

Supporting Information

Clarifying Stereochemical Outcomes in Radical-Initiated Vinyl Cyclopropane Cycloadditions within the Beckwith-Houk Framework

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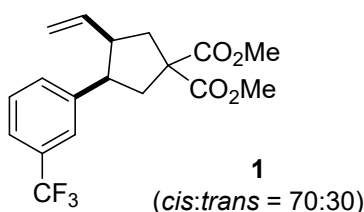
Experimental Section

Preparation of Known Compounds

The synthesis of compounds **1** and **2** were carried out according to the literature procedure reported by Miyake et al. with no modifications. The synthesis of compounds **3-5** were carried out according to the literature procedure reported by Merad et al. with no modifications. The synthesis of compounds **6-10** were carried out according to the literature procedure reported by Sharma et al. with no modifications.

Characterization of Products

For these studies, ^1H NMR chemical shifts and coupling constants were recorded again using Bruker 500 MHz NEO NMR spectrometer (operating at 499.79 MHz for ^1H) equipped with a multinuclear TCI Prodigy Cryoprobe.



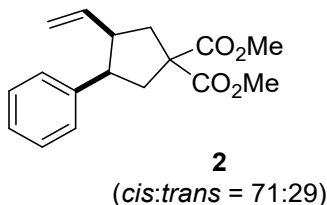
Colorless oil (49.6 mg, 70% yield) as a mixture of diastereomers (*cis* : *trans* = 70:30). R_f = 0.40 (10% EtOAc in hexane).

^1H NMR (500 MHz, CDCl_3) δ 7.91 – 7.71 (m, 6H), 5.73 (ddd, J = 17.1, 10.3, 8.2 Hz, 1H), 5.34 – 5.18 (m, 3H), 4.17 (t, J = 4.3 Hz, 8H), 3.90 (dt, J = 10.9, 7.4 Hz, 1H), 3.50 – 3.42 (m, 1H), 3.24 – 3.10 (m, 2H), 3.10 – 3.03 (m, 1H), 2.99 (dd, J = 13.7, 10.9 Hz, 1H), 2.85 – 2.72 (m, 2H), 2.65 – 2.55 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 172.9, 172.8, 172.7, 172.5, 142.6, 141.7, 138.2, 137.5, 131.7, 131.7, 131.7, 131.0, 130.9, 130.8, 130.5, 130.5, 130.2, 129.9, 128.8, 128.5, 125.6, 125.1, 125.1, 125.0, 125.0, 124.4, 124.4, 124.3, 123.5, 123.4, 123.4, 123.2, 123.2, 123.1, S24 123.1, 122.9, 116.2, 116.1, 58.9, 58.1, 53.0, 52.9, 52.8, 51.1, 51.0, 47.9, 47.3, 42.2, 40.3, 38.9, 37.9.

^{19}F NMR (376 MHz, CDCl_3) δ -62.60, -62.61.

DART-TOF LC/MS m/z calcd. for $\text{C}_{18}\text{H}_{19}\text{F}_3\text{O}_4$ [$\text{M}+\text{H}^+$] 357.1314, found 357.1314.

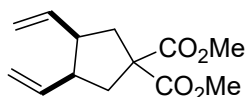


Colorless oil (50.4 mg, 88% yield) as a mixture of diastereomers (*cis* : *trans* = 71:29). R_f = 0.35 (10% EtOAc in hexane).

^1H NMR (500 MHz, CDCl_3) δ 7.75 – 7.67 (m, 3H), 7.67 – 7.54 (m, 4H), 5.79 (ddd, J = 17.1, 10.4, 8.0 Hz, 1H), 5.44 – 5.18 (m, 3H), 3.87 (dt, J = 10.7, 7.5 Hz, 1H), 3.45 (p, J = 7.3 Hz, 1H), 3.22 (dd, J = 13.6, 7.7 Hz, 1H), 3.19 – 3.12 (m, 2H), 3.12 – 2.97 (m, 2H), 2.87 – 2.74 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 173.1, 173.0, 172.9, 172.7, 141.5, 140.8, 138.7, 138.2, 128.4, 128.3, 128.1, 127.6, 126.6, 126.3, 115.6, 115.4, 59.0, 58.1, 52.9, 52.8, 51.5, 50.9, 48.0, 47.3, 42.5, 40.3, 39.0, 38.1.

DART-TOF LC/MS m/z calcd. for $\text{C}_{17}\text{H}_{21}\text{O}_4$ [$\text{M}+\text{H}^+$] 289.1440, found 289.1442.



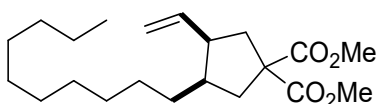
3
(*cis:trans* = 57:43)

Colorless oil: (27 mg, 0.12 mmol, 60%) as an unseparable mixture of two diastereomers : (*cis trans* = 57:43).

^1H NMR (500 MHz, CDCl_3) δ 5.75 – 5.59 (m, 4H), 5.05 – 4.95 (m, 8H), 2.76 (dt, J = 7.5, 5.3 Hz, 2H), 2.60 – 2.51 (m, 2H), 2.47 (ddt, J = 12.2, 7.1, 5.2 Hz, 2H), 2.36 – 2.26 (m, 2H), 2.25 – 2.16 (m, 2H), 2.08 – 1.98 (m, 2H).

^{13}C NMR (75 MHz, CDCl_3) δ 173.2, 173.0, 172.9, 139.2, 138.4, 115.6, 115.4, 59.1, 58.3, 53.0, 52.9, 49.8, 47.2, 40.2, 38.9;

HRMS (ESI+, m/z): [$\text{M}+\text{H}$] + calculated for [$\text{C}_{13}\text{H}_{19}\text{O}_4$] + : 239.1278, found 239.1276.



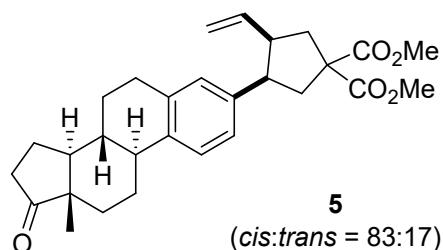
4
(*cis:trans* = 68:32)

Colorless oil: (12.5 mg, 0.035 mmol, 18%) as an unseparable mixture of two diastereomers: (*cis : trans* = 68:32).

^1H NMR (500 MHz, CDCl_3) δ 5.81 – 5.56 (m, 1H), 5.06 – 4.91 (m, 3H), 2.69 (p, J = 7.0 Hz, 1H), 2.47 (dd, J = 14.0, 7.3 Hz, 1H), 2.36 (dd, J = 12.3, 5.6 Hz, 1H), 2.18 (dd, J = 14.0, 5.4 Hz, 1H), 2.05 – 1.92 (m, 2H), 1.18 – 1.07 (m, 2H), 0.95 – 0.75 (m, 6H).

^{13}C NMR (75 MHz, CDCl_3) δ 173.5, 173.4, 173.31, 173.29, 140.5, 138.5, 115.4, 115.3, 59.07, 59.06, 52.9, 52.8, 50.6, 46.5, 45.4, 43.1, 40.7, 40.4, 39.4, 33.3, 32.1, 30.6, 29.9, 29.8 (4C), 29.5, 28.3, 22.8, 14.3

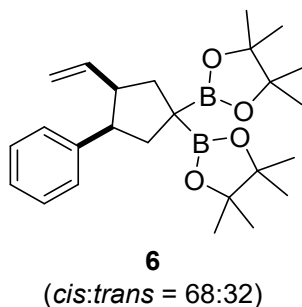
HRMS (ESI+, m/z): $[\text{M}+\text{Na}]^+$ calculated for $[\text{C}_{21}\text{H}_{36}\text{NaO}_4]^+$: 375,2506 found 375.2509.



Colorless oil: (72 mg, 0.15 mmol, 77%) as an unseparable mixture of two diastereomers: (*cis* : *trans* = 83:17).

^1H NMR (500 MHz, CDCl_3) δ 7.94 – 7.71 (m, 1H), 7.58 (dq, J = 22.9, 9.1 Hz, 1H), 7.44 – 7.29 (m, 1H), 7.27 (d, J = 23.0 Hz, 1H), 5.84 – 5.69 (m, 1H), 5.34 – 5.15 (m, 3H), 4.13 (d, J = 5.5 Hz, 9H), 3.83 – 3.67 (m, 1H), 3.37 (tt, J = 24.4, 8.0 Hz, 2H), 3.26 (dd, J = 7.6, 4.2 Hz, 1H), 3.24 – 3.09 (m, 2H), 3.05 (ddd, J = 13.8, 7.0, 2.5 Hz, 2H), 3.02 – 2.85 (m, 5H), 2.85 – 2.75 (m, 2H), 2.75 – 2.61 (m, 2H), 2.51 (tdd, J = 28.0, 12.9, 7.3 Hz, 4H), 2.43 – 2.35 (m, 2H), 2.35 – 2.21 (m, 2H), 2.21 – 2.06 (m, 2H), 2.06 – 1.89 (m, 4H), 1.89 – 1.84 (m, 1H), 1.84 – 1.76 (m, 1H), 1.56 (s, 1H), 1.39 – 1.25 (m, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 173.3, 173.20, 173.19, 173.1, 172.9, 139.1, 139.0, 138.5, 138.3, 138.2, 138.12, 138.10, 137.7, 136.6, 136.5, 136.2, 129.3, 128.9, 128.5, 128.1, 126.2, 125.8, 125.6, 125.5, 125.3, 125.1, 124.9, 115.7, 115.4, 68.1, 59.1, 58.2, 53.1, 53.0, 51.04, 51.02, 50.7, 50.5, 50.4, 48.2, 47.7, 47.6, 47.23, 47.20, 44.5, 44.4, 42.8, 42.8, 41.0, 40.4, 39.2, 38.44, 38.37, 38.29, 38.27, 36.0, 31.7, 29.59, 29.55, 26.7, 25.8, 21.7, 14.0. According to literature data. ^[34]



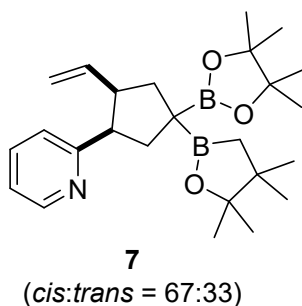
Colorless oil; 71% yield (93 mg), as a mixture of diastereomers (*cis* : *trans* = 68:32). R_f (EtOAc/Hexane, 10:90) = 0.5

^1H NMR (500 MHz, CDCl_3) δ 7.35 – 7.17 (m, 3H), 4.99 – 4.82 (m, 1H), 2.59 – 2.40 (m, 1H), 2.40 – 2.21 (m, 1H), 2.14 – 2.03 (m, 1H), 1.32 (dd, J = 5.4, 2.9 Hz, 13H).

^{13}C NMR (100 MHz, CDCl_3) δ 144.3, 142.9, 141.3, 139.6, 128.6, 128.1, 127.81, 127.8, 125.9, 125.7, 114.4, 114.0, 83.33, 83.3, 83.25, 83.2, 53.4, 53.1, 50.2, 49.1, 39.1, 37.1, 35.4, 33.7, 24.8, 24.76, 24.73, 24.7.

^{11}B NMR (128 MHz, CDCl_3) δ 34.6.

HRMS (ASAP): m/z $[\text{M}+\text{H}]^+$ for $\text{C}_{25}\text{H}_{39}\text{B}_2\text{O}_4$, calculated 425.3029; observed 425.3043.



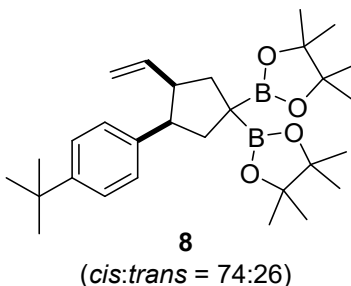
Brown oil; 46% Yield (60 mg), as a mixture of diastereomers (*cis* : *trans* = 67:33) R_f (EtOAc/Hexane, 20:80) = 0.2

^1H NMR (500 MHz, CDCl_3) δ 8.49 (dd, J = 5.1, 1.8 Hz, 1H), 7.57 – 7.48 (m, 1H), 7.14 – 6.99 (m, 2H), 4.92 – 4.75 (m, 2H), 2.46 – 2.19 (m, 3H), 2.17 – 1.97 (m, 1H), 1.23 (dd, J = 9.5, 2.8 Hz, 29H).

^{13}C NMR (100 MHz, CDCl_3) δ 163.7, 162.8, 149.0, 148.7, 141.3, 139.5, 136.0, 135.6, 122.7, 122.3, 121.1, 120.8, 114.3, 113.8, 83.3, 83.25, 83.23, 83.2, 55.5, 52.6, 52.1, 49.2, 38.4, 36.8, 35.4, 33.5, 24.8, 24.76, 24.72, 24.7.

^{11}B NMR (128 MHz, CDCl_3) δ 34.5.

HRMS (ASAP): m/z $[\text{M}+\text{H}]^+$ for $\text{C}_{24}\text{H}_{38}\text{B}_2\text{NO}_4$, calculated 426.2981; observed 426.2992.



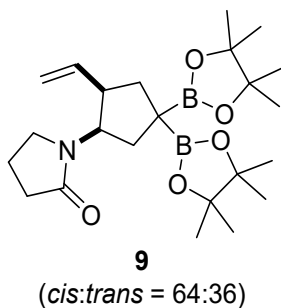
Colorless oil; 68% Yield (101 mg), as a mixture of diastereomers (*cis* : *trans* = 74:26) R_f (EtOAc/Hexane, 10:90) = 0.5

¹H NMR (500 MHz, CDCl₃) δ 7.30 – 7.25 (m, 2H), 7.15 (dd, *J* = 16.8, 8.3 Hz, 2H), 4.97 – 4.89 (m, 1H), 4.82 (dt, *J* = 10.4, 1.6 Hz, 1H), 3.16 (dt, *J* = 10.2, 6.9 Hz, 1H), 2.94 – 2.85 (m, 1H), 2.44 – 2.34 (m, 1H), 2.28 – 2.14 (m, 2H), 2.10 – 2.01 (m, 1H), 1.30 (s, 10H), 1.29 – 1.21 (m, 28H).

¹³C NMR (100 MHz, CDCl₃) δ 148.4, 148.3, 141.7, 141.1, 139.7, 128.2, 127.3, 125.0, 124.7, 114.4, 113.8, 83.31, 83.3, 83.2, 83.16, 52.8, 52.6, 49.6, 48.8, 39.1, 37.0, 35.3, 34.4, 33.7, 31.5, 24.8, 24.78, 24.75, 24.73, 24.7.

¹¹B NMR (128 MHz, CDCl₃) δ 35.2.

HRMS (ASAP): *m/z* [M+H]⁺ for C₂₉H₄₇B₂O₄, calculated 481.3655; observed 481.3669.



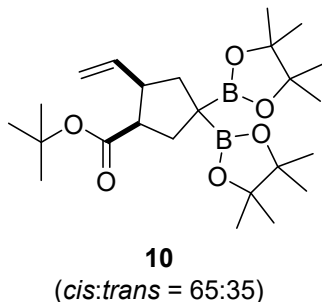
Yellow oil; 37% Yield (49 mg), as a mixture of diastereomers (*cis* : *trans* = 64:36) *R_f* (EtOAc/Hexane, 10:90) = 0.3.

¹H NMR (500 MHz, CDCl₃) δ 5.83 (ddd, *J* = 17.0, 10.5, 6.4 Hz, 0H), 5.74 (ddd, *J* = 17.2, 10.4, 6.6 Hz, 1H), 5.23 – 5.08 (m, 1H), 5.07 – 4.91 (m, 2H), 4.83 (ddt, *J* = 12.3, 8.1, 4.0 Hz, 0H), 4.44 (q, *J* = 7.9 Hz, 1H), 3.87 (q, *J* = 7.1 Hz, 0H), 3.36 (dt, *J* = 9.5, 7.1 Hz, 2H), 3.28 (dt, *J* = 10.6, 7.1 Hz, 2H), 2.75 (p, *J* = 7.3 Hz, 1H), 2.58 – 2.29 (m, 4H), 2.20 (ddd, *J* = 28.0, 12.9, 7.4 Hz, 2H), 2.02 – 1.82 (m, 3H), 1.76 (dd, *J* = 12.7, 7.6 Hz, 1H), 1.23 (d, *J* = 4.6 Hz, 17H), 1.21 (s, 15H), 1.19 (s, 21H).

¹³C NMR (100 MHz, CDCl₃) δ 175.2, 137.8, 135.7, 116.9, 115.3, 83.4, 83.3, 55.7, 53.4, 47.4, 46.2, 45.8, 43.6, 41.7, 34.0, 31.5, 31.3, 24.7, 24.6, 24.5, 18.4, 18.3.

¹¹B NMR (128 MHz, CDCl₃) δ 33.5.

HRMS (ASAP): *m/z* [M+H]⁺ for C₂₃H₄₀B₂NO₅, calculated 432.3087; observed 432.3102.



Colorless oil; 48% Yield (67 mg), as a mixture of diastereomers (*cis* : *trans* = 65:35) R_f (EtOAc/Hexane, 10:90) = 0.3.

¹H NMR (500 MHz, CDCl₃) δ 5.75 (ddt, *J* = 17.7, 10.3, 7.5 Hz, 1H), 5.08 – 4.85 (m, 2H), 2.77 – 2.67 (m, 1H), 2.36 – 2.15 (m, 1H), 2.10 (dd, *J* = 17.1, 6.8 Hz, 2H), 1.96 – 1.88 (m, 1H), 1.39 (d, *J* = 6.7 Hz, 9H), 1.23 – 1.17 (m, 24H).

¹³C NMR (100 MHz, CDCl₃) δ 174.7, 173.7, 140.9, 138.9, 114.9, 114.0, 83.4, 83.33, 83.3, 83.2, 79.9, 79.8, 52.3, 50.3, 49.4, 48.2, 36.8, 35.8, 34.4, 32.3, 28.4, 28.3, 24.8, 24.77, 24.74, 24.7.

¹¹B NMR (128 MHz, CDCl₃) δ 34.1.

HRMS (ASAP): *m/z* [M+H]⁺ for C₂₄H₄₃B₂O₆, calculated 449.3240; observed 449.3243

NMR Acquisition Parameters

NMR Parameters for 1D qNOE experiments

1D NOESY experiments were acquired on a Bruker 500 MHz NEO NMR spectrometer (operating at 499.79 MHz for ¹H) equipped with a multinuclear TCI Prodigy Cryoprobe. Data were acquired using the Bruker TopSpin pulse program "selnpgp.2" with a spectral width of 10 ppm and 32 scans. The mixing time for each experiment increased in 100 msec increments from 300 to 800 msec, utilizing a 80 msec Gaussian-shaped pulse for selective excitation. qNOE experiments for compound **10** were acquired with a 40 msec Gaussian-shaped pulse.

NMR Parameters for 2D Undecoupled ¹H-¹³C HSQC-NOESY

The HSQC-NOESY spectrum of **3** was acquired on a Bruker 500 MHz NEO NMR spectrometer (Operating at 499.79 MHz for ^1H and 125.67 MHz for ^{13}C) equipped with a multinuclear TCI Prodigy Cryoprobe using the Bruker pulse program "hsqcetgpnosp". 3k data points were acquired in F2 (SW=10 ppm) and 128 points were acquired in F1 (SW=70 ppm). 1024 scans were acquired per increment with a 1 s relaxation delay. CNST2 was set to 145 Hz and a mixing time of 600 msec was used for the NOESY pulse sequence module.

NMR Parameters for 1D PSYCHE

The 1D PSYCHE spectrum of **10** was acquired on a Bruker 500 MHz NEO NMR spectrometer (operating at 499.79 MHz for ^1H) equipped with a multinuclear TCI Prodigy Cryoprobe using the Bruker pulse program "reset_psyche_1d". 10 k points were acquired in F2 and 64 points were acquired in F1 with 64 scans per increment. SW was set to 10 ppm in F2 and 1.5 ppm in F1. L31 was set to 100.

DFT Methods

Chemical Shift calculations

For NMR δ prediction analysis of **1-10**, structures were energy-minimized using MMFF94 in Chem3D and extended mixed torsional/low-mode (MTLMOD) conformational searches were performed using the OPLS4³³ force field in the Schrödinger MacroModel software package. NMR predictions were based on the DELTA50 methodology; ^{13}C δ predictions were performed at the PCM- ω B97X-D/def2-SVP//PCM-B3LYP-D3/6-311G(d,p) level of theory, and ^1H δ predictions were performed at the PCM-WP04/6-311++G(2d,p)//PCM-B3LYP-D3/6-311G(d,p) level of theory, both of which were performed in the Gaussian³⁴ software package.

Activation Energy Calculations

Activation Energy calculations, geometry optimizations and frequency calculations were conducted at the B3LYP-D3(BJ)/6-31+G** level of theory under solvation (DMSO for **1**, **2**, methanol for **4** and **5**, and dichloroethane for **7**, **9** and **10**). Single-point energy calculations were done at the M06-2X-D3/def2-TZVP level of theory under solvation using the solvents listed above. Conformation analysis for stationary and saddle points was performed using the Global Optimizer Algorithm (GOAT) feature in the ORCA software.³⁵ All quantum mechanical calculations were performed using *Gaussian 16*.³⁴ Geometry optimizations and frequency calculations were performed using the hybrid B3LYP^{36,37} functional applied with Grimme's D3³⁸ dispersion correct with Beck-Johnson (BJ)³⁹ damping and the 6-31+G(d,p)⁴⁰⁻⁴⁴ basis set. Single-point energy calculations were performed on all optimized structures using the hybrid meta-GGA M06-2X⁴⁵ functional applied with D3 dispersion and the def2-TZVP^{46,47} basis sets. Solvation effects were accounted for geometry optimizations and single-point energy calculations using the SMD⁴⁸ variation of the integral equation formalism variant of the polarizable continuum model.⁴⁹⁻⁵³ A truncated model of **4** and **5** was used to simplify conformation analysis and computational cost.

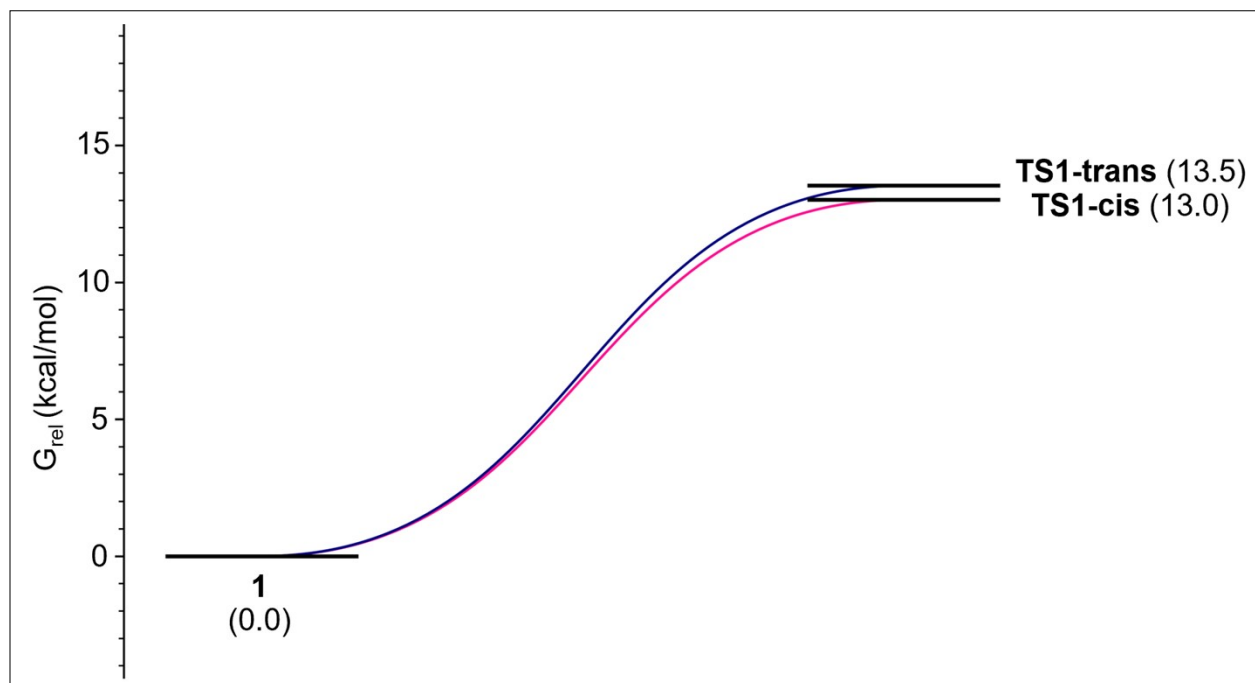


Figure S1. Gibbs free energy profile for the key intermediate and transition state structures for compound **1** computed at the (SMD=DMSO) M06-2X-D3/def2-TZVP//((SMD=DMSO) B3LYP-D3(BJ)/6-31+G** level of theory.

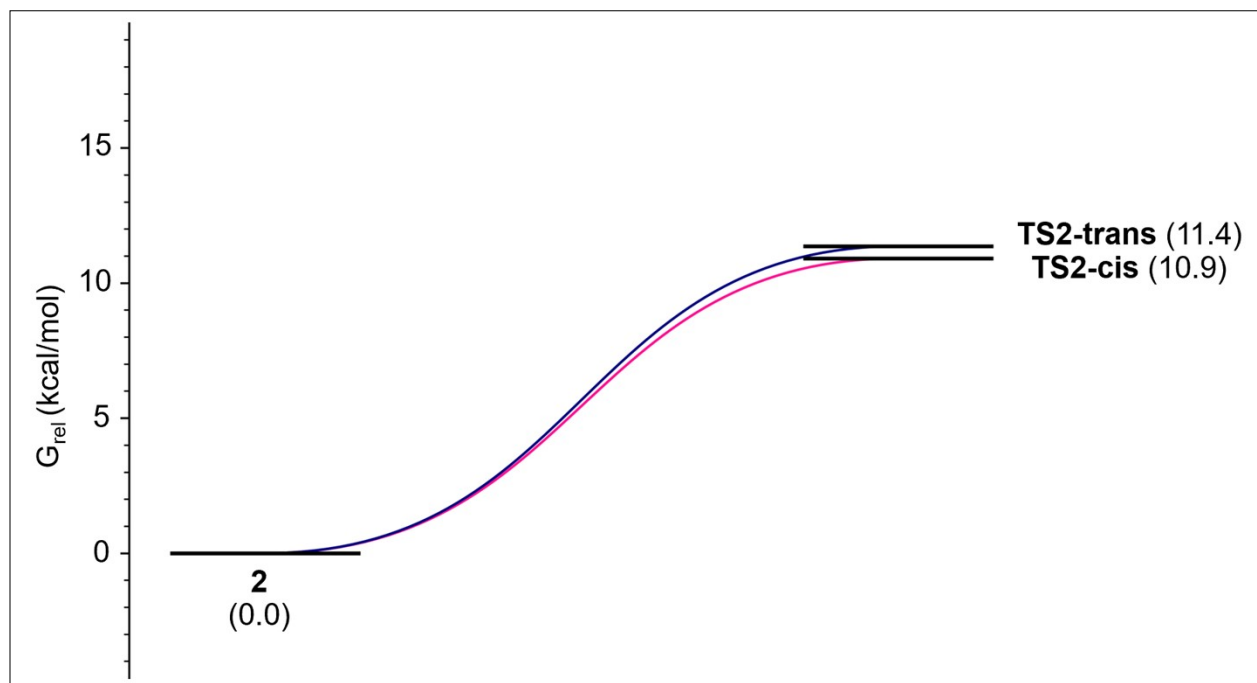


Figure S2. Gibbs free energy profile for the key intermediate and transition state structures for compound **2** computed at the (SMD=DMSO) M06-2X-D3/def2-TZVP//((SMD=DMSO) B3LYP-D3(BJ)/6-31+G** level of theory.

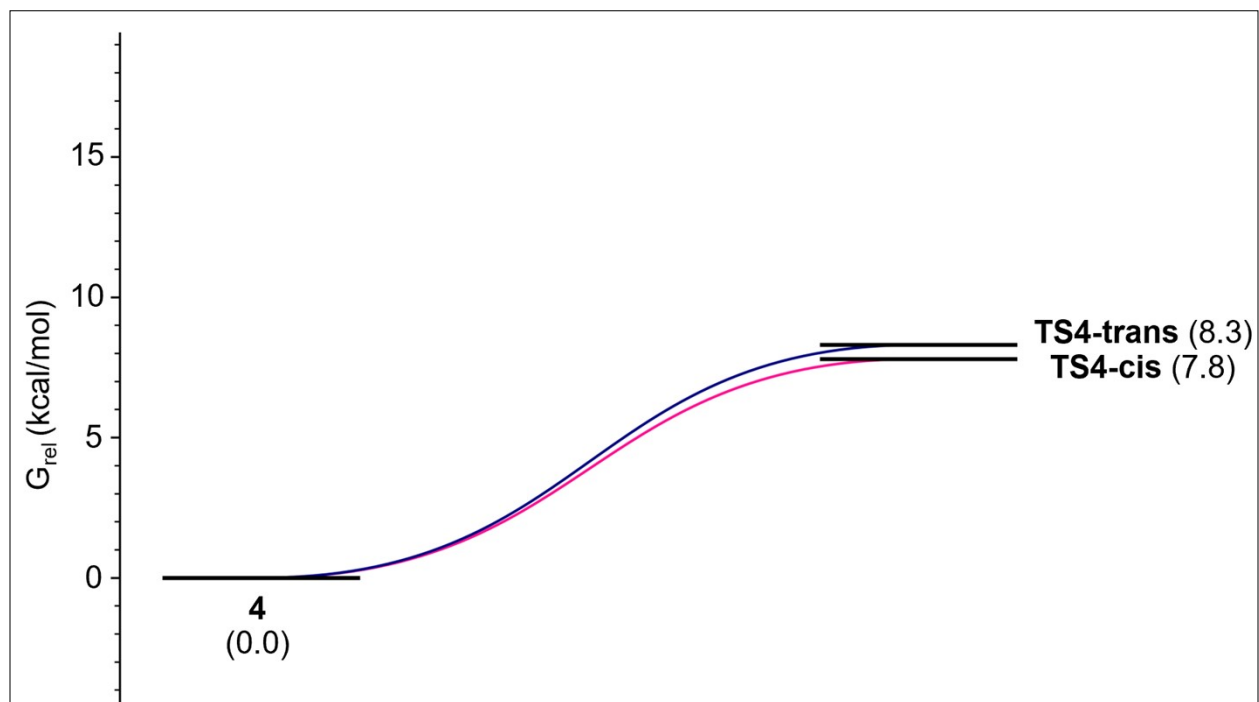


Figure S3. Gibbs free energy profile for the key intermediate and transition state structures for compound **4** computed at the (SMD=methanol) M06-2X-D3/def2-TZVP//((SMD=methanol) B3LYP-D3(BJ)/6-31+G** level of theory.

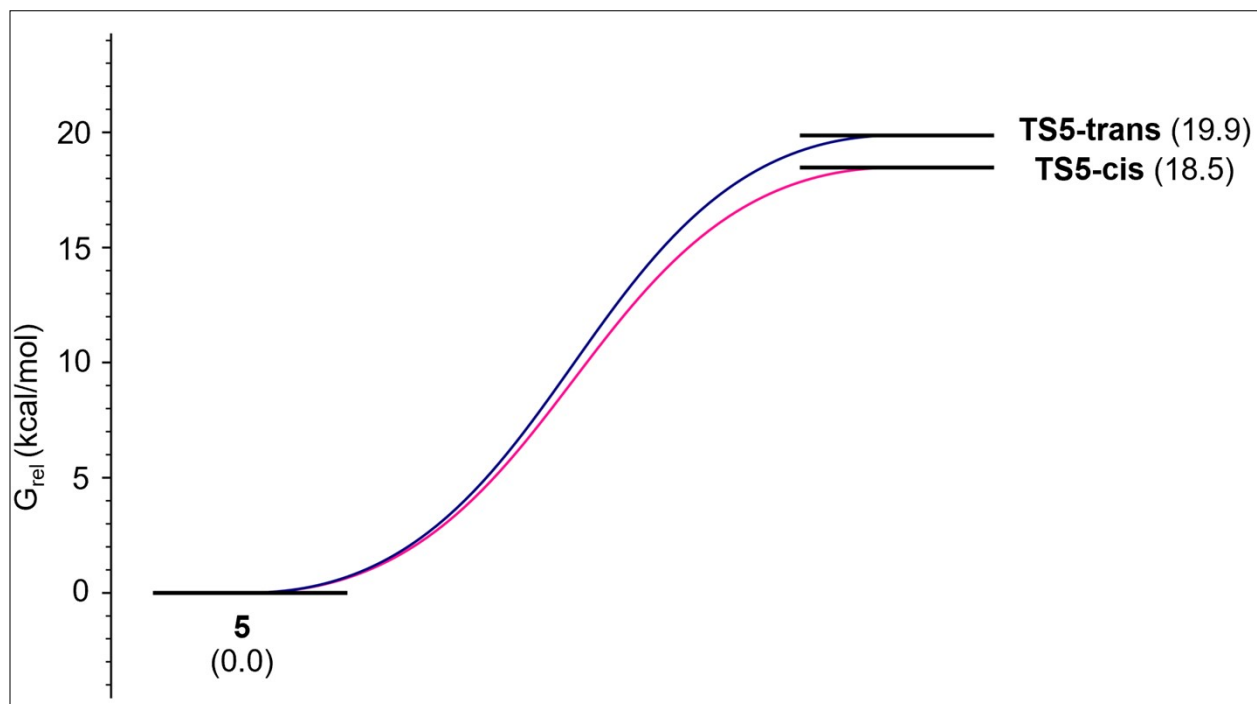


Figure S4. Gibbs free energy profile for the key intermediate and transition state structures for compound **5** computed at the (SMD=methanol) M06-2X-D3/def2-TZVP//((SMD=methanol) B3LYP-D3(BJ)/6-31+G** level of theory.

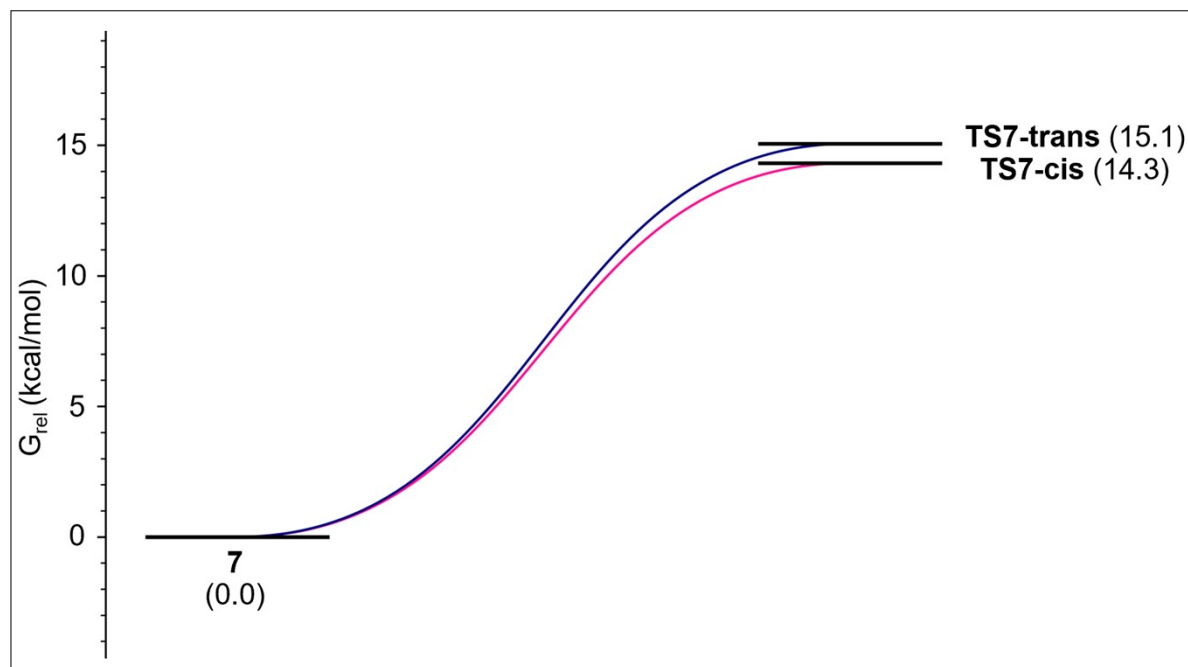


Figure S5. Gibbs free energy profile for the key intermediate and transition state structures for compound **7** computed at the (SMD=dichloroethane) M06-2X-D3/def2-TZVP//((SMD=dichloroethane) B3LYP-D3(BJ/6-31+G** level of theory.

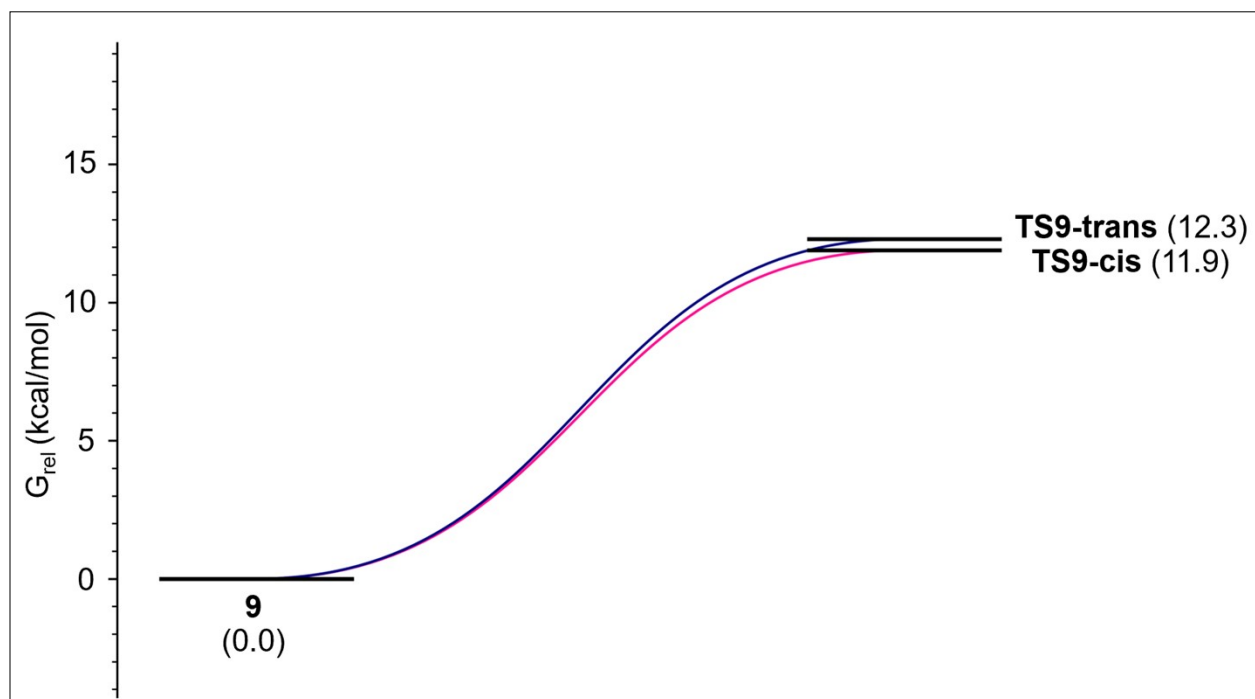


Figure S6. Figure Sx. Gibbs free energy profile for the key intermediate and transition state structures for compound **9** computed at the (SMD=dichloroethane) M06-2X-D3/def2-TZVP//((SMD=dichloroethane) B3LYP-D3(BJ/6-31+G**) level of theory.

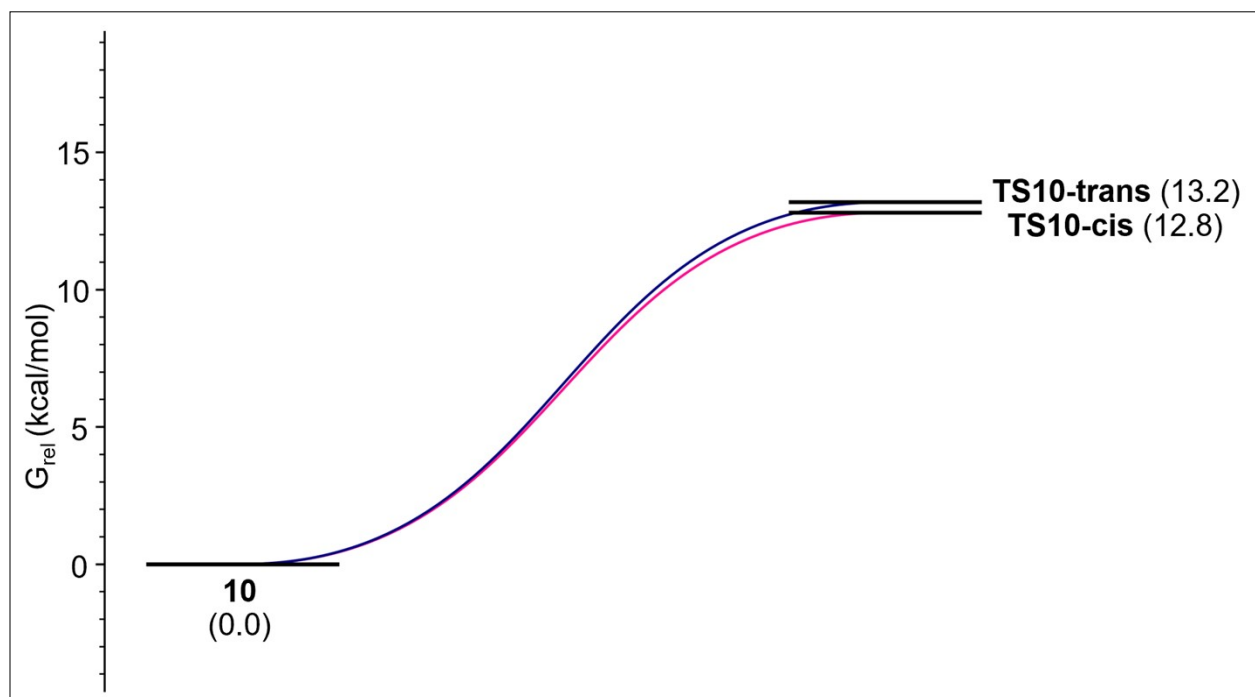


Figure S7. Gibbs free energy profile for the key intermediate and transition state structures for compound **10** computed at the (SMD=dichloroethane) M06-2X-D3/def2-TZVP//((SMD=dichloroethane) B3LYP-D3(BJ/6-31+G** level of theory.

DFT-Predicted vs. Experimental Chemical Shifts

1

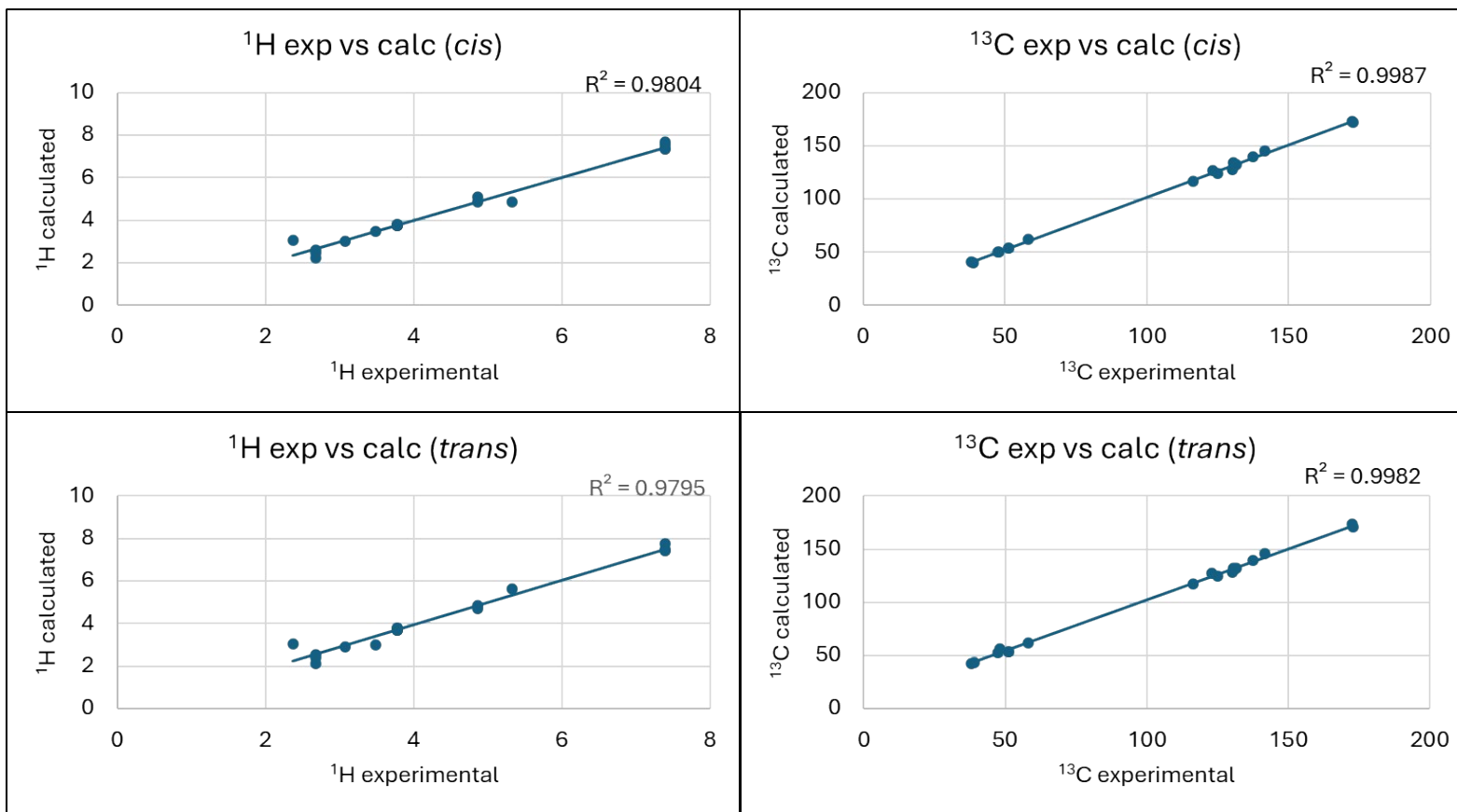


Figure S8. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **1**.

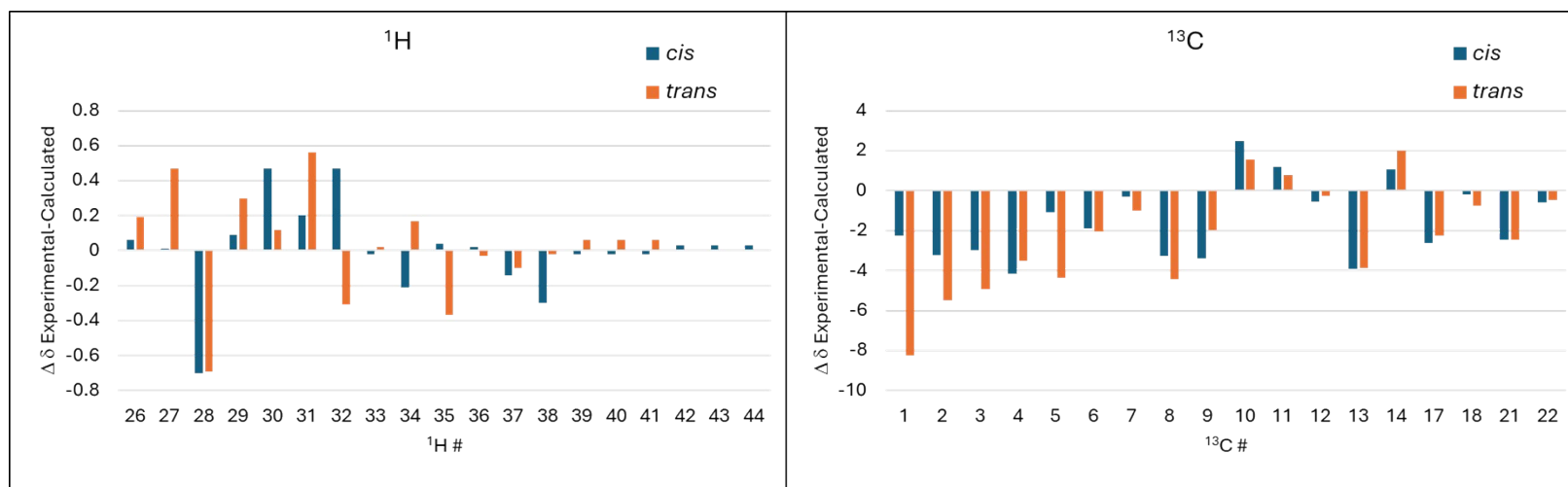


Figure S9. $\Delta \delta$ for ^1H and ^{13}C experimental-calculated of **1**.

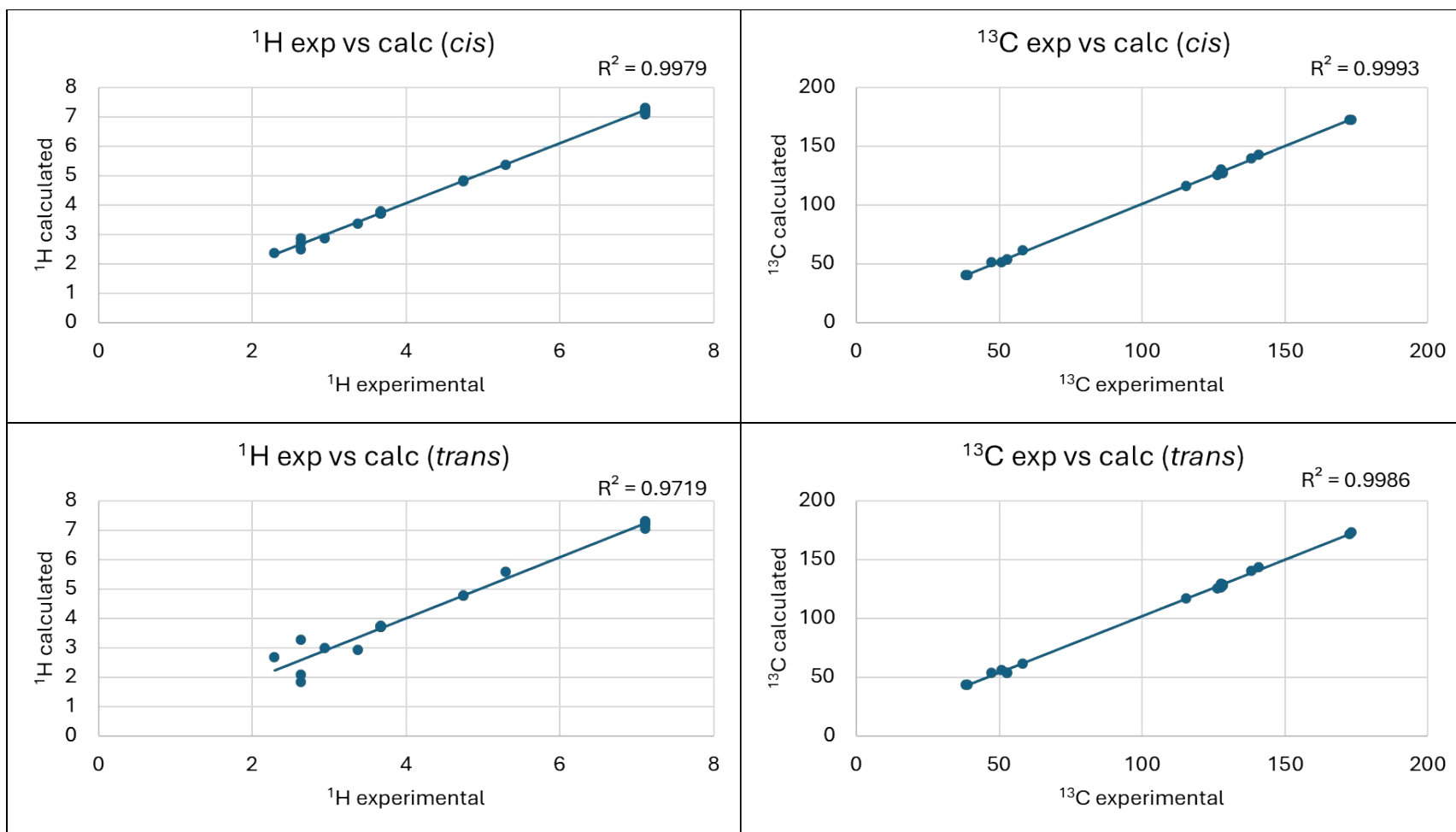


Figure S10. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **2**.

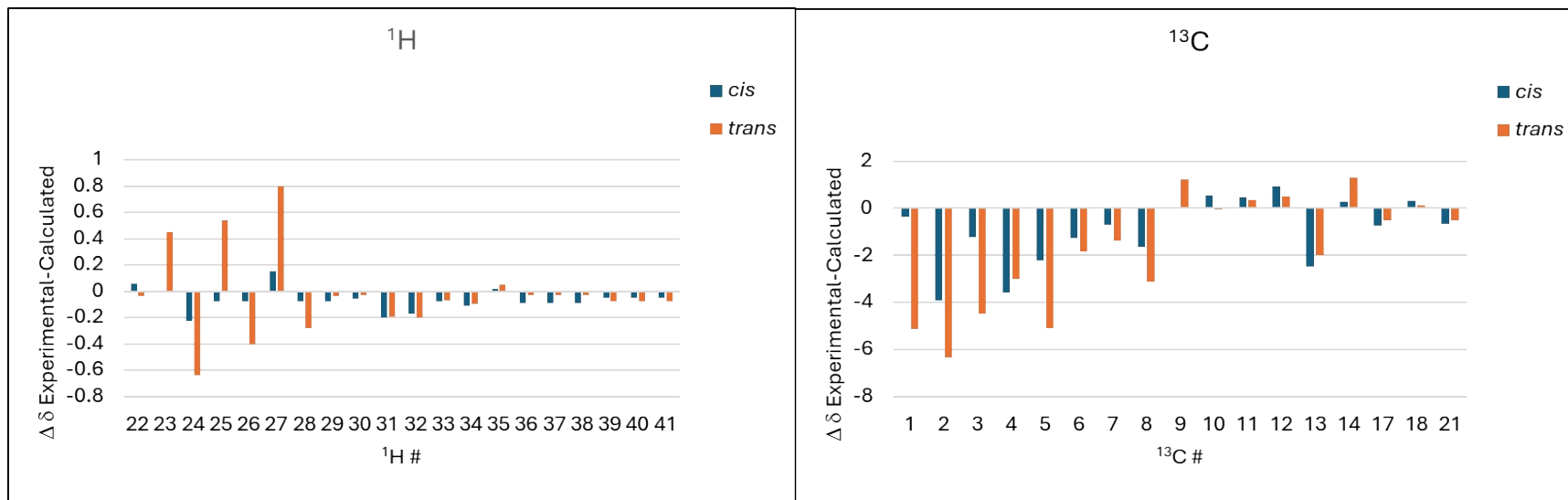


Figure S11. $\Delta\delta$ for ^1H and ^{13}C experimental-calculated of **2**.

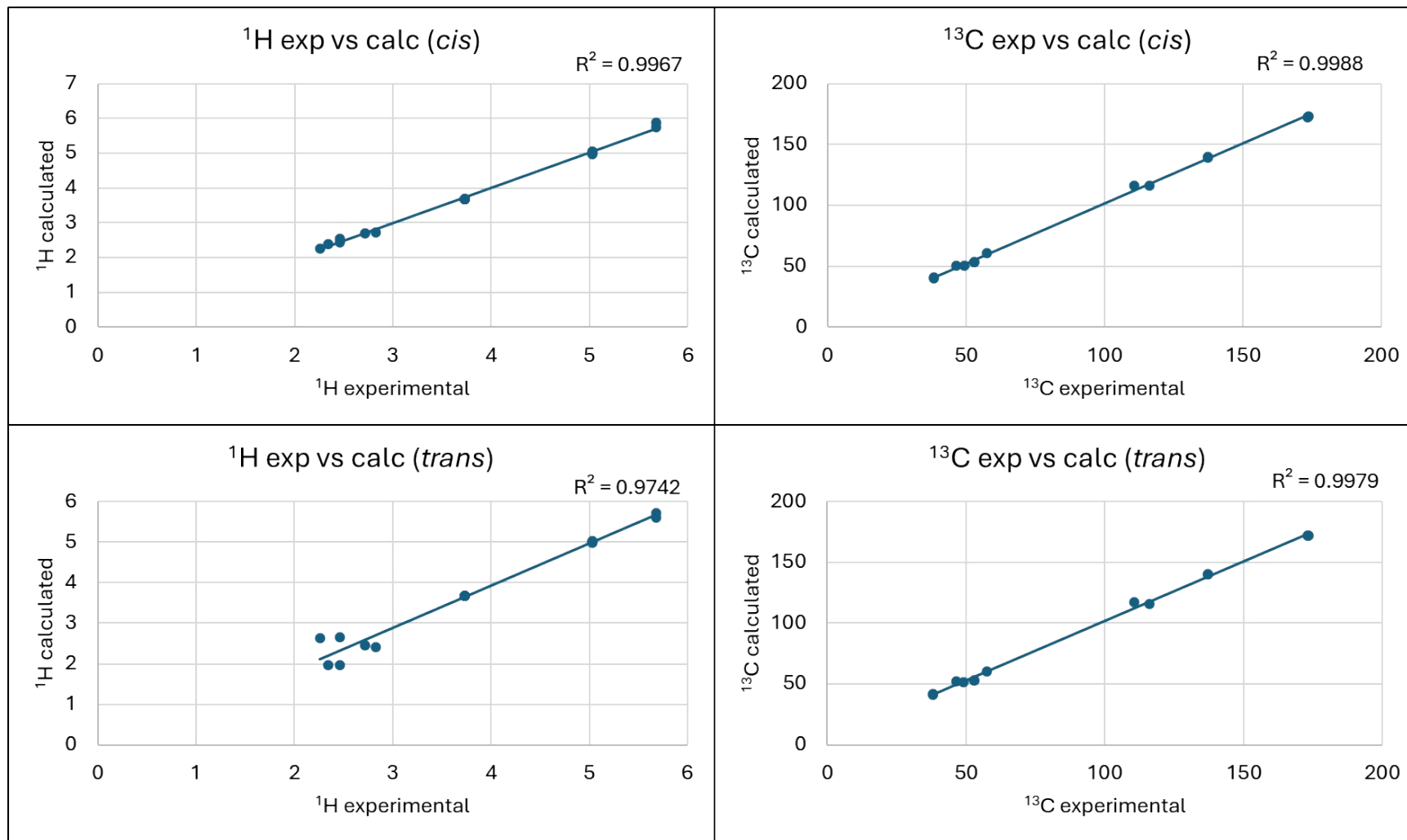


Figure S12. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **3**.

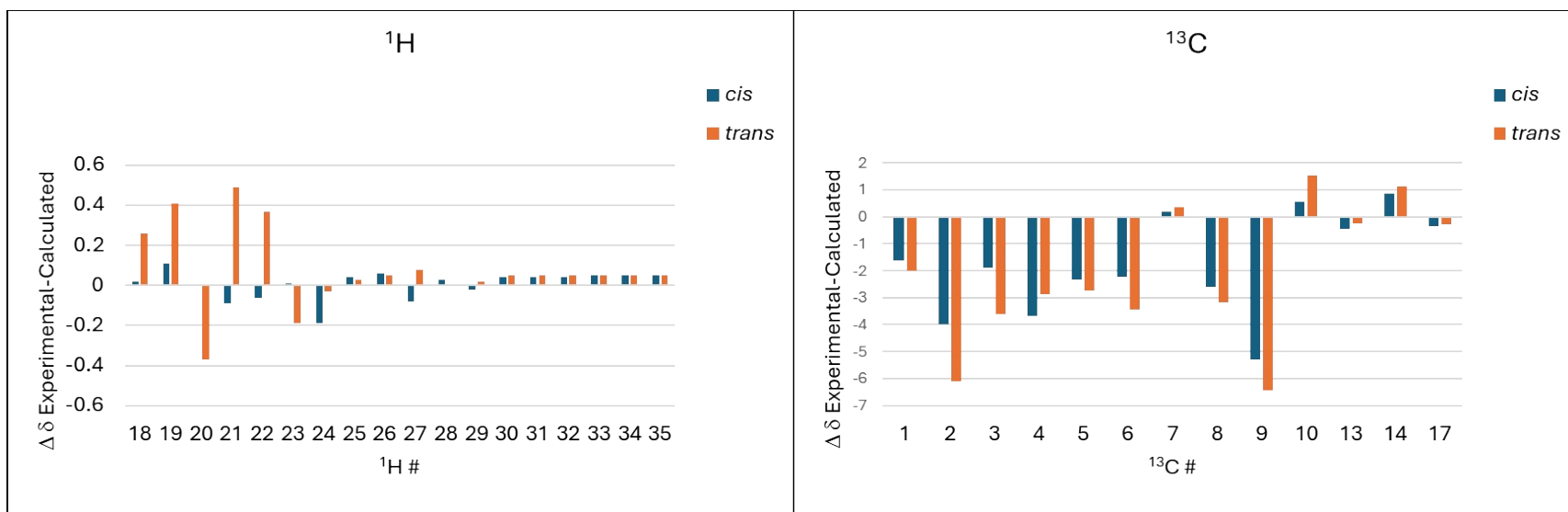


Figure S13. $\Delta\delta$ for ^1H and ^{13}C experimental-calculated of **3**.

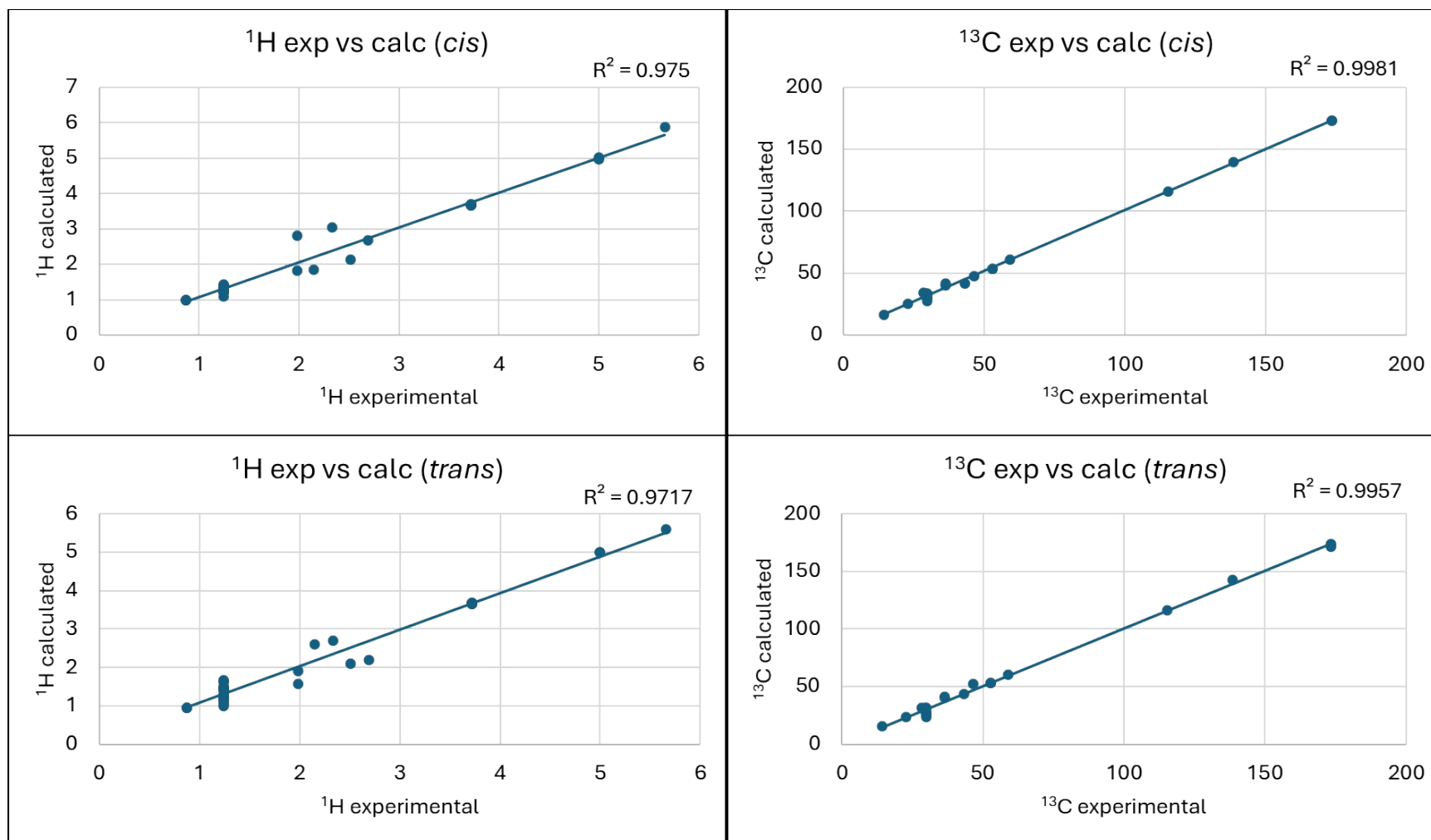


Figure S14. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **4**.

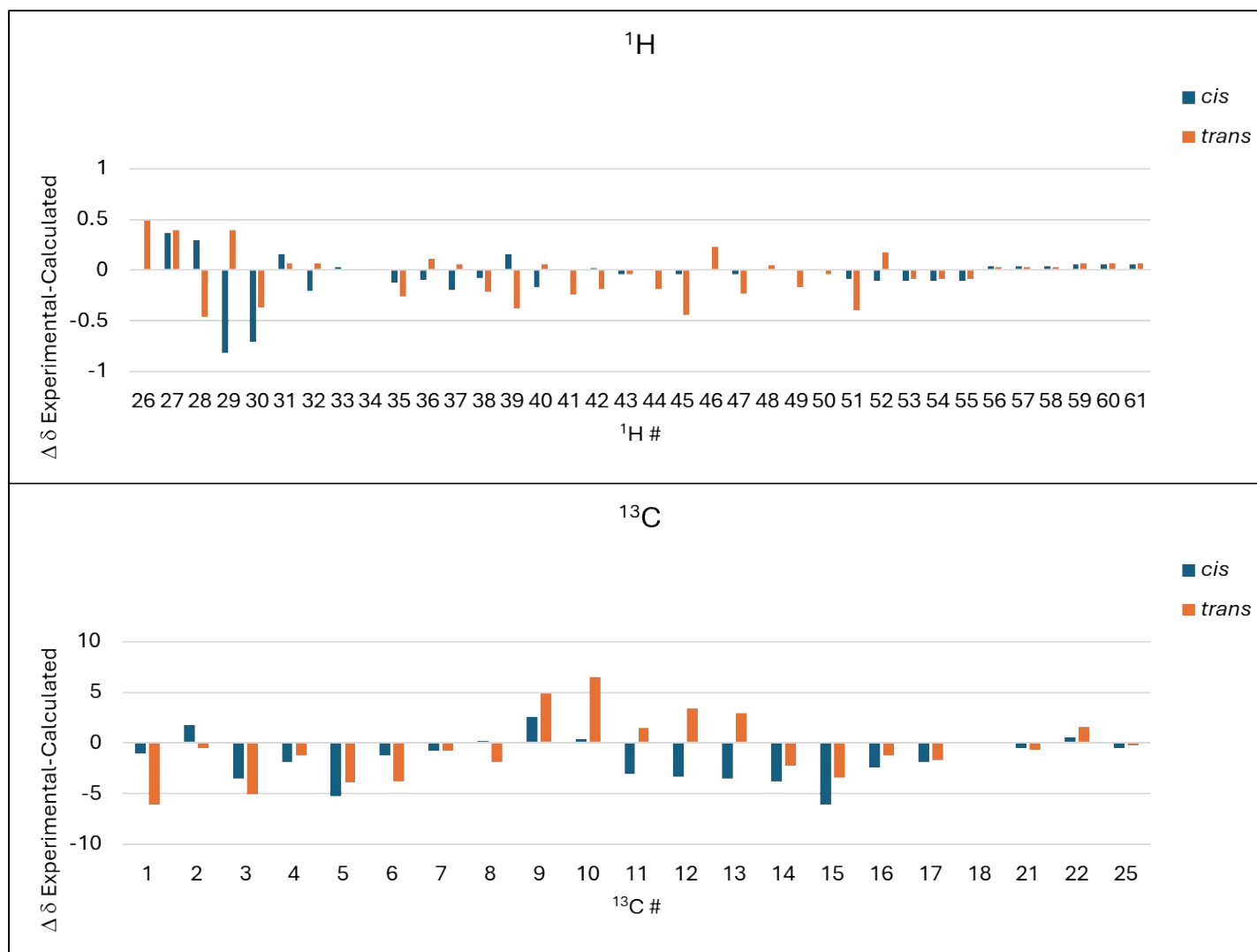


Figure S15. $\Delta\delta$ for ^1H and ^{13}C experimental-calculated of **4**.

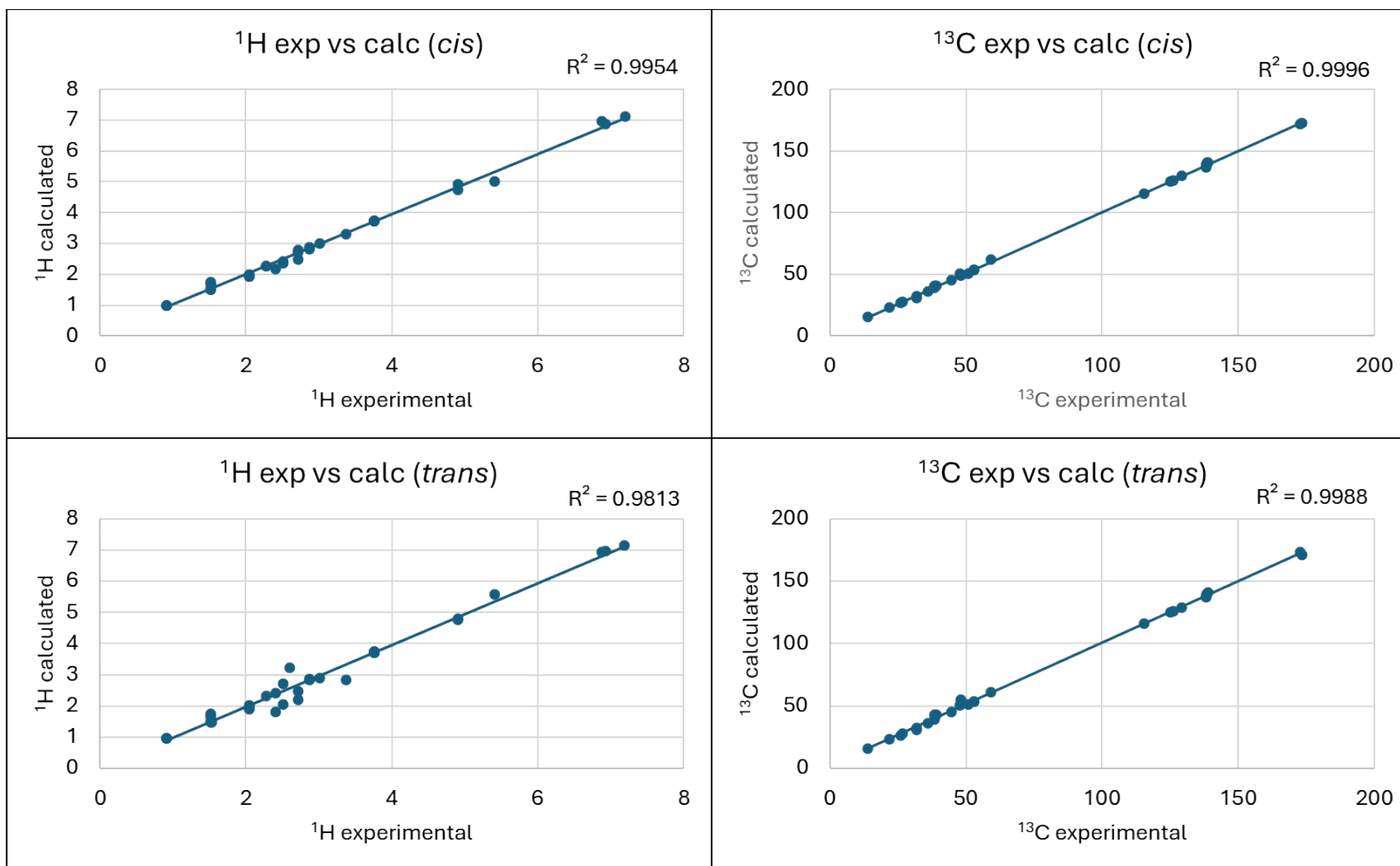


Figure S16. ¹H and ¹³C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **5**.

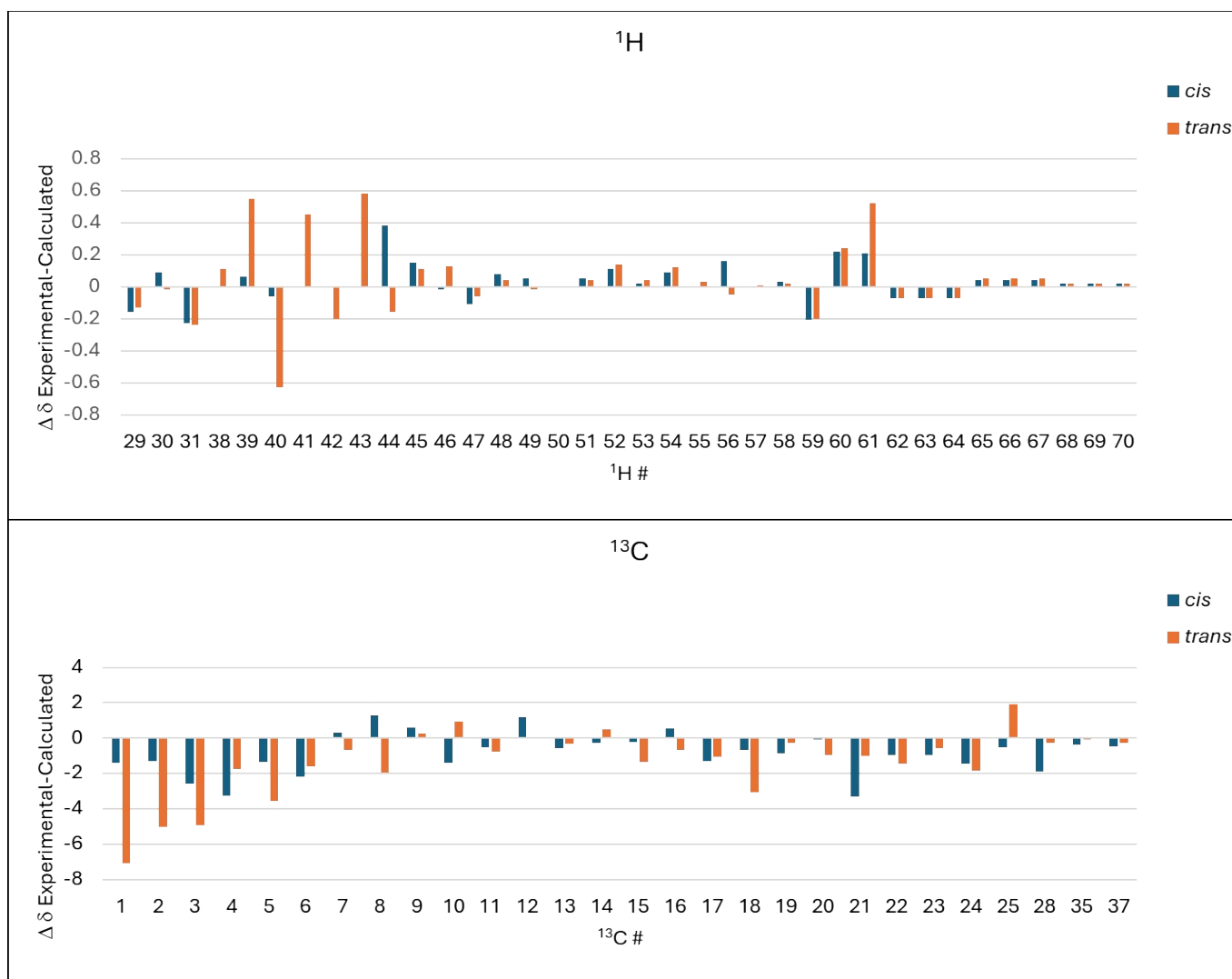


Figure S17. $\Delta \delta$ for ¹H and ¹³C experimental-calculated of **5**.

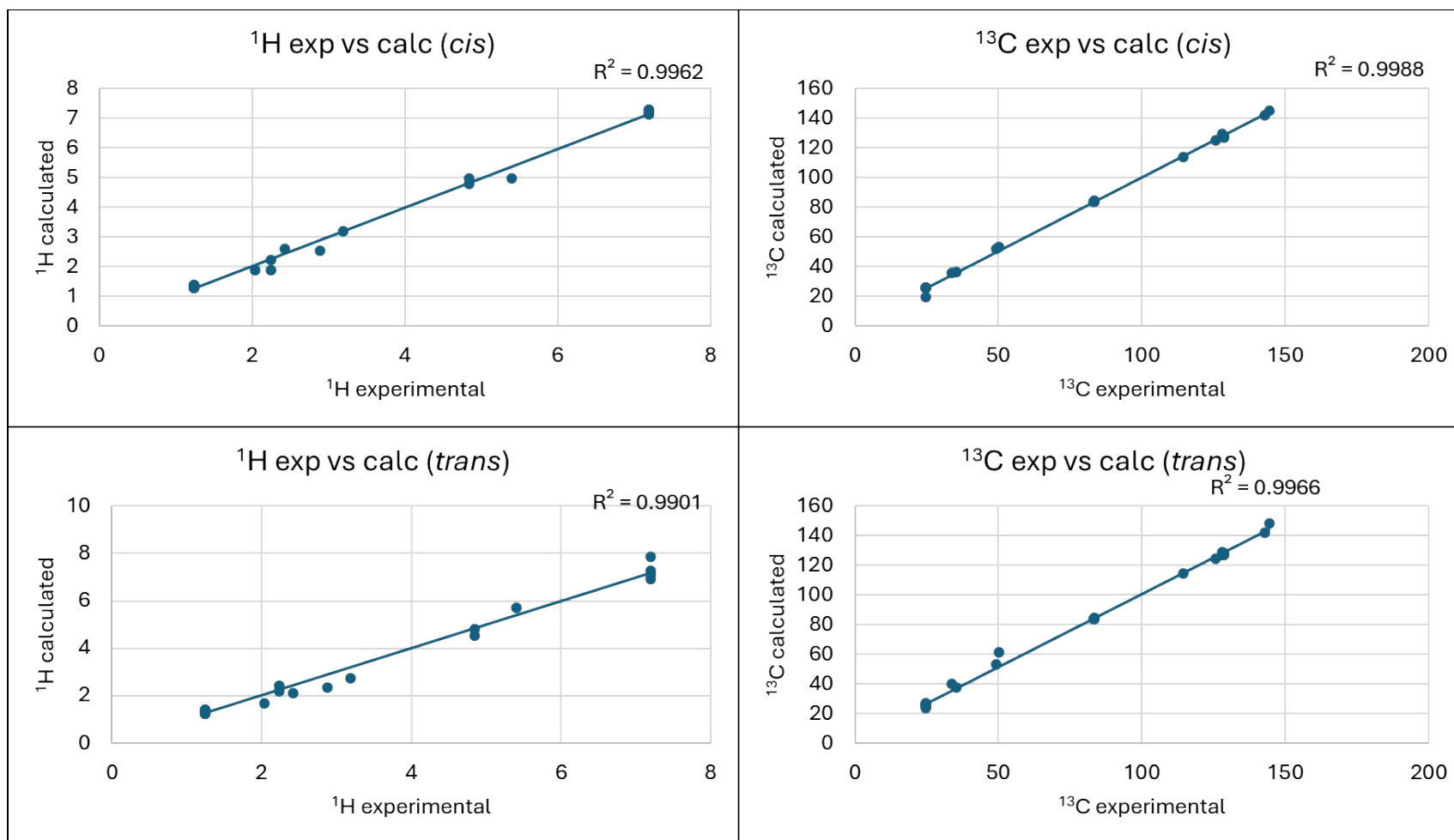


Figure S18. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **6**.

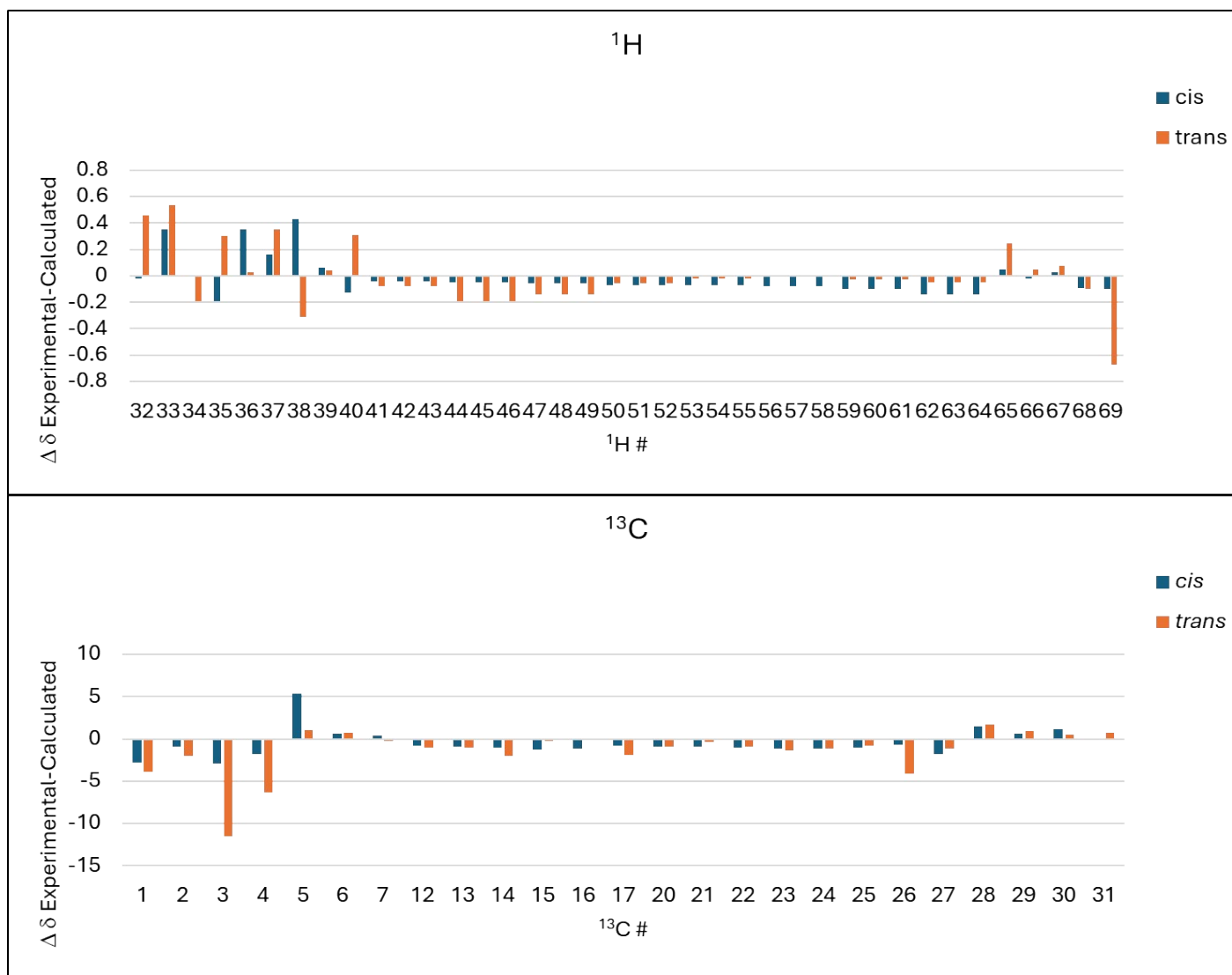


Figure S19. $\Delta \delta$ for ¹H and ¹³C experimental-calculated of **6**.

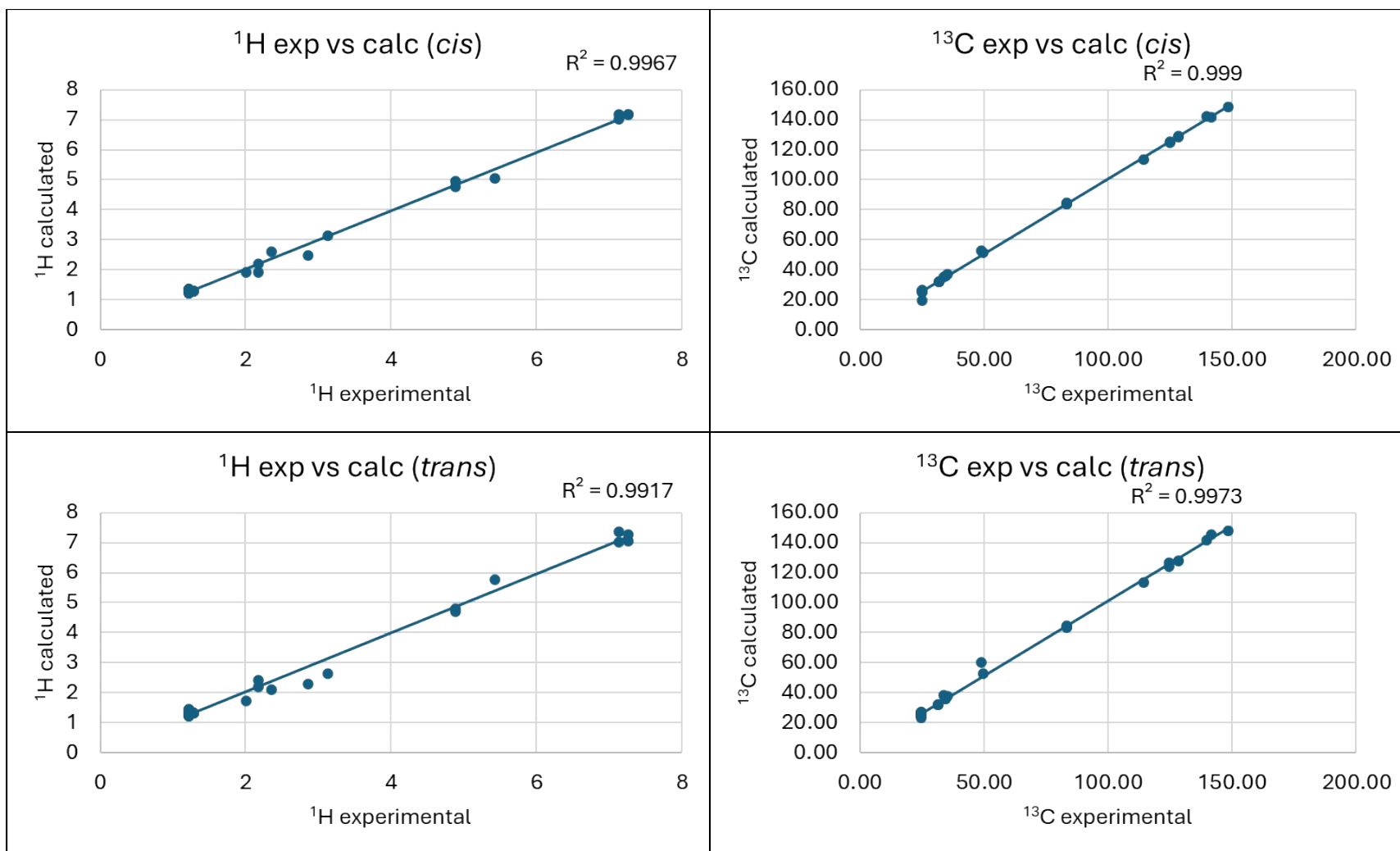


Figure S20. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **7**.

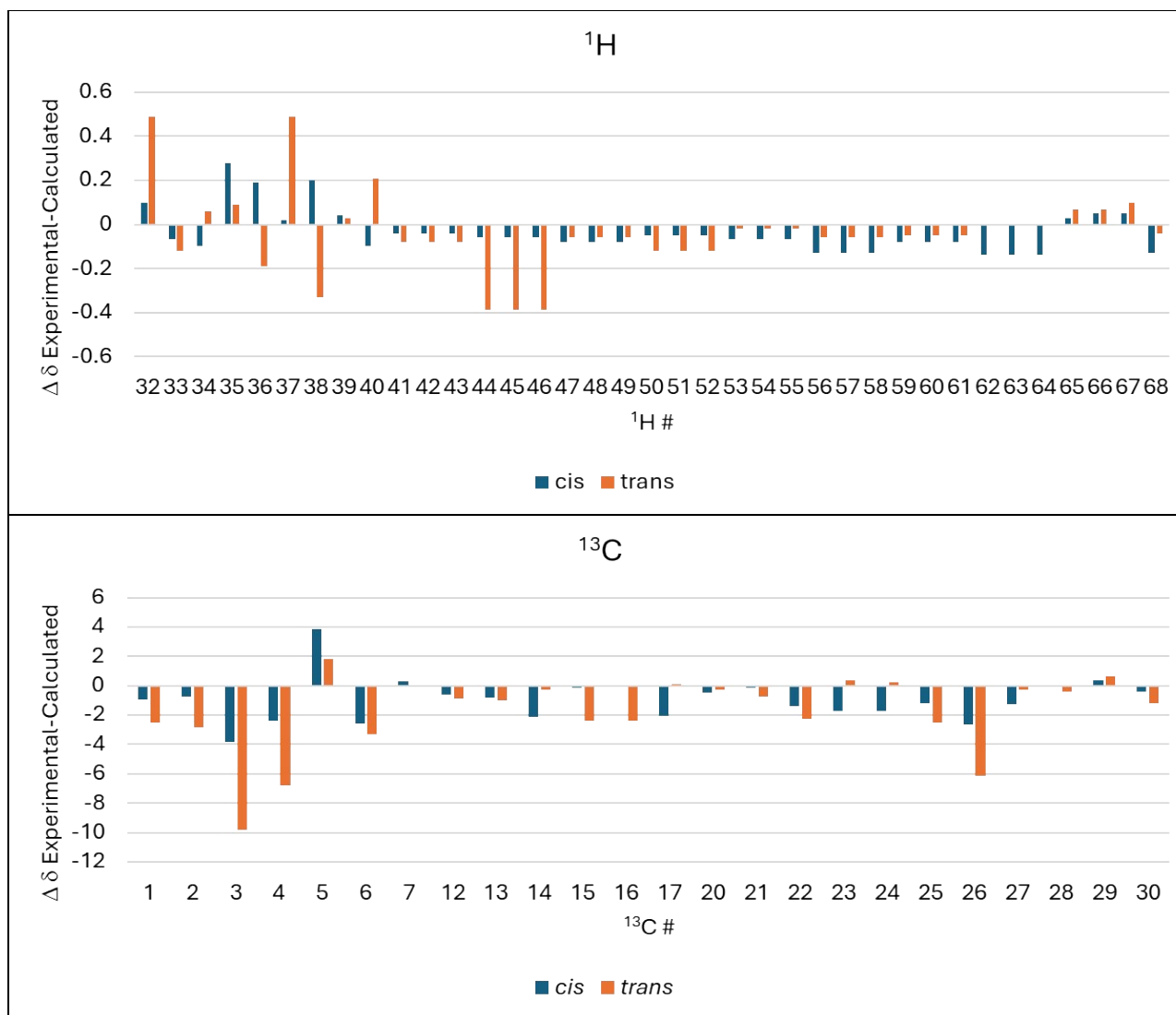


Figure S21. $\Delta \delta$ for ¹H and ¹³C experimental-calculated of 7.

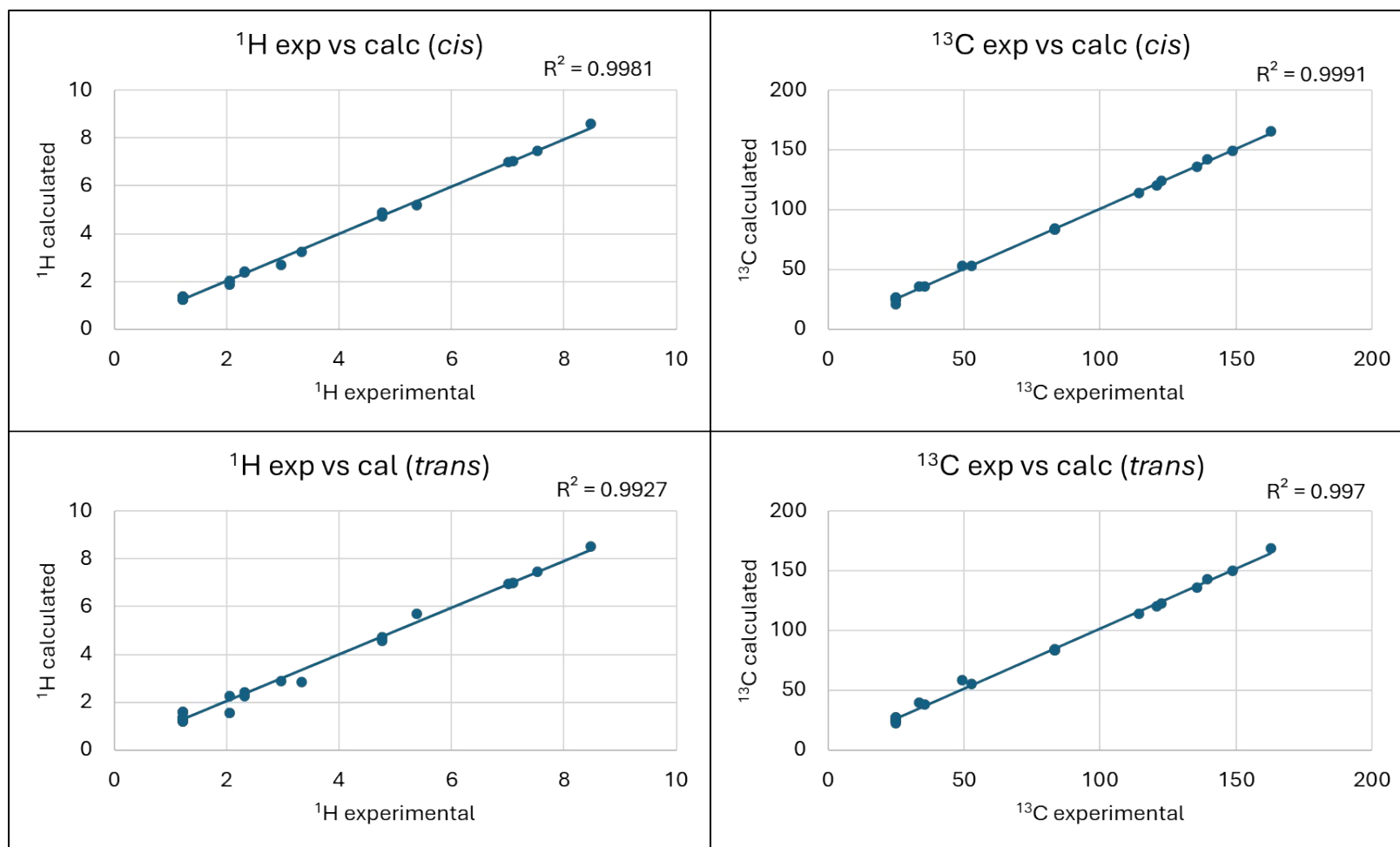


Figure S22. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **8**.

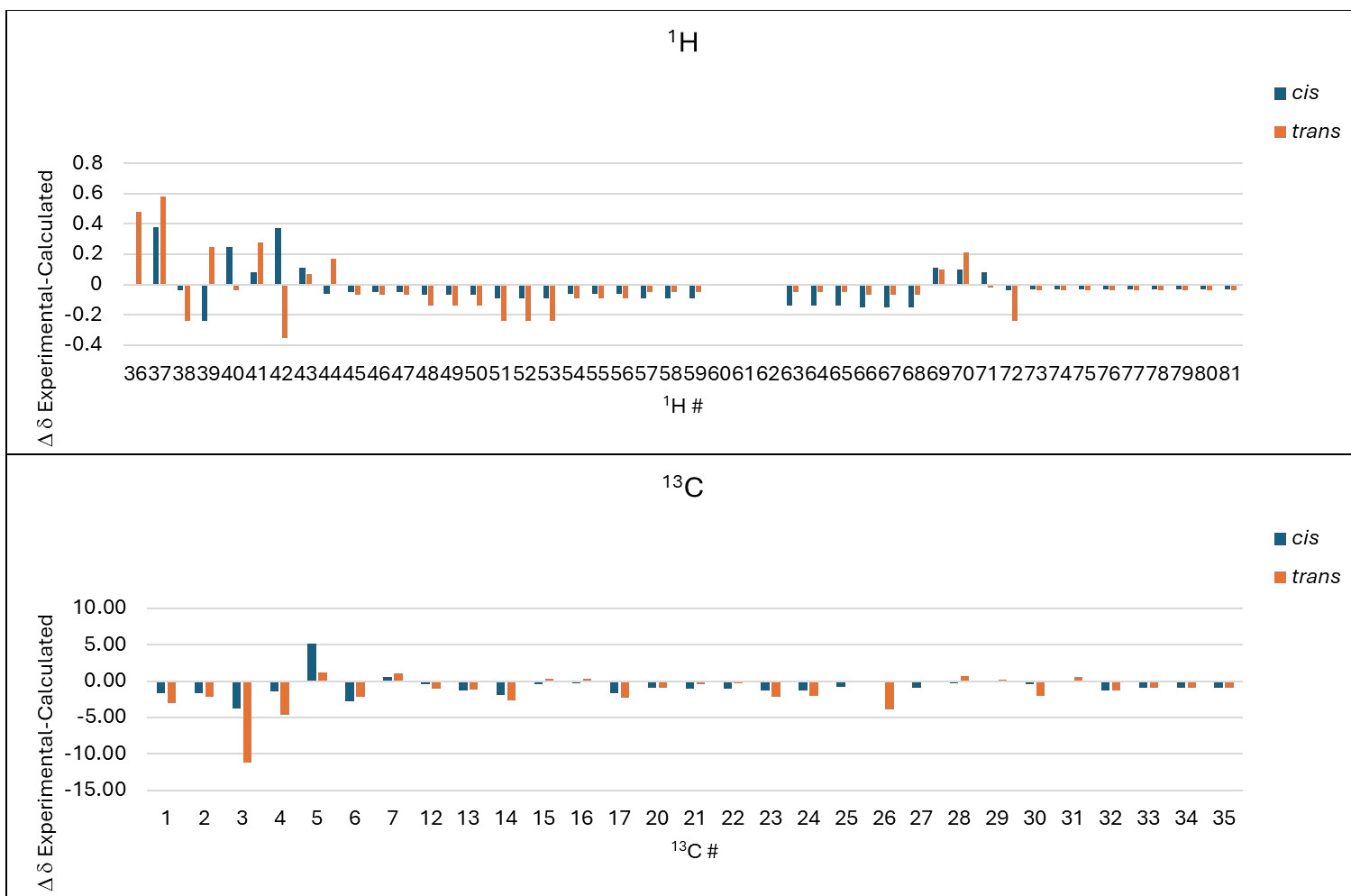


Figure S23. $\Delta \delta$ for ¹H and ¹³C experimental-calculated of **8**.

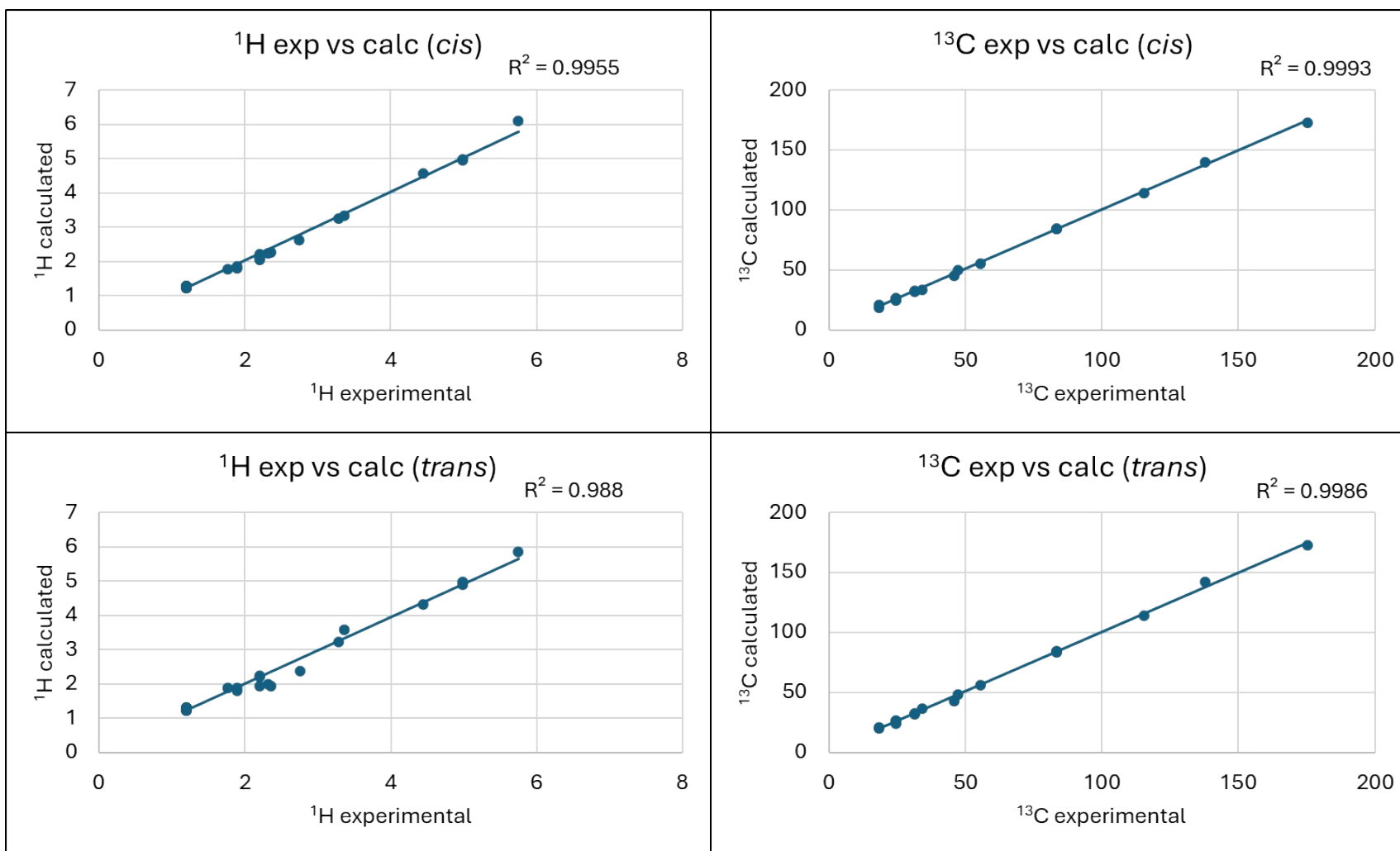


Figure S24. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **9**.

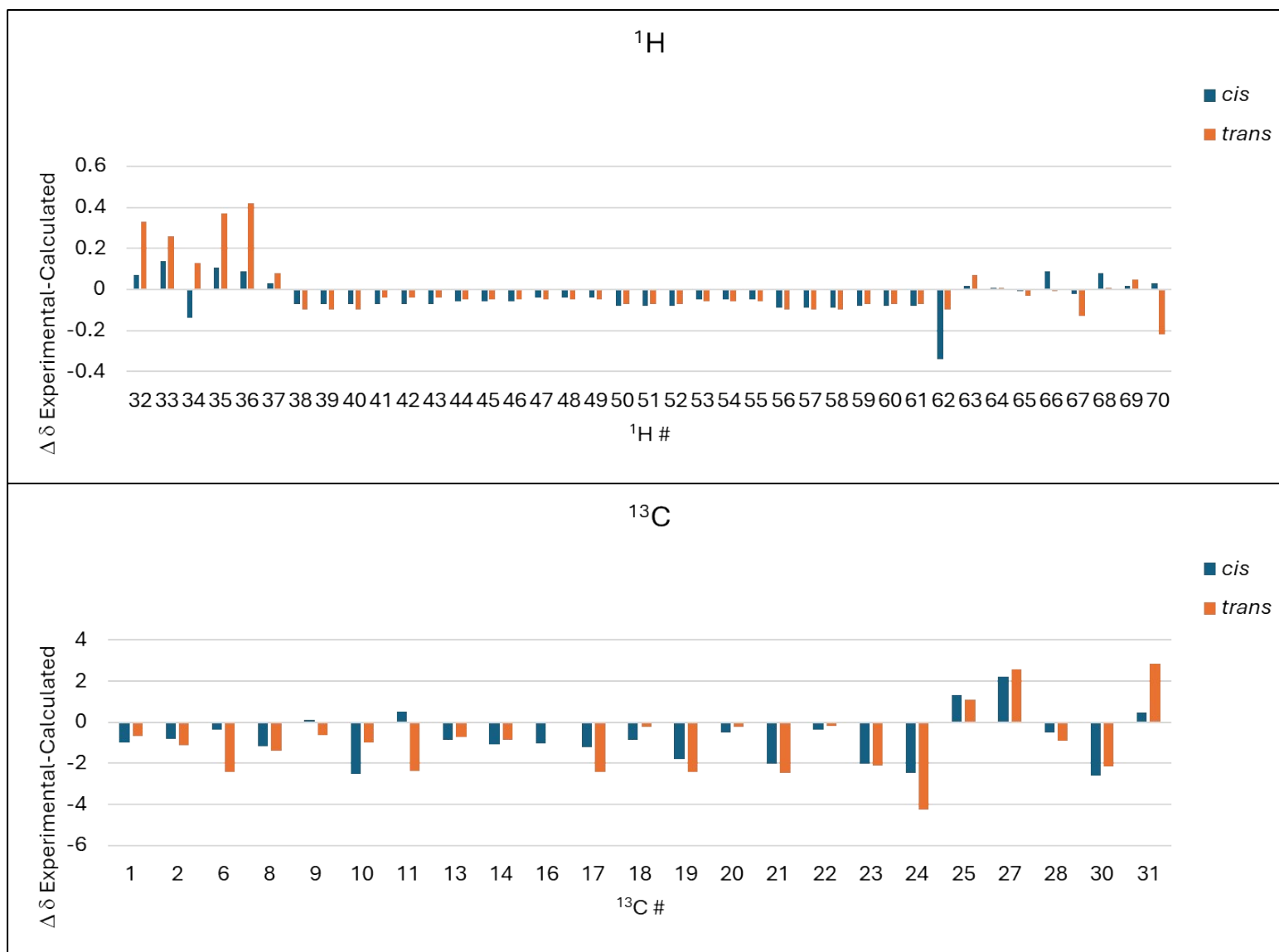


Figure S25. $\Delta \delta$ for ^1H and ^{13}C experimental-calculated of **9**.

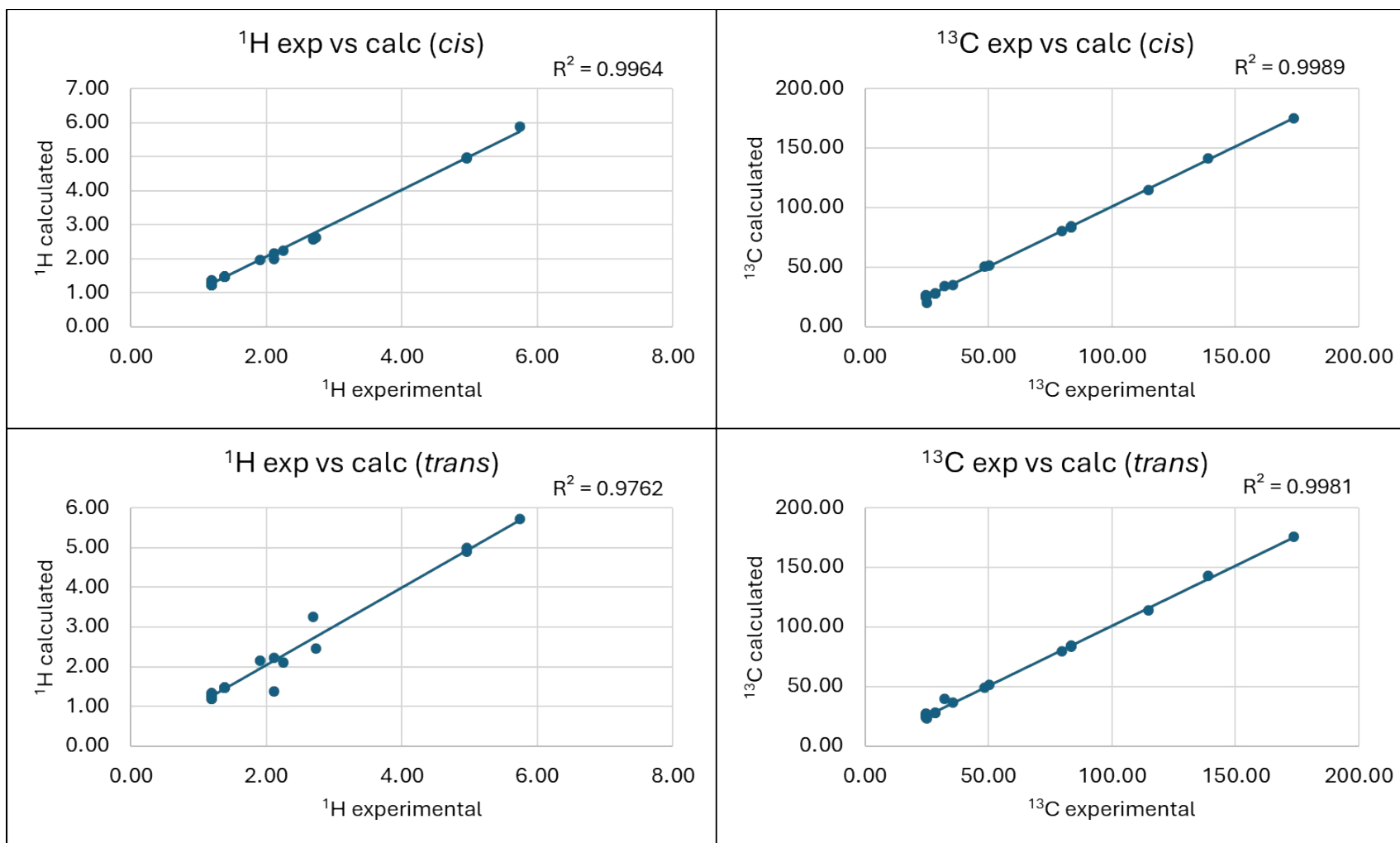


Figure S26. ^1H and ^{13}C experimental vs. calculated chemical shift plots for the *cis* and *trans* configurations of **10**.

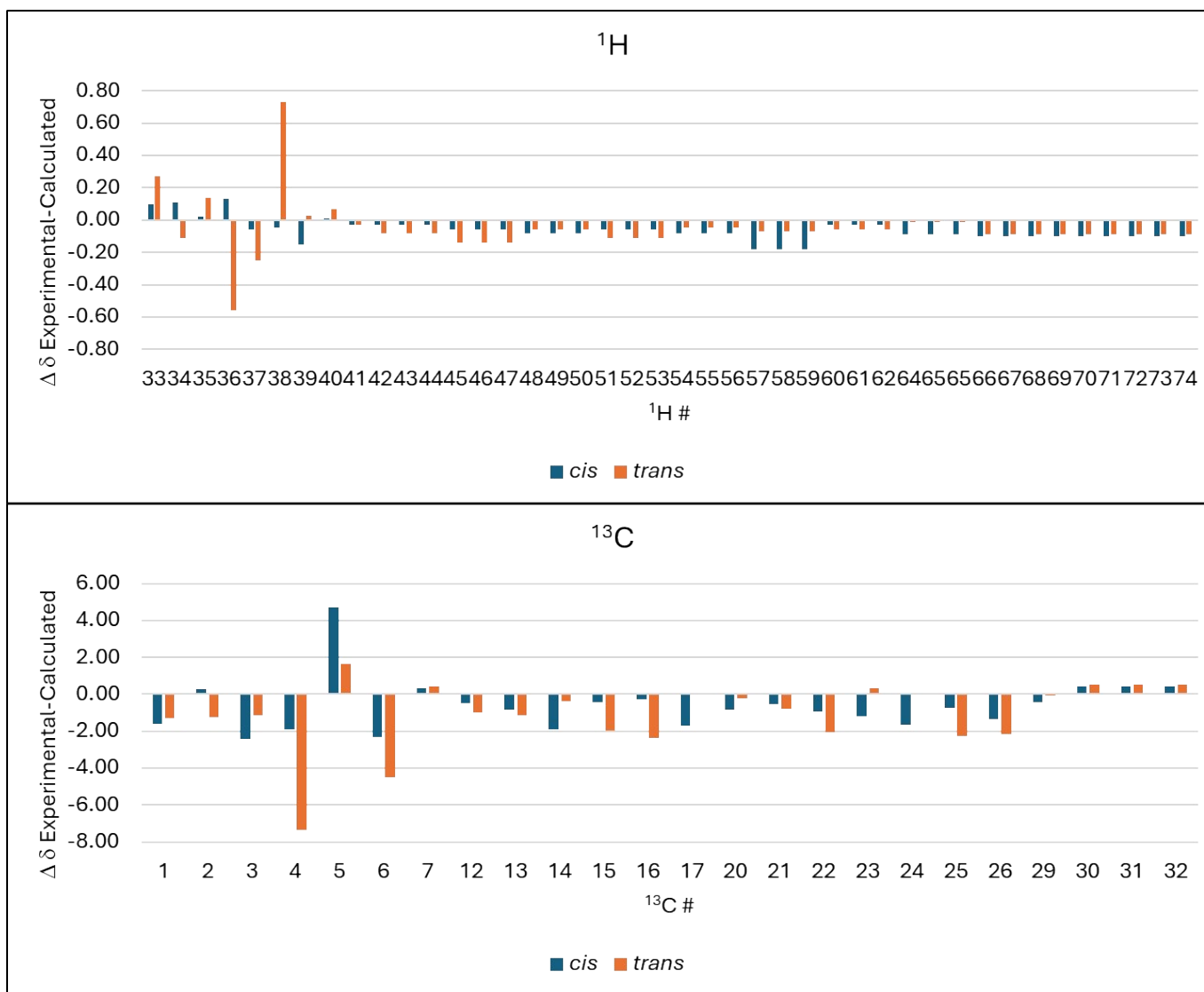


Figure S27. $\Delta \delta$ for ¹H and ¹³C experimental-calculated of **10**.

Table S1. ¹H RMSD and MAE values for 1-10.

Compound #	RMSD <i>cis</i>	RMSD <i>trans</i>	MAE <i>cis</i>	MAE <i>trans</i>
1	0.25	0.27	0.15	0.19
2	0.07	0.31	0.09	0.21
3	0.07	0.21	0.05	0.14
4	0.22	0.23	0.12	0.18
5	0.12	1.42	0.08	1.14
6	0.14	0.21	0.10	0.14
7	0.10	0.19	0.09	0.13
8	0.12	0.17	0.09	0.12
9	0.09	0.14	0.07	0.10
10	0.09	0.17	0.08	0.11

Table S2. ¹³C RMSD and MAE values for 1-10.

Compound #	RMSD <i>cis</i>	RMSD <i>trans</i>	MAE <i>cis</i>	MAE <i>trans</i>
1	2.43	3.47	2.09	2.79
2	1.69	2.93	1.26	2.18
3	2.52	3.25	2.01	2.61
4	2.69	3.17	2.12	2.56
5	0.23	2.31	0.15	1.58
6	1.68	3.06	1.32	1.88
7	1.73	3.14	1.34	2.06
8	1.61	2.73	1.20	1.74
9	1.43	1.86	1.21	1.53
10	1.54	2.14	1.18	1.42

Cartesian Coordinates

In xyz format (unit: Ångstrom)

Structure 1

Eopt = -3869.682378 a.u.

45 atoms

Br	2.785156	3.222085	-0.967006
C	1.734219	2.021082	0.256953
C	0.646356	1.347068	-0.481351
C	-0.647965	1.574219	-0.227720
C	-1.769654	0.869294	-0.928876
C	-2.603514	-0.037840	0.016154
C	-3.236399	0.810256	1.127762
O	-4.099311	1.698207	0.612392
C	-4.768165	2.573900	1.551062
O	-2.984653	0.717575	2.313144
C	-3.740629	-0.686637	-0.784386
O	-4.583486	-1.338917	0.029733
C	-5.695429	-2.021083	-0.597596
O	-3.859467	-0.645948	-1.993290
C	-1.719952	-1.146203	0.662511
C	-1.043222	-2.006930	-0.350732
H	1.374102	2.674095	1.050488
H	2.488629	1.337618	0.639547
H	0.936625	0.624370	-1.240304
H	-0.913134	2.305164	0.537247
H	-1.373149	0.242505	-1.730983
H	-2.443454	1.601310	-1.384935
H	-5.405609	3.214405	0.942856
H	-4.035716	3.171791	2.097367
H	-5.369536	1.987774	2.249432

H	-5.328750	-2.780091	-1.291831
H	-6.327887	-1.303953	-1.125316
H	-6.245480	-2.486007	0.219576
H	-2.365188	-1.757413	1.305296
H	-1.003837	-0.651075	1.317823
H	-1.673783	-2.490731	-1.094176
C	0.346909	-2.239561	-0.462158
C	0.842997	-3.023914	-1.546131
C	1.304746	-1.719428	0.457858
C	2.201289	-3.251869	-1.715150
H	0.131698	-3.436766	-2.255825
C	2.657796	-1.965265	0.275873
H	0.978886	-1.126491	1.301576
C	3.129228	-2.723556	-0.810090
H	2.549682	-3.844452	-2.555405
H	4.191561	-2.899186	-0.941585
C	3.664166	-1.397724	1.232522
F	3.106988	-0.827658	2.328979
F	4.533787	-2.343801	1.690353
F	4.442843	-0.434987	0.652836

TS1-cis

Eopt = -3869.667448

45 atoms

C	0.407579	-0.383573	1.434237
C	0.765733	1.111973	-0.102061
C	1.779183	0.290698	-0.859115
C	1.398755	-1.386067	0.913420
H	0.768159	0.227455	2.255925
H	0.918990	-2.111632	0.252317

H	2.496896	0.937869	-1.372805
H	1.267030	-0.304967	-1.617763
H	1.149761	1.798793	0.651642
C	-0.458033	1.426510	-0.668465
C	-1.400064	2.339450	-0.035572
H	-0.788154	0.900159	-1.561219
H	-2.441093	2.034224	-0.108925
H	-1.136166	2.619473	0.981018
C	2.510188	-0.668341	0.104844
H	1.846714	-1.941097	1.744925
C	3.445389	0.113638	1.039877
O	3.368795	0.141673	2.252780
O	4.371161	0.778054	0.334424
C	5.336837	1.544729	1.091981
H	5.988856	2.001742	0.348543
H	4.831355	2.313402	1.680488
H	5.908904	0.885590	1.748728
C	3.376387	-1.727553	-0.577222
O	4.202118	-2.392127	0.025383
O	3.099854	-1.880713	-1.875115
C	3.834819	-2.916536	-2.572514
H	3.632035	-3.890472	-2.122161
H	3.469289	-2.885729	-3.598109
H	4.905490	-2.704216	-2.540795
C	-1.024973	-0.626707	1.464115
C	-1.675532	-1.441563	0.516447
C	-1.826237	0.081107	2.385790
C	-3.066199	-1.537062	0.505654
H	-1.098605	-1.975707	-0.228990
C	-3.214780	-0.027616	2.373966

H	-1.342103	0.724270	3.115185
C	-3.850916	-0.840339	1.433523
Br	-1.445674	4.162785	-1.007831
H	-4.931793	-0.923656	1.417402
H	-3.807549	0.527377	3.094493
C	-3.730569	-2.438971	-0.491249
F	-4.971058	-2.010059	-0.844738
F	-3.022566	-2.567260	-1.644373
F	-3.897514	-3.710248	-0.012170

TS1-trans

Eopt = -3869.665423

45 atoms

C	-0.654837	-0.992126	0.016565
C	-0.638233	1.153940	-0.375413
C	-2.138558	1.353215	-0.266692
C	-2.019974	-1.120855	-0.588780
H	-0.629117	-0.972824	1.105908
H	-2.464174	-2.099015	-0.369921
H	-2.491718	1.776927	-1.212314
H	-2.380743	2.060516	0.527551
H	-0.268372	0.965242	-1.383679
C	0.257654	1.711990	0.513368
C	1.692350	1.742897	0.241683
H	-0.086587	2.083930	1.475577
H	2.322801	1.477956	1.087517
H	1.988202	1.212536	-0.659457
H	-1.986869	-1.010109	-1.673625
C	-2.891402	0.014029	-0.005232
C	-4.292917	0.115777	-0.601742
O	-5.202206	0.720617	-0.059547

O	-4.396795	-0.474885	-1.795516
C	-5.674987	-0.353325	-2.466882
H	-5.558086	-0.894481	-3.405005
H	-6.463427	-0.803579	-1.860386
H	-5.901692	0.697970	-2.656430
C	-3.079155	-0.200918	1.507394
O	-2.743156	0.575816	2.379440
O	-3.659271	-1.385114	1.745981
C	-3.901265	-1.719942	3.132844
H	-4.372615	-2.701840	3.114251
H	-2.957653	-1.759656	3.681292
H	-4.568355	-0.984219	3.587287
Br	2.318380	3.676359	-0.118482
C	0.567911	-1.472281	-0.582892
C	1.731889	-1.511263	0.216740
C	0.694254	-1.806604	-1.951384
C	2.960041	-1.869757	-0.332337
H	1.657802	-1.253664	1.268052
C	1.927443	-2.167256	-2.487452
H	-0.176456	-1.781918	-2.597784
C	3.075379	-2.197009	-1.689067
H	2.001734	-2.424878	-3.539437
H	4.034427	-2.470473	-2.113952
C	4.180616	-1.822684	0.536406
F	5.181738	-2.625119	0.091781
F	4.711828	-0.563295	0.610082
F	3.927740	-2.192633	1.821005

Structure 2

Eopt = -3532.610973

42 atoms

Br	-5.130343	0.362991	0.328396
C	-4.355608	-1.452681	-0.132833
C	-3.130145	-1.293511	-0.944500
C	-1.908563	-1.573111	-0.477436
C	-0.653840	-1.413893	-1.280047
C	0.347810	-0.367469	-0.707306
C	-0.391582	0.963202	-0.560664
O	-1.079030	1.022310	0.586835
C	-1.926816	2.175017	0.758357
O	-0.420752	1.827068	-1.414420
C	0.919183	-0.856823	0.623029
O	1.500746	0.137818	1.304007
C	2.205334	-0.237746	2.502761
O	0.911543	-2.016123	0.990191
C	1.519582	-0.217182	-1.738358
C	2.597777	0.739371	-1.356840
H	-5.175485	-1.939663	-0.659443
H	-4.177465	-1.926951	0.830984
H	-3.258765	-0.922667	-1.960403
H	-1.795533	-1.925992	0.546209
H	-0.901354	-1.114809	-2.303522
H	-0.113347	-2.365830	-1.327984
H	-2.407977	2.039580	1.726278
H	-2.678786	2.213497	-0.031201
H	-1.327398	3.088752	0.752434
H	1.513505	-0.662409	3.234632
H	2.641689	0.685669	2.883519
H	2.990732	-0.960410	2.270819
H	1.050262	0.121735	-2.667583

H	1.914908	-1.220982	-1.920253
H	2.392187	1.795364	-1.508440
C	3.828966	0.398951	-0.748267
C	4.202070	-0.939279	-0.428520
C	4.751280	1.430307	-0.403661
C	5.411099	-1.214517	0.196141
H	3.530312	-1.758092	-0.663589
C	5.956082	1.143549	0.219179
H	4.488806	2.459690	-0.635054
C	6.298798	-0.181388	0.526519
H	5.668188	-2.243946	0.431851
H	6.636845	1.952130	0.472298
H	7.242042	-0.404709	1.016351

TS2-cis

Eopt = -3532.601385

42 atoms

C	-0.306641	1.174420	0.514617
C	0.285886	-0.899865	0.193729
C	-1.026535	-1.356642	-0.400429
C	-1.541846	1.053575	-0.328529
H	-0.466137	1.071979	1.587006
H	-1.305330	1.146005	-1.389342
H	-1.298430	-2.343521	-0.015591
H	-0.924105	-1.432387	-1.487399
H	0.404490	-1.017248	1.268241
C	1.434251	-0.873426	-0.574504
C	2.743042	-0.572474	-0.004685
H	1.363219	-0.959522	-1.656663
H	3.338840	0.124182	-0.590259
H	2.714255	-0.285847	1.043039

C	-2.157589	-0.342741	-0.091733
H	-2.263463	1.841664	-0.082203
C	-2.624543	-0.484200	1.364567
O	-2.236194	-1.328198	2.148673
O	-3.519511	0.464892	1.671276
C	-4.053177	0.441530	3.015813
H	-3.249091	0.570918	3.743488
H	-4.748894	1.278391	3.064491
H	-4.574947	-0.500633	3.197835
C	-3.362949	-0.668300	-0.970771
O	-4.166290	-1.545007	-0.701121
O	-3.409150	0.067494	-2.085422
C	-4.478763	-0.235309	-3.014310
H	-5.448105	-0.083078	-2.535176
H	-4.346876	0.462637	-3.840160
H	-4.391972	-1.265714	-3.365543
C	0.817084	2.026502	0.175451
C	1.695729	2.447616	1.198795
C	1.144681	2.366781	-1.155884
C	2.844890	3.180180	0.908967
H	1.465377	2.186619	2.228655
C	2.295236	3.099204	-1.443855
H	0.506180	2.041133	-1.970296
C	3.152741	3.510672	-0.416227
H	3.503693	3.490679	1.715153
Br	3.960597	-2.235001	0.003249
H	4.050743	4.076530	-0.646091
H	2.529821	3.343670	-2.476214

TS2-trans

Eopt = -3532.599870

42 atoms

C	-0.142908	1.323544	-0.689675
C	0.355519	-0.717591	-0.050311
C	-1.038755	-1.186929	-0.368923
C	-1.392900	1.285646	0.132254
H	-0.267063	1.085456	-1.743247
H	-2.084631	2.082422	-0.161858
H	-1.273088	-2.092773	0.197330
H	-1.090371	-1.444961	-1.430842
H	0.525627	-0.361857	0.965546
C	1.459560	-1.108650	-0.769835
C	2.812809	-0.772225	-0.343218
H	1.337238	-1.597756	-1.734295
H	3.472452	-0.446485	-1.143430
H	2.859033	-0.101951	0.511413
H	-1.157341	1.439248	1.188228
C	-2.099857	-0.093761	-0.031344
C	-2.832361	-0.405412	1.276140
O	-2.536099	-1.282059	2.064867
O	-3.836123	0.464219	1.466055
C	-4.596904	0.321929	2.689011
H	-3.948005	0.464759	3.555859
H	-5.355628	1.102659	2.648756
H	-5.065123	-0.663894	2.729322
C	-3.124103	-0.058201	-1.166909
O	-3.234196	0.828092	-1.991846
O	-3.867800	-1.174924	-1.163011
C	-4.850492	-1.305303	-2.217570
H	-4.358293	-1.314764	-3.192559
H	-5.347219	-2.257054	-2.032530

H	-5.568462	-0.483885	-2.167910
Br	3.828044	-2.452682	0.320094
C	1.020745	2.115821	-0.375421
C	2.026965	2.270257	-1.360972
C	1.264152	2.665262	0.905973
C	3.213896	2.941911	-1.081500
H	1.862003	1.849172	-2.349095
C	2.453570	3.336547	1.180554
H	0.522696	2.560284	1.691136
C	3.437357	3.478305	0.192835
H	3.969029	3.045711	-1.855826
H	2.617963	3.749540	2.171989
H	4.363608	4.000460	0.413658

Structure 4

Eopt = -1665.054984

59 atoms

C	2.061108	-1.658431	-1.058046
C	2.656071	-0.357465	-0.409525
C	2.455006	0.929100	-1.270305
C	1.155714	1.037936	-2.014219
C	0.615528	-1.901072	-0.760956
H	2.243473	-1.607201	-2.135400
H	2.652683	-2.495351	-0.669097
H	2.637294	1.799363	-0.638351
H	3.246136	0.919261	-2.031396
H	1.000696	0.290948	-2.787208
C	1.888059	-1.129946	3.151736
O	2.407521	-1.167289	1.797189
O	1.297579	0.725713	1.315663

C	6.093015	0.410140	0.818289
O	4.864244	-1.315148	-0.837875
O	4.658733	0.408781	0.601759
C	0.230965	2.001340	-1.918607
H	-0.607639	1.979455	-2.612002
C	0.250313	3.148564	-0.955179
H	0.592875	4.075865	-1.429727
C	-0.512212	-1.762208	-1.726176
H	0.364706	-2.187856	0.258655
H	0.870110	2.972123	-0.075813
S	-1.446917	3.648111	-0.399278
C	-2.079827	2.157007	0.233008
C	-3.590931	0.664116	0.945906
C	-2.306467	0.130549	1.146606
N	-3.399887	1.917854	0.368357
N	-1.404557	1.092889	0.692984
H	-4.137686	2.546050	0.065564
H	-0.383076	1.020003	0.769899
C	-2.116655	-1.134163	1.700989
C	-4.744032	-0.037737	1.291847
C	-4.555824	-1.302292	1.848287
H	-5.423736	-1.889440	2.130724
C	-3.267650	-1.839295	2.049162
H	-3.168669	-2.829036	2.483137
H	-5.731666	0.379629	1.130160
H	-1.125249	-1.542963	1.850775
H	6.610485	0.608088	-0.122622
H	6.271434	1.212742	1.532307
H	6.406288	-0.550897	1.231219
H	2.251053	-0.233869	3.659144

H	0.797140	-1.142303	3.133423
H	2.277104	-2.028052	3.628551
C	2.042975	-0.185615	0.978504
C	4.172811	-0.506678	-0.242205
H	-1.037225	-0.811054	-1.543028
H	-0.128628	-1.697958	-2.752798
C	-1.539027	-2.905604	-1.631694
H	-1.862860	-3.011302	-0.587665
H	-1.045424	-3.847452	-1.904188
C	-2.772398	-2.697269	-2.521966
H	-2.448774	-2.555465	-3.562782
H	-3.372946	-3.616165	-2.508814
C	-3.656706	-1.521392	-2.092638
H	-4.550066	-1.450941	-2.724413
H	-3.130086	-0.563497	-2.164093
H	-3.989604	-1.641672	-1.055906

TS4-cis

Eopt = -1665.048813

59 atoms

C	2.043533	-1.113229	0.503685
C	0.014653	-1.077814	-0.560956
C	0.288699	0.229302	-1.255236
C	2.527610	0.123134	-0.185081
H	1.593977	-0.972097	1.486086
H	3.003090	-0.136261	-1.134129
H	-0.637979	0.804536	-1.341319
H	0.667210	0.045977	-2.266531
H	-0.422576	-0.999306	0.429145
C	-0.148135	-2.257352	-1.241119
C	-0.714891	-3.449079	-0.604507

H	0.130263	-2.325979	-2.291056
H	-0.387230	-4.394369	-1.040864
H	-0.607383	-3.466343	0.480170
S	-2.652742	-3.591533	-0.895399
C	-3.085811	-1.996584	-0.355961
N	-3.294626	-1.607970	0.918284
N	-3.169649	-0.905131	-1.138567
C	-3.497015	-0.234825	0.967624
H	-3.270500	-2.237564	1.715592
C	-3.420692	0.219085	-0.365261
H	-2.993284	-0.919297	-2.138339
C	-3.717338	0.643961	2.030820
C	-3.555158	1.569389	-0.693515
C	-3.848640	1.989767	1.702990
H	-3.771243	0.290893	3.054573
C	-3.768860	2.444397	0.366572
H	-3.487431	1.910623	-1.720349
H	-4.013165	2.712670	2.495388
H	-3.871815	3.505467	0.163897
H	3.272795	0.658845	0.417634
C	1.340852	1.065759	-0.490288
C	0.748950	1.626957	0.806810
O	-0.399386	1.466196	1.183542
O	1.661749	2.320656	1.492644
C	1.228836	2.908857	2.743921
H	0.419208	3.618669	2.560895
H	0.899488	2.125025	3.429124
H	2.106193	3.419813	3.137963
C	1.775254	2.239924	-1.362511
O	2.841213	2.323416	-1.947287

O	0.814029	3.165501	-1.433501
C	1.079387	4.328960	-2.257274
H	0.182081	4.941455	-2.182368
H	1.946629	4.867524	-1.869675
H	1.251918	4.021614	-3.290603
C	2.705834	-2.436308	0.282588
H	1.953115	-3.232539	0.360544
H	3.104063	-2.484296	-0.737343
C	3.822129	-2.754785	1.304745
H	3.374450	-2.786898	2.306923
H	4.192225	-3.768028	1.093847
C	5.007590	-1.779865	1.312998
H	4.661493	-0.778722	1.602211
H	5.708831	-2.097779	2.095667
C	5.755110	-1.696695	-0.020344
H	5.117959	-1.306816	-0.820383
H	6.627645	-1.037884	0.057243
H	6.111554	-2.686597	-0.332956

TS4-trans

Eopt = -1665.048554

59 atoms

C	1.587266	1.207174	-0.024475
C	1.269169	0.361195	2.111298
C	2.007091	-0.934961	1.843520
C	2.683799	0.222110	-0.277529
H	0.607933	0.964962	-0.434287
H	3.611593	0.559191	0.195318
H	1.436596	-1.786846	2.219018
H	2.966394	-0.918250	2.370357
H	1.872223	1.230158	2.362468

C	-0.056514	0.369412	2.454002
C	-0.807610	1.586376	2.799843
H	-0.625109	-0.553560	2.383465
H	-1.617100	1.412157	3.509002
H	-0.170915	2.402532	3.150714
C	2.307900	-1.145986	0.330119
H	2.889745	0.104188	-1.350297
C	1.908402	2.661555	0.101176
H	1.089353	3.182270	0.611495
H	2.809163	2.789549	0.716634
C	2.137322	3.341423	-1.266838
H	2.963495	2.840380	-1.788709
H	1.242349	3.203951	-1.889262
C	2.445401	4.836409	-1.138872
H	1.619724	5.329359	-0.607280
H	3.339188	4.967430	-0.513568
C	2.662357	5.517240	-2.492137
H	2.882238	6.584502	-2.372093
H	3.501231	5.062292	-3.033234
H	1.770992	5.429321	-3.125645
C	1.084289	-1.694541	-0.406929
O	-0.031387	-1.828723	0.075382
O	1.370219	-1.983609	-1.675125
C	0.282215	-2.477052	-2.499146
H	0.725924	-2.650729	-3.478249
H	-0.106527	-3.407232	-2.080656
H	-0.505534	-1.723897	-2.560688
C	3.447872	-2.151267	0.185447
O	4.594757	-1.868927	-0.118610
O	3.039167	-3.388548	0.483263

C	4.031570	-4.444450	0.417883
H	3.496676	-5.354011	0.687115
H	4.429171	-4.516459	-0.596572
H	4.835198	-4.244117	1.129330
S	-1.667660	2.457740	1.304893
C	-2.656917	1.180218	0.658064
N	-3.989357	1.271755	0.470470
N	-2.256049	-0.019034	0.198047
C	-4.467116	0.109190	-0.122979
H	-4.549747	2.071304	0.748967
C	-3.349071	-0.729375	-0.285082
H	-1.296395	-0.368033	0.193199
C	-5.746986	-0.285444	-0.515701
C	-3.459192	-2.003778	-0.844312
C	-5.857875	-1.556091	-1.074714
H	-6.604874	0.365025	-0.386787
C	-4.735810	-2.398509	-1.236205
H	-2.594019	-2.645001	-0.963860
H	-6.833080	-1.909632	-1.393750
H	-4.872894	-3.380320	-1.677918

Structure 5

Eopt = -1894.979620

67 atoms

C	-2.028738	-0.411227	-1.339418
C	-3.255950	-0.280385	-0.388621
C	-3.929115	1.118838	-0.601872
C	-3.066222	2.257561	-0.141556
C	-0.974808	-1.388548	-0.928080
H	-2.430817	-0.650603	-2.336834
H	-1.586285	0.581917	-1.433777

H	-4.142075	1.205603	-1.671574
H	-4.885334	1.125323	-0.071640
H	-3.040116	2.459490	0.927858
C	-4.621274	-3.699028	-0.904007
O	-3.737415	-2.591681	-0.633528
O	-5.446744	-1.168347	-0.999335
C	-3.403258	-1.074843	3.250040
O	-1.830006	0.189626	1.516960
O	-3.695741	-1.018359	1.832940
C	-2.309085	2.998713	-0.956479
H	-2.322067	2.823528	-2.031034
C	-1.420758	4.094873	-0.472315
H	-1.435118	4.207798	0.614166
H	-1.286146	-2.298787	-0.425199
H	-1.673332	5.059739	-0.926149
S	0.348467	3.903462	-1.021420
C	0.993297	2.698120	0.057600
C	2.575217	1.525260	1.129675
C	1.323642	0.965174	1.432901
N	2.318717	2.596326	0.280280
N	0.375761	1.723413	0.743420
H	3.017903	3.229806	-0.094507
H	-0.618245	1.482452	0.715725
C	1.203031	-0.147199	2.264688
C	3.761418	1.009361	1.646656
C	3.641200	-0.097574	2.482363
H	4.536833	-0.536189	2.910080
C	2.386967	-0.665219	2.782614
H	2.342428	-1.533089	3.432798
H	4.722252	1.449572	1.405316

H	0.235854	-0.579884	2.485156
H	-2.468609	-1.614782	3.417919
H	-3.331793	-0.065413	3.660013
H	-4.240187	-1.612686	3.693650
H	-5.438641	-3.717397	-0.178848
H	-5.026940	-3.625222	-1.915852
H	-4.005109	-4.592639	-0.805590
C	-4.288935	-1.370677	-0.700235
C	-2.827562	-0.358350	1.072083
C	0.408704	-1.193316	-1.138034
C	0.947320	-0.075908	-1.842414
C	1.345521	-2.123659	-0.608428
C	2.315022	0.087063	-1.959908
H	0.284764	0.657077	-2.290304
C	2.721899	-1.955945	-0.722167
H	0.962599	-2.989354	-0.070939
C	3.228589	-0.828249	-1.403565
H	2.703108	0.952618	-2.493102
C	3.654853	-2.963303	-0.077405
C	4.714900	-0.597946	-1.576109
C	5.079149	-2.902861	-0.636774
C	5.578922	-1.456315	-0.646585
H	4.986178	-0.820025	-2.619797
H	5.534104	-1.056168	0.374616
H	5.739973	-3.538923	-0.036179
H	3.689997	-2.763671	1.003498
H	3.236948	-3.971383	-0.186889
H	5.093992	-3.300524	-1.661398
H	6.626303	-1.405673	-0.966344
H	4.936327	0.467544	-1.432188

TS5-cis

Eopt = -1894.951463

67 atoms

C	-1.367573	0.160072	-1.785909
C	0.191739	-0.342060	-0.428448
C	-0.158103	0.805244	0.485561
C	-1.188380	1.655315	-1.667645
H	-0.881725	-0.307043	-2.636729
H	-2.152596	2.168427	-1.678443
H	0.644159	0.999241	1.203303
H	-1.055734	0.550783	1.058791
H	0.901070	-0.122271	-1.225297
C	0.121339	-1.655175	0.001175
C	0.710263	-2.770887	-0.770395
H	-0.461583	-1.909183	0.883755
H	0.000191	-3.584140	-0.952743
H	1.141429	-2.453842	-1.722343
S	2.058338	-3.736521	0.146343
C	3.355721	-2.584663	0.242207
N	3.296858	-1.243162	0.176674
N	4.640654	-2.938341	0.443523
C	4.572272	-0.704793	0.340046
H	2.435487	-0.711796	0.089019
C	5.437847	-1.796483	0.519164
H	4.973661	-3.895955	0.495534
C	5.031199	0.611201	0.348966
C	6.806861	-1.624012	0.715988
C	6.399969	0.786676	0.549033
H	4.353944	1.445737	0.208314
C	7.270157	-0.308665	0.727923

H	7.471272	-2.470097	0.851789
H	6.805948	1.792967	0.567391
H	8.328867	-0.123549	0.878610
C	-0.429580	2.072166	-0.352893
H	-0.628655	2.014892	-2.533757
C	0.887974	2.747203	-0.740810
O	1.994702	2.243424	-0.637201
O	0.671975	3.963602	-1.250071
C	1.833982	4.705041	-1.700095
H	1.442498	5.654192	-2.062881
H	2.519553	4.864124	-0.865194
H	2.332907	4.160686	-2.504592
C	-1.229539	3.070862	0.486935
O	-2.362431	3.455589	0.254454
O	-0.521849	3.457209	1.554273
C	-1.156475	4.398761	2.456315
H	-2.063526	3.958716	2.875685
H	-0.421290	4.582439	3.238427
H	-1.392121	5.322154	1.923091
C	-2.560992	-0.517012	-1.314470
C	-2.797040	-1.856847	-1.701531
C	-3.468722	0.068251	-0.411015
C	-3.891343	-2.552194	-1.206907
H	-2.110496	-2.339259	-2.392472
C	-4.573684	-0.627921	0.094048
H	-3.321463	1.095209	-0.091683
C	-4.796523	-1.959817	-0.306762
H	-4.059198	-3.580551	-1.520145
C	-5.492192	0.061335	1.086579
C	-5.998805	-2.745731	0.176274

C	-6.850847	-0.630337	1.231809
H	-4.994834	0.077028	2.067523
H	-5.619966	1.110198	0.794813
C	-6.659816	-2.137967	1.417322
H	-6.738464	-2.784936	-0.637450
H	-5.703018	-3.784870	0.364279
H	-7.397009	-0.198332	2.078042
H	-7.456352	-0.450893	0.332326
H	-6.027485	-2.315367	2.298563
H	-7.618891	-2.633846	1.605171

TS5-trans

Eopt = -1894.950019

67 atoms

C	1.809120	0.856811	0.817290
C	0.040878	0.417163	-0.297259
C	-0.193014	1.809837	-0.859572
C	2.113674	2.085205	0.008382
H	1.312516	1.035780	1.764021
H	2.534898	1.821486	-0.962688
H	-1.221239	2.136149	-0.694187
H	-0.016762	1.787755	-1.939193
H	0.660055	-0.235748	-0.902405
C	-0.887024	-0.198718	0.529904
C	-0.810554	-1.634033	0.854084
H	-1.672061	0.391068	0.995126
H	0.201627	-2.036466	0.771358
H	-1.216853	-1.896170	1.832472
C	0.788825	2.839936	-0.229862
H	2.840171	2.728729	0.519099
C	0.234569	3.364074	1.102954

O	-0.851859	3.075993	1.576281
O	1.108263	4.177484	1.701121
C	0.709500	4.747350	2.972708
H	1.546622	5.372991	3.279011
H	-0.193942	5.347169	2.844259
H	0.537874	3.950531	3.699424
C	0.901776	4.042314	-1.159362
O	0.117398	4.981556	-1.132325
O	1.896296	3.933758	-2.037047
C	2.021874	4.994782	-3.018786
H	1.118875	5.042559	-3.630815
H	2.192493	5.948404	-2.515337
H	2.884092	4.719052	-3.624135
S	-1.706402	-2.765762	-0.413557
C	-3.331323	-2.179178	-0.298510
N	-4.258927	-2.345515	-1.262115
N	-3.906456	-1.517046	0.722565
C	-5.469996	-1.788235	-0.855652
H	-4.086286	-2.795714	-2.155245
C	-5.240735	-1.246138	0.419846
H	-3.445906	-1.281283	1.594608
C	-6.713641	-1.702089	-1.478606
C	-6.242869	-0.590485	1.132283
C	-7.719410	-1.047679	-0.767941
H	-6.883460	-2.121686	-2.463939
C	-7.488983	-0.503232	0.512147
H	-6.058338	-0.174153	2.116371
H	-8.705041	-0.954449	-1.212459
H	-8.302012	-0.003243	1.028538
C	2.644436	-0.329634	0.808166

C	2.594027	-1.222329	1.904488
C	3.463950	-0.685963	-0.282000
C	3.335113	-2.396457	1.895245
H	1.966292	-0.979816	2.758033
C	4.210051	-1.869322	-0.300010
H	3.519030	-0.032075	-1.148284
C	4.152035	-2.743878	0.805020
H	3.285276	-3.067573	2.750060
C	5.041111	-2.204290	-1.525430
C	4.970195	-4.018401	0.854943
C	6.101938	-3.277074	-1.261735
H	4.364579	-2.561228	-2.315774
C	5.481923	-4.463134	-0.518556
H	5.832134	-3.852201	1.518394
H	4.377637	-4.812767	1.324286
H	6.545182	-3.598926	-2.210896
H	6.914127	-2.854550	-0.653781
H	4.649226	-4.865434	-1.112418
H	6.210288	-5.272817	-0.396877
H	5.503563	-1.288815	-1.912183

Structure 7

Eopt = -2432.142497

80 atoms

C	0.976303	1.200643	-0.857697
C	1.297928	0.181002	0.283889
C	0.976668	0.750893	1.700936
C	-0.405992	1.324902	1.815263
C	1.669177	2.508147	-0.693619
H	1.290256	0.745257	-1.806580
H	-0.099673	1.362027	-0.928060

H	1.116034	-0.040428	2.442950
H	1.700786	1.541741	1.936613
H	-0.585233	2.253199	1.274950
C	-0.473070	-2.894168	-1.093589
C	-0.531510	-3.157572	0.454668
B	0.495940	-1.154145	0.033412
O	0.399433	-2.153183	0.973569
O	-0.117409	-1.474662	-1.151820
C	-1.897828	-2.849024	1.066801
H	-2.254485	-1.860667	0.770970
H	-2.641856	-3.592634	0.767567
H	-1.812999	-2.868768	2.157061
C	-0.050443	-4.534972	0.887238
H	-0.118503	-4.622368	1.976088
H	-0.679172	-5.314040	0.443982
H	0.985985	-4.712221	0.592775
C	-1.791797	-3.098547	-1.823328
H	-2.574781	-2.452215	-1.427634
H	-1.663926	-2.868913	-2.885746
H	-2.116150	-4.140737	-1.736098
C	0.652211	-3.654031	-1.798002
H	1.609785	-3.515379	-1.289530
H	0.434968	-4.724912	-1.849373
H	0.750803	-3.273636	-2.819125
C	4.975590	-0.685104	0.817075
C	4.725972	-1.168079	-0.657014
B	2.808784	-0.261987	0.207186
O	3.612369	-0.461377	1.303076
O	3.452972	-0.521152	-0.981019
C	5.696212	0.661943	0.900866

H	5.222183	1.411271	0.260105
H	5.657329	1.020516	1.933721
H	6.746129	0.567779	0.608847
C	5.654182	-1.706415	1.718721
H	5.777924	-1.286382	2.721683
H	5.068484	-2.623968	1.801481
H	6.646520	-1.957189	1.330203
C	5.773687	-0.717860	-1.664665
H	6.756137	-1.120495	-1.397781
H	5.511367	-1.092349	-2.658991
H	5.843724	0.370509	-1.715858
C	4.492275	-2.676162	-0.767724
H	4.135524	-2.906015	-1.775680
H	5.418140	-3.232558	-0.595484
H	3.741063	-3.019415	-0.050653
C	-1.416893	0.784871	2.506849
H	-1.276232	-0.154732	3.039648
C	-2.774085	1.407203	2.605809
H	-2.811928	2.395886	2.141225
C	1.028663	3.767193	-0.620307
C	1.792925	4.958658	-0.444028
C	1.150383	6.183117	-0.364992
C	-0.931583	5.012164	-0.635487
C	-0.247962	6.224070	-0.461805
H	1.721955	7.096611	-0.229227
H	-2.017773	5.010784	-0.713620
H	-0.795493	7.158766	-0.405053
H	2.754138	2.504860	-0.606720
H	-3.078086	1.526477	3.651836
S	-4.141416	0.350104	1.949116

C	-3.893996	0.359660	0.186277
C	-4.615480	-0.548758	-0.609576
C	-3.036886	1.253411	-0.476305
C	-4.500970	-0.569688	-1.997780
C	-2.904968	1.231173	-1.864088
H	-2.461224	1.974120	0.085820
C	-3.636522	0.323624	-2.631423
H	-5.076370	-1.288448	-2.571037
H	-2.222238	1.929707	-2.336963
H	-3.535004	0.301077	-3.711562
Cl	-5.712465	-1.706876	0.147181
H	2.874066	4.887593	-0.372802
N	-0.340473	3.822201	-0.713300

TS7-cis

Eopt = -2432.123382

80 atoms

C	0.300638	1.916693	-0.939430
C	0.708655	1.079468	0.960772
C	-0.736359	0.802938	1.317884
C	-1.191006	1.698500	-0.915382
H	0.860427	1.188884	-1.521199
H	-1.555128	1.508632	-1.932999
H	-1.160775	1.674100	1.831735
H	-0.789728	-0.043626	2.011666
H	1.228798	0.246953	0.491011
C	1.491891	1.920733	1.738643
C	2.979255	2.075547	1.641809
H	1.007381	2.639813	2.398375
H	3.233487	3.077789	1.270592
H	3.454888	1.995245	2.627468

C	-1.527710	0.506549	0.022095
H	-1.683143	2.606173	-0.552397
S	3.864092	0.989412	0.461403
C	-0.608498	-3.114224	-0.709627
C	-0.016981	-2.372623	-1.961013
B	-1.037918	-0.867163	-0.577299
O	-0.683039	-1.069371	-1.888886
O	-0.905959	-2.000193	0.191635
C	1.483397	-2.098156	-1.841467
H	1.729769	-1.634720	-0.882917
H	2.064243	-3.019213	-1.939627
H	1.786387	-1.415492	-2.640311
C	-0.339970	-3.015737	-3.301047
H	-1.416753	-3.072273	-3.473000
H	0.106914	-2.427147	-4.108289
H	0.076448	-4.027275	-3.347467
C	0.360368	-4.057217	-0.011161
H	1.247039	-3.531457	0.346631
H	-0.133112	-4.521198	0.848592
H	0.675558	-4.853720	-0.693158
C	-1.936459	-3.817932	-0.993969
H	-2.380723	-4.133595	-0.045307
H	-2.642327	-3.152563	-1.498996
H	-1.787763	-4.705918	-1.615289
C	-5.101110	0.266292	1.316387
C	-5.276240	-0.044412	-0.213900
B	-3.071613	0.359396	0.258664
O	-3.991644	0.390596	-0.765136
O	-3.650550	0.159413	1.489004
C	-5.398096	-1.539379	-0.517277

H	-4.604782	-2.113185	-0.030074
H	-6.364873	-1.932036	-0.188970
H	-5.315416	-1.689124	-1.597866
C	-6.391460	0.730189	-0.901099
H	-6.431949	0.454453	-1.959439
H	-7.358583	0.487253	-0.449104
H	-6.234553	1.808603	-0.833905
C	-5.778408	-0.724633	2.252258
H	-5.398173	-1.738297	2.110996
H	-5.597242	-0.431639	3.291037
H	-6.860205	-0.728764	2.083788
C	-5.480891	1.699933	1.691826
H	-5.000297	2.427840	1.031510
H	-6.563665	1.848438	1.646141
H	-5.150582	1.896528	2.716155
C	3.747773	-0.627585	1.194145
C	3.129698	-0.885916	2.429311
C	4.292843	-1.725053	0.503508
C	3.059540	-2.181557	2.940822
H	2.684306	-0.073882	2.989558
C	4.229526	-3.021998	1.007126
C	3.606550	-3.254372	2.234102
H	2.567530	-2.347653	3.894183
H	4.660182	-3.838889	0.438245
H	3.548132	-4.264618	2.625792
Cl	5.085623	-1.475745	-1.053229
C	0.879194	3.252316	-0.975633
C	2.139607	3.464428	-1.578485
C	2.719600	4.726123	-1.538798
H	2.641157	2.635251	-2.066262

C	0.793978	5.473998	-0.327972
C	2.036740	5.764050	-0.894991
H	3.687429	4.900756	-2.000216
H	0.230899	6.255791	0.178711
H	2.448276	6.766171	-0.834585
N	0.221463	4.264027	-0.356390

TS7-trans

Eopt = -2432.124340

80 atoms

C	-0.013814	2.135327	-0.446768
C	-0.090783	1.661771	1.627868
C	1.268323	0.973458	1.707039
C	1.435459	1.765208	-0.616487
H	-0.716782	1.409773	-0.855619
H	2.067643	2.616508	-0.346202
H	1.217056	0.106551	2.371554
H	1.990697	1.672957	2.142030
H	-0.109306	2.714614	1.912836
C	-1.254306	0.932805	1.862540
C	-2.598851	1.557649	1.950611
H	-1.204053	-0.152699	1.838110
H	-3.134546	1.324181	2.875825
H	-2.540435	2.646966	1.873230
S	-3.706682	1.093320	0.528694
C	1.748288	0.551895	0.291200
H	1.636316	1.525260	-1.668306
C	-0.092455	-2.164413	-1.641702
C	0.095936	-2.843061	-0.236947
B	0.991288	-0.734517	-0.220025
O	0.480621	-1.707384	0.604846

O	0.811370	-1.016496	-1.553170
C	-1.165996	-3.467829	0.338087
H	-0.952041	-3.892448	1.323806
H	-1.963567	-2.733796	0.448489
H	-1.521098	-4.275078	-0.310518
C	1.259684	-3.834226	-0.190729
H	1.027569	-4.743728	-0.752420
H	2.175594	-3.396518	-0.598724
H	1.448047	-4.111154	0.850818
C	-1.496943	-1.598181	-1.855135
H	-1.812115	-0.977701	-1.013150
H	-1.496897	-0.976726	-2.755263
H	-2.230440	-2.397254	-1.989549
C	0.322107	-3.023424	-2.827399
H	0.163458	-2.467837	-3.756865
H	1.375033	-3.307301	-2.773006
H	-0.284953	-3.933733	-2.867570
C	5.311150	-0.422468	-0.590104
C	5.325053	-0.557525	0.974841
B	3.265742	0.147267	0.261474
O	3.898568	-0.493715	1.300911
O	4.088900	0.350305	-0.820963
C	5.886852	-1.871527	1.498377
H	5.318372	-2.728582	1.131888
H	6.931916	-1.986990	1.193158
H	5.849527	-1.877137	2.592158
C	5.989895	0.626036	1.680048
H	7.073834	0.616125	1.533404
H	5.597407	1.580711	1.317577
H	5.787889	0.557810	2.753152

C	5.123326	-1.759341	-1.310545
H	4.278486	-2.320502	-0.900185
H	4.922669	-1.565986	-2.368413
H	6.022207	-2.378365	-1.237593
C	6.490102	0.338209	-1.179010
H	6.388364	0.387556	-2.267557
H	6.545933	1.358105	-0.793253
H	7.428543	-0.176241	-0.948023
C	-4.102488	-0.611322	0.855256
C	-3.860069	-1.255250	2.081054
C	-4.717717	-1.370428	-0.157521
C	-4.212748	-2.590036	2.277102
H	-3.387755	-0.717845	2.893171
C	-5.072886	-2.704474	0.028552
C	-4.817979	-3.321610	1.253780
H	-4.004634	-3.056647	3.234916
H	-5.542391	-3.250625	-0.782490
H	-5.088351	-4.362287	1.399861
Cl	-5.072930	-0.629403	-1.718523
C	-0.474707	3.510760	-0.548326
C	-1.785709	3.795897	-0.994920
C	-0.082509	5.767273	-0.198129
C	-2.230012	5.111322	-1.032509
H	-2.428385	2.980909	-1.309889
C	-1.362530	6.130940	-0.624102
H	0.620902	6.532159	0.126010
H	-3.233951	5.341855	-1.377453
H	-1.662924	7.173388	-0.635023
N	0.361573	4.506061	-0.152215

Structure 9

Eopt = -2470.483762

82 atoms

C	-0.603501	-0.923342	0.379055
C	0.252059	0.230953	1.045661
C	-0.318968	0.595133	2.450974
C	-1.727121	1.104764	2.367915
C	0.147830	-2.161242	0.023944
H	-1.379214	-1.208670	1.096796
H	-1.131384	-0.533397	-0.493417
H	-0.280651	-0.285060	3.104068
H	0.325409	1.359151	2.903245
H	-1.873565	2.041450	1.826578
C	3.980960	-0.380330	0.617098
C	3.747441	-0.911802	2.079751
B	1.771417	-0.191017	1.183324
O	2.396237	-0.438209	2.376822
O	2.620978	-0.262655	0.103775
C	3.707092	-2.437284	2.174976
H	3.348001	-2.718951	3.170604
H	3.036979	-2.874736	1.428997
H	4.705120	-2.867095	2.039703
C	4.696550	-0.341925	3.124953
H	4.450777	-0.754402	4.109320
H	5.731455	-0.614936	2.892206
H	4.627779	0.746943	3.184701
C	4.762244	-1.324688	-0.286377
H	4.841412	-0.892197	-1.289482
H	5.777299	-1.469652	0.099590
H	4.276785	-2.298786	-0.368264
C	4.583851	1.024986	0.569575

H	4.572947	1.383080	-0.464699
H	4.005124	1.726451	1.178567
H	5.620464	1.027924	0.920396
C	0.784527	3.693391	-0.408864
C	0.606819	2.824887	-1.705042
B	0.361108	1.517085	0.149871
O	0.920768	2.677891	0.630428
O	0.003598	1.604687	-1.173301
C	-0.457681	4.513520	-0.057271
H	-0.340647	4.920816	0.952097
H	-0.595419	5.348753	-0.751081
H	-1.361144	3.895049	-0.073034
C	2.027197	4.571514	-0.394729
H	2.939784	3.977679	-0.487493
H	1.994987	5.295615	-1.215971
H	2.075642	5.128519	0.547036
C	-0.322002	3.419446	-2.753054
H	0.099750	4.349749	-3.148946
H	-0.434961	2.717066	-3.585645
H	-1.313167	3.633930	-2.348781
C	1.931964	2.408527	-2.346606
H	2.593499	1.935267	-1.616146
H	1.730533	1.683457	-3.141999
H	2.446670	3.266260	-2.790383
C	-2.795409	0.466268	2.857197
H	-2.663864	-0.478329	3.385120
C	-4.202420	0.922569	2.674598
H	-4.263203	1.928259	2.252151
H	0.429972	-2.884120	0.780330
H	-4.767095	0.915699	3.613769

S	-5.175648	-0.268072	1.626722
C	-4.301493	-0.214244	0.071841
C	-4.087917	-1.380277	-0.680380
C	-3.844627	0.998007	-0.470545
C	-3.453959	-1.347730	-1.922655
C	-3.196260	1.039776	-1.700946
H	-4.008006	1.919896	0.076472
C	-3.003195	-0.132726	-2.432901
H	-3.308132	-2.270140	-2.474405
H	-2.847552	1.989342	-2.089515
H	-2.500223	-0.106929	-3.394352
Cl	-4.624063	-2.951043	-0.081286
C	1.810340	-3.251298	-1.360030
C	0.632987	-1.443971	-2.338097
C	2.339796	-3.093366	-2.775383
C	1.903581	-1.676316	-3.167345
H	0.499420	-0.403396	-2.046784
H	-0.270409	-1.778570	-2.864624
H	3.420937	-3.254162	-2.799986
H	1.875579	-3.855757	-3.416563
H	2.667627	-0.954772	-2.861375
H	1.720836	-1.554657	-4.237872
N	0.843854	-2.289342	-1.153960
O	2.154618	-4.086577	-0.520068

TS9-cis

Eopt = -2470.468842

82 atoms

C	3.150092	-0.990563	0.528507
C	2.039065	-0.006254	0.486078
H	2.226897	0.991210	0.876743

C	0.769359	-0.337181	0.056212
C	-0.290376	-1.260810	1.740206
C	-1.421414	-0.274856	1.769092
C	-1.672951	0.224762	0.323930
C	-0.295398	0.704291	-0.205785
H	3.750688	-0.936122	1.440230
H	2.775521	-2.014241	0.441208
H	0.667718	-1.263955	-0.508274
H	-1.173299	0.574808	2.413033
H	-2.326123	-0.738069	2.184411
H	-0.008096	1.640335	0.291064
H	-0.353478	0.913930	-1.279490
N	0.573606	-1.386510	2.821042
C	0.907334	-0.286696	3.736699
C	1.321940	-2.517355	3.047772
C	2.231718	-0.735252	4.381963
H	0.107165	-0.163813	4.475907
H	1.006756	0.646007	3.177173
C	2.220062	-2.264391	4.243570
O	1.238190	-3.557950	2.386291
H	2.312791	-0.395626	5.416575
H	3.072499	-0.318259	3.819661
H	1.773927	-2.755309	5.118284
H	3.206045	-2.706432	4.081920
H	-0.478098	-2.220119	1.267892
S	4.333964	-0.907499	-0.921316
C	5.219049	0.611977	-0.656887
C	5.137644	1.369703	0.524895
C	6.071517	1.094590	-1.667569
C	5.866212	2.548697	0.679909

H	4.503096	1.038907	1.336512
C	6.805826	2.269495	-1.521815
C	6.701683	3.006210	-0.341227
H	5.776943	3.108075	1.606168
H	7.450293	2.600941	-2.328929
H	7.269305	3.923840	-0.226008
Cl	6.244098	0.194077	-3.176369
C	-3.733665	-2.531679	-1.290076
C	-2.531032	-2.411923	-2.294094
C	-3.925824	3.182446	-0.481712
C	-4.618358	2.585026	0.796458
B	-2.265739	-0.929274	-0.572149
B	-2.755889	1.362197	0.270249
O	-3.582243	1.689334	1.318123
O	-2.995348	2.115360	-0.855174
O	-3.234666	-1.797283	-0.125071
O	-1.907771	-1.153370	-1.878215
C	-1.474693	-3.502981	-2.108934
H	-1.840758	-4.471810	-2.460758
H	-0.587271	-3.238643	-2.691496
H	-1.178701	-3.602962	-1.060642
C	-2.928333	-2.299145	-3.758676
H	-2.029605	-2.213777	-4.377191
H	-3.474845	-3.193653	-4.074572
H	-3.554350	-1.423408	-3.940834
C	-4.073087	-3.952288	-0.863782
H	-4.366115	-4.550263	-1.732794
H	-3.228218	-4.439401	-0.372918
H	-4.914205	-3.934871	-0.163783
C	-4.991409	-1.799051	-1.761719

H	-4.766042	-0.774377	-2.071088
H	-5.461833	-2.320655	-2.600206
H	-5.708096	-1.759217	-0.936328
C	-3.077719	4.421670	-0.189707
H	-3.706469	5.285690	0.043983
H	-2.393712	4.251070	0.646970
H	-2.481979	4.659932	-1.075820
C	-4.862066	3.443090	-1.652930
H	-4.292509	3.847400	-2.495400
H	-5.359473	2.528930	-1.982895
H	-5.625148	4.177060	-1.374500
C	-4.970065	3.604078	1.870400
H	-5.682337	4.337723	1.479269
H	-5.437378	3.096164	2.719740
H	-4.085883	4.133329	2.231205
C	-5.829852	1.707699	0.475479
H	-5.595467	0.965864	-0.292827
H	-6.131872	1.175604	1.382397
H	-6.675336	2.311200	0.132769

TS9-trans

Eopt = -2470.468936

82 atoms

C	0.025853	2.646074	0.218953
C	-0.520159	1.197314	-1.397121
C	0.938074	0.871321	-1.618715
C	1.364933	2.038101	0.567836
H	0.033298	3.561802	-0.368191
H	1.443112	1.832814	1.638981
H	1.401233	1.654781	-2.232492
H	1.027606	-0.067362	-2.176560

H	-1.037282	0.537557	-0.695646
C	-1.291551	1.849024	-2.318896
C	-2.775344	2.064442	-2.249967
H	-0.805131	2.397747	-3.126691
H	-2.994643	3.117902	-2.028167
H	-3.260142	1.845159	-3.208941
S	-3.697319	1.206425	-0.919485
C	1.659369	0.738223	-0.257487
H	2.129793	2.787433	0.336805
C	5.212875	-0.021196	-1.395219
C	5.426930	0.372715	0.110818
B	3.206095	0.515414	-0.430574
O	4.145740	0.995818	0.450696
O	3.761317	-0.202873	-1.463396
C	5.584804	-0.835495	1.035636
H	5.526540	-0.497140	2.074334
H	4.792707	-1.571392	0.872111
H	6.551936	-1.324207	0.886353
C	6.540487	1.380153	0.357370
H	7.502584	0.971607	0.031790
H	6.361363	2.317872	-0.172494
H	6.608405	1.597734	1.427796
C	5.887172	-1.318035	-1.819205
H	6.972511	-1.239479	-1.698939
H	5.531005	-2.168265	-1.234178
H	5.675390	-1.514100	-2.874832
C	5.559008	1.104649	-2.371331
H	5.204580	0.829690	-3.369189
H	5.079214	2.045015	-2.084152
H	6.639600	1.266176	-2.423109

C	0.174753	-2.595667	0.823809
C	0.860101	-2.108162	2.151311
B	1.170855	-0.562865	0.486607
O	1.145440	-0.703031	1.853447
O	0.758830	-1.696564	-0.172064
C	-0.026654	-2.171361	3.386737
H	0.524577	-1.797087	4.254966
H	-0.929425	-1.569176	3.267635
H	-0.321134	-3.205850	3.590544
C	2.206618	-2.780152	2.421202
H	2.853818	-2.744256	1.540525
H	2.710106	-2.252882	3.236824
H	2.075066	-3.825427	2.715436
C	-1.334854	-2.354332	0.787744
H	-1.865056	-3.041189	1.453567
H	-1.586494	-1.330147	1.074494
H	-1.691129	-2.518290	-0.230965
C	0.488826	-4.031777	0.430230
H	0.133492	-4.723818	1.200580
H	-0.022734	-4.274136	-0.506390
H	1.560037	-4.187175	0.287072
C	-3.717896	-0.494291	-1.433079
C	-3.073233	-0.970329	-2.587171
C	-4.413398	-1.433303	-0.650246
C	-3.134710	-2.318272	-2.940346
H	-2.504813	-0.285998	-3.203967
C	-4.487291	-2.779414	-0.998000
C	-3.843205	-3.227796	-2.152133
H	-2.620167	-2.654197	-3.835394
H	-5.036747	-3.467397	-0.364502

H	-3.892444	-4.277323	-2.423495
Cl	-5.220238	-0.912336	0.831930
N	-1.018480	2.647743	1.138669
C	-1.153334	1.682385	2.238543
C	-2.071517	3.527284	1.070543
C	-2.620794	1.821815	2.680751
H	-0.453308	1.939434	3.042002
H	-0.907823	0.679882	1.890581
C	-3.029083	3.223609	2.206700
O	-2.182933	4.428091	0.228618
H	-2.730157	1.682975	3.758460
H	-3.228555	1.068625	2.174189
H	-2.889184	3.984013	2.986242
H	-4.063658	3.291364	1.861103

Structure 10

Eopt =

-2530.878578

86 atoms

C	-1.218921	1.329481	0.939151
C	-1.468931	0.245469	-0.158603
C	-0.880250	0.678799	-1.532847
C	0.617126	0.608767	-1.637155
C	0.212102	1.589232	1.234278
H	-1.712857	2.260368	0.650831
H	-1.700713	0.981124	1.863469
H	-1.298987	0.018727	-2.301812
H	-1.222242	1.694751	-1.767154
H	1.055806	-0.374829	-1.483791
C	-0.198547	-2.883127	1.611665
C	-0.376271	-3.389440	0.133594

B	-0.939029	-1.173948	0.281386
O	-0.523843	-2.135347	-0.606313
O	-0.901576	-1.596781	1.587354
C	0.819274	-4.144391	-0.430376
H	0.609905	-4.444913	-1.461578
H	1.721094	-3.529547	-0.430702
H	1.010995	-5.048857	0.155915
C	-1.665067	-4.182028	-0.088309
H	-2.535698	-3.648286	0.303370
H	-1.810332	-4.329134	-1.162556
H	-1.613145	-5.164297	0.390125
C	1.254181	-2.574574	1.969943
H	1.280645	-2.044782	2.926252
H	1.841303	-3.491533	2.069087
H	1.726507	-1.940992	1.216498
C	-0.838036	-3.766233	2.672735
H	-1.914530	-3.867065	2.520346
H	-0.386820	-4.763641	2.659338
H	-0.670364	-3.330488	3.662563
C	-5.197764	-0.333442	0.342019
C	-5.067700	-0.444718	-1.220255
B	-3.025403	0.011326	-0.290062
O	-3.923021	0.286117	0.713001
O	-3.617077	-0.533733	-1.403331
C	-5.242474	-1.690631	1.046670
H	-4.428683	-2.341816	0.715066
H	-5.135895	-1.533567	2.124022
H	-6.193147	-2.200130	0.865276
C	-6.333584	0.554818	0.828240
H	-7.296822	0.158529	0.491168

H	-6.339362	0.577306	1.922369
H	-6.230189	1.578981	0.464469
C	-5.710837	-1.681999	-1.829575
H	-6.788444	-1.685127	-1.636295
H	-5.559554	-1.678320	-2.913384
H	-5.279988	-2.600621	-1.426515
C	-5.524480	0.814855	-1.958191
H	-5.065108	1.714125	-1.537156
H	-5.227237	0.737480	-3.008212
H	-6.611793	0.926036	-1.916012
C	1.416499	1.628725	-1.963882
H	0.987337	2.620038	-2.111356
C	2.904474	1.579451	-2.182205
H	3.138438	1.990540	-3.171705
C	0.876211	2.869045	1.128162
C	0.534103	5.232095	0.459896
H	0.840798	0.776005	1.581426
H	3.440402	2.212878	-1.466604
S	3.690816	-0.074392	-2.234822
C	3.929855	-0.504889	-0.523668
C	4.523012	-1.741404	-0.210823
C	3.597691	0.339538	0.547038
C	4.803634	-2.116134	1.101394
C	3.876116	-0.026635	1.863232
H	3.116415	1.291878	0.371720
C	4.484927	-1.250086	2.147941
H	5.266267	-3.077770	1.295731
H	3.603330	0.653239	2.663941
H	4.699211	-1.539649	3.171546
Cl	4.950231	-2.864704	-1.504750

C	-0.705867	5.923158	-0.104277
H	-0.491534	6.980992	-0.283859
H	-1.006283	5.464021	-1.051421
H	-1.541613	5.852323	0.598980
C	0.913987	5.828801	1.815718
H	1.102581	6.900732	1.695714
H	0.092550	5.704603	2.529121
H	1.810940	5.360001	2.222699
C	1.684580	5.288283	-0.546200
H	1.390053	4.820219	-1.490382
H	1.930156	6.336124	-0.748127
H	2.575569	4.788825	-0.164016
O	0.075391	3.840495	0.633496
O	2.055371	3.046017	1.457168

TS10-cis

Eopt = -2530.866402

86 atoms

C	0.042169	1.809052	-1.524569
C	1.113075	0.304785	-0.345935
C	-0.008604	0.127728	0.648415
C	-1.204757	1.815228	-0.690180
H	0.022680	1.221777	-2.437791
H	-2.076262	2.040804	-1.317367
H	0.157931	0.797110	1.501202
H	0.020119	-0.898754	1.030693
H	1.087040	-0.357835	-1.208328
C	2.353028	0.784476	0.025850
C	3.563025	0.664454	-0.822480
H	2.463143	1.307468	0.973664
H	3.346553	0.240080	-1.804649

H	4.064133	1.626288	-0.974140
C	-1.372068	0.425741	-0.013221
H	-1.136057	2.595512	0.072370
S	4.908000	-0.319775	0.018749
C	-2.879787	-1.741769	-2.752157
C	-1.739093	-2.672547	-2.201966
B	-1.745212	-0.681787	-1.071662
O	-1.363528	-1.996872	-0.958436
O	-2.517305	-0.442021	-2.182342
C	-2.174902	-4.092844	-1.871945
H	-1.320257	-4.660071	-1.490542
H	-2.961126	-4.107423	-1.114544
H	-2.543656	-4.596730	-2.771189
C	-0.490236	-2.689936	-3.085706
H	-0.672579	-3.234599	-4.016496
H	-0.158705	-1.677899	-3.335275
H	0.317583	-3.193068	-2.546924
C	-4.263638	-2.088970	-2.200222
H	-4.960543	-1.287648	-2.462748
H	-4.636896	-3.024274	-2.627125
H	-4.248279	-2.184521	-1.110606
C	-2.927956	-1.614472	-4.267671
H	-3.744555	-0.944550	-4.553967
H	-1.996383	-1.210640	-4.669216
H	-3.112943	-2.591467	-4.725717
C	-4.510700	0.963533	2.073692
C	-3.900838	-0.333907	2.717595
B	-2.557095	0.404118	1.018874
O	-2.538962	-0.334355	2.178055
O	-3.734485	1.088779	0.837682

C	-3.825362	-0.319754	4.237268
H	-4.828610	-0.233334	4.666935
H	-3.382844	-1.255742	4.591867
H	-3.215411	0.508329	4.603667
C	-4.562331	-1.623548	2.227389
H	-4.620494	-1.653928	1.135426
H	-3.964385	-2.476700	2.561144
H	-5.572120	-1.730538	2.633920
C	-4.241911	2.229481	2.889255
H	-3.184124	2.318471	3.154047
H	-4.519481	3.101935	2.290316
H	-4.834284	2.241357	3.808717
C	-5.986290	0.866214	1.713671
H	-6.318632	1.809094	1.268494
H	-6.175061	0.063911	0.997600
H	-6.585838	0.683877	2.611376
C	4.105494	-1.875670	0.359982
C	3.134242	-2.421269	-0.496667
C	4.445599	-2.615736	1.505172
C	2.508398	-3.630621	-0.202164
H	2.864535	-1.894300	-1.403155
C	3.836755	-3.835464	1.801661
C	2.855750	-4.341404	0.949183
H	1.752349	-4.017018	-0.877997
H	4.126401	-4.375852	2.696331
H	2.372840	-5.284395	1.184553
Cl	5.680448	-2.022716	2.617878
C	0.976950	2.925803	-1.606377
O	1.801354	3.052154	-2.513942
O	0.878435	3.763924	-0.551399

C	1.756956	4.936980	-0.382821
C	3.213897	4.491342	-0.251204
H	3.585177	4.062306	-1.182419
H	3.830953	5.358925	0.005370
H	3.316245	3.752056	0.549070
C	1.259757	5.539144	0.930167
H	0.205549	5.822772	0.850558
H	1.367257	4.820745	1.749048
H	1.842557	6.432701	1.173453
C	1.548264	5.916437	-1.538331
H	2.086776	6.845549	-1.324071
H	1.917165	5.507870	-2.480126
H	0.485073	6.155464	-1.646472

TS10-trans

Eopt = -2530.866984

C	-0.098073	1.605447	-2.112749
C	-0.914348	-0.207591	-1.185386
C	0.435018	-0.875520	-1.109166
C	1.357060	1.297117	-1.885668
H	-0.500544	1.476898	-3.110956
H	1.890289	2.199590	-1.566430
H	0.626487	-1.404795	-2.051745
H	0.407659	-1.629904	-0.314414
H	-1.218029	0.320431	-0.284943
C	-1.918799	-0.655169	-2.020732
C	-3.330168	-0.213831	-1.910709
H	-1.674930	-1.341007	-2.830569
H	-3.449285	0.635094	-1.239675
H	-3.756893	0.059076	-2.881702
C	1.550313	0.160786	-0.829389

H	1.793485	0.976842	-2.836461
S	-4.461927	-1.599517	-1.375348
C	2.249623	1.634892	2.608152
C	0.829491	0.988941	2.832931
B	1.496137	0.693037	0.656902
O	0.651987	0.193543	1.618665
O	2.380780	1.620821	1.152086
C	0.733146	0.060014	4.036307
H	1.430246	-0.776901	3.960704
H	0.942343	0.609099	4.960128
H	-0.281047	-0.344846	4.104220
C	-0.309171	2.009418	2.860500
H	-0.274269	2.614801	3.771238
H	-0.272935	2.664816	1.988761
H	-1.262189	1.471806	2.844992
C	3.395634	0.783993	3.158324
H	4.345388	1.202144	2.812687
H	3.398430	0.784177	4.252327
H	3.330516	-0.249303	2.808528
C	2.379537	3.072409	3.093118
H	1.666070	3.731285	2.594630
H	2.214390	3.127753	4.174080
H	3.389574	3.438704	2.884362
C	5.007814	-1.095947	-1.821495
C	4.736803	-1.895615	-0.495487
B	2.963056	-0.520473	-0.966025
O	3.305556	-1.665995	-0.284537
O	3.971165	-0.061973	-1.778168
C	4.980630	-3.394977	-0.590704
H	4.757003	-3.864303	0.372386

H	4.351536	-3.859831	-1.352391
H	6.029632	-3.595840	-0.831170
C	5.461099	-1.314833	0.719779
H	6.537889	-1.498224	0.660711
H	5.293388	-0.238636	0.810057
H	5.080057	-1.797753	1.624054
C	4.750903	-1.915966	-3.087229
H	4.770775	-1.246901	-3.952663
H	5.520298	-2.680811	-3.226642
H	3.773458	-2.406552	-3.055323
C	6.368900	-0.418899	-1.895453
H	7.168527	-1.165133	-1.847325
H	6.460956	0.116905	-2.845251
H	6.508643	0.297131	-1.083228
C	-3.842563	-1.988013	0.251899
C	-3.336800	-0.999126	1.112447
C	-3.872151	-3.308424	0.731605
C	-2.854812	-1.321125	2.378883
H	-3.316125	0.033634	0.786334
C	-3.404176	-3.640166	2.003457
C	-2.884129	-2.643216	2.828362
H	-2.455871	-0.535853	3.012403
H	-3.442298	-4.671714	2.336127
H	-2.508832	-2.901577	3.813336
Cl	-4.522672	-4.608835	-0.268162
C	-0.762509	2.616935	-1.302277
O	-0.274743	3.132248	-0.295903
O	-2.005217	2.891732	-1.771740
C	-2.917687	3.825041	-1.083846
C	-4.169145	3.777635	-1.958846

H	-4.933663	4.444650	-1.549000
H	-3.939134	4.098674	-2.979692
H	-4.577635	2.763118	-1.995936
C	-2.318470	5.232150	-1.076693
H	-1.434253	5.286140	-0.440217
H	-2.043148	5.532605	-2.093087
H	-3.065044	5.940189	-0.701920
C	-3.230842	3.320473	0.326139
H	-3.995957	3.963494	0.773586
H	-3.627027	2.300653	0.291950
H	-2.346640	3.335821	0.963425

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