025500	-3.30801000	1.33327500	H	4.83372000	3.53059600	2.22755400
Cl	2.12470300	-5.32831000	0.40349700	H	4.43463800	1.85079800	1.81416700
C	4.45917900	-2.95646300	3.98555700	H	3.74568700	4.23551100	0.04417400
H	5.44037100	-2.79820500	4.44405000	C	5.60308500	3.27359700	-0.26888400
H	3.74876700	-3.25242600	4.76248200	C	6.36991900	4.41710400	0.00224200
H	4.52900600	-3.75144800	3.23590500	C	7.71183900	4.49924000	-0.37015900
O	4.18720500	-0.86957700	-1.95886900	C	8.31961900	3.43330100	-1.03948000
C	4.42325800	-2.28847600	-1.75259900	C	7.56736300	2.29246400	-1.32825600
C	4.52118200	-2.89620200	-3.15170700	C	6.22495000	2.21680000	-0.94341700
C	5.09919700	-1.73271700	-3.97154800	H	5.63341100	1.33888700	-1.18950600
C	4.39018300	-0.52774700	-3.35301100	H	8.02175200	1.46726100	-1.87374600
H	3.41207000	-0.35158200	-3.81599300	H	9.35967300	3.50038200	-1.34911300
H	4.96633600	0.40038800	-3.39471900	H	8.28129600	5.39930700	-0.15012500
H	4.90991700	-1.81967100	-5.04554400	H	5.90126700	5.26142100	0.50597800
H	6.18355600	-1.65979600	-3.82319500	H	2.65958900	3.78218100	-1.86275200
H	3.52451100	-3.16701600	-3.51922700	H	3.79066700	2.63635800	-2.56251400
H	5.14110500	-3.79687700	-3.16945400	H	1.90782500	0.83701200	-2.26869100
H	5.36356500	-2.40383100	-1.19731100	H	1.76747900	2.04837100	-3.53785800
H	3.61021200	-2.69774100	-1.15051800	H	-0.38294200	1.86817600	-2.65074800
C	4.12255400	3.19708700	0.17760100	H	0.26884600	3.40953300	-2.14501000
C	4.10722600	2.88979500	1.69504100	O	-0.07414900	-1.44020000	-1.43946400
N	2.77420800	3.00272500	2.32860100	C	0.11284500	-2.86146200	-1.19114700
C	2.78571600	2.28703200	3.62383600	C	-0.39578300	-3.57881700	-2.44147200
C	1.44168500	2.36922000	4.34810200	C	-0.13974300	-2.53475200	-3.53875000
C	1.03780900	3.82750100	4.58615300	C	-0.46752700	-1.22873900	-2.81411200
H	1.73536800	4.28739000	5.30237900	H	-1.54457700	-1.01538000	-2.84977300
H	0.03905600	3.88704400	5.03576300	H	0.07250300	-0.35889700	-3.19290300
C	1.07916800	4.59550000	3.26089200	H	-0.75288100	-2.68076300	-4.43336300
C	2.42740800	4.42362100	2.55591700	H	0.91443400	-2.54859400	-3.84286400
H	2.41062700	4.93514600	1.58945700	H	-1.46931100	-3.78776200	-2.36128900
H	3.22210200	4.90241200	3.16291200	H	0.12485400	-4.52680500	-2.59873400
H	0.28005200	4.24064500	2.60051600	H	1.17434400	-3.05662900	-1.02314300
H	0.90005300	5.66633400	3.41884300	H	-0.43429500	-3.13207000	-0.28393000
H	1.51143800	1.81442700	5.29046400				



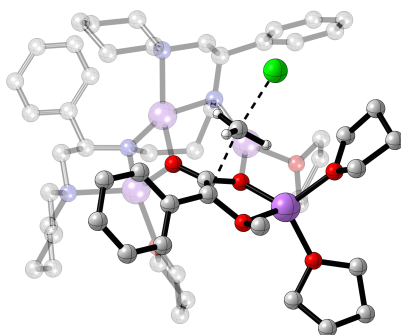
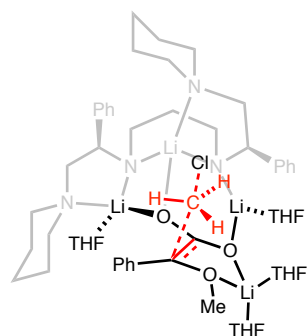
**TS VI**

G = -3381.902018

G<sub>MP2</sub> = -3371.584094

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-12.0306640	2.42906600	-1.63761300
O	-1.73307400	0.16834500	-0.68539300	H	-10.4013970	0.63591400	-2.12484900
Li	-5.23999500	-0.71447400	-1.66476500	C	-6.14565200	1.74419800	-3.26171400
N	-6.27887100	1.00520900	-2.01098400	C	-4.73856100	2.25658600	-3.60104400
C	-7.67337100	0.64468100	-1.85934800	C	-4.23445900	3.42229200	-2.73121100
C	-7.84773700	-0.42659900	-0.76463400	N	-3.69454700	2.97149000	-1.45644000
N	-7.15595500	-1.71009400	-1.04112000	Li	-4.93015500	1.63547100	-0.59903300
C	-7.26002700	-2.55900700	0.16495000	N	-4.66243200	2.90101400	1.37663700
H	-6.80489000	-2.01311500	0.99603800	C	-4.35765900	2.12785800	2.59887500
H	-8.32695600	-2.70963900	0.42431000	C	-5.59171000	1.43614800	3.17671400
C	-6.59776200	-3.92694200	-0.01329900	C	-6.69478600	2.45207200	3.48773600
H	-6.71672500	-4.50516200	0.91167500	H	-6.36611000	3.11259500	4.30443100
H	-5.51919200	-3.80028900	-0.17254200	H	-7.60440100	1.94717700	3.83622400
C	-7.19924500	-4.67379000	-1.20809100	C	-6.98557900	3.28578000	2.23691700
C	-7.13202200	-3.77794900	-2.44861400	C	-5.70635400	3.90698800	1.66978100
C	-7.77431200	-2.41172900	-2.18798800	H	-5.93717200	4.44726300	0.74765300
H	-7.67827500	-1.78099500	-3.07521100	H	-5.31038000	4.65085300	2.39093300
H	-8.85907400	-2.54436900	-2.00286900	H	-7.44996100	2.65434400	1.47103400
H	-7.63916000	-4.24999500	-3.30018900	H	-7.69935800	4.09050100	2.45476700
H	-6.08343900	-3.62838800	-2.73284500	H	-5.29759200	0.87795900	4.07216000
H	-8.24788900	-4.92699900	-0.99263000	H	-5.95663100	0.69722100	2.45217300
H	-6.67010600	-5.61817600	-1.38162700	H	-3.59842100	1.38323700	2.34712400
H	-8.92087000	-0.61561800	-0.58676300	H	-3.92211100	2.79686900	3.36953800
H	-7.43199000	-0.02913100	0.17037100	C	-3.42637200	3.55944900	0.90169300
H	-8.06666300	0.20701700	-2.80533700	H	-3.14110400	4.37752400	1.59019100
C	-8.67095000	1.79281900	-1.56298500	H	-2.62785500	2.80822700	0.94158600
C	-10.0470130	1.59695800	-1.75377700	C	-3.51749300	4.08319000	-0.54500200
C	-10.9686030	2.60917100	-1.48662300	H	-4.38913300	4.76882200	-0.59415300
C	-10.5266530	3.85537500	-1.03522600	C	-2.30590000	4.98295800	-0.85546000
C	-9.15971000	4.07139600	-0.85912900	C	-2.48713400	6.31102200	-1.26161700
C	-8.24412000	3.04824500	-1.12085400	C	-1.40415300	7.13001800	-1.59442800
H	-7.17746400	3.21516500	-1.00202100	C	-0.10355200	6.63322600	-1.52131400
H	-8.80212000	5.04268600	-0.52389000	C	0.09806200	5.31009300	-1.11549500
H	-11.2400220	4.65058100	-0.83301200	C	-0.98951200	4.49680800	-0.79097400

H	-0.81202100	3.46590100	-0.49005300	H	-2.41937200	-1.48050900	-2.93887100
H	1.10953300	4.91213300	-1.05850700	H	-3.01911400	-3.15497200	-2.87864900
H	0.74326500	7.26449400	-1.77850600	O	1.02478900	1.51758800	0.78063000
H	-1.57933000	8.15480500	-1.91339300	C	2.22797100	2.19482800	0.34525500
H	-3.49861400	6.70816300	-1.32197500	C	2.50368400	3.29072400	1.38376500
Li	-2.32814900	1.60442100	-1.77828700	C	1.80393200	2.74555600	2.63928400
O	-3.90064600	-0.28248700	-0.26782000	C	0.56830900	2.08328600	2.03884400
C	-2.66355800	-0.38325000	0.05830400	H	-0.21948700	2.81770000	1.83260900
C	-2.23170100	-1.15250000	1.20796600	H	0.14757000	1.26546600	2.62571900
C	-3.06870700	-1.40394800	2.39623400	H	1.54859000	3.52669500	3.36096500
C	-2.63279700	-1.06037300	3.69563200	H	2.43287200	2.00282800	3.14487500
C	-3.38784100	-1.37385600	4.82622100	H	2.04092200	4.23452100	1.07654100
C	-4.60953600	-2.03653300	4.70304900	H	3.57423500	3.46638600	1.52403800
C	-5.06506700	-2.37166700	3.42468800	H	3.03816100	1.45714000	0.30739700
C	-4.30945100	-2.06570000	2.29596000	H	2.06453500	2.58706000	-0.66388600
H	-4.66658700	-2.35122500	1.31608100	O	1.35664800	-1.18156200	-0.96008700
H	-6.01203100	-2.89334100	3.30622700	C	1.06243600	-2.07790000	-2.06246600
H	-5.19381000	-2.29034500	5.58328900	C	1.76811700	-3.38013800	-1.70931500
H	-3.01644400	-1.09365900	5.80963700	C	3.06523500	-2.86630300	-1.06135300
H	-1.69387200	-0.52882400	3.81655000	C	2.62607500	-1.56349700	-0.36822000
O	-1.06754200	1.81916500	-3.32101000	H	3.34510700	-0.74944900	-0.51283900
C	-0.08600500	0.84793400	-3.74480500	H	2.46171300	-1.69721600	0.70531900
C	0.56002900	1.41648900	-5.01445400	H	3.81756500	-2.65379000	-1.82925700
C	0.37109400	2.92991200	-4.82940900	H	3.50251000	-3.57842900	-0.35591000
C	-1.00307600	2.99458800	-4.16884900	H	1.94777900	-4.00522400	-2.58835000
H	-1.81118500	2.94176600	-4.90883600	H	1.15810400	-3.96109300	-1.01042700
H	-1.15547400	3.86735800	-3.53388500	H	-0.02197300	-2.16311300	-2.14150400
H	0.41032600	3.48866600	-5.76909200	H	1.45895500	-1.64378400	-2.99119500
H	1.13556000	3.33750700	-4.15703400	C	-0.10981100	-1.96350700	2.10981600
H	0.02133700	1.07432300	-5.90574400	O	-0.84429300	-0.88105400	1.53185600
H	1.60717600	1.11599100	-5.11835500	H	-5.08861300	4.11976600	-2.58684600
H	0.64276900	0.72226300	-2.93534600	H	-3.50438400	4.01227400	-3.32721200
H	-0.58861800	-0.11027500	-3.90780000	H	-4.01830700	1.42169900	-3.56402400
O	-4.43881000	-1.67655500	-3.29275100	H	-4.76099700	2.59152900	-4.64936800
C	-3.08955700	-2.20489200	-3.41455100	H	-6.49210800	1.12638700	-4.12540700
C	-2.82235100	-2.35828000	-4.92129400	H	-6.81019200	2.63084100	-3.30038500
C	-3.85753300	-1.41725100	-5.55866500	C	-2.12035900	-3.14833200	-0.02212900
C	-5.03533600	-1.56651200	-4.60026000	H	-2.08757900	-3.66596400	0.92129700
H	-5.60915000	-2.47853400	-4.81935600	H	-3.07972700	-2.90729500	-0.44680300
H	-5.71245400	-0.71127300	-4.58294500	H	-1.23795900	-2.68076700	-0.41519800
H	-4.11410300	-1.68907800	-6.58732300	Cl	-1.78803300	-4.97963400	-1.23923500
H	-3.50107000	-0.38051100	-5.55416100	H	-0.67364600	-2.44602100	2.91274200
H	-3.00165900	-3.39216500	-5.23642200	H	0.16250700	-2.71421600	1.36092400
H	-1.79043500	-2.10742200	-5.18753100	H	0.80076500	-1.52829200	2.53503200



### TS VII

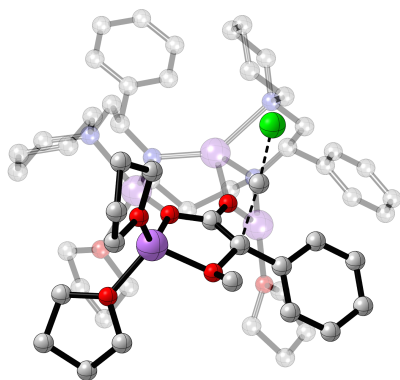
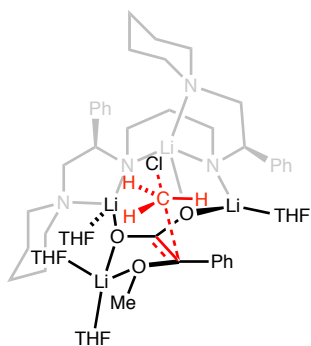
G = -3381.897949

G<sub>MP2</sub> = -3371.581335

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-10.2891800	0.81911200	-1.79657300
O	-1.77988000	0.57424900	-0.17303300	C	-5.92720200	1.99701100	-2.55154900
Li	-5.20356400	-0.33918600	-0.77386200	C	-4.52020900	2.59270400	-2.70316900
N	-6.20891300	1.35028600	-1.27668300	C	-4.22025300	3.83169300	-1.83130200
C	-7.60260900	0.95835500	-1.26724200	N	-3.81683300	3.47866000	-0.47834400
C	-7.86532300	-0.03865100	-0.11940900	Li	-4.99828900	2.03734400	0.23611700
N	-7.14006900	-1.32463800	-0.26345300	N	-5.18964300	3.32111200	2.18957500
C	-7.24235800	-2.07882400	1.00495400	C	-5.00244600	2.65928200	3.49930200
H	-6.77688200	-1.47690800	1.79188100	C	-6.20303000	1.79772200	3.89253200
H	-8.30877600	-2.21095800	1.27646700	C	-7.48132800	2.64128200	3.94715400
C	-6.56711000	-3.44906800	0.93228500	H	-7.40403900	3.36091700	4.77544300
H	-6.69881900	-3.95890400	1.89276000	H	-8.35752100	2.01377300	4.15334600
H	-5.48679000	-3.31132300	0.80192200	C	-7.65442700	3.39462300	2.62432500
C	-7.13291800	-4.29015300	-0.21616800	C	-6.39263600	4.17954300	2.25442400
C	-7.05837400	-3.49032200	-1.52015100	H	-6.53050800	4.66184600	1.28385900
C	-7.72292700	-2.12071800	-1.36512000	H	-6.23067800	4.98602300	2.99743900
H	-7.62400600	-1.55310300	-2.29378900	H	-7.88349000	2.68573100	1.82080500
H	-8.80824900	-2.26175200	-1.18876700	H	-8.50066500	4.09082600	2.67601600
H	-7.54711400	-4.02972700	-2.34218200	H	-6.00140800	1.32664500	4.86320400
H	-6.00899700	-3.34293000	-1.80275100	H	-6.32172400	0.98856100	3.15840600
H	-8.18202700	-4.54498100	-0.00478200	H	-4.09756800	2.04957800	3.45037500
H	-6.58992400	-5.23952000	-0.30758400	H	-4.82561100	3.41786100	4.28609300
H	-8.94671500	-0.23215100	-0.01079400	C	-3.98453800	4.12906400	1.88713700
H	-7.52553500	0.42505300	0.81505000	H	-3.92380500	4.98987300	2.57757600
H	-7.86905300	0.43787200	-2.21587800	H	-3.11787100	3.49440900	2.10062300
C	-8.65774800	2.08960800	-1.18416400	C	-3.89518200	4.61601000	0.42869200
C	-10.0008060	1.82437800	-1.49107700	H	-4.81027300	5.20642200	0.21370300
C	-10.9722480	2.82283600	-1.42131900	C	-2.73643500	5.61427500	0.26007900
C	-10.6130370	4.12302500	-1.05712800	C	-2.86317600	6.67220700	-0.65421900
C	-9.27767300	4.40654600	-0.76890700	C	-1.80823300	7.55503400	-0.90088000
C	-8.31288900	3.39739000	-0.83229300	C	-0.59924900	7.40965400	-0.21896500
H	-7.26961900	3.61121800	-0.62191900	C	-0.46148700	6.37538900	0.71083300
H	-8.98274200	5.41892700	-0.50094900	C	-1.51334600	5.48605800	0.94188900
H	-11.3648640	4.90697300	-1.00906400	H	-1.38186300	4.70426500	1.68611100
H	-12.0078800	2.58919700	-1.65830500	H	0.46326200	6.26972000	1.27399200



H	0.21932700	8.10297300	-0.39616700	H	-3.48359900	-3.02516200	-1.04697000
H	-1.93719300	8.36451800	-1.61604200	O	1.33548300	1.22064900	0.89216000
H	-3.81030600	6.80835100	-1.17178000	C	2.27594600	0.94630400	1.96062200
Li	-2.28400800	2.29503400	-0.75239800	C	3.14006300	2.19904200	2.06031600
O	-3.87823500	0.21860900	0.58291100	C	2.10461000	3.30168600	1.78789300
C	-2.62518200	-0.05676500	0.60407800	C	1.19811600	2.66487700	0.73002300
C	-2.07557800	-1.01186800	1.54045700	H	1.50376100	2.90848800	-0.29319000
C	-2.89019100	-2.02688800	2.23264900	H	0.14721300	2.93020800	0.85973800
C	-2.63836400	-3.40973500	2.09334400	H	2.55271300	4.23541800	1.43527000
C	-3.33423200	-4.35843300	2.84465400	H	1.52673000	3.50300800	2.69499600
C	-4.31789500	-3.95995900	3.74956100	H	3.92309500	2.19035300	1.29161800
C	-4.61059800	-2.59751500	3.87280200	H	3.61742700	2.29413100	3.03977500
C	-3.91255600	-1.64903900	3.13018200	H	1.72472100	0.78144000	2.89351000
H	-4.13997800	-0.59621600	3.25558500	H	2.82601400	0.03844500	1.69322000
H	-5.37807900	-2.26813700	4.56941900	O	1.12159000	-0.93169100	-1.36541100
H	-4.85026000	-4.69518400	4.34702900	C	2.46871000	-0.56256000	-1.75440000
H	-3.10511200	-5.41435400	2.71802200	C	3.10880300	-1.82841300	-2.34518700
H	-1.88650400	-3.74096900	1.38223500	C	2.26733400	-2.95704200	-1.72654400
O	-0.85461800	2.73526200	-2.11287500	C	0.88122200	-2.31973100	-1.68686000
C	-0.57026900	1.88056900	-3.22812000	H	0.21340400	-2.71577500	-0.91929000
C	-1.01644100	2.68326400	-4.45354700	H	0.38493600	-2.38463400	-2.66573300
C	-0.72968800	4.14982800	-4.03928600	H	2.61023500	-3.18423300	-0.71011200
C	-0.49438600	4.07660300	-2.51286900	H	2.29098000	-3.88205300	-2.30996300
H	-1.10851400	4.76208600	-1.93024700	H	4.17359800	-1.90270800	-2.10671100
H	0.56215800	4.24399100	-2.26369700	H	3.00865500	-1.83723000	-3.43645100
H	-1.57443500	4.79999700	-4.27980700	H	2.41463400	0.26245500	-2.47226900
H	0.15277300	4.54948700	-4.54866800	H	2.98766400	-0.20855100	-0.85842500
H	-2.08698200	2.53641700	-4.62185700	C	0.10483100	-1.94051400	2.14971300
H	-0.48396700	2.38444700	-5.36190000	O	-0.76450800	-1.46714200	1.11683200
H	0.51026400	1.66784000	-3.26072200	H	-5.13398600	4.46593100	-1.83290700
H	-1.10910500	0.94425900	-3.06797300	H	-3.46415500	4.45033700	-2.36739900
O	-4.24971400	-1.47074600	-2.17341000	H	-3.76638900	1.80825300	-2.51584500
C	-3.17823900	-2.39847500	-1.88944100	H	-4.40501000	2.87865300	-3.76022200
C	-2.95506100	-3.17191000	-3.18990800	H	-6.08373400	1.28911900	-3.40259600
C	-3.29481700	-2.11329100	-4.25030300	H	-6.63198400	2.82378500	-2.77055800
C	-4.46623500	-1.37234700	-3.59917600	C	-1.49383500	0.73097400	2.99862700
H	-5.42570300	-1.84810500	-3.83932000	H	-0.65028200	0.79104600	2.33747300
H	-4.52507000	-0.31490500	-3.86632500	H	-2.40298300	1.24119400	2.73643900
H	-3.55957300	-2.53925500	-5.22270700	H	-1.51205600	0.03204500	3.81817600
H	-2.44579800	-1.43435500	-4.39731400	Cl	-0.68704600	2.41834800	4.23035000
H	-3.64829900	-4.01854700	-3.25971000	H	1.05330300	-2.18933500	1.66265600
H	-1.93587100	-3.56214300	-3.27579000	H	0.27817600	-1.17929600	2.91569100
H	-2.29118500	-1.82571400	-1.59621600	H	-0.29367000	-2.83767100	2.63152700



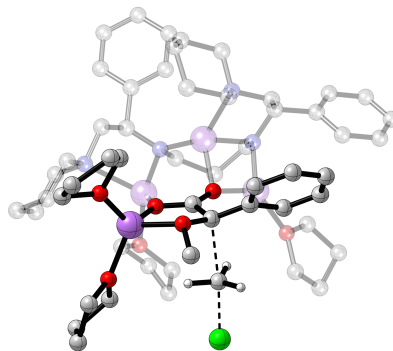
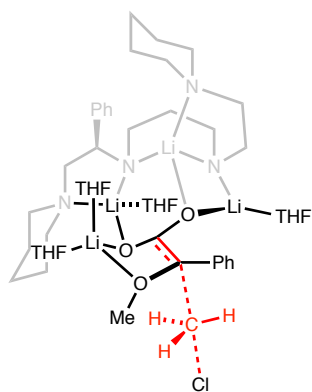
**TS VIII**

G = -3381.897059

G<sub>MP2</sub> = -3371.580887

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	4.21753200	7.19005600	-1.92142900
O	1.73861600	0.70574100	-0.17154200	C	5.20654500	2.82253000	-2.75102900
Li	2.56107600	2.19206700	-1.30641800	C	5.89134400	1.45138100	-2.88318700
N	4.43915500	3.07091000	-1.52888700	C	7.11381000	1.21790500	-1.96979000
C	4.13674000	4.48784400	-1.48377200	N	6.72680700	0.82761300	-0.62402400
C	3.06172900	4.77164200	-0.41552200	Li	5.14314200	1.88459400	-0.01547400
N	1.72169800	4.22234800	-0.74250100	N	6.25673900	2.00826400	2.06677400
C	0.87602900	4.28961500	0.46770000	C	5.40598800	1.59803400	3.20307100
H	1.34843000	3.67683900	1.24280300	C	4.35748900	2.65681400	3.54572700
H	0.84576200	5.32971600	0.84773900	C	5.03100600	3.99151100	3.88558700
C	-0.55506600	3.80840100	0.21613500	H	5.59323400	3.88277900	4.82476100
H	-1.13366800	3.92712400	1.14073900	H	4.28139900	4.77413500	4.05762900
H	-0.53735800	2.73687500	-0.01673000	C	5.98930100	4.39700000	2.75892500
C	-1.21641600	4.57574000	-0.93356900	C	6.95759300	3.26263800	2.41506500
C	-0.31152100	4.52560600	-2.16788800	H	7.59105200	3.55434300	1.57342600
C	1.09750100	5.01265800	-1.82448700	H	7.62916700	3.08099200	3.27819700
H	1.73760100	4.95991600	-2.70780800	H	5.42036700	4.66470400	1.86076600
H	1.04938500	6.07961200	-1.52798000	H	6.57078300	5.28506800	3.03727800
H	-0.71653400	5.14629700	-2.97746400	H	3.73248000	2.29522400	4.37002000
H	-0.25228100	3.49584000	-2.54311400	H	3.69315800	2.78885300	2.67894800
H	-1.36898500	5.62348300	-0.63698400	H	4.92242800	0.65566000	2.93176100
H	-2.20987600	4.16422300	-1.15581300	H	6.02836900	1.39583800	4.09706100
H	2.97754300	5.85462600	-0.22175900	C	7.23532400	0.94075400	1.75996400
H	3.38996900	4.30256500	0.52017600	H	8.05527300	0.94808700	2.50034200
H	3.72314800	4.83231800	-2.46045400	H	6.71483800	-0.01738800	1.87455200
C	5.31859500	5.46354800	-1.24414000	C	7.80316000	1.00394600	0.32587400
C	5.16526500	6.83024800	-1.52168100	H	8.28019300	2.00079700	0.19907900
C	6.20223400	7.73701100	-1.30324100	C	8.96113600	-0.00403000	0.19384200
C	7.43103800	7.28765900	-0.81345100	C	10.2462180	0.41889500	-0.16559600
C	7.60502900	5.92839300	-0.55201800	C	11.2980050	-0.48961900	-0.31419700
C	6.55734900	5.02827600	-0.76570100	C	11.0839120	-1.85018200	-0.09554000
H	6.69479900	3.96778900	-0.57996700	C	9.80769500	-2.29154600	0.26680400
H	8.56304900	5.56311200	-0.18842800	C	8.76139400	-1.37829100	0.40195300
H	8.24551500	7.98855100	-0.64805600	H	7.77158400	-1.74046200	0.67328100
H	6.05483500	8.79238300	-1.52154200	H	9.62944900	-3.34941200	0.44838700

H	11.8996050	-2.56042900	-0.20552400	H	1.29592400	-0.47021200	-2.90618300
H	12.2843780	-0.13231800	-0.60125200	O	-1.38106500	0.51623000	1.39451100
H	10.4234470	1.47951100	-0.33477100	C	-2.77693800	0.16362900	1.25116300
Li	5.41722000	-0.61678600	-0.62863900	C	-3.45324500	0.54913100	2.57121400
O	3.89063100	0.17238500	0.15833600	C	-2.56509100	1.69819900	3.07195000
C	2.64495400	-0.12741400	0.24369200	C	-1.17791900	1.21985200	2.65749100
C	2.23081000	-1.38095400	0.85308100	H	-0.75130100	0.53518300	3.39763900
C	3.12763600	-2.54884200	0.90666800	H	-0.46015900	2.02166900	2.47682600
C	2.74352800	-3.81031000	0.39618100	H	-2.63653200	1.86162600	4.15059000
C	3.57449100	-4.92710100	0.50178600	H	-2.82330000	2.63454700	2.56259200
C	4.82520900	-4.82929000	1.11325600	H	-3.42164300	-0.28785400	3.27802300
C	5.22783900	-3.59016500	1.62175200	H	-4.50016300	0.83457400	2.43114000
C	4.39709500	-2.47592400	1.52840600	H	-3.19106700	0.72544700	0.40468200
H	4.71584000	-1.53772600	1.96805200	H	-2.84918800	-0.90554300	1.02647400
H	6.18897300	-3.49474100	2.12182700	O	-1.19784200	-0.40875400	-1.54989200
H	5.46633100	-5.70129600	1.20827000	C	-1.45147600	-1.76203300	-1.99191800
H	3.23675100	-5.88139600	0.10273300	C	-1.73976300	-1.65351800	-3.48884500
H	1.78356900	-3.90947900	-0.10100300	C	-2.43423000	-0.28512800	-3.57897800
O	5.58390400	-2.04797700	-1.99611600	C	-1.66863800	0.54082300	-2.54000800
C	4.62612400	-2.90030500	-2.64150400	H	-2.29245300	1.28491600	-2.03443100
C	5.37815100	-4.21012600	-2.95185600	H	-0.79398800	1.04281100	-2.96622200
C	6.87718600	-3.80918400	-2.87070200	H	-3.48993700	-0.37601900	-3.29825200
C	6.83975500	-2.28951800	-2.66188000	H	-2.38838200	0.15914300	-4.57751200
H	6.84588300	-1.74820500	-3.61870600	H	-2.35788100	-2.47772400	-3.85645100
H	7.63019700	-1.89584300	-2.02352200	H	-0.80364500	-1.64853600	-4.05910800
H	7.43806600	-4.07979700	-3.77028200	H	-0.57290700	-2.36152600	-1.74177500
H	7.35952600	-4.29509800	-2.01762600	H	-2.31963500	-2.15781600	-1.44667800
H	5.10335900	-4.59965100	-3.93713200	C	0.12426800	-2.46124700	1.47456100
H	5.13800800	-4.97490200	-2.20894400	O	0.86139900	-1.70344200	0.50596100
H	3.78461400	-3.02492500	-1.95940800	H	7.70895900	2.15700700	-1.96759600
H	4.28168100	-2.41233400	-3.56668400	H	7.77933300	0.47859900	-2.46720800
O	1.74470300	1.52646800	-3.16955400	H	4.56957600	2.96204300	-3.65794800
C	2.03414300	0.13314200	-3.43951300	H	6.01151300	3.56961900	-2.88621900
C	1.99140400	-0.01310600	-4.96141300	H	6.22291100	1.36205200	-3.92964100
C	2.49013300	1.36369600	-5.42582000	H	5.15821100	0.64290300	-2.73022400
C	1.86204100	2.29801000	-4.38992700	C	2.04195700	-0.52812400	2.98147500
H	0.85687000	2.62124800	-4.69283100	H	2.03273600	-1.54490800	3.33189000
H	2.47228800	3.17923800	-4.18029800	H	2.98112800	-0.01202300	2.88950800
H	2.19170600	1.61321500	-6.44854800	H	1.15752400	-0.06964800	2.58432000
H	3.58262200	1.41397800	-5.36447200	Cl	1.58045800	0.28045900	5.03203700
H	0.96432900	-0.18597800	-5.30801000	H	-0.75045600	-2.86140100	0.95196000
H	2.61198600	-0.84099200	-5.31802700	H	0.71486700	-3.29657900	1.85996500
H	3.02897200	-0.10143300	-3.04432100	H	-0.20949800	-1.83743400	2.30857700



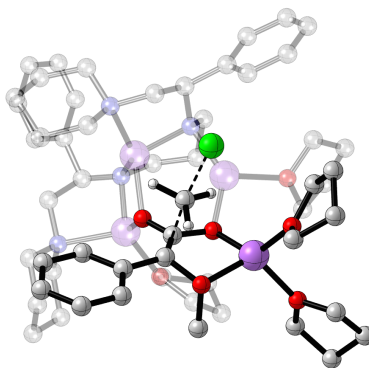
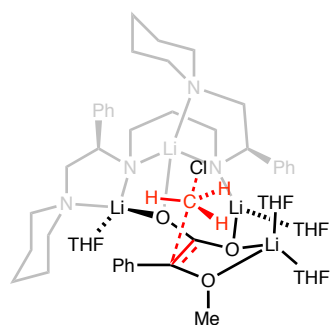
### TS IX

G = -3381.901457

G<sub>MP2</sub> = -3371.586417

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	3.39259900	6.96724300	-2.54592600
O	1.65623200	0.45334900	-0.77718100	C	5.05874500	2.78834300	-3.44695200
Li	2.44625800	1.69997800	-2.22941200	C	5.93329400	1.52661000	-3.54881700
N	4.15852800	2.89102100	-2.29455700	C	7.08072000	1.41906600	-2.52332100
C	3.65599800	4.24979100	-2.26254800	N	6.61547300	0.91486400	-1.24289800
C	2.40736300	4.34717300	-1.36175900	Li	4.87663000	1.75121900	-0.76513000
N	1.21291800	3.65032300	-1.89848500	N	5.72682600	1.88542200	1.41735500
C	0.18520900	3.59223000	-0.84110500	C	4.83596000	1.31875900	2.44969500
H	0.59924600	3.02411600	-0.00208300	C	3.63807300	2.22827000	2.73176500
H	-0.03551000	4.61408800	-0.47078600	C	4.09484400	3.62657400	3.16387800
C	-1.11888300	2.94522700	-1.31539400	H	4.58551300	3.55828700	4.14600100
H	-1.84368900	2.96735500	-0.49285500	H	3.23628800	4.29962700	3.28616000
H	-0.93288100	1.89116000	-1.55507300	C	5.08246200	4.19071600	2.13661300
C	-1.68188200	3.65369300	-2.55133600	C	6.22087800	3.20461200	1.86260900
C	-0.59615500	3.72669500	-3.62716300	H	6.88406700	3.60688100	1.09326800
C	0.67690200	4.36993000	-3.07301200	H	6.82801500	3.08145100	2.78208300
H	1.44618100	4.39560300	-3.84728100	H	4.56292700	4.40818200	1.19616200
H	0.46021300	5.42307900	-2.80158500	H	5.50992300	5.13909900	2.48497600
H	-0.93908900	4.30602400	-4.49377000	H	3.01482000	1.76354800	3.50745000
H	-0.36451200	2.71502300	-3.98352600	H	3.02358300	2.30086400	1.82319300
H	-1.99810800	4.67151300	-2.28035000	H	4.49505100	0.34008600	2.10410600
H	-2.57353300	3.13474300	-2.92639800	H	5.39640600	1.15650200	3.39206800
H	2.15565200	5.40218600	-1.15526800	C	6.86073300	0.95886600	1.18322300
H	2.65227100	3.88158400	-0.39841900	H	7.59034400	1.03523700	2.00948500
H	3.34163200	4.57218700	-3.28095100	H	6.45167000	-0.05651000	1.21432000
C	4.65028800	5.36345200	-1.83900000	C	7.56284000	1.15950000	-0.17502000
C	4.33529500	6.71250400	-2.06266900	H	7.93269000	2.20826500	-0.21285500
C	5.20771000	7.73442100	-1.68852700	C	8.83489200	0.29444300	-0.24411700
C	6.43335400	7.42401600	-1.09391500	C	10.0483440	0.85020600	-0.66881000
C	6.77020300	6.08643200	-0.88519800	C	11.2029070	0.07273500	-0.79457700
C	5.88511100	5.06949100	-1.25439400	C	11.1685820	-1.28648000	-0.48456800
H	6.14961800	4.02649700	-1.11036100	C	9.96777800	-1.85866800	-0.05384000
H	7.73082000	5.83066300	-0.44310800	C	8.81641400	-1.07774300	0.05628500
H	7.12126400	8.21602800	-0.80830900	H	7.89097100	-1.54294900	0.38880200
H	4.93598700	8.77224700	-1.86846300	H	9.93096600	-2.91527100	0.20338900

H	12.0653390	-1.89452600	-0.57413300	H	1.76638300	-1.25566800	-3.90534300
H	12.1291590	0.53148800	-1.13312200	O	-0.94589800	0.91513100	1.54355700
H	10.0853640	1.91169400	-0.90666800	C	-2.27248900	1.35354400	1.86922100
Li	5.49293000	-0.67490900	-1.39158100	C	-2.50238500	0.89525500	3.31831600
O	3.81512100	-0.12066600	-0.80927600	C	-1.06693300	0.81857600	3.91037200
C	2.61731600	-0.33201600	-0.39076100	C	-0.15284300	1.17183400	2.72195300
C	2.31343900	-1.47225500	0.44975400	H	0.74353100	0.55839800	2.64167500
C	3.31569100	-2.07534700	1.34735800	H	0.12937600	2.23357900	2.73342400
C	3.10403600	-2.16029100	2.74212900	H	-0.85322300	-0.18848700	4.27945000
C	4.04437900	-2.74331000	3.59118700	H	-0.92111700	1.51297900	4.74265400
C	5.23508200	-3.26533100	3.08433200	H	-2.98273400	-0.08765800	3.33937900
C	5.46247600	-3.20092100	1.70713900	H	-3.14825100	1.59089800	3.86177600
C	4.51953100	-2.62772300	0.85589800	H	-2.32384500	2.44875600	1.78594800
H	4.70244900	-2.63488400	-0.21219100	H	-2.95844100	0.91322100	1.14304300
H	6.37479300	-3.61879400	1.28714000	O	-1.30296800	-0.80464500	-1.29914900
H	5.96725800	-3.72016600	3.74547100	C	-1.02646300	-0.90313000	-2.72726800
H	3.84603300	-2.78064600	4.66009500	C	-2.40218200	-0.95750400	-3.38110800
H	2.19710000	-1.73825300	3.16408400	C	-3.18739800	-1.80876100	-2.37067200
O	5.98595700	-2.21841600	-2.54894600	C	-2.62184900	-1.33428100	-1.02475600
C	7.27627400	-2.08554600	-3.20855300	H	-2.53530500	-2.13996600	-0.28812000
C	7.68797200	-3.50988900	-3.56640600	H	-3.22836600	-0.52836400	-0.59361900
C	6.33431400	-4.15735800	-3.89344100	H	-2.96930000	-2.87101700	-2.52491100
C	5.40171400	-3.51456300	-2.86307800	H	-4.27099500	-1.67212700	-2.43359300
H	5.35913500	-4.10104900	-1.93752500	H	-2.36897300	-1.40238200	-4.37967100
H	4.38305800	-3.37299900	-3.23227400	H	-2.83330100	0.04770600	-3.46292700
H	6.33984900	-5.24839700	-3.81658600	H	-0.41452600	-0.04247400	-3.00354700
H	6.02101700	-3.89339800	-4.91031200	H	-0.46284100	-1.82326100	-2.92195100
H	8.15451900	-3.99961100	-2.70320900	C	0.31000900	-2.56714500	1.30066700
H	8.39691900	-3.54014100	-4.39927200	O	1.00121900	-1.34354400	1.04133400
H	7.14782100	-1.46498900	-4.10427200	H	7.53481400	2.42962400	-2.42515400
H	7.95135900	-1.57927300	-2.51773500	H	7.89075000	0.80266200	-2.97125700
O	1.96750400	0.81041200	-4.07294300	H	4.48995300	2.87241800	-4.40333900
C	2.45945000	-0.53334100	-4.33784000	H	5.76325900	3.64147300	-3.48844300
C	2.57642900	-0.64608200	-5.85822300	H	6.37087300	1.52564000	-4.55905100
C	2.87798400	0.80216800	-6.26948200	H	5.30292700	0.62392100	-3.49347200
C	2.01397200	1.59406200	-5.28854400	C	1.98512700	-2.87106700	-1.43207800
H	0.99050500	1.71707800	-5.66847100	H	2.12445200	-3.71376100	-0.77533600
H	2.42415900	2.57610000	-5.04261000	H	1.04061800	-2.36092400	-1.45719300
H	2.62940000	1.02076400	-7.31269700	H	2.85062800	-2.38789400	-1.84812500
H	3.93680100	1.03544200	-6.11193500	Cl	1.53221400	-4.06899500	-3.23120200
H	1.62749100	-0.98277300	-6.29218400	H	0.00025000	-3.06008900	0.37336500
H	3.35210800	-1.35573300	-6.15953300	H	0.92732100	-3.25641700	1.88504200
H	3.43373800	-0.64103300	-3.84815200	H	-0.57667000	-2.30289200	1.88543300



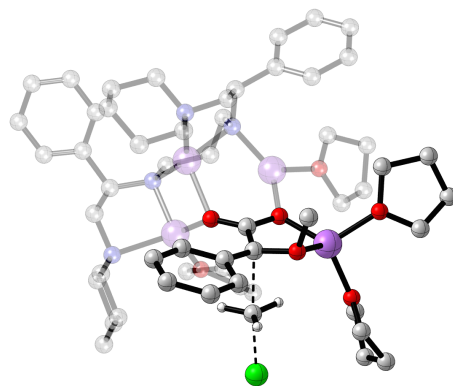
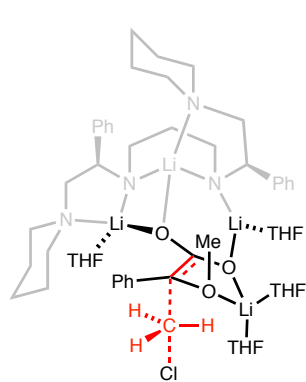
**TS X**

G = -3381.899169

G<sub>MP2</sub> = -3371.582026

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-10.2657450	1.11576700	-2.07078500
O	-1.82710400	0.46343300	-0.35048400	C	-5.93890900	2.24150700	-2.62552100
Li	-5.24714100	-0.18068200	-0.92630100	C	-4.49835200	2.74857300	-2.79876800
N	-6.21942200	1.53437300	-1.38290000	C	-4.09344200	3.93618100	-1.89936400
C	-7.61937300	1.16455800	-1.36868200	N	-3.69535700	3.51472500	-0.56567000
C	-7.90474600	0.19333700	-0.20210300	Li	-5.00076700	2.17623000	0.12755600
N	-7.18291500	-1.09999600	-0.29298700	N	-5.11730700	3.36697700	2.08730800
C	-7.25538500	-1.79094500	1.01287800	C	-4.96668000	2.54001200	3.30629900
H	-6.81042200	-1.13495900	1.76593900	C	-6.26244200	1.83375300	3.70539200
H	-8.31518800	-1.94298700	1.29843200	C	-7.39508700	2.84095500	3.92285700
C	-6.53657800	-3.14106000	0.99836500	H	-7.16135500	3.46919200	4.79486100
H	-6.62509200	-3.60343400	1.98855200	H	-8.33928700	2.32796200	4.14466800
H	-5.46568100	-2.97447000	0.82643300	C	-7.53506100	3.71882200	2.67530500
C	-7.10946600	-4.05632600	-0.08940000	C	-6.19802900	4.35844200	2.29146200
C	-7.09955900	-3.32348000	-1.43572700	H	-6.31479000	4.93910500	1.37196800
C	-7.79119500	-1.96110800	-1.32951000	H	-5.89605400	5.06959200	3.08556800
H	-7.74332500	-1.43858200	-2.28811100	H	-7.90393600	3.11608300	1.83765300
H	-8.86498400	-2.11389100	-1.10179700	H	-8.27128100	4.51658000	2.83611700
H	-7.60335700	-3.91786200	-2.20926200	H	-6.07642300	1.23978600	4.60847100
H	-6.06345200	-3.16980300	-1.76116700	H	-6.54657300	1.12920500	2.91171100
H	-8.14249000	-4.33156200	0.16948100	H	-4.19108400	1.79620600	3.10997900
H	-6.53974900	-4.99204900	-0.15133500	H	-4.61729700	3.16507300	4.15008200
H	-8.98932500	0.00996400	-0.11029800	C	-3.83359200	4.06266700	1.82035300
H	-7.58172000	0.68409800	0.72376100	H	-3.68148700	4.86672000	2.56140000
H	-7.89744500	0.63510400	-2.31150400	H	-3.03400200	3.33263700	1.98180700
C	-8.65355000	2.31370200	-1.28926300	C	-3.70925800	4.61814500	0.38972300
C	-9.98004800	2.09509100	-1.68802100	H	-4.59235000	5.26333300	0.20129700
C	-10.9368820	3.10729600	-1.61198000	C	-2.50016500	5.56097300	0.27186700
C	-10.5774700	4.37415700	-1.14551800	C	-2.56073600	6.65299000	-0.60844300
C	-9.25743600	4.61127900	-0.76061500	C	-1.46308500	7.49571100	-0.80323300
C	-8.30738600	3.58890700	-0.83208300	C	-0.27770600	7.27469500	-0.09987800
H	-7.27521300	3.77018900	-0.54716400	C	-0.20726600	6.20637900	0.79834900
H	-8.96286600	5.59793900	-0.40976600	C	-1.30099500	5.35591000	0.97750700
H	-11.3170080	5.16929800	-1.09204300	H	-1.21420200	4.55006500	1.70291200
H	-11.9603420	2.91081800	-1.92349400	H	0.69632200	6.04138900	1.38107500

H	0.57347900	7.93788100	-0.23439200	H	-3.13348000	-2.76124100	-2.19624700
H	-1.54103700	8.33403900	-1.49218000	O	1.46443000	1.09161500	0.79880200
H	-3.48939900	6.84876900	-1.14052500	C	1.70877600	2.50449900	0.55259900
Li	-2.23016400	2.25353300	-0.87683500	C	2.76380900	2.94498500	1.57784800
O	-3.91580400	0.28018900	0.47943400	C	3.42548700	1.61966800	1.98996400
C	-2.66775000	-0.00664300	0.54656400	C	2.23848100	0.66340600	1.94895600
C	-2.08359100	-0.75724300	1.64213100	H	1.62743500	0.76084300	2.85124600
C	-2.77420000	-1.45320600	2.73386300	H	2.50610700	-0.38547100	1.78973000
C	-2.03750000	-2.26147200	3.63284300	H	3.88483800	1.66506700	2.98153000
C	-2.64224700	-2.87508700	4.72760600	H	4.19335500	1.31738000	1.26600000
C	-4.00342400	-2.70050400	4.98122700	H	2.26712500	3.39434100	2.44204200
C	-4.74316100	-1.89018900	4.11739600	H	3.47125800	3.66628900	1.15744000
C	-4.14761900	-1.27850500	3.01554100	H	2.05924900	2.59739000	-0.48260700
H	-4.73160200	-0.65086100	2.35705300	H	0.76924600	3.05167600	0.66120600
H	-5.80304600	-1.72763200	4.30230500	O	1.11427700	-0.96674100	-1.40892300
H	-4.47427200	-3.17520700	5.83770500	C	0.65686400	-1.73030100	-2.54998300
H	-2.03788300	-3.48735700	5.39330000	C	1.89493800	-2.43075100	-3.12173600
H	-0.97050300	-2.38860100	3.47930700	C	3.03118100	-1.49139200	-2.69030300
O	-0.72229900	2.69811700	-2.14079700	C	2.55666600	-1.04865100	-1.30886200
C	-0.56765500	1.93488300	-3.35014600	H	2.92047400	-0.07046400	-0.99260300
C	-0.65791500	2.95828300	-4.47888400	H	2.81994400	-1.78961500	-0.54116400
C	0.08020300	4.15858800	-3.86350900	H	3.09855800	-0.63006100	-3.36552100
C	-0.29738000	4.07465700	-2.37617300	H	4.00949000	-1.97975500	-2.66096500
H	-1.13418000	4.72285600	-2.11290200	H	1.83069900	-2.56811700	-4.20499700
H	0.53947500	4.29812100	-1.70959500	H	2.02441000	-3.41808800	-2.66363600
H	-0.21478800	5.11432200	-4.30530100	H	-0.11754400	-2.42720200	-2.21777800
H	1.16271900	4.04710600	-3.99783000	H	0.21457800	-1.03226900	-3.26995000
H	-1.70674000	3.20785700	-4.67341300	C	-0.85473500	-2.59347400	0.70713500
H	-0.20647300	2.60342700	-5.41076200	O	-0.78727500	-1.29574600	1.31272500
H	0.41048200	1.43069100	-3.34262100	H	0.17285300	-2.89627200	0.48385100
H	-1.35439500	1.17564800	-3.36457300	H	-1.30907900	-3.31810300	1.38904300
O	-4.53219600	-1.25707200	-2.52116100	H	-1.44182400	-2.56038600	-0.21972500
C	-3.19472500	-1.78201800	-2.68736800	H	-4.95808500	4.63441900	-1.86748300
C	-2.94850800	-1.88077500	-4.20794500	H	-3.30370700	4.51215400	-2.43576300
C	-4.06626500	-1.00796700	-4.80576400	H	-3.79608500	1.90871300	-2.65510400
C	-5.19283700	-1.22079500	-3.80029800	H	-4.39062300	3.05951600	-3.84960600
H	-5.71004700	-2.17541400	-3.97734600	H	-6.17288800	1.60337600	-3.51299400
H	-5.92466500	-0.41293000	-3.76701400	H	-6.59331000	3.12418800	-2.76694400
H	-4.34297200	-1.30219200	-5.82269600	C	-1.24672200	1.01757200	2.79624600
H	-3.77583200	0.04840200	-4.81825000	H	-0.96978100	1.44573400	1.85051200
H	-3.05291400	-2.91658100	-4.54990500	H	-2.20251600	1.24540500	3.23452600
H	-1.94733700	-1.53949900	-4.48920200	H	-0.63186300	0.26234500	3.25521500
H	-2.51686200	-1.08902200	-2.18194200	Cl	-0.19918000	2.70443000	3.88026700



**TS XI**

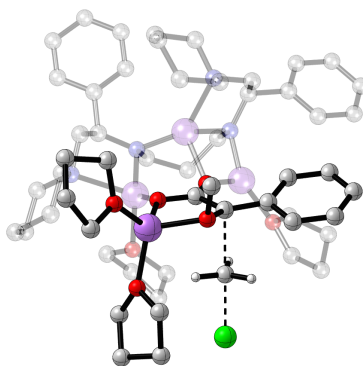
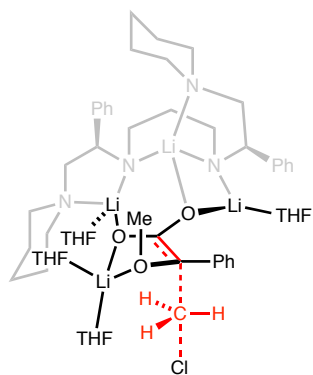
G = -3381.907557

G<sub>MP2</sub> = -3371.589862

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-10.1539060	-0.27803300	-2.99034200
O	-1.78011700	0.51995300	-0.44983400	C	-6.05435600	1.63268800	-3.28969800
Li	-4.99329800	-0.77909700	-1.78107200	C	-4.72923500	2.40907700	-3.33915700
N	-6.25242900	0.78308000	-2.12161100	C	-4.59430200	3.55316400	-2.31539000
C	-7.56213000	0.17360900	-2.22129200	N	-4.14744800	3.08439500	-1.01139000
C	-7.70926000	-0.97039800	-1.19592200	Li	-5.22528000	1.47045200	-0.49938600
N	-6.76354800	-2.09708000	-1.38553100	N	-5.56470600	2.56726000	1.60057400
C	-6.83547300	-2.97737900	-0.19889000	C	-5.35039800	1.75170600	2.81626200
H	-6.59200100	-2.37729700	0.68095400	C	-6.54940800	0.86356900	3.15087000
H	-7.87452600	-3.34001900	-0.06804900	C	-7.82291400	1.69542900	3.32325800
C	-5.89277900	-4.17642800	-0.29758100	H	-7.72371300	2.34254200	4.20755400
H	-5.99498100	-4.78601200	0.60826300	H	-8.69104300	1.04828400	3.49947000
H	-4.85544400	-3.82068000	-0.32036700	C	-8.03124400	2.55471700	2.07378900
C	-6.18689400	-5.00197300	-1.55457900	C	-6.78669000	3.38785200	1.75928800
C	-6.18029900	-4.08587800	-2.78309600	H	-6.94720200	3.95346900	0.83816000
C	-7.11011200	-2.88296400	-2.58991200	H	-6.63062700	4.12825500	2.56999800
H	-7.05877200	-2.22585000	-3.46189900	H	-8.26335900	1.91216100	1.21673300
H	-8.15833800	-3.23530900	-2.51487700	H	-8.88437500	3.23353700	2.19787200
H	-6.49327500	-4.63442700	-3.68116200	H	-6.32040600	0.28678100	4.05455200
H	-5.16100200	-3.72271500	-2.96056700	H	-6.69546900	0.13814700	2.34014100
H	-7.17418700	-5.47778100	-1.45726600	H	-4.46086200	1.13389900	2.65802200
H	-5.45251500	-5.80762400	-1.66983600	H	-5.14173700	2.41313100	3.68155700
H	-8.74622500	-1.34966400	-1.19462200	C	-4.38603700	3.43934600	1.39937300
H	-7.51983400	-0.55164000	-0.19911400	H	-4.34375700	4.20710600	2.19485700
H	-7.70969700	-0.27404700	-3.23179200	H	-3.50017400	2.80279100	1.51715400
C	-8.78754400	1.10723600	-2.06242900	C	-4.32820200	4.10232900	0.01072100
C	-10.0506040	0.69558200	-2.51245500	H	-5.28893600	4.63406900	-0.14539500
C	-11.1736340	1.50991800	-2.36720000	C	-3.26314900	5.21136700	-0.03315200
C	-11.0509740	2.77058400	-1.77742900	C	-3.50386500	6.37914800	-0.77302400
C	-9.79751200	3.20126300	-1.34155200	C	-2.53191700	7.37461000	-0.90435500
C	-8.67914700	2.37505700	-1.48350800	C	-1.29307800	7.23267300	-0.27763700
H	-7.69638200	2.70859900	-1.16291700	C	-1.03993500	6.08377200	0.47776200
H	-9.68717500	4.18770400	-0.89603500	C	-2.01006100	5.08569500	0.58890100
H	-11.9216290	3.41268500	-1.66882900	H	-1.79318800	4.20208700	1.18447900
H	-12.1429480	1.16491000	-2.72012600	H	-0.08896200	5.97427800	0.99580000



H	-0.53952600	8.01146400	-0.36386600	H	-2.22660000	-2.58863400	-3.03780500
H	-2.74838100	8.26702500	-1.48706500	O	1.33572400	1.44461000	0.34451300
H	-4.47457600	6.50924200	-1.24640300	C	2.75812200	1.24224000	0.45944600
Li	-2.47688100	2.08399700	-1.25478200	C	3.36957100	2.59098400	0.09284800
O	-3.89647500	-0.22863700	-0.23038400	C	2.37119200	3.56929400	0.73552900
C	-2.67552500	-0.22095000	0.16740100	C	1.02173700	2.84133600	0.59553700
C	-2.19057000	-1.08367700	1.22098900	H	0.42817500	3.19716100	-0.24963300
C	-2.96235700	-1.79281600	2.24830100	H	0.41348900	2.90871500	1.50309600
C	-2.28306800	-2.54035100	3.24100100	H	2.35978400	4.55018700	0.25203900
C	-2.97339800	-3.26001100	4.21324000	H	2.61939800	3.72164400	1.79168900
C	-4.36907900	-3.27091200	4.23437200	H	3.38895300	2.71263200	-0.99657400
C	-5.05635400	-2.54615100	3.25879000	H	4.39016800	2.70937500	0.46839900
C	-4.37220000	-1.82022300	2.28457800	H	3.00962900	0.95862500	1.49218000
H	-4.91562100	-1.26077500	1.53569800	H	3.02242900	0.42071600	-0.20828900
H	-6.14420000	-2.53822700	3.25712000	O	1.22778000	-1.34468600	-0.87626900
H	-4.90870500	-3.83372200	4.99106600	C	1.83582900	-2.43856200	-0.13271100
H	-2.41231800	-3.82167800	4.95684000	C	2.87496800	-3.03076500	-1.07989400
H	-1.19758900	-2.56135100	3.23597500	C	2.17382600	-2.88176200	-2.43935300
O	-1.03024000	2.80407600	-2.45047400	C	1.45364000	-1.53706200	-2.29742800
C	-0.00125500	2.00256700	-3.07674800	H	0.48692700	-1.51954900	-2.80862500
C	0.57496500	2.85545400	-4.21539000	H	2.06364500	-0.69759500	-2.65684600
C	0.27189300	4.28655100	-3.74438400	H	1.43875800	-3.68191700	-2.56716400
C	-1.08949700	4.11121100	-3.07830100	H	2.86595000	-2.89111800	-3.28684300
H	-1.90031000	4.11413600	-3.81644000	H	3.10638500	-4.07093300	-0.83433600
H	-1.31552500	4.84150800	-2.30059400	H	3.80729500	-2.45238100	-1.04950400
H	0.24758700	5.01401100	-4.56095900	H	2.25063800	-2.01848100	0.78809100
H	1.01719100	4.62021000	-3.01208500	H	1.06344000	-3.17287000	0.11203800
H	0.05037000	2.64782400	-5.15508400	C	-0.75652200	0.19539700	2.65979200
H	1.64043700	2.66547300	-4.37759100	O	-0.83652000	-0.78380900	1.61200300
H	0.75279500	1.76983400	-2.31579000	H	-5.58453700	4.05557900	-2.24826000
H	-0.44718900	1.06505500	-3.42337300	H	-3.92904500	4.33176200	-2.74926800
O	-3.93330400	-1.43948800	-3.39404400	H	-3.88432500	1.70709300	-3.23263500
C	-2.49163100	-1.61028800	-3.44952800	H	-4.64376400	2.83603700	-4.35009100
C	-2.09502900	-1.47535300	-4.93434000	H	-6.12558500	1.03961200	-4.23320200
C	-3.34127700	-0.84925900	-5.58475600	H	-6.85593900	2.39028300	-3.40205700
C	-4.46024400	-1.43939900	-4.73243500	H	-1.24899200	-0.16819300	3.56627200
H	-4.69328600	-2.46941000	-5.03968500	H	0.30595600	0.36095200	2.86342600
H	-5.37723500	-0.84803300	-4.72446600	H	-1.22592100	1.13637400	2.34525600
H	-3.44220000	-1.09485600	-6.64645100	C	-1.70997100	-2.86042400	-0.17166100
H	-3.33366300	0.24155100	-5.48018300	H	-1.41519400	-3.35289500	0.73959800
H	-1.89458900	-2.46227800	-5.36520600	H	-2.74331600	-2.89641900	-0.47339400
H	-1.19495200	-0.86684400	-5.07233000	H	-1.02847000	-2.19602300	-0.66993400
H	-2.06048900	-0.82840300	-2.81611900	Cl	-1.08158000	-4.57097200	-1.47575600



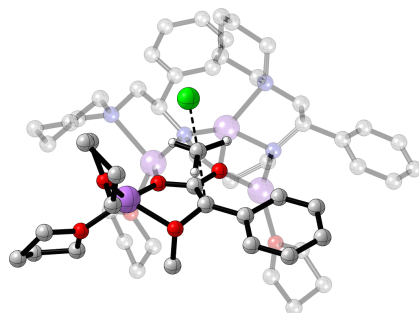
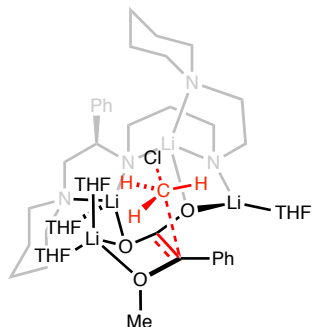
### TS XII

G = -3381.904155

G<sub>MP2</sub> = -3371.587695

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-3.75521400	6.90495600	2.77206600
O	-1.69738000	0.57946000	0.62834400	C	-5.27572100	2.63760900	3.55566200
Li	-2.62362400	1.65782900	2.29136100	C	-6.05336100	1.31344500	3.64842900
N	-4.37149100	2.80835200	2.41467400	C	-7.18639500	1.13010100	2.61942100
C	-3.92175000	4.18584800	2.42768100	N	-6.68365100	0.70571000	1.32145600
C	-2.67053300	4.35636200	1.54167700	Li	-5.01514500	1.67812600	0.85496000
N	-1.45904100	3.68837300	2.07214300	N	-5.84885300	1.79727600	-1.30853200
C	-0.42995500	3.65469500	1.01807500	C	-4.93795000	1.29409200	-2.35684300
H	-0.84005500	3.08454600	0.17993900	C	-3.76188500	2.24520500	-2.59476800
H	-0.21871700	4.68192200	0.65562300	C	-4.25254400	3.64783400	-2.97393700
C	0.87456600	3.01295900	1.49599500	H	-4.73077300	3.60698400	-3.96365600
H	1.60167000	3.02448700	0.67555700	H	-3.41059100	4.34680100	-3.05977000
H	0.67680200	1.96226700	1.74165500	C	-5.26517000	4.14510800	-1.93612400
C	1.43176700	3.72845300	2.73001600	C	-6.37672300	3.11815400	-1.71061300
C	0.34470100	3.79067500	3.80524800	H	-7.05804600	3.47119800	-0.93310300
C	-0.93907600	4.41264800	3.25070300	H	-6.97184100	3.01112100	-2.63960800
H	-1.71048600	4.42173400	4.02332700	H	-4.76137900	4.34261500	-0.98299400
H	-0.74157700	5.47058200	2.98274500	H	-5.71615500	5.09313500	-2.25394200
H	0.67924900	4.37750800	4.67005700	H	-3.12283200	1.82978800	-3.38586600
H	0.12954300	2.77653500	4.16277800	H	-3.15470900	2.29374000	-1.67981300
H	1.73931100	4.74845300	2.45673800	H	-4.56954000	0.31222000	-2.04745300
H	2.32754700	3.21821400	3.10711400	H	-5.48893000	1.15239400	-3.30794000
H	-2.45671000	5.42502700	1.36468200	C	-6.96358200	0.83849400	-1.10782800
H	-2.89063800	3.90786900	0.56440200	H	-7.71059900	0.95129200	-1.91348300
H	-3.62675400	4.48773100	3.45828200	H	-6.54960700	-0.16929000	-1.20525000
C	-4.95476900	5.27292500	2.02906400	C	-7.64947000	0.94284800	0.27284400
C	-4.68797400	6.62709800	2.28246000	H	-8.07381700	1.96844700	0.35628500
C	-5.59578900	7.62532200	1.92896000	C	-8.87712000	0.01064200	0.27630700
C	-6.80928900	7.28489900	1.32598300	C	-10.1782790	0.52424000	0.31779400
C	-7.09889500	5.94102400	1.08839500	C	-11.2929310	-0.31895000	0.32397200
C	-6.17836700	4.94852800	1.43679000	C	-11.1239360	-1.70275700	0.28215600
H	-6.40462600	3.89993100	1.26952700	C	-9.83123000	-2.23330700	0.24002700
H	-8.04988000	5.66125700	0.63996800	C	-8.72482300	-1.38361900	0.24332200
H	-7.52448500	8.05815700	1.05653500	H	-7.72176800	-1.80424400	0.22938100
H	-5.36091200	8.66798300	2.13129400	H	-9.68753900	-3.31127000	0.20347800

H	-11.9878850	-2.36262800	0.28579300	H	-1.63202800	-1.24727400	4.04022500
H	-12.2929440	0.10674200	0.36472100	O	1.12348100	1.05152000	-1.34163900
H	-10.3194820	1.60320400	0.35177400	C	2.57131700	0.98093200	-1.39584400
Li	-5.41711000	-0.77066500	1.58368300	C	3.01710500	2.00322200	-2.45386000
O	-3.79385500	-0.12742800	0.90793500	C	1.81817300	2.96249400	-2.53288700
C	-2.62917400	-0.29166900	0.37803400	C	0.64825000	2.00858100	-2.31388400
C	-2.29550600	-1.48578800	-0.36922500	H	0.38327300	1.48500000	-3.24261900
C	-3.20696400	-2.47639300	-0.95550400	H	-0.24954900	2.47657300	-1.90587900
C	-2.66987500	-3.64165300	-1.55833100	H	1.75387800	3.49348900	-3.48705500
C	-3.48597400	-4.63086300	-2.10025900	H	1.85896000	3.70536600	-1.72867000
C	-4.87709800	-4.50838300	-2.06548600	H	3.17332900	1.51249500	-3.42106600
C	-5.43029300	-3.36727200	-1.48228900	H	3.95060100	2.50146400	-2.17738800
C	-4.61509200	-2.37317500	-0.94023000	H	2.95166900	1.21833000	-0.39758200
H	-5.06667200	-1.48061600	-0.53057600	H	2.86729000	-0.04246400	-1.64734800
H	-6.50962700	-3.23295300	-1.46345100	O	1.40428800	-0.92883900	1.09639800
H	-5.51358400	-5.28001300	-2.48924800	C	2.02795500	-2.13699000	0.57913300
H	-3.02812000	-5.50923600	-2.54952900	C	2.46638100	-2.94038500	1.80364500
H	-1.59147300	-3.76693700	-1.59030700	C	2.74848900	-1.83573800	2.83399200
O	-5.70715200	-2.36953300	2.68881400	C	1.64109600	-0.82866200	2.52994600
C	-5.01635300	-3.65463200	2.68473600	H	1.90840200	0.20797100	2.75272800
C	-5.93125100	-4.63117000	3.43675700	H	0.71579900	-1.08669700	3.05524700
C	-7.31607700	-3.97734100	3.30856900	H	3.73661400	-1.38755500	2.67086600
C	-6.97072300	-2.49440300	3.38757500	H	2.69816800	-2.19681400	3.86478700
H	-6.83903000	-2.16562800	4.42738800	H	3.33903300	-3.56607300	1.59261000
H	-7.68775000	-1.83820300	2.89190600	H	1.64906900	-3.57724600	2.15646200
H	-8.01493800	-4.28629600	4.09177000	H	1.29366600	-2.64864400	-0.04850000
H	-7.76767500	-4.20706100	2.33637400	H	2.88471800	-1.83969200	-0.04008900
H	-5.63795400	-4.69705900	4.49067900	C	-1.06920100	-1.04024500	-2.38945600
H	-5.88729300	-5.63899700	3.01430800	O	-1.00676500	-1.41806100	-1.00517300
H	-4.86765200	-3.94281600	1.63991400	H	-1.61650400	-1.78696800	-2.97177700
H	-4.04024900	-3.53811500	3.16354900	H	-1.56059100	-0.06611400	-2.50339200
O	-2.11139900	0.78225000	4.12273000	H	-0.03821000	-0.98058600	-2.74788700
C	-2.42365100	-0.60597600	4.43066900	H	-7.72835000	2.09813300	2.54950000
C	-2.55689700	-0.68400700	5.95359500	H	-7.93737100	0.43096200	3.04948400
C	-3.01010000	0.73709400	6.31728700	H	-4.72622400	2.76387600	4.51752300
C	-2.20822900	1.57745100	5.32643000	H	-6.04380400	3.43480100	3.59073500
H	-1.19655200	1.77582100	5.70652900	H	-6.49511700	1.27395000	4.65579700
H	-2.68458200	2.52426600	5.06537600	H	-5.35500900	0.46101200	3.59836300
H	-2.80332600	1.00865200	7.35728800	C	-1.62803100	-2.65480800	1.50394200
H	-4.08325500	0.86065300	6.13467200	H	-1.64195300	-3.52115100	0.86493000
H	-1.58642800	-0.90792500	6.41164800	H	-0.77116000	-2.00466300	1.50827000
H	-3.26119100	-1.46062800	6.26529800	H	-2.53658700	-2.34153200	1.98596500
H	-3.36541100	-0.85787500	3.92981200	Cl	-0.91275000	-3.81426800	3.28133600



### TS XIII

G = -3381.900631

G<sub>MP2</sub> = -3371.584664

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.00000000	0.00000000	0.00000000	H	-4.29867300	7.45474600	0.14822600
O	-1.78634400	0.73126300	0.29608200	C	-5.41684200	3.44589100	1.94380700
Li	-2.72822000	2.46039800	0.90248600	C	-6.15123700	2.16185900	2.36799100
N	-4.59169500	3.37232800	0.73797900	C	-7.30596600	1.70666100	1.45240100
C	-4.24897100	4.72509600	0.34750500	N	-6.82298300	0.97144800	0.29552300
C	-3.14203200	4.69931400	-0.72648800	Li	-5.20739900	1.85715700	-0.47624400
N	-1.82363500	4.23645900	-0.22526900	N	-6.14122900	1.41299000	-2.55719800
C	-0.96904600	3.88925600	-1.38089900	C	-5.19184100	0.73320200	-3.46641100
H	-1.45687800	3.07811500	-1.93082100	C	-4.12262700	1.68866300	-3.99626600
H	-0.89858500	4.75354100	-2.06968900	C	-4.76465000	2.86853800	-4.73411500
C	0.44047000	3.46516900	-0.96405100	H	-5.24909200	2.50049600	-5.65043000
H	1.02578700	3.25695400	-1.86732600	H	-4.00288300	3.59199500	-5.05051200
H	0.37781100	2.53177600	-0.39090200	C	-5.81055800	3.54107800	-3.83643300
C	1.12296500	4.53845700	-0.10846300	C	-6.80538300	2.52014100	-3.27866500
C	0.20977100	4.91445700	1.06250200	H	-7.50155200	3.01238000	-2.59418000
C	-1.17831100	5.31145100	0.55684200	H	-7.40702100	2.10597100	-4.11209700
H	-1.82763900	5.56943200	1.39656300	H	-5.31650300	4.05316300	-3.00231300
H	-1.08625200	6.22325300	-0.06637200	H	-6.36741500	4.30889100	-4.38845600
H	0.63259200	5.74717900	1.63917700	H	-3.43082000	1.13504100	-4.64102300
H	0.11227900	4.06020400	1.74549400	H	-3.53253800	2.06280300	-3.14690800
H	1.31386700	5.43119900	-0.72104200	H	-4.72428800	-0.08392500	-2.91034900
H	2.10007200	4.18865900	0.25017800	H	-5.73385500	0.28092400	-4.31980300
H	-3.02936600	5.68908800	-1.20090600	C	-7.15133800	0.44721200	-2.06606800
H	-3.45965200	4.00235700	-1.51080100	H	-7.91242400	0.25908000	-2.84416200
H	-3.84686800	5.30039100	1.21557400	H	-6.63486700	-0.50437600	-1.89714800
C	-5.39728600	5.62750500	-0.17279100	C	-7.82625100	0.86798600	-0.74198700
C	-5.23081200	7.01968600	-0.21151600	H	-8.31388100	1.85259900	-0.91521700
C	-6.23473800	7.85849400	-0.69524300	C	-8.98623700	-0.09619900	-0.43017800
C	-7.44285600	7.31644300	-1.14060600	C	-10.2966310	0.37491800	-0.28784900
C	-7.62964000	5.93465100	-1.09191900	C	-11.3518800	-0.48815100	0.02108300
C	-6.61522200	5.10120200	-0.61279600	C	-11.1149080	-1.85246700	0.18640500
H	-6.76486600	4.02743200	-0.55601500	C	-9.81283300	-2.34212300	0.04642100
H	-8.57253300	5.50199500	-1.41916400	C	-8.76421300	-1.47092400	-0.25035200
H	-8.23199500	7.96560500	-1.51178900	H	-7.75445800	-1.86519000	-0.34360600
H	-6.07800200	8.93461900	-0.71842200	H	-9.61643300	-3.40584200	0.16386100

H	-11.9331420	-2.52856500	0.42147800	H	-1.94293900	0.47607000	3.56782300
H	-12.3589110	-0.09258400	0.13218100	O	1.36205200	-0.38609800	-1.44962800
H	-10.4914510	1.43781300	-0.41873400	C	1.86285100	-1.74165000	-1.55930900
Li	-5.50678300	-0.37512200	0.78359900	C	2.10953700	-1.96512100	-3.04835100
O	-3.92722700	0.18941800	-0.09632000	C	2.57111400	-0.57312200	-3.50598200
C	-2.69429200	-0.15170000	0.00085300	C	1.70688700	0.36140900	-2.65407400
C	-2.25313800	-1.50642000	-0.29531100	H	0.77802200	0.61621900	-3.17123300
C	-3.09673600	-2.69509200	-0.45380900	H	2.23044600	1.27326800	-2.34937200
C	-2.54901200	-3.99273300	-0.30558300	H	2.40256800	-0.40803600	-4.57299500
C	-3.31757300	-5.13972200	-0.49584300	H	3.63691700	-0.42560200	-3.29174000
C	-4.66148300	-5.05051600	-0.86287000	H	1.17829400	-2.22639200	-3.55972600
C	-5.21055500	-3.78227800	-1.06529500	H	2.85148000	-2.74845700	-3.23256700
C	-4.44983000	-2.63080200	-0.87005900	H	2.79725600	-1.82310700	-0.98291700
H	-4.88755000	-1.66420000	-1.08203800	H	1.11403100	-2.40309700	-1.11827900
H	-6.24182600	-3.68268600	-1.39701900	O	1.32191700	0.51567200	1.41616900
H	-5.25729100	-5.94566200	-1.01690700	C	0.99133300	0.99876500	2.73993700
H	-2.85300800	-6.11470300	-0.36586100	C	2.19143000	1.83778500	3.17427800
H	-1.49819500	-4.10004600	-0.06022100	C	3.35610200	1.07818100	2.52165100
O	-5.71250600	-1.55235600	2.33954300	C	2.74967200	0.63179600	1.18747200
C	-4.89726300	-2.66637800	2.78667100	H	3.12774400	-0.33280600	0.83970500
C	-5.68459800	-3.33877000	3.91776900	H	2.90991300	1.37354700	0.39721000
C	-7.13728200	-2.97500300	3.57276300	H	3.63193200	0.20888700	3.13014600
C	-6.98628800	-1.55512100	3.03564200	H	4.25201600	1.69048700	2.38374200
H	-6.94777500	-0.81667500	3.84710900	H	2.27893800	1.91256600	4.26240700
H	-7.75420300	-1.25908600	2.31976900	H	2.11578000	2.85223200	2.76616400
H	-7.81233500	-3.02713500	4.43220000	H	0.05283100	1.55267100	2.67117500
H	-7.52631900	-3.63731900	2.79076800	H	0.85413500	0.13555300	3.40685600
H	-5.40900500	-2.91173100	4.88951100	C	-0.90849600	-2.06430000	1.61915100
H	-5.50495700	-4.41707600	3.95920000	O	-0.93329100	-1.77220800	0.21409100
H	-4.74030900	-3.33458500	1.93536400	H	-1.26151200	-1.20159800	2.19682700
H	-3.92671700	-2.27596900	3.11032000	H	-1.53225800	-2.93369100	1.84695700
O	-2.14486900	2.45162900	3.00540500	H	0.13095600	-2.28245800	1.88328100
C	-2.57274100	1.33405300	3.81814900	H	-7.87252100	2.61511500	1.15316900
C	-2.43524900	1.79863300	5.26822800	H	-8.02864700	1.12811600	2.06967200
C	-2.76522800	3.29380900	5.14907800	H	-4.81433000	3.78193500	2.82221100
C	-2.12909000	3.65976100	3.80557900	H	-6.20101800	4.22116000	1.85446700
H	-1.08549200	3.97923400	3.92449800	H	-6.55739900	2.34632200	3.37460800
H	-2.68068400	4.43365500	3.26733500	H	-5.43198100	1.33420700	2.48279000
H	-2.37053100	3.89432300	5.97411100	C	-1.73444700	-1.14012400	-2.47075400
H	-3.84972600	3.44085000	5.10463300	H	-1.37657800	-0.15728700	-2.21844600
H	-1.40686600	1.65750800	5.62344800	H	-1.09883400	-2.00094200	-2.35672100
H	-3.10565300	1.25951500	5.94422400	H	-2.76588700	-1.28006500	-2.74396300
H	-3.61212300	1.09226100	3.57014400	Cl	-1.10490100	-0.85314800	-4.63850100

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