Supporting Information

Oxa-Michael-based divergent synthesis of artificial glutamate analogs

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General methods
All reactions susceptible to moisture and air were carried out in an atmosphere of argon gas, using the glassware oven-dried over 3 h. CH₂Cl₂ and THF were purified by Glass Contour Solvent Dispensing System (Nikko Hansen). All other reagents were purchased at the highest commercial grade and used directly. Analytical thin-layer chromatography (TLC) was performed using Merck silica gel 60 F254 plate (0.25-mm thickness). Flash column chromatography was carried out using Kanto Chemical silica gel 60N (40-50 mesh) or Yamazen silica gel HiFlash (SiOH-30µ Premium, 30 µm, 60 Å) with automated flash column systems EPCLC-Wprep2XY-10VW (Yamazen Corporation). Reversed-phase silica gel column chromatography was carried out using Fuji Silysia Chromatorex DM1020T (ODS, 100-200 mesh). For high-performance liquid chromatography (HPLC), a JASCO LC-2000Plus series was used. Optical rotations were recorded on a JASCO P-1030 polarimeter. IR spectra were recorded on a JASCO FT/IR-400 spectrometer. ESI mass spectra were recorded on a Thermo Fisher Scientific Q Exactive Focus mass spectrometer. ¹H and ¹³C NMR spectra were recorded on a BRUKER AVANCE 400 spectrometer or BRUKER AVANCE III HD 400 spectrometer. Chemical shift values are reported in δ (ppm) with reference to internal residual solvent [¹H NMR, CDCl₃ (7.24), D₂O (4.70), CD₃OD (3.30); ¹³C NMR, CDCl₃ (77.0), D₂O (-), CD₃OD (49.0)]. Coupling constants (J) are reported in Hertz (Hz). The following abbreviations were used to designate the multiplicities; s = singlet, d = doublet, dd = double doublet, ddd = double double double doublet, m = multiplet, br = broad.

Benzyl (2R*,3R*,3aR*,6S*,6aS*)-6a-(2-(benzyloxy)-2-oxoethyl)-3-hydroxy-4-oxo-2-vinylhexahydro-2H-furo[2,3-c]pyrrole-6-carboxylate (7)
A suspension of diester 5 (68.7 mg, 0.230 mmol) in hydrochloric acid (6 M, 15 mL) was stirred at 65 °C for 20 h. The mixture was then
concentrated to dryness by blowing of air to give a residue (70.6 mg), which was mainly composed of dicarboxylic acid 6.

A portion of the residue thus obtained above (19.5 mg), without purification, was dissolved in DMF (3.5 mL). To the stirred mixture at rt were added Cs$_2$CO$_3$ (70.3 mg, 0.216 mmol) and BnBr (0.0427 mL, 0.360 mmol). After stirring at 50 °C for 7 h, the mixture was cooled to rt, poured into saturated aqueous NH$_4$Cl (4 mL), and extracted with EtOAc (4 × 4 mL). Combined extracts were dried over Na$_2$SO$_4$ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 750 mg, EtOAc/hexane = 5:5) to give dibenzyl ester 7 (20.2 mg, 72%) as a yellow foam.

Data for dibenzyl ester 7: IR (ATR) 3526, 3185, 2889, 1739, 1715, 1703, 1457, 1362, 1207, 1076, 1038 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.37–7.27 (m, 10H), 6.11 (brs, 1H), 5.85 (ddd, $J$ = 16.9, 10.6, 6.0 Hz, 1H), 5.39 (d, $J$ = 16.9 Hz, 1H), 5.34 (d, $J$ = 10.6 Hz, 1H), 5.11 (d, $J$ = 12.0 Hz, 1H), 5.08 (d, $J$ = 12.0 Hz, 1H), 5.05 (d, $J$ = 12.3 Hz, 1H), 5.02 (d, $J$ = 12.3 Hz, 1H), 4.41 (d, $J$ = 3.3 Hz, 1H), 4.39–4.34 (m, 2H), 3.25 (s, 1H), 2.97 (d, $J$ = 17.0 Hz, 1H), 2.90 (d, $J$ = 17.0 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 173.9, 170.4, 169.6, 135.2, 134.5, 131.6, 128.8 ($\times$3), 128.7 ($\times$2), 128.6 ($\times$2), 128.5 ($\times$3), 119.7, 86.7, 84.3, 76.7, 67.8, 66.9, 65.6, 58.4, 39.3; HRMS (ESI, positive) calcd for C$_{25}$H$_{25}$NO$_7$Na$^+$ [(M+Na)$^+$] 474.1523, found 474.1523.

Benzyl (2R$^*$,3R$^*$,3aR$^*$,6S$^*$,6aS$^*$)-6a-(2-(benzyloxy)-2-oxoethyl)-3-hydroxy-4-oxo-2-((E)-3-oxobut-1-en-1-yl)hexahydro-2H-furo[2,3-c]pyrrole-6-carboxylate (10)

To a stirred solution of alkene 7 (5.97 mg, 0.0132 mmol) and 3-buten-2-one (0.0054 mL, 0.066 mmol) in CH$_2$Cl$_2$ (0.300 mL) at rt was added Hoveyda-Grubbs catalyst second generation (0.2 mg, 0.0003 mmol). After stirring at 50 °C in a sealed tube for 70 h, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 600 mg, EtOAc/hexane = 4:6) to give enone 10 (5.37 mg, 82%) as a colorless oil: IR (ATR) 3587, 3299, 3180, 3030, 1747, 1734, 1716, 1679, 1557, 1456, 1364 cm$^{-1}$; $^1$H
NMR (400 MHz, CDCl$_3$) $\delta$ 7.40–7.26 (m, 10H), 6.69 (dd, $J$ = 16.1, 4.9 Hz, 1H), 6.28 (d, $J$ = 16.1 Hz, 1H), 6.07 (b(rs, 1H), 5.12 (s, 2H), 5.09 (d, $J$ = 12.2 Hz, 1H), 5.03 (d, $J$ = 12.2 Hz, 1H), 4.55 (d, $J$ = 3.5 Hz, 1H), 4.52 (m, 1H), 4.34 (s, 1H), 3.26 (s, 1H), 2.99 (d, $J$ = 17.2 Hz, 1H), 2.84 (d, $J$ = 17.2 Hz, 1H), 2.24 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 197.9, 173.7, 170.4, 169.5, 139.6, 135.0, 134.6, 130.0, 134.4, 132.5, 128.9, 128.9 ($\times$2), 128.8 ($\times$2), 128.6 ($\times$2), 128.6, 128.5 ($\times$2), 87.1, 82.7, 77.0, 67.9, 67.1, 65.6, 58.7, 39.0, 27.3; HRMS (ESI, positive) calcd for C$_{27}$H$_{27}$NO$_8$Na$^+$ [(M+Na)$^+$] 516.1629, found 516.1625.

Benzyl (4$S*$,4$R*$,5$S*$,6$S*$,8$R*$,8$R$*)-5a-(2-(benzyloxy)-2-oxoethyl)-8-oxo-4-(2-oxopropyl)octahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylate (11r)

To a stirred solution of enone 10 (8.46 mg, 0.0171 mmol) in CH$_2$Cl$_2$ (0.300 mL) at rt were added parafomaldehyde (0.6 mg, 0.02 mmol) and MsOH (0.0022 mL, 0.034 mmol). After 16 h, the mixture was poured into water (0.5 mL) and extracted with EtOAc (6 × 0.5 mL). Combined extracts were dried over Na$_2$SO$_4$ and concentrated under reduced pressure to give a residue (8.82 mg), which is mainly a mixture composed of 1,3-dioxane 11r and N-hydroxymethylated 1,3-dioxane 12r ($11r/12r = 2.2:1$).

A portion of the residue thus obtained above (1.01 mg), without purification, was dissolved in EtOH (0.500 mL). To the stirred mixture at rt was added ammonium hydroxide (28%, 0.0006 mL, 0.009 mmol). After 2 h, the mixture was concentrated under reduced pressure to give a residue (0.92 mg), which is a mixture composed of 1,3-dioxane 11r and N-hydroxymethylated 1,3-dioxane 12r ($11r/12r = 2.9:1$).

The residue thus obtained, without purification, was dissolved in EtOH (0.250 mL). To the stirred mixture at rt was added ammonium hydroxide (28%, 0.0006 mL, 0.009 mmol). After 29 h, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 500 mg, EtOAc/hexane = 7:3) to give 1,3-dioxane 11r (0.75 mg, 73%) as a colorless oil: IR (ATR) 3566, 2935, 1742, 1732, 1718, 1696, 1520, 1363, 1208, 1077, 883 cm$^{-}$
1H NMR (400 MHz, CDCl₃) δ 7.37–7.25 (m, 10H), 5.99 (brs, 1H), 5.05 (d, J = 12.1 Hz, 1H), 5.02 (d, J = 12.3 Hz, 1H), 5.00 (d, J = 12.3 Hz, 1H), 4.93 (d, J = 6.7 Hz, 1H), 4.91 (d, J = 12.1 Hz, 1H), 4.63 (d, J = 6.7 Hz, 1H), 4.49 (d, J = 2.3 Hz, 1H), 4.42 (s, 1H), 4.18 (ddd, J = 7.0, 6.0, 2.3 Hz, 1H), 3.81 (dd, J = 2.3, 2.3 Hz, 1H), 3.38 (d, J = 17.4 Hz, 1H), 3.24 (s, 1H), 2.95 (d, J = 17.4 Hz, 1H), 2.79 (dd, J = 17.5, 7.0 Hz, 1H), 2.68 (dd, J = 17.5, 6.0 Hz, 1H), 2.10 (s, 3H); 13C NMR (100 MHz, CDCl₃) δ 205.8, 172.7, 169.9, 169.5, 135.6, 134.6, 128.7, 128.7 (×2), 128.6 (×2), 128.5 (×2), 128.3, 128.2 (×2), 91.7, 87.7, 77.8, 76.3, 71.4, 67.7, 66.4, 64.8, 56.1, 44.7, 40.0, 30.7; HRMS (ESI, positive) calcd for C₂₈H₂₉NO₉Na⁺ [(M+Na)⁺] 546.1735, found 546.1733.

(4S*,4aR*,5aS*,6S*,8aR*,8bR*)-5a-(Carboxymethyl)-8-oxo-4-(2-oxopropyl)octahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylic acid (1ar, (2R*,7R*)-TKM-50)

A mixture of dibenzyl ester 11r (4.55 mg, 0.0087 mmol) and Pd/C (5%, 0.9 mg) in MeOH (1 mL) was stirred under hydrogen atmosphere (balloon) at rt. After 43 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure to give glutamate analog 1ar ((2R*,7R*)-TKM-50, 2.55 mg, 86%) as a colorless oil which was sufficiently pure for characterization.

Data for (2R*,7R*)-TKM-50 (1ar): IR (ATR) 3360, 2929, 2843, 1739, 1722, 1709, 1692, 1359, 1175, 1078, 1020 cm⁻¹; 1H NMR (400 MHz, D₂O) δ 4.94 (d, J = 6.9 Hz, 1H), 4.77 (d, J = 6.9 Hz, 1H), 4.57 (d, J = 2.2 Hz, 1H), 4.43 (s, 1H), 4.38 (ddd, J = 8.8, 4.1, 2.2 Hz, 1H), 3.87 (dd, J = 2.2, 2.2 Hz, 1H), 3.32 (s, 1H), 3.25 (d, J = 17.1 Hz, 1H), 2.95 (dd, J = 17.7, 8.8 Hz, 1H), 2.93 (d, J = 17.1 Hz, 1H), 2.82 (dd, J = 17.7, 4.1 Hz, 1H), 2.19 (s, 3H); 13C NMR (100 MHz, D₂O) δ 211.8, 175.2, 173.9, 173.6, 91.3, 87.4, 77.6, 76.4, 71.2, 66.4, 56.6, 44.6, 40.0, 29.8; HRMS (ESI, negative) calcd for C₁₄H₁₄NO₆⁻ [(M–H)⁻] 342.0831, found 342.0844.

Benzyl (2S*,3S*,3aS*,6bR*,6aR*)-6a-((2-((benzyloxy)2-oxoethyl)-3-hydroxy-4-oxo-2-((E)-3-oxooct-1-en-1-yl)hexahydro-2H-furo[2,3-
c]pyrrole-6-carboxylate (S10b)

To a stirred solution of alkene 7 (14.8 mg, 0.0328 mmol) and 1-octene-3-one (0.0249 mL, 0.164 mmol) in CH₂Cl₂ (0.400 mL) at rt was added Hoveyda-Grubbs catalyst second generation (1.0 mg, 0.0016 mmol). After stirring at 50 °C in a sealed tube for 18 h, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 600 mg, EtOAc/hexane = 5:5) to give enone S10b (13.9 mg, 77%) as a brown oil: IR (ATR) 3545, 3382, 3223, 2951, 1742, 1716, 1704, 1682, 1387, 1191, 1038 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.39–7.25 (m, 10H), 6.71 (dd, J = 16.0, 4.8 Hz, 1H), 6.50 (brs, 1H), 6.30 (dd, J = 16.0, 1.4 Hz, 1H), 5.11 (d, J = 12.0 Hz, 1H), 5.09 (d, J = 12.0 Hz, 1H), 5.06 (d, J = 12.3 Hz, 1H), 5.03 (d, J = 12.3 Hz, 1H), 4.57–4.47 (m, 2H), 4.36 (s, 1H), 3.78 (d, J = 7.1 Hz, 1H), 3.25 (s, 1H), 2.98 (d, J = 17.2 Hz, 1H), 2.89 (d, J = 17.2 Hz, 1H), 2.50 (t, J = 7.3 Hz, 2H), 1.57 (tt, J = 7.3, 7.3 Hz, 2H), 1.36–1.19 (m, 4H), 0.86 (t, J = 6.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 200.2, 174.0, 170.3, 169.6, 138.6, 135.1, 134.5, 131.6, 128.8, 128.8 (×2), 128.7 (×2), 128.6 (×2), 128.5, 128.4 (×2), 87.1, 82.9, 76.8, 67.8, 67.0, 65.7, 58.7, 40.6, 39.1, 31.4, 23.6, 22.4, 13.9; HRMS (ESI, positive) calcd for C₃₁H₃₅NO₈Na⁺ [(M+Na)⁺] 572.2255, found 572.2247.

Benzyl (4R*,4aS*,5aR*,6R*,8aS*,8bS*)-5a-[(2-(benzyloxy)-2-oxoethyl)-8-oxo-4-(2-oxoheptyl)octahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylate (S11br), and

benzyl (4S*,4aS*,5aR*,6R*,8aS*,8bS*)-5a-[(2-(benzyloxy)-2-oxoethyl)-8-oxo-4-(2-oxoheptyl)octahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylate (S11bs)

To a stirred solution of enone S10b (2.98 mg, 0.0054 mmol) in CH₂Cl₂ (0.500 mL) at -20 °C were added paraformaldehyde (0.2 mg, 0.007 mmol) and MsOH (0.0007 mL, 0.01 mmol). After stirring for 22 h, the mixture was allowed to warm to 0 °C, and stirring was continued for 30 h. The mixture was then poured into water (0.5 mL) and extracted with EtOAc (6 × 0.5 mL). Combined extracts were dried over Na₂SO₄ and concentrated under reduced pressure to give a residue (2.82 mg), which is a mixture composed of N-hydroxymethylated 1,3-dioxanes S12br,
S12bs and 1,3-dioxanes S11br, S11bs ((S12br, S12bs)/(S11br, S11bs) = 1:9.7).

The residue thus obtained above, without purification, was dissolved in EtOH (0.500 mL). To the stirred mixture at rt was added ammonium hydroxide (28%, 0.0016 mL, 0.023 mmol). After 13 h, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 500 mg, EtOAc/hexane = 3:7) to give a mixture of 1,3-dioxane S11br and S11bs (2.37 mg, S11br/S11bs = 2.8:1) as a colorless oil.

Purification of a portion of the mixture (2.05 mg) by HPLC (XTerra™ MS, 4.6 × 150 mm, MeOH/H₂O = 8:2, 1.0 mL/min, 40 °C; detected at 254 nm) gave diastereomerically pure 1,3-dioxanes S11br (7R*, 1.40 mg, 51%, t_R 4.9 min) and S11bs (7S*, 0.61 mg, 22%, t_R 4.2 min).

Data for 1,3-dioxide S11br (7R*): retention time 4.9 min; IR (ATR) 3297, 2926, 2870, 1740, 1730, 1689, 1456, 1386, 1190, 1093 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.36–7.26 (m, 10H), 5.89 (brs, 1H), 5.04 (d, J = 12.1 Hz, 1H), 5.02 (d, J = 12.3 Hz, 2H), 5.00 (d, J = 12.3 Hz, 1H), 4.93 (d, J = 6.7 Hz, 1H), 4.90 (d, J = 12.1 Hz, 1H), 4.62 (d, J = 6.7 Hz, 1H), 4.49 (d, J = 2.3 Hz, 1H), 4.40 (s, 1H), 4.20 (dd, J = 7.1, 6.0, 2.3 Hz, 1H), 3.81 (dd, J = 2.3, 2.3 Hz, 1H), 3.38 (d, J = 17.4 Hz, 1H), 3.24 (s, 1H), 2.96 (d, J = 17.4 Hz, 1H), 2.77 (dd, J = 17.3, 7.1 Hz, 1H), 2.64 (dd, J = 17.3, 6.0 Hz, 1H), 2.34 (t, J = 7.4 Hz, 2H), 1.57–1.46 (m, 1H), 1.34–1.15 (m, 4H), 0.86 (t, J = 7.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 208.2, 172.6, 169.9, 169.4, 135.6, 134.6, 128.7, 128.7 (×2), 128.6 (×2), 128.5 (×2), 128.3, 128.2 (×2), 91.7, 87.7, 77.8, 76.4, 71.6, 67.7, 66.4, 64.8, 56.1, 43.9, 43.6, 40.0, 31.3, 23.2, 22.4, 13.9; HRMS (ESI, positive) calcd for C₃₂H₄₇NO₉Na⁺ [(M+Na)⁺] 602.2361, found 602.2341.

Data for 1,3-dioxide S11bs (7S*): retention time 4.2 min; IR (ATR) 3222, 2921, 2898, 2850, 1738, 1724, 1712, 1696, 1532, 1379, 1217 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.35–7.25 (m, 10H), 5.88 (s, 1H), 5.04 (d, J = 12.1 Hz, 2H), 5.01 (d, J = 12.1 Hz, 1H), 4.90 (d, J = 12.1
Hz, 1H), 4.79 (d, J = 6.2 Hz, 1H), 4.75 (d, J = 6.2 Hz, 1H), 4.52–4.45 (m, 3H), 3.69 (dd, J = 2.4, 2.4 Hz, 1H), 3.38 (d, J = 17.4 Hz, 1H), 3.28 (s, 1H), 2.98 (d, J = 17.4 Hz, 1H), 2.82 (dd, J = 16.3, 7.9 Hz, 1H), 2.62 (dd, J = 16.3, 6.7 Hz, 1H), 2.40 (t, J = 7.5 Hz, 2H), 1.60–1.47 (m, 2H), 1.33–1.18 (m, 4H), 0.86 (t, J = 7.0 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 206.9, 172.7, 169.9, 169.4, 135.5, 134.6, 128.7, 128.7 (×2), 128.6 (×2), 128.5 (×2), 128.3 (×3), 87.9, 86.5, 78.5, 75.6, 69.0, 67.7, 66.5, 64.7, 56.0, 43.1, 43.1, 40.0, 31.3, 23.2, 22.4, 13.9; HRMS (ESI, positive) calcd for C32H37NO9Na+ [(M+Na)+] 602.2361, found 602.2340.

(4S*,4aR*,5aS*,6S*,8aR*,8bR*)-5a-(Carboxymethyl)-8-oxo-4-(2-oxoheptyl)octahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylic acid (1br, (2R*,7R*)-TKM-86)
A mixture of dibenzyl ester S11br (2.53 mg, 0.0044 mmol) and Pd/C (5%, 0.5 mg) in MeOH (0.250 mL) and THF (0.250 mL) was stirred under hydrogen atmosphere (balloon) at rt. After 20 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure. The residue was purified by trituration with water three times to give glutamate analog 1br ((2R*,7R*)-TKM-86, 1.69 mg, 97%) as a colorless oil: IR (ATR) 3543, 3273, 3192, 1737, 1722, 1708, 1687, 1412, 1368, 1190, 1033 cm⁻¹; ¹H NMR (400 MHz, D2O) δ 4.92 (d, J = 6.9 Hz, 1H), 4.74 (d, J = 6.9 Hz, 1H), 4.55 (d, J = 2.3 Hz, 1H), 4.36 (ddd, J = 8.7, 4.4, 2.3 Hz, 1H), 4.30 (s, 1H), 3.83 (dd, J = 2.3, 2.3 Hz, 1H), 3.24 (s, 1H), 3.15 (d, J = 16.0 Hz, 1H), 2.93 (dd, J = 17.6, 8.7 Hz, 1H), 2.85 (d, J = 16.0 Hz, 1H), 2.78 (dd, J = 17.6, 4.4 Hz, 1H), 2.57–2.40 (m, 2H), 1.49 (tt, J = 7.3, 7.3 Hz, 2H), 1.27–1.12 (m, 4H), 0.79 (t, J = 7.0 Hz, 3H); 13C NMR (100 MHz, D2O) δ 214.6, 175.2 (×3), 91.2, 87.7, 77.8, 76.3, 71.4, 67.9, 56.6, 43.7, 42.9, 41.0, 30.5, 22.9, 21.7, 13.2; HRMS (ESI, negative) calcd for C18H24NO− [(M−H)−] 398.1457, found 398.1458.

(4R*,4aR*,5aS*,6S*,8aR*,8bR*)-5a-(Carboxymethyl)-8-oxo-4-(2-oxoheptyl)octahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylic acid (1bs, (2R*,7S*)-TKM-86)
A mixture of dibenzyl ester S11bs (0.87 mg, 0.0015 mmol) and Pd/C
(5%, 0.16 mg) in MeOH (0.250 mL) and THF (0.250 mL) was stirred under hydrogen atmosphere (balloon) at rt. After 20 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure. The residue was purified by trituration with water three times to give glutamate analog \( \text{1bs} \) ((2R*,7S*)-TKM-86, 0.59 mg, 98%) as a colorless oil: IR (ATR) 3504, 3263, 3193, 2931, 1723, 1709, 1701, 1689, 1586, 1412, 1291 cm\(^{-1} \); \(^1\)H NMR (400 MHz, D\(_2\)O) δ 4.86 (d, \( J = 7.0 \) Hz, 1H), 4.76 (d, \( J = 7.0 \) Hz, 1H), 4.56 (m, 1H), 4.50 (d, \( J = 2.5 \) Hz, 1H), 4.23 (s, 1H), 3.68 (m, 1H), 3.31 (s, 1H), 3.14 (dd, \( J = 17.1 \), 9.2 Hz, 1H), 2.97 (d, \( J = 15.7 \) Hz, 1H), 2.83 (dd, \( J = 17.1 \), 5.0 Hz, 1H), 2.77 (d, \( J = 15.7 \) Hz, 1H), 2.50 (t, \( J = 7.3 \) Hz, 2H), 1.48 (tt, \( J = 7.3 \), 7.3 Hz, 2H), 1.31-1.13 (m, 4H), 0.78 (t, \( J = 7.0 \) Hz, 3H); \(^{13}\)C NMR (100 MHz, D\(_2\)O) δ 214.0, 175.5 (×3), 88.0, 85.4, 76.7, 75.4, 69.0, 68.6, 56.8, 42.8 (×2), 41.8, 30.5, 22.8, 21.7, 13.2; HRMS (ESI, negative) calcd for C\(_{18}\)H\(_{24}\)NO\(_9\) [(M-H)-] 398.1457, found 398.1458.

**Benzyl (2S*,3S*,3aS*,6aR*,6aR*)-6a-(2-(benzyloxy)-2-oxoethyl)-3-hydroxy-2-((E)-3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)-4-oxohexahydro-2H-furo[2,3-c]pyrrole-6-carboxylate (S10c)**

To a stirred solution of alkene 7 (10.41 mg, 0.0231 mmol) and 4-methoxyphenyl vinyl ketone (18.7 mg, 0.115 mmol) in CH\(_2\)Cl\(_2\) (0.400 mL) at rt was added Hoveyda-Grubbs catalyst second generation (0.7 mg, 0.001 mmol). After stirring at 50 °C in a sealed tube for 12 h, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 600 mg, EtOAc/hexane = 6:4) to give enone S10c (8.92 mg, 66%) as a brown oil: IR (ATR) 3628, 3276, 2893, 1747, 1735, 1716, 1599, 1456, 1259, 1210 cm\(^{-1} \); \(^1\)H NMR (400 MHz, CDCl\(_3\)) δ 7.92 (d, \( J = 8.9 \) Hz, 2H), 7.37-7.26 (m, 10H), 7.16 (dd, \( J = 15.5 \), 1.6 Hz, 1H), 6.94-6.85 (m, 3H), 5.92 (brs, 1H), 5.14 (d, \( J = 11.9 \) Hz, 1H), 5.09 (d, \( J = 11.9 \) Hz, 1H), 5.07 (s, 2H), 4.66 (m, 1H), 4.62 (m, 1H), 4.41 (s, 1H), 3.85 (s, 3H), 3.29 (s, 1H), 3.21 (brs, 1H), 3.04 (d, \( J = 17.0 \) Hz, 1H), 2.99 (d, \( J = 17.0 \) Hz, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) δ 188.3, 173.7, 170.2, 169.6, 163.6, 139.7, 135.2, 134.5, 131.1, 130.3, 128.8, 128.8 (×2), 128.7 (×2), 128.6 (×2), 128.5 (×2), 127.6, 113.9 (×2), 87.3, 83.3, 76.7, 67.8, 66.9, 65.4, 58.4, 55.5, 39.4; HRMS (ESI, positive)
calcd for C$_{33}$H$_{31}$NO$_9$Na$^+$ [(M+Na)$^+$] 608.1891, found 608.1882.

Benzyl (4R*,4aS*,5aR*,6R*,8aS*,8bS*)-5a-(2-(benzylxylo)-2-oxoethyl)-4-(2-(4-methoxyphenyl)-2-oxoethyl)-8-oxooctahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylate (S11cr), and benzyl (4S*,4aS*,5aR*,6R*,8aS*,8bS*)-5a-(2-(benzylxylo)-2-oxoethyl)-4-(2-(4-methoxyphenyl)-2-oxoethyl)-8-oxooctahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylate (S11cs)

To a stirred solution of enone S10c (7.71 mg, 0.0132 mmol) in CH$_2$Cl$_2$ (0.500 mL) at rt were added paraformaldehyde (0.5 mg, 0.02 mmol) and MsOH (0.0017 mL, 0.026 mmol). After 2 h, the mixture was poured into water (0.5 mL) and extracted with EtOAc (6 × 0.5 mL). Combined extracts were dried over Na$_2$SO$_4$ and concentrated under reduced pressure to give a residue (8.22 mg), which is a mixture composed of N-hydroxymethylated 1,3-dioxanes S12cr, S12cs and 1,3-dioxanes S11cr, S11cs ((S12cr, S12cs)/(S11cr, S11cs) = 1:1.7).

The residue thus obtained, without purification, was dissolved in EtOH (0.500 mL). To the stirred mixture at rt was added ammonium hydroxide (28%, 0.0043 mL, 0.064 mmol). After 19 h, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (60N, 600 mg, EtOAc/hexane = 4:6) to give an inseparable mixture of 1,3-dioxanes S11cr and S11cs (6.75 mg, S11cr/S11cs = 1:2:1) as a brown oil.

Purification of a portion of the mixture (5.39 mg) by HPLC (XTerra™ MS, 4.6 × 150 mm, MeOH/H$_2$O = 7:3, 1.0 mL/min, 40 °C, detected at 254 nm) gave diastereomerically pure 1,3-dioxanes S11cr (7R*, 1.65 mg, 26%, $t_R$ 8.8 min) and S11cs (7S*, 1.26 mg, 19%, $t_R$ 7.4 min).

Data for 1,3-dioxane S11cr (7R*): retention time 8.8 min; IR (ATR) 3312, 2931, 1739, 1724, 1714, 1700, 1261, 1173, 1073, 1032, 822 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.88 (d, $J = 8.9$ Hz, 2H), 7.34-7.25 (m, 10H), 6.89 (d, $J = 8.9$ Hz, 2H), 5.90 (brs, 1H), 5.03 (d, $J = 12.1$ Hz, 1H), 5.02 (s, 2H), 4.97 (d, $J = 6.7$ Hz, 1H), 4.89 (d, $J = 12.1$ Hz,
1H), 4.69 (d, J = 6.7 Hz, 1H), 4.54 (d, J = 2.3 Hz, 1H), 4.40 (ddd, J = 6.9, 6.6, 2.3 Hz, 1H), 4.38 (s, 1H), 3.94 (ddd, J = 2.3, 2.3 Hz, 1H), 3.84 (s, 3H), 3.82 (dd, J = 2.3, 2.3 Hz, 1H), 3.40 (d, J = 17.4 Hz, 1H), 3.31 (dd, J = 17.2, 6.9 Hz, 1H), 3.28 (s, 1H), 3.20 (dd, J = 17.2, 6.6 Hz, 1H), 3.00 (d, J = 17.4 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 195.6, 172.7, 169.9, 169.5, 163.8, 135.6, 134.7, 130.6 (×2), 129.9, 128.7, 128.7 (×2), 128.6 (×2), 128.5 (×2), 128.2, 128.1 (×2), 113.8 (×2), 91.8, 87.7, 77.9, 75.6, 72.2, 67.7, 66.4, 64.9, 56.1, 55.5, 40.1, 39.7; HRMS (ESI, positive) calcd for C$_{34}$H$_{33}$NO$_{10}$Na$^+$ [(M+Na)$^+$] 638.1997, found 638.1988.

Data for 1,3-dioxane S11cs (7S*): retention time 7.4 min; IR (ATR) 3390, 2921, 2849, 1741, 1722, 1714, 1674, 1601, 1261, 1177, 1073 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.88 (d, J = 8.9 Hz, 2H), 7.34–7.25 (m, 10H), 6.92 (d, J = 8.9 Hz, 2H), 5.93 (s, 1H), 5.04 (d, J = 12.1 Hz, 1H), 5.02 (d, J = 12.4 Hz, 1H), 4.99 (d, J = 12.4 Hz, 1H), 4.90 (d, J = 12.1 Hz, 1H), 4.85 (d, J = 6.5 Hz, 1H), 4.83 (d, J = 6.5 Hz, 1H), 4.67 (m, 1H), 4.54 (d, J = 2.3 Hz, 1H), 4.50 (s, 1H), 3.85 (s, 3H), 3.82 (dd, J = 2.3, 2.3 Hz, 1H), 3.40 (d, J = 17.4 Hz, 1H), 3.34 (dd, J = 16.4, 6.7 Hz, 1H), 3.30 (s, 1H), 3.18 (dd, J = 16.4, 7.3 Hz, 1H), 3.00 (d, J = 17.4 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 194.5, 172.7, 169.9, 169.4, 163.9, 135.5, 134.6, 130.4 (×2), 129.5, 128.7, 128.7 (×2), 128.6 (×2), 128.5 (×2), 128.3 (×2), 128.3, 113.9 (×2), 87.8, 86.7, 78.6, 75.7, 69.5, 67.7, 66.5, 64.7, 56.1, 55.5, 40.1, 38.7; HRMS (ESI, positive) calcd for C$_{34}$H$_{33}$NO$_{10}$Na$^+$ [(M+Na)$^+$] 638.1997, found 638.1987.

(4S*,4aR*,5aS*,6S*,8aR*,8bR*)-5a-(Carboxymethyl)-4-(2-(4-methoxyphenyl)-2-oxoethyl)-8-oxooctahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylic acid (1cr, (2R*,7R*)-TKM-99)

A mixture of dibenzyl ester S11cr (1.65 mg, 0.0027 mmol) and Pd/C (5%, 0.3 mg) in MeOH (0.250 mL) and THF (0.250 mL) was stirred under hydrogen atmosphere (balloon) at rt. After 22 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure to give a residue.
The residue and Pd/C (5%, 0.3 mg) were suspended in MeOH (0.250 mL) and THF (0.250 mL), and stirred under hydrogen atmosphere (balloon) at rt. After 14 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure to give a residue.

The residue and Pd/C (5%, 0.3 mg) were suspended in MeOH (0.250 mL) and THF (0.250 mL), and stirred under hydrogen atmosphere (balloon) at rt. After 16 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure to give a mixture mainly composed of glutamate analog 1cr ((2R*,7R*)-TKM-99). Other products generated by over-reduction at the benzylic position were also obtained.

Purification of the mixture by HPLC (XTerra™ MS, 4.6 x 150 mm, CH$_3$CN (0.05% TFA)/H$_2$O (0.05% TFA) = 3:7, 1.0 mL/min, 40 °C, detected at 220 nm) gave glutamate analog 1cr ((2R*,7R*)-TKM-99, 0.50 mg, 43%) as a colorless oil: retention time 13.8 min; IR (ATR) 3418, 3369, 2923, 2851, 1713, 1704, 1693, 1684, 1599, 1512, 1417 cm$^{-1}$; $^1$H NMR (400 MHz, D$_2$O) $\delta$ 7.99 (d, $J = 8.9$ Hz, 2H), 7.05 (d, $J = 8.9$ Hz, 2H), 4.92 (d, $J = 6.8$ Hz, 1H), 4.77 (d, $J = 6.8$ Hz, 1H), 4.53 (m, 1H), 4.50 (d, $J = 2.3$ Hz, 1H), 4.23 (brs, 1H), 3.88-3.83 (m, 4H), 3.57 (dd, $J = 17.3$, 8.9 Hz, 1H), 3.32 (s, 1H), 3.26 (dd, $J = 17.3$, 3.9 Hz, 1H), 2.92 (d, $J = 14.9$ Hz, 1H), 2.77 (d, $J = 14.9$ Hz, 1H); $^{13}$C NMR (100 MHz, D$_2$O) $\delta$ 199.8, 175.2 (x2), 173.7, 164.0, 131.1 (x2), 129.4, 114.1 (x2), 91.4, 87.4, 77.7, 76.5, 72.1, 66.7, 56.6, 55.6, 40.3, 39.7; HRMS (ESI, negative) calcd for C$_{20}$H$_{20}$NO$_{10}$ $^-$ [(M-H)$^-$] 434.1093, found 434.1091.

(4R*,4aR*,5aS*,6S*,8aR*,8bR*)-5a-(Carboxymethyl)-4-((2-(4-methoxyphenyl)-2-oxoethyl)-8-oxooctahydro-[1,3]dioxino[4',5':4,5]furo[2,3-c]pyrrole-6-carboxylic acid (1cs, (2R*,7S*)-TKM-99)

A mixture of dibenzyl ester S11cs (1.26 mg, 0.0010 mmol) and Pd/C (5%, 0.2 mg) in MeOH (0.250 mL) and THF (0.250 mL) was stirred under hydrogen atmosphere (balloon) at rt. After 22 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure to give a residue.
The residue and Pd/C (5%, 0.3 mg) were suspended in MeOH (0.250 mL) and THF (0.250 mL), and stirred under hydrogen atmosphere (balloon) at rt. After 14 h, the mixture was filtered through a pad of Celite and concentrated under reduced pressure to give a residue.

The residue and Pd/C (5%, 0.3 mg) were suspended in MeOH (0.250 mL) and THF (0.250 mL), and the suspension stirred under hydrogen atmosphere (balloon) at rt. After 16 h, the mixture was filtered through a pad of Celite and the filtrate concentrated under reduced pressure to give a mixture mainly composed of glutamate analog 1cs ((2R*,7S*)-TKM-99). Other products generated by over-reduction at the benzylic position were also obtained.

Purification of the mixture by HPLC (XTerra™ MS, 4.6 × 150 mm, CH3CN (0.05% TFA)/ H2O (0.05% TFA) = 3:7, 1.0 mL/min, 40 °C, detected at 220 nm) gave glutamate analog 1cs ((2R*,7S*)-TKM-99), 0.50 mg, 56% as a colorless oil: retention time 13.1 min; IR (ATR) 3428, 3294, 2930, 2852, 1733, 1724, 1714, 1685, 1542, 1471, 1291 cm\(^{-1}\); \(^1\)H NMR (400 MHz, D2O) \(\delta\) 7.96 (d, \(J = 8.9\) Hz, 2H), 7.04 (d, \(J = 8.9\) Hz, 2H), 4.93 (d, \(J = 6.9\) Hz, 1H), 4.84-4.61 (m, 2H), 4.54 (s, 1H), 4.23 (brs, 1H), 3.85 (s, 3H), 3.79 (s, 1H), 3.63 (dd, \(J = 16.9, 8.6\) Hz, 1H), 3.38 (dd, \(J = 16.8, 5.3\) Hz, 1H), 3.37 (s, 1H), 2.92 (m, 1H), 2.82 (m, 1H); \(^13\)C NMR (100 MHz, D2O) \(\delta\) 199.1, 175.0 (×2), 173.6, 164.0, 130.9 (×2), 129.1, 114.2 (×2), 87.2, 85.6, 77.6, 75.0, 69.6, 66.9, 56.8, 55.6, 40.2, 37.6; HRMS (ESI, negative) calcd for C20H20NO10- [(M-H)⁻] 434.1093, found 434.1094.

Methyl (2R*,3R*,3aR*,6S*,6aS*)-3-hydroxy-6a-(2-methoxy-2-oxoethyl)-4-oxo-2-((E)-3-oxobut-1-en-1-yl)hexahydro-2H-furo[2,3-c]pyrrole-6-carboxylate (13)

To a stirred solution of homoallylic alcohol 5 (7.87 mg, 0.0263 mmol) and 3-buten-2-one (0.0107 mL, 0.1316 mmol) in CH2Cl2 (0.5 mL) at rt was added Hoveyda-Grubbs catalyst second generation (0.3 mg, 0.0005 mmol). After stirring at 50 °C in a sealed tube for 20 h, the mixture was concentrated under reduced pressure. The residue was purified by
column chromatography on silica gel (60N, 600 mg, EtOAc) to give enone 13 (8.06 mg, 90%) as a brown oil: IR (ATR) 3627, 2923, 1747, 1733, 1718, 1707, 1544, 1457, 1373, 1171, 1093 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.11 (brs, 1H), 6.73 (dd, J = 16.0, 4.1 Hz, 1H), 6.28 (d, J = 16.0 Hz, 1H), 4.57–4.53 (m, 2H), 4.36 (s, 1H), 3.73 (s, 3H), 3.66 (s, 3H), 3.28 (s, 1H), 3.03 (d, J = 17.5 Hz, 1H), 2.98 (d, J = 17.5 Hz, 1H), 2.25 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 198.3, 174.3, 170.9, 170.2, 140.4, 132.2, 87.1, 82.7, 76.6, 65.5, 58.7, 52.8, 52.1, 39.1, 27.3; HRMS (ESI, positive) calcd for C₁₅H₁₉NO₈Na⁺ [(M+Na)⁺] 364.1003, found 364.1003.

(2R*,4R*,5aR*,6S*,8aR*,8bR*)-5a-(Carboxymethyl)-2-hydroxy-4-methoxy-2-methyl-8-oxodecahydropyrano[2',3':4,5]furo[2,3-c]pyrrole-6-carboxylic acid (2, TKM-15)

To a stirred solution of enone 13 (8.11 mg, 0.0238 mmol) in MeOH (2 mL) at rt was added aqueous LiOH (1 M, 1.31 mL, 1.31 mmol). After 70 h, to the mixture was added Amberlyst 15 ion-exchange resin (wet, 2 g). After stirring at rt for 1 h, insoluble materials were removed by filtration. The filtrate was concentrated by blowing of air at 50 °C. The residue was purified by column chromatography on reversed-phase silica gel (DM1020T, 500 mg, water) to give glutamate analog 2 (TKM-15, 4.35 mg, 53%) as a brown oil: IR (ATR) 3411, 3310, 2950, 2906, 2841, 1722, 1705, 1694, 1442, 1408, 1216 cm⁻¹; ¹H NMR (400 MHz, D₂O) δ 4.59 (s, 1H), 4.54 (m, 1H), 4.17 (m, 1H), 3.87 (ddd, J = 12.5, 4.6, 4.6 Hz, 1H), 3.37 (s, 1H), 3.29 (s, 3H), 3.18 (d, J = 16.2 Hz, 1H), 2.95 (d, J = 16.2 Hz, 1H), 1.86 (dd, J = 12.5, 4.6 Hz, 1H), 1.64 (dd, J = 12.5, 12.5 Hz, 1H), 1.40 (s, 3H); ¹³C NMR (100 MHz, D₂O) δ 175.4, 173.6, 171.8, 98.0, 85.3, 74.7, 74.5, 71.9, 65.2, 56.9, 54.7, 41.3, 34.1, 28.2; HRMS (ESI, negative) calcd for C₁₄H₁₈NO₅⁻ [(M–H)⁻] 344.0987, found 344.0984.
[CONFIGURATIONAL AND CONFORMATIONAL ANALYSIS OF CYCLIC HEMIACETAL 2 (TKM-15)]

The planar structure of TKM-15 (2) was analyzed using 1D and 2D NMR data. As shown in Figure S1A, formation of the hemiacetal ring was confirmed by HMBC correlations from H14 to C8/C9, in addition to the C4-C8 spin system established by COSY, TOCSY, and HSQC spectra.

![Figure S1. Structure analysis of hemiacetal product TKM-15 (2). (A) COSY and HMBC correlations observed. (B) J_{H,H} values. (C) NOESY correlations observed.]

The relative configuration of the hemiacetal ring in TKM-15 (2) was established to be (7S*,9R*) as shown in Figures S1B and S1C. The 7S* stereochemistry was determined by the vicinal coupling constants (\(^3J_{H6,H7} = 5\) Hz, \(^3J_{H7,H8a} = 5\) Hz, \(^3J_{H7,H8b} = 12\) Hz) and NOE correlations (H5/H7). Additional NOE correlations at H8a/H14 and H8b/H14 were observed in the same intensity, which suggested equatorial orientation of the 14-Me group, since the axial orientation of the 14-Me group should exhibit stronger NOE effects with H8a than H8b.

Oxa-Michael reaction and acetalization are known as thermodynamically controlled reactions. Therefore, the analysis that the structure of the product is the one illustrated in Figure S1 is consistent with its thermodynamic stability; the 7-methoxy and the 9-hydroxy groups take equatorial and axial orientations, respectively.
This analysis was supported by density functional theory (DFT) calculation\cite{1} of the possible diastereomers, S2A, S2B, S2C, and S2D (for structures, see Figure S2). The calculations were performed with Spartan '18 (Wavefunction, Irvine, CA, U.S.A.).\cite{2} The theoretical $^{13}$C NMR shifts for four hemiacetals S2A, S2B-S2D were independently obtained by the calculation sequence; 1) conformational search with MMFF94,\cite{3} 2) structural optimizations with HF/3-21G level, 3) energy calculations at $\omega$B97X-D/6-31G* level, 4) structural optimizations with $\omega$B97X-D/6-31G* level, 5) energy calculations at $\omega$B97X-V/6-311+G(2df,2p){6-311+G*} level fixing the geometries to generate Boltzmann distribution, 6) empirically corrected calculations of the $^{13}$C NMR chemical shifts at $\omega$B97X-D/6-31G* level with $\omega$B97X-D/6-31G* model,\cite{4} and 7) correction of the $^{13}$C NMR shift values based on the Boltzmann weighting. Parameters regarding solvents (D$_2$O) were not added in these calculations.

The experimental $^{13}$C values for TKM-15 (2) (\textit{2}_{\text{obs}}), and the calculated $^{13}$C values for S2A (S2A\text{calc}), S2B (S2B\text{calc}), S2C (S2C\text{calc}), and S2D (S2D\text{calc}) are summarized in Table S1. The calculated $^{13}$C NMR shifts of S2A were consistent well with the experimental values for TKM-15 (2); the root mean square deviation (RMS) value of correct structure S2A was the smallest among those of the candidates (S2A, 1.79 ppm; 7-\textit{epi} stereoisomer S2B, 2.29 ppm; 9-\textit{epi} stereoisomer S2C, 2.73 ppm; 7,9-\textit{epi} stereoisomer S2D, 2.71 ppm). Furthermore, analysis using DP4 probability statistics\cite{1a, 5} revealed that S2A was by far the highest probability (S2A, 98.4%; 7-\textit{epi} stereoisomer S2B, 1.6%;
9-epi stereoisomer S2C, 0.0%; 7,9-epi stereoisomer S2D, 0.0%). The relative configuration of the hemiacetal TKM-15 (2) was thus unambiguously assigned to be (7S*,9R*).

**Table S1.** Comparison of experimental $^{13}$C shifts of TKM-15 (2), and calculated $^{13}$C shifts for four candidates S2A and S2B–S2D.

| Position $^a$ | Experimental $^{13}$C NMR data were collected at 100 MHz in D$_2$O. | Calculated $^c$ |
|--------------|---------------------------------------------------------------------|-----------------|
|              | $^{13}$C NMR data were obtained employing ωB97X-V/6-311+G(2df,2p)-[6-311+G*]//ωB97X-D/6-31G* model. For detail, see text. |
|              |                                                                     |
| $a$          | 85.3                                                                | 89.3 (S2A$_{calc}$) |
|             | 89.7                                                                | 90.3 (S2B$_{calc}$) |
|             | 90.3                                                                | 90.0 (S2C$_{calc}$) |
|             |                                                                     | 90.0 (S2D$_{calc}$) |
| $b$          | 54.7                                                                | 55.0 (S2A$_{calc}$) |
|             | 55.4                                                                | 54.9 (S2B$_{calc}$) |
|             | 55.0                                                                | 55.0 (S2D$_{calc}$) |
| $c$          | 74.5                                                                | 76.8 (S2A$_{calc}$) |
|             | 73.3                                                                | 77.3 (S2B$_{calc}$) |
|             |                                                                     | 76.9 (S2C$_{calc}$) |
| $d$          | 74.7                                                                | 77.8 (S2A$_{calc}$) |
|             | 77.4                                                                | 80.5 (S2B$_{calc}$) |
|             |                                                                     | 80.3 (S2D$_{calc}$) |
| $e$          | 171.8                                                               | 172.4 (S2A$_{calc}$) |
|             | 172.3                                                               | 172.6 (S2B$_{calc}$) |
|             |                                                                     | 173.4 (S2C$_{calc}$) |
| $f$          | 65.2                                                                | 65.2 (S2A$_{calc}$) |
|             | 65.3                                                                | 65.8 (S2B$_{calc}$) |
|             |                                                                     | 67.9 (S2D$_{calc}$) |
| $g$          | 71.9                                                                | 72.2 (S2A$_{calc}$) |
|             | 76.7                                                                | 74.2 (S2B$_{calc}$) |
|             |                                                                     | 75.1 (S2C$_{calc}$) |
| $h$          | 34.1                                                                | 34.6 (S2A$_{calc}$) |
|             | 30.3                                                                | 35.7 (S2B$_{calc}$) |
|             |                                                                     | 31.9 (S2C$_{calc}$) |
| $i$          | 98                                                                  | 98.3 (S2A$_{calc}$) |
|             | 97.5                                                                | 99.6 (S2B$_{calc}$) |
|             |                                                                     | 98.3 (S2C$_{calc}$) |
| $j$          | 173.6                                                               | 173.0 (S2A$_{calc}$) |
|             | 173.0                                                               | 173.0 (S2B$_{calc}$) |
|             |                                                                     | 173.1 (S2C$_{calc}$) |
| $k$          | 41.3                                                                | 39.1 (S2A$_{calc}$) |
|             | 39.6                                                                | 39.6 (S2B$_{calc}$) |
|             |                                                                     | 41.2 (S2C$_{calc}$) |
| $l$          | 175.4                                                               | 174.1 (S2A$_{calc}$) |
|             | 173.4                                                               | 174.8 (S2B$_{calc}$) |
|             |                                                                     | 174.8 (S2C$_{calc}$) |
| $m$          | 28.2                                                                | 30.1 (S2A$_{calc}$) |
|             | 28.4                                                                | 23.4 (S2B$_{calc}$) |
|             |                                                                     | 24.1 (S2C$_{calc}$) |
| $n$          | 56.9                                                                | 55.3 (S2A$_{calc}$) |
|             | 56.3                                                                | 57.2 (S2B$_{calc}$) |
|             |                                                                     | 55.9 (S2C$_{calc}$) |
| RMS/ppm      |                                                                     | 1.79 (S2A$_{calc}$) |
|             |                                                                     | 2.29 (S2B$_{calc}$) |
|             |                                                                     | 2.73 (S2C$_{calc}$) |
| DP4/%        |                                                                     | 98.4 (S2A$_{calc}$) |
|             |                                                                     | 1.6 (S2B$_{calc}$) |
|             |                                                                     | 0.0 (S2C$_{calc}$) |

$^a$ For numbering, see Figure S2.

$^b$ Experimental $^{13}$C NMR data were collected at 100 MHz in D$_2$O.

$^c$ Calculated $^{13}$C NMR data were obtained employing ωB97X-V/6-311+G(2df,2p)-[6-311+G*]//ωB97X-D/6-31G* model. For detail, see text.
Final geometries used for NMR calculations ($\omega$B97X-D/6-31G*)

(7S*,9R*)-S2A, M0003:M0001

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.0834830380 | 0.3767716184 | -1.2526613461 |
| 2 | C    | -1.5450285438  | 0.0454700098  | -0.9040640582  |
| 3 | C    | -1.4813492209  | -0.4396060073  | 0.5358788120   |
| 4 | C    | -0.1634221875  | -1.2205914809  | 0.5331578063   |
| 5 | O    | 0.6987249970   | -0.4371176551  | -0.3295136230  |
| 6 | C    | -1.8967348930  | -1.1276022031  | -1.8091367097  |
| 7 | N    | -0.9024365382  | -1.2544474283  | -2.7206775027  |
| 8 | C    | 0.1460043413   | -0.2401057358  | -2.6479981958  |
| 9 | C    | 0.4813200949   | -1.3591713949  | 1.9067201077   |
|10 | C    | 0.5105906006   | -0.0133678173  | 2.6130833183   |
|11 | C    | -0.8851933874  | 0.5757794216   | 2.6747213054   |
|12 | O    | -1.3857903791  | 0.7526375059   | 1.3400257309   |
|13 | O    | -2.8718139042  | -1.8403974910  | -1.6962683959  |
|14 | C    | -0.0324619572  | 0.6748488315   | -3.8317473612  |
|15 | O    | -0.2289961984  | 1.8601504461   | -3.8594869593  |
|16 | O    | 0.0528684090   | -0.0675988885  | -4.9630097929  |
|17 | C    | 0.3294768314   | 1.8174011960   | -1.0330694446  |
|18 | C    | 1.7632014304   | 2.0230436535   | -1.4097977801  |
|19 | O    | 2.3940406481   | 1.374640538    | -2.2069468001  |
|20 | O    | 2.2891017040   | 3.0910848460   | -0.7719378675  |
|21 | H    | -2.2341515099  | 0.8674886208   | -1.0207067060  |
|22 | H    | -2.3286657512  | -1.0406774696  | 0.8178815971   |
|23 | H    | -0.3343722085  | -2.1899371744  | 0.0859050586   |
|24 | C    | -0.9568271203  | 1.9449268400   | 3.3261780872   |
|25 | O    | -1.6885674526  | -0.3855069035  | 3.3545618501   |
|26 | O    | 1.8465801997   | -1.7790139472  | 1.8432308072   |
|27 | C    | 2.1310737207   | -2.9876205442  | 1.1213464781   |
|28 | H    | 1.1349842285   | -0.6576054906  | -2.6817147901  |
|29 | H    | -0.1123611944  | -2.0599059736  | 2.4787632790   |
|30 | H    | -0.9195843698  | -1.9379908478  | -3.4459928678  |
|31 | H    | 0.8998984628   | -0.1423077916  | 3.6116397797   |
(7S*,9R*)-S2A, M0003:M0002

| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 1 C  | 0.1315534715 | 0.2777574217 | -1.2231962281 |
| 2 C  | -1.3031732893  | -0.1323065890  | -0.8460033275  |
| 3 C  | -1.1837982305  | -0.5971056581  | 0.5935098011   |
| 4 C  | 0.1853071533   | -1.2807237047  | 0.5867347336   |
| 5 O  | 0.9817677899   | -0.4223489154  | -0.271000064   |
| 6 C  | -1.6281969385  | -1.3072518748  | -1.7488310266  |
| 7 N  | -0.6389554531  | -1.4062733900  | -2.6739380065  |
| 8 O  | 0.3922578921   | -0.3962305387  | -2.6062878719  |
| 9 C  | 0.3979901268   | -1.3750248248  | 1.9588072769   |
| 10 O | 0.7978779791   | -0.0218281270  | 2.6498226310   |
| 11 C | -0.6304946539  | 0.4860342404   | 2.7113189831   |
| 12 O | -1.1505410724  | 0.6130833511   | 1.3802018144   |
| 13 O | -2.5802557162  | -2.0489529989  | -1.6352527584  |
| 14 C | 0.3938342574   | 0.5323353738   | -3.793192993   |
| 15 O | 1.1268212732   | 1.4847442236   | -3.8942349246  |
| 16 O | -0.4344723717  | 0.1401652335   | -4.7734044243  |
| 17 C | 0.4625318040   | 1.7509903015   | -1.0817208927  |
| 18 C | -0.4280795051  | 2.6467969852   | -1.8774832054  |
| 19 O | -1.3723188149  | 2.3110079746   | -2.5528062226  |
| 20 O | -0.0740072011  | 3.9377309342   | -1.7297438152  |
| 21 H | -2.0233733704  | 0.6558145412   | -0.9713049166  |
(7S*, 9R*)-S2A, M0003:M0003

| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 1    | 0.0821918796 | 0.2366940958 | -1.2524271021 |
| 2    | -1.3476984061 | -0.1716680592 | -0.8783909851 |
| 3    | -1.2347708690 | -0.6195122515 | 0.5677429146 |
| 4    | 0.1265535190 | -1.3205058545 | 0.5651008532 |
| 5    | 0.9315624330 | -0.4919791640 | -0.3142119970 |
| 6    | -1.6462454186 | -1.3746117850 | -1.7565346129 |
| 7    | -0.6456735611 | -1.4797660970 | -2.6702804417 |
| 8    | 0.3425999756 | -0.4216907785 | -2.6382789470 |
| 9    | 0.7840340142 | -1.4028503205 | 1.936329826 |
| 10   | 0.7546469080 | -0.0439928188 | 2.6164711747 |
| 11   | -0.6698798434 | 0.4744440621 | 2.6780904550 |
| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 12   | -1.1914766714 | 0.59540555357 | 1.3466341760 |
| 13   | -2.5817020986 | -2.1336380726 | -1.6261815141 |
| 14   | 0.1978880383  | 0.4396555941  | -3.8640819799 |
| 15   | -0.5203454863 | 0.2385834634  | -4.7994747369 |
| 16   | 1.1087065039  | 1.4515103339  | -3.8398422115 |
| 17   | 0.4396865959  | 1.6998605751  | -1.0735356306 |
| 18   | -0.4042620406 | 2.6292775944  | -1.8753964077 |
| 19   | -1.3802131452 | 2.3433785170  | -2.5264239859 |
| 20   | 0.0304235046  | 3.9023144689  | -1.7620353289 |
| 21   | -2.0718022953 | 0.6094423745  | -1.0264316861 |
| 22   | -2.0414077160 | -1.2604011065 | 0.8800597305 |
| 23   | 0.0141495163  | -2.3028428094 | 0.1279860526 |
| 24   | -0.8050241838 | 1.8514301659  | 3.3028097496 |
| 25   | -1.4158530480 | -0.5097659657 | 3.3894954174 |
| 26   | 2.1642031004  | -1.7706406238 | 1.8695506431 |
| 27   | 2.4651682075  | -3.0627196885 | 1.3206958158 |
| 28   | 1.3552328293  | -0.7973362348 | -2.6174705011|
| 29   | 0.2240420747  | -2.1162588678 | 2.5268474323 |
| 30   | -0.6951994431 | -2.1393260762 | -3.4168020766|
| 31   | 1.1552620280  | -0.1350498984 | 3.6148528931 |
| 32   | 1.3660040766  | 0.6301396619  | 2.0368336010 |
| 33   | 1.0720263701  | 1.9909605212  | -4.643839870 |
| 34   | 1.4762254264  | 1.8740435734  | -3.143735982 |
| 35   | 0.2752201040  | 1.9263611961  | -0.030560286 |
| 36   | -0.5346089486 | 4.5236099250  | -2.245044747 |
| 37   | -1.8373425076 | 2.1754785438  | 3.2442655581 |
| 38   | -0.4962646955 | 1.8130798030  | 4.3386507170 |
| 39   | -0.1936652430 | 2.5643183373  | 2.7679263481 |
| 40   | -2.3419741985 | -0.2445519295 | 3.4793069685 |
| 41   | 2.2817018407  | -3.0931229532 | 0.254203080 |
| 42   | 1.8878923488  | -3.8449646095 | 1.8046756871 |
| 43   | 3.5149885250  | -3.2327933376 | 1.5033479354 |

(7S*, 9R*)-S2A, M0003:M0004
| Atom | X Coordinates | Y Coordinates | Z Coordinates |
|------|---------------|---------------|---------------|
| C    | -1.3155567113 | -0.2236266224 | -1.0351429139 |
| C    | -1.2183258270 | -0.6791461645 | 0.4088445083  |
| C    | 0.1684730503  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| O    | 0.9582385032  | -0.4119920605 | -0.3673561574 |
| C    | -1.5978208227 | -1.4081398771 | -1.9391591826 |
| N    | -0.5735221741 | -1.5077000882 | -2.8239716591 |
| C    | 0.4525509098  | -0.4937000247 | 0.4088445083  |
| C    | 0.7587961501  | -1.3211246394 | 0.4436132058  |
| I | Atom | X           | Y           | Z           |
|---|------|-------------|-------------|-------------|
| 1 | C    | -0.2812499823 | -0.1071453205 | -1.3317450215 |
| 2 | C    | -1.6219736791  | 0.2959703531  | -0.7150505563 |
| 3 | C    | -1.5073531369  | -0.0641239289  | 0.7504848383 |
| 4 | C    | -0.5631054976  | -1.2856410866  | 0.7435834013 |
| 5 | O    | 0.0813173400   | -1.2870485104  | -0.5554726475 |
| 6 | C    | -2.6168793949  | -0.6320666721  | -1.4041012646 |
| 7 | N    | -2.0223144044  | -1.1004151553  | -2.5270034343 |
| 8 | C    | -0.6391387900  | -0.6826602543  | -2.716436358 |
| 9 | C    | 0.4730026032   | -1.205447987   | 1.8764656851 |
|10 | C    | -0.1983819655  | -0.6019882411  | 3.1059657709 |
|11 | C    | -0.6560168964  | 0.8358877237  | 2.8229926962 |
|12 | O    | -0.8685543199  | 1.0351231834  | 1.4185892536 |
|13 | O    | -3.7277030901  | -0.9039038686  | -1.0008214842 |
|14 | C    | -0.5792702184  | 0.2855338162  | -3.8692290295 |
|15 | O    | -0.0670979976  | 1.3724743850  | -3.9134399723 |
|16 | O    | -1.1890344021  | -0.2664159696  | -4.9454475019 |
|17 | C    | 0.8198480532   | 0.9262772205  | -1.2167178298 |
|18 | C    | 2.0560175483   | 0.4933332865  | -1.9349091763 |
|19 | O    | 2.1643304558   | -0.4124542433 | -2.7241429461 |
|20 | O    | 3.1125356512   | 1.2709392458  | -1.5959927229 |
|21 | H    | -1.8878369033  | 1.3336541529  | -0.8494566859 |
|22 | H    | -2.4662992058  | -0.2756886970  | 1.1950792848 |
|23 | H    | -1.1324017064  | -2.1984640914  | 0.8390007684 |
|24 | C    | 0.3526204122   | 1.8916554336  | 3.2343845184 |
|25 | O    | -1.8969061825  | 0.9722218509  | 3.5101127638 |
|26 | O    | 1.5880263553   | -0.3758340928  | 1.5249251297 |

(7S*,9R*)-S2A, M0003:M0005
| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | 0.3173399356 | 0.1378331367 | -1.4334478176 |
| 2 | C    | -0.1078752716 | 1.5779086634 | -1.0911581580 |
| 3 | C    | -0.5748678499 | 1.4816703343 | 0.3525698735 |
| 4 | C    | -1.2678680260 | 0.1173236553 | 0.3602277151 |
| 5 | O    | -0.3972451456 | -0.6910493874 | -0.4707766589 |
| 6 | C    | -1.3130540641 | 1.8481514906 | -1.9815128215 |
| 7 | N    | -1.4045001421 | 0.8283153228 | -2.8678878082 |
| 8 | C    | -0.3264954582 | -0.1559824533 | -2.8049423642 |
| 9 | C    | -1.3782380312 | -0.4918027334 | 1.7429566805 |
| 10| C    | -0.0030084531 | -0.5204691121 | 2.3986409510 |
| 11| C    | 0.5455044655 | 0.8971933046 | 2.4585726185 |
| 12| O    | 0.6381818094 | 1.4443570920 | 1.1374245641 |
| 13| O    | -2.0741346795 | 2.7869099649 | -1.8743853303 |
| 14| C    | 0.5375160081 | 0.0579719455 | -4.0207909728 |
| 15| O    | 1.7022382254 | 0.3462526706 | -4.0921943838 |

(7S*,9R*)-$S_{2A}$, M0003:M0006
(7S*,9R*)-S2A, M0003:M0007

| ATOM | X        | Y        | Z        |
|------|----------|----------|----------|
| 1    | C        | -0.3652723446 | 0.1166362923 | -1.3433452839 |
| 2    | C        | 0.0052831040  | 1.4686637178  | -0.7352998428  |
| 3    | C        | -0.3060209542 | 1.3326728635  | 0.7368309493   |
| 4    | C        | -1.4863139106 | 0.3398339998  | 0.7674560959   |
| 5    | O        | -1.4914957217 | -0.3172987359 | -0.5270384378  |
6 C -0.9559581036  2.4372861627  -1.4038411206
7 N -1.4423313323  1.8260327568  -2.5152486086
8 C -1.0110923452  0.4621492648  -2.7150871185
9 C -1.3369334534  -0.6868892450  1.9024986963
10 C -0.7112608789  0.0054791392  3.1089615225
11 C  0.6977410919  0.5143233442  2.7726897056
12 O  0.8388527896  0.7287202014  1.3629447315
13 O  0.1596527606  1.4107851748  4.5659048308
14 C  0.0832345826  -0.7944383920  -3.881767294
15 O  0.3545200222  0.7287202014  -4.2172115540
16 O  0.5143233442  0.7287202014  -4.5659048308
17 C  0.6926520424  -0.9690446560  3.1089615225
18 C  2.0017542271  -0.5794409038  2.7726897056
19 O  0.3545200222  -0.7944383920  1.3629447315
20 O  0.1596527606  1.4107851748  4.5659048308
21 H  0.6926520424  -0.9690446560  -1.2972580929
22 H  0.0832345826  -0.7944383920  -3.881767294
23 H  0.6926520424  -0.9690446560  -4.2172115540
24 O  0.8167450183  1.7603313389  3.453543029
25 O  0.8167450183  1.7603313389  3.453543029
26 O  0.1596527606  1.4107851748  1.3629447315
27 C  0.1596527606  1.4107851748  4.5659048308
28 H  0.6926520424  -0.9690446560  3.1089615225
29 H  0.6926520424  -0.9690446560  4.5659048308
30 H  0.6926520424  -0.9690446560  3.1089615225
31 H  0.1596527606  1.4107851748  4.5659048308
32 H  0.1596527606  1.4107851748  3.1089615225
33 H  0.1596527606  1.4107851748  4.5659048308
34 H  0.1596527606  1.4107851748  3.1089615225
35 H  0.1596527606  1.4107851748  4.5659048308
36 H  0.1596527606  1.4107851748  3.1089615225
37 H  0.1596527606  1.4107851748  4.5659048308
38 H  0.1596527606  1.4107851748  3.1089615225
39 H  0.1596527606  1.4107851748  4.5659048308
40 H  0.1596527606  1.4107851748  3.1089615225
41 H  0.1596527606  1.4107851748  4.5659048308
(7S*, 9R*)-S2A, M0003:M0008

| I | Atom | X            | Y            | Z            |
|---|------|--------------|--------------|--------------|
| 1 | C    | 0.0840193440 | 0.2974278596 | -1.2986902749 |
| 2 | C    | -1.4084749485| -0.0374565970| -1.1217872690 |
| 3 | C    | -1.5399098640| -0.3642863606| 0.3594026457  |
| 4 | C    | -0.2244264587| -1.1055988318| 0.6221620653  |
| 5 | O    | 0.7377353475 | -0.3949696410| -0.196334664  |
| 6 | C    | -1.6152574064| -1.3091199605| -1.9322778396 |
| 7 | N    | -0.4893212764| -1.5171916406| -2.6584880922 |
| 8 | C    | 0.5082780605 | -0.4576869283| -2.5773702084 |
| 9 | C    | 0.2310707173 | -1.0704182303| 2.0748785508  |
|10 | C    | 0.1657071194 | 0.3514721115 | 2.6076608990  |
|11 | C    | -1.2354366976| 0.9044162296 | 2.4291554999  |
|12 | O    | -1.5724760293| 0.9099949687 | 1.0316578298  |
|13 | O    | -2.5942496139| -2.0237962378| -1.8921288975 |
|14 | C    | 0.5000772064 | 0.3213328619 | -3.8716307435 |
|15 | O    | 0.5372199970 | 1.5093997610 | -4.045376744  |
|16 | O    | 0.4926102876 | -0.5513831359| -4.9120964703 |
|17 | C    | 0.4291274705 | 1.7669768380 | -1.1580904972 |
|18 | C    | 1.9030994021 | 1.9805458343 | -0.9987405595 |
|19 | O    | 2.4265181078 | 2.7842045865 | -0.2767870220 |
|20 | O    | 2.6326078752 | 1.1808464377 | -1.8251295996 |
|21 | H    | -2.0856853157| 0.7491079124 | -1.4166518227 |
|22 | H    | -2.4108093400| -0.9545745667| 0.5869597638  |
|23 | H    | -0.3197325430| -2.1217215089| 0.2662039588  |
|24 | C    | -1.4068319543| 2.3378910864 | 2.8971215490  |
|25 | O    | -2.1022251878| 0.0041473419 | 3.1145528908  |
|26 | O    | 1.5928893032 | -1.4759515908| 2.2341125314  |
|27 | C    | 1.9314092351 | -2.8098686618| 1.8246001456  |
|28 | H    | 1.5039180888 | -0.8289568322| -2.4146109618 |
|29 | H    | -0.4316874577| -1.7061107890| 2.6465198548  |
|30 | H    | -0.4156133286| -2.2501654795| -3.3295379047 |
|   |   |       |       |       |
|---|---|-------|-------|-------|
|31| H | 0.4276749885 | 0.3526937363 | 3.6546998200 |
|32| H | 0.8710559909 | 0.9486107188 | 2.0510197128 |
|33| H | 0.5177901347 | -0.1009078017 | -5.7688657495 |
|34| H | -0.0536962157 | 2.1212157045 | -0.2650841194 |
|35| H | 0.0938330066 | 2.3329458616 | -2.0119379530 |
|36| H | 3.5845842551 | 1.3160598689 | -1.7103279308 |
|37| H | -2.4122180838 | 2.6738124144 | 2.673248322 |
|38| H | -1.2340623165 | 2.9806301230 | 2.3811470441 |
|39| H | -3.5845842551 | 1.3160598689 | -1.7103279308 |
|40| H | -0.0536962157 | 2.1212157045 | -0.2650841194 |
|41| H | -0.0536962157 | 2.1212157045 | -0.2650841194 |
|42| H | -0.0536962157 | 2.1212157045 | -0.2650841194 |

\[(7S^*, 9R^*)-S2A, \text{ M0003:M0009}\]

| ATOM | X   | Y   | Z   |
|------|-----|-----|-----|
| 1    | C   | 0.0774679415 | 0.1741998448 | -1.4096165030 |
| 2    | C   | -1.3605135918 | -0.2555756074 | -1.0662875384 |
| 3    | C   | -1.2673863316 | -0.6922542693 | 0.3843141494 |
| 4    | C   | 0.1058580696 | -1.3650365240 | 0.4184928585 |
| 5    | O   | 0.9104719584 | -0.4933031717 | -0.418682579 |
| 6    | C   | -1.6246323325 | -1.4697624436 | -1.9391747603 |
| 7    | N   | -0.5144463286 | -1.5850410374 | -2.8130226736 |
| 8    | C   | 0.3923029777 | -0.5231248343 | -2.7652695753 |
| 9    | C   | 0.7041642690 | -1.4478038938 | 1.8074206502 |
| 10   | C   | 0.6990132457 | -0.0666290505 | 2.4515374271 |
| 11   | C   | -0.7272219505 | 0.4617964249 | 2.4819077531 |
| 12   | O   | -1.2503730905 | 0.5354277032 | 1.1506897814 |
| 13   | O   | -2.5636115165 | -2.2284302793 | -1.8322454341 |
| 14   | C   | 0.3017271392 | 0.2986631144 | -4.0230745888 |
| 15   | O   | -0.3531898626 | 0.0515930904 | -4.9936661256 |
| 16   | O   | 1.1853095996 | 1.3339469247 | -3.9781294876 |
| 17   | C   | 0.3847285879 | 1.6519744856 | -1.2691164403 |
| 18   | C   | -0.4487142572 | 2.5270671155 | -2.1399016430 |
| 19   | O   | -1.3892024159 | 2.1880657940 | -2.8172396719 |
| 20   | O   | -0.0532244475 | 3.8157524975 | -2.0613558769 |


(7S*,9R*)-S2A, M0003:M0010

| I | Atom | X           | Y           | Z           |
|---|------|-------------|-------------|-------------|
| 1 | C    | 0.1162122054 | 0.3868246450| -1.4393307726|
| 2 | C    | -1.3528065573 | 0.1112635903| -1.0428582935|
| 3 | C    | -1.2611906544 | -0.4690048260| 0.3695678079|
| 4 | C    | 0.0836296921  | -1.2020050161| 0.3157798700|
| 5 | O    | 0.9170501759  | -0.2938538593| -0.4505090607|
| 6 | C    | -1.8336253210 | -0.9803422113| -1.9786299137|
| 7 | N    | -0.8432799622 | -1.2323366810| -2.8741962800|
| 8 | C    | 0.3100532745  | -0.3644497382| -2.8045794350|
| 9 | C    | 0.7247265233  | -1.4371887540| 1.6757824519|
10  C  0.7265669642  -0.143179318  2.4718255401
11  C  -0.6917252896  0.3811091841  2.5895098950
12  O  -1.2108507708  0.6511608809  1.2731319522
13  O  -2.8890176424  -1.5694521610  -1.8994825536
14  C  0.3489263850  0.5425750880  -4.0052048659
15  O  -0.5358507963  0.7506110736  -4.7870508544
16  O  1.5748581278  1.1132924662  -4.1074042741
17  C  0.5623024636  1.8522129364  -1.4793837193
18  O  -0.5358507963  0.7506110736  -4.7870508544
19  O  1.5748581278  1.1132924662  -4.1074042741
20  O  -1.0825155280  3.0059407245  -0.286431417
21  H  -1.9819304631  0.9836623158  -1.0729668379
22  H  -2.0872229542  -1.1191870443  0.6021804985
23  H  -0.0399972337  -2.1274562496  -0.2307545302
24  C  -0.8015538040  1.6869196721  3.3511648020
25  O  -1.4610414631  -0.6615849437  3.1842044856
26  O  2.0911518271  -1.8453624848  1.5727803890
27  C  2.3374633116  -3.1334591730  0.9911248618
28  H  1.2453888588  -0.8964766286  -2.7461168756
29  H  0.1395649910  -2.1849150356  2.1953809271
30  H  -0.9810916631  -1.8814429303  -3.6192261849
31  H  1.1308218699  -0.3292383018  3.4557717940
32  H  1.3282296652  0.5838737655  1.951266816
33  H  1.6454688126  1.7117487051  -4.8661797518
34  H  0.0668191826  2.3664239229  -2.2877653570
35  H  1.6310490776  1.8745419313  -1.6109371071
36  H  -1.4204227334  3.2997285973  0.5709535403
37  H  -1.8316913515  2.0285871707  3.3450813464
38  H  -0.4891443433  1.5338276972  4.3793945781
39  H  -0.1742491243  2.4284195225  2.8850828878
40  H  -2.3741160886  -0.3774012746  3.3302781871
41  H  2.1252989113  -3.1407012598  -0.0711575510
42  H  1.7490750724  -3.9074975644  1.4752337332
43  H  3.3861334727  -3.3393898407  1.1407122607

(7S*,9R*)-S2A, M0003:M0011
| I | Atom | X         | Y         | Z         |
|---|------|-----------|-----------|-----------|
| 1 | C    | -0.3134043437 | 0.1085020779 | -1.2547513873 |
| 2 | C    | -1.7459222489 | 0.0886541025 | -0.6916074143 |
| 3 | C    | -1.5548073977 | -0.2401853794 | 0.7806927118  |
| 4 | C    | -0.4044302361 | -1.2481549200 | 0.7278462531  |
| 5 | O    | 0.4531835548  | -0.6941354711 | -0.3093908265 |
| 6 | C    | -2.4167945480 | -1.0917592810 | -1.3799068641 |
| 7 | N    | -1.5865032688 | -1.5200852062 | -2.3614002478 |
| 8 | C    | -0.3821619149 | -0.7208218423 | 2.5092046187  |
| 9 | C    | 0.3520868153  | -1.3686551363 | 2.0418478887  |
|10 | C    | 0.38438441321 | 0.0198302296  | 2.5092046187  |
|11 | C    | -0.4547921852 | 0.8937157041  | 2.5092046187  |
|12 | O    | -1.1229474239 | 0.9967828611  | 1.388668272   |
|13 | O    | -3.4821082154 | -1.5795612134 | -1.0674321468 |
|14 | C    | -0.5392795166 | 0.0463965678  | -3.8459424022 |
|15 | O    | -0.4399505765 | 1.2273469043  | -4.0471119856 |
|16 | O    | -0.8157966454 | -0.8315711082 | -4.8403962394 |
|17 | C    | 0.3453106155  | 1.4707093430  | -1.3098254598 |
|18 | C    | 1.7302449425  | 1.3752772284  | -1.8679694001 |
|19 | O    | 2.1776086543  | 0.4800978289  | -2.5396157935 |
|20 | O    | 2.4545660878  | 2.4728977946  | -1.5556842101 |
|21 | H    | -2.2971176029 | 1.0058282279  | -0.8290679734 |
|22 | H    | -2.4431030300 | -0.6258727402 | 1.2505506714  |
|23 | H    | -0.7654982470 | -2.2186849100 | 0.4211332087  |
|24 | C    | -0.1565147527 | 2.3206617633  | 3.0794597630  |
|25 | O    | -1.3031698934 | 0.2279713544  | 3.5852821043  |
|26 | O    | 1.4037227151  | -2.3350278776 | 1.9907977536  |
|27 | C    | 2.5807381220  | -2.0694831962 | 1.1965306342  |
|28 | H    | 0.5097714294  | -1.316851038  | -2.6248928597 |
|29 | H    | -0.3382745732 | -1.7591810043 | 2.7713493816  |
|30 | H    | -1.8205435578 | -2.2704366794 | -2.9744048847 |
|31 | H    | 1.2828764474  | -0.0549220907 | 3.4645254653  |
|32 | H    | 1.4376928987  | 0.4764714078  | 1.7830657347  |
|33 | H    | -0.9128016459 | -0.3965486872 | -5.7002341350 |
|34 | H    | 0.3776609897  | 1.8575740311  | -0.3066299576 |
| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.0466812055 | -0.0313368387 | -1.2309408590 |
| 2 | C    | -1.4945925169 | -0.0318379854 | -0.7079253351 |
| 3 | C    | -1.3500625119 | -0.3711827484 | 0.7629493573 |
| 4 | C    | -0.1968452166 | -1.3756405620 | 0.7475545786 |
| 5 | O    | 0.7017414411 | -0.8037184064 | -0.2490736455 |
| 6 | C    | -2.1833677401 | -1.1673681580 | -1.4409314717 |
| 7 | N    | -1.3411377055 | -1.6052498935 | -2.4121933389 |
| 8 | C    | -0.0863784177 | -0.8981475396 | -2.5288150662 |
| 9 | C    | 0.4979633127 | -1.5106676651 | 2.0938815122 |
|10 | C    | 0.9136703148 | -0.1288162842 | 2.5939714640 |
|11 | C    | -0.3255437784 | 0.7515907036 | 2.6853844268 |
|12 | O    | -0.9341696309 | 0.8633004853 | 1.3922440068 |
|13 | O    | -3.2735599877 | -1.6254699298 | -1.176544677 |
|14 | C    | 0.0511301698 | -0.1373272001 | -3.8282034829 |
|15 | O    | 0.9787025591 | 0.5907976142 | -4.0757714378 |
|16 | O    | -0.9134627819 | -0.4270154964 | -4.708866783 |
|17 | C    | 0.6286068847 | 1.3254530431 | -1.2998651762 |
|18 | C    | -0.0942396230 | 2.3130125431 | -2.155028545 |
|19 | O    | -1.1520376423 | 2.1440642603 | -2.7137440255 |
|20 | O    | 0.5710054150 | 3.4823238034 | -2.2117845174 |
|21 | H    | -2.0106922041 | 0.8963919382 | -0.8737945975 |
|22 | H    | -2.2517151760 | -0.7584728354 | 1.2058303091 |
|23 | H    | -0.5409623641 | -2.3429656543 | 0.4110847320 |

(7S*,9R*)-S2A, M0003:M0012
| I | Atom | X         | Y         | Z         |
|---|------|-----------|-----------|-----------|
| 24 | C    | -0.0364872197 | 2.1738981848 | 3.1317739310 |
| 25 | O    | -1.2187292873 | 0.0898084904 | 3.5758724904 |
| 26 | O    | 1.5449815363  | -2.4846079767 | 2.0846089058 |
| 27 | C    | 2.7759172707  | -2.1928419513 | 1.3898527142 |
| 28 | H    | 0.7648548804  | -1.5618807944 | -2.4670305819 |
| 29 | H    | -0.2303447798 | -1.9035857115 | 2.7847994421 |
| 30 | H    | -1.6339834454 | -2.2773695630 | -3.0874361852 |
| 31 | H    | 1.3651434488  | 0.3292528175  | 1.9048601845 |
| 32 | H    | -0.8205214597 | 0.0794073888  | -5.5293290229 |
| 33 | H    | 1.6414099924  | 1.2364908115  | -1.6615743281 |
| 34 | H    | 0.6423846888  | 1.7084539682  | -0.2899506303 |
| 35 | H    | 0.1216125633  | 4.1312552935  | -2.7731525178 |
| 36 | H    | 0.3539626995  | 2.1655319195  | 4.1403950708 |
| 37 | H    | 0.7637471960  | 0.4596299222  | -0.3612279072 |
| 38 | H    | -0.9505876339 | 2.7550280749  | 3.1027927167 |
| 39 | H    | 1.5262912151  | 0.5953630517  | 3.6849934396 |
| 40 | H    | 1.6414099924  | 1.2364908115  | -1.6615743281 |
| 41 | H    | -0.8205214597 | 0.0794073888  | -5.5293290229 |
| 42 | H    | 1.6414099924  | 1.2364908115  | -1.6615743281 |
| 43 | H    | 0.3539626995  | 2.1655319195  | 4.1403950708 |

(7S*, 9R*) - S2A, M0003:M0013
| ATOM | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| 1    | 0.1831644476 | 0.4149875513 | -1.4172918905 |
| 2    | -1.2891313413 | 0.1313561325 | -1.0351322726 |
|   |   |   |   |
|---|---|---|---|
| C | -1.2132612714 | -0.4371186640 | 0.3838928035 |
| C | 0.1342311017 | -1.1663159340 | 0.3514498391 |
| O | 0.9734112503 | -0.2664301763 | -0.4166218484 |
| C | -1.7473670297 | -0.9798256743 | -1.9600422161 |
| N | -0.7326487997 | -1.2565321586 | -2.8203969026 |
| C | 0.3975138310 | -0.3586070777 | -2.7690392422 |
| C | 0.7624539929 | -1.3845725655 | 1.7205185185 |
| C | 0.7454285361 | -0.0844819607 | 2.5065081999 |
| C | 0.6780826901 | 0.4294324609 | 2.604994419 |
| O | 1.1826353290 | 0.6882358922 | 1.2805494419 |
| O | -2.8084231924 | -1.5616887409 | -1.8996069774 |
| C | 0.5075635461 | 0.4958231528 | -4.0116497742 |
| O | 1.3403448504 | 1.3479668722 | -4.182035637 |
| O | -0.3997936801 | 0.1709004713 | -4.9548558749 |
| C | 0.6398669236 | 1.8770915706 | -1.443016604 |
| C | 0.2419456077 | 2.5917337665 | -0.1865008272 |
| O | 0.9208877730 | 2.8194773046 | 0.7792684713 |
| O | -1.0420621920 | 3.0245754526 | -0.2947233086 |
| H | -1.9254000584 | 0.9977893656 | -1.0813487619 |
| H | -2.0394156958 | -1.0897169321 | 0.609547733 |
| H | 0.0178871799 | -2.0984390225 | -0.184843219 |
| O | -0.8084344098 | 1.7379573866 | 3.3625245204 |
| O | -1.4468608113 | -0.615835367 | 3.1947829237 |
| O | 2.1332941252 | -1.7822693667 | 1.6358928047 |
| O | 2.3976847603 | -3.0670642466 | 1.0551509474 |
| H | 1.338547622 | -0.8791811856 | -2.6614542213 |
| H | 0.1779522488 | -2.1331922503 | 2.239493696 |
| H | -0.8638153257 | -1.8933733177 | -3.5765297535 |
| H | 1.1404240409 | -0.2599271586 | 3.4961052013 |
| H | 1.3468938724 | 0.6436165637 | 1.9871551485 |
| H | -0.2953076439 | 0.7051246650 | -5.7566865478 |
| H | 0.1958073549 | 2.3995010616 | -2.2719838358 |
| H | 1.7135471290 | 1.8886924840 | -1.5326259098 |
| H | -1.3962836205 | 3.3290817172 | 0.5524689098 |
| H | -1.841951737 | 2.0685708848 | 3.3402133389 |
| H | -0.5048512130 | 1.5934874022 | 4.3907461786 |
| I | Atom | X            | Y            | Z            |
|---|------|--------------|--------------|--------------|
| 1 | C    | 0.0692631549 | 0.2892839905 | -1.6095177054 |
| 2 | C    | -1.3884269387 | -0.055599617 | -1.2220676659 |
| 3 | C    | -1.2765558286 | -0.5908953275 | 0.2060740982  |
| 4 | C    | 0.1100025132  | -1.2403566640 | 0.1899113964  |
| 5 | O    | 0.8911148744  | -0.2830650699 | -0.5726752969 |
| 6 | C    | -1.8015109507 | -1.1953287846 | -2.1318105350 |
| 7 | N    | -0.7853172928 | -1.4271072161 | -3.0020638006 |
| 8 | C    | 0.3338601296  | -0.5156042228 | -2.9326381713 |
| 9 | C    | 0.7286482053  | -1.4122330042 | 1.5606369941  |
| 10| O    | 0.6898852837  | -0.0808512234 | 2.3014921600  |
| 11| C    | -0.7555010578 | 0.3814782223  | 2.3955443589  |
| 12| O    | -1.2935527997 | 0.5619019057  | 1.0744421660  |
| 13| O    | -2.8308712807 | -1.8293023798 | -2.0521895559 |
| 14| C    | 0.3835572923  | 0.3371405580  | -4.1719092144 |
| 15| O    | -0.4763186336 | 0.4714811589  | -4.9967234662 |
| 16| O    | 1.5884989640  | 0.9543178729  | -4.2552820467 |
| 17| C    | 0.4228750355  | 1.7760331194  | -1.7171356481 |
| 18| C    | 0.0176790066  | 2.5142868239  | -0.4767253179 |
| 19| O    | 0.7065731376  | 2.8000027627  | 0.4667179663  |
| 20| O    | -1.2861808632 | 2.8817945054  | -0.5677759226 |
| 21| H    | -2.0630691067 | 0.7805721446  | -1.2795415091 |
| 22| H    | -2.0680144844 | -1.2768893682 | 0.455519649  |
| 23| H    | 0.0815297784  | -2.1880840357 | -0.3282750801 |
| 24| C    | -0.9268849531 | 1.7145014877  | 3.1009773110  |
| 25| O    | -1.4683765410 | -0.6670590992 | 3.0502098641  |
| 26| O    | 2.0579806124  | -1.8978735142 | 1.3410982967  |
| 27| C    | 2.7030414420  | -2.4945988606 | 2.4768267582  |
| I | Atom | X    | Y    | Z    |
|---|------|------|------|------|
| 1 | C    | -0.0981338205 | -0.2994484501 | -1.2244218658 |
| 2 | C    | 1.3344342997 | 0.1159036826 | -0.8509794864 |
| 3 | C    | 1.2197797640 | 0.5786537601 | 0.5906175928 |
| 4 | C    | -0.1448086490 | 1.2699898334 | 0.5867318598 |
| 5 | O    | -0.9430546213 | 0.4196223101 | -0.275897651 |
| 6 | C    | 1.6403989734 | 1.3035188664 | -1.7474832383 |
| 7 | N    | 0.6393108677 | 1.4067512129 | -2.6584810303 |
| 8 | C    | -0.3776307545 | 0.3779550970 | -2.5991319254 |
| 9 | C    | -0.7977408655 | 1.3592724596 | 1.9590676624 |
| 10| C    | -0.7707345915 | 0.0014782640 | 2.6409031134 |
| 11| C    | 0.6540347335 | -0.5162019882 | 2.7036115303 |
| 12| O    | 1.1774216601 | -0.6350659256 | 1.3716291713 |
| 13| O    | 2.5865334518 | 2.0527588116 | -1.6328688975 |
| 14| C    | -0.3250722473 | -0.4714357615 | -3.8376799471 |
| 15| O    | 0.3241571064 | -0.2657818917 | -4.8223708512 |
| 16| O    | -1.2443012062 | -1.4719547217 | -3.7595762708 |
(7S*,9R*)-S2A, M0003:M0017

| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
| 1 | C    | -0.2049537705 | 0.3292574888 | -1.4480982247 |
| 2 | C    | -1.6209374512  | -0.1541355807 | -1.0941805479 |
| 3 | C    | -1.4962883828  | -0.5919134668 | 0.3597862342 |
| 4 | C    | -0.1110456845  | -1.2450974979 | 0.3665237772 |
| 5 | O    | 0.6561621132   | -0.3969172074 | -0.5241696224 |

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| # | At. | X      | Y      | Z      |
|---|-----|--------|--------|--------|
| 6 | C   | -1.8302644366 | -1.3795741054 | -1.9738402298 |
| 7 | N   | -0.8127768211  | -1.4183318211  | -2.8701956090 |
| 8 | C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 9 | C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 10| C   | 0.5471300335   | 0.1377198014   | 2.3192293659 |
| 11| C   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 12| O   | -0.8127768211  | -1.4183318211  | -2.8701956090 |
| 13| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 14| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 15| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 16| O   | -0.8127768211  | -1.4183318211  | -2.8701956090 |
| 17| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 18| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 19| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 20| O   | -0.8127768211  | -1.4183318211  | -2.8701956090 |
| 21| H   | -2.3981010894  | 0.5820962869   | -4.0460821585 |
| 22| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 23| O   | -0.8127768211  | -1.4183318211  | -2.8701956090 |
| 24| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 25| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 26| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 27| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 28| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 29| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 30| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 31| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 32| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 33| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 34| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 35| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 36| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 37| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 38| C   | 0.5469922651   | -1.2683187377  | 1.7309130132 |
| 39| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| 40| C   | 0.0917045364   | -0.2743237143  | -2.834533585 |
| 41| O   | -0.8910961128  | 0.6228828793   | 2.4189803641 |
| I | Atom | X          | Y          | Z          |
|---|------|------------|------------|------------|
| 1 | C    | -0.0936692912 | 0.3644017924 | -1.3093109735 |
| 2 | C    | -1.5270737092 | -0.0550292586 | -0.9596362435 |
| 3 | C    | -1.4212905726 | -0.5272288949 | 0.4833249904 |
| 4 | C    | -0.0610903451 | -1.2361213185 | 0.4738771112 |
| 5 | O    | 0.7423442827  | -0.4301218532 | -0.4272430134 |
| 6 | C    | -1.8012168618 | -1.2365513209 | -1.8742701249 |
| 7 | N    | -0.8166021934 | -1.2676765815 | -2.8100429178 |
| 8 | C    | 0.1530640581  | -0.1770076250 | -0.7334599695 |
| 9 | C    | 0.6280122504  | -1.2941145641 | 1.8301457633 |
|10 | C    | 0.6239381381  | 0.0860057843 | 2.4666196303 |
|11 | C    | -0.8046159857 | 0.5844548289 | 2.5822862025 |
|12 | O    | -1.3884613847 | 0.6802783240 | 1.2722866308 |
|13 | O    | -2.7054590119 | -2.0351691011 | -1.7573686340 |
|14 | C    | -0.1736553473 | 0.8059622255 | -3.8234672571 |
|15 | O    | 0.4625626688  | 1.0395738954 | -4.8113298211 |
|16 | O    | -1.3815281320 | 1.3910416619 | -3.5799543510 |
|17 | C    | 0.2317705229  | 1.8271967920 | -1.0409126374 |
|18 | C    | 1.7129221383  | 1.9716595147 | -0.9094871748 |
|19 | O    | 2.3271939481  | 2.3738707006 | 0.0392966067 |
|20 | O    | 2.3166945231  | 1.5776580414 | -2.0642000740 |
|21 | H    | -2.2561469503 | 0.7262499070 | -1.908584889 |
|22 | H    | -2.2290719681 | -1.1726159313 | 0.7835027244 |
|23 | H    | -0.1865063800 | -2.2232023787 | 0.0514149604 |
|24 | C    | -0.9320697048 | 1.9688819949 | 3.1912625210 |
|25 | O    | -1.5109631937 | -0.3994009943 | 3.3340606928 |
|26 | O    | 2.0030385001  | -1.6727801478 | 1.7316979534 |
|27 | C    | 2.2857080993  | -2.9685217640 | 1.1827285952 |
|28 | H    | 1.1661344834  | -0.5079162785 | -2.8404080679 |
|29 | H    | 0.0806552433  | -1.9877384284 | 2.4542313727 |
|30 | H    | -0.7686230610 | -1.9906108213 | -3.4953139816 |


(7S*,9R*)-S2A, M0003:M0019

| ATOM | X      | Y      | Z      |
|------|--------|--------|--------|
| 1    | 0.1331105198 | 0.2622081914 | -1.2529069620 |
| 2    | -1.3155810366 | -0.0975203245 | -0.8848606816 |
| 3    | -1.2174646714 | -0.5699358215 | 0.555804855 |
| 4    | 0.1310751190  | -1.2926662935 | 0.555824608 |
| 5    | 0.9568353243  | -0.4498909372 | -0.2907656245 |
| 6    | -1.6726927507 | -1.2605125922 | -1.7887943779 |
| 7    | -0.6875289599 | -1.3840310676 | -2.7167926147 |
| 8    | 0.3832421499  | -0.4155974808 | -2.6400455746 |
| 9    | 0.7116904073  | -1.4133639731 | 1.9317443630 |
| 10   | 0.7645240186  | -0.0640337379 | 2.6313433641 |
| 11   | -0.6488979253 | 0.4845091687  | 2.6842397373 |
| 12   | -1.1523476936 | 0.6344256553  | 1.3487618967 |
| 13   | -2.6407422707 | -1.9806932440 | -1.6748562988 |
| 14   | 0.3126558978  | 0.5757800021  | -3.7653996653 |
| 15   | -0.6435501688 | 0.8393019027  | -4.4398827849 |
| 16   | 1.5087409868  | 1.1968052848  | -3.873088750 |
| 17   | 0.5301721706  | 1.7349517021  | -1.1092892627 |
| 18   | -0.1890682715 | 2.7193038138  | -1.9884009464 |
| 19   | 0.3195103469  | 3.4813264066  | -2.7703226320 |
| 20   | -1.5295028173 | 2.7030342709  | -1.7892544409 |
|   |   |   |   |
|---|---|---|---|
| 21 | H | -1.9974779323 | 0.7252447723 | -0.9998200590 |
| 22 | H | -2.0387090814 | -1.1981703532 | 0.8553589072 |
| 23 | H | 0.0123705340 | -2.2624446421 | 0.0923787288 |
| 24 | C | -0.7605385487 | 1.8556441317 | 3.3260254907 |
| 25 | O | -1.4248732927 | -0.4925685822 | 3.3736097720 |
| 26 | O | 2.1436883519 | -1.8109549924 | 1.8726946226 |
| 27 | C | 2.4219037012 | -3.1053012304 | 1.3173161239 |
| 28 | H | 1.3640693721 | -0.8582831474 | -2.6189544011 |
| 29 | H | 0.1893705179 | -2.1228947325 | 2.5053124508 |
| 30 | H | -0.7518424800 | -2.0617687210 | -3.4457068041 |
| 31 | H | 1.1526484757 | -0.1772796411 | 3.6323716993 |
| 32 | H | 1.3953258808 | 0.6047829063 | 2.0669477842 |
| 33 | H | 1.4707243638 | 2.0187553997 | -4.3850744121 |
| 34 | H | 1.5860439771 | 1.8330025542 | -1.2959867749 |
| 35 | H | 0.3002953843 | 1.9789459482 | -0.0825623949 |
| 36 | H | -1.9943485447 | 3.3155804681 | -2.3797632252 |
| 37 | H | -1.7836573475 | 2.2054459171 | 3.2565989353 |
| 38 | H | -0.4684242767 | 1.7948996219 | 4.3655761513 |
| 39 | H | -0.1242832576 | 2.5609231471 | 2.8105481946 |
| 40 | H | -2.3442885398 | -0.2047807182 | 3.4626980126 |
| 41 | H | 2.2457708263 | -3.1255413560 | 0.2492780186 |
| 42 | H | 1.8253705994 | -3.8787163147 | 1.7920216548 |
| 43 | H | 3.4666809416 | -3.2979213616 | 1.5059386493 |
(7R*,9R*)-S2B, M0004:M0001

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.4856692755 | 0.1627061765 | -1.3821669079 |
| 2 | C    | -0.6764245119  | -1.2887640374 | -0.9028329824  |
| 3 | C    | -0.1122434127  | -1.2847901841 | 0.5104702086   |
| 4 | C    | 1.0938085317   | -0.3593763007 | 0.3392481261   |
| 5 | O    | 0.6160291625   | 0.6648684212  | -0.564539961   |
| 6 | C    | 0.2324545498   | -2.1104211499 | 1.8066866662   |
| 7 | N    | 0.6657656277   | -1.2971844076 | -2.8029184347  |
| 8 | C    | 0.0822823988   | 0.0372284697  | -2.8133636994  |
| 9 | C    | 1.5440068096   | 0.3188653322  | 1.6212012580   |
|10 | C    | 0.3591192736   | 0.8726230566  | 2.4099917522   |
|11 | C    | -0.7002990398  | -0.2124117697 | 2.6318397962   |
|12 | O    | -1.1161029265  | -0.6526624305 | 1.316730140    |
|13 | O    | 0.5467144710   | -3.2687559694 | -1.6347222702  |
|14 | C    | -0.9150503913  | 0.1222649987  | -3.9440746548  |
|15 | O    | -2.0329912414  | 0.5643281399  | -3.9326353238  |
|16 | O    | -0.3466310192  | -0.3591647364 | -5.0762562177  |
|17 | C    | -1.6662542353  | 1.0837813950  | -1.1601544529  |
|18 | C    | -1.3939473983  | 2.4584786905  | -1.6834570924  |
|19 | O    | -0.5204919365  | 2.7866847480  | -2.4460528349  |
|20 | O    | -2.3020939223  | 3.3398794094  | -1.2076383778  |
|21 | H    | -1.6965525102  | -1.6394604865 | -0.9223037173  |
|22 | H    | 0.1417259250   | -2.2645644745 | 0.8767261682   |
|23 | H    | 1.9120947225   | -0.9009602182 | -0.1124498317  |
|24 | C    | -1.9622875822  | 0.2931787603  | 3.2976304321   |
|25 | O    | -0.1976101437  | -1.2836942275 | 3.3927597496   |
|26 | O    | 2.1738347786   | -0.6873630909 | 2.4549381187   |
|27 | C    | 3.5822687770   | -0.9291080359 | 2.2651925608   |
|28 | H    | 0.8131746751   | 0.8147191431  | -2.9509050263  |
|29 | H    | 2.2499091429   | 1.1050812635  | 1.3874985619   |
|30 | H    | 1.2219341390   | -1.6296643373 | -3.5603338148  |
|31 | H    | 0.7093802452   | 1.2376350477  | 3.3655606755   |
|32 | H    | -0.0791567588  | 1.6825102210  | 1.8468850683   |
|33 | H    | -0.9412058445  | -0.2976189181 | 5.8383762179   |
|   |   |   |   |
|---|---|---|---|
| 34 | H  | -1.8509092838 | 1.1211454742 | -0.1006376828 |
| 35 | H  | -2.5523720936 | 0.7225711565 | -1.6578929008 |
| 36 | H  | -2.1736811210 | 4.2273058107 | -1.5735682286 |
| 37 | H  | -2.6493638340 | -0.5362292257 | 3.3857759528 |
| 38 | H  | -1.7286280853 | 0.6647493567 | 4.2861374255 |
| 39 | H  | -2.4170507587 | 1.0747155649 | 2.7053132839 |
| 40 | H  | 0.76577378251 | -1.3609938330 | 3.2795432246 |
| 41 | H  | 4.1416828520  | -0.0068639133 | 2.364285689 |
| 42 | H  | 3.7838831497  | -1.3679217354 | 1.2969263571 |
| 43 | H  | 3.8812102700  | -1.6176161357 | 3.0394440281 |

(7R*, 9R*)-S2B, M0004:M0002

| ATOM | X     | Y     | Z     |
|------|-------|-------|-------|
| 1 C  | -0.2826456991 | 0.3581832103 | -1.3693833025 |
| 2 C  | -0.4530829054 | -1.1010263290 | -0.9090364448 |
| 3 C  | 0.0860037962  | -1.1006101657 | 0.5102634927 |
| 4 C  | 1.2650791989  | -0.1363774351 | 0.3810968001 |
| 5 O  | 0.7658381089  | 0.8947671680 | -0.5067719673 |
| 6 C  | 0.4538352106  | -1.9051580684 | -1.8217953257 |
| 7 N  | 0.8767793632  | -1.0825118416 | -2.818432836 |
| 8 C  | 0.3521269404  | 0.2629440422  | -2.7907697964 |
| 9 C  | 1.6758011337  | 0.5226971877  | 1.6857725551 |
| 10 C | 0.4635195183  | 1.0314062346  | 2.4629958826 |
| 11 C | -0.5754912711 | -0.0820730027 | 2.6373487673 |
| 12 O | -0.9513059005 | -0.5052070803 | 1.3062476411 |
| 13 O | 0.7788951702  | -3.0620617529 | -1.6669498220 |
| 14 C | -0.5805225546 | 0.5686870408  | -3.9345292222 |
| 15 O | -1.1583629191 | 1.6201057677  | -4.0579348469 |
| 16 O | -0.6327277978 | -0.4083422473 | -4.8516579426 |
| 17 C | -1.4883167109 | 1.2600268977  | -1.1866440894 |
| 18 C | -2.7148549106 | 0.7712693482  | -1.8840313456 |
| 19 O | -2.8309395396 | -0.2602117986 | -2.5024038617 |
| 20 O | -3.7394485507 | 1.6281218856  | -1.7148046137 |
| 21 H | -1.4669983570 | -1.4534095486 | -0.966318043 |
| 22 H | 0.3614180204  | -2.0766111694 | 0.8711343800 |
| 23 H | 2.1057248472  | -0.6415257127 | -0.0728919036 |
| ATOM | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -1.8623890145 | 0.3829300642 | 3.2854428881 |
| O    | -0.0662167780  | -1.1554235534 | 3.3915605559 |
| C    | 2.3119849050   | -0.4930346434 | 2.5031188482 |
| C    | 3.7349660254   | -0.6719502793 | 2.3593810458 |
| H    | 1.1332247971   | 1.0095184431  | -2.8181884749 |
| H    | 2.3691329291   | 1.3295208934  | 1.4866216025 |
| H    | 1.3807221219   | -1.4387429971 | -3.6010628580 |
| C    | 0.7849354120   | 1.384860186  | 3.4338592509 |
| H    | 0.0182464149   | 1.8436842175  | 1.908838191 |
| H    | -1.2577339121  | -0.2068728673 | -5.563673504 |
| H    | -1.2777803199  | 2.2627544299  | -1.526579743 |
| C    | -1.6966146592  | 1.2752507453  | -0.1272675392 |
| O    | -4.5434437973  | 1.3282523513  | -2.164011306 |
| H    | -2.5323084354  | -0.4630191688 | 3.3448492940 |
| H    | -1.6577050262  | 0.7418433814  | 4.2849838316 |
| C    | -2.3231276048  | 1.1648056450  | 2.6978678650 |
| H    | 0.8993670489   | -1.2163532060 | 3.2899019652 |
| C    | 4.2560054747   | 0.2567501089  | 2.5575623958 |
| C    | 3.9929628074   | -1.0235585307 | 1.3688772988 |
| C    | 0.8993670489   | -1.2163532060 | 3.2899019652 |
| C    | 4.0254473287   | -1.4119532321 | 3.0880521202 |

(7R*, 9R*) - S2B, M0004:M0003
|    | Atom | X            | Y            | Z            |
|----|------|--------------|--------------|--------------|
| 14 | C    | -0.4472130727 | 0.4244915027 | -4.0549340886|
| 15 | O    | -1.0883342193 | 1.4347774119 | -4.2077081898|
| 16 | O    | -0.3962659863 | -0.5558092508| -4.9687124968|
| 17 | C    | -1.5010554695 | 1.0777309932 | -1.3525089144|
| 18 | C    | -2.6633551850 | 0.4931161036 | -2.0850930315|
| 19 | O    | -2.6790241593 | -0.5460636733| -2.7011288472|
| 20 | O    | -3.7567326775 | 1.267986320  | -1.9535307422|
| 21 | H    | -1.3050281887 | -1.6191322439| -1.0688776760|
| 22 | H    | 0.5154590494  | -2.0957941132| 0.8162274120 |
| 23 | H    | 2.1935155152  | -0.5406854784| -0.0742666017|
| 24 | C    | -1.9363901383 | 0.2176217235 | 3.1468251917 |
| 25 | O    | -0.0289795038 | -1.1716680919| 3.3057158033 |
| 26 | O    | 2.3424389854  | -0.3769516242| 2.411467383 |
| 27 | C    | 3.3867874985  | 0.1235010037 | 3.2726713991|
| 28 | H    | 1.1937524320  | 0.9786336654 | -2.8817879495|
| 29 | H    | 2.2547935654  | 1.4606363687 | 1.4206394414|
| 30 | H    | 1.6083769330  | -1.4606938457| -3.631362580 |
| 31 | H    | 0.6002681533  | 1.4352418793 | 3.3431541810|
| 32 | H    | -0.1373161281 | 1.803702456  | 1.7846911019|
| 33 | H    | -1.0033916278 | -0.3987648403| -5.7068467937|
| 34 | H    | -1.3491189384 | 2.0870461491 | -1.7037508683|
| 35 | H    | -1.7484159405 | 1.0940640124 | -0.3016198759|
| 36 | H    | -4.5204788195 | 0.9060525628 | -2.4266562338|
| 37 | H    | -2.5398758656 | -0.6774148857| 3.1971921889|
| 38 | H    | -1.7819727084 | 0.5966155768 | 4.1480161355|
| 39 | H    | -2.4428143700 | 0.9585117613 | 2.5440178755|
| 40 | H    | 0.9319497658  | -1.2076682089| 3.1580110713|
| 41 | H    | 2.9881737128  | 0.7870023005 | 4.0299288622|
| 42 | H    | 4.1356366106  | 0.6486002791 | 2.6929971522|
| 43 | H    | 3.8329834224  | -0.7370087066| 3.7451997841|

(7R*, 9R*)-S2B, M0004:M0004

| I | Atom | X            | Y            | Z            |
|---|------|--------------|--------------|--------------|
| 1 | C    | -0.4160528617 | 0.0404329451 | -1.4975018555|
| 2 | C    | -0.5239233785 | -1.4124709544| -0.9981884424|
|   |   |   |   |   |
|---|---|---|---|---|
| 3 | C | -0.0086608821 | -1.3477483308 | 0.4319945828 |
| 4 | C | 1.1332525680 | -0.3399867734 | 0.2898779175 |
| 5 | O | 0.6152220292 | 0.6321659025 | -0.6494806182 |
| 6 | C | 0.4662904537 | -2.1867339845 | -1.8574933780 |
| 7 | N | 0.8770619253 | -2.8539182334 | 0.4319945828 |
| 8 | C | 0.2144730279 | 0.2898779175 | 1.5702558579 |
| 9 | C | 0.4662904537 | -2.1867339845 | -1.8574933780 |
| 10| C | 0.2382402305 | 0.873411200 | 2.3104443768 |
| 11| C | -0.7443206851 | -0.0625878373 | 2.5133808709 |
| 12| O | -1.0825346145 | -0.7736458134 | -1.8663937124 |
| 13| O | 0.8467791878 | 0.873411200 | 2.3104443768 |
| 14| C | -0.7375785544 | -0.0625878373 | 2.5133808709 |
| 15| O | -1.8982477741 | 0.2484168483 | -1.4035109697 |
| 16| O | -0.0680111748 | -0.4577781613 | -1.3352051241 |
| 17| C | -1.6655106374 | 0.8797714417 | -1.850781972 |
| 18| C | -1.4649457227 | 2.2636084197 | -1.8663937124 |
| 19| O | -0.6071762322 | 2.6312323383 | -2.629104600 |
| 20| O | -2.4217084593 | 3.0995357049 | -1.4035109697 |
| 21| H | -1.5169273939 | -1.8319743544 | -1.0421392867 |
| 22| H | 0.2993085789 | -2.3024113634 | 0.8220410247 |
| 23| H | 2.0164851603 | -0.8202832049 | -1.016668168 |
| 24| C | -2.0598357261 | 0.1265759600 | 3.1365229885 |
| 25| O | -0.1846549771 | -1.3062857829 | 3.3068932091 |
| 26| O | 2.1927956024 | -0.5951846173 | 2.3703826191 |
| 27| C | 3.2753524761 | -0.1097738717 | 3.1925189231 |
| 28| H | 0.9017229871 | 0.7524822044 | -3.0258358146 |
| 29| H | 2.1427113517 | 1.2191630797 | 1.334093421 |
| 30| H | 1.4920650545 | -1.6632660010 | -3.578353940 |
| 31| H | 0.5096392440 | 1.2875170722 | 3.272962165 |
| 32| H | -0.2369171616 | 1.6370056238 | 1.7136366472 |
| 33| H | -0.6310567561 | -0.4526406611 | -5.9732525212 |
| 34| H | -1.8978005158 | 0.9155273033 | -0.2854109874 |
| 35| H | -2.5011627441 | 0.4525852315 | -1.8673675260 |
| 36| H | -2.3397639522 | 3.9887090869 | -1.7782900122 |
| 37| H | -2.6841831493 | -0.7519828252 | 3.2136945511 |
| 38| H | -1.8856392264 | 0.5245447699 | 4.1270032349 |
|     |     |        |        |        |
|-----|-----|--------|--------|--------|
| 39  | H   | -2.5539746811 | 0.8654198974 | 2.5214516257 |
| 40  | H   | 0.7734660933  | -1.3676139077 | 3.1511185697 |
| 41  | H   | 2.9206555515  | 0.5893428253  | 3.9394005555 |
| 42  | H   | 4.0286670749  | 0.3702064463  | 2.5805625556 |
| 43  | H   | 3.7007366261  | -0.9729569806 | 3.6790470094 |

\((7R^*, 9R^*)-S2B, \text{ M0004:M0005}\)

| I  | Atom | X       | Y       | Z       |
|----|------|---------|---------|---------|
| 1  | C    | -0.3546473918 | 0.0775506142 | -1.4993634621 |
| 2  | C    | -0.5441897418 | -1.3834217821 | -1.0617040678 |
| 3  | C    | -0.0822384108 | -1.3922045215 | 0.3884107742 |
| 4  | C    | 1.1050882493 | -0.4253384161 | 0.339276391 |
| 5  | O    | 0.6573043787 | 0.5953432628 | -0.691851787 |
| 6  | C    | 0.4419866091 | -2.1750231893 | -1.9085123645 |
| 7  | N    | 0.9302244206 | -1.3319626707 | -2.8537482769 |
| 8  | C    | 0.3298133197 | 0.0040582578 | -2.882004535 |
| 9  | C    | 1.4278852396 | 0.3226310457 | 1.6208640182 |
| 10 | C    | 0.1684165195 | 0.7588200071 | 2.3605244958 |
| 11 | C    | -0.8071493482 | -0.4159620922 | 2.4706252431 |
| 12 | O    | -1.1612539270 | -0.7798331068 | 1.1210341093 |
| 13 | O    | 0.7737723525 | -3.3258904950 | -1.7320260200 |
| 14 | C    | -0.6514100391 | 0.0125618491 | -4.0203169792 |
| 15 | O    | -1.7943632884 | -0.3574893666 | -3.9686021703 |
| 16 | O    | -0.0607575513 | 0.4093495929 | -5.1648366505 |
| 17 | C    | -1.5955606107 | 0.9323675346 | -1.3664067766 |
| 18 | C    | -1.4085976734 | 2.2960205107 | -1.9419263790 |
| 19 | O    | -0.533360825 | 2.6432497807 | -2.6928901684 |
| 20 | O    | -2.3994758361 | 3.1268154526 | -1.5485855484 |
| 21 | H    | -1.5517612204 | -1.7492652824 | -1.1487485779 |
| 22 | H    | 0.1578651565 | -2.3618471744 | 0.7722919878 |
| 23 | H    | 1.9910568601 | -0.9263535711 | -0.0113086638 |
| 24 | C    | -2.1081951335 | -0.0803047934 | 3.1658314762 |
| 25 | O    | -0.1926301835 | -1.5485978384 | 3.0616179161 |
| 26 | O    | 2.1849400138 | -0.5925133959 | 2.4614355419 |
| 27 | C    | 3.2857368695 | -0.0353842637 | 3.2148229598 |
| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
| 28| H    | 1.0410873875 | 0.7905419345 | -2.9970189103 |
| 29| H    | 2.0345746689  | 1.1713294815  | 1.3441560304  |
| 30| H    | 1.6236251126  | -1.6173433815 | -3.508142476  |
| 31| H    | 0.4340438883  | 1.1152511925  | 3.3470626098  |
| 32| H    | -0.3149665515 | 1.5552422891  | 1.8208659476  |
| 33| H    | -0.6495237834 | 0.389473803   | -5.9315814920 |
| 34| H    | -1.8094918354 | 0.9908661403  | -0.3154769179 |
| 35| H    | -2.4362892902 | 0.4737218423  | -1.8606188109 |
| 36| H    | -2.3303554200 | 4.0136745489  | -1.9264709175 |
| 37| H    | -2.7266477866 | -0.9635817356 | 3.1539073277  |
| 38| H    | -1.9134008776 | 0.2096604288  | 4.1881811902  |
| 39| H    | -2.6083837689 | 0.7223210586  | 2.6453483618  |
| 40| H    | 0.7483317347  | -1.4134018967 | 3.2353836537  |
| 41| H    | 0.4477768555  | -0.9742967228 | -1.8172063931 |
| 42| O    | 0.8773150119  | -1.1585417586 | -2.8176577508 |
| 43| O    | 0.3103479224  | 0.1736872133  | -2.8239972149 |
| 44| O    | 1.7123165152  | 0.4639332891  | 1.6310546364  |
| 45| O    | 0.5179964786  | 1.0017425247  | 2.4162637637  |
| 46| H    | -0.5353707102 | -0.0932787002 | 2.6196442901  |
| 47| O    | -0.9350701819 | -0.5279229442 | 1.2987509838  |
| 48| O    | 0.7791754539  | -3.1262169780 | -1.6439156026 |
| 49| C    | -0.6276418564 | 0.3265381103  | -3.9913648083 |
| 50| O    | -0.8023615064 | -0.4607228815 | -4.8748372659 |
| 51| O    | -1.1803018875 | 1.5708166549  | -3.9929890709 |

(7R*,9R*)-S2B, M0004:M0006
|   |   | X                  | Y                  | Z                  |
|---|---|--------------------|--------------------|--------------------|
| 17| C | -1.4656316894      | 1.2211633623       | -1.1736703818      |
| 18| C | -2.7157215467      | 0.7846454627       | -1.8569072877      |
| 19| O | -2.8953086045      | -0.2557859136      | -2.442259424       |
| 20| O | -3.6930759559      | 1.7043805332       | -1.7147360692      |
| 21| H | -1.4833739786      | -1.5117936949      | -0.9722469105      |
| 22| H | 0.3450859935       | -2.1262961734      | 0.8685456011       |
| 23| H | 2.1059023825       | -0.7407044449      | -0.1064138621      |
| 24| C | -1.8066058136      | 0.3998818621       | 3.277267753        |
| 25| O | -0.0332465505      | -1.1638528303      | 3.3818257400       |
| 26| O | 2.3415824783       | -0.5506833077      | 2.4556195180       |
| 27| C | 3.7575805467       | -0.7613796279      | 2.2859749553       |
| 28| H | 1.0619875277       | 0.9450007999       | -2.9085160982      |
| 29| H | 2.4154715412       | 1.2567121465       | 1.412233209        |
| 30| H | 1.3991311748       | -1.5173012462      | -3.5881573756      |
| 31| H | 0.8576682457       | 1.3605009863       | 3.3780643525       |
| 32| H | 0.0781758157       | 1.8140261509       | 1.8574834100       |
| 33| H | -1.7529850843      | 1.7109788691       | -4.7618945443      |
| 34| H | -1.2267629800      | 2.2240949892       | -1.4908496882      |
| 35| H | -1.6569549212      | 1.2167758897       | -0.1109633715      |
| 36| H | -4.5264634741      | 1.4111182230       | -2.1122166126      |
| 37| H | -2.4892122227      | -0.4344099494      | 3.3547442340       |
| 38| H | -1.5841007251      | 0.7666918933       | 4.2705757538       |
| 39| H | -2.2618252856      | 1.1826254080       | 2.6869511096       |
| 40| H | 0.9301457089       | -1.2405305694      | 3.2697865204       |
| 41| H | 4.3034839536       | 0.1529843390       | 2.4836361837       |
| 42| H | 3.9898954821       | -1.1088252516      | 1.2877112747       |
| 43| H | 4.0428947811       | -1.5151485423      | 3.002405778        |

(7R*, 9R*)-S2B, M0004:M0007

| I | Atom | X             | Y             | Z             |
|---|------|---------------|---------------|---------------|
| 1 | C    | -0.1832479216 | 0.2184032638  | -1.5049124553 |
| 2 | C    | -0.3460037752 | -1.2383105155 | -1.0363799816 |
| 3 | C    | 0.1256387562  | -1.2115622252 | 0.4071761031  |
| 4 | C    | 1.2965432832  | -0.2317407323 | 0.3215712573  |
| 5 | O    | 0.8302624187  | 0.7745661917  | -0.6128036727 |
| 6  | C   | 0.6376446150 | -2.0272153778 | -1.8834711575 |
| 7  | N   | 1.1051355642 | -1.1982639926 | -2.8555974266 |
| 8  | C   | 0.5064850237 | 0.1194650288  | -2.8953452387 |
| 9  | C   | 1.6326517759 | 0.4624668429  | 1.6276421400  |
| 10 | C   | 0.3789094651 | 0.9604902735  | 2.3455979204  |
| 11 | C   | -0.6424106067 | -0.1749817256 | 2.4895309423  |
| 12 | O   | -0.9550770882 | -0.6208091007 | 1.1505542212  |
| 13 | O   | 0.9810805755 | -3.1729248488 | -1.6955853915 |
| 14 | C   | -0.3606779529 | 0.2516184001  | -4.1186063591 |
| 15 | O   | -0.4568513296 | -0.5347725542 | -5.0147128018 |
| 16 | O   | -0.9485714798 | 1.4796102350  | -4.1500643673 |
| 17 | C   | -1.3999022001 | 1.1108422564  | -1.3584151159 |
| 18 | C   | -2.5895214697 | 0.6365840624  | -2.1197894212 |
| 19 | O   | -2.6990149713 | -0.4089585346 | -2.7133127133 |
| 20 | O   | -3.6021088130 | 1.5257116492  | -2.0426111902 |
| 21 | H   | -1.3469918474 | -1.616408954  | -1.1435983995 |
| 22 | H   | 0.3971356778  | -2.1799898425 | 0.7903364401  |
| 23 | H   | 2.1768194825  | -0.7266462086 | -0.058912545  |
| 24 | C   | -1.9624084556 | 0.2638961333  | 3.0857146935  |
| 25 | O   | -0.1375096801 | -1.2274721551 | 3.2770154425  |
| 26 | O   | 2.2888682904  | -0.5632611246 | 2.4223172576  |
| 27 | C   | 3.3424592666  | -0.1190096594 | 3.3033463457  |
| 28 | H   | 1.2419622732  | 0.9095509909  | -2.932193298  |
| 29 | H   | 2.3187915748  | 1.2757673052  | 1.4315127698  |
| 30 | H   | 1.6834297382  | -1.5413112604 | -3.5921112711 |
| 31 | H   | 0.6346905344  | 1.3396619526  | 3.3266491441  |
| 32 | H   | -0.0566093941 | 1.7545939123  | 1.7581030928  |
| 33 | H   | -1.4741851153 | 1.6082713674  | -4.9537624734 |
| 34 | H   | -1.1737378789 | 2.1217361143  | -1.6586843507 |
| 35 | H   | -1.6573097973 | 1.0969703085  | -0.3096861925 |
| 36 | H   | -4.3983848291 | 1.2070670698  | -2.4930428479 |
| 37 | H   | -2.6158248151 | -0.5960123158 | 3.1225397995  |
| 38 | H   | -1.8048192203 | 0.6312362215  | 4.0906602140  |
| 39 | H   | -2.4159512494 | 1.0335459592  | 2.4768201764  |
| 40 | H   | 0.8208211357  | -1.3204577953 | 3.1409653544  |
| 41 | H   | 2.9665508342  | 0.5678446709  | 4.0513501212  |
(7R*, 9R*)-S2B, M0004:M0008

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.3137061187 | 0.2316885413 | -1.7016288605 |
| 2 | C    | -0.5386573290 | -1.2051615021 | -1.1756342877 |
| 3 | C    | 0.0267945151 | -1.1843000478 | 0.2466761733 |
| 4 | C    | 1.1667547353 | -0.1712852823 | 0.1064595556 |
| 5 | O    | 0.6069453811 | 0.8405342668 | -0.7682092894 |
| 6 | C    | 0.3410192929 | -2.0951181908 | -2.0328117090 |
| 7 | N    | 0.9105858213 | -1.3204076241 | -2.9959669999 |
| 8 | C    | 0.4515268166 | 0.0471263582 | -3.0588890057 |
| 9 | C    | 1.5723758468 | 0.5221023421 | 1.3924518743 |
|10 | C    | 0.3533816562 | 0.957205428 | 2.2022217417 |
|11 | C    | -0.5958959395 | 0.249661990 | -4.2741779683 |
|12 | O    | -1.0075570124 | -0.6593172523 | 1.0904238048 |
|13 | O    | -0.9132734310 | -0.5974762704 | -4.9593918960 |
|14 | C    | -0.5569350732 | 1.5767247087 | -4.5173632323 |
|15 | C    | -1.5451905551 | 1.1362909606 | -1.8129283035 |
|16 | C    | -2.3099443682 | 1.1631704622 | -0.5225716740 |
|17 | O    | -2.2434568799 | 1.9905661353 | 0.3475693439 |
|18 | O    | -3.1581187743 | 0.1072849789 | -0.4767317191 |
|19 | H    | -1.5695879298 | -1.5134682754 | -1.1816376705 |
|20 | H    | 0.3531813788 | -2.1550171172 | 0.5781451543 |
|21 | H    | 2.0306803873 | -0.6340811937 | -0.3459833214 |
|22 | C    | -1.8741035336 | 0.1510702693 | 3.1307507295 |
|23 | O    | 0.0162488636 | -1.2811519934 | 3.1174014937 |
|24 | O    | 2.3412035553 | -0.4776640231 | 2.1178886966 |
|25 | O    | 3.4117661555 | 0.0172091105 | 2.9490338441 |
|26 | H    | 2.514337784 | 0.7684760900 | -3.0815353851 |
|27 | H    | 2.2022838337 | 1.3676933361 | 1.149529094 |
|28 | H    | 1.4870990163 | -1.7263296146 | -3.7014337532 |
|   |   | X               | Y               | Z               |
|---|---|-----------------|-----------------|-----------------|
|31 | H | 0.6611990801    | 1.3491317335    | 3.1631899026    |
|32 | H | -0.1763850647   | 1.7169056417    | 1.6496444743    |
|33 | H | -1.1150805869   | 1.7557738184    | -5.2889482314   |
|34 | H | -2.2089976411   | 0.7579348713    | -2.5740987062   |
|35 | H | -1.2135712486   | 2.1314288713    | -2.0569343685   |
|36 | H | -3.4825901268   | -0.0693885997   | 0.4175334089    |
|37 | H | -2.4978230173   | -0.7307056299   | 3.1963953856    |
|38 | H | -1.6403581722   | 0.4845180901    | 4.1327914542    |
|39 | H | -2.3818361088   | 0.9336694879    | 2.5877724651    |
|40 | H | 0.9675967932    | -1.3125054545   | 2.9191043100    |
|41 | H | 3.0345351008    | 0.6523414856    | 3.7405203856    |
|42 | H | 4.1265846993    | 0.5717985410    | 2.3537799763    |
|43 | H | 3.8920338687    | -0.8477871136   | 3.3781859114    |

(7R*,9R*) -S2B, M0004:M0009
| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 20 | O    | -0.6496379761 | 2.5877452142 | -2.5237036355 |
| 21 | H    | -1.5874309784 | -1.8392574246 | -1.0185119700 |
| 22 | H    | 0.2464569494 | -2.3089207300 | 0.8185130468  |
| 23 | H    | 1.9684109959 | -0.8406483987 | -0.1062775638 |
| 24 | C    | -2.0989048457 | 0.1576613853 | 3.1296681087  |
| 25 | O    | -0.2122630328 | -1.2581748524 | 3.3179037396  |
| 26 | O    | 2.151881443  | -0.563361551 | 2.354932546   |
| 27 | C    | 3.2267700964 | -0.066039593 | 3.180935134   |
| 28 | H    | 0.7826646086 | 0.744254626  | -3.047516139  |
| 29 | H    | 2.0936089538 | 1.229505300  | 1.283179980   |
| 30 | H    | 1.3738145983 | -1.6762626932| -3.607624782  |
| 31 | H    | 0.4616304926 | 1.3490236460 | 3.217608103   |
| 32 | H    | -0.2946783452| 1.6451044056 | 1.651936334   |
| 33 | H    | -0.7854184343| -0.528931740 | -5.965176582  |
| 34 | H    | -2.0397259870| 0.712195822  | -0.257510336  |
| 35 | H    | -2.5048791600| 0.6390626745 | -1.966206448  |
| 36 | H    | -0.4484030192| 3.529604782  | -2.622666827  |
| 37 | H    | -2.7156398416| -0.724298651 | 3.222545692   |
| 38 | H    | -1.9236235970| 0.5724012551 | 4.112749662   |
| 39 | H    | -2.5974284424| 0.847183081  | 2.505081463   |
| 40 | H    | 0.7438114008 | -1.0323435094| 3.152010367   |
| 41 | H    | 2.8650454379 | 0.635521593  | 3.921591781   |
| 42 | H    | 3.9815128600 | 0.413798662  | 2.570885668   |
| 43 | H    | 3.6524234461 | -0.924916081 | 3.674905240   |

(7R*, 9R*)-S2B, M0004:M0010

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.4026433105 | 0.3353608528 | -1.5796307377 |
| 2 | C    | -0.7187033456 | -1.0831688282 | -1.0500034304 |
| 3 | C    | -0.0863497449 | -1.1213377062 | 0.3439022438  |
| 4 | C    | 1.1271464504 | -0.2072979536 | 0.1481596477  |
| 5 | O    | 0.6152655665 | 0.855535929  | -0.6932652525 |
| 6 | C    | 0.0470908943 | -2.0326830111 | -1.9514349447 |
| 7 | N    | 0.6293573745 | -1.2979121317 | -2.9380779164 |
| 8 | C    | 0.2726002817 | 0.1010200260 | -2.9761171005 |
|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 9  | C  | 1.6542171684 | 0.4319312602 | 1.4203257335 |
| 10 | C  | 0.5179199986 | 0.9563555474 | 2.2933819039 |
| 11 | C  | -0.5179966868 | -0.1418700155 | 2.5460858842 |
| 12 | O  | -1.0292560658 | -0.5217864840 | 1.2400421872 |
| 13 | O  | 0.1768499322  | -3.2245048967 | -1.7855595235 |
| 14 | C  | -0.6384972153 | 0.3731806477 | -4.1435539533 |
| 15 | C  | -0.5179966868 | -0.1418700155 | 2.5460858842 |
| 16 | O  | -0.6907168012 | 1.7073958684 | -4.3823494375 |
| 17 | O  | -1.5566420644 | 1.3419467023 | -1.6212360239 |
| 18 | O  | -2.2514561519 | 1.4195149838 | -0.2939142826 |
| 19 | O  | -2.0750981312 | 2.2325315223 | 0.5745433498 |
| 20 | O  | -3.1796084523 | 0.4356471322 | -0.2112935035 |
| 21 | H  | -1.7703701879 | -1.3074248547 | -1.0094520386 |
| 22 | H  | 0.1751200359  | -2.1179118260 | 0.6556754811 |
| 23 | H  | 1.9119724464  | -0.7439547028 | -0.3617299292 |
| 24 | C  | -1.7244915146 | 0.3397188777 | 3.3239570351 |
| 25 | O  | 0.0308344341  | -1.2546456362 | 3.2095299504 |
| 26 | O  | 2.3432928950  | -0.6016583979 | 2.1705845128 |
| 27 | C  | 3.7479148638  | -0.7850574094 | 1.9081966665 |
| 28 | H  | 1.1222970329  | 0.7599439576 | -3.0411878001 |
| 29 | H  | 2.3406802481  | 1.2286957562 | 1.1653612557 |
| 30 | H  | 1.1326015492  | -1.7430849028 | -3.6756275940 |
| 31 | H  | 0.9232777742  | 1.2988386358 | 3.2356166165 |
| 32 | H  | 0.0268559992  | 1.7668811444 | 1.7786433230 |
| 33 | H  | -1.2748630139 | 1.9311809639 | -5.1223718526 |
| 34 | H  | -2.2876581777 | 1.0302922048 | -2.3502327106 |
| 35 | H  | -1.1539534351 | 2.3080508918 | -1.8750596690 |
| 36 | H  | -3.4691671740 | 0.2743056600 | 0.6977212388 |
| 37 | H  | -2.4171784426 | -0.4863724132 | 3.4178868719 |
| 38 | H  | -1.4151735965 | 0.6449729572 | 4.3144855070 |
| 39 | H  | -2.1892657555 | 1.1663265378 | 2.8085945688 |
| 40 | H  | 0.9877731040  | -1.3139787016 | 3.0451193919 |
| 41 | H  | 4.2943171129  | 0.1280610043 | 2.1099904156 |
| 42 | H  | 3.9237524545  | -1.0875756398 | 0.8835747627 |
| 43 | H  | 4.0860167804  | -1.5634561305 | 2.5736787454 |
(7R*, 9R*)-S2B, M0004:M0011

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.5541909875 | 0.1739055375 | -1.3780866380 |
| 2 | C    | -0.7467023709  | -1.2784307210 | -0.9015326482 |
| 3 | C    | -0.1688928336  | -1.2823043176  | 0.5079941529 |
| 4 | C    | 1.0417124636   | -0.3621286725  | 0.3300950949 |
| 5 | O    | 0.5684879387   | 0.6595105069   | -0.5794983361 |
| 6 | C    | 0.1496678793   | -2.1001044509  | -1.8169917904 |
| 7 | N    | 0.5704901168   | -1.2850763757  | -2.8169337617 |
| 8 | C    | -0.0134107873  | 0.0493120744   | 2.6359026111 |
| 9 | C    | 1.4941965635   | 0.3283698058   | 1.6047640369 |
| 10 | O   | 0.3107494331   | 0.8888734540   | 2.3915154943 |
| 11 | C   | -0.7407289424  | -0.1991925466  | 2.6359026111 |
| 12 | O   | -1.1646121992  | -0.6534993973  | 1.3254462061 |
| 13 | O   | 0.4655702644   | -3.2588561689  | -1.6509555846 |
| 14 | C   | -1.0214850152  | 0.1410618594   | -3.9405182786 |
| 15 | O   | -2.1264832114  | 0.6117575784   | -3.9363238242 |
| 16 | O   | -0.4700284039  | -0.3757308998  | -5.0683835855 |
| 17 | C   | -1.7205526723  | 1.1021738017   | -1.0999993594 |
| 18 | C   | -1.3391879950  | 2.5401000054   | -1.2689820705 |
| 19 | O   | -1.6871936924  | 3.4541372507   | -0.5726556554 |
| 20 | O   | -0.5598591198  | 2.7414060619   | -2.3691920400 |
| 21 | H   | -1.7687286797  | -1.6237573060  | -0.9072725307 |
| 22 | H   | 0.0851276664   | -2.2651807500  | 0.8650759451 |
| 23 | H   | 1.8569190548   | -0.9096541443  | -0.1194050829 |
| 24 | C   | -2.0016937266  | 0.3059050736   | 3.3030729091 |
| 25 | O   | -0.2287192622  | -1.2623285647  | 3.3999475285 |
| 26 | O   | 2.1311388034   | -0.6678404807  | 2.4451683195 |
| 27 | C   | 3.5393498646   | -0.9115770638  | 2.2550094459 |
| 28 | H   | 0.7157825754   | 0.8261192599   | -2.9605682845 |
| 29 | H   | 2.1981789915   | 1.1127123247   | 1.3600388634 |
| 30 | H   | 1.1080252013   | -1.6197553013  | -3.5861631870 |
| 31 | H   | 0.6655168575   | 1.2689767420   | 3.3391737728 |
| 32 | H   | -0.1370654873  | 1.6876188874   | 1.8201243975 |
| 33 | H   | -1.0674152741  | -0.3186588910  | -5.8282899538 |
Table 3

| I  | Atom | X     | Y     | Z     |
|----|------|-------|-------|-------|
| 34 | H    | -2.0040496641 | 0.9497139761 | -0.0746723180 |
| 35 | H    | -2.5511289228 | 0.8923985794 | -1.7544226601 |
| 36 | H    | -0.3317698581 | 3.6756448233 | -2.4820098427 |
| 37 | H    | -2.6846189835 | -0.5258235033 | 3.3978526618 |
| 38 | H    | -1.7646249093 | 0.6827106495 | 4.2885658560 |
| 39 | H    | -2.4594310583 | -0.5258235033 | 3.3978526618 |
| 40 | H    | 0.7340611005  | -1.3374961954 | 3.2820710070 |
| 41 | H    | 4.0963144249  | 0.0151988123 | 2.3178690142 |
| 42 | H    | 3.736395278   | -1.3834401571 | 1.3015207068 |
| 43 | H    | 3.8448853312  | -1.5709655484 | 3.0513069993 |

(7R*, 9R*)-S2B, M0004:M0012
| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 1    | 0.4107678900 | 0.4082639736 | -1.5613152419 |
| 2    | -1.0126861854 | 0.7245830983 | -1.0426895832 |
| 3    | -1.0626558359 | 0.0976438230 | 0.3540938680 |
| 4    | -0.1477865415 | -1.1168540690 | 0.1700259599 |
| 5    | 0.9210234554 | -0.6096570952 | -0.6652863759 |
| 6    | -1.9557311625 | -0.0492352163 | -1.9445097966 |
| 7    | -1.2120386471 | -0.6599568806 | -2.9071536798 |
| 8    | 0.1822499433 | -0.2905104490 | -2.9502085579 |
| 9    | 0.4815543159 | -1.6390661880 | 1.4492505741 |
| 10   | 0.9958293448 | -0.4998269899 | 2.3245203146 |
| 11   | -0.1057713814 | 0.5356200647 | 2.5639711651 |
| 12   | -0.4743432354 | 1.0436766269 | 1.2534465552 |
| I | Atom | X               | Y               | Z               |
|---|------|-----------------|-----------------|-----------------|
| 13 | O    | -3.1523828956  | -0.1598466158  | -1.7977302255  |
| 14 | C    | 0.5230405214   | 0.5468929526   | -4.1619898406  |
| 15 | O    | 1.6264922249   | 0.9579956090   | -4.4117989897  |
| 16 | O    | -0.5323056410  | 0.7585938925   | -4.9726081648  |
| 17 | C    | 1.4288336069   | 1.5523223370   | -1.5892162975  |
| 18 | C    | 1.4823418336   | 2.2533295080   | -0.2643491589  |
| 19 | O    | 2.2781677936   | 2.084687092    | 0.6214199091   |
| 20 | O    | 0.4965743382   | 3.1831949501   | -0.2046645927  |
| 21 | H    | -1.2385683504  | 1.7760342451   | -1.0069208163  |
| 22 | H    | -2.0623112220  | -0.1634328106  | 0.6567523092   |
| 23 | H    | -0.6814434964  | -1.9034691428  | -0.3447011311  |
| 24 | C    | 0.3672791499   | 1.7444722399   | 3.3433493852   |
| 25 | O    | -1.2245447217  | -0.0130357319  | 3.2178639244   |
| 26 | O    | -0.5565151936  | -2.3294624325  | 2.1922932020   |
| 27 | C    | -0.7335255689  | -3.7348827469  | 1.9304555693   |
| 28 | H    | 0.8416255924   | -1.1460285883  | -2.9641296689  |
| 29 | H    | 1.2823096243   | -2.329867230   | 1.2026015962   |
| 30 | H    | -1.6536348589  | -1.1384500660  | -3.6624934449  |
| 31 | H    | 1.3294270520   | -0.9025418856  | 3.2711514351   |
| 32 | H    | 1.8109843717   | -0.0092169864  | 1.8168777764   |
| 33 | H    | -0.2911283279  | 1.2766251216   | -5.7554084622  |
| 34 | H    | 1.1583561157   | 2.2794197215   | -2.3350374605  |
| 35 | H    | 2.3969476975   | 1.1367760315   | -1.8149183193  |
| 36 | H    | 0.3261744507   | 3.4825795920   | 0.6995584747   |
| 37 | H    | -0.4605300205  | 2.4362858782   | 3.4284125614   |
| 38 | H    | 0.6644006392   | 1.4377921870   | 4.3372353132   |
| 39 | H    | 1.1974851398   | 2.2094258891   | 2.8339417552   |
| 40 | H    | -1.2801715644  | -0.9706092393  | 3.0563087092   |
| 41 | H    | 0.1793280662   | -4.2783796072  | 2.1412797553   |
| 42 | H    | -1.0262224941  | -3.9131109566  | 0.9033430964   |
| 43 | H    | -1.5168928225  | -4.0744360296  | 2.5894372289   |

(7R*, 9R*)-S2B, M0004:M0014

| I | Atom | X               | Y               | Z               |
|---|------|-----------------|-----------------|-----------------|
| 1 | C    | -0.3738032629  | 0.0756052948   | -1.5566181463  |
|   |   |   |   |   |
|---|---|---|---|---|
| 2 | C | -0.5019448772 | -1.3880090768 | -1.1168247833 |
| 3 | C | -0.0037511505 | -1.3742688791 | 0.3225342549 |
| 4 | C | 1.1603646433 | -0.3815625131 | 0.2304026046 |
| 5 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 6 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 7 | N | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 8 | C | 0.1792799192 | 0.0253724687 | -2.9956411630 |
| 9 | C | 1.4685722676 | -0.3815625131 | 0.2304026046 |
| 10 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 11 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 12 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 13 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 14 | C | 0.1792799192 | 0.0253724687 | -2.9956411630 |
| 15 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 16 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 17 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 18 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 19 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 20 | C | 0.1792799192 | 0.0253724687 | -2.9956411630 |
| 21 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 22 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 23 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 24 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 25 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 26 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 27 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 28 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 29 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 30 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 31 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 32 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 33 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 34 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
| 35 | C | 0.4771315809 | -2.1270391756 | -2.0133630352 |
| 36 | O | 0.7074993171 | 0.5999535620 | -0.7364477798 |
| 37 | O | 0.8370281203 | -1.2783615310 | -3.0145031231 |
\[(7R^*, 9R^*)-S2B, \text{ M0004:M0015}\]

| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
|  1 | C    | -0.4618707559 | 0.1550237351 | -1.4499625957 |
|  2 | C    | -0.6525736639 | -1.2969235408 | -0.9912936459 |
|  3 | C    | -0.0994370801 | -1.3015765790 | 0.4275051113 |
|  4 | C    | 1.1151052939 | -0.3789255896 | 0.2763367681 |
|  5 | O    | 0.6854993360 | 0.6202251389 | -0.6828264044 |
|  6 | O    | 0.6315958734 | -3.2306467843 | -1.7476722366 |
|  7 | N    | 0.0196031614 | 0.0615471597 | -0.6828264044 |
|  8 | C    | 1.5195046983 | 0.3498086632 | 1.5460081284 |
|  9 | C    | 0.3042714898 | 0.9225938084 | 2.2724575959 |
| 10 | C    | -0.7369684338 | -0.1737244573 | 2.5233384989 |
| 11 | O    | -1.1217410150 | -0.6823809970 | 1.2215914010 |
| 12 | O    | 0.6315958734 | -3.2306467843 | -1.7476722366 |
| 13 | C    | -1.0947257407 | 0.1094114839 | -3.9219200815 |
| 14 | O    | -1.1153123849 | 0.7221813545 | -4.9518171673 |
| 15 | O    | -2.1105876565 | -0.7151176146 | -3.5432034182 |
| 16 | C    | -1.6215930645 | 1.0983408695 | -1.1436815303 |
| 17 | C    | -1.0979063092 | 2.4974535341 | -1.1179584619 |
| 18 | O    | -1.1071344982 | 3.2668682022 | -0.1948511746 |
| 19 | O    | -0.5738457079 | 2.8206660026 | -2.3311596386 |
| 20 | H    | -1.6721639029 | -1.6398939381 | -1.0387673119 |
| 21 | H    | 0.1543360490 | -2.2821565865 | 0.7929612364 |
| 22 | H    | 1.9474636515 | -0.9365541067 | -0.1282650618 |
| 23 | C    | -2.0215290849 | 0.3403627595 | 3.1384532970 |
| 24 | O    | -0.2373275159 | -1.2028588382 | 3.3407466048 |
| 25 | O    | 2.1413962174 | -0.6204479491 | 2.4272808210 |
| I  | Atom | X      | Y      | Z      |
|----|------|--------|--------|--------|
| 1  | C    | -0.4203760712 | 0.2060312572 | -1.4316050605 |
| 2  | C    | -0.6155245903 | -1.2525765472 | -0.9853454937 |
| 3  | C    | -0.0670494025 | -1.2749701070 | 0.4328831745 |
| 4  | C    | 1.1439908485 | -0.3503158586 | 0.2936358684 |
| 5  | O    | 0.6777804320 | 0.6918269235 | -0.5975372012 |
| 6  | C    | 0.3055235226 | -2.0524033080 | -1.890896744 |
| 7  | N    | 0.7116328860 | -1.2311391388 | -2.8914976348 |
| 8  | C    | 0.1582171025 | 0.1264995222 | -2.8670979801 |
| 9  | C    | 1.5816038796 | 0.2960100622 | 1.5954987094 |
| 10 | C    | 0.3929024396 | 0.8452769201 | 2.3812839637 |
| 11 | C    | -0.6773833760 | -0.2365772924 | 2.5688334444 |
| 12 | O    | -1.0746996658 | -0.6438177022 | 1.2357427342 |
| 13 | O    | 0.6575407884 | -3.1998111061 | -1.7175397749 |
| 14 | C    | -0.8349670792 | 0.1858025084 | -3.9940968327 |
| 15 | O    | -0.6398188902 | 0.6078936147 | -5.0974009900 |
|   | Atom | X         | Y         | Z         |
|---|------|-----------|-----------|-----------|
| 16| O    | -1.9991504378 | -0.4370808050 | -3.6526775873 |
| 17| C    | -1.6161203113  | 1.1062295673  | -1.1889851463 |
| 18| C    | -1.3805749440  | 2.4832968818  | -1.7188365521 |
| 19| O    | -0.7095369304  | 2.7556529112  | -2.6845785291 |
| 20| O    | -2.0630445913  | 3.4186752166  | -1.0278007498 |
| 21| H    | -1.6346738601  | -1.5979988852 | -1.0337198085 |
| 22| H    | 0.1763390974   | -2.2610120076 | 0.7877223175 |
| 23| H    | 1.9685869338   | -0.885043805  | -0.1552760757 |
| 24| C    | -1.9478951559  | 0.2631713543  | 3.2225808957 |
| 25| O    | -0.1962633643  | -1.3261816158 | 3.3148319499 |
| 26| O    | 2.1852938569   | -0.7466701891 | 2.4060195665 |
| 27| C    | 3.6021196626   | -0.9740933430 | 2.2654940811 |
| 28| H    | 0.9042883909   | 0.8801603992  | -3.0153405758 |
| 29| H    | 2.3033349843   | 1.0762655549  | 1.3927178349 |
| 30| H    | 1.3758616577   | -1.5296911951 | -3.5733781527 |
| 31| H    | 0.7342378097   | 1.1923909492  | 3.3466979294 |
| 32| H    | -0.0336930863  | 1.6662099552  | 1.8255612800 |
| 33| H    | -2.6116615172  | -0.5041141396 | -4.4005722533 |
| 34| H    | -1.8028920836  | 1.1304028344  | -0.1326113128 |
| 35| H    | -2.4823527571  | 0.7007794681  | -1.6913881017 |
| 36| H    | -1.9494532450  | 4.3058314244  | -1.4004663454 |
| 37| H    | -2.6371638875  | -0.5663943717 | 3.2871068980 |
| 38| H    | -1.7293407525  | 0.6195761395  | 4.2200930982 |
| 39| H    | -2.3907040651  | 1.0547683020  | 2.6348469848 |
| 40| H    | 0.7659756490   | -1.4191253813 | 3.2027198803 |
| 41| H    | 4.1566679081   | -0.0720631793 | 2.4925460013 |
| 42| H    | 3.8539172154   | -1.3071907104 | 1.2670630432 |
| 43| H    | 3.8585249999   | -1.7447005025 | 2.9747586771 |

(7R*, 9R*) -S2B, M0004:M0017

| I | Atom | X         | Y         | Z         |
|---|------|-----------|-----------|-----------|
|   | C    | 0.1209755088 | 0.3543792823 | -1.5743867316 |
| 2 | C    | -1.3448109535 | 0.5043843513 | -1.1400521740 |
| 3 | C    | -1.3515601924 | -0.0018982195 | 0.2941306413 |
| 4 | C    | -0.3717485027 | -1.1748040785 | 0.2021877028 |
| Atom | Charge | X   | Y   | Z   |
|------|--------|-----|-----|-----|
| O    | 0      | 0.6427330829 | -0.7053134393 | -0.7204713039 |
| C    | -2.0978059892 | -0.4722487548 | -2.0293862780 |
| N    | -1.2442610981 | -0.8820536579 | -3.004631943 |
| C    | 0.0642522938  | -0.2306074786 | -3.0026054123 |
| C    | 0.3191220925  | -1.5249685778 | 1.5059428347 |
| C    | 0.8127704972  | -0.2770344630 | 2.2371066487 |
| C    | -0.3313077932 | 0.7313096379  | 2.4029857339 |
| O    | -0.7789880057 | 1.0653115460  | 1.0684101209 |
| O    | -3.2347604767 | -0.8570600231 | -1.8650526453 |
| C    | 0.0273754013  | 0.8085218464  | -0.916077127 |
| O    | 0.5738451495  | 0.7736043335  | -5.156163811 |
| O    | -0.8141713974 | 1.8256975206  | -3.7406955814 |
| C    | 0.9949363426  | 1.5744323138  | -1.359336483 |
| C    | 2.4242138770  | 1.2263578374  | -1.6425053757 |
| O    | 2.8040249770  | 0.5128761299  | -2.536875143 |
| O    | 3.2780250397  | 1.8369130410  | -0.791719637 |
| C    | -1.7298436598 | 1.505721860  | -1.2260899346 |
| H    | -2.3280260556 | -0.2810362074 | 0.6503362672 |
| H    | -0.8661249406 | -2.0509119703 | -0.1873191599 |
| C    | 0.0964197909  | 2.0448755915  | 3.0260531050 |
| O    | -1.3811828009 | 0.2046219275  | 3.178185483 |
| O    | -0.7051704795 | -2.1960560866 | 2.2908085671 |
| C    | -0.2689777007 | -3.2812901375 | 3.136932838 |
| H    | 0.8766109115  | -0.9071112602 | -3.1736202053 |
| H    | 1.1343477597  | -2.2056703636 | 1.3001315387 |
| H    | -1.5089052854 | -1.5675572066 | -3.678859921 |
| H    | 1.2025498391  | -0.5428167626 | 3.212970241 |
| H    | 1.5970243566  | 0.1747690032  | 1.6481166368 |
| H    | -0.9399594495 | 2.4660789815  | -4.4567162372 |
| H    | 0.8786014446  | 1.8875948053  | -0.3395870526 |
| H    | 0.6825713867  | 2.3721096158  | -2.018885903 |
| H    | 4.2025026729  | 1.6331063923  | -0.9982059813 |
| H    | -0.7687009117 | 2.6907507820  | 3.0652738707 |
| H    | 0.4616683963  | 1.8735688286  | 4.0240980759 |
| H    | 0.8649684457  | 2.5122892045  | 2.4213546932 |
| H    | -1.4644917548 | -0.7526218704 | 3.0276283318 |
(7R*,9R*)-S2B, M0004:M0018

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.4501329964 | 0.1738716310 | -1.4762126297 |
| 2 | C    | -0.6769360446  | -1.2756448913 | -1.0303883638 |
| 3 | C    | -0.1204217522  | -1.3050312372 | 0.3873247897 |
| 4 | C    | 1.1164606809   | -0.4129697045 | 0.2392930824 |
| 5 | O    | 0.6986782610   | 0.6129010981 | -0.6934683846 |
| 6 | C    | 0.2152072362   | -2.0840193777 | -1.9596743704 |
| 7 | N    | 0.6241031994   | -1.2583074287 | -2.9608167893 |
| 8 | C    | 0.0510247037   | 0.0878296649 | -2.931266987 |
| 9 | C    | 1.5505456338   | 0.2864204847 | 1.5146918328 |
| 10| C    | 0.3554613642   | 0.8855114212 | 2.253563344 |
| 11| C    | -0.7179706741  | -0.1824000434 | 2.4941244959 |
| 12| O    | -1.1217043293  | -0.6586058018 | 1.1873319102 |
| 13| O    | 0.5458574015   | -3.239641806  | -1.8075285452 |
| 14| C    | -1.0308948401  | 0.1192519874 | -3.977071277 |
| 15| O    | -0.9672553185  | 0.6145010986 | -5.0650330977 |
| 16| O    | -2.1132763248  | -0.6067136219 | -3.5707360226 |
| 17| C    | -1.5810531877  | 1.1478492726 | -1.1918925614 |
| 18| C    | -1.0534526305  | 2.5313315611 | -1.4082783877 |
| 19| O    | -0.5503290523  | 2.9202689868 | -2.4322007192 |
| 20| O    | -1.1845420923  | 3.3180521540 | -0.3168134143 |
| 21| H    | -1.7037363650  | -1.5955043796 | -1.0760412417 |
| 22| H    | 0.1058789190   | -2.2942691422 | 0.7463527131 |
| 23| H    | 1.9305327821   | -0.9846651591 | -0.1814703044 |
| 24| C    | -1.9839305107  | 0.3582575438 | 3.1242208770 |
| 25| O    | -0.2422460961  | -1.2358214584 | 3.2947590063 |
| 26| O    | 2.1462219673   | -0.7091129673 | 2.3850186218 |
| 27| C    | 3.5565515107   | -0.9677517525 | 2.2355740089 |
| 28| H    | 0.7686721020   | 0.8569657365 | -3.1359455890 |
| 29| H    | 2.2748849557   | 1.0533604087 | 1.2736204299 |
(7R*,9R*)-S2B, M0004:M0019

| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
|   | C    | 0.1339585467 | 0.2970449247 | -1.5486821219 |
|   | C    | -1.3298086422 | 0.4736126455 | -1.1124625748 |
|   | C    | -1.3337654310 | 0.019507569 | 0.3389455433 |
|   | C    | -0.3635585203 | -1.162451587 | 0.2846610150 |
|   | O    | 0.6602973140 | -0.7175683315 | -0.6391228032 |
|   | C    | -2.1022246129 | -0.5291178355 | -1.9529132231 |
|   | N    | -1.2647918864 | -0.9867086372 | -2.9177644691 |
|   | C    | 0.0723814510 | -0.38667444418 | -2.9380697537 |
|   | C    | 0.3055673431 | -1.4836715575 | 1.6070841816 |
|   | C    | 0.8074679981 | -0.2245394480 | 2.3125538393 |
|   | O    | -0.3209402184 | 0.8085911460 | 2.4270010687 |
|   | O    | -0.7393943945 | 1.1023117395 | 1.0723951998 |
|   | O    | -3.2427134291 | -0.8924220447 | -1.7613510284 |
|   | C    | 0.0938849101 | 0.5268409767 | -4.1319539109 |
|   | O    | 0.5292669489 | 0.2760491843 | -5.2186930315 |
|   | O    | -0.5821332461 | 1.6829463256 | -3.8721936230 |
|   | C    | 0.9915499814 | 1.5383711057 | -1.3982356468 |
|   | C    | 2.3779222426 | 1.3093520079 | -1.9066724386 |
| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
| 1 | C    | 0.3249030365 | -0.2042244257 | -1.4579974014 |
| 2 | C    | 0.3986478595 | 1.2420708398 | -0.9314875308 |
| 3 | C    | -0.1636014373 | 1.1526874682 | 0.4767438905 |
| 4 | C    | -1.2485163734 | 0.0904159368 | 0.311522808 |
| 5 | O    | -0.6340599869 | -0.8704590947 | -0.5815738683 |
| 6 | C    | -0.5079243237 | 2.0532553480 | -1.8350422180 |
| 7 | N    | -0.9082486539 | 1.2463812355 | -2.8538865261 |
|   |   |   |   |   |
|---|---|---|---|---|
| 8 | C | -0.3733090228 | -0.0986801137 | -2.8495094755 |
| 9 | C | -1.6128499984 | -0.6430680175 | 1.5875851599 |
| 10 | C | -0.3673179147 | -1.0659427271 | 2.3661913904 |
| 11 | C | 0.5622846589 | 0.1349830022 | 2.5815339238 |
| 12 | O | 0.9158319214 | 0.6218199184 | 1.2668273697 |
| 13 | O | -0.8427973553 | 3.2046824493 | -1.6631143637 |
| 14 | C | -0.3673179147 | -1.0659427271 | 2.3661913904 |
| 15 | O | 0.4890040334 | 0.3649217123 | -5.0571817026 |
| 16 | O | 1.0427491155 | -1.557579778 | -4.0872892008 |
| 17 | C | 1.602834059 | -1.0116565382 | -3.220252159 |
| 18 | C | 2.7445491160 | -0.5816362254 | -2.1869074614 |
| 19 | O | 3.7710343580 | -1.1749460937 | -2.3646410758 |
| 20 | O | 2.5127809901 | 0.6351996423 | -2.7637592226 |
| 21 | H | 1.3938371721 | 1.6452689349 | 0.9272637220 |
| 22 | H | -0.5228091806 | 2.0911399282 | 0.8620750577 |
| 23 | H | -2.1360069466 | 0.5182439474 | -0.1299349576 |
| 24 | C | 1.8746259137 | -0.2182007020 | 3.2465607083 |
| 25 | O | -0.0599207617 | 1.1386589494 | 3.3489061615 |
| 26 | O | -2.3840495526 | 0.3225449766 | 2.3536987550 |
| 27 | C | -3.4578303143 | -0.2032438515 | 3.1631293992 |
| 28 | H | -1.1511277041 | -0.8497694673 | -2.8419917821 |
| 29 | H | -2.2278593071 | -1.4983257869 | 1.3412611716 |
| 30 | H | -1.4112319639 | 1.6085007189 | -3.6351742369 |
| 31 | H | -0.6469899058 | -1.4807794974 | 3.3258945552 |
| 32 | H | 0.1539108871 | -1.8140203111 | 1.7890225619 |
| 33 | H | 1.5186494394 | -1.7763063258 | -4.8465818288 |
| 34 | H | 1.4045216552 | -2.0508714935 | -1.5311842673 |
| 35 | H | 1.9004427927 | -0.9104133948 | -0.2870770290 |
| 36 | H | 3.2462624087 | 0.9361576648 | -3.3205620722 |
| 37 | H | 2.4598591300 | 0.6859662118 | 3.3324500840 |
| 38 | H | 1.6875715846 | -0.6135674779 | 4.2355750694 |
| 39 | H | 2.4158767378 | -0.9420855564 | 2.6538777693 |
| 40 | H | -1.0141154004 | 1.1632273680 | 3.163957804 |
| 41 | H | -3.0841028922 | -0.8738195931 | 3.9265660814 |
| 42 | H | -4.1751701984 | -0.7277653414 | 2.5445998816 |
| 43 | H | -3.9332948635 | 0.6450393368 | 3.6286026926 |
| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 1    | -0.2998143984 | 0.3081286447 | -1.3964971325 |
| 2    | -0.4781923427  | -1.1367432883 | -0.9000689255  |
| 3    | 0.0849437831   | -1.1063124805 | 0.5114252838   |
| 4    | 1.2638940870   | -0.148360591  | 0.3453001965   |
| 5    | 0.7481025626   | 0.8670462383  | -0.5514006858  |
| 6    | 0.4046336278   | -1.9703296593 | -1.8071472171  |
| 7    | 0.8062178070   | -1.1794592196 | -2.8395639321  |
| 8    | 0.3162020975   | 0.1797432139  | -2.8275848572  |
| 9    | 1.6996117662   | 0.5321230012  | 1.6306857328   |
| 10   | 0.5024398909   | 1.059955239   | 2.4183756677   |
| 11   | -0.5379627568  | -0.0456750021 | 2.6298145643   |
| 12   | -0.9359838221  | -0.4886995075 | 1.3112732114   |
| 13   | 0.7332497067   | -3.122212099  | -1.626093306   |
| 14   | -0.7062905399  | 0.4095763223  | -3.9032458394  |
| 15   | -1.352927831   | -0.4173518726 | -4.4826430766  |
| 16   | -0.8390176359  | 1.7427457768  | -4.092857049   |
| 17   | -1.5002199203  | 1.2435422053  | -1.2280446123  |
| 18   | -2.7388606171  | 0.8991575920  | -2.0068177052  |
| 19   | -3.3204205238  | 1.6232753911  | -2.7740232691  |
| 20   | -3.1881413956  | -0.3481323228 | -1.7325731356  |
| 21   | -1.5009576022  | -1.4663074479 | -0.9203502013  |
| 22   | 0.3621538997   | -2.0755417199 | 0.8886428592   |
| 23   | 2.0959276163   | -0.6625576913 | -0.1145847764  |
| 24   | -1.8124981973  | 0.4350621455  | 3.2903752096   |
| 25   | -0.0204124513  | -1.1086211191 | 3.3930221397   |
| 26   | 2.3426939371   | -0.4759268587 | 2.4521264502   |
| 27   | 3.7629143022   | -0.6606162501 | 2.2880104719   |
| 28   | 1.0942085674   | 0.9181672117  | -2.920025627   |
| 29   | 2.3942985602   | 1.3314502049  | 1.4074338156   |
| 30   | 1.3512229196   | -1.5510527201 | -3.5877082167  |
| 31   | 0.8409683037   | 1.4280075865  | 3.3770563485   |
| 32   | 0.0508839054   | 1.8632591500  | 1.8561041757   |
| 33   | -1.6458877644  | 1.9848182586  | -4.5720302310  |
|   |   |   |   |
|---|---|---|---|
| 34 | H | -1.2084519681 | 2.2436624869 | -1.5005117494 |
| 35 | H | -1.7420204301 | 1.1859440735 | -0.1768608017 |
| 36 | H | -3.9712156572 | -0.5816300778 | -2.2543282129 |
| 37 | H | -2.4853678645 | -0.4066170353 | 3.3718072035 |
| 38 | H | -1.5913955392 | 0.8080268389 | 4.2812674468 |
| 39 | H | -2.2782754074 | 1.2102324326 | 2.6979329855 |
| 40 | H | 0.9438392983 | -1.1728865844 | 3.2809720631 |
| 41 | H | 4.2913454407 | 0.2625005319 | 2.4921027024 |
| 42 | H | 4.0057989283 | -0.9989204263 | 1.2889854957 |
| 43 | H | 4.0587636997 | -1.4124762783 | 3.0022451514 |
### (7S*,9S*)-S2C, M001: M0001

| I  | Atom | X             | Y             | Z             |
|----|------|---------------|---------------|---------------|
| 1  | C    | -0.0204326187 | -0.1348656184 | -1.3585004227 |
| 2  | C    | 0.4731422526  | -1.4752306644 | -0.8118805584 |
| 3  | C    | 0.8871358237  | -1.1908280316 | 0.6173845558  |
| 4  | C    | 1.3921216360  | 0.2668101654  | 0.5455090600  |
| 5  | O    | 0.8463740069  | 0.8214029226  | -0.675743885  |
| 6  | C    | 1.7047276442  | -1.7642169188 | -1.6629458101 |
| 7  | N    | 1.6124102192  | -1.004956736  | -2.7802028905 |
| 8  | C    | 0.4785014971  | 0.0907983345  | 2.8196572966  |
| 9  | C    | 0.9494817000  | 1.0738618488  | 1.7743877358  |
| 10 | C    | 0.9469847156  | 0.1271989592  | 2.9758052154  |
| 11 | O    | -0.1910474584 | 0.8994529645  | 2.8196572966  |
| 12 | O    | -0.2910617945 | 1.2533493359  | 1.3702994823  |
| 13 | C    | -0.4964675517 | -0.5571432328 | -3.8667645041 |
| 14 | O    | -1.6850067099 | -0.7111415392 | -3.7716038050 |
| 15 | O    | 0.1651696420  | -0.7590486321 | 5.0306953993  |
| 16 | C    | -1.4660572143 | 0.1978725893  | -1.057168240  |
| 17 | C    | -1.8703567431 | 1.4923921498  | 1.6833454400  |
| 18 | O    | -1.2809448197 | 2.1048249247  | -2.5398892891 |
| 19 | O    | -3.0380566305 | 1.9389377411  | 1.1642292141  |
| 20 | H    | -0.2459431486 | -2.2786458239 | -0.8604961016 |
| 21 | H    | 1.6551121360  | -1.8765544874 | 0.9420457595  |
| 22 | H    | 2.4698676218  | 0.2807508992  | 0.4747615650  |
| 23 | O    | -0.3906572997 | 1.5784972634  | 1.6213128910  |
| 24 | C    | -0.5182697433 | 2.8855886660  | 1.0069859758  |
| 25 | H    | 0.7630659637  | 0.9217357842  | -3.0434625894 |
| 26 | H    | 1.6244852958  | 1.9048600210  | 1.9375529403  |
| 27 | H    | 2.2838522733  | -1.0429384122 | -3.5149050057 |
| 28 | H    | 1.9098888089  | -0.3647117731 | 3.046880783   |
| 29 | H    | 0.7673557766  | 0.6695169594  | 3.8924329546  |
| 30 | H    | -0.4257498637 | -1.0370725702 | -5.7457752903 |
| 31 | H    | -1.5640909580 | 0.2677145003  | 0.0119136949  |
| 32 | H    | -2.1327989627 | -0.5643208793 | -1.4278132195 |
| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 34   | H       | -3.3528687549 | 2.7382102857 | -1.6115727583 |
| 35   | H       | -0.0241387761 | 2.8957277149 | 0.0512409438  |
| 36   | H       | -0.1017597734 | 3.6463432799 | 1.6563298242  |
| 37   | H       | -1.5766158267 | 3.0484685784 | 0.8799156322  |
| 38   | O       | -1.4177955185 | -0.3227185174 | 3.1813937436  |
| 39   | H       | -1.5194116095 | 0.4972834885 | 2.6708982403  |
| 40   | C       | -0.0055584735 | -0.3227185174 | 3.1813937436  |
| 41   | H       | -1.5194116095 | 0.4972834885 | 2.6708982403  |

(7S*, 9S*)-S2C, M0001:M0002
| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
|  1 | C    | -0.0790672802 | -0.5793809150 | -1.4161201906 |
|  2 | C    | 1.3724220791  | -0.2367363080 | -1.0098405423 |
|  3 | C    | 1.2291482641  | 0.4183239473  | 0.3660520348  |
|  4 | C    | -0.1127247192 | 1.1376274290  | 0.2208698971  |
|  5 | O    | -0.9176052418 | 0.1751747772  | -0.5094071834 |
|  6 | C    | 1.8315976924  | 0.8182129931  | -1.9979080618 |
|  7 | N    | 0.8517139063 | 0.9770143381  | -2.9271019989 |
|  8 | C    | -0.2518355018 | 0.0476366672  | -2.8425070899 |
|  9 | C    | -0.7689483275 | 1.4511665084  | 1.5553759210  |
| 10 | C    | -0.8543163172 | 0.1893403750  | 2.3967661112  |
| 11 | C    | 0.5082699879  | -0.4689062976  | 2.6040122337  |
| 12 | O    | 1.1392283685  | -0.6570260540  | 1.3062460153  |
| I | Atom | X             | Y             | Z             |
|---|------|---------------|---------------|---------------|
| 1 | C    | -0.1274932541 | -0.6297069691 | -1.3883509018 |
| # | Symbol | X     | Y     | Z     |
|---|--------|-------|-------|-------|
| 2 | C      | 1.3222664348 | -0.2706724877 | -0.9874207659 |
| 3 | C      | 1.1789627220  | 0.3935982882  | 0.3852184018  |
| 4 | C      | -0.1690551404 | 1.1010851655  | 0.2377950922  |
| 5 | O      | -0.9678385906 | 0.1259703456  | -0.4809378345 |
| 6 | C      | 1.7687366008  | 0.7863220661  | -1.9796835190 |
| 7 | N      | 0.7747069648  | 0.9531730725  | -2.8919734321 |
| 8 | C      | -0.3148435451 | 0.0090680109  | -2.8107703982 |
| 9 | C      | -0.8945498962 | 1.1010851655  | 0.2377950922  |
| 10| C      | -0.1690551404 | 1.1010851655  | 0.2377950922  |
| 11| C      | 1.7687366008  | 0.7863220661  | -1.9796835190 |
| 12| O      | 1.1047680531  | -0.6723258755 | 1.336012936  |
| 13| O      | 2.8001296391  | 1.4190497342  | -1.9268631623|
| 14| C      | -0.3220567898 | -0.9656453293 | -3.966352449 |
| 15| O      | -1.1308576719 | -1.8461688840 | -4.1048315099|
| 16| O      | 0.6520406792  | -0.7253013310 | -4.8660030949|
| 17| C      | -0.5425437489 | -2.1054350824 | -1.2988876425|
| 18| C      | -0.2240360880 | -2.6539235610 | 0.0576701094 |
| 19| O      | -0.9850407777 | -2.7541227788 | 0.991541841  |
| 20| O      | 1.0596641507  | -3.064149963  | 0.1161339135 |
| 21| H      | 1.9887512059  | -1.1146721725 | -0.9483768647|
| 22| H      | 1.9962970806  | 1.0663507655  | 0.5939805543 |
| 23| H      | -0.0466758897 | 1.9881937349  | -0.367558316 |
| 24| O      | -2.1726866882 | 1.8727006908  | 1.4352026394 |
| 25| C      | -2.3717388990 | 3.1427437876  | 0.7958273435 |
| 26| H      | -1.2826525313 | 0.4885104444  | -2.794407246 |
| 27| H      | -0.2232960329 | 2.1892427377  | 2.051014603  |
| 28| H      | 0.9072451773  | 1.5367602120  | -3.6897915957|
| 29| H      | -1.3335255374 | 0.3977279292  | 3.8340640567 |
| 30| H      | -1.5319229945 | -0.5301048759 | 1.9017979632 |
| 31| H      | 0.6165392858  | -1.3411908842 | -5.6349991146|
| 32| H      | -0.0115859768 | -2.6899612743 | -2.0297549595|
| 33| H      | -1.6036855427 | -2.1697732171 | -1.4724591389|
| 34| H      | 1.3916501687  | -3.1106071004 | 1.0266576400 |
| 35| H      | -2.1391223712 | 3.1014719948  | -0.2610612815|
| 36| H      | -1.7717037103 | 3.9195368709  | 1.2607276026 |
| 37| H      | -3.4168117385 | 3.3814085401  | 0.9167126726 |
| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
| 38| O    | 0.3496013120 | -1.7634203622 | 3.1893691093 |
| 39| H    | -0.2945578341 | -2.2835492476 | 2.6783393748 |
| 40| C    | 1.4073358110 | 0.2968894218 | 3.5510107176 |
| 41| H    | 1.6008901521 | 1.2962208809 | 3.1842154135 |
| 42| H    | 2.3409074684 | -0.2434543167 | 3.6184239041 |
| 43| H    | 0.9661502616 | 0.3579611360 | 4.5358461461 |

(7S*,9S*)-S2C, M0001:M0005

| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
| 1 | C    | -0.4955211249 | 0.0565820154 | -1.5895521277 |
| 2 | C    | -0.1451080704 | -1.4011808620 | -1.2112923405 |
| 3 | C    | 0.4811629309 | -1.2789429635 | 0.1792703213 |
| 4 | C    | 1.1821836235 | 0.0753565417 | 0.0836232270 |
| 5 | O    | 0.2069242797 | 0.8801667680 | -0.6311060888 |
| 6 | C    | 0.9339946119 | -1.8277988229 | -2.1875679633 |
| 7 | N    | 1.1074525083 | -0.8231602250 | -3.085533107 |
| 8 | C    | 0.1786514315 | 0.2795536179 | -2.9878747588 |
| 9 | C    | 1.4679637369 | 0.6941487500 | 1.4348739089 |
| 10| C    | 0.1784738698 | 0.7760460968 | 2.2392015969 |
| 11| C    | -0.4731060937 | -0.5996158494 | 2.4064006326 |
| 12| O    | -0.6185025327 | -1.2168106540 | 1.0989322457 |
| 13| O    | 1.5756093570 | -2.8533060880 | -2.1314884304 |
| 14| C    | -0.7882696821 | 0.2426698177 | -4.1420029372 |
| 15| O    | -0.9829420995 | -0.6683979234 | -4.8963660362 |
| 16| O    | -1.4383529454 | 1.4295432475 | -4.2333640549 |
| 17| C    | -1.9807362188 | 0.4476429599 | -1.5591451142 |
| 18| C    | -2.5760363175 | 0.1136668433 | -0.2265936694 |
| 19| O    | -2.7076158866 | 0.8690007579 | 0.7087729092 |
| 20| O    | -2.9814595859 | -1.1705417808 | -0.1900591319 |
| 21| H    | -0.9886463607 | -2.0692115424 | -1.2076575534 |
| 22| H    | 1.1466129127 | -2.0987720740 | 0.3996105514 |
| 23| H    | 2.0934892764 | 0.0030088650 | -0.4909155578 |
| 24| O    | 2.0400253513 | 1.9799489995 | 1.1731888369 |
| 25| C    | 2.7067659363 | 2.6148956265 | 2.2761498335 |
| 26| H    | 0.6585846999 | 1.2439262937 | -2.9654142444 |
|   | X               | Y               | Z               |
|---|-----------------|-----------------|-----------------|
|1  | 0.112221208     | 0.0859013551    | -1.3984781966   |
|2  | 0.6240388724    | -1.2495978974   | -0.8598570335   |
|3  | 0.9840313255    | -0.9728645939   | 0.5821924886    |
|4  | 1.4709094419    | 0.4898579903    | 0.5421791881    |
|5  | 0.9168921305    | 1.0628424528    | -0.6697872625   |
|6  | 1.8845811141    | -1.4936441030   | -1.6749874398   |
|7  | 1.8231591893    | -0.6969796266   | -2.7731543258   |
|8  | 0.6626701836    | 0.1647136813    | -2.8461285003   |
|9  | 1.0164162598    | 1.2684908369    | 1.7866179250    |
|10 | 0.9791703480    | 0.2928071768    | 2.9641050363    |
|11 | -0.1561601419   | -0.7275993481   | 2.7532604178    |
|12 | -0.2215684781   | -1.0820800633   | 1.3485032752    |
|13 | 2.7905016911    | -2.2409360656   | -1.376147150    |
|14 | -0.2595279861   | -0.3020086878   | -3.9400039290   |
|15 | -0.0703959491   | -1.1965213203   | -4.7104744695   |
|16 | -1.3377677455   | 0.5261006619    | -4.0205739350   |

(7S*, 9S*)-S2C, M0001-M0006
| I  | Atom | X        | Y        | Z        |
|----|------|----------|----------|----------|
| 17 | C    | -1.3443977119 | 0.4161285074 | -1.1422176972 |
| 18 | C    | -2.3011287918 | -0.5996735638 | -1.6628440871 |
| 19 | O    | -2.0343163130 | -1.6607038253 | -2.1736854878 |
| 20 | O    | -3.5764291207 | -0.1987210715 | -1.4752176328 |
| 21 | H    | -0.0793647761 | -2.0562421494 | -0.9700439093 |
| 22 | H    | 1.7472553229 | -1.6506904787 | 0.9338244333 |
| 23 | H    | 2.5485779829 | 0.5164428155 | 0.4714126150 |
| 24 | O    | -0.3143622775 | 1.7986220225 | 1.6288724426 |
| 25 | C    | -0.4016095223 | 3.1256605544 | 1.0569737370 |
| 26 | H    | 0.9202930652 | 1.1959391483 | -3.0388570945 |
| 27 | H    | 1.7003362271 | 2.0847055440 | 1.9847024708 |
| 28 | H    | 2.5002901549 | -0.7575457824 | -3.5019259072 |
| 29 | H    | 1.9395709564 | -0.2011589058 | 3.0521890368 |
| 30 | H    | 0.7738269151 | 0.8162457059 | 3.8864310450 |
| 31 | H    | -1.9418373052 | 0.2631392433 | -4.7309369612 |
| 32 | H    | -1.5974585940 | 1.3705153197 | -1.5782614818 |
| 33 | H    | -1.4617800612 | 0.4779090394 | -0.0713740312 |
| 34 | H    | -4.2135361144 | -0.8720848081 | -1.7563643520 |
| 35 | H    | 0.0480886856 | 3.1374074914 | 0.0796087349 |
| 36 | H    | 0.0872375514 | 3.8450208198 | 1.7039967644 |
| 37 | H    | -1.4530085437 | 3.3590702743 | 0.9907852441 |
| 38 | H    | -1.3908306379 | -0.1527063553 | 3.0976061185 |
| 39 | H    | -1.4681593293 | 0.6871540281 | 2.6160490357 |
| 40 | C    | 0.0035644026 | -1.9900016998 | 3.5756350202 |
| 41 | H    | 0.9107552558 | -2.5147777877 | 3.3047700628 |
| 42 | H    | -0.8485695245 | -2.6257141637 | 3.3832362624 |
| 43 | H    | 0.0278197271 | -1.7424223714 | 4.6283647277 |

$\left(7S^*,9S^*\right)$-S2C, M0001:M0007

| I  | Atom | X        | Y        | Z        |
|----|------|----------|----------|----------|
| 1  | C    | -0.0975272505 | -0.1559127888 | -1.3471506099 |
| 2  | C    | 0.4392288444 | -1.4781788835 | -0.7904004241 |
| 3  | C    | 0.8435495521 | -1.1692642106 | 0.6356292449 |
| 4  | C    | 1.3218143982 | 0.2938520993 | 0.5438482044 |
| 5  | O    | 0.7152570131 | 0.8390323806 | -0.6554102053 |
|    |   |   |   |   |   |   |   |   |
|----|---|---|---|---|---|---|---|---|
|    | 6 | C | 1.6864372548 | -1.7360383072 | -1.6283658677 |
|    | 7 | N | 1.5968642160 | -0.9621230827 | -2.7351157090 |
|    | 8 | C | 0.4151516048 | -0.1106130723 | -2.8006424336 |
|    | 9 | C | 0.9147056150 | 1.0933651643 | 1.7917011832 |
|    | 10| C | 0.9108163118 | 0.1380952454 | 2.9871340883 |
|    | 11| C | -0.2410728082 | -0.8729712807 | 2.8363761857 |
|    | 12| O | -0.3329963869 | -1.2768118555 | 1.4418311511 |
|    | 13| C | 0.4151516048 | -0.1106130723 | -2.8006424336 |
|    | 14| O | -0.3329963869 | -1.2768118555 | 1.4418311511 |
|    | 15| O | 2.5971811444 | -2.4801453129 | -3.3314254930 |
|    | 16| O | 0.1887909201 | -0.7906126264 | -5.055042994 |
|    | 17| C | -1.5627322334 | 0.1012972986 | -1.0512752334 |
|    | 18| C | -2.0234020309 | 1.4621869715 | -1.4684839312 |
|    | 19| O | -2.8383679957 | 2.1447802656 | -0.9076926822 |
|    | 20| O | -1.4425455265 | 1.8782162443 | -2.630708050 |
|    | 21| H | -0.2550519824 | -2.3034886964 | -0.832634222 |
|    | 22| H | 1.6239556058 | -1.8363183186 | 0.9690940760 |
|    | 23| H | 2.3951163517 | 0.3208956921 | 0.4290959526 |
|    | 24| O | -0.4151348386 | 1.6230307692 | 1.6591861191 |
|    | 25| C | -0.5097085106 | 2.9681063676 | 1.1279953499 |
|    | 26| H | 0.6497102659 | 0.9079835399 | -3.0463107028 |
|    | 27| H | 1.6092909484 | 1.9079727813 | 1.9546825393 |
|    | 28| H | 2.2689427565 | -0.8754438880 | -3.4696293837 |
|    | 29| H | 1.8674946524 | -0.3661818801 | 3.6011848322 |
|    | 30| H | 0.7431293626 | 0.6808410475 | 3.9057749224 |
|    | 31| H | -0.3572852649 | -1.1362836736 | -5.7362979716 |
|    | 32| H | -1.6995387517 | 0.0072200040 | 0.0111900165 |
|    | 33| H | -2.1748288207 | -0.6192061481 | -1.5717690340 |
|    | 34| H | -1.7838804236 | 2.7391982649 | -2.9141317042 |
|    | 35| H | 0.0139289774 | 3.0284523361 | 0.1879329978 |
|    | 36| H | -0.0946647951 | 3.6779363197 | 1.8334773359 |
|    | 37| H | -1.5573805082 | 3.1568059937 | 0.9754037661 |
|    | 38| O | -1.4620495593 | -0.2785001478 | 3.8159138688 |
|    | 39| H | -1.5462214827 | 0.5445692868 | 2.6710639128 |
|    | 40| C | -0.0774406887 | -2.1128218254 | 3.6913844450 |
|    | 41| H | 0.8197718570 | -2.6531710448 | 3.4188921734 |
| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
| 1 | C    | -0.0275720889 | 0.0559064014 | -1.4004712002 |
| 2 | C    | -0.5228353040 | 1.4095492479 | -0.8947869115 |
| 3 | C    | -0.9203060626 | 1.1691475539 | 0.5460793596 |
| 4 | C    | -1.4274562172 | -0.2902034695 | 0.5244789031 |
| 5 | O    | -0.8939950973 | -0.8822477080 | -0.686839448 |
| 6 | C    | -1.7674094316 | 1.6572169983 | -1.7355182730 |
| 7 | N    | -1.6709200939 | 0.8784045313 | -2.8407771807 |
| 8 | C    | -0.5299841228 | -0.0443316844 | -2.8577050689 |
| 9 | C    | -0.9795864068 | -1.0565357736 | 1.7775504301 |
|10 | C    | -0.9670988544 | -0.0689383335 | 2.9452776214 |
|11 | C    | 0.1734103365 | 0.9478893630 | 2.7467921292 |
|12 | O    | 0.2657783257 | 1.2873047909 | 1.3380867516 |
|13 | O    | -2.6842883750 | 2.3964180077 | -1.4469548653 |
|14 | C    | 0.3977821224 | 0.4432373731 | -3.9352191090 |
|15 | O    | 0.3270163921 | 0.1467366627 | -5.0941358183 |
|16 | O    | 1.2701527514 | 1.3830056942 | -3.4816716129 |
|17 | C    | 1.4225739296 | -0.2523794024 | -1.073340289 |
|18 | C    | 1.9117388113 | -1.4624219790 | -1.7982190867 |
|19 | O    | 1.5173377501 | -1.8601585753 | -2.8678391342 |
|20 | O    | 2.9167049903 | -2.0831627395 | -1.1368082199 |
|21 | H    | 0.1919464070 | 2.2102822363 | -0.9927328072 |
|22 | H    | -1.6846813025 | 1.8647303081 | 0.8581495296 |
|23 | H    | -2.5059187374 | -0.3045629797 | 0.4632698481 |
|24 | O    | 0.3572740655 | -1.5732061655 | 1.6330265666 |
|25 | C    | 0.4691301214 | -2.9030474219 | 1.0639811998 |
|26 | H    | -0.8254394485 | -1.0496261063 | -3.0830407859 |
|27 | H    | -1.6569268993 | -1.8782110639 | 1.9741456551 |
|28 | H    | -2.4019905646 | 0.8312941691 | -3.5176956141 |
|29 | H    | -1.9277436061 | 0.4290857426 | 3.0032963377 |
|30 | H    | -0.7851118443 | -0.5795517452 | 3.8795725328 |
| I | Atom | X      | Y      | Z      |
|---|------|--------|--------|--------|
| 31 | H    | 1.8080813120 | 1.7518221149 | -4.1985102212 |
| 32 | H    | 1.4936297834 | -0.3984710751 | -0.0126756503 |
| 33 | H    | 2.0501246314 | 0.5763166198 | -1.3656729218 |
| 34 | H    | 3.2822962149 | -2.8240256670 | -1.6439123574 |
| 35 | H    | -0.1388367989 | -2.9759375300 | 0.1777525444 |
| 36 | H    | 1.1701137744 | -3.6473101203 | 3.1216497991 |
| 37 | H    | 1.5063254667 | -3.0273146682 | 0.8034601125 |
| 38 | O    | 1.4009912046 | 0.3802926207 | 3.1216497991 |
| 39 | H    | 1.4979875578 | -0.4575977951 | 2.6403989961 |
| 40 | C    | -0.0047751346 | 2.2205346373 | 3.5497731019 |
| 41 | H    | -0.9053466097 | 2.7415359307 | 3.2512152194 |
| 42 | H    | 0.8525504691 | 2.8527914018 | 3.3703019759 |
| 43 | H    | -0.0547234164 | 1.9857395970 | 4.6045135681 |

(7S*, 9S*)-S2C, M0001:M0009
|     | Atom | X            | Y            | Z            |
|-----|------|--------------|--------------|--------------|
| 20  | O    | -3.0167400167 | -1.1371498049 | -0.1065331971 |
| 21  | H    | -1.0511261152 | -2.0317932246 | -1.1475976081 |
| 22  | H    | 1.1195579496  | -2.0532109759 | 0.4116765382  |
| 23  | H    | 2.0380190841  | 0.0496203164  | -0.5022599260 |
| 24  | O    | 2.0147805061  | 2.0283409342  | 1.1580264978  |
| 25  | C    | 2.6986528340  | 2.6705175134  | 2.2462117616  |
| 26  | H    | 0.6263845515  | 1.2676843254  | -2.8736675423 |
| 27  | H    | 2.1914851034  | 0.1173342512  | 1.9271542953  |
| 28  | H    | 1.1195579496  | -2.0532109759 | 0.4116765382  |
| 29  | H    | 2.0380190841  | 0.0496203164  | -0.5022599260 |
| 30  | C    | 2.6986528340  | 2.6705175134  | 2.2462117616  |
| 31  | H    | 0.6263845515  | 1.2676843254  | -2.8736675423 |
| 32  | H    | 2.1914851034  | 0.1173342512  | 1.9271542953  |
| 33  | H    | 1.1195579496  | -2.0532109759 | 0.4116765382  |
| 34  | H    | 2.0380190841  | 0.0496203164  | -0.5022599260 |
| 35  | C    | 2.6986528340  | 2.6705175134  | 2.2462117616  |
| 36  | H    | 0.6263845515  | 1.2676843254  | -2.8736675423 |
| 37  | H    | 2.1914851034  | 0.1173342512  | 1.9271542953  |
| 38  | H    | 1.1195579496  | -2.0532109759 | 0.4116765382  |
| 39  | H    | 2.0380190841  | 0.0496203164  | -0.5022599260 |
| 40  | C    | 2.6986528340  | 2.6705175134  | 2.2462117616  |
| 41  | H    | 0.6263845515  | 1.2676843254  | -2.8736675423 |
| 42  | H    | 2.1914851034  | 0.1173342512  | 1.9271542953  |
| 43  | H    | 1.1195579496  | -2.0532109759 | 0.4116765382  |

(7S*,9S*)-S2C, M0001:M0010

| I | Atom | X            | Y            | Z            |
|---|------|--------------|--------------|--------------|
| 1 | C    | -0.3805902033 | -0.0243999860 | -1.4484526975 |
| 2 | C    | 0.0239334939  | -1.4614797613 | -1.0480709572 |
| 3 | C    | 0.6643186495  | -1.2973734431 | 0.3307738268  |
| 4 | C    | 1.3171078200  | 0.0788755260  | 0.2153494768  |
| 5 | O    | 0.3050600819  | 0.8385327046  | -0.5100124481 |
| 6 | C    | 1.0952797301  | -1.8765181924 | -2.0369637591 |
| 7 | N    | 1.2159629798  | -0.8886873438 | -2.9628918676 |
| 8 | C    | 0.2678365833  | 0.1959804119  | -2.8602694530 |
### (7S*,9S*)-S2C, M0001:M0011

| I | Atom | X            | Y            | Z            |
|---|------|--------------|--------------|--------------|
| 1 | C    | -0.2975121526 | -0.0607782422 | -1.4541463682 |
| 2 | C    | 0.4836481802  | -1.3258162112 | -1.0288415844 |
| 3 | C    | 0.9398349733  | -1.0226894385 | 0.4000196630  |
| 4 | C    | 1.1616204564  | 0.4879183419  | 0.3455014628  |
| 5 | O    | 0.0264208576  | 0.9354607160  | -0.4524979253 |
| 6 | C    | 1.7061967214  | -1.3759173277 | -1.9243544060 |
| 7 | N    | 1.6161424923  | -0.3544016677 | -2.8157254072 |
| 8 | C    | 0.3838311110  | 0.3963481304  | -2.7942901959 |
| 9 | C    | 1.1472421877  | 1.1301190840  | 1.7227465616  |
| 10| C    | -0.1516292011 | 0.7737358500  | 2.4355752405  |
| 11| C    | -0.3263540549 | -0.7436440968 | 2.5582245232  |
| 12| O    | -0.1747839807 | -1.3434409919 | 1.2422483830  |
| 13| O    | 2.6288805259  | -2.1533488509 | -1.8216208918 |
| 14| C    | -0.4399964127 | 0.1968146140  | -4.0465648600 |
| 15| O    | -1.5174782481 | 0.6993936747  | -4.2347424426 |
| 16| O    | 0.1780048209  | -0.5666063572 | -4.9679403428 |
| 17| C    | -1.8273388212 | -0.1768332315 | -1.5255899065 |
| 18| C    | -2.3624673919 | -0.6869886845 | -0.2230102631 |
| 19| O    | -2.7840696514 | -0.0175752298 | 0.6920652408  |
| 20| O    | -2.3344593634 | -2.0338635830 | -0.1889208216 |
| 21| H    | -0.0967143888 | -2.2312757692 | -1.0700190008 |
| 22| H    | 1.8239007400  | -1.5789639164 | 0.6695480638  |
| 23| H    | 2.0828768964  | 0.7248754446  | -0.1665743233 |
| 24| O    | 1.4331012806  | 2.5308589715  | 1.6777911726  |
| 25| C    | 0.4119260774  | 3.4340667095  | 1.197505539  |
| 26| H    | 0.5471773035  | 1.4599699420  | -2.6948575527 |
| 27| H    | 1.9870902824  | 0.7157167513  | 2.2639982666  |
| 28| H    | 2.2779025405  | -0.2595538055 | -3.5556990216 |
| 29| H    | -0.1712866316 | 1.2089374417  | 3.4254082917  |
| 30| H    | -0.9839015274 | 1.1511610692  | 1.8617491906  |
| 31| H    | -0.3474012479 | -0.6584117010 | -5.7772291916 |
| 32| H    | -2.1140317964 | -0.8655118916 | -2.3016875182 |
| 33| H    | -2.2364848646 | 0.7986362454  | -1.7272290560 |
|   |   |   |   |   |
|---|---|---|---|---|
| 34 | H | -2.3429739240 | -2.3831317135 | 0.7166357915 |
| 35 | H | -0.4268709211 | 3.4801886244 | 1.8803177433 |
| 36 | H | 0.0608474785 | 3.1447126113 | 0.2208413440 |
| 37 | H | 0.8832880580 | 4.4041325953 | 1.1542609307 |
| 38 | O | -1.6349938345 | -1.0648713313 | 2.9672422883 |
| 39 | H | -2.2821366920 | -0.5966192098 | 2.4119075982 |
| 40 | C | 0.6084375933 | -1.4148143263 | 3.5483124903 |
| 41 | H | 1.6487551118 | -1.2648959314 | 3.2934521925 |
| 42 | H | 0.3932914614 | -2.4739443049 | 3.5493698163 |
| 43 | H | 0.4224679555 | -1.0191490033 | 4.5367742707 |
(7R*, 9S*) - S2D, M0002:M0001

| I  | Atom | X              | Y              | Z              |
|----|------|----------------|----------------|----------------|
| 1  | C    | 0.0967376891   | 0.3544905798   | -1.7416824008 |
| 2  | C    | -1.2818471377  | -0.0898115111  | -1.1983343633 |
| 3  | C    | -0.9928449474  | -0.5186089475  | 0.2436200323  |
| 4  | C    | 0.4172047858   | -1.0815572788  | 0.1183671896  |
| 5  | O    | 1.0632698777   | -0.1515238445  | -0.7908673354 |
| 6  | C    | -1.6609811717  | -1.3160699471  | -2.0055485326 |
| 7  | N    | -0.7069864249  | -1.5020429246  | -2.9580672041 |
| 8  | C    | 0.2814664352   | -0.4553737469  | -3.0716882210 |
| 9  | C    | 1.1820684230   | -1.1068423306  | 1.4251028045  |
| 10 | C    | 1.1178714386   | 0.2482842145   | 2.1183479117  |
| 11 | O    | -0.3094695762  | 0.7778213694   | 2.2870383788  |
| 12 | O    | -0.985391724   | 0.6964780796   | 1.0043913857  |
| 13 | O    | -2.6086822814  | -2.0393058791  | -1.7986206304 |
| 14 | C    | 0.0324632940   | 0.3594337903   | -4.3137842139 |
| 15 | O    | -0.9610098716  | 0.3748376796   | -4.9840610393 |
| 16 | O    | 1.1287522464   | 1.1059429919   | -4.5994533177 |
| 17 | C    | 0.3274215466   | 1.8639689363   | -1.911279436 |
| 18 | C    | 0.0491083456   | 2.578898267    | -0.6250230845 |
| 19 | O    | 0.8662280111   | 2.8802687358   | 0.2147461663  |
| 20 | O    | -1.2590609894  | 2.8764126469   | -0.5133341781 |
| 21 | H    | -2.0344736392  | 0.6786165634   | -1.2355255913 |
| 22 | H    | -1.7045252833  | -1.2331539590  | 0.6202635558  |
| 23 | H    | 0.3910741347   | -2.0735362935  | -0.3049944466 |
| 24 | C    | -1.1289740674  | 0.901644160    | 3.3611510562  |
| 25 | O    | -0.2901516062  | 2.1529699483   | 2.6078763956  |
| 26 | O    | 0.5334273888   | -2.1615010848  | 2.1606501707  |
| 27 | C    | 1.2840575213   | -2.7386813352  | 3.243033826  |
| 28 | H    | 1.2943568015   | -0.8213082589  | -3.0936885215 |
| 29 | H    | 2.2153124396   | -1.3682657972  | 1.2274272364  |
| 30 | H    | -0.7949318114  | -2.232391699   | -3.6321946344 |
| 31 | H    | 1.5957119684   | 0.2212150915   | 3.0884107253  |
| 32 | H    | 1.6534905673   | 0.9437233636   | 1.4881787453  |
| 33 | H    | 1.0109206674   | 1.6528584132   | -5.3907168223 |
| ATOM | X       | Y       | Z       |
|------|---------|---------|---------|
| 1    | -0.4187 | 0.1457  | -1.7239 |
| 2    | 0.0401  | -1.2317 | -1.1869 |
| 3    | 0.4803  | -0.9456 | 0.2531  |
| 4    | 1.0325  | 0.4686  | 0.1270  |
| 5    | 0.0895  | 1.1113  | -0.7699 |
| 6    | 1.2657  | -1.6008 | -2.0041 |
| 7    | 1.4567  | -0.6293 | -2.9342 |
| 8    | 0.4006  | 0.3477  | -3.0484 |
| 9    | 1.0667  | 1.2288  | 1.4363  |
| 10   | -0.2795 | 1.1504  | 2.1449  |
| 11   | -0.7947 | -0.2819 | 2.3151  |
| 12   | -0.7246 | -0.9533 | 1.0287  |
| 13   | 1.9828  | -2.5579 | -1.8134 |
| 14   | -0.3903 | 0.1989  | -4.3288 |
| 15   | -1.3235 | 0.8961  | -6.3324 |
| 16   | 0.0814  | -0.7746 | -5.1315 |
| 17   | -1.9296 | 0.3775  | -1.8734 |
| 18   | -2.6256 | 0.0804  | -0.5819 |
| 19   | -2.9253 | 0.8833  | 0.2722  |
| 20   | -2.9111 | -1.2327 | -0.4810 |
| 21   | -0.7233 | -1.9896 | -1.2190 |
| 22   | 1.2051  | 1.6535  | 0.6178  |
| 23   | 2.0204  | 0.4500  | -0.3060 |

(7R*, 9S*)-S2D, M0002:M0002

ATOM    X       Y       Z
1       -0.4187228330 0.1457027963 -1.7239784571
2       0.0401764728 -1.2316711443 -1.1869038211
3       0.4803520124 -0.9456301594 0.2531440107
4       1.0324930825  0.4685976157  0.1270848791
5       0.0895112185  1.1113296229 -0.7695678431
6       1.2657093470 -1.6007944202 -2.0004129266
7       1.4568898451 -0.6293300004 -2.9342612666
8       0.4005992108  0.3477327305 -3.0484926701
9       1.0666939120  1.2288125544  1.4363242702
10      -0.2795221246 1.1504395775  2.1449425112
11      -0.7947661930 -0.2819984119  2.3151914125
12      -0.7246149520 -0.9533564546  1.0287187099
13      1.9827943815 -2.5578995709 -1.8134792156
14      -0.3902823029  0.1989655368 -4.3288440334
15      -1.3234870509  0.8961821198 -6.3324063237
16      0.08140008481 -0.7746914742 -5.1315745657
17      -1.9295894165  0.3775451662 -1.8737387074
18      -2.6256338571  0.0804821516 -0.5819241894
19      -2.9252959862  0.8833723339  0.2722322587
20      -2.911253925  -1.2327603523 -0.4810105201
21      -0.7233626062 -1.9895661851 -1.2190179882
22      1.2051787487 -1.6535503377  0.6178359400
23      2.0204354447  0.4500889113 -0.3060498510
| I | Atom | X         | Y         | Z         |
|---|------|-----------|-----------|-----------|
| 1 | C    | -0.4687322742 | 0.1821176318 | -1.6118834463 |
| 2 | C    | -0.1359429728  | -1.2392580325 | -1.0995548167 |
| 3 | C    | 0.3607842399   | -1.0129668421 | 0.3317954500 |
| 4 | C    | 1.0505921398   | 0.3394603680  | 0.2026184646 |
| 5 | O    | 0.1597327754   | 1.0837618585  | -0.6692713629 |
| 6 | C    | 1.0266020436   | -1.7138609048 | -1.9491763088 |
| 7 | N    | 1.2653661925   | -0.7694988649 | -2.8994247750 |
| 8 | C    | 0.3080473883   | 0.309356447   | -2.9678905410 |
| 9 | C    | 1.1862814862   | 1.0788738807  | 1.5198307117 |
| 10 | C  | -0.1413261091  | 1.1257143757  | 2.2611831329  |
| 11 | C  | -0.8010445947  | -0.2468290240 | 2.4267785047  |
| 12 | O  | -0.8213235260  | -0.9057835215 | 1.130860603  |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| 13   | 1.6732228363 | 2.7214793436 | -1.7721813981 |
| 14   | -0.5660196500 | 0.1512202402 | -4.1844375872 |
| 15   | -0.6785589339 | -0.8225099032 | -4.8740993027 |
| 16   | -1.2366500676 | 1.3064551916 | -4.4204251882 |
| 17   | -1.9550371372 | 0.5538785428 | -1.7246627483 |
| 18   | -2.6481139067 | 0.3310512401 | -0.4155969694 |
| 19   | -2.8389580777 | 1.1642237673 | 0.4402368880 |
| 20   | -3.0638927184 | -0.9444214641 | -0.3025677551 |
| 21   | -0.9707398238 | -1.9183493808 | -1.1225595671 |
| 22   | 1.0176760458  | -1.7941705292 | 0.6751281569  |
| 23   | 2.0142165729  | 0.2178166422 | -0.2707401763 |
| 24   | -0.1709389493 | -1.1447571429 | 3.4726841897 |
| 25   | -2.1612037542 | -0.1002998624 | 2.7802517002 |
| 26   | 2.1486674687  | 0.3545628961 | 2.3104698608 |
| 27   | 3.5230723914  | 0.7650414059 | 2.195615022  |
| 28   | 0.7637058114  | 1.2856130202 | -2.9940386864 |
| 29   | 1.5309745260  | 2.0886791571 | 1.3316311304 |
| 30   | 1.9584357440  | -0.917161163 | -3.601974592 |
| 31   | -0.0017432021 | 1.5684322294 | 3.2371107211 |
| 32   | -0.8031851397 | 1.7433217269 | 1.6781907360 |
| 33   | -1.8189795035 | 1.2472661915 | -5.1927887515 |
| 34   | -2.4315458533 | -0.0719388941 | -2.4628170781 |
| 35   | -2.0269678719 | 1.5927266674 | -1.9988353755 |
| 36   | -3.1638465777 | -1.2198173635 | 0.6234204275 |
| 37   | 0.8841065262  | -1.2587463442 | 3.2940650995 |
| 38   | -0.6732735478 | -2.1019895621 | 3.4468502974 |
| 39   | -0.3221313740 | -0.6987921922 | 4.4461791437 |
| 40   | -2.5953469810 | 0.5358599302 | 2.1867716978 |
| 41   | 3.6380760676  | 1.8112032794 | 2.4557974041 |
| 42   | 3.9104766160  | 0.6063947407 | 1.1958267882 |
| 43   | 4.0814659379  | 0.1589953420 | 2.8916116402 |

$(7^R, 9^S) - S2D$, M0002:M0004

| I | Atom | X           | Y           | Z           |
|---|------|-------------|-------------|-------------|
| 1 | C    | -0.5154962521 | 0.2363472491 | -1.5941997912 |
2  C  -0.1708132364  -1.1853005900  -1.0883623172
3  C  0.3279373822  -0.9645084631   0.3441198897
4  C  1.0069274619   0.3940325582   0.2211407922
5  O  0.1089870547   1.1362669643  -0.6440937805
6  C  0.9962711237  -1.6480636563 -1.9390022732
7  N  1.2469579556  -0.6862936949 -2.8685199658
8  C  0.2790825278   0.3815735709  -2.9412590132
9  C  1.1408453278   1.1271633655  1.5420207943
10 C  -0.1829074929  1.1543980040  2.2909421808
11 C  -0.8269645811  -0.2261476416  2.4517502032
12 O  -0.8502462079  -0.8755537113  1.1504417228
13 O  1.6350475213  -2.6640819272  -1.7796400806
14 C  -0.5616447344   0.3191676960  -4.1964843372
15 O  -1.4221606556   1.114113375  -4.4734678036
16 O  -0.2260099005  -0.7020527701  -5.008896111
17 C  -2.0017572148   0.6098123361  -1.6963746521
18 C  -2.6861219331   0.3653129794  -0.3870681509
19 O  -2.8869782149   1.1844979493   0.479933525
20 O  -3.0862395207  -0.9175916308  -0.287504837
21 H  -1.0042555999  -1.8706687960  -1.1121898999
22 H  0.9936147719   1.1844979493   0.479933525
23 H  1.9708438617   0.2819916447  -0.2541754737
24 C  -0.1771551410  -1.1245897230   3.4852125582
25 O  -2.1844939322  -0.0971062164   2.8187373012
26 O  2.1173395565   0.4090508791   2.3214202756
27 C  3.4838355505   0.8446464345   2.2066951237
28 H  0.7341708931   1.3607410082  -2.9147675721
29 H  1.4724865079   2.1420712048   1.3577327032
30 H  1.9173098693  -0.8398892229  -3.5907401387
31 H  -0.0435321114   1.5923756197   3.2691245608
32 H  -0.8607412267   1.7677989110   1.7151730998
33 H  -0.7581391669  -0.7122076293  -5.8181052231
34 H  -2.4876103255   0.0113481610  -2.4475537979
35 H  -2.0737353784   1.6539311163  -1.9509568681
36 H  -3.1888477561  -1.2018304611   0.6352908390
37 H  0.8772403895  -1.2268713492   3.2953977436
| I | Atom | X     | Y     | Z     |
|---|------|-------|-------|-------|
| 1 | C    | -0.3031246063 | -0.0383504383 | -1.5906870178 |
| 2 | C    | 0.5788478218  | -1.1864847303 | -1.0715231654 |
| 3 | C    | 0.9819805069  | -0.7901425987 | 0.3446701263  |
| 4 | O    | 0.0734452004  | 1.1019063533  | -0.7974314422 |
| 5 | O    | 1.8212269225  | -1.1334790236 | -1.9507102498 |
| 6 | N    | 1.5659334668  | -0.2918753467 | -2.9838451251 |
| 7 | C    | 0.2256341353  | 0.2424249482  | 1.6004720717  |
| 8 | C    | 0.6939269100  | 0.4368667339  | 2.7829176159  |
| 9 | C    | -0.0168194437 | -0.9126832025 | 2.6250706897  |
| 10| O    | -0.0206261815 | -1.3011881964 | 1.2272919908  |
| 11| O    | 2.8677867618  | -1.6982480757 | -1.7260039568 |
| 12| C    | -0.5752580627 | -0.4606851737 | -4.0972590024 |
| 13| O    | -0.3230210138 | -1.5093675197 | -4.619468435  |
| 14| C    | -1.6763597898 | 0.2715109622  | -4.400140712  |
| 15| C    | -1.8286057075 | -0.2335395623 | -1.5273162108 |
| 16| O    | -2.2593821050 | -0.5216520645 | -0.1208179265 |
| 17| O    | -2.4718955876 | 0.3074913454  | 0.7377532055  |
| 18| O    | -2.3806408082 | -1.8395101933 | 0.0941451424  |
| 19| H    | 0.1071003035  | -2.1560245519 | -1.0878453506 |
| 20| C    | 1.9559142706  | -1.1832430910 | 0.5908119952  |
| 21| C    | 1.9424914598  | 1.1430106415  | 0.1143985244  |
| 22| C    | 0.6124693330  | -2.0190133467 | 3.4472404558  |
| 23| O    | -1.3808271000 | -0.8575398602 | 2.9968558487  |
| 24| O    | 1.0553492873  | 2.6059396463  | 1.8892299654  |
27  C  0.6009773979  3.7189147170  1.0927392398
28  H  0.1932327003  1.3051030115 -3.2034134969
29  H  -0.6507662124  1.4992596761  3.6933406181
30  H  2.2395686157 -0.1378207915 -3.7029409459
31  H  1.7651825879  0.2993655192  2.8632307035
32  H  0.3457963110  0.9012526650  3.6933406181
33  H  -2.2306285960 -0.1497437166 -5.0743297628
34  H  -2.1229012332 -1.0647998993 -2.1454141137
35  H  -2.2938034807  0.6778426763 -1.8662897707
36  H  -2.3309466733  2.0651092179  1.0380703385
37  H  1.6414342350 -2.1760495459  3.1513309678
38  H  0.0508175686 -2.9280692431  3.2873519765
39  H  0.5735633338 -1.7606444036  4.4967828180
40  H  -1.8727618271 -0.2218672690  2.4489545121
41  H  -0.4457154940  3.9265803075  1.2849765438
42  H  0.7254778874  3.5243144754  0.0353442656
43  H  1.1984885948  4.5689305847  1.3841548141

(7R*,9S*)-S2D, M0002:M0006

I  Atom         X          Y          Z
    -----------------------------------------------
  1  C  -0.3702329510  0.0024083689 -1.5759694976
  2  C  0.5072691960 -1.1510920041 -1.0596901815
  3  C  0.9286963876 -0.7566495612  0.3533036855
  4  C  0.9073235679  0.7810676038  0.3209039489
  5  O  0.0180466060  1.1401265059 -0.7807770740
  6  C  1.7450606026 -1.1105143563 -1.9467899614
  7  N  1.5024531100 -0.2498658947 -2.9665019714
  8  C  0.1689694022  0.2952441757 -3.0167248504
  9  C  0.3671536491  1.3908149102  1.6148794137
 10  C  0.6830635152  0.4749837128  2.7938276749
 11  C  -0.0233385879 -0.8788072824  2.6532254727
 12  O  -0.0556428176 -1.2699645090  1.2551491791
 13  O  2.7803066546 -1.7024875607 -1.7377339150
 14  C  -0.6675515178 -0.2990797492 -4.1249053993
 15  O  -1.7750503406  0.0834648685  4.4030676622
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| 16 O | -0.0543441633 | -1.2995688902 | -4.7834458566 |
| 17 C | -1.8972090077 | -0.1695257941 | -1.4987636351 |
| 18 C | -2.3050464500 | -0.4981771060 | -0.0949231242 |
| 19 O | -2.5234492495 | 0.3004746774 | 0.7900756342 |
| 20 O | -2.3928859689 | 1.8257004447 | 0.0846529569 |
| 21 H | 0.0268010908 | -2.1163474574 | -1.067429299 |
| 22 H | 1.9067369060 | -1.1501344704 | 0.5824180425 |
| 23 H | 1.8913475923 | 1.1757186035 | 0.1209469760 |
| 24 C | 0.6311030384 | -1.9800128090 | 3.4627632616 |
| 25 O | -1.3774297335 | -0.8291228135 | 3.0553082893 |
| 26 O | 0.9991695815 | 2.6477685711 | 1.8891549524 |
| 27 C | 0.5164873202 | 3.7514318280 | 1.0961167165 |
| 28 H | 0.1572284263 | 1.3676425934 | -3.1366735858 |
| 29 H | -0.6969254198 | 1.5139486757 | 1.4917578012 |
| 30 H | 2.1612310112 | -0.1303708568 | -3.7050424218 |
| 31 H | 1.7566951212 | 0.3449555221 | 2.8535066847 |
| 32 H | 0.3489160191 | 0.9390094052 | 3.7096029664 |
| 33 H | -0.6053628323 | -1.6566752435 | -5.4964615251 |
| 34 H | -2.2247016887 | -0.9650730836 | -2.1433811306 |
| 35 H | -2.3505006254 | 0.7619987216 | -1.7973899510 |
| 36 H | -2.3354356232 | -2.0753347250 | 1.0214784636 |
| 37 H | 1.6545568255 | -2.1311094571 | 3.1451932922 |
| 38 H | 0.0714826072 | -2.8926587498 | 3.3166948380 |
| 39 H | 0.6131698096 | -1.7202230704 | 4.5125742547 |
| 40 H | -1.8917911471 | -0.2229554738 | 2.4946230112 |
| 41 H | -0.5300302543 | 3.9446175333 | 1.3038534594 |
| 42 H | 0.6277172053 | 3.5547960384 | 0.0377755984 |
| 43 H | 1.1059431322 | 4.6109844471 | 1.3758813990 |

(7R*, 9S*) - S2D, M0002: M0007

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| 1 C  | -0.3698305666 | 0.0737504809 | -1.7512018881 |
| 2 C  | 0.0555139489 | -1.3149489001 | -1.2153243496 |
| 3 C  | 0.5325351166 | -1.0389092817 | 0.2119205666 |
| 4 C  | 1.0928504114 | 0.3719100807 | 0.0895691103 |
| I | Atom | X          | Y          | Z          |
|---|------|------------|------------|------------|
| 1 | C    | 0.2788090558 | -0.0446166582 | -1.7416386508 |
| 2 | C    | -0.6232695264 | 1.1112142002  | -1.2759876350 |
| 3 | C    | -1.0163726800 | 0.7712205422  | 0.1571830791  |
| 4 | C    | -0.9680917888 | -0.7653662619 | 0.1913288477  |
| 5 | O    | -0.0653778789 | -1.1503462751 | -0.8903506268 |
| 6 | C    | -1.8663114888 | 0.9955901502  | -2.1481474464 |
| 7 | N    | -1.5997538939 | 0.1078798005  | -3.1382773216 |
| 8 | C    | -0.2512816843 | -0.4080032483 | -3.166135606  |
| 9 | C    | -0.4203873606 | -1.3099168543 | 1.5060539530  |
| 10| C    | -0.7038910060 | -0.3287827093 | 2.6465492813  |
| 11| C    | -0.0065494954 | 1.0177066198  | 2.4221668234  |
| 12| O    | -0.0146789240 | 1.3381364827  | 1.0092266028  |
| 13| O    | -2.9210136581 | 1.5550562215  | -1.9484280133 |
| 14| C    | 0.5343874552  | 0.2508105380  | -4.2682763477 |
| 15| O    | 0.2652757187  | 1.2682154715  | -4.8417582919 |
| 16| O    | 1.6445580248  | -0.4799724917 | -4.5405406624 |
| 17| C    | 1.8007979597  | 0.1813292756  | -1.6972208275 |
| 18| C    | 2.2298677643  | 0.5355029182  | -0.3061452043 |
| 19| O    | 2.4495126013  | -0.2513084894 | 0.5902908851  |
| 20| O    | 2.3408204919  | 1.8628116760  | -0.150877510  |
| 21| H    | -0.1693685111 | 2.0874131836  | -1.3370185533 |
| 22| H    | -1.9943012490 | 1.1615991513  | 0.3913735864  |
| 23| H    | -1.9395954094 | -1.1949469127 | 0.0107691278  |
| 24| C    | -0.6441609100 | 2.1546754390  | 3.1947953110  |
| 25| O    | 1.3585948255  | 0.9904103611  | 2.7935917405  |
| 26| O    | -1.0992486930 | -2.5540408889 | 1.7480103019  |
| 27| C    | -0.3700501288 | -3.5258486908 | 2.5153164610  |
| 28| H    | -0.2027457108 | -1.4776110218 | -3.2785627914 |
| 29| H    | 0.6375676606  | -1.4668875433 | 1.3735453965  |
| I | Atom | X       | Y       | Z       |
|---|------|---------|---------|---------|
|   | C    | -0.3595454076 | 0.0705327559 | -1.7213706294 |
|   | C    | 0.5402098539  | -1.0885139467 | -1.2568153769 |
|   | C    | 0.9593246828  | -0.7425674440 | 0.1690770774  |
|   | C    | 0.9130887087  | 0.7944981185  | 0.1970567370  |
|   | O    | -0.0004870521 | 1.1777157349  | -0.8739737613 |
|   | C    | 1.7739469103  | -0.9921595145 | -2.1448809927 |
|   | N    | 1.5163974125  | -0.0905355688 | -3.1237923722 |
|   | C    | 0.1764640293  | 0.4417452000  | -3.1452405682 |
|   | C    | 0.3824855136  | 1.3433907204  | 1.5161638032  |
|   | C    | 0.7017556679  | 0.3747413017  | 2.6569714193  |
|   | C    | 0.0067947642  | -0.9772321505 | 2.4596580754  |
|   | O    | -0.0189531615 | -1.3088098297 | 1.0483569054  |
|   | O    | 2.8171628152  | -1.5805129228 | -1.9656531940 |
|   | C    | -0.6483419199 | -0.0969187665 | -4.2903651992 |
|   | O    | -1.7798909610 | 0.2450739183  | -4.5208840016 |
|   | O    | 0.0114930982  | -0.9888456016 | -5.0526937625 |
|   | C    | -1.8829474442 | -0.1343799457 | -1.6534194360 |
|   | C    | -2.2800557819 | -0.5205308359 | -0.2619699088 |
| I  | Atom | X               | Y               | Z               |
|----|------|-----------------|-----------------|-----------------|
| 19 | O    | -2.4990386082   | 0.2405270763    | 0.6562210471    |
| 20 | O    | -2.3585080288   | -1.8546167486   | -0.1336200031   |
| 21 | H    | 0.0765598576    | -2.0609883435   | -1.300877628    |
| 22 | H    | 1.9427519532    | -1.1309873759   | 0.3831190134    |
| 23 | H    | 1.8836361407    | 1.2212944510    | 0.0042605957    |
| 24 | C    | 0.6711172261    | -2.1045532372   | 3.2241152515    |
| 25 | O    | -1.3472404017   | -0.9531787195   | 2.8656563091    |
| 26 | O    | 1.0476830400    | 2.5991231740    | 1.7339671570    |
| 27 | C    | 0.3166371418    | 3.5690102993    | 2.5019852421    |
| 28 | H    | 0.1548499340    | -2.0609883435   | -1.3008877195   |
| 29 | H    | -0.6802327498   | 1.4837052708    | 1.4034878754    |
| 30 | H    | 2.1705865685    | 0.0723229894    | -3.8580034957   |
| 31 | H    | 1.7766082017    | 0.2486109793    | 2.7052151074    |
| 32 | H    | 0.3690283249    | 0.7754167331    | 3.6041411951    |
| 33 | H    | -0.5303036496   | -1.3050846209   | -5.7915199921   |
| 34 | H    | -2.1959497393   | -0.9110988654   | -2.3271588290   |
| 35 | H    | -2.3529975649   | 0.7993678320    | -1.9165141973   |
| 36 | H    | -2.2989673513   | -2.1402454744   | 0.7924707763    |
| 37 | H    | 1.6965809722    | -2.2315838020   | 2.9026704117    |
| 38 | H    | 0.1215707282    | -3.0161713573   | 3.0384256099    |
| 39 | H    | 0.6483884232    | -1.8897015180   | 4.2839498293    |
| 40 | H    | -1.8703590217   | -0.3438538414   | 2.3155213257    |
| 41 | H    | 0.1447360517    | 3.2330595007    | 3.5184656152    |
| 42 | H    | -0.6385103928   | 3.7915960235    | 2.0398661414    |
| 43 | H    | 0.9224712156    | 4.4618724659    | 2.5227585479    |

(7R*, 9S*)-S2D, M0002:M0010

| I  | Atom | X               | Y               | Z               |
|----|------|-----------------|-----------------|-----------------|
| 1  | C    | -0.4879154757   | 0.1616039669    | -1.6251654027   |
| 2  | C    | -0.1671280015   | -1.2645752470   | -1.1148214509   |
| 3  | C    | 0.3753968919    | -1.0048324392   | 0.2995928157    |
| 4  | C    | 1.0534221731    | 0.3094221269    | 0.1680675981    |
| 5  | O    | 0.1529727085    | 1.0573334154    | -0.6843015536   |
| 6  | C    | 0.9593716721    | -1.7764327013   | -1.9914922020   |
| 7  | N    | 1.2061470338    | -0.8386612796   | -2.9445649582   |
|   |   |   |   |   |
|---|---|---|---|---|
|  8 | C  | 0.2962175644 | 0.2837129837 | -2.9813869282 |
|  9 | C  | 1.2020947250 | 1.0430285344 | 1.4883196244 |
| 10 | C  | -0.1306560267 | 1.1150430553 | 2.2206094429 |
| 11 | C  | -0.7731960235 | -0.2582076592 | 2.3863285328 |
| 12 | O  | -0.7829859027 | -0.9703308109 | 1.1413005265 |
| 13 | O  | 1.5795023652 | -2.8033986522 | -1.8268066304 |
| 14 | C  | -0.5787548626 | 0.2022598724 | -4.2034740107 |
| 15 | O  | -0.7664902719 | -0.7580056739 | -4.8965152890 |
| 16 | O  | -1.1427408174 | 1.4111324957 | -4.4453842215 |
| 17 | C  | -1.9769483142 | 0.5114584842 | -1.7546924358 |
| 18 | C  | -2.7285069471 | 0.2039371578 | -0.4888570966 |
| 19 | O  | -3.3098043531 | -0.8334623529 | -0.2862950628 |
| 20 | O  | -2.6824034004 | 1.2141638249 | 0.3919958241 |
| 21 | H  | -1.0194415135 | -1.9251638236 | -1.1043270627 |
| 22 | H  | 1.0460877236 | -1.8294976839 | 0.6152742363 |
| 23 | H  | 2.0124513122 | 0.1890886527 | -0.3164857670 |
| 24 | C  | -0.1793680456 | -1.1167957198 | 3.4908823935 |
| 25 | O  | -2.1701624862 | -0.0247391424 | 2.655116435 |
| 26 | O  | 2.1461660621 | 0.3021279447 | 2.2853381073 |
| 27 | C  | 3.5321866302 | 0.6709828269 | 2.1631231001 |
| 28 | H  | 0.7934605421 | 1.2396856742 | -2.9795665442 |
| 29 | H  | 1.5629243689 | 2.0476713931 | 1.303759983 |
| 30 | H  | 1.8783953579 | -1.0070284954 | -3.6624017821 |
| 31 | H  | 0.0015045476 | 1.5705413297 | 3.1913280379 |
| 32 | H  | -0.7912394010 | 1.7142032910 | 1.616612799 |
| 33 | H  | -1.7299220015 | 1.4025240000 | -5.2161919823 |
| 34 | H  | -2.4110082269 | -0.0980722919 | -2.5322021773 |
| 35 | H  | -2.0672885880 | 1.5575735471 | -1.9948709422 |
| 36 | H  | -2.7801498158 | 0.9022882024 | 1.3204226257 |
| 37 | H  | 0.8860918058 | -1.2028654773 | 3.3607000216 |
| 38 | H  | -0.6371460343 | -2.0987541413 | 3.4668799234 |
| 39 | H  | -0.3858111290 | -0.6513995393 | 4.4455015581 |
| 40 | H  | -2.6486718327 | -0.8670347289 | 2.5972452328 |
| 41 | H  | 3.6752512952 | 1.7197307749 | 2.3977347481 |
| 42 | H  | 3.9156836753 | 0.4762585752 | 1.1684340710 |
| 43 | H  | 4.0724110158 | 0.0669776839 | 2.8751941583 |
(7R*,9S*)-S2D, M0002:M0011

| I | Atom | X             | Y             | Z             |
|---|------|---------------|---------------|---------------|
| 1 | C    | -0.4088146972 | 0.1353878612  | -1.7352362589 |
| 2 | C    | 0.0271699736  | -1.2543864198 | -1.2096356096 |
| 3 | C    | 0.5097466041  | -0.9871181059 | 0.2180974026  |
| 4 | C    | 1.0545179917  | 0.4305070982  | 0.1064434534  |
| 5 | O    | 0.1079944616  | 1.0860408778  | -0.7719579601 |
| 6 | C    | 1.2153174280  | -1.6690995502 | -2.0554326883 |
| 7 | N    | 1.4202118866  | -0.7037123289 | -2.9899822169 |
| 8 | C    | 0.4236654166  | 0.3379684951  | -3.0572377728 |
| 9 | C    | 1.0923962777  | 1.1748838351  | 1.4255697163  |
| 10| C    | -0.2679604301 | 1.1231768353  | 2.1124672823  |
| 11| C    | -0.7776137002 | -0.3062375435 | 2.2632758828  |
| 12| O    | -0.6773559029 | -1.0199795591 | 1.0251890510  |
| 13| O    | 1.9005690745  | -2.6532399756 | -1.8861693830 |
| 14| C    | -0.3852966747 | 0.2938768654  | -4.3320027884 |
| 15| O    | -1.1867224245 | 1.1343905571  | -4.6469757421 |
| 16| O    | 0.1070781739  | -0.7752968609 | -5.1042301126 |
| 17| C    | -1.9185824652 | 0.3481769626  | -1.9126857784 |
| 18| C    | -2.6743839514 | -0.0254166183 | -0.6676122920 |
| 19| O    | -3.1596873729 | -1.1132879368 | -0.4751267205 |
| 20| O    | -2.7557847932 | 0.9864000913  | 0.2094211652  |
| 21| H    | -0.7630209493 | -1.9880949353 | -1.2142268258 |
| 22| H    | 1.2425669227  | -1.6997573141 | 0.5559648718  |
| 23| H    | 2.0417217026  | 0.4149946257  | -0.3302048092 |
| 24| C    | -0.1323298311 | -1.1021142767 | 3.3857226058  |
| 25| O    | -2.1979025632 | -0.2144918756 | 2.4897539017  |
| 26| O    | 2.1342685520  | 0.5032289042  | 2.1591446496  |
| 27| C    | 2.7593093438  | 1.2591930379  | 3.2122107683  |
| 28| H    | 0.8456328766  | 1.3295812211  | -2.9903051195 |
| 29| H    | 1.3652223038  | 2.2073726776  | 1.2420585039  |
| 30| H    | 2.1042814527  | -0.8275253877 | -3.7047575231 |
| 31| H    | -0.2458768749 | 1.5998911826  | 3.0827994933  |
| 32| H    | -0.9553254587 | 1.6482488420  | 1.4703070812  |
| I  | Atom | X     | Y     | Z     |
|----|------|-------|-------|-------|
| 33 | H    | -0.6285428680 | -0.7786204101 | -5.9215631549 |
| 34 | H    | -2.2761150464 | -0.2913282032 | -2.7030892071 |
| 35 | H    | -2.0975796977 | 1.3812435594  | -2.1613700550 |
| 36 | H    | -2.8722283634 | 0.6681453461  | 1.1323771299  |
| 37 | H    | 0.9361069356  | -1.1237654022 | 3.2503795974  |
| 38 | H    | -0.5214000081 | -2.1131770101 | 3.3792165260  |
| 39 | H    | -0.3698537398 | -0.6376620998 | 4.333725182  |
| 40 | H    | -2.5917147159 | 0.6681453461  | 1.1323771299  |
| 41 | H    | -2.8722283634 | 0.6681453461  | 1.1323771299  |
| 42 | H    | -0.5214000081 | -2.1131770101 | 3.3792165260  |
| 43 | H    | -0.3698537398 | -0.6376620998 | 4.333725182  |

(7R*, 9S*) - S2D, M0002:M0012
|   |   |   |   |   |
|---|---|---|---|---|
| 22 | H | 1.0293773560 | -1.7774061993 | 0.6104849335 |
| 23 | H | 1.9844003678 | 0.2567252996 | -0.2924617593 |
| 24 | C | -0.2045237796 | -1.1027889260 | 3.4981749176 |
| 25 | O | -2.2016749143 | -0.0173417565 | 2.6682801457 |
| 26 | O | 2.1151485363 | 0.3434759726 | 2.3071353056 |
| 27 | C | 3.4963239486 | 0.7327462275 | 2.195835174 |
| 28 | H | 0.7980365126 | -2.9027837559 |   |
| 29 | H | 1.5178915332 | 2.0955796014 | 1.3455077273 |
| 30 | H | -0.0421918782 | 1.3267556263 | -2.9027837559 |
| 31 | H | 1.8588018224 | -0.9211788547 | 3.6548306401 |
| 32 | H | -0.8327500821 | 1.7421720564 | 1.6517138294 |
| 33 | H | -0.9593441937 | -0.6691806681 | 5.7673454933 |
| 34 | H | -2.4370189934 | -0.0038178421 | 2.5311423445 |
| 35 | H | -2.0894578702 | 1.6332986290 | 1.9629308248 |
| 36 | H | -2.8147802983 | 0.9184494803 | 1.340927875 |
| 37 | H | 0.8614568015 | -1.1826977613 | 3.3672514324 |
| 38 | H | -0.6575020055 | -2.0867949365 | 3.4666646396 |
| 39 | H | -0.4132152488 | -0.6459756655 | 4.4564674504 |
| 40 | H | -2.6738528440 | -0.8621142352 | 2.5972695785 |
| 41 | H | 3.6262157551 | 1.7767162370 | 2.4578369742 |
| 42 | H | 3.8821205283 | 0.5690127375 | 1.1962699397 |
| 43 | H | 4.0440409898 | 0.1170950711 | 2.8921181602 |
Summary of $^{13}$C chemical shift calculations ($\delta^{13}$C: $\omega$B97X-D/6-31G*, Boltzmann distribution; $\omega$B97X-V/6-311+G(2df,2p)[6-311G*])

| (7S*,9R*)-S2A, M0003 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Energy (kJ/mol)         | Relative Energy (kJ/mol) | Boltzmann a | b | c | d | e | f | g | h | i | j | k | l | m | n | o | p | q | r | s | t | u |
| M0003: M0001 | -3351089.57 | 0 | 25.4% | 89.20 | 55.83 | 76.90 | 76.57 | 171.66 | 64.08 | 72.04 | 35.26 | 98.54 | 173.62 | 38.93 | 174.34 | 30.01 | 54.33 |
| M0003: M0002 | -3351089.1 | 0.47 | 21.0% | 89.27 | 54.36 | 76.70 | 75.76 | 172.88 | 66.27 | 72.12 | 35.45 | 98.31 | 173.02 | 39.01 | 175.00 | 29.99 | 54.39 |
| M0003: M0003 | -3351087.05 | 2.53 | 9.1% | 88.58 | 54.91 | 76.81 | 75.56 | 173.36 | 66.45 | 72.10 | 35.52 | 98.28 | 170.67 | 39.89 | 174.63 | 30.00 | 54.40 |
| M0003: M0004 | -3351085.47 | 4.1 | 4.8% | 89.02 | 54.53 | 77.38 | 78.34 | 172.48 | 66.05 | 73.42 | 31.55 | 98.38 | 173.26 | 39.20 | 175.09 | 30.32 | 55.82 |
| M0003: M0005 | -3351085.18 | 4.4 | 4.3% | 89.27 | 55.60 | 77.64 | 79.86 | 171.27 | 66.27 | 72.12 | 36.18 | 96.76 | 173.26 | 37.48 | 175.41 | 30.93 | 55.96 |
| M0003: M0006 | -3351084.49 | 5.09 | 3.2% | 91.56 | 52.64 | 74.82 | 82.48 | 172.34 | 64.31 | 72.81 | 36.12 | 96.62 | 173.27 | 36.35 | 175.07 | 30.91 | 60.11 |
| M0003: M0007 | -3351083.7 | 5.88 | 2.4% | 89.18 | 55.70 | 77.01 | 76.64 | 172.04 | 64.42 | 72.21 | 34.70 | 99.05 | 174.28 | 39.94 | 170.05 | 29.88 | 54.27 |
| M0003: M0008 | -3351083.27 | 6.3 | 2.0% | 88.48 | 54.79 | 77.51 | 78.86 | 172.77 | 66.23 | 73.44 | 31.57 | 98.34 | 170.71 | 40.02 | 174.58 | 30.34 | 55.91 |
| M0003: M0010 | -3351085.35 | 4.22 | 4.6% | 88.78 | 54.58 | 77.08 | 76.38 | 174.03 | 68.25 | 72.37 | 33.25 | 99.35 | 173.56 | 40.74 | 170.54 | 28.96 | 54.39 |
| M0003: M0011 | -3351084.07 | 5.51 | 2.7% | 90.11 | 54.68 | 78.33 | 83.91 | 171.35 | 64.06 | 68.18 | 31.94 | 98.89 | 173.96 | 38.99 | 174.34 | 30.42 | 52.22 |
| M0003: M0012 | -3351083.33 | 6.25 | 2.0% | 89.96 | 53.52 | 78.13 | 83.02 | 172.21 | 66.29 | 68.19 | 32.00 | 98.54 | 173.09 | 39.30 | 174.88 | 30.39 | 52.27 |
| M0003: M0013 | -3351081.6 | 7.97 | 1.0% | 89.22 | 56.66 | 77.03 | 76.48 | 172.35 | 66.03 | 72.03 | 35.15 | 98.57 | 170.26 | 39.78 | 172.16 | 29.99 | 54.38 |
| M0003: M0014 | -3351083.56 | 6.01 | 2.0% | 88.50 | 54.42 | 76.98 | 76.55 | 174.09 | 69.28 | 72.36 | 33.17 | 99.43 | 172.45 | 40.44 | 170.61 | 28.91 | 54.36 |
| M0003: M0015 | -3351083.11 | 6.47 | 1.9% | 88.68 | 54.40 | 77.76 | 79.72 | 173.59 | 67.84 | 73.43 | 29.65 | 99.37 | 173.58 | 40.66 | 170.77 | 29.11 | 55.76 |
| M0003: M0016 | -3351081.1 | 8.47 | 0.8% | 88.46 | 56.09 | 77.04 | 75.49 | 172.91 | 66.82 | 72.11 | 35.36 | 98.46 | 171.74 | 41.53 | 169.58 | 29.90 | 54.48 |
| M0003: M0017 | -3351080.69 | 8.89 | 0.7% | 88.97 | 55.38 | 77.66 | 80.03 | 172.00 | 64.35 | 73.62 | 30.78 | 99.05 | 174.50 | 40.05 | 170.46 | 30.18 | 55.72 |
| M0003: M0018 | -3351080.49 | 9.08 | 0.6% | 88.48 | 55.82 | 76.91 | 76.69 | 172.57 | 66.86 | 72.32 | 34.51 | 99.02 | 171.14 | 41.08 | 169.84 | 29.80 | 54.14 |
| M0003: M0019 | -3351081.95 | 7.62 | 1.2% | 88.37 | 52.86 | 77.05 | 76.37 | 173.82 | 65.58 | 72.15 | 35.50 | 98.32 | 173.08 | 41.58 | 171.56 | 30.00 | 54.43 |

Boltzmann averaged 89.32 55.00 76.75 77.82 172.37 65.24 72.19 34.57 98.32 173.03 39.11 174.11 30.09 55.27
|        | Energy (kJ/mol) | Relative Energy (kJ/mol) | Boltzmann Weights | a | b | c | d | e | f | g | h | i | j | k | l | m | n |
|--------|----------------|-------------------------|-------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| M0004: M0001 | -3351096.98 | 1.4 | 9.8% | 90.02 | 55.95 | 73.08 | 74.52 | 171.62 | 63.64 | 76.11 | 34.59 | 96.98 | 173.40 | 38.98 | 174.35 | 28.87 | 56.90 |
| M0004: M0002 | -3351096.43 | 1.95 | 7.9% | 90.06 | 54.41 | 72.71 | 73.84 | 172.92 | 65.86 | 75.84 | 34.91 | 97.01 | 172.97 | 39.17 | 174.89 | 28.73 | 56.59 |
| M0004: M0003 | -3351097.55 | 0.84 | 12.3% | 89.76 | 54.77 | 73.06 | 78.22 | 172.40 | 65.84 | 76.70 | 29.15 | 97.31 | 173.12 | 39.39 | 174.81 | 28.51 | 56.05 |
| M0004: M0004 | -3351098.38 | 0 | 17.3% | 89.59 | 56.26 | 73.45 | 78.88 | 171.45 | 63.76 | 77.06 | 35.03 | 96.96 | 170.57 | 40.05 | 174.32 | 28.73 | 56.93 |
| M0004: M0005 | -3351098.23 | 0.15 | 16.3% | 89.54 | 54.76 | 72.85 | 73.69 | 173.34 | 65.87 | 76.24 | 35.03 | 96.96 | 170.57 | 40.05 | 174.32 | 28.73 | 56.93 |
| M0004: M0006 | -3351093.93 | 4.46 | 2.9% | 89.07 | 55.05 | 73.12 | 78.04 | 173.07 | 66.01 | 75.84 | 29.45 | 97.14 | 170.59 | 39.98 | 174.34 | 28.66 | 56.97 |
| M0004: M0007 | -3351094.74 | 3.64 | 4.0% | 89.82 | 54.66 | 73.37 | 74.78 | 174.14 | 67.68 | 76.32 | 33.00 | 98.22 | 175.24 | 40.73 | 170.66 | 27.73 | 56.82 |
| M0004: M0008 | -3351094.26 | 5.93 | 1.6% | 90.05 | 55.64 | 73.04 | 74.45 | 170.03 | 63.84 | 76.56 | 34.18 | 97.30 | 170.43 | 39.60 | 170.73 | 28.74 | 56.83 |
| M0004: M0009 | -3351095.38 | 3 | 5.2% | 89.19 | 54.67 | 73.51 | 79.15 | 173.57 | 68.81 | 76.59 | 27.08 | 98.21 | 172.50 | 40.47 | 170.89 | 27.53 | 55.71 |
| M0004: M0010 | -3351093.68 | 4.7 | 2.6% | 89.44 | 54.63 | 73.34 | 74.91 | 173.97 | 68.90 | 76.35 | 32.92 | 97.94 | 172.36 | 40.47 | 170.65 | 27.71 | 56.84 |
| M0004: M0011 | -3351091.55 | 6.84 | 1.1% | 89.18 | 55.99 | 73.73 | 79.12 | 172.21 | 66.39 | 76.96 | 28.17 | 97.88 | 170.98 | 40.70 | 170.72 | 28.38 | 55.94 |
| M0004: M0012 | -3351090.79 | 8.59 | 0.5% | 89.40 | 55.79 | 72.99 | 74.53 | 172.34 | 66.39 | 76.43 | 34.06 | 97.35 | 170.90 | 40.57 | 170.50 | 28.67 | 56.81 |
| M0004: M0013 | -3351089.4 | 8.98 | 0.5% | 89.53 | 55.86 | 72.88 | 74.27 | 172.55 | 65.58 | 76.25 | 34.63 | 97.05 | 170.38 | 39.68 | 171.79 | 28.81 | 56.88 |
| M0004: M0014 | -3351089.48 | 7.55 | 0.8% | 89.48 | 55.30 | 73.40 | 78.83 | 172.00 | 65.77 | 76.86 | 28.67 | 97.52 | 170.08 | 39.93 | 172.58 | 28.51 | 56.11 |
| M0004: M0015 | -3351089.61 | 8.78 | 0.5% | 90.19 | 55.72 | 72.99 | 74.19 | 172.21 | 66.39 | 76.39 | 34.48 | 97.01 | 169.87 | 39.70 | 172.61 | 28.85 | 56.87 |
| M0004: M0016 | -3351090.14 | 8.24 | 0.6% | 89.00 | 56.02 | 73.15 | 78.72 | 172.36 | 65.70 | 76.39 | 29.09 | 97.36 | 170.39 | 39.86 | 171.85 | 28.68 | 55.97 |
| M0004: M0017 | -3351089.45 | 9.37 | 0.5% | 88.92 | 54.99 | 73.35 | 77.99 | 172.41 | 66.43 | 76.53 | 30.89 | 97.53 | 171.63 | 41.07 | 169.32 | 28.48 | 56.93 |
| M0004: M0018 | -3351088.91 | 9.47 | 0.4% | 89.22 | 53.04 | 73.22 | 74.32 | 173.73 | 65.27 | 76.21 | 34.99 | 97.04 | 172.79 | 41.78 | 171.31 | 28.69 | 56.97 |

Boltsmann averaged: 89.67 55.39 73.29 77.40 172.31 65.27 76.67 30.33 97.49 172.98 39.57 173.41 28.37 56.28
|   | Energy (kJ/mol) | Relative Energy (kJ/mol) | Boltzmann Weights |
|---|----------------|-------------------------|-------------------|
| M0001: M0001 | -3351088.85 | 0 | 31.3% 91.24 55.72 76.74 83.04 171.18 62.55 73.66 36.64 98.73 173.07 37.85 175.39 24.76 60.76 |
| M0001: M0002 | -3351085.44 | 3.41 | 7.9% 92.13 52.95 76.68 82.78 172.26 64.48 73.98 36.68 98.70 173.10 36.99 174.71 24.62 60.26 |
| M0001: M0003 | -3351087.76 | 1.09 | 20.2% 89.43 54.89 77.58 76.15 173.95 67.80 74.98 36.34 100.22 173.48 41.23 174.59 22.28 54.59 |
| M0001: M0004 | -3351086.31 | 2.54 | 11.2% 89.06 54.93 77.46 76.21 173.65 68.97 74.84 36.26 100.25 172.28 40.89 174.56 22.30 54.52 |
| M0001: M0005 | -3351085.74 | 3.11 | 8.9% 89.20 54.70 77.85 79.89 173.45 67.54 75.94 32.95 100.22 173.48 41.18 174.81 22.39 55.68 |
| M0001: M0006 | -3351082.46 | 6.39 | 2.4% 91.41 53.25 76.84 82.74 172.59 64.50 74.04 36.64 98.74 170.38 37.88 174.47 24.58 60.16 |
| M0001: M0007 | -3351081.71 | 7.14 | 1.8% 91.80 55.58 76.60 83.29 171.80 63.05 73.68 36.53 98.80 173.54 38.87 171.45 24.85 62.12 |
| M0001: M0008 | -3351081.72 | 7.13 | 1.8% 90.84 55.53 76.49 82.79 172.22 64.03 73.70 36.50 98.88 171.04 37.60 172.83 24.89 60.37 |
| M0001: M0009 | -3351084.23 | 4.62 | 4.9% 88.91 54.70 77.75 79.87 173.12 68.69 75.87 32.82 100.13 172.53 40.88 174.82 22.40 55.68 |
| M0001: M0010 | -3351084.79 | 4.06 | 6.1% 90.00 53.87 78.46 83.65 173.18 67.70 71.04 33.46 100.82 173.30 41.29 174.83 22.01 52.22 |
| M0001: M0011 | -3351083.45 | 5.4  | 3.5% 89.76 53.78 78.38 83.62 173.03 68.84 71.09 33.31 100.95 172.32 41.15 174.94 21.98 52.20 |
| Boltzmann averaged | 90.28 | 54.86 | 77.29 | 80.47 | 172.65 | 65.84 | 74.15 | 35.71 | 99.60 | 172.98 | 39.59 | 174.81 | 23.38 | 57.25 |
| Energy (kJ/mol) | Relative Energy (kJ/mol) | Boltzmann Weights |
|----------------|--------------------------|-------------------|
|                |                          | $a$   | $b$   | $c$   | $d$   | $e$   | $f$   | $g$   | $h$   | $i$   | $j$   | $k$   | $l$   | $m$   | $n$   |
| M0002: M0001   | -3351095.03              | 0     | 38.2% | 89.75 | 55.01 | 76.79 | 79.62 | 173.58 | 67.52 | 74.93 | 30.00 | 97.85 | 173.54 | 41.19 | 174.94 | 23.19 | 55.48 |
| M0002: M0002   | -3351093.95              | 1.08  | 24.7% | 89.42 | 55.14 | 76.76 | 79.71 | 173.11 | 68.81 | 74.95 | 29.92 | 97.94 | 172.50 | 41.22 | 175.15 | 23.14 | 55.46 |
| M0002: M0003   | -3351091.48              | 3.55  | 9.1%  | 90.04 | 55.19 | 76.41 | 75.27 | 173.77 | 67.59 | 74.96 | 35.67 | 98.53 | 173.48 | 41.23 | 174.76 | 23.97 | 56.90 |
| M0002: M0004   | -3351090.4               | 4.63  | 5.9%  | 89.72 | 55.13 | 76.42 | 75.44 | 173.56 | 68.77 | 75.00 | 35.58 | 98.63 | 172.48 | 41.01 | 174.85 | 23.83 | 57.01 |
| M0002: M0005   | -3351091.04              | 3.98  | 7.7%  | 92.13 | 54.87 | 77.88 | 89.40 | 173.30 | 66.46 | 76.02 | 38.38 | 99.90 | 173.60 | 41.19 | 175.67 | 27.22 | 56.36 |
| M0002: M0006   | -3351090.22              | 4.81  | 5.5%  | 91.75 | 55.26 | 77.77 | 89.34 | 173.14 | 67.77 | 75.90 | 38.38 | 99.89 | 172.40 | 41.21 | 175.74 | 27.24 | 56.59 |
| M0002: M0007   | -3351088.84              | 6.18  | 3.2%  | 89.95 | 54.64 | 76.98 | 79.01 | 173.20 | 68.08 | 74.57 | 26.67 | 98.25 | 173.31 | 41.88 | 171.49 | 26.09 | 55.62 |
| M0002: M0008   | -3351085.93              | 9.1   | 1.0%  | 91.76 | 54.96 | 77.60 | 88.89 | 173.10 | 66.40 | 77.31 | 35.12 | 99.97 | 173.59 | 41.31 | 176.00 | 27.39 | 55.91 |
| M0002: M0009   | -3351085.04              | 9.99  | 0.7%  | 91.55 | 55.25 | 77.56 | 88.88 | 172.82 | 67.71 | 77.33 | 35.18 | 99.97 | 172.60 | 41.22 | 176.15 | 27.33 | 56.04 |
| M0002: M0010   | -3351086.47              | 8.56  | 1.2%  | 90.18 | 54.67 | 76.60 | 74.53 | 173.72 | 68.24 | 74.57 | 32.74 | 98.58 | 173.38 | 42.08 | 171.50 | 26.81 | 57.22 |
| M0002: M0011   | -3351087.76              | 7.26  | 2.0%  | 89.67 | 54.48 | 76.91 | 79.03 | 173.16 | 69.16 | 74.55 | 26.57 | 98.20 | 172.34 | 41.61 | 171.74 | 26.08 | 55.56 |
| M0002: M0012   | -3351085.34              | 9.69  | 0.8%  | 90.10 | 54.41 | 76.66 | 74.74 | 173.69 | 69.14 | 74.42 | 32.62 | 98.77 | 172.26 | 41.81 | 171.71 | 26.85 | 57.14 |

Boltsmann averaged

90.03 55.04 76.88 80.31 173.41 67.91 75.09 31.89 98.32 173.11 41.24 174.85 24.11 55.87
[MOUSE BEHAVIORAL ASSAY]
The mouse behavioral assay was performed under approval by the Ethical Committee of Experimental Animal Care at Hokkaido University (14-0081).

[REFERENCES AND NOTES]

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[NMR SPECTRA OF ALL NEW COMPOUNDS]
$^1$H NMR (400 MHz, CDCl$_3$)
\[ ^{13}C \text{ NMR} (100 \text{ MHz, CDCl}_3) \]

The spectrum shows various peaks at different ppm values. The peaks correspond to different chemical shifts, indicating the presence of various functional groups and chemical structures in the molecule. The structure of the molecule is also depicted, showing the connectivity of atoms and functional groups such as carbonyls (\(\text{O} = \text{C}\)), amides (\(\text{CONH}\)), and hydroxyl groups (\(\text{OH}\)).
$^{13}$C NMR (100 MHz, CDCl$_3$)
$^{1}H$ NMR (400 MHz, CDCl$_3$)
$^{13}$C NMR (100 MHz, CDCl$_3$)
1H NMR (400 MHz, D\textsubscript{2}O)

1ar ((2R\textsuperscript{a},7R\textsuperscript{a})-TKM-50)
$^{13}$C NMR (100 MHz, D$_2$O) of 1ar ((2$^R$,7$^R$)-TKM-50)
$^{1}$H NMR (400 MHz, CDCl$_3$)
$^{13}$C NMR (100 MHz, CDCl$_3$)
$\text{H NMR (400 MHz, CDCl}_3$)
$^{13}$C NMR (100 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

![NMR Spectrum](image-url)
$^{13}$C NMR (100 MHz, CDCl$_3$)

- 128.68, 128.62, 128.53, 128.29, 134.61, 135.52
- 172.70, 169.90, 169.36
- 51.4, 56.0, 66.5, 67.69, 69.04, 75.6, 78.5, 86.53, 87.86
- 13.87, 206.93

NH, O, H, CH$_3$
$^{1}H$ NMR (400 MHz, D$_2$O)

1H NMR spectra of the compound 1br ((2R*,7R*)-TKM-86)
13C NMR (100 MHz, D2O)

1br ((2R*,7R*)-TKM-86)
1H NMR (400 MHz, D$_2$O)

1bs ((2R*,7S*)-TKM-86)
$^{13}$C NMR (100 MHz, D$_2$O)

1bs ((2$R^*$,7$S^*$)-TKM-86)
$^1$H NMR (400 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)
\[ 1\text{H NMR (400 MHz, D}_2\text{O)} \]

1cr (\((2R^*,7R^*)\)-TKM-99)

\[ \text{NH} \]

\[ \text{O} \]

\[ \text{H} \]

\[ \text{H} \]

\[ \text{H} \]

\[ \text{O} \]

\[ \text{O} \]

\[ \text{O} \]

\[ \text{O} \]

\[ \text{O} \]

\[ \text{OH} \]

\[ \text{OH} \]

\[ 1\text{H NMR (400 MHz, D}_2\text{O)} \]

1cr (\((2R^*,7R^*)\)-TKM-99)
$1cr ((2R^*,7R^*)-TKM-99)$
$^1$H NMR (400 MHz, D$_2$O)

1cs ((2$^R$,7$^S$)-TKM-99)
1cs ((2R*,7S*)-TKM-99)
$^1$H NMR (400 MHz, CDCl$_3$)

13
13C NMR (100 MHz, CDCl$_3$)
$^{1}H$ NMR (400 MHz, D$_2$O)
13C NMR (100 MHz, D$_2$O)

2 (TKM–15)