SUPPORTING INFORMATION

Functionalization of *N*-[(Silyl)methyl]-β-lactam Carbanions with Carbon Electrophiles.

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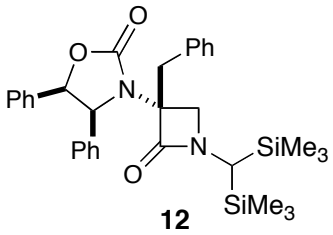
General

All reactions were carried out under an atmosphere of nitrogen in oven or flame-dried glassware with magnetic stirring. Solvents were distilled prior to use. Tetrahydrofuran (THF) was distilled from sodium metal/benzophenone ketyl. Dichloromethane (CH_2Cl_2) was distilled from calcium hydride. Purification of reaction products was carried out by flash chromatography using silicagel 60 (230-400 mesh). Analytical thin layer chromatography was performed on 0.25 mm silica gel 60-F plates. Visualization was accomplished with UV light and phosphomolybdic acid-ammonium cerium (IV) nitrate sulfuric acid-water reagent, followed by heating. Melting points are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded at 500 MHz and 75 MHz respectively and are reported as δ values (ppm) relative to residual $CHCl_3$ δH (7.26 ppm) and $CDCl_3$ δC (77.16 ppm) as internal standards, respectively. Mass spectra were either under EI (70 eV) or CI conditions after direct injection (HRMS) or using GC-MS coupling (column: fused silica gel, 15 m, 0.25mm, 0.25 nm phase SPB-5).

Preparation Details and Physical and Spectroscopic Data of Compounds 12, 16-36:

Preparation and physical data of compounds **10**,[8(b)] **11**,[9(a)] **13**,[8(a)] **14**,[8(a)] and **15**,[9(b)] was previously described.



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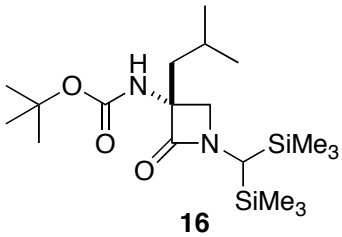
(3*R*)-3-Benzyl-1-[bis(trimethylsilyl)-methyl]-3[(4*S*,5*R*)-4,5-diphenyl-2-oxo-oxazolidin-3-yl]azetidin-2-one (**12**): This compound was prepared in 74% yield from **9** (R= Ph; R^2= H) and benzyl bromide, following the reported protocol for α-alkylation.[8(a)] M.p: 204-6ºC; $[\alpha]_D^{25}$ = + 0.99 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1734.2; 1699.5 (C=O); 845.7 (C-Si); MS m/z (Ion Source Type: ESI, positive polarity): MS +1: 557.3; MS2(557.0): 513.2,188.1; MS3(511.1): 406.4, 354.3, 262.1, 188.0. ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.52-7.38 (m, 5H); 7.23-7.08 (m, 5H); 5.91 (d, 1H, *J* = 7.3 Hz); 5.44 (d, 1H, *J* = 7.3 Hz); 3.58 (d, 1H, *J* = 6.2 Hz); 3.48 (d, 1H, *J* = 6.8 Hz); 2.96 (d, 1H, *J* = 13.7 Hz); 2.56 (s, 1H); 2.37 (d, 1H, *J* = 13.7 Hz); 0.02 (s, 9H); -0.16 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 164.3; 156.7; 135.5; 134.9; 133.8; 130.7; 128.7; 128.2; 127.9; 127.6; 127.0; 125.7; 81.2; 72.3; 65.3; 52.4; 37.4; 37.3; -0.45; -0.64. Anal. Calcd. for $C_{32}H_{40}N_2O_3Si_2$: C, 69.02; H, 7.24; N, 5.03. Found: C, 68.74; H, 7.23; N, 5.10.



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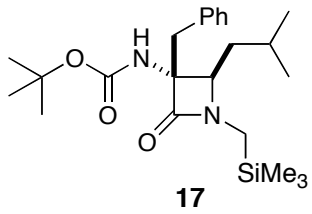
(3*R*)-1-[Bis(trimethylsilyl)-methyl]-3-*tert*-butoxycarbonylamino-3-isobutylazetidin-2-one (**16**): This compound was prepared in 64% overall yield from **11** following the reported phenyloxazolidinone deprotection and Boc-protection protocol.[8(a)] M.p: 67ºC; $[\alpha]_D^{25}$ = –

26.1 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 3260.0 (NH); 1733.5; 1701.2 (C=O); MS m/z (int): 329 (37), 188 (26), 172 (30), 157 (50), 101 (100), 73 (47), 57 (64). ^{1}H-NMR (δ, ppm, $CDCl_3$): 5.13 (s, 1H); 3.67 (d, 1H, *J* = 5.2 Hz); 3.29 (d, 1H, *J* = 5.5 Hz); 2.69 (s, 1H); 1.95-1.52 (m, 3H); 1.43 (s, 9H); 0.99 (d, 3H, *J* = 5.1 Hz); 0.96 (d, 3H, *J* = 4.9 Hz); 0.13 (s, 9H); 0.12 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 167.8; 154.3; 79.6; 67.2; 56.2; 36.6;28.2; 24.4; 24.1; 23.4; -0.30. Anal. Calcd. for $C_{19}H_{40}N_2O_3Si_2$: C, 56.95; H, 10.06; N, 6.99. Found: C, 57.11; H, 9.94; N, 7.05.



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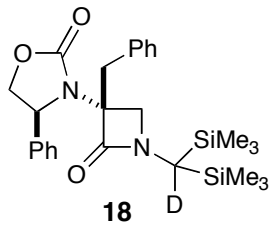
(3*R*,4*R*)-3-Benzyl-4-isobutyl-3-(*tert*-butoxycarbonylamino)-1-(trimethylsilylmethyl)azetidin-2-one (**17**): This compound was prepared in 70% overall yield from (3*R*,4*R*)-3-benzyl-1-[bis(trimethylsilyl)methyl]-3-*tert*butoxycarbonylamino-4-isobutyl azetidin-2-one,[9(a)] following the described CsF-mediated monodesilylation procedure.[8(a)] M.p.: Oil; $[\alpha]_D^{25}$ = +27.6 (c= 0.5, Cl_2CH_2); IR(cm^{-1}, KBr): 1748.2 (CO), 1699.0 (CO), 853 (C-Si); MS m/z (int): 348 (11), 289 (11), 233 (52), 232 (13), 177 (100), 173 (53), 146 (42), 129 (47), 91 (12); ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.32-7.24 (m, 5H); 4.93 (bs, 1H); 3.78 (t, 1H, *J* = 6.3 Hz); 3.33 (d, 1H, *J* = 13.3 Hz); 3.17 (d, 1H, *J* = 13.6 Hz); 2.78 (d, 1H, *J* = 15.9 Hz); 2.51 (d, 1H, *J* = 15.9 Hz), 2.00 (m, 1H); 1.68 (m, 1H); 1.54 (m, 1H); 1.42 (s, 9H); 1.03 (t, 6H), 0.16 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 167.8, 154.7; 135.8; 130.8; 130.3; 128.5; 127.9; 127.1; 126.5; 79.7; 68.2; 64.2; 45.1; 38.4; 35.3; 32.4; 29.8; 25.8; 22.8; –1.1. HRMS (*m/z*) 418.2637; $C_{23}H_{38}N_2O_3Si$ requires 418.2653.



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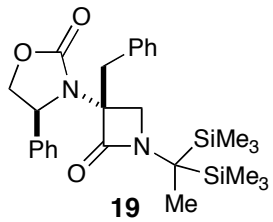
(3*R*)-3-Benzyl-1-[bis(trimethylsilyl)-deutero-methyl]-3-[(4*S*)-4-phenyl-2-oxo-oxazolidin-3-yl]azetidin-2-one (**18**): The general procedure was followed at a 0.5 scale from **10** (0.5 mmol, 247 mg), sBuLi (0.65 mmol. 0.5 mL) and MeOD (5.0 mmol, 0.2 mL). The reaction mixture was warmed overnight from –78ºC to 20ºC. Eluent: EtOAc/hexanes 1:10. Yield: 197 mg (82%). M.p.: 154-7ºC (CH_2Cl_2-hexanes); $[\alpha]_D^{25}$ = +20.5 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1737 (CO), 1730 (CO), 846 (C-Si); MS m/z (int): 279 (17), 172 (3), 104 (23), 91 (22), 73 (100); ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.70-7.17 (m, 10H); 5.18 (dd, 1H, *J* = 8.1 and 1.8 Hz); 4.64 (t, 1H, *J* = 8.5 Hz); 4.43 (dd, 1H, *J* =8.7 and 1.9 Hz); 3.52 (d, 1H, *J* = 6.4 Hz); 3.44 (d, 1H); 2.85 (d, 1H, *J* = 13.7 Hz); 2.52 (s, 1H); 2.24 (d, 1H, *J* = 13.7 Hz); 0.00 (s, 9H); – 0.12 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 164.1, 156.7; 140.2; 134.8; 130.5; 129.0; 128.4; 127.7; 126.9; 72.3; 71.1; 59.6; 52.1; 37.3; – 0.6; –0.8. Anal. Calcd. for $C_{26}H_{35}DN_2O_3Si_2$: C, 64.82; H, 7.74; N, 5.81. Found: C, 64.89; H, 7.60; N, 5.91.



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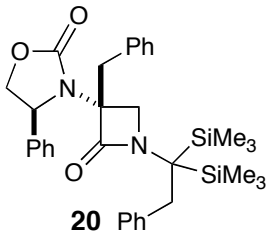
(3*R*) 3-Benzyl-1-[1,1-bis(trimethylsilyl)ethyl]-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**19**): The general procedure was followed at a 0.5 scale from **10** (0.5 mmol, 247 mg), sBuLi (0.65 mmol. 0.5 mL)/TMEDA (0.65 mmol, 98 μL) and methyl iodide (1.5 mmol, 94

μL). Eluent: EtOAc/hexanes 1:5. Yield: 126 mg (51%). M.p.: 170-1ºC (CH_2Cl_2-hexanes); $[\alpha]_D^{25}$ = +36.5 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1762.5; 1734.8 (C=O); MS m/z (int): 73 (100); 91 (27); 104 (24); 114 (24); 115 (29); 193 (37); 279 (47); 352 (25); 393 (88); 394 (30); 421 (21); 480 (20). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.66-7.63 (m, 2H); 7.44-7.35 (m, 3H); 7.20-7.15 (m, 3H); 7.09-7.06 (m, 2H); 5.19 (dd, 1H, *J* = 1.6 and 8.0 Hz); 4.63 (t, 1H, *J* = 8.3 Hz); 4.44 (dd, 1H, *J* = 1.6 and 8.6 Hz); 3.55 (d, 1H, *J* = 6.6 Hz); 3.39 (d, 1H, *J* = 6.7 Hz); 2.80 (d, 1H, *J* = 13.6 Hz); 2.23 (d, 1H, *J* = 13.6 Hz); 1.15 (s, 3H); 0.05 (s, 9H); –0.12 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 164.0; 156.8; 140.3; 134.9; 130.7; 129.1; 128.5; 127.8; 126.9; 71.3; 68.2; 59.7; 49.7; 40.4; 37.4; –1.2; –1.5. Anal. Calcd. for $C_{27}H_{38}N_2O_3Si_2$: C, 65.54; H, 7.74; N, 5.66. Found: C, 65.82; H, 7.91; N, 5.78.



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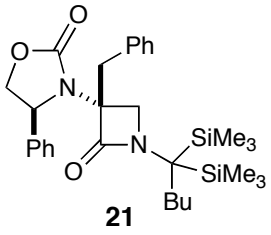
(3*R*)-3-Benzyl-1-[1,1-bis(trimethylsilyl)-2-phenylethyl]-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**20**): The general procedure was followed at a 0.25 mmol scale from **10** (0.25 mmol, 120 mg) nBuLi (0.30 mmol, 0.12 mL)/TMEDA (0.30 mmol, 45 μL) and benzyl bromide (0.50 mmol, 61 μL). The reaction mixture was warmed overnight from –100ºC to 20ºC. Eluent: EtOAc/hexanes 1:5. Yield: 100 mg (70%). M.p.: 173-5ºC (CH_2Cl_2-hexanes); $[\alpha]_D^{25}$ = +13.0 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1761.3; 1736.0 (C=O); MS m/z (int): 465(15.3), 352(13.1), 280(22.5), 279(100), 234(16.3), 220(22.4), 158(16.7), 144(54.2,) 117(20.9), 104(41.4). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.66 (d, 2H, *J* = 7.3 Hz); 7.44-7.35 (m, 3H); 7.26-7.25 (m, 3H); 7.14-7.08 (m, 5H); 6.82 (d, 2H, *J* = 6.8 Hz); 5.26 (d, 1H, *J* = 6.8 Hz); 4.72 (t, 1H, *J* = 8.3 Hz); 4.51 (d, 1H, *J* = 7.8 Hz); 3.87 (d, 1H, *J* = 6.8 Hz); 3.62 (d, 1H, *J* = 6.8 Hz); 3.12 (d, 1H, *J* = 15.6 Hz); 2.94 (d, 1H, *J* = 15.6 Hz); 2.85 (d, 1H, *J* = 13.7 Hz); 2.35 (d, 1H, *J* = 13.7 Hz); 0.05 (s, 9H); –0.06 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 165.0; 156.7; 140.2; 139.4; 134.8; 130.9; 129.8; 129.1; 128.7; 128.1; 127.9; 127.2; 126.4: 71.2; 69.3; 59.8; 50.7; 47.5; 37.6; 36.8; 0.9; 0.6. Anal. Calcd. for $C_{33}H_{42}N_2O_3Si_2$: C, 69.43; H, 7.42; N, 4.91. Found: C, 69.86; H, 7.59; N, 5.10.



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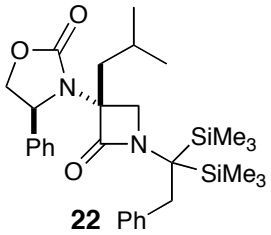
(3*R*)-3-Benzyl-1-[1,1-bis(trimethylsilyl)-2-n-butyl]-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**21**): The general procedure was followed at a 0.5 mmol scale from **10** (0.5 mmol, 240 mg) nBuLi (0.60 mmol, 0.24 mL)/TMEDA (0.60 mmol, 90 μL) and n-butyl iodide (1.50 mmol, 170 μL). The reaction mixture was warmed overnight from –100ºC to 20ºC. Eluent: EtOAc/hexanes 1:5. Yield: 107 mg (40%). M.p.: 123-4ºC (CH_2Cl_2); $[\alpha]_D^{25}$ = +6.4 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1753; 1726 (C=O); 845(C-Si). MS m/z (int): 435(28), 156(18), 91(12), 73(100), 69(11). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.67 (d, 2H, *J* = 8.4 Hz); 7.43 (m, 2H); 7.37 (m, 1H); 7.22-7.15 (m, 3H); 7.08 (d, 2H, *J* = 6.8 Hz); 5.23 (d, 1H, *J* = 8.9 Hz); 4.64 (t, 1H, *J* = 8.3 Hz); 4.46 (dd, 1H, J_1 = 8.6 Hz, J_2=1.5 Hz); 3.53 (d, 1H, *J* = 6.7 Hz); 3.37 (d, 1H, *J* = 6.7 Hz); 2.79 (d, 1H, *J* = 13.6 Hz); 2.24 (d, 1H, *J* = 13.6 Hz); 1.47 2.35 (m, 2H); 1.05 (m, 2H); 0.82 (m, 1H); 0.77 (m, 3H); 0.107 (s, 9H); 0.09 (s, 9H) . ^{13}C-NMR (δ, ppm,

$CDCl_3$): 164.2; 156.7; 140.3; 134.8; 130.6; 129.0; 128.4; 127.7; 126.8; 71.2; 68.2; 59.5; 45.2; 31.1; 28.3; 23.1; 13.6; 1.0; -0.2. HRMS (*m/z*) 536.2897; $C_{30}H_{44}N_2O_3Si_2$ requires 536.2891.



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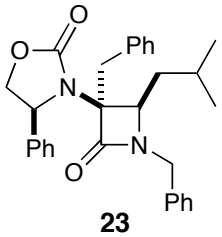
(3*R*)-1-[1,1-Bis(trimethylsilyl)-2-phenylethyl]-3-isobutyl-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**22**): The general procedure was followed at a 0.25 mmol scale from **11** (0.25 mmol, 111 mg), nBuLi (0.30 mmol, 0.12 mL)/TMEDA (0.30 mmol, 45 μL) and benzyl bromide (0.50 mmol, 61 μL). The reaction mixture was warmed overnight from –100ºC to 20ºC. Eluent: EtOAc/hexanes 1:5. Yield: 103 mg (77%). M.p.: 76-78ºC (CH_2Cl_2-hexanes); $[\alpha]_D^{25}$ = –32.9 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1743.4 (C=O); MS m/z (int): 407(12), 321(28), 320(100), 244(8), 218(7), 115(9), 75(13), 73(14). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.65-7.62 (m, 2H); 7.46-7.39 (m, 3H); 7.30-7.25 (m, 5H); 5.33 (dd, 1H, *J* = 2.0 and 8.4 Hz); 4.72 (t, 1H, *J* = 8.6 Hz); 4.49 (dd, 1H, *J* = 2.1 and 8.7 Hz); 4.18 (d, 1H, *J* = 6.9 Hz); 3.64 (d, 1H, *J* = 7.0 Hz); 3.28 (d, 1H, *J* = 15.1 Hz); 3.16 (d, 1H, *J* = 15.0 Hz); 1.63-1.57 (m, 1H); 1.39-1.33 (m, 1H); 1.29-1.08 (m, 1H); 0.97 (d, 3H, *J* = 6.4 Hz); 0.48 (d, 3H, *J* = 6.7 Hz); 0.17 (s, 9H); 0.14 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 167.0; 157.1; 140.6; 139.6; 129.8; 129.0; 128.9; 128.1; 127.7; 126.7; 71.1; 68.1; 59.4; 53.3; 47.1; 42.0; 36.3; 24.0; 23.0; 1.0; 0.9. Anal. Calcd. for $C_{30}H_{44}N_2O_3Si_2$: C, 67.12; H, 8.26; N, 5.22. Found: C, 67.52; H, 8.69; N, 5.22.



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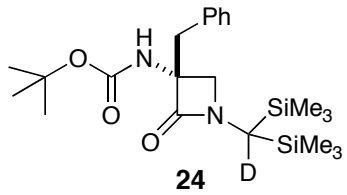
(3*S*)-1,3-Dibenzyl-4-isobutyl-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**23**): The general procedure was followed at a 0.25 scale from **14** (0.25 mmol, 116 mg), nBuLi (0.30 mmol, 0.12 mL)/TMEDA (0.30 mmol, 45 μL) and benzyl bromide (0.50 mmol, 61 μL). The reaction mixture was warmed overnight from –100ºC to 20ºC. Eluent: EtOAc/hexanes 1:5. Yield: 58 mg (50%). MS m/z (int): 468.2(2), 335.2(2), 294.1(6), 293.1(42), 174.1(2), 149.0(3), 130.1(10), 129.1(6), 105.1(10), 104.1(100), 103.1(12), 97.1(11), 91.1(67), 83.1(11), 71.1(12), 57.1(20), 55.1(16). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.49 (d, 2H, *J* = 7.0 Hz); 7.38-7.22 (m, 7H); 7.19-7.13 (m, 4H); 6.65 (d, 2H, *J* = 7.0 Hz); 4.78 (dd, 1H, *J* = 3.0 and 9.0 Hz); 4.21-4.13 (m, 3H); 3.96 (d, 1H, *J* = 15.5 Hz); 3.71 (d, 1H, *J* = 13.5 Hz); 3.48 (dd, 1H, *J* = 3.0 and 9.0 Hz); 3.32 (d, 1H, *J* = 13.5 Hz); 1.50 (ddd, 1H, *J* = 3.0, 12.5 and 14.0 Hz); 1.26 (m, 1H); 0.82 (m, 1H); 0.67 (d, 3H, *J* = 6.5 Hz); 0.53 (d, 3H, *J* = 6.5 Hz). HRMS (*m/z*) 468.2425; $C_{30}H_{32}N_2O_3$ requires 468.2413.



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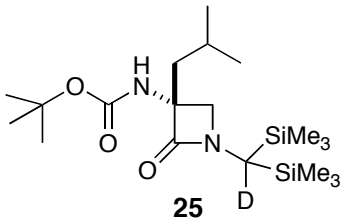
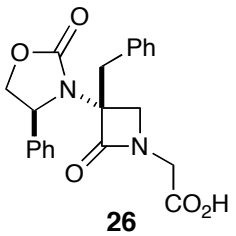
(3*R*)-3-Benzyl-1-[bis(trimethylsilyl)-deutero-methyl]-3-(*tert*-butoxycarbonylamino)azetidin-2-one (**24**): The general procedure was followed at a 0.5 mmol scale from **15** (0.5 mmol, 247 mg), sBuLi (0.65 mmol, 0.5 mL) and MeOD (5.0 mmol, 0.2 mL). The reaction mixture was warmed overnight from –78ºC to

20ºC. Eluent: EtOAc/hexanes 1:10. Yield: 197 mg (82%). Oil; $[\alpha]_D^{25}$ = + 30.7 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 3290, 2951 (NH), 1733, 1700, (CO), 846 (C-Si); MS m/z (int): 365(16), 347 (18), 283 (26), 234 (18), 208 (21), 177 (100), 92 (40), 73 (33). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.30-7.24 (m, 5H); 5.38 (s, 1H); 3.54 (d, 1H, *J* = 5.4 Hz); 3.40 (d, 1H, *J* = 5.3 Hz); 3.27 (s, 2H); 1.48 (s, 9H); 0.06 (s, 9H); –0.08 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 167.1; 154.6; 135.5; 130.4; 129.2; 126.6; 78.4; 68.3; 54.0; 39.2; 37.3; 28.5; – 0.3; – 0.6. Anal. Calcd. for $C_{22}H_{37}DN_2O_3Si_2$: C, 60.64; H, 9.02; N, 6.43. Found: C, 60.83; H, 8.84; N, 6.05.



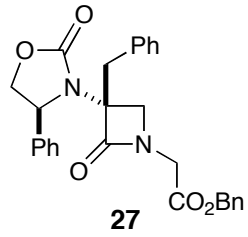
25

(3*R*)-1-[Bis(trimethylsilyl)-deutero-methyl]-3-(*tert*-butoxy carbonylamino)-3-isobutylazetidin-2-one (**25**): The general procedure was followed at a 0.5 scale from **16** (0.5 mmol, 247 mg), 1.3M sBuLi (0.65 mmol, 0.5 mL in cyclohexane) and MeOD (5.0 mmol, 0.2 mL). The reaction mixture was warmed overnight from –78ºC to 20ºC. Eluent: EtOAc/hexanes 1:10. Yield: 197 mg (67%). M.p: 63ºC; $[\alpha]_D^{25}$ = –27.8 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 3260.0 (NH); 1733.5; 1701.2 (CO); MS m/z (int): 330 (29), 189 (28), 172 (30), 158 (64), 101 (100), 73 (55), 57 (40). ^{1}H-NMR (δ, ppm, $CDCl_3$): 5.13 (s, 1H); 3.67 (d, 1H, *J* = 5.2 Hz); 3.29 (d, 1H, *J* = 5.5 Hz); 1.95-1.52 (m, 3H); 1.43 (s, 9H); 0.99 (d, 3H, *J* = 5.1 Hz); 0.96 (d, 3H, *J* = 4.9 Hz); 0.13 (s, 9H); 0.12 (s, 9H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 167.8; 154.5; 79.4; 67.2; 56.1; 42.6; 36.7; 28.2; 24.5; 24.3; 23.2; –0.3. Anal. Calcd. for $C_{19}H_{39}DN_2O_3\ Si_2$: C, 56.81; H, 10.29; N, 6.97. Found: C, 56.52; H, 11.03; N, 7.03.



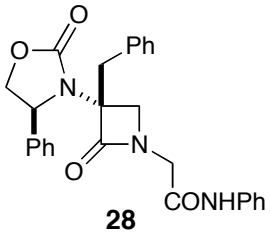
26

(3*R*)-3-Benzyl-1-(carboxymethyl)-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**26**): To a solution of **10** (1.0 mmol, 0.48 g) in THF (8 mL) cooled to –78ºC under nitrogen was added 1.3M sBuLi (1.2 mmol, 0.92 mL in cyclohexane) and the mixture was stirred at –78ºC for 30min. Then, CO_2 gas was collected in a balloon, dried through a molecular sieves tube and bubbled into the carbanion solution until color vanishment. The cooling bath was removed and the reaction mixture was allowed to warm to 0ºC, while the excess of carbon dioxide was vented. After work-up, the product was purified by column chromatography (eluent: EtOAc/hexanes 1:5). Yield: 220 mg (58%). Oil; $[\alpha]_D^{25}$ = +27.2 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): $3500\text{-}2900_{(broad)}$ (OH); 1749.9; 1770.8 (CO); MS m/z (int): 307 (12), 279 (100), 235 (14), 220 (29), 194 (12), 144 (74), 117 (21), 115 (24), 104 (58), 103 (24), 91 (27). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.52-7.38 (m, 5H); 7.23-7.07 (m, 3H); 7.08-7.06 (m, 2H); 5.09 (dd, 1H, *J* = 2.4 and 8.3 Hz); 4.71 (t, 1H, *J* = 8.6 Hz); 4.36 (dd, 1H, *J* = 2.4 and 8.8 Hz); 3.96 (d, 1H, *J* = 18.1 Hz); 3.73 (d, 1H, *J* = 5.9 Hz); 3.44 (d, 1H, *J* = 18.1 Hz); 3.32 (d, 1H, *J* = 6.4 Hz); 2.97 (d, 1H, *J* = 13.7 Hz); 2.63 (d, 1H, *J* = 13.2 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 170.1; 165.7; 157.0; 139.9; 134.1; 130.0; 129.1; 129.0; 128.2; 127.1; 71.5; 71.2; 59.5; 51.0; 42.4; 37.7. Anal. Calcd. for $C_{21}H_{20}N_2O_5$: C, 66.31; H, 5.30; N, 7.36. Found: C, 66.26; H, 5.36; N, 7.31.



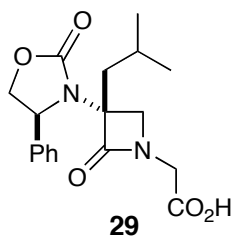
27

(3*R*)-3-Benzyl-1-(benzyloxycarbonylmethyl)-3-[(4*S*)-4-phenyl-2-oxo-oxazolidin-3-yl]-azetidin-2-one (**27**): To a solution of **10** (1.0 mmol, 0.48 g) in THF (8 mL) cooled to –78ºC under nitrogen was added 1.3M sBuLi (1.2 mmol, 0.92 mL in cyclohexane) and the mixture was stirred at –78ºC for 30min. Benzyl chloroformate (2 mmol, 0.29 mL) was added and, after stirring for 30 min at the same temperature, the cooling bath was removed and the reaction mixture was allowed to warm to 0ºC. After the work-up, the crude was purified by column chromatography (silicagel-60, eluent: EtOAc/hexanes 1:1). Yield: 211 mg (45%). Oil; $[\alpha]_D^{25}$ = +30.9 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1815; 1769; 1747 (C=O); MS m/z (int): 465(17.6), 280(22.4), 279(100), 234(16.3), 220(24.5), 158(14.6), 144(42.7), 104(31.7), 73(36.3). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.54-7.44 (m, 2H); 7.44-7.31 (m, 8H); 7.30-7.21 (m, 3H); 7.20-7.08 (m, 2H); 5.12 (d, 1H); 5.08 (d, 1H); 5.04 (dd, 1H); 4.60 (t, 1H); 4.30 (dd, 1H, *J* = 2.4 and 8.4 Hz); 3.98 (d, 1H, *J* = 18.1 Hz); 3.73 (d, 1H, *J* = 5.9 Hz); 3.43 (d, 1H, *J* = 18.1 Hz); 3.36 (d, 1H, *J* = 6.3 Hz); 2.98 (d, 1H, *J* = 13.7 Hz); 2.52 (d, 1H, *J* = 13.7 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 167.2; 165.2; 156.6; 140.1; 134.8; 130.1; 129.1; 128.7; 128.6; 128.4; 128.3; 128.2; 127.4; 127.0; 126.5; 72.1; 71.1; 67.2; 59.7; 51.0; 42.4; 37.8. Anal. Calcd. for $C_{28}H_{26}N_2O_5$: C, 71.47; H, 5.57; N, 5.95. Found: C, 71.52; H, 5.50; N, 5.86.



28

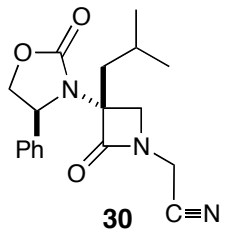
(3*R*)-3-Benzyl-1-[(*N*-phenylaminocarbonyl)methyl]-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**28**): The general procedure was followed from **10** (1.0 mmol, 0.48 g), 0.60M nBuLi/TMEDA solution (1.2 mmol, 2.00 mL), and phenyl isocyanate (2.0 mmol, 0.24 mL). Eluent: EtOAc/hexanes 1:1. Yield: 287 mg (63%). M.p.: 165-7ºC; $[\alpha]_D^{25}$ = +34.1 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1763; 1729; 1683 (C=O); MS m/z (int): 280(13), 279(100), 234(6), 220 (8), 158(5), 144(22), 104(19), 103(4); ^{1}H-NMR (δ, ppm, $CDCl_3$): 9.01 (s, 1H); 7.75 (d, 2H); 7.52-7.08 (m, 13H); 5.04 (dd, 1H, *J* = 2.7 and 8.6 Hz); 4.78 (t, 1H, *J* = 8.7 Hz); 4.29 (dd, 1H, *J* = 2.6 and 8.7 Hz); 4.18 (d, 1H, *J* = 17.6 Hz); 3.70 (d, 1H, *J* = 5.6 Hz); 3.26 (d, 1H, *J* = 13.3 Hz); 3.02-2.95 (3d, 3H). ^{13}C-NMR (δ, ppm, $CDCl_3$): 166.7; 165.2; 157.3; 139.9; 137.9; 132.7; 130.1; 129.9; 129.5; 128.8; 128.5; 127.8; 126.0; 124.4; 120.4; 71.1; 70.9; 58.9; 51.2; 45.5; 36.8. Anal. Calcd. for $C_{27}H_{25}N_3O_4$: C, 71.19; H, 5.53; N, 9.22. Found: C, 70.79; H, 5.53; N, 9.28.



29

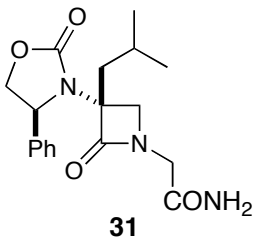
(3*R*)-1-(Carboxymethyl)-3-isobutyl-3-[(4*S*)-4-phenyl-2-oxo-oxazolidin-3-yl]-azetidin-2-one (**29**): The general procedure was followed at a 3 mmol scale from **11** (3.0 mmol, 1.34 g) and 0.60M nBuLi/TMEDA solution (3.6 mmol, 6.0 mL), using CO_2 gas as electrophile. Yield: 0.934 g (90%). Oil; $[\alpha]_D^{25}$ = –4.4 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 3400-3100 (broad, OH); 1741.3; 1739.5(CO); HPLC-MS (ESI): MS: 345.2; MS2(345.2): 162.0, 132.1; MS3(162.0): 132.0; ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.51-7.34 (m, 5H); 5.10 (dd, 1H, *J* = 8.6

and 2.5 Hz); 4.70 (t, 1H, *J* = 8.6 Hz); 4.37 (dd, 1H, *J* = 8.8 and 2.6 Hz); 4.10 (d, 1H, *J* = 18.2 Hz); 4.03 (d, 1H, *J* = 18.2 Hz); 3.95 (d, 1H, *J* = 6.3 Hz); 3.55 (d, 1H, *J* = 6.2 Hz); 1.68-1.60 (m, 1H); 1.45 (dd, 1H, *J* = 14.5 and 3.5 Hz); 1.25 (dd, 1H, *J* = 14.5 and 3.5 Hz); 0.90 (d, 3H, *J* = 6.6 Hz); 0.62 (d, 3H, *J* = 6.7 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 170.8; 167.1; 157.2; 140.1; 129.1; 127.4; 71.3; 71.0; 59.6; 52.9; 42.8; 41.4; 27.3; 24.2; 24.0; 23.0. Anal. Calcd. for $C_{18}H_{22}N_2O_5$: C, 62.42; H, 6.40; N, 8.09. Found: C, 62.24; H, 6.26; N, 7.55.



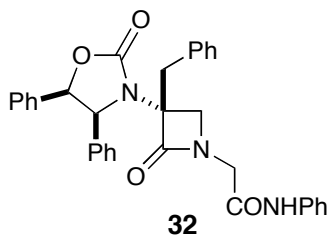
30

(3*R*)-1-Cyanomethyl-3-isobutyl-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**30**): The general procedure was followed at a 0.5 mmol scale from **11** (0.5 mmol, 0.22 g), 0.60M nBuLi/TMEDA solution (0.6 mmol, 1.00 mL) and trimethylsilyl isocyanate (1.0 mmol, 0.13 mL). After the addition of the isocyanate the reaction temperature was slowly raised to 0ºC and the mixture was stirred for 5h. Eluent: EtOAc/hexanes 1:2. Yield: 98 mg (60%). Oil; $[\alpha]_D^{25}$ = –10.6 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 3448; 2958; 2922; 2328; 1769; 1746; HPLC-MS (ESI): MS+1: 328.2; MS2(328.2): 300.1, 273.1; MS3(300.1): 273.1, 137.0; MS4(273.1): 242.2, 198.0, 110.1; ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.46- 7.41 (m, 5H); 5.00 (dd, 1H, *J* = 8.5 and 2.3 Hz); 4.71 (t, 1H); 4.38 (dd, 1H, J = 8.5 and 2.3 Hz); 4.31 (d, 1H, *J* = 17.8 Hz); 4.11 (d, 1H, *J* = 17.8 Hz); 3.91 (d, 1H, *J* = 6.1 Hz); 3.48 (d, 1H, *J* = 6.1 Hz); 1.62 (m, 1H); 1.45 (dd, 1H, *J* = 3.8 and 14.5 Hz); 1.26 (dd, 1H, *J* = 3.8 and 14.5 Hz); 0.92 (d, 3H, *J* = 6.5 Hz); 0.67 (d, 3H, *J* = 6.5 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 166.4; 156.7; 139.9; 129.3; 127.2; 113.3; 71.8; 70.9; 59.5; 52.6; 41.3; 31.9; 29.8; 24.2; 23.0. HRMS (*m/z*) 327.1576; $C_{18}H_{21}N_3O_3$ requires 327.1583.



31

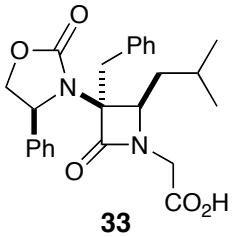
(3*R*)-1-[(Aminocarbonyl)methyl]-3-isobutyl-3-[(4*S*)-4-phenyl-2-oxo-oxazolidin-3-yl]-azetidin-2-one (31): The general procedure was followed at a 4 mmol scale from **11** (4 mmol, 1.79 g), 0.60M nBuLi/TMEDA solution (4.8 mmol, 8.00 mL) and trimethylsilyl isocyanate (12.0 mmol, 1.60 mL). After the addition of the isocyanate, the reaction mixture was stirred at –78ºC for 2h and quenched with saturated aqueous NH_4Cl solution at the same temperature. Eluent: EtOAc. Yield: 1.10 g (80%). For characterization data, see ref. 9(a)



32

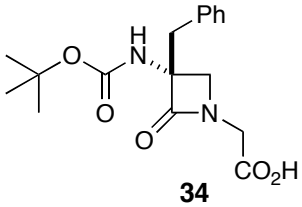
(3*R*)-3-Benzyl-1-[(*N*-phenylaminocarbonyl)methyl]-3-[(4*S*,5*R*)-4,5-diphenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**32**): The general procedure was followed from **12** (1.0 mmol, 0.557 g), 0.60M nBuLi/TMEDA solution (1.2 mmol, 2.08 mL) and phenyl isocyanate (2.0 mmol, 0.24 mL). Eluent: EtOAc/hexanes 1:1. Yield: 394 mg (74%). M.p.: 74-75ºC; $[\alpha]_D^{25}$ = –41.5 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 1767; 1731; 1683; HPLC-MS (ESI) m/z (int): MS:

530.4; MS2(530.4): 324.1, 291.1; MS3(291.1): 248.0, 172.0, 144.1, 115.1; MS4(172.0): 157.0. ^{1}H-NMR (δ, ppm, $CDCl_3$): 9.14 (s, 1H); 7.82-6.98 (m, 20 H); 6.04 (d, 1H, *J* = 7.5 Hz); 5.21 (d, 1H, *J* = 7.3 Hz); 4.21 (d, 1H, *J* = 17.7 Hz); 3.89 (d, 1H, *J* = 5.8 Hz); 3.35 (d, 1H, *J* = 13.2 Hz); 3.03 (d, 1H, *J* = 5.5 Hz); 2.98 (d, 1H, *J* = 17.6Hz); 2.94 (d, 1H, *J* = 13.4 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 166.9; 165.3; 157.2; 137.9; 135.1; 133.2; 132.6; 130.1; 128.0; 127.8; 127.2; 125.9; 124.4; 120.4; 80.9; 71.2; 64.4; 50.9; 45.4; 36.9. Anal. Calcd. for $C_{33}H_{29}N_3O_4$: C, 74.56; H, 5.50; N, 7.90. Found: C, 74.43; H, 5.61; N, 8.41.



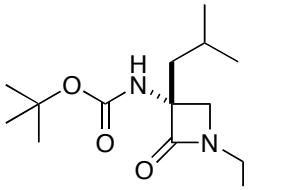
33

(3*S*,4*R*)-3-Benzyl-1-carboxylmethyl-4-isobutyl-3-[(4*S*)-4-phenyl-2-oxo-1,3-oxazolidin-3-yl]azetidin-2-one (**33**): The general procedure was followed from **14** (1.0 mmol, 0.45 g), TMEDA (1.2 mmol, 0.19 mL) and 1.5M tBuLi (1.2 mmol, 0.84 mL in pentane) at –78ºC, using CO_2 gas as electrophile. Yield: 353 mg (81%). Oil; $[\alpha]_D^{25}$ = +0.84 (c= 0.1, Cl_2CH_2); IR(cm^{-1}, KBr): 3500-2700 (broad, OH); 1749; 1738; 1718 (CO); MS m/z (int): 378(13.7), 294(13.1), 293(57.1), 130(16.2), 104(100), 91(13.9). ^{1}H-NMR (δ, ppm, $CDCl_3$): 7.47-7.30 (m, 10H); 4.50 (d, 1H, *J* = 6.8 Hz); 4.14 (dd, 1H, *J* = 2.7 and 8.5 Hz); 4.08 (d, 1H, *J* = 18.1 Hz); 4.00 (t, 1H, *J* = 8.5 Hz); 3.93 (d, 1H, *J* = 14.2 Hz); 3.84 (dd, 1H, *J* = 9.8 Hz); 3.45 (d, 1H, *J* = 18.1 Hz); 3.38 (d, 1H, *J* = 14.2 Hz); 1.63-1.58 (m, 1H); 1.40 (m, 1H); 0.96 (m, 1H); 0.89 (d, 3H, *J* = 6.4 Hz); 0.80 (d, 3H, *J* = 6.4 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 171.4; 166.1; 157.4; 140.3; 135.0; 130.8; 128.7; 128.6; 128.2; 127.9; 127.3; 72.3; 71.5; 62.6; 59.0; 41.8; 38.7; 38.1; 25.8; 23.7; 21.4. Anal. Calcd. for $C_{25}H_{28}N_2O_5$: C, 68.79; H, 6.47; N, 6.42. Found: C, 69.03; H, 6.39; N, 6.55.



34

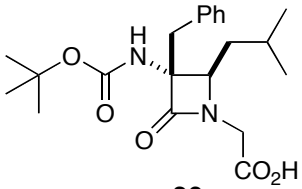
(*R*)-3-Benzyl-3-*tert*-butoxycarbonylamino-1-carboxymethyl azetidin-2-one (**34**): The general procedure was followed from **15** (1.0 mmol, 0.43 g) and 0.60M nBuLi/TMEDA solution (2.5 mmol, 4.17 mL) using CO_2 gas as electrophile. Yield: 214 mg (64%). For characterization data, see ref. 9(b)



35

(*R*)-3-*tert*-Butoxycarbonylamino-1-carboxymethyl-3-isobutyl-azetidin-2-one (**35**): The general procedure was followed from **16** (1.0 mmol, 0.40 g) and 0.60M nBuLi/TMEDA solution (2.5 mmol, 4.17 mL) using CO_2 gas as electrophile. Yield: 204 mg (68 %). Oil; $[\alpha]_D^{25}$ = + 18.9 (c= 1.0, Cl_2CH_2); IR(cm^{-1}, KBr): 3550-2910 (OH); 1765; 1743; 1716 (CO); MS m/z (int): 279.2(32), 167.0(78), 150.0(12), 149.9(24), 149.0(100), 113.1(13). ^{1}H-NMR (δ, ppm, $CDCl_3$): 5.06 (s, 1H); 4.07 (m, 2H); 3.78 (bs, 1H); 3.52 (bs, 1H); 1.88 (m, 2H); 1.75 (m, 1H); 1.44 (s, 9H); 1.00 (d, 3H, *J* = 5.0 Hz); 0.97 (d, 3H, *J* = 5.0 Hz). ^{13}C-NMR (δ, ppm, $CDCl_3$): 169.7; 154.8; 81.3; 68.3; 54.1; 50.7; 42.1; 28.2; 24.4; 24.1; 23.4;

–0.30. Anal. Calcd. for $C_{14}H_{24}N_2O_5$: C, 55.98; H, 8.05; N, 9.33. Found: C, 55.56; H, 7.89; N, 9.28.



36

(3*R*,4*R*)-3-Benzyl-3-*tert*-butoxycarbonylamino-1-carboxymethyl-4-isobutylazetidin-2-one (**36**): The general procedure was followed from **17** (1.0 mmol, 0.42 g), TMEDA (2.5 mmol, 0.38 mL) and 1.5M tBuLi (2.5 mmol, 1.67 mL in pentane) at –78ºC, using CO_2 gas as electrophile. Yield: 0.176 g (45%). For characterization data, see ref. 9(a)

COMPUTATIONAL DATA

Cartesian Coordinates and Total Energies of Structures 37-39:

Structure 37:

```
COMPND  Structure_37.PDB
HETATM    1  C                  -1.716   2.156  -1.021
HETATM    2  C                  -1.330   1.871  -2.514
HETATM    5  N                  -0.379   0.847  -2.000
HETATM    6  N                  -3.118   1.869  -0.681
HETATM    7  C                  -1.287   3.523  -0.485
HETATM    8  C                  -0.695   1.030  -0.712
HETATM    9  O                  -0.218   0.500   0.306
HETATM   10  C                   0.633  -0.037  -2.551
HETATM   14  C                   4.530   1.403   1.306
HETATM   15  C                   1.064  -3.805  -0.334
HETATM   23  C                   3.050   1.271   0.951
HETATM   24 Si                  -0.047  -1.513  -3.419
HETATM   25  O                   2.913  -0.049   0.372
HETATM   26 Si                   2.119   0.800  -3.245
HETATM   27  C                  -4.092   2.459  -1.469
HETATM   28  C                  -3.606   0.629  -0.072
HETATM   30  C                  -5.136   0.824  -0.265
HETATM   31  C                  -3.263   0.418   1.391
HETATM   32  O                  -3.950   3.386  -2.232
HETATM   33  O                  -5.284   1.820  -1.282
HETATM   36  C                  -2.817  -0.043   4.125
HETATM   37  C                  -3.110  -0.885   1.877
HETATM   38  C                  -3.198   1.488   2.290
HETATM   39  C                  -2.969   1.260   3.647
HETATM   40  C                  -2.892  -1.117   3.236
HETATM   46  C                  -0.104  -3.974   1.743
HETATM   49  C                   0.583  -2.612   1.665
HETATM   51  C                   4.210  -0.572   0.002
HETATM   52 Li                   1.214  -0.676  -0.427
HETATM   54  C                   0.745  -4.813   0.775
HETATM   62  C                   5.196   0.586   0.187
HETATM   66  O                   1.059  -2.505   0.303
HETATM    3  H                  -0.841   2.698  -3.037
HETATM    4  H                  -2.128   1.459  -3.137
HETATM   11  H                  -1.946   4.300  -0.880
HETATM   12  H                  -0.258   3.745  -0.788
HETATM   13  H                  -1.334   3.529   0.608
HETATM   19  H                   4.733   0.953   2.285
HETATM   50  H                   4.861   2.445   1.334
HETATM   47  H                   2.045  -3.962  -0.795
HETATM   56  H                   0.304  -3.805  -1.122
HETATM   18  H                   2.748   2.015   0.204
HETATM   22  H                   2.374   1.333   1.807
HETATM   20  H                   1.060  -2.461  -3.753
HETATM   64  H                  -1.024  -2.258  -2.551
HETATM   67  H                  -0.806  -1.314  -4.704
HETATM   55  H                   1.981   1.602  -4.510
HETATM   58  H                   2.710   1.781  -2.273
HETATM   61  H                   3.174  -0.221  -3.539
HETATM   29  H                  -3.259  -0.242  -0.648
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HETATM   34  H                    -5.602   1.190   0.656
HETATM   35  H                    -5.642  -0.088  -0.588
HETATM   45  H                    -2.643  -0.220   5.183
HETATM   41  H                    -3.160  -1.724   1.186
HETATM   42  H                    -3.320   2.503   1.921
HETATM   43  H                    -2.911   2.102   4.332
HETATM   44  H                    -2.780  -2.135   3.600
HETATM   57  H                    -0.125  -4.376   2.760
HETATM   59  H                    -1.137  -3.900   1.381
HETATM   16  H                     1.443  -2.556   2.346
HETATM   53  H                    -0.079  -1.764   1.855
HETATM   17  H                     4.443  -1.416   0.663
HETATM   21  H                     4.157  -0.933  -1.030
HETATM   48  H                     1.664  -5.149   1.269
HETATM   60  H                     0.225  -5.697   0.394
HETATM   63  H                     5.258   1.180  -0.731
HETATM   65  H                     6.202   0.239   0.440
CONECT    1    2    6    7    8
CONECT    2    1    5    3    4
CONECT    5    2    8   10
CONECT    6    1   27   28
CONECT    7    1   11   12   13
CONECT    8    1    5    9
CONECT    9    8   52
CONECT   10    5   24   26
CONECT   14   23   62   19   50
CONECT   15   54   66   47   56
CONECT   23   14   25   18   22
CONECT   24   10   20   64   67
CONECT   25   23   51   52
CONECT   26   10   55   58   61
CONECT   27    6   32   33
CONECT   28    6   30   31   29
CONECT   30   28   33   34   35
CONECT   31   28   37   38
CONECT   32   27
CONECT   33   27   30
CONECT   36   39   40   45
CONECT   37   31   40   41
CONECT   38   31   39   42
CONECT   39   36   38   43
CONECT   40   36   37   44
CONECT   46   49   54   57   59
CONECT   49   46   66   16   53
CONECT   51   25   62   17   21
CONECT   52    9   25   66
CONECT   54   15   46   48   60
CONECT   62   14   51   63   65
CONECT   66   15   49   52
CONECT    3    2
CONECT    4    2
CONECT   11    7
CONECT   12    7
CONECT   13    7
CONECT   19   14
CONECT   50   14
CONECT   47   15
CONECT   56   15
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CONECT   18   23
CONECT   22   23
CONECT   20   24
CONECT   64   24
CONECT   67   24
CONECT   55   26
CONECT   58   26
CONECT   61   26
CONECT   29   28
CONECT   34   30
CONECT   35   30
CONECT   45   36
CONECT   41   37
CONECT   42   38
CONECT   43   39
CONECT   44   40
CONECT   57   46
CONECT   59   46
CONECT   16   49
CONECT   53   49
CONECT   17   51
CONECT   21   51
CONECT   48   54
CONECT   60   54
CONECT   63   62
CONECT   65   62
END
```

Total Energy (Hartree)

(37): –1931.59825174

Structure 38:

```
COMPND  Structure_38.PDB
HETATM    1  C                -1.279   0.466   1.935
HETATM    2  C                -0.135   1.281   1.253
HETATM    5  N                 0.800   0.654   2.203
HETATM    6  N                -1.889  -0.575   1.085
HETATM    7  C                -2.332   1.257   2.700
HETATM    8  C                -0.136  -0.103   2.820
HETATM    9  O                -0.080  -0.957   3.702
HETATM   10  C                 2.248   0.600   2.204
HETATM   20  C                 3.718  -3.024  -2.454
HETATM   23  C                 4.606  -1.754  -2.340
HETATM   24 Si                 3.109   1.929   1.271
HETATM   25  O                 2.435  -3.100   1.834
HETATM   26 Si                 3.052   0.157   3.812
HETATM   27  C                -1.149  -1.542   0.474
HETATM   28  C                -3.300  -0.651   0.683
HETATM   30  C                -3.327  -2.098   0.126
HETATM   31  C                -3.730   0.405  -0.326
HETATM   32  O                 0.067  -1.678   0.462
HETATM   33  O                -1.960  -2.397  -0.206
HETATM   36  C                -4.611   2.291  -2.212
HETATM   37  C                -4.958   1.056  -0.163
HETATM   38  C                -2.947   0.708  -1.447
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HETATM   39  C                  -3.384   1.645  -2.383
HETATM   40  C                  -5.400   1.993  -1.100
HETATM   46  C                   1.539  -3.741   2.787
HETATM   48  C                   2.449  -4.429   3.805
HETATM   51  O                   2.909  -1.612  -0.723
HETATM   52 Li                   1.988  -1.330   1.036
HETATM   56  C                   3.696  -4.756   2.968
HETATM   62  C                   3.795  -3.528   2.062
HETATM   65  C                   2.504  -2.717  -1.549
HETATM   66  C                   3.730  -0.773  -1.547
HETATM    3  H                  -0.200   2.372   1.345
HETATM    4  H                   0.056   1.011   0.209
HETATM   11  H                  -3.046   1.761   2.041
HETATM   12  H                  -1.827   2.019   3.300
HETATM   13  H                  -2.876   0.603   3.391
HETATM   14  H                   4.258  -3.911  -2.109
HETATM   18  H                   3.400  -3.215  -3.484
HETATM   19  H                   4.895  -1.348  -3.314
HETATM   22  H                   5.524  -1.973  -1.785
HETATM   57  H                   4.535   1.544   1.053
HETATM   64  H                   2.505   2.134  -0.090
HETATM   67  H                   3.165   3.327   1.836
HETATM   55  H                   2.582   0.908   5.023
HETATM   58  H                   2.998  -1.282   4.213
HETATM   61  H                   4.510   0.463   3.662
HETATM   29  H                  -3.946  -0.585   1.561
HETATM   34  H                  -3.930  -2.198  -0.777
HETATM   35  H                  -3.665  -2.815   0.882
HETATM   45  H                  -4.949   3.023  -2.940
HETATM   41  H                  -5.574   0.833   0.706
HETATM   42  H                  -1.990   0.215  -1.592
HETATM   43  H                  -2.764   1.874  -3.245
HETATM   44  H                  -6.353   2.493  -0.955
HETATM   59  H                   0.926  -4.465   2.235
HETATM   60  H                   0.900  -2.968   3.218
HETATM   47  H                   2.704  -3.734   4.612
HETATM   49  H                   1.982  -5.315   4.248
HETATM   50  H                   4.598  -4.900   3.570
HETATM   63  H                   3.534  -5.662   2.372
HETATM   53  H                   4.255  -3.732   1.090
HETATM   54  H                   4.346  -2.714   2.549
HETATM   17  H                   2.219  -3.528  -0.878
HETATM   21  H                   1.627  -2.422  -2.140
HETATM   15  H                   4.280  -0.100  -0.889
HETATM   16  H                   3.091  -0.176  -2.214
CONECT    1    2    6    7    8
CONECT    2    1    5    3    4
CONECT    5    2    8   10
CONECT    6    1   27   28
CONECT    7    1   11   12   13
CONECT    8    1    5    9
CONECT    9    8
CONECT   10    5   24   26
CONECT   20   23   65   14   18
CONECT   23   20   66   19   22
CONECT   24   10   57   64   67
CONECT   25   46   52   62
CONECT   26   10   55   58   61
```

```
CONECT   27    6   32   33
CONECT   28    6   30   31   29
CONECT   30   28   33   34   35
CONECT   31   28   37   38
CONECT   32   27   52
CONECT   33   27   30
CONECT   36   39   40   45
CONECT   37   31   40   41
CONECT   38   31   39   42
CONECT   39   36   38   43
CONECT   40   36   37   44
CONECT   46   25   48   59   60
CONECT   48   46   56   47   49
CONECT   51   52   65   66
CONECT   52   25   32   51
CONECT   56   48   62   50   63
CONECT   62   25   56   53   54
CONECT   65   20   51   17   21
CONECT   66   23   51   15   16
CONECT    3    2
CONECT    4    2
CONECT   11    7
CONECT   12    7
CONECT   13    7
CONECT   14   20
CONECT   18   20
CONECT   19   23
CONECT   22   23
CONECT   57   24
CONECT   64   24
CONECT   67   24
CONECT   55   26
CONECT   58   26
CONECT   61   26
CONECT   29   28
CONECT   34   30
CONECT   35   30
CONECT   45   36
CONECT   41   37
CONECT   42   38
CONECT   43   39
CONECT   44   40
CONECT   59   46
CONECT   60   46
CONECT   47   48
CONECT   49   48
CONECT   50   56
CONECT   63   56
CONECT   53   62
CONECT   54   62
CONECT   17   65
CONECT   21   65
CONECT   15   66
CONECT   16   66
END
```

Total Energy (Hartree)

(38): –1931.59111128

Structure 39:

```
COMPND  Structure_39.PDB
HETATM    1  C                  -1.656   1.061   0.167
HETATM    2  C                  -0.665   1.964  -0.647
HETATM    5  N                   0.364   1.632   0.366
HETATM    6  N                  -2.016  -0.212  -0.477
HETATM    7  C                  -2.868   1.750   0.783
HETATM    8  C                  -0.446   0.855   1.107
HETATM    9  O                  -0.204   0.129   2.080
HETATM   10  C                   1.809   1.744   0.404
HETATM   24 Si                   2.680   1.840  -1.210
HETATM   25  O                   2.652  -1.656   1.748
HETATM   26 Si                   2.526   2.613   1.861
HETATM   27  C                  -1.114  -1.213  -0.725
HETATM   28  C                  -3.288  -0.463  -1.174
HETATM   30  C                  -3.139  -1.982  -1.432
HETATM   31  C                  -3.491   0.371  -2.431
HETATM   32  O                   0.079  -1.260  -0.457
HETATM   33  O                  -1.724  -2.235  -1.378
HETATM   36  C                  -3.924   1.879  -4.760
HETATM   37  C                  -4.665   1.116  -2.590
HETATM   38  C                  -2.535   0.386  -3.457
HETATM   39  C                  -2.750   1.136  -4.613
HETATM   40  C                  -4.883   1.866  -3.748
HETATM   47  C                   4.075  -1.402   1.678
HETATM   48  C                   4.500  -1.149   3.121
HETATM   49  C                   2.291  -2.093   3.089
HETATM   52 Li                   1.407  -0.482   0.855
HETATM   54  C                   3.600  -2.131   3.890
HETATM    3  H                  -0.909   3.031  -0.700
HETATM    4  H                  -0.426   1.584  -1.645
HETATM   11  H                  -2.538   2.657   1.297
HETATM   12  H                  -3.347   1.100   1.522
HETATM   22  H                  -3.606   2.041   0.029
HETATM   17  H                   4.150   1.819  -0.958
HETATM   20  H                   2.367   0.690  -2.125
HETATM   23  H                   2.428   3.043  -2.083
HETATM   13  H                   2.181   1.977   3.173
HETATM   19  H                   4.016   2.581   1.750
HETATM   21  H                   2.148   4.057   2.060
HETATM   29  H                  -4.126  -0.285  -0.494
HETATM   34  H                  -3.505  -2.289  -2.412
HETATM   35  H                  -3.626  -2.575  -0.650
HETATM   45  H                  -4.088   2.465  -5.661
HETATM   41  H                  -5.416   1.109  -1.803
HETATM   42  H                  -1.620  -0.193  -3.359
HETATM   43  H                  -2.000   1.140  -5.398
HETATM   44  H                  -5.800   2.441  -3.855
HETATM   14  H                   4.224  -0.548   1.012
HETATM   18  H                   4.573  -2.284   1.254
HETATM   46  H                   4.273  -0.115   3.402
HETATM   53  H                   5.568  -1.327   3.281
HETATM   15  H                   1.804  -3.070   3.013
HETATM   16  H                   1.574  -1.368   3.488
HETATM   50  H                   3.450  -1.845   4.935
HETATM   51  H                   4.034  -3.137   3.874
CONECT    1    2    6    7    8
CONECT    2    1    5    3    4
```

```
CONECT    5    2    8   10
CONECT    6    1   27   28
CONECT    7    1   11   12   22
CONECT    8    1    5    9
CONECT    9    8
CONECT   10    5   24   26
CONECT   24   10   17   20   23
CONECT   25   47   49   52
CONECT   26   10   13   19   21
CONECT   27    6   32   33
CONECT   28    6   30   31   29
CONECT   30   28   33   34   35
CONECT   31   28   37   38
CONECT   32   27   52
CONECT   33   27   30
CONECT   36   39   40   45
CONECT   37   31   40   41
CONECT   38   31   39   42
CONECT   39   36   38   43
CONECT   40   36   37   44
CONECT   47   25   48   14   18
CONECT   48   47   54   46   53
CONECT   49   25   54   15   16
CONECT   52   25   32
CONECT   54   48   49   50   51
CONECT    3    2
CONECT    4    2
CONECT   11    7
CONECT   12    7
CONECT   22    7
CONECT   17   24
CONECT   20   24
CONECT   23   24
CONECT   13   26
CONECT   19   26
CONECT   21   26
CONECT   29   28
CONECT   34   30
CONECT   35   30
CONECT   45   36
CONECT   41   37
CONECT   42   38
CONECT   43   39
CONECT   44   40
CONECT   14   47
CONECT   18   47
CONECT   46   48
CONECT   53   48
CONECT   15   49
CONECT   16   49
CONECT   50   54
CONECT   51   54
END
```

Total Energy (Hartree)

(THF): –232.44928908

(39): –1699.12875805

(39 + THF): –1931.57804713