SUPPORTING INFORMATION (JO-060537g)

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

C. Palomo^{*,†}, *J. M. Aizpurua*^{*,†,#}, *A. Benito*[†], *L. Cuervo*[†], *R. M. Fratila*[†], *J. I. Miranda*[†] and *A. Linden*[‡]

[†] Departamento de Química Organica-I. Universidad del Pais Vasco. Facultad de Química. Apdo 1072. 20080 San Sebastian. Spain.

[‡] Organisch-chemisches Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

[#] jesusmaria.aizpurua@ehu.es

LIST OF CONTENTS

	page
1.- Preparation Details and Physical and Spectroscopic Data of Compounds 12, 16-36.	
1.1. General	S2
1.2. Starting materials and <i>N</i> -[silyl(methyl)]- β -lactam models 10-17 .	S2
1.3. Compounds collected in Table 1: 18-25 .	S3
1.4. Compounds collected in Table 2: 26-36 .	S6
2.- Computational Data: Cartesian Coordinates and Total Energies.	
2.1. Structure 37 .	S10
2.2. Structure 38 .	S12
2.3. Structure 39 .	S15

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. ^1H 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.

(3R)-3-Benzyl-1-[bis(trimethylsilyl)-methyl]-3-[(4S,5R)-4,5-diphenyl-2-oxo-oxazolidin-3-yl]azetidin-2-one (12): This compound was prepared in 74% yield from **9** ($\text{R} = \text{Ph}$; $\text{R}^2 = \text{H}$) and benzyl bromide, following the reported protocol for α -alkylation.^{8(a)} M.p: 204-6°C; $[\alpha]_{\text{D}}^{25} = +0.99$ ($c = 1.0$, 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. ^1H -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 $\text{C}_{32}\text{H}_{40}\text{N}_2\text{O}_3\text{Si}_2$: C, 69.02; H, 7.24; N, 5.03. Found: C, 68.74; H, 7.23; N, 5.10.

(3R)-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: 67°C; $[\alpha]_{\text{D}}^{25} = -$

26.1 (c= 1.0, Cl₂CH₂); 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). ¹H-NMR (δ, ppm, CDCl₃): 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). ¹³C-NMR (δ, ppm, CDCl₃): 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 C₁₉H₄₀N₂O₃Si₂: C, 56.95; H, 10.06; N, 6.99. Found: C, 57.11; H, 9.94; N, 7.05.

(3R,4R)-3-Benzyl-4-isobutyl-3-(tert-butoxycarbonylamino)-1-(trimethylsilylmethyl)azetidin-2-one (17): This compound was prepared in 70% overall yield from (3R,4R)-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; [α]_D²⁵ = +27.6 (c= 0.5,

Cl₂CH₂); 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); ¹H-NMR (δ, ppm, CDCl₃): 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). ¹³C-NMR (δ, ppm, CDCl₃): 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; C₂₃H₃₈N₂O₃Si requires 418.2653.

(3R)-3-Benzyl-1-[bis(trimethylsilyl)-deutero-methyl]-3-[(4S)-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 -78°C to 20°C. Eluent: EtOAc/hexanes 1:10. Yield: 197 mg (82%). M.p.: 154-7°C (CH₂Cl₂-hexanes); [α]_D²⁵ = +20.5 (c= 1.0, Cl₂CH₂); 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); ¹H-NMR (δ, ppm, CDCl₃): 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). ¹³C-NMR (δ, ppm, CDCl₃): 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 C₂₆H₃₅DN₂O₃Si₂: C, 64.82; H, 7.74; N, 5.81. Found: C, 64.89; H, 7.60; N, 5.91.

(3R) 3-Benzyl-1-[1,1-bis(trimethylsilyl)ethyl]-3-[(4S)-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.: 170-1°C (CH₂Cl₂-hexanes); $[\alpha]_{\text{D}}^{25} = +36.5$ ($c = 1.0$, Cl₂CH₂); 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). ¹H-NMR (δ , ppm, CDCl₃): 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). ¹³C-NMR (δ , ppm, CDCl₃): 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 C₂₇H₃₈N₂O₃Si₂: C, 65.54; H, 7.74; N, 5.66. Found: C, 65.82; H, 7.91; N, 5.78.

(3R)-3-Benzyl-1-[1,1-bis(trimethylsilyl)-2-phenylethyl]-3-[(4S)-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 -100°C to 20°C. Eluent: EtOAc/hexanes 1:5. Yield: 100 mg (70%). M.p.: 173-5°C (CH₂Cl₂-hexanes); $[\alpha]_{\text{D}}^{25} = +13.0$ ($c = 1.0$, Cl₂CH₂); 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). ¹H-NMR (δ , ppm, CDCl₃): 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). ¹³C-NMR (δ , ppm, CDCl₃): 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 C₃₃H₄₂N₂O₃Si₂: C, 69.43; H, 7.42; N, 4.91. Found: C, 69.86; H, 7.59; N, 5.10.

(3R)-3-Benzyl-1-[1,1-bis(trimethylsilyl)-2-n-butyl]-3-[(4S)-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 -100°C to 20°C. Eluent: EtOAc/hexanes 1:5. Yield: 107 mg (40%). M.p.: 123-4°C (CH₂Cl₂); $[\alpha]_{\text{D}}^{25} = +6.4$ ($c = 1.0$, Cl₂CH₂); 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). ¹H-NMR (δ , ppm, CDCl₃): 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). ¹³C-NMR (δ , ppm,

CDCl₃): 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; C₃₀H₄₄N₂O₃Si₂ requires 536.2891.

(3R)-1-[1,1-Bis(trimethylsilyl)-2-phenylethyl]-3-isobutyl-3-[(4S)-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), *n*BuLi (0.30 mmol, 0.12 mL)/TMEDA (0.30 mmol, 45 μ L) and benzyl bromide (0.50 mmol, 61 μ L). The reaction mixture was warmed overnight from -100°C to 20°C . Eluent: EtOAc/hexanes 1:5. Yield: 103 mg (77%). M.p.: $76-78^{\circ}\text{C}$ (CH₂Cl₂-hexanes); $[\alpha]_{\text{D}}^{25} = -32.9$ ($c = 1.0$, CH₂CH₂); 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). ¹H-NMR (δ , ppm, CDCl₃): 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). ¹³C-NMR (δ , ppm, CDCl₃): 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 C₃₀H₄₄N₂O₃Si₂: C, 67.12; H, 8.26; N, 5.22. Found: C, 67.52; H, 8.69; N, 5.22.

(3S)-1,3-Dibenzyl-4-isobutyl-3-[(4S)-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), *n*BuLi (0.30 mmol, 0.12 mL)/TMEDA (0.30 mmol, 45 μ L) and benzyl bromide (0.50 mmol, 61 μ L). The reaction mixture was warmed overnight from -100°C to 20°C . 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). ¹H-NMR (δ , ppm, CDCl₃): 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; C₃₀H₃₂N₂O₃ requires 468.2413.

(3R)-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), *s*BuLi (0.65 mmol, 0.5 mL) and MeOD (5.0 mmol, 0.2 mL). The reaction mixture was warmed overnight from -78°C to

20°C. Eluent: EtOAc/hexanes 1:10. Yield: 197 mg (82%). Oil; $[\alpha]_D^{25} = +30.7$ ($c = 1.0$, CH_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). $^1\text{H-NMR}$ (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). $^{13}\text{C-NMR}$ (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 $\text{C}_{22}\text{H}_{37}\text{DN}_2\text{O}_3\text{Si}_2$: C, 60.64; H, 9.02; N, 6.43. Found: C, 60.83; H, 8.84; N, 6.05.

(3R)-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 *s*BuLi (0.65 mmol, 0.5 mL in cyclohexane) and MeOD (5.0 mmol, 0.2 mL). The reaction mixture was warmed overnight from -78°C to 20°C. Eluent: EtOAc/hexanes 1:10. Yield: 197 mg (67%).

M.p: 63°C; $[\alpha]_D^{25} = -27.8$ ($c = 1.0$, CH_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). $^1\text{H-NMR}$ (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). $^{13}\text{C-NMR}$ (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 $\text{C}_{19}\text{H}_{39}\text{DN}_2\text{O}_3\text{Si}_2$: C, 56.81; H, 10.29; N, 6.97. Found: C, 56.52; H, 11.03; N, 7.03.

(3R)-3-Benzyl-1-(carboxymethyl)-3-[(4S)-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 -78°C under nitrogen was added 1.3M *s*BuLi (1.2 mmol, 0.92 mL in cyclohexane) and the mixture was stirred at -78°C 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 0°C, 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; $[\alpha]_D^{25} = +27.2$ ($c = 1.0$, CH_2CH_2); IR(cm^{-1} , KBr): 3500-2900(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). $^1\text{H-NMR}$ (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). $^{13}\text{C-NMR}$ (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 $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}_5$: C, 66.31; H, 5.30; N, 7.36. Found: C, 66.26; H, 5.36; N, 7.31.

(3R)-3-Benzyl-1-(benzyloxycarbonylmethyl)-3-[(4S)-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 -78°C under nitrogen was added 1.3M sBuLi (1.2 mmol, 0.92 mL in cyclohexane) and the mixture was stirred at -78°C 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 0°C . After the work-up, the crude was purified by column chromatography (silicagel-60, eluent: EtOAc/hexanes 1:1). Yield: 211 mg (45%). Oil; $[\alpha]_{\text{D}}^{25} = +30.9$ ($c = 1.0$, 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). ^1H -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 $\text{C}_{28}\text{H}_{26}\text{N}_2\text{O}_5$: C, 71.47; H, 5.57; N, 5.95. Found: C, 71.52; H, 5.50; N, 5.86.

(3R)-3-Benzyl-1-[(N-phenylaminocarbonyl)methyl]-3-[(4S)-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.: $165-7^{\circ}\text{C}$; $[\alpha]_{\text{D}}^{25} = +34.1$ ($c = 1.0$, 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); ^1H -

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 $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_4$: C, 71.19; H, 5.53; N, 9.22. Found: C, 70.79; H, 5.53; N, 9.28.

(3R)-1-(Carboxymethyl)-3-isobutyl-3-[(4S)-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; $[\alpha]_{\text{D}}^{25} = -4.4$ ($c = 1.0$, 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; ^1H -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 $\text{C}_{18}\text{H}_{22}\text{N}_2\text{O}_5$: C, 62.42; H, 6.40; N, 8.09. Found: C, 62.24; H, 6.26; N, 7.55.

(3R)-1-Cyanomethyl-3-isobutyl-3-[(4S)-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 *n*BuLi/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 0°C and the mixture was stirred for 5h. Eluent: EtOAc/hexanes 1:2. Yield: 98 mg (60%). Oil; $[\alpha]_{\text{D}}^{25} = -10.6$ ($c = 1.0$, 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; ^1H -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; $\text{C}_{18}\text{H}_{21}\text{N}_3\text{O}_3$ requires 327.1583.

(3R)-1-[(Aminocarbonyl)methyl]-3-isobutyl-3-[(4S)-4-phenyl-2-oxo-1,3-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 *n*BuLi/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 -78°C 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)

(3R)-3-Benzyl-1-[(N-phenylaminocarbonyl)methyl]-3-[(4S,5R)-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 *n*BuLi/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.: 74-75°C; $[\alpha]_{\text{D}}^{25} = -41.5$ ($c = 1.0$, 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. ¹H-NMR (δ, ppm, CDCl₃): 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* = 17.6 Hz); 2.94 (d, 1H, *J* = 13.4 Hz). ¹³C-NMR (δ, ppm, CDCl₃): 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 C₃₃H₂₉N₃O₄: C, 74.56; H, 5.50; N, 7.90. Found: C, 74.43; H, 5.61; N, 8.41.

(3*S*,4*R*)-3-Benzyl-1-carboxymethyl-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 *t*BuLi (1.2 mmol, 0.84 mL in pentane) at -78°C, using CO₂ gas as electrophile. Yield: 353 mg (81%). Oil; [α]_D²⁵ = +0.84 (c = 0.1, Cl₂CH₂); 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). ¹H-NMR (δ, ppm, CDCl₃): 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). ¹³C-NMR (δ, ppm, CDCl₃): 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 C₂₅H₂₈N₂O₅: C, 68.79; H, 6.47; N, 6.42. Found: C, 69.03; H, 6.39; N, 6.55.

(*R*)-3-Benzyl-3-*tert*-butoxycarbonylamino-1-carboxymethylazetidin-2-one (34): The general procedure was followed from **15** (1.0 mmol, 0.43 g) and 0.60M *n*BuLi/TMEDA solution (2.5 mmol, 4.17 mL) using CO₂ gas as electrophile. Yield: 214 mg (64%). For characterization data, see ref. 9(b)

(*R*)-3-*tert*-Butoxycarbonylamino-1-carboxymethyl-3-isobutylazetidin-2-one (35): The general procedure was followed from **16** (1.0 mmol, 0.40 g) and 0.60M *n*BuLi/TMEDA solution (2.5 mmol, 4.17 mL) using CO₂ gas as electrophile. Yield: 204 mg (68 %). Oil; [α]_D²⁵ = +18.9 (c = 1.0, Cl₂CH₂); 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). ¹H-NMR (δ, ppm, CDCl₃): 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). ¹³C-NMR (δ, ppm, CDCl₃): 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 C₁₄H₂₄N₂O₅: C, 55.98; H, 8.05; N, 9.33. Found: C, 55.56; H, 7.89; N, 9.28.

(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 *t*BuLi (2.5 mmol, 1.67 mL in pentane) at –78°C, using CO₂ 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

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						

CONNECT	18	23
CONNECT	22	23
CONNECT	20	24
CONNECT	64	24
CONNECT	67	24
CONNECT	55	26
CONNECT	58	26
CONNECT	61	26
CONNECT	29	28
CONNECT	34	30
CONNECT	35	30
CONNECT	45	36
CONNECT	41	37
CONNECT	42	38
CONNECT	43	39
CONNECT	44	40
CONNECT	57	46
CONNECT	59	46
CONNECT	16	49
CONNECT	53	49
CONNECT	17	51
CONNECT	21	51
CONNECT	48	54
CONNECT	60	54
CONNECT	63	62
CONNECT	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

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			

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

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

END

Total Energy (Hartree)

(THF): -232.44928908

(39): -1699.12875805

(39 + THF): -1931.57804713