SUPPORTING INFORMATION

Oxidation of 8-Thioguanosine Gives Redox-Responsive Hydrogels and Reveals Intermediates in a Desulfurization Pathway

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General Experimental. Chemicals and solvents were purchased from Aldrich, Alfa Aesar, or Carbosynth. Deuterated solvents were purchased from Cambridge Isotope Labs. NMR spectra were recorded on a Bruker AVIII-600 spectrometer. Chemical shifts are reported in ppm relative to the residual solvent peak. ESI-MS experiments were done with a JEOL AccuTOF spectrometer. CD spectroscopy was performed on a Jasco J-810 spectropolarimeter. UV-Vis spectroscopy was done on a Varian Cary 100 spectrometer. X-ray single crystal diffraction was measured on a Bruker Smart Apex2 diffractometer. MALDI-TOF mass spectra were performed on a Bruker Autoflex Speed spectrometer using 2,5-dihydroxybenzoic acid as the matrix. IR spectra were collected on a Thermo Nicolet Nexus 670 FT-IR with ATR module.

Preparation of hydrogels from 8-disulfideG 1: Disulfide **1** was weighed into a vial and the appropriate amount of deionized water was added to attain a desired concentration. The suspension, which contained small chunks of solid, was repeatedly sonicated and shaken until visible particles had broken up to give an opaque suspension. The vial was placed on the bench at rt. Periodically, the vial was inverted to determine if a self-standing gel had formed.

Circular Dichroism Procedure: Hydrogels made from 8-disulfideG **1** were prepared using the above procedure. Hydrogel samples were allowed to stand at ambient temperature for 1 day before making the CD measurements at 25 °C using a Hellma 106-QS quartz cell with an optical path length of 0.01 mm (scanning speed 200 nm/min; response time 2 s). Measurements were made in triplicate and the CD curves were averaged and smoothed.

UV-Vis Spectroscopy of Guanosine Analogs: Guanosine analogs **1-5** (2 mg) were added to deionized water (10 mL). The suspension (0.5 mL) was diluted with 2.5 mL of deionized water. Compound **1-3** appeared soluble at this dilute concentration and the solution was used for measurement. Due to the poor solubility of cyclosulfinate **4**, solid particles still remained in the diluted sample. This sample was ultracentrifuged and the supernatant was used for measurement. To obtain the UV-vis of sulfinate **5**, cyclosulfinate **4** (2 mg) was suspended in 0.5 mL of deionized water and then 2 eq of LiOH was added to that solution. The sample was allowed to sit for 15 min and then diluted with deionized water. Measurements were made in triplicate.

MAS Solid-State NMR. Solid-state natural abundance ^{13}C and ^{15}N NMR spectra of magic angle spinning (MAS) samples were acquired on a Bruker AVANCE NEO 500 MHz NMR spectrometer using the combination of standard cross-polarization (CP) with proton spinal-64 decoupling. Samples were packed in 3.2 mm o.d. rotors and run in Bruker 3.2 mm HCN triple resonance probe. Proton 90° pulse widths of 2.5 μs, contact times of 2 ms and pulse delays of 5 s were used to acquire both ^{13}C and ^{15}N NMR spectra. Carbon-13 chemical shifts were referenced with respect to TMS by setting $\delta(^{13}C) = 0$ ppm and nitrogen-15 chemical shifts were referenced with respect to α-glycine by setting $\delta(^{15}N) = 33.4$ ppm. Spectra of MAS samples were acquired at ambient temperature with spinning frequency of 8 to 13 kHz and spinning sidebands were confirmed by running experiments with a different spinning rate. ^{13}C CP/MAS NMR experiment was acquired with a total scan of 2k and ^{15}N CP/MAS NMR experiment was acquired with a total scan of 32k. ^{1}H-^{13}C HETCOR NMR spectra were acquired with proton 90° pulse widths of 2.5 μs and a spinning frequency of 10 kHz.

Background on G-Quartets and Guanosine Conformation

Figure S1. The G-quartet is formed by 4 guanines that use Watson-Crick and Hoogsteen edges to form a planar H-bonded macrocycle. The process is typically templated by K^+. Individual G-quartets stack to give a G-quadruplex, which extends to form nanotubes. Entangled columnar structures give a matrix that traps water, resulting in a hydrogel.[1]

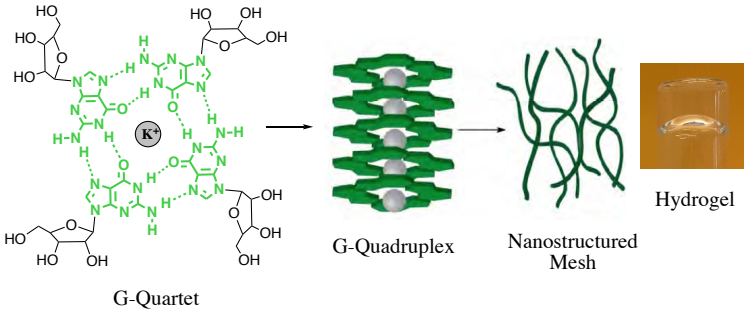


Figure S2. Guanines form various self-assembled motifs,[1] including ribbons and the G-quartet. Note that the G-ribbon II uses the "sugar" edge (N3 and NH_2) of the purine to form H-bonds. This motif would not be possible for a G analog that was in its *syn* conformation (see Fig. S3 below). The G-ribbon I motif is, however, an alternative self-assembly motif to the G-quartet, for hydrogel formation.

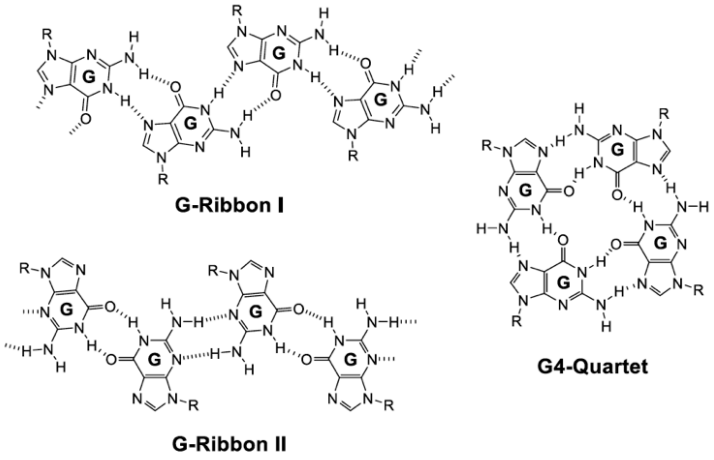
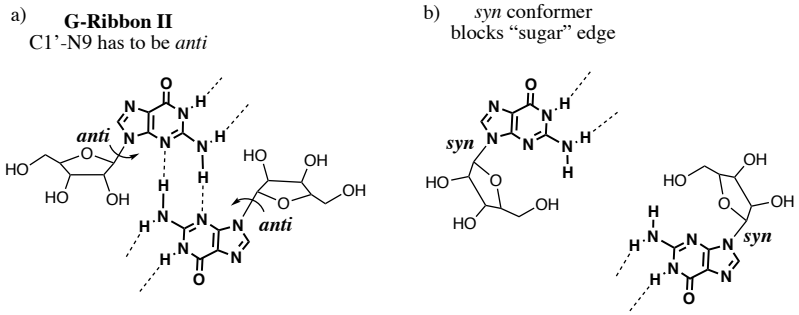
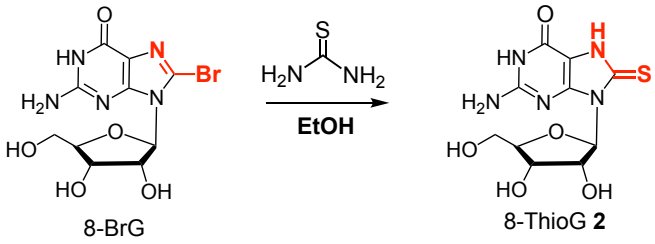


Figure S3. This H-bond ribbon uses the "sugar" edge of the nucleobase to make intermolecular H-bonds. When the sugar is "*anti*" relative to the base (left) H-bonding is possible. When the compound adopts a "*syn*" conformation (on right) the "sugar" edge is blocked and formation of this H-bonded ribbon is not possible.



Synthesis and Characterization of Guanosine Analogs

8-thioG **2**



8-thioG **2** was prepared from 8-bromoguanosine and thiourea using a literature procedure.[2] Solution ^{1}H, ^{13}C and ^{15}N NMR data for **2** was consistent with values from the literature.[3,4] Material made via this procedure was subsequently used to prepare 8-thioG disulfide **1**.

^{1}H NMR (600 MHz, DMSO-d_6): δ 12.91 (s, 1H, N7H), 11.03 (s, 1H, N1H), 6.54 (s, 2H, N2H), 6.24 (d, J = 5.5 Hz, 1H, H1′), 5.25 (d, J = 6.0 Hz, 1H, 2′-OH), 4.95 (m, 1H, H2′), 4.88 (d, J = 5.7 Hz, 1H, 3′-OH), 4.77 (t, J = 5.9 Hz, 1H, 5′-OH), 4.21 (m, 1H, H3′), 3.79 (m, 1H, H4′), 3.65 (m, 1H, H5′), 3.49 (m, 1H, H5″). This data is consistent with literature assignments.[3]

^{13}C NMR (151 MHz, DMSO-d_6): δ 165.71 (C8), 153.51 (C6), 150.90 (C2), 149.52 (C4), 104.08 (C5), 88.73 (C1′), 85.10 (C4′), 70.54 (C3′), 70.30 (C2′), 62.35 (C5′). Data is consistent with literature assignments.[4]

^{15}N NMR (60. 8 MHz, DMSO-d_6): δ 169.10 (N9), 166.79 (N3), 149.34 (N7), 147.08 (N1), 75.39 ($NH_2$2). This data is consistent with literature assignments.[3]

ESI-MS ($[M + H]^+$): m/z = 316.11 (MW=315.30)

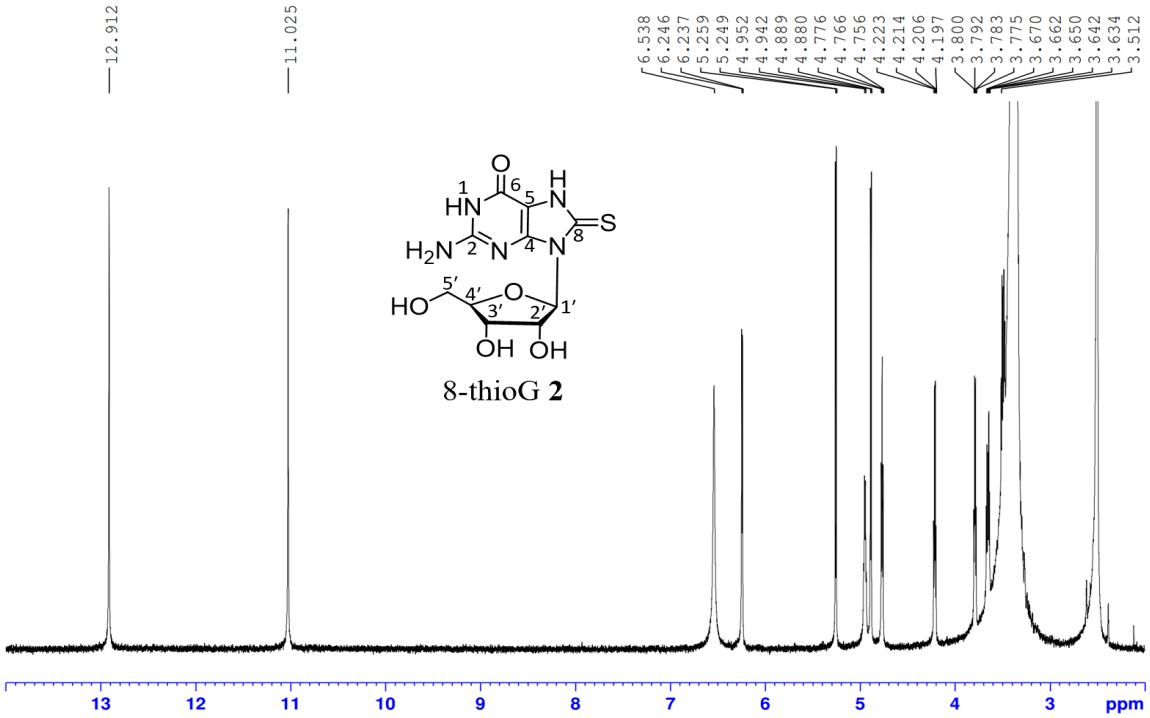


Figure S4: ^{1}H NMR spectrum of 8-thioG **2** in DMSO-d_6.

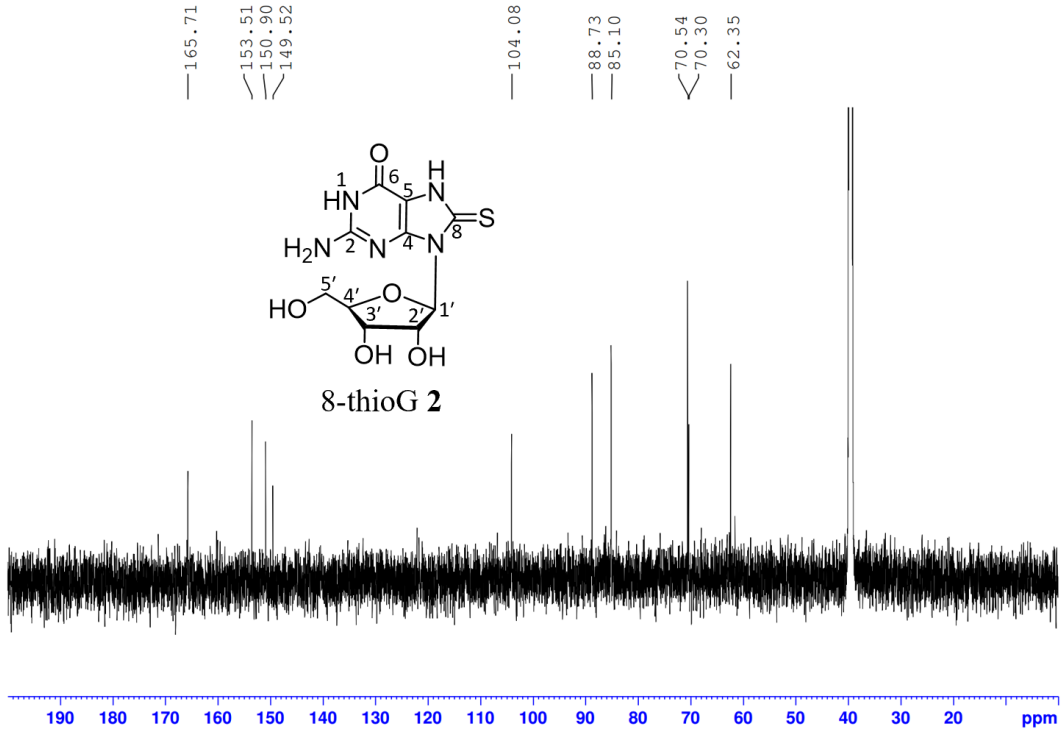


Figure S5: ^{13}C NMR spectrum of 8-thioG **2** in DMSO-d_6.

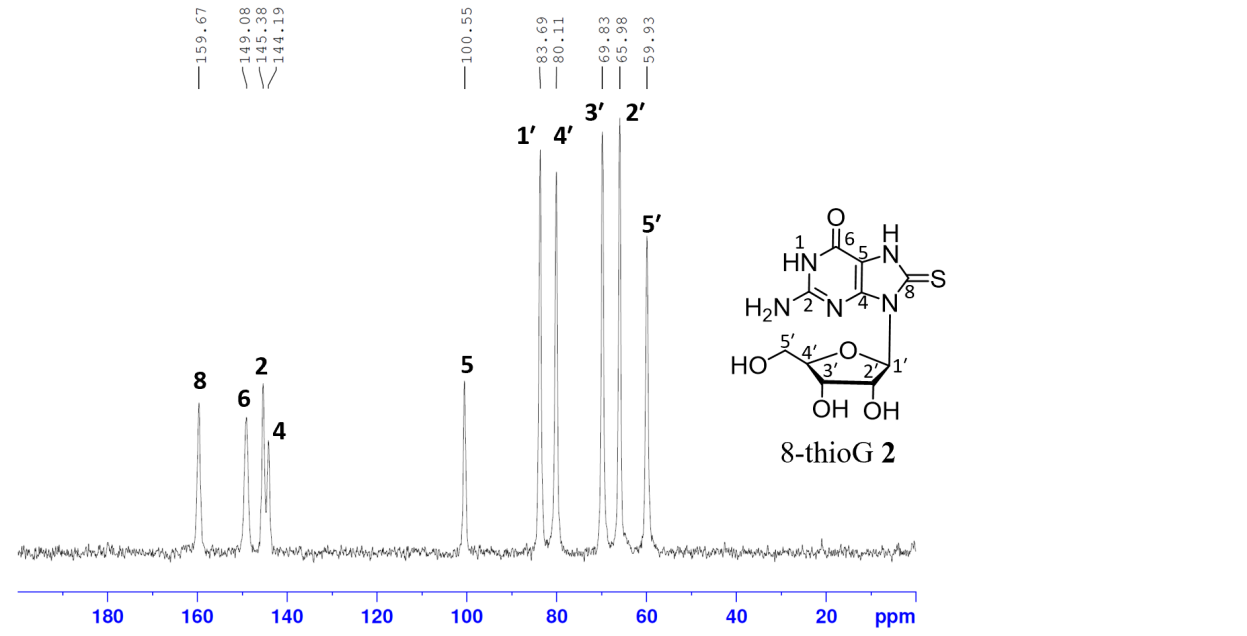


Figure S6: MAS solid-state ^{13}C NMR (125.7 MHz) spectrum of 8-thioG **2**.

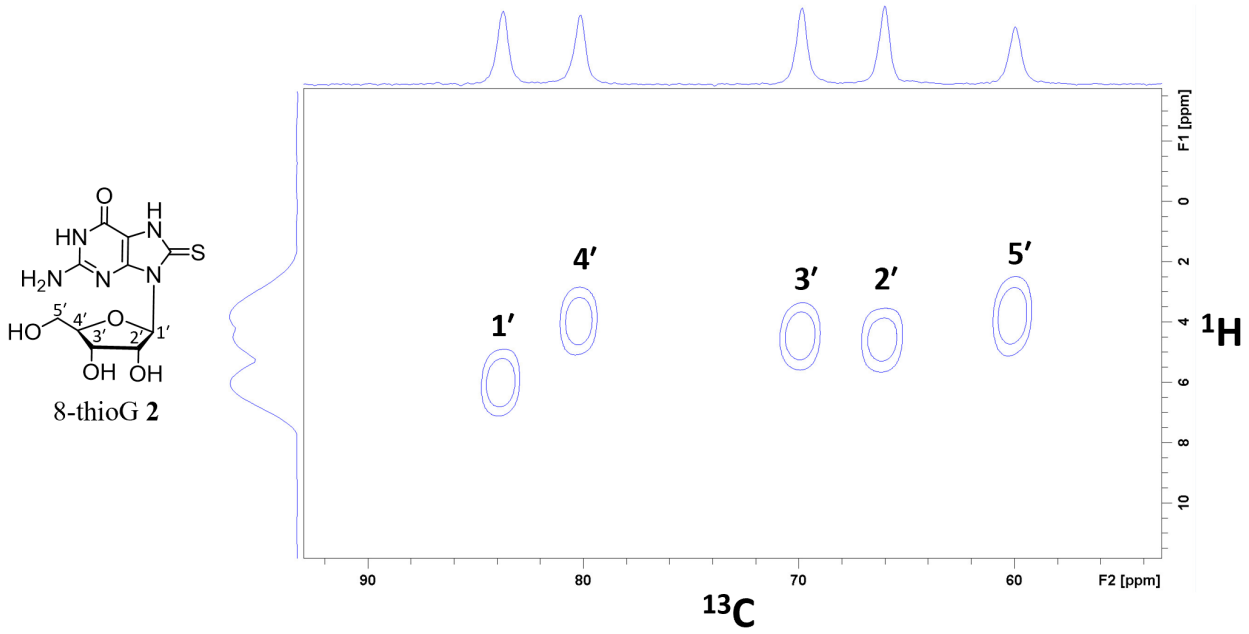


Figure S7: MAS solid-state ^{13}C-^{1}H HETCOR 2D NMR spectrum of 8-thioG **2**. This experiment allowed us to assign ribose ^{13}C resonances.

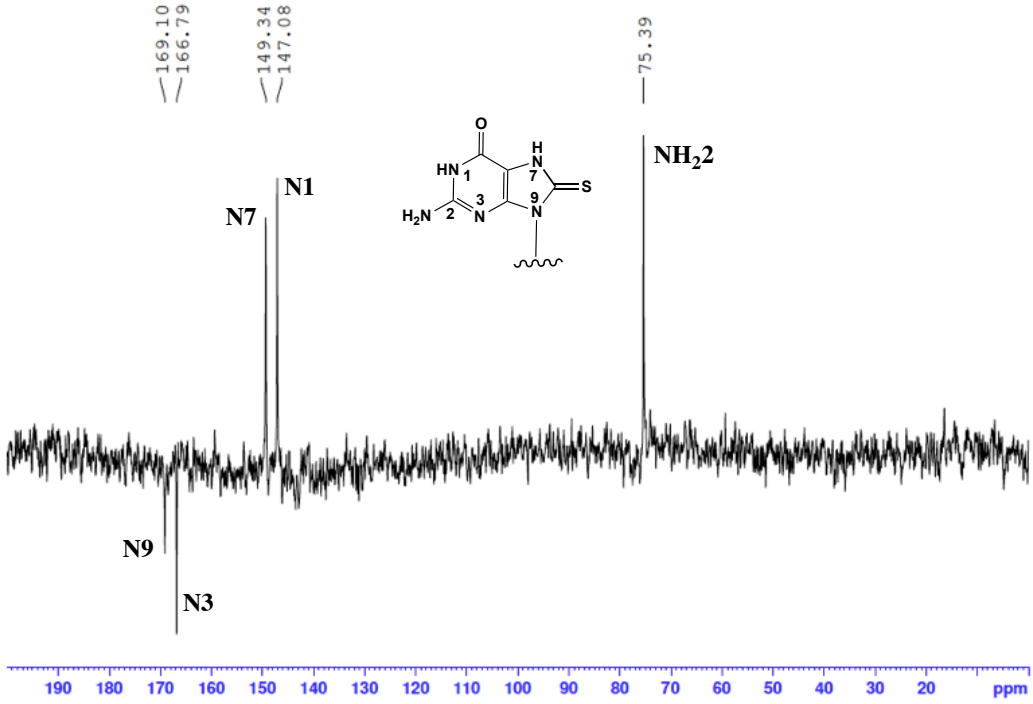


Figure S8: Solution ^{15}N NMR spectrum (60.8 MHz) of 8-thioG **2** in DMSO-d_6.

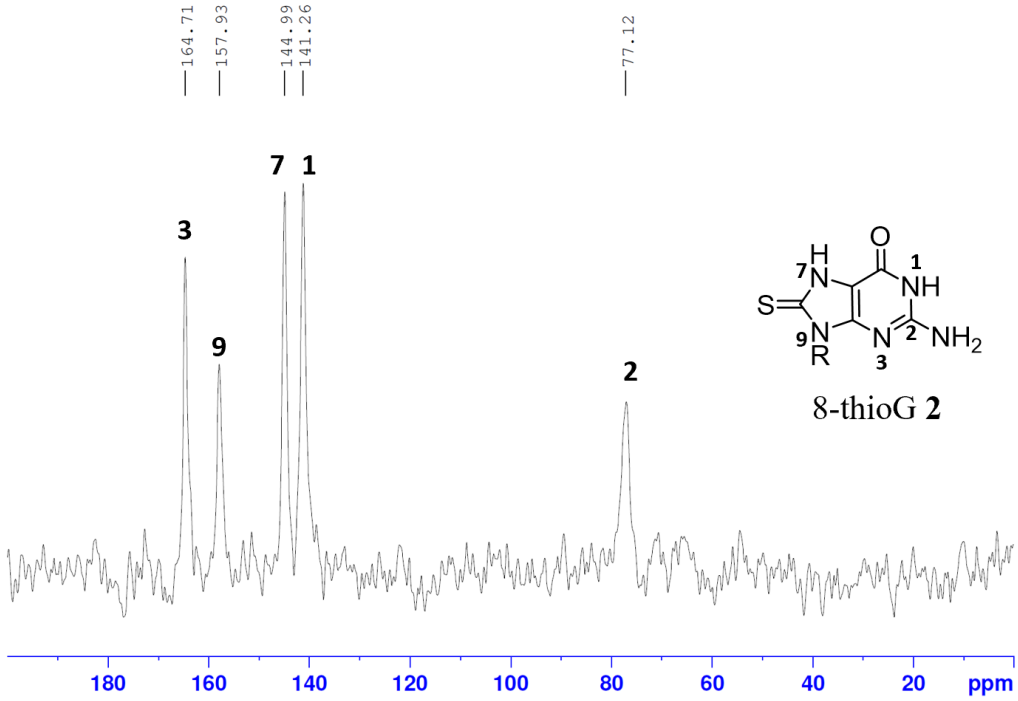
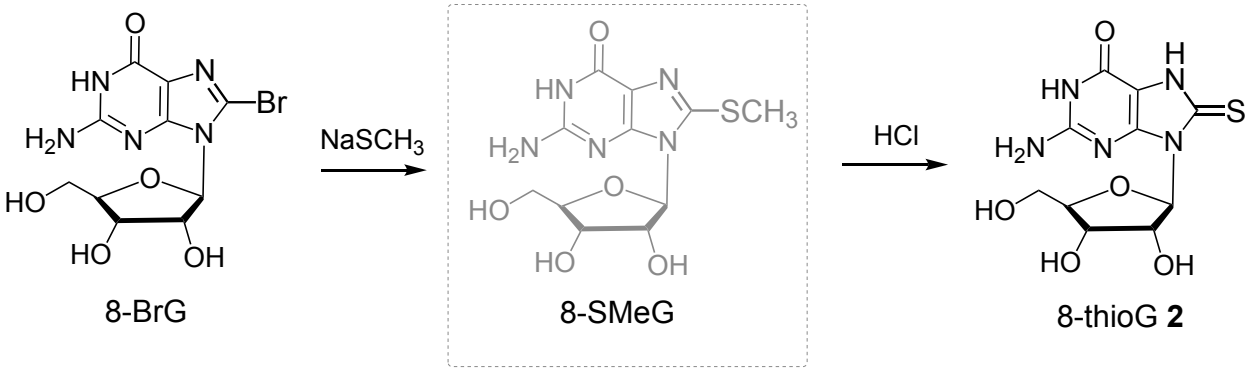


Figure S9: MAS solid-state ^{15}N NMR spectrum (50.7 MHz) of 8-thioG **2**.

Single Crystals of 8-thioG 2



We also attempted to synthesize 8-thiomethylG from 8-bromoG and sodium thiomethoxide (see above). After the acid work-up, we isolated 8-thioG **2** instead. This material was much more crystalline than material made using the literature procedure with thiourea. Thus, we obtained diffraction-quality crystals for X-ray analysis using material obtained from the following procedure: 8-bromoguanosine (100 mg, 0.28 mmol) was added to 1 mL of sodium thiomethoxide solution (21 wt%, 3 mmol) and the mixture was heated at reflux for 18 h. The reaction mixture was filtered to remove insoluble particles and allowed to cool to rt. The filtrate was carefully acidified to pH=2 by adding concentrated HCl, with stirring in a well-ventilated hood. The resulting suspension was cooled on ice and filtered. The solid was rinsed with 1 mL of cold water and 2 mL of acetone. Recrystallization in water give 8-thioG **2** as a crystalline solid (81 mg, 0.26 mmol, 92%). Both solution ^{1}H and ^{13}C NMR spectra of this material were identical to spectra of material made according to the literature approach.

Experimental and Summary of Crystal Structure Data for 8-thioG 2 • 2H$_2$O. A suitable single crystal of $C_{10}H_{17}N_5O_7S$ (UM3255) was selected and measured on a Bruker APEX 2 SMART diffractometer. The crystal was kept at 120(2) K during data collection. The integral intensity was corrected for absorption using SADABS software,[5] via the multi-scan method. Resulting minimum and maximum transmission were 0.862 and 0.990, respectively. The structure was solved with the ShelXT-2014 program,[6] and refined with the ShelXL-2015 program,[7] and least-square minimization using ShelX software.[6] Number of restraints used = 2. The H atoms were located from difference Fourier maps and freely refined. Crystal structure data for 8-thioG **2** • $2H_2O$ was deposited with Cambridge Crystallographic Data Centre as CCDC-1960382.

Table S1 Crystal and Structure Refinement Data for 8-thioG **2** • $2H_2O$

Identification code	UM3255
Empirical formula	$C_{10}H_{17}N_5O_7S$
Formula weight	351.34
Temperature/K	120(2)
Crystal system	monoclinic
Space group	C2
a/Å	23.123(2)
b/Å	9.7734(9)
c/Å	6.3397(6)
α/°	90
β/°	91.2914(14)
γ/°	90
Volume/$Å^3$	1432.3(2)
Z	4
$\rho_{calc}g/cm^3$	1.629
μ/mm^{-1}	0.275
F(000)	736.0
Crystal size/mm^3	0.31 × 0.09 × 0.035
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.524 to 59.968
Index ranges	-32 ≤ h ≤ 32, -13 ≤ k ≤ 13, -8 ≤ l ≤ 8
Reflections collected	8608
Independent reflections	4064 [R_{int} = 0.0213, R_{sigma} = 0.0400]
Data/restraints/parameters	4064/2/242
Goodness-of-fit on F^2	1.186
Final R indexes [I>=2σ (I)]	R_1 = 0.0367, wR_2 = 0.0587
Final R indexes [all data]	R_1 = 0.0452, wR_2 = 0.0596
Largest diff. peak/hole / e $Å^{-3}$	0.30/-0.30
Flack parameter	-0.05(5)

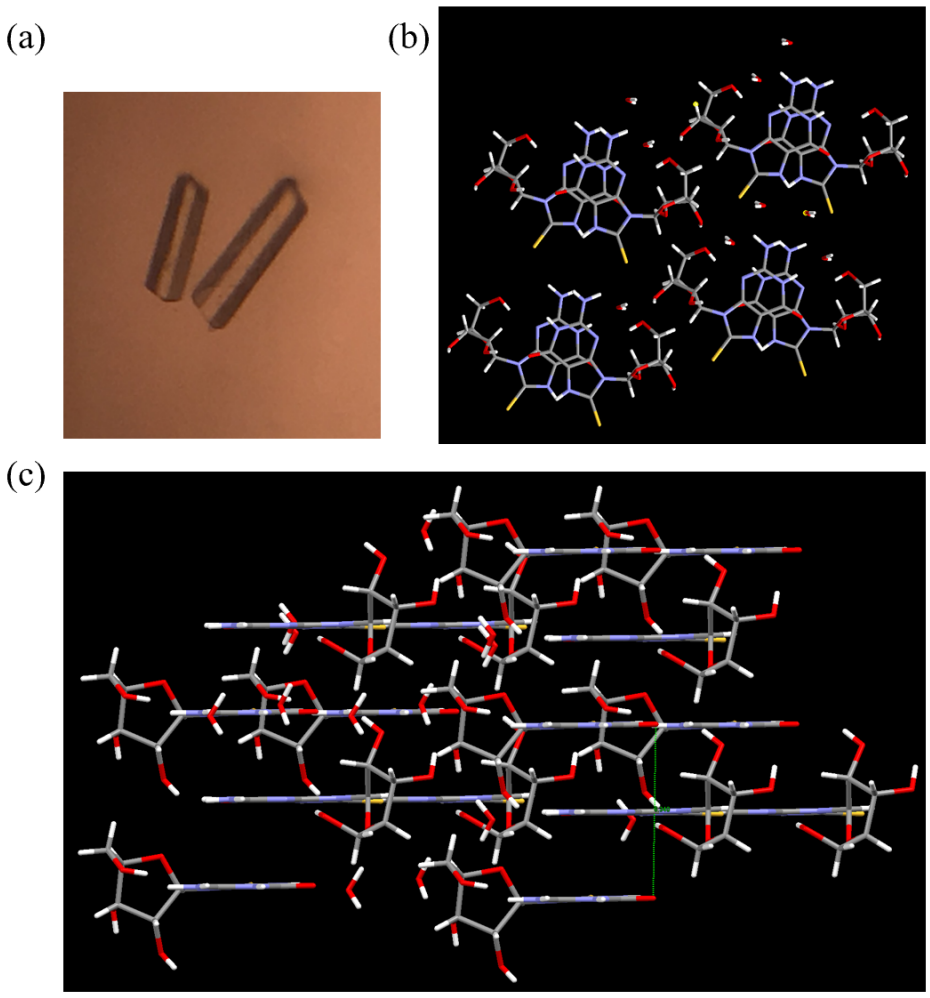
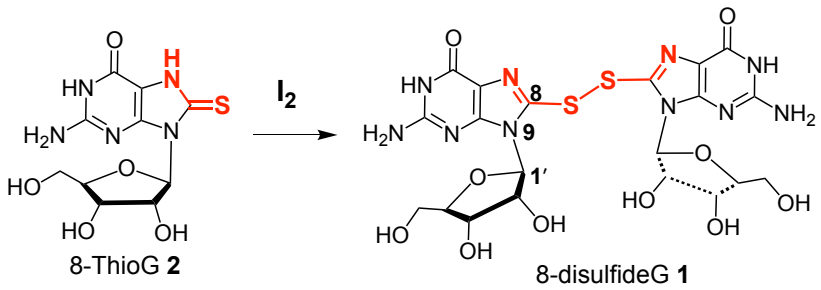


Figure S10: (a) A photo of the crystals of 8-thioG **2** • $2H_2O$ used for X-ray crystallography analysis. (b) Top view and (c) side view showing packing of individual molecules of **2** obtained from the crystal structure of 8-thioG **2** • $2H_2O$.

8-disulfideG 1



To a suspension of 8-thioG **2** (250 mg, 0.80 mmol) in a mixture of methanol (2.5 mL) and acetonitrile (7.5 mL) was added a solution of I_2 in DMSO (10 M, 180 µL, 1.8 mmol). A dark gelatinous mixture formed upon addition of I_2. The mixture was repeatedly shaken and sonicated until we obtained a fine red suspension, which was then stirred at rt for 12 h. The mixture was ultracentrifuged and the solid residue was washed with 15 mL of dichloromethane, followed by 15 mL of diethyl ether. This brown solid contained both disulfide **1** and I_2, as determined by an iodine-starch test. The solid was suspended in 5 mL of deionized water and then concentrated formic acid (88 wt%, 0.83 mL) was added. The mixture was stirred for 1 h. Then, LiOH (75 mg) was added to neutralize any HI and the mixture was stirred overnight at rt. A bright yellow solid, obtained upon ultracentrifugation, was washed with 3 x 5 mL of 12.5 wt% formic acid and 3 x 5 mL of deionized water. The resulting gelatinous solid was lyophilized to give a solid powder that was stirred in 5 mL of diethyl ether for 1 h. The bright yellow solid obtained upon ultracentrifugation was dried in air to afford disulfide **1** (221 mg, 0.35 mmol, 88%).

^{1}H NMR (600 MHz, DMSO-d_6) δ 10.91 (s, 2H, N1H), 6.60 (s, 4H, N2H), 5.93 (d, J = 6.2 Hz, 2H, H1′), 4.99 (t, J = 5.9 Hz, 2H, H2′), 4.18 (dd, J = 5.0, 3.7 Hz, 2H, H3′), 3.82 (dd, J = 4.8 Hz, J = 3.6 Hz, 2H, H4′), 3.66 (dd, J = 11.8, 4.9 Hz, 2H, H5′), 3.54 (dd, J = 11.8, 5.5 Hz, 2H, H5″).

^{13}C NMR (151 MHz, DMSO-d_6) δ 156.19 (C6), 153.82 (C2), 152.54 (C4), 139.41 (C8), 118.59 (C5), 88.77 (C1′), 85.69 (C4′), 71.08 (C2′), 70.60 (C3′), 61.96 (C5′).

MALDI-MS: m/z = 631.019 ($M + Li^+$), 650.925 ($M + Na^+$), 666.974 ($M + K^+$)

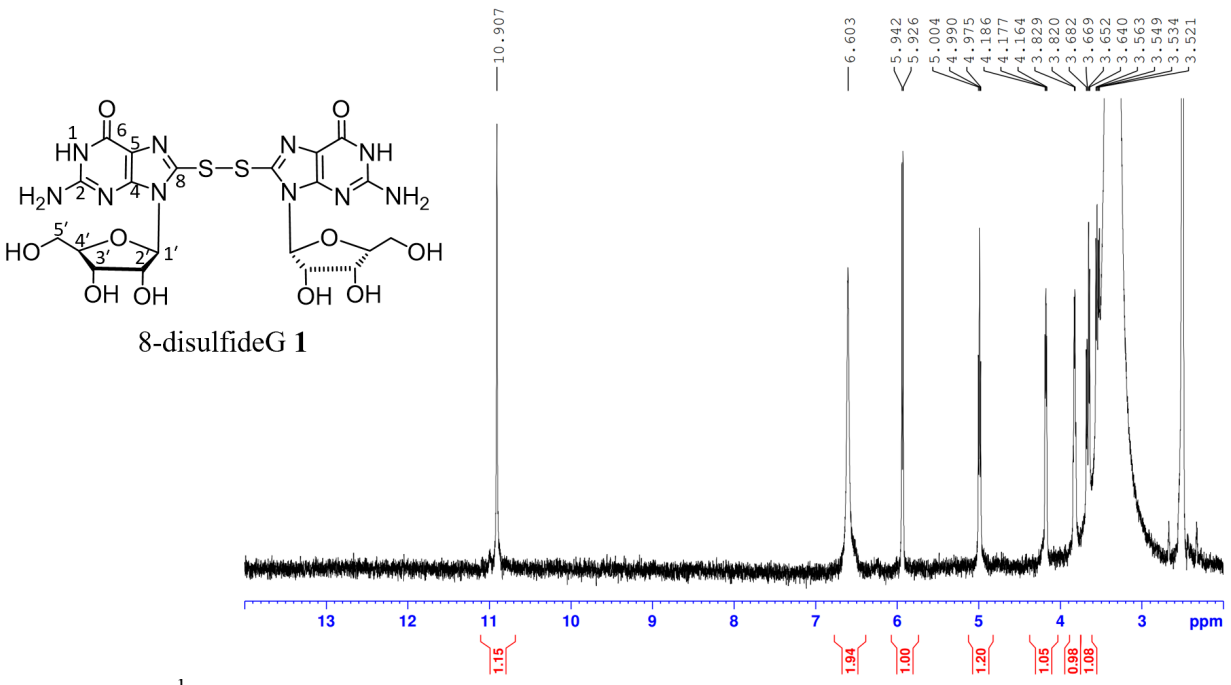


Figure S11: ^{1}H NMR spectrum of 8-disulfideG **1** in DMSO-d_6

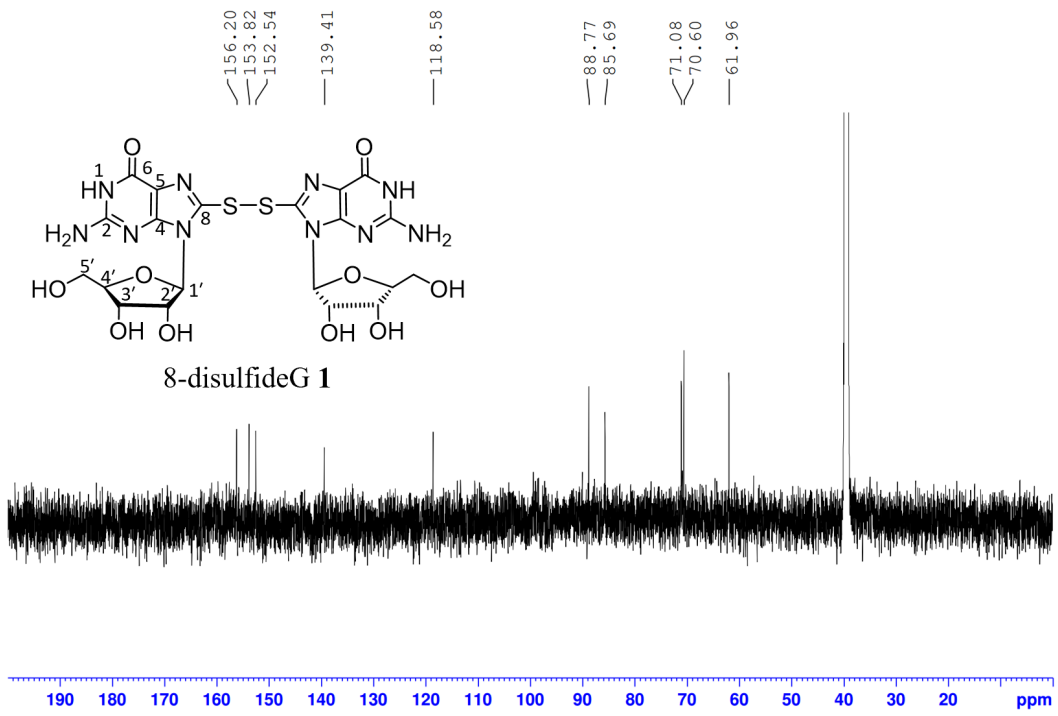


Figure S12: ^{13}C NMR spectrum of 8-disulfideG **1** in DMSO-d_6

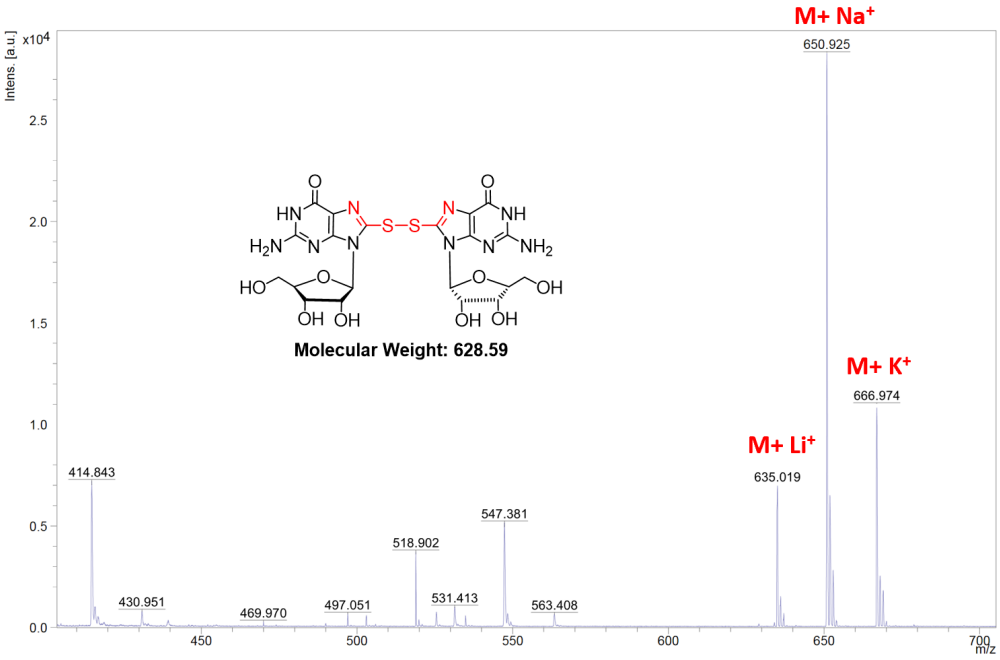


Figure S13: MALDI-TOF mass spectrum of 8-disulfideG **1** (mw 628.59) shows peaks that correspond to the mass of **1** + Li^+, Na^+ and K^+, respectively.

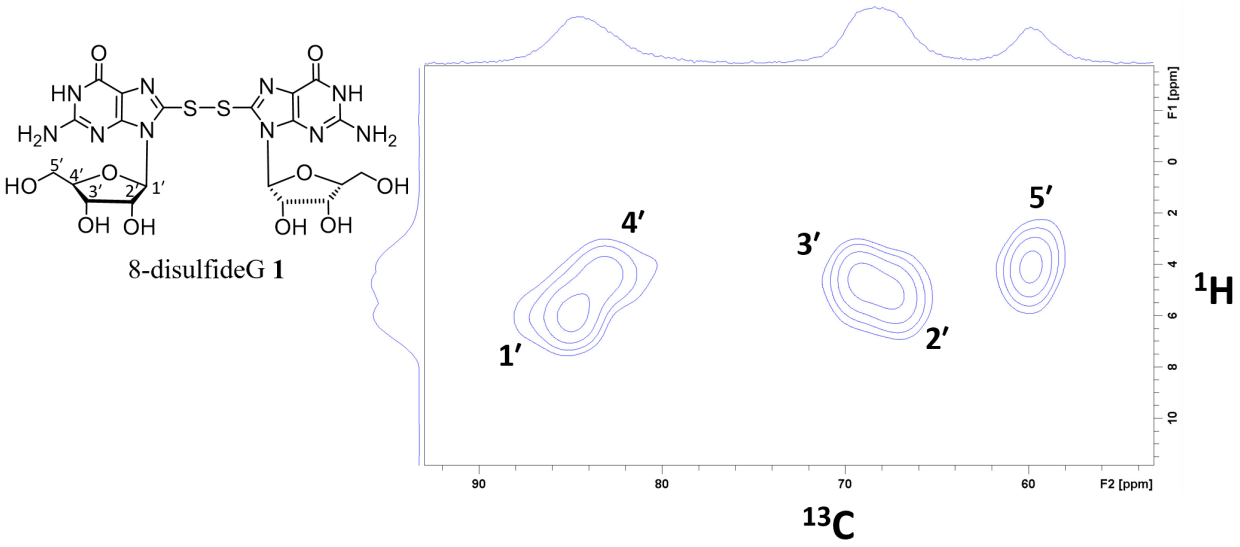


Figure S14: MAS solid-state ^{13}C-^{1}H HETCOR 2D NMR spectrum of disulfide **1**. This experiment allowed us to assign ribose ^{13}C resonances.

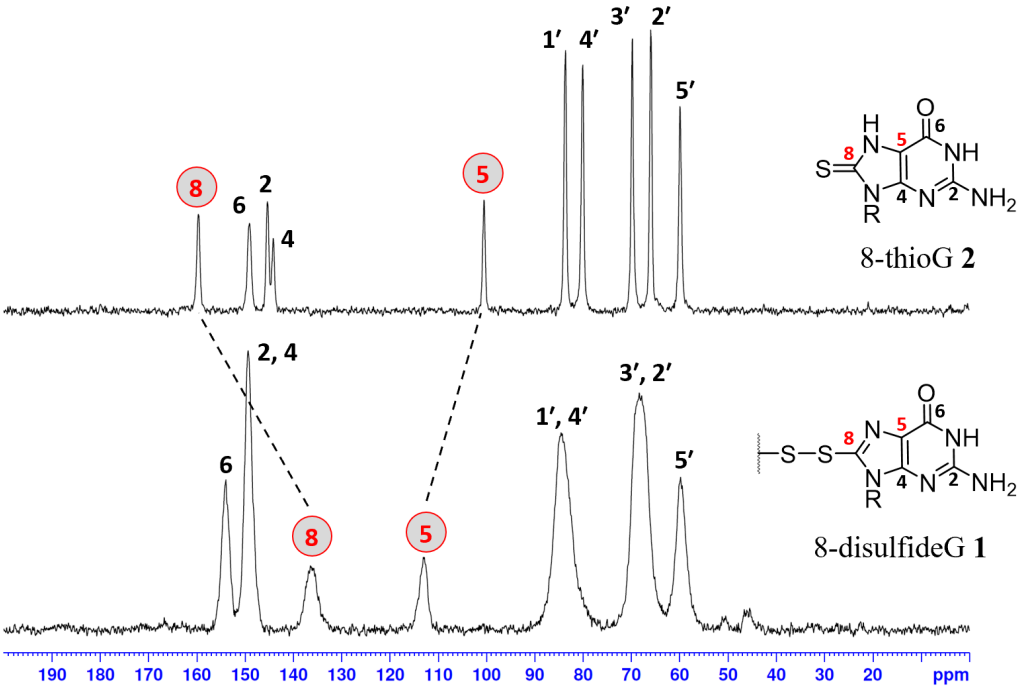


Figure S15: A comparison of MAS solid-state ^{13}C NMR spectra for 8-thioG **2** (above) and disulfide **1** (below). Note the significant changes in chemical shifts for C8 and C5, consistent with the change in chemical environment at those atoms upon oxidation of **2** to disulfide **1**.[8]

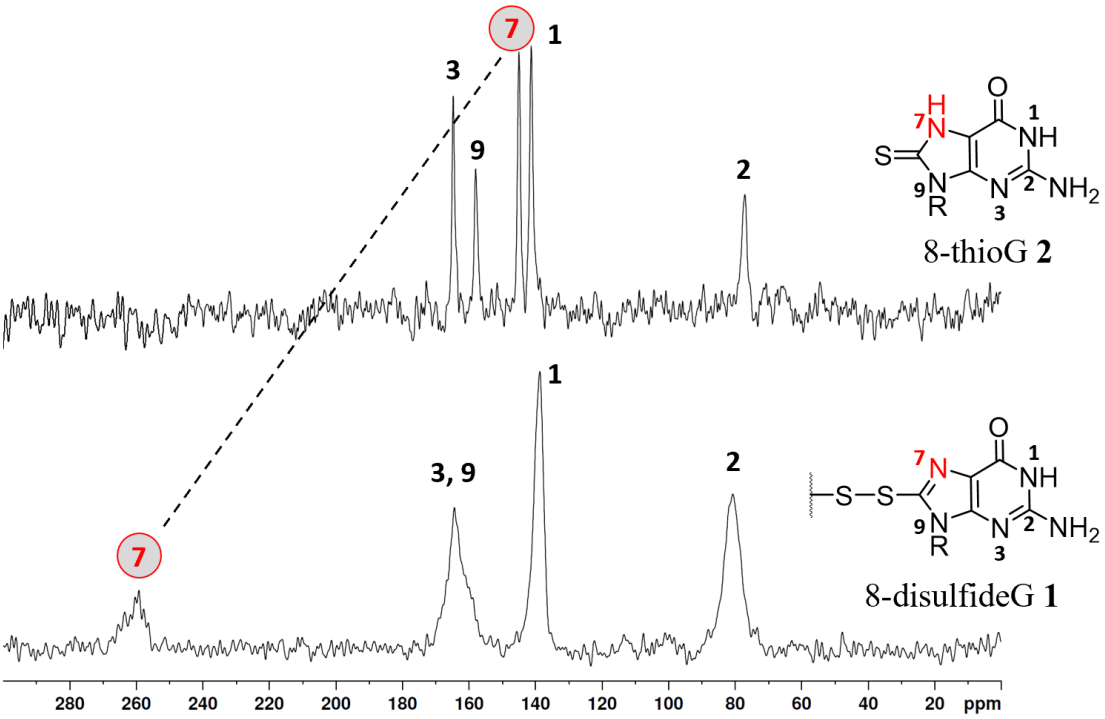


Figure S16: A comparison of MAS solid-state ^{15}N NMR spectra for 8-thioG **2** (above) and disulfide **1** (below). Note the significant changes in chemical shift for N7, which is consistent with the change in hybridization at that nitrogen atom upon oxidation to disulfide **1**.[9]

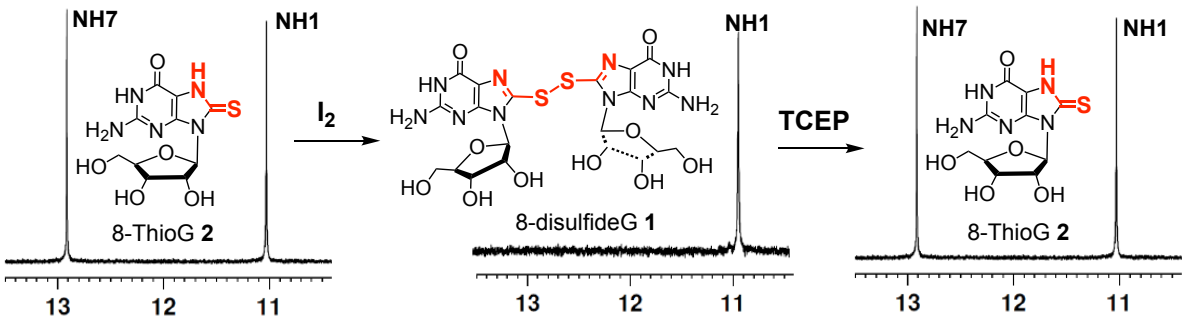


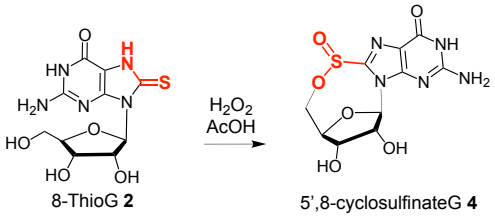
Figure S17: ^{1}H NMR spectra showing resonances for NH protons, as 8-thioG **2** (left) was oxidized to disulfide **1** and then reduced back to 8-thioG **2** with TCEP. In this experiment, 8-disulfide 1 (10 mg) was suspended in water (0.5 mL) after which a stock solution containing 1 eq TCEP relative to was added to the suspension. The mixture was vigorously shaken. The yellow color for compound 1 disappears within 1 min and white crystals form at the same time. The resulting solid was dried in air and dissolved in DMSO-d_6 for NMR analysis.

8, 5′-cyclosulfinateG 4

Compound **4** can be made by oxidation of either 8-thioG **2** or disulfide **1** using excess H_2O_2.

Method 1 from 8-thioG **2**:

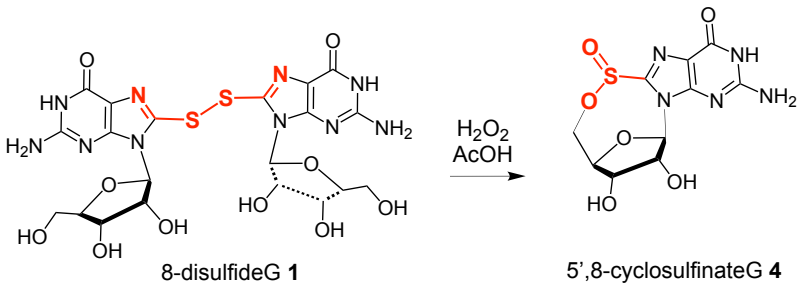
To a suspension of 8-thioG **2** (85 mg, 0.258 mmol) in deionized water (7 mL) was added glacial acetic acid (425 µL, 0.874 mmol) and concentrated H_2O_2 (50 wt%, 111 µL, 1.95 mmol). The heterogeneous mixture was stirred at 65 °C for 48 h. The suspension turned yellow after 30 min, indicating formation of disulfide **1**, and then became off-white over time. The mixture was filtered and washed with 5 mL of deionized water and then 3 mL of acetone. The white solid was dried to give **4** (36.2 mg, 0.110 mmol, 42.6%).



8-ThioG **2** 5',8-cyclosulfinateG **4**

Method 2 from disulfide **1**:

To a suspension of 8-disulfideG **1** (10 mg, 16 µmol) in deionized water (1 mL) was added glacial acetic acid (50 µL) and an aqueous stock solution of H_2O_2 (400 mM, 0.56 mL). The heterogeneous mixture was stirred at rt for 4 days. The reaction mixture was ultracentrifuged and the resulting solid was washed with 0.5 mL deionized water and 0.5 mL acetone. The white solid was dried in air to give **4**.



8-disulfideG **1** 5',8-cyclosulfinateG **4**

^{1}H NMR (600 MHz, DMSO-d_6) δ 10.78 (s, 1H, N1H), 6.76 (s, 2H, N2H), 5.79 (s, 1H, H1′), 5.62 (d, J = 4.0 Hz, 1H, 2′-OH), 5.43 (d, J = 5.6 Hz, 1H, 3′-OH), 4.74 (dd, J = 13.0, 2.7 Hz, 1H, H5′), 4.40 (d, J = 13.1 Hz, 1H, H5″), 4.33 (t, J = 3.8 Hz, 1H, H2′), 4.24 (dd, J = 7.5, 2.6 Hz, 1H, H4′), 4.06 (m, 1H, H3′).

^{13}C NMR (151 MHz, DMSO-d_6) δ 156.75 (C6), 154.67 (C2), 151.79 (C4), 146.98 (C8), 117.28 (C5), 91.65 (C1′), 82.92 (C4′), 74.48 (C2′), 69.17 (C3′), 68.59 (C5′).

ESI-MS ($[M + H]^+$): m/z = 330.07 (MW=329.29)

IR: 1140 cm^{-1} corresponds to S=O stretch in a sulfinate ester.[8]

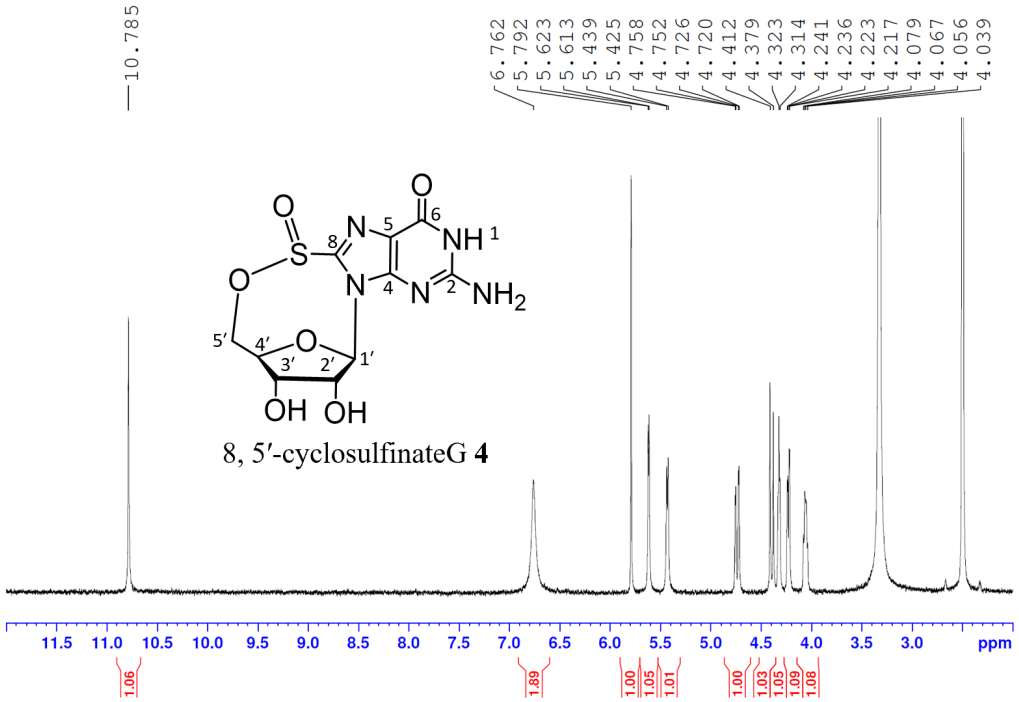


Figure S18: ^{1}H NMR spectrum of 8, 5′-cyclosulfinateG **4** in DMSO-d$_6$

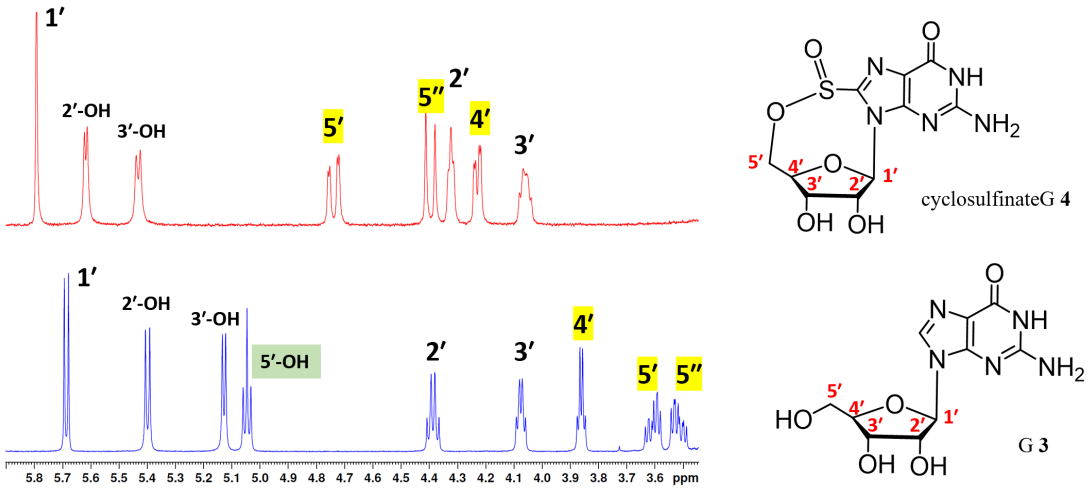
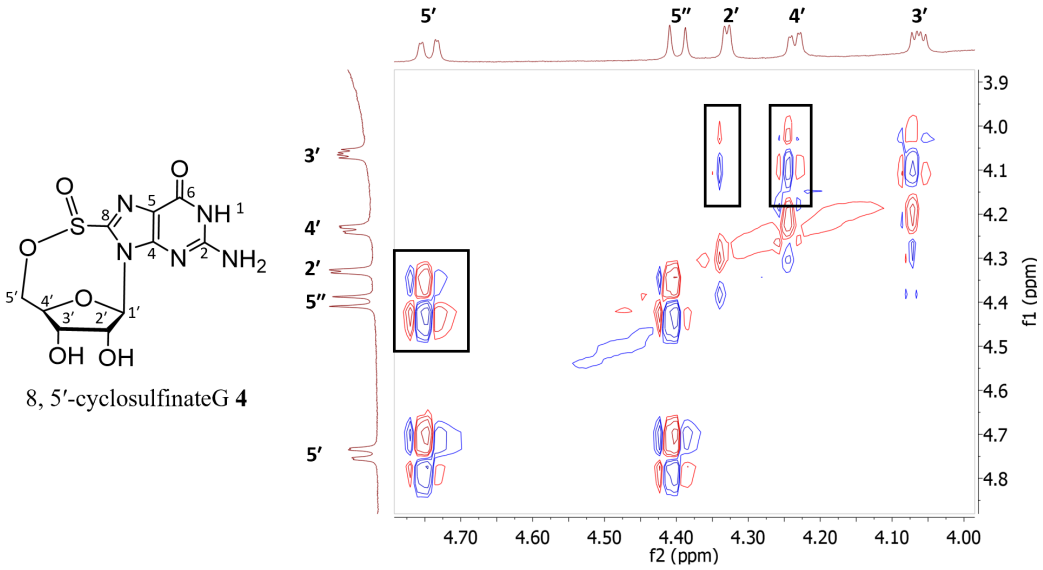
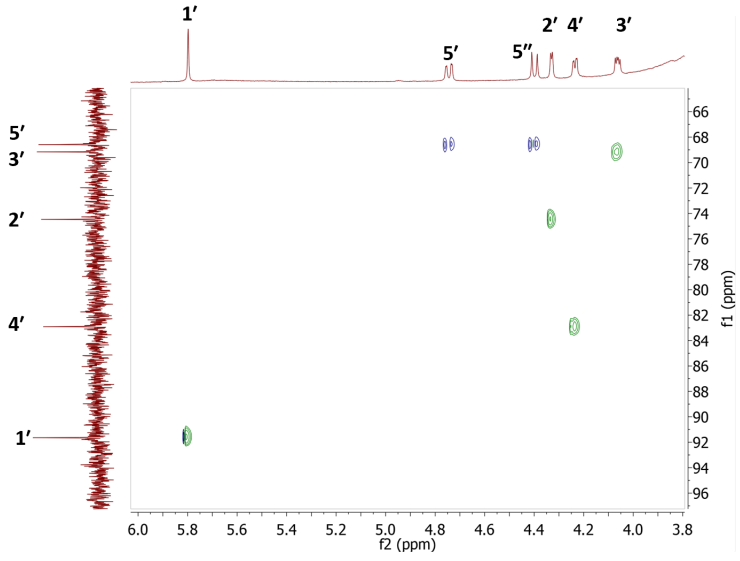


Figure S19: ^{1}H NMR spectra comparing the ribose region for cyclosulfinateG **4** and G **3**. Signals for diastereotopic H5′ and H5″ in **4** are shifted downfield, consistent with an electron withdrawing substituent at C5′; 2) H5′ and H5″ resonances are 0.34 ppm apart and show distinct ^{3}J couplings to H4′, consistent with these hydrogens being constrained in unique environments by the 8,5′ ring; 3) although signals for 2′-OH and 3′-OH exist, there is no resonance for 5′-OH.



8, 5′-cyclosulfinateG **4**

Figure S20: ^{1}H-^{1}H COSY spectra of 8,5′-cyclosulfinateG **4** in DMSO-d$_6$. This experiment, combined with ^{1}H-^{13}C HSQC, allowed us to assign the ribose protons.



8, 5′-cyclosulfinateG **4**

Figure S21: ^{1}H-^{13}C HSQC spectrum of 8,5′-cyclosulfinateG **4** in DMSO-d$_6$ Blue cross peaks correspond to CH_2 groups while green cross peaks correspond to CH groups.

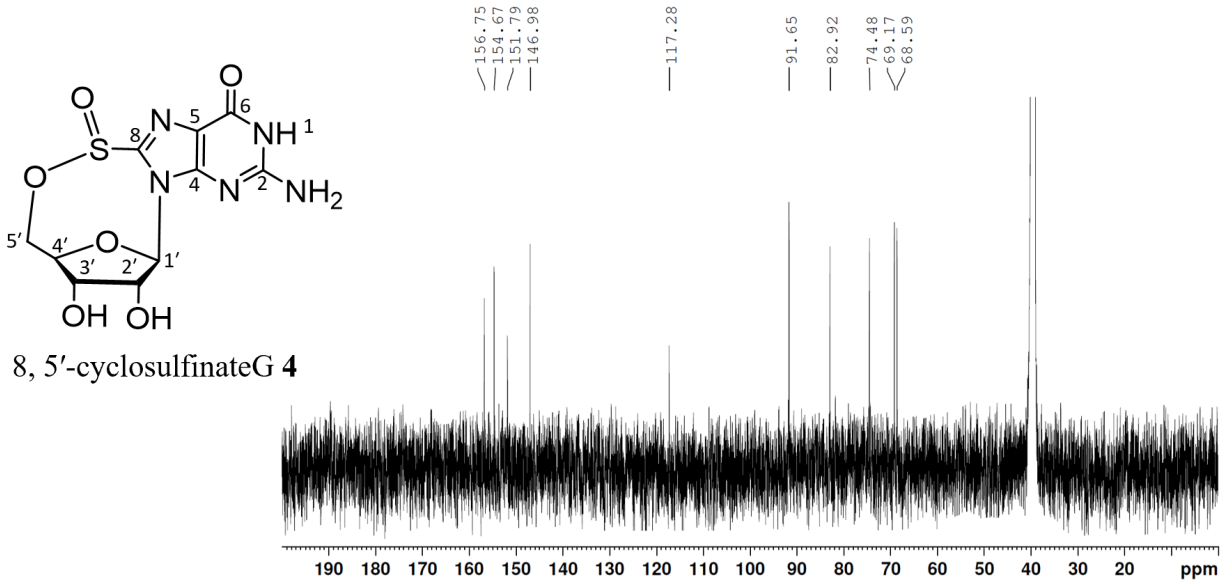


Figure S22: ^{13}C NMR spectrum of 8, 5′-cyclosulfinateG **4** in DMSO-d_6

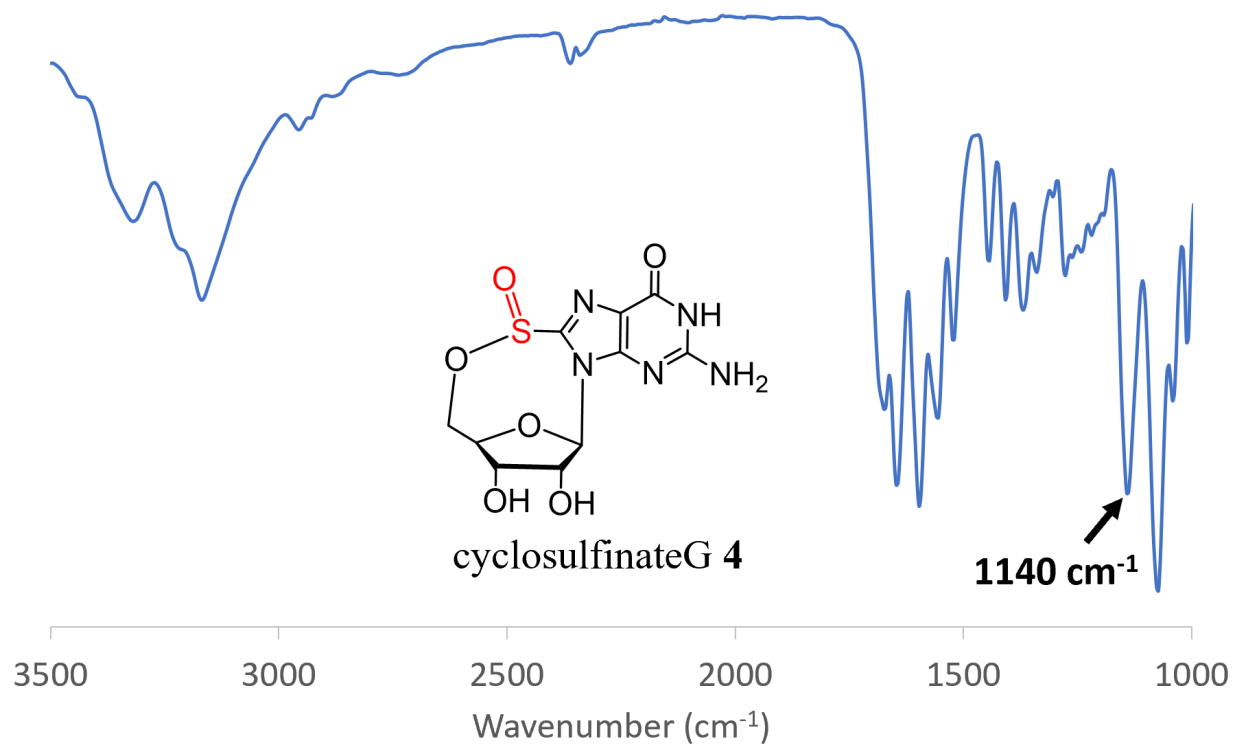
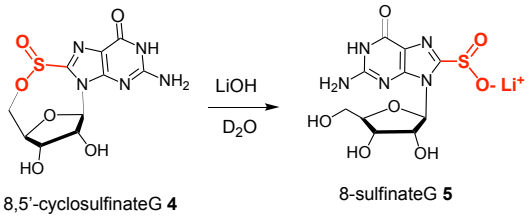


Figure S23: IR spectrum of cyclosulfinateG **4** contains a peak at 1140 cm^{-1} that corresponds to an S=O stretching frequency in a sulfinate ester.[10]

8-sulfinateG 5

To a suspension of 8,5′-cyclosulfinateG **4** (5 mg, 0.015 mmol) in D_2O (0.5 mL) was added a stock solution of 400 mM LiOH in D_2O (76 µL, 2 eq). The mixture was sonicated and transferred to an NMR tube. Hydrolysis of **4** was followed *in situ* by ^1H and ^{13}C NMR. For ^{13}C NMR analysis, 1 mg of TMSP-d_4 (3-(trimethylsilyl)propionic-2,2,3,3-d_4 acid sodium salt) was added to the solution as a chemical shift standard, and the chemical shift for the methyl carbons in TMSP-d_4 was set to δ=0 ppm.



^1H NMR (600 MHz, D_2O): δ 6.51 (d, J = 7.3 Hz, 1H, H1′), 4.96 (dd, J = 7.3, 5.4 Hz, 1H, H2′), 4.46 (dd, J = 2.0, 5.4 Hz, 1H, H3′), 4.30 (q, J = 2.2 Hz, 1H, H4′), 3.94 (dd, J = 13.0, 2.3 Hz, 1H, H5′), 3.85 (dd, J = 13.0, 2.6 Hz, 1H, H5″).

^{13}C NMR (150 MHz, D_2O): δ 170.39, 163.12, 158.88, 154.78, 120.02, 90.88, 89.09, 75.49, 74.08, 65.12.

ESI-MS ($[M - H]^-$): m/z = 345.88 (MW=346.29)

IR: Intense and broad peaks at 1040 cm^{-1} and 977 cm^{-1} are characteristic of asymmetric and symmetric stretches for aromatic sulfinate anions.

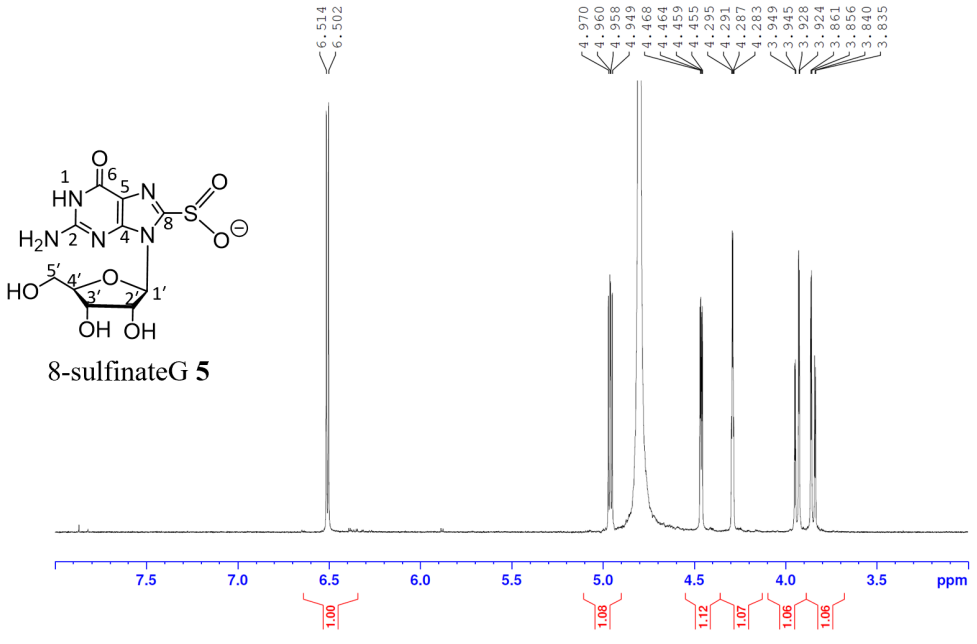


Figure S24: ^1H NMR spectrum of 8-sulfinateG **5** in D_2O.

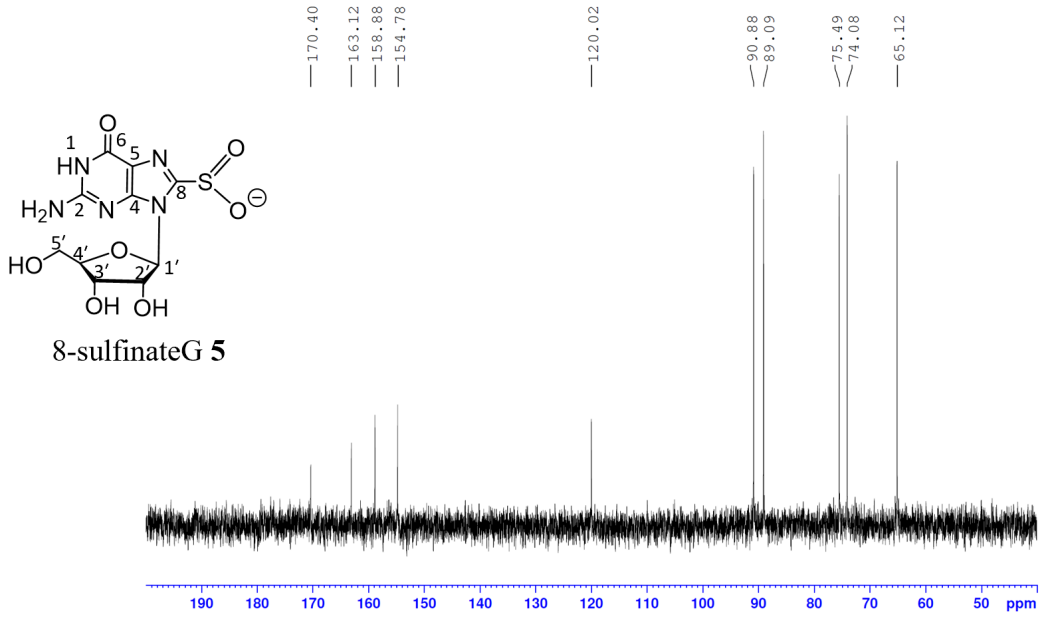


Figure S25: ^{13}C NMR spectrum of 8-sulfinateG **5** in D_2O.

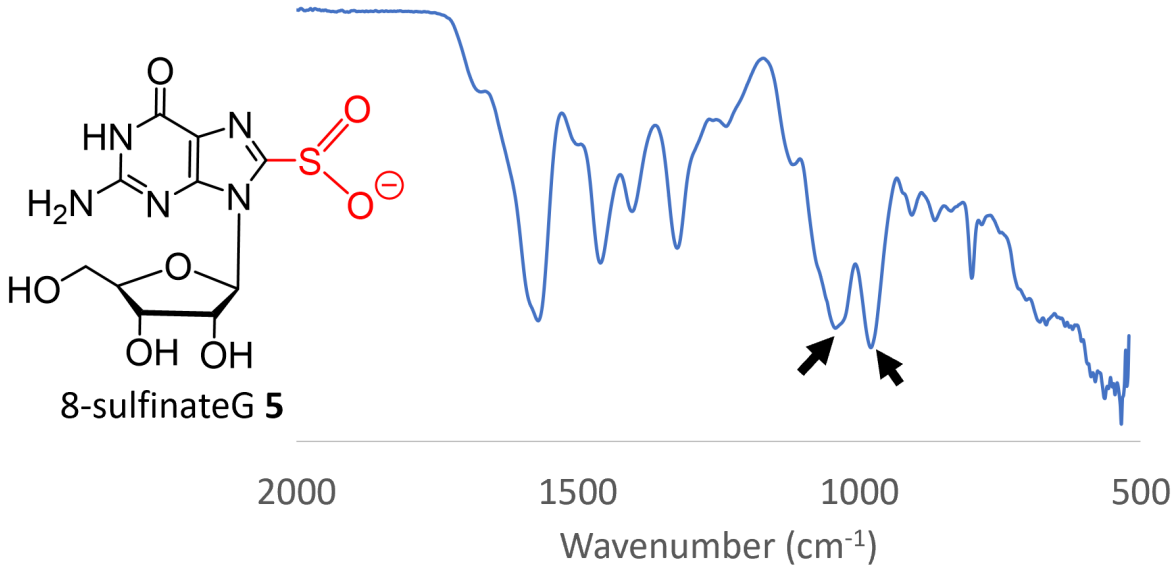


Figure S26: IR spectrum of the Li^+ salt of 8-sulfinateG **5** (lyophilized sample) shows two peaks at 1040 and 977 cm^{-1} (see arrows) which correspond to the asymmetric and symmetric stretch for a sulfinate ester. [11]

Hydrogel Section

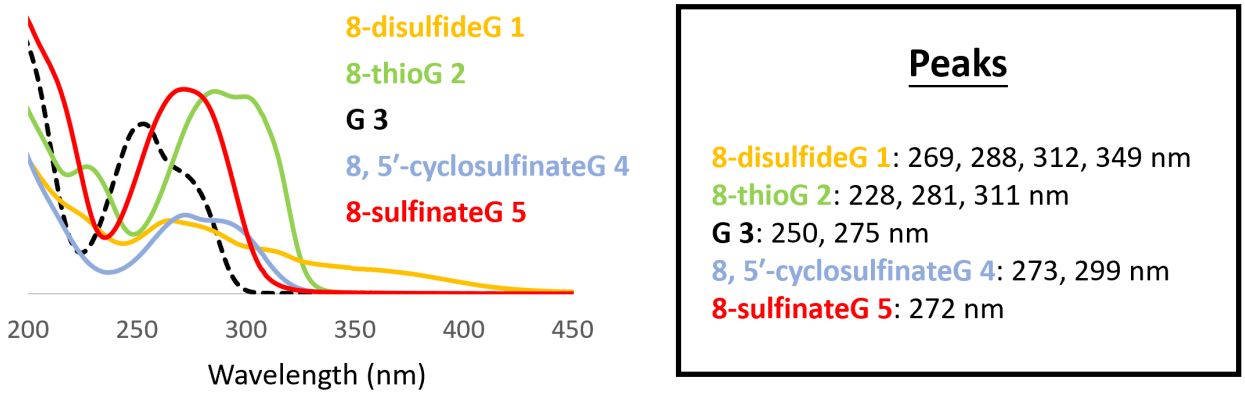


Figure S27: UV-vis spectra and absorption peaks of all compounds **1-5** in this work.

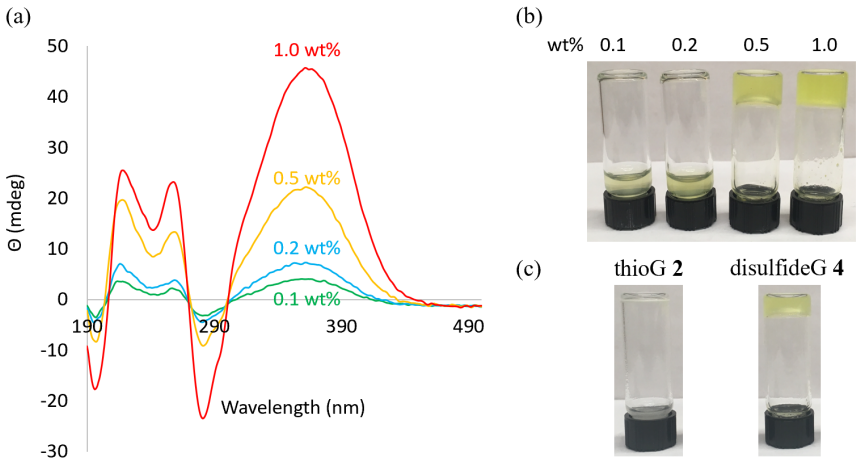


Figure S28: (a) CD spectra of hydrogels (0.5 and 1 wt %) or solutions (0.2 and 0.1 wt %) containing 8-disulfideG **1.** Spectra were taken 24 h after making the solutions/hydrogels. (b) Photos of solutions/hydrogels of 8-disulfideG **1** hydrogels used for CD analysis. (c) Photos show that 8-disulfideG **1** (0.5 wt %) gives a self-standing hydrogel, whereas 8-thioG **2** (0.5 wt %) gives a suspension in water.

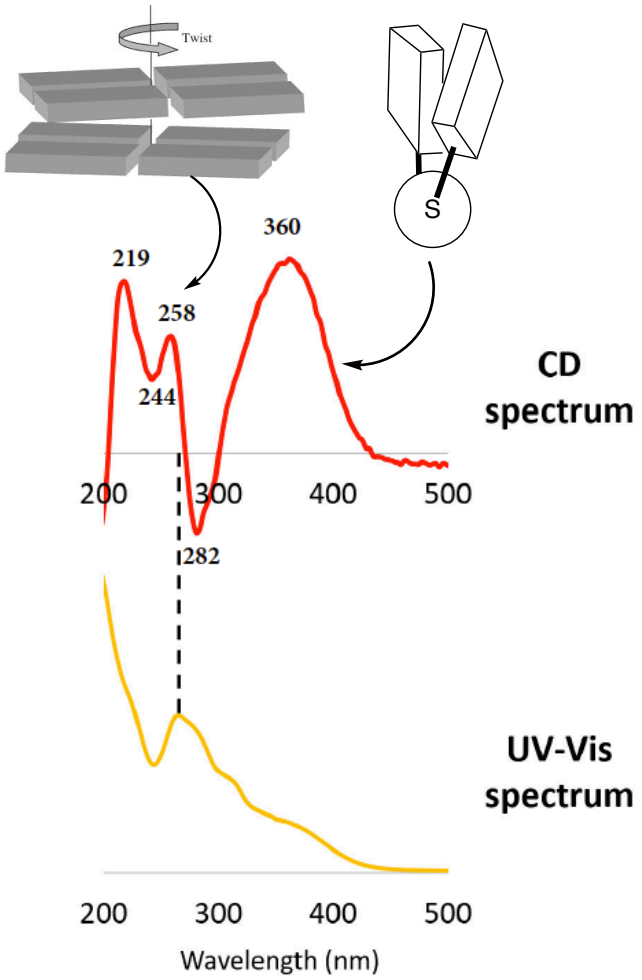


Figure S29: Stack plot of the CD spectrum of a hydrogel made from 8-disulfideG **1** (0.5 wt %, 8 mM) on top of a UV spectrum of a dilute aqeous solution of 8-disulfideG **1**. The exciton centered at 270 nm (peak at 258 nm and trough at 282 nm) in the CD spectrum is diagnostic of a chirality axis down the middle of a stack of twisted G-quartets.[12] The peak at 360 nm indicates axial chirality about the S-S bond.

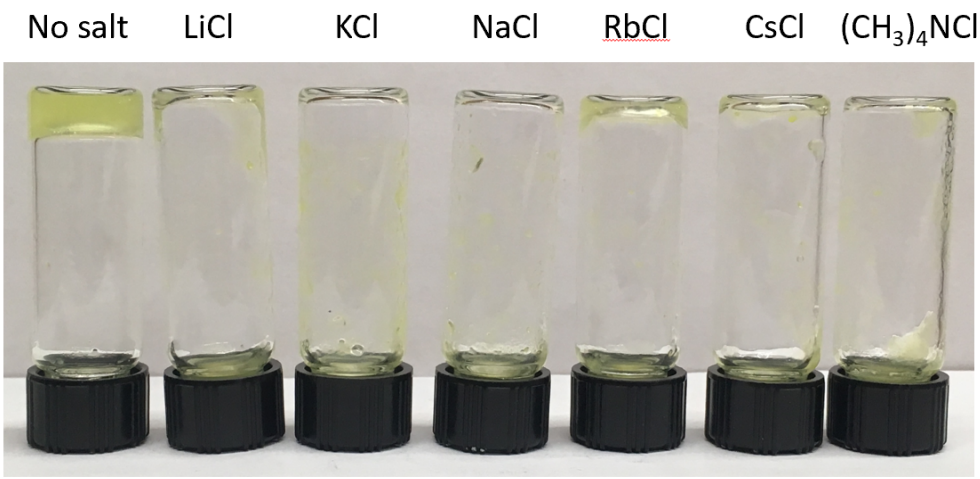


Figure S30: Addition of salts containing monovalent cations apparently inhibit formation of hydrogels by 8-disulfideG **1**. Each vial contained disulfide **1** (8 mM, 0.5 wt%) and 1 mol equiv of salt (8 mM) in 0.5 mL of water. All samples had been thoroughly sonicated and shaken to break up visible aggregates. The resulting suspensions were allowed to sit at ambient temperature for 30 min before inverting the vials and taking this photograph. The sample of disulfide **1** on the left, without added salt, formed a self-standing hydrogel. All the other samples contained free-flowing suspensions with noticeable aggregates. We observed no gelation of the samples containing added salt even after 1 week.

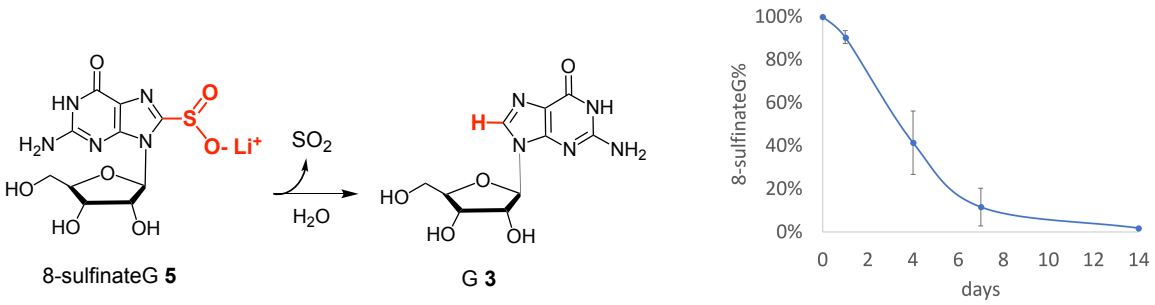


Figure S31: The 8-sulfinateG **5** loses SO_2 to give guanosine **3**. The amount of **5** as a function of time was determined by ^{1}H NMR. The above graph shows the % 8-sulfinateG **5** (30 mM) in a basic solution containing 2 equiv of LiOH at rt as a function of time. Complete desulfurization to give G **3** takes 2 weeks. TMSP-d_4 (3-(trimethylsilyl)propionic-2,2,3,3-d_4 acid sodium salt) was added as an internal standard for NMR analysis. Experiments were done in triplicate.

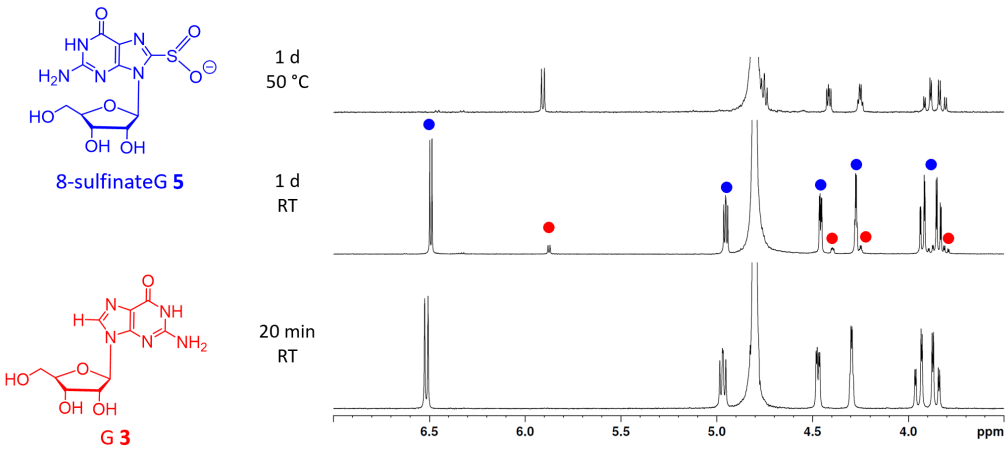


Figure S32: ^{1}H NMR shows conversion of 8-sulfinateG **5** (blue dots, 30 mM) to G **3** (red dots) at 50 °C and at rt. After 1 day at 50 °C conversion of 8-sulfinateG **5** to G **3** was complete.

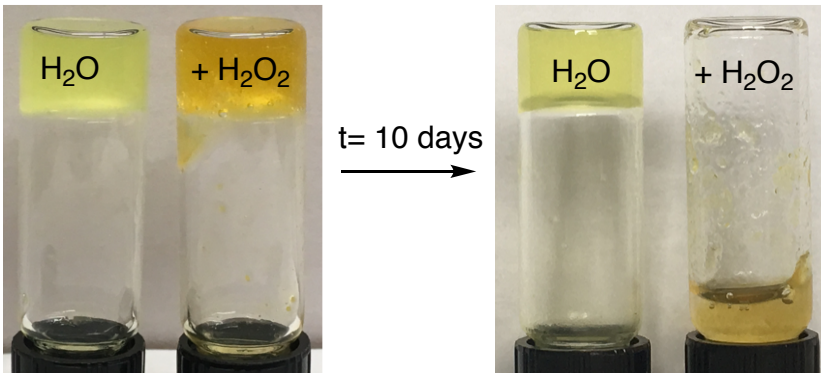


Figure S33: Photographs of hydrogels made from 8-disulfideG **1** (0.5 wt%, 8 mM) and either water (vial on left) or an aqeuous solution of H_2O_2 (112 mM) and acetic acid (51 mM). After 10 days the self-standing hydrogel containing H_2O_2 had completely disassembled to give a solution.

Section on Computation

Computational Methods and Results. All optimizations were carried out using DFT calculation with the B3LYP method and 6-31g(d) basis set.[13] Dispersion was included and the solvent water using CPCM model was selected.[14] Vibrational frequencies were computed at the same level to obtain enthalpic and free energy corrections at 298 K and to characterize the minima (zero imaginary frequencies). This method provided excellent agreement with available X-ray structural information (see manuscript). Further, to refine energetics, we carried out single point energy calculations using a larger basis set Def2-SVP,[15] with other settings unchanged. Structural figures were generated using CLYview.[16]

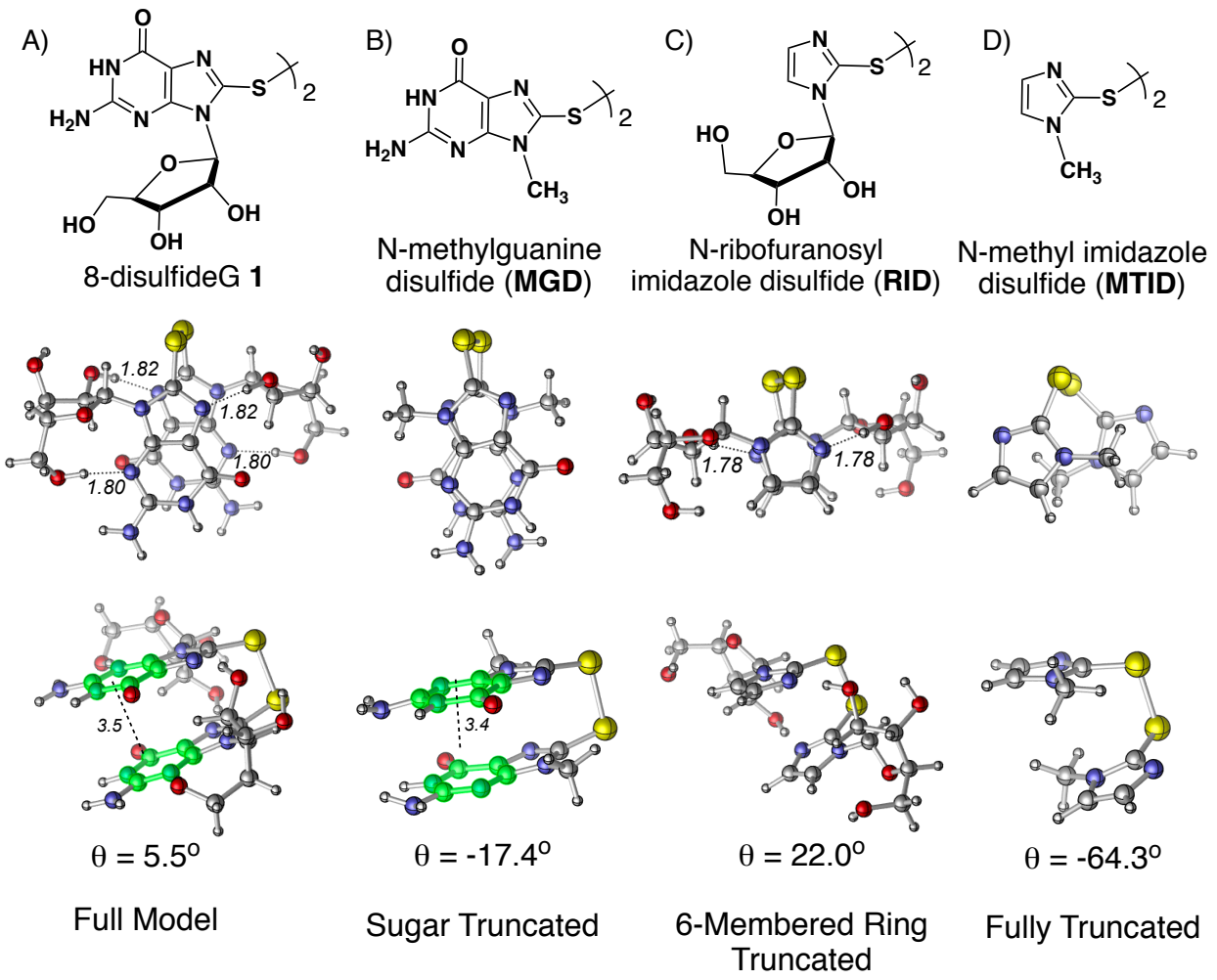


Figure S34. We performed optimizations using B3LYP-D3/6-31G(d)-CPCM (water) and carried out single point energy calculations using a larger basis set B3LYP-D3/Def2SVP-CPCM (water) to refine energetics for 4 different compounds 8-thioguanosine disulfide **1** and 3 model compounds: N-methylguanine disulfide (**MGD**), N-ribofuranosyl imidazole disulfide (**RID**) and N-methyl imidazole disulfide (**MTID**). These model compounds were chosen to probe the impact of the sugar and the purine's 6-membered ring on the conformation of 8-thioguanosine disulfide **1**. The lowest energy conformers for the full and truncated models are shown above in both top and side views. A) The C-S-S-C dihedral angle for 8-thioguanosine disulfide **1** is θ= 5.5° with 4 hydrogen bonds. This nearly eclipsed conformation results in significant π stacking between the 2 purine rings. B) The C-S-S-C dihedral angle for **MGD** is θ= -17.4° and shows significant π-stacking interactions between the 2 purine rings. C) **RID** has θ= 22.0° with 2 hydrogen bonds and still maintains significant π-stacking interactions. D) The lowest energy structure for the fully truncated **MTID** has θ= -64.3°, more in line with a typical disulfide bond.

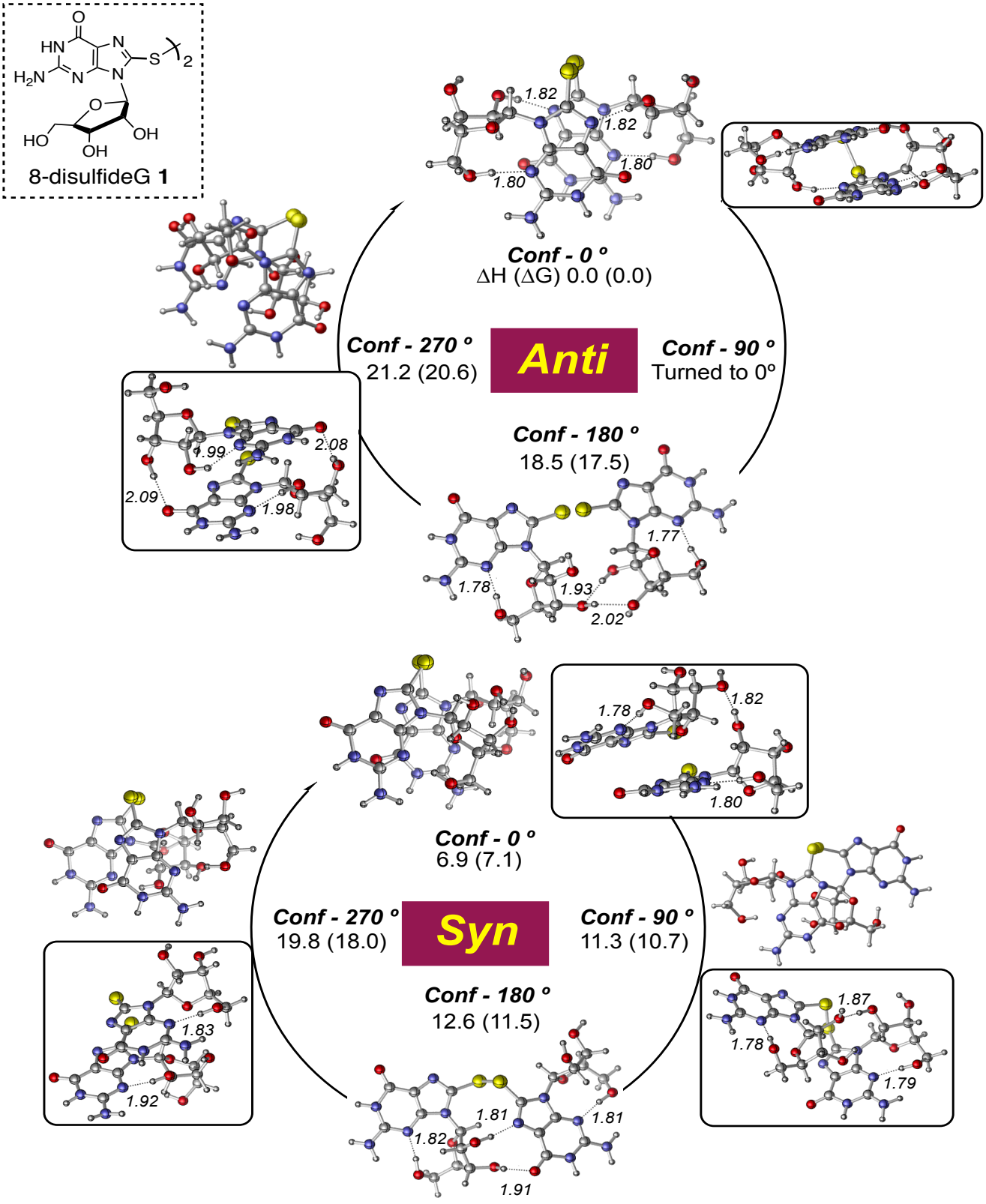


Figure S35. Conformational search of the dihedral angle for the C8-S-S-C8 bond in 8-disulfide G **1**. The **Anti-Conf-0º** is lowest in energy. The next lowest energy conformer is the **Syn-Conf-0º**. *Anti/syn* refers to the orientation of the purine C6 carbonyl group, either pointing in opposite directions (*anti*-parallel) or in the same direction (*syn* or parallel alignment). Level of theory B3LYP-D3/Def2SVP-CPCM(water)//B3LYP-D3/6-31G(d)-CPCM(water).

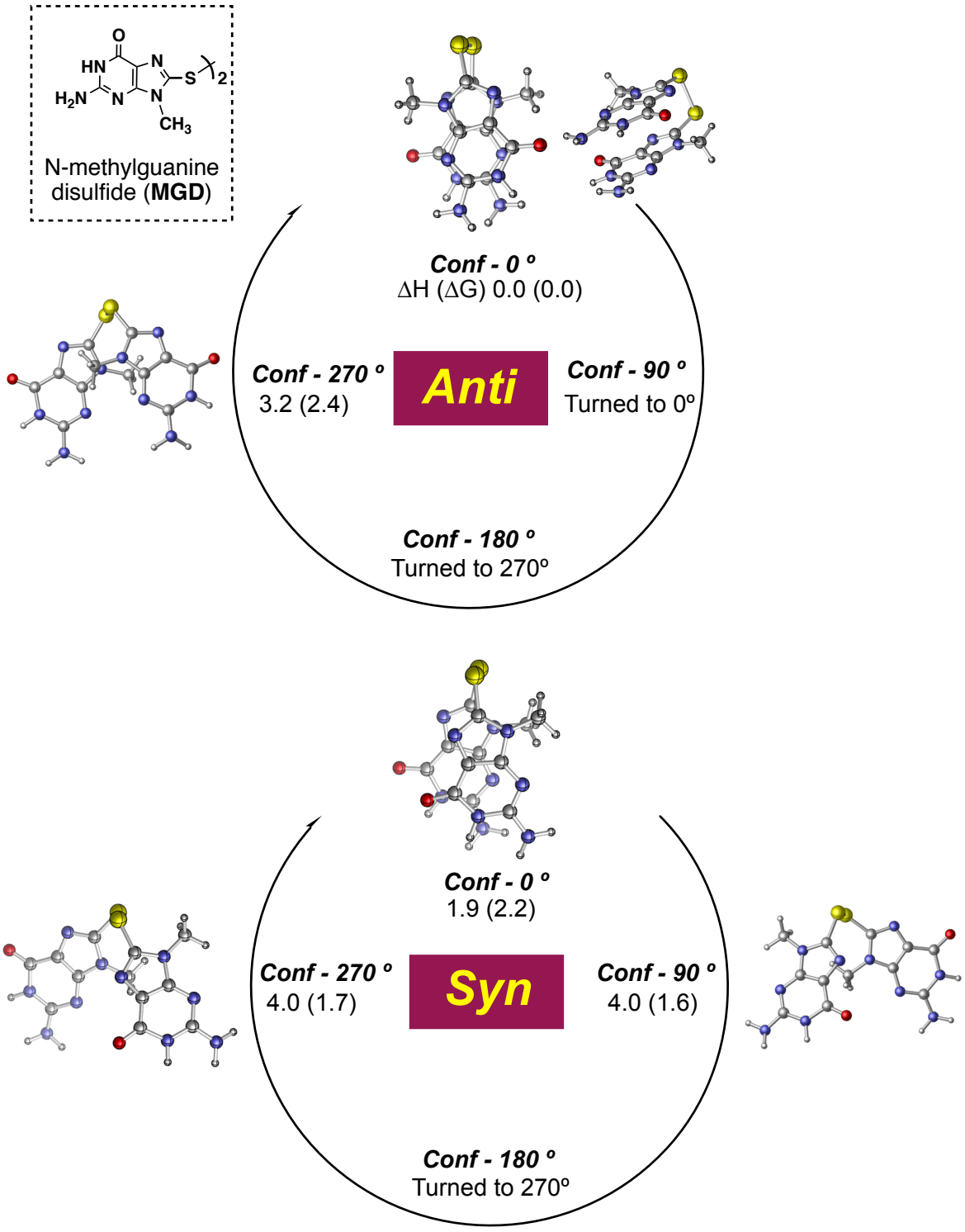


Figure S35. Conformational search of the dihedral angle for the C8-S-S-C8 bond in N-methyl-guanine disulfide (**MGD**). The **Anti-Conf-0º** is lowest in energy. The next lowest energy conformer is the **Syn-Conf-0º**. *Anti/syn* refers to the orientation of the purine C6 carbonyl group, either pointing in opposite directions (*anti*-parallel) or in the same direction (*syn* or parallel alignment). Level of theory B3LYP-D3/Def2SVP-CPCM(water)//B3LYP-D3/6-31G(d)-CPCM(water).

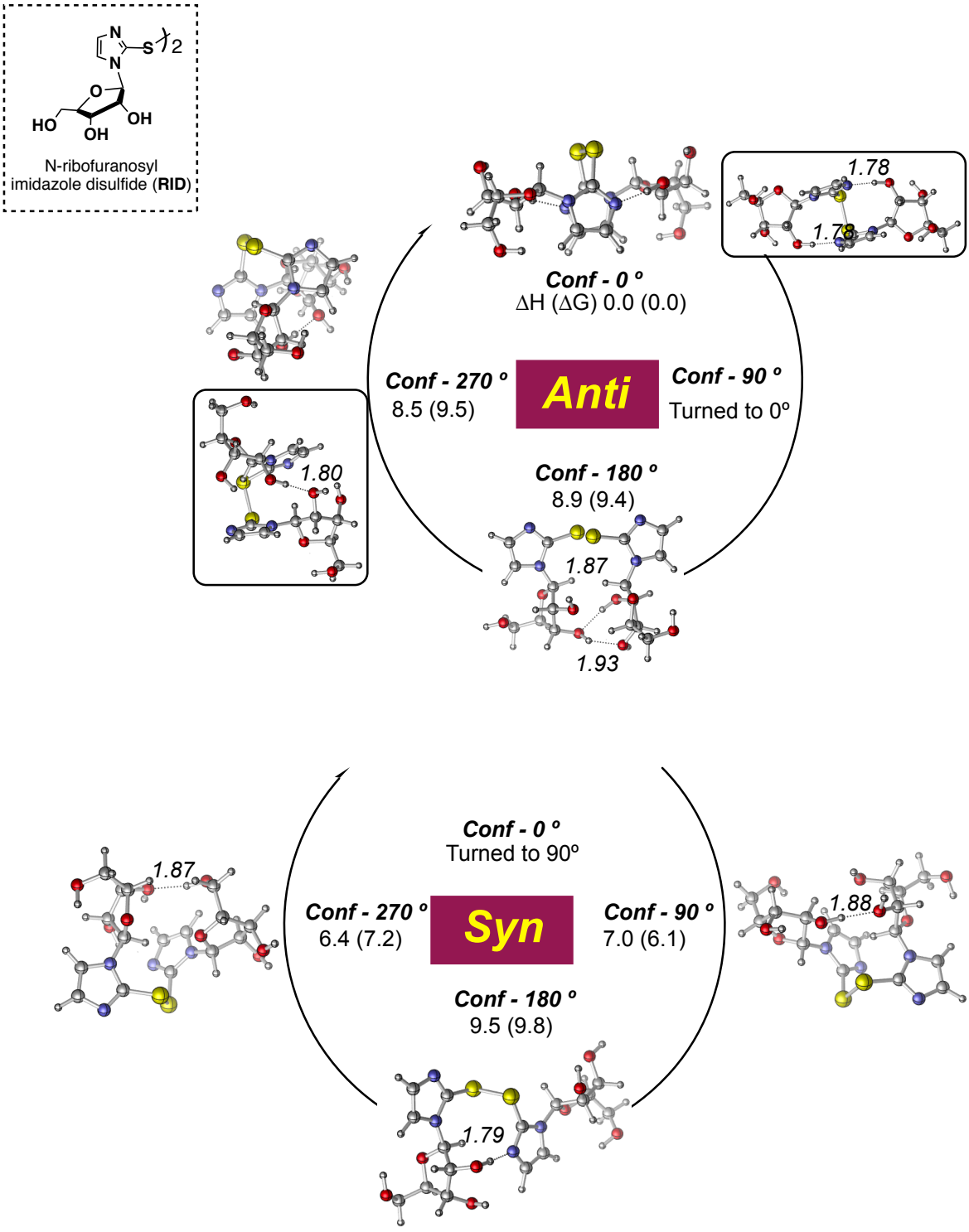


Figure S36. Conformational search of the dihedral angle for the C8-S-S-C8 bond in N-ribofuranosyl-imidazole disulfide (**RID**). The **Anti-Conf-0º** is lowest in energy. *Anti/syn* refers to the orientation of the 2 N-ribose groups, either pointing in opposite directions (*anti*-parallel) or in the same direction (*syn* or parallel alignment). Level of theory B3LYP-D3/Def2SVP-CPCM(water)//B3LYP-D3/6-31G(d)-CPCM(water).

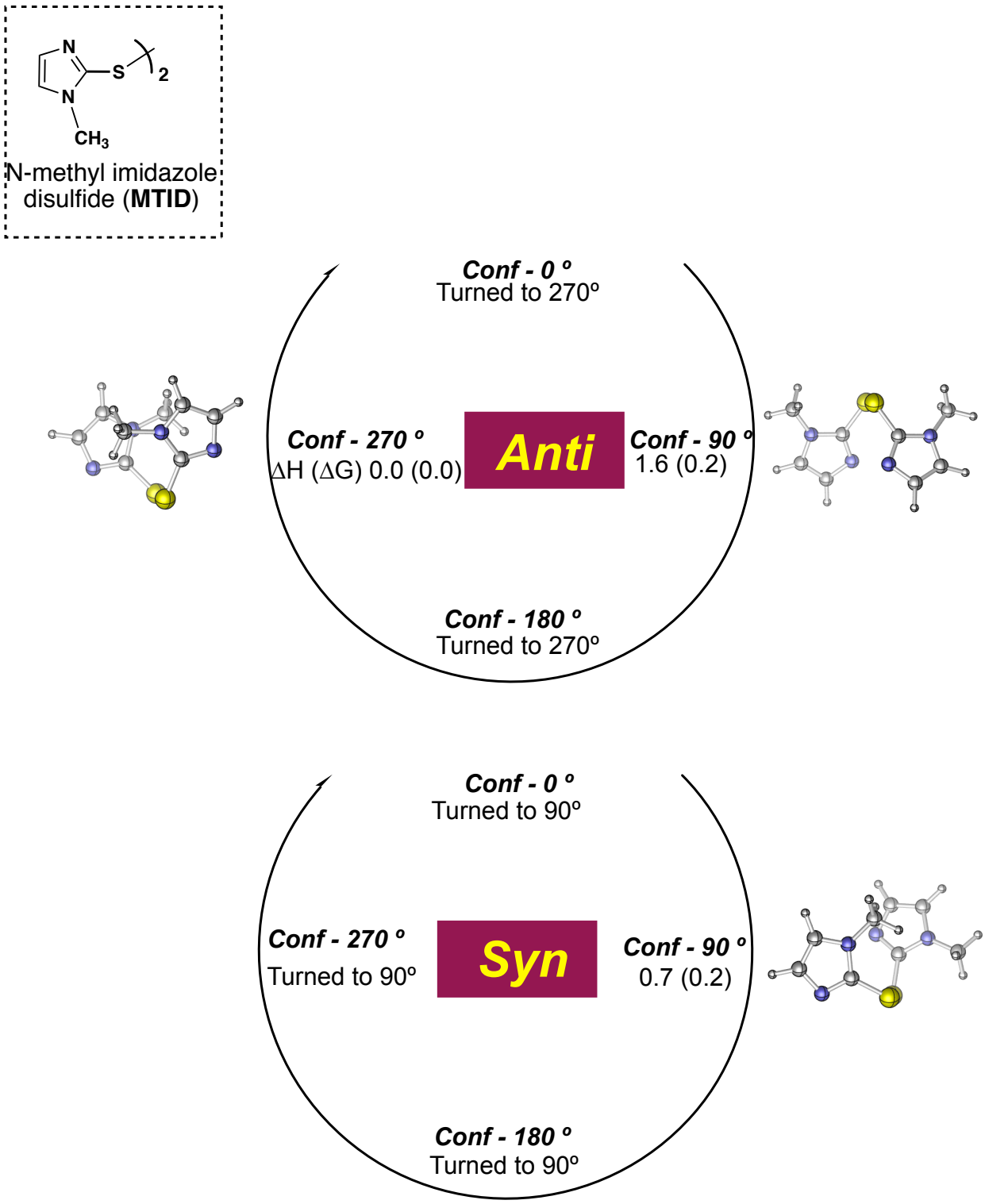
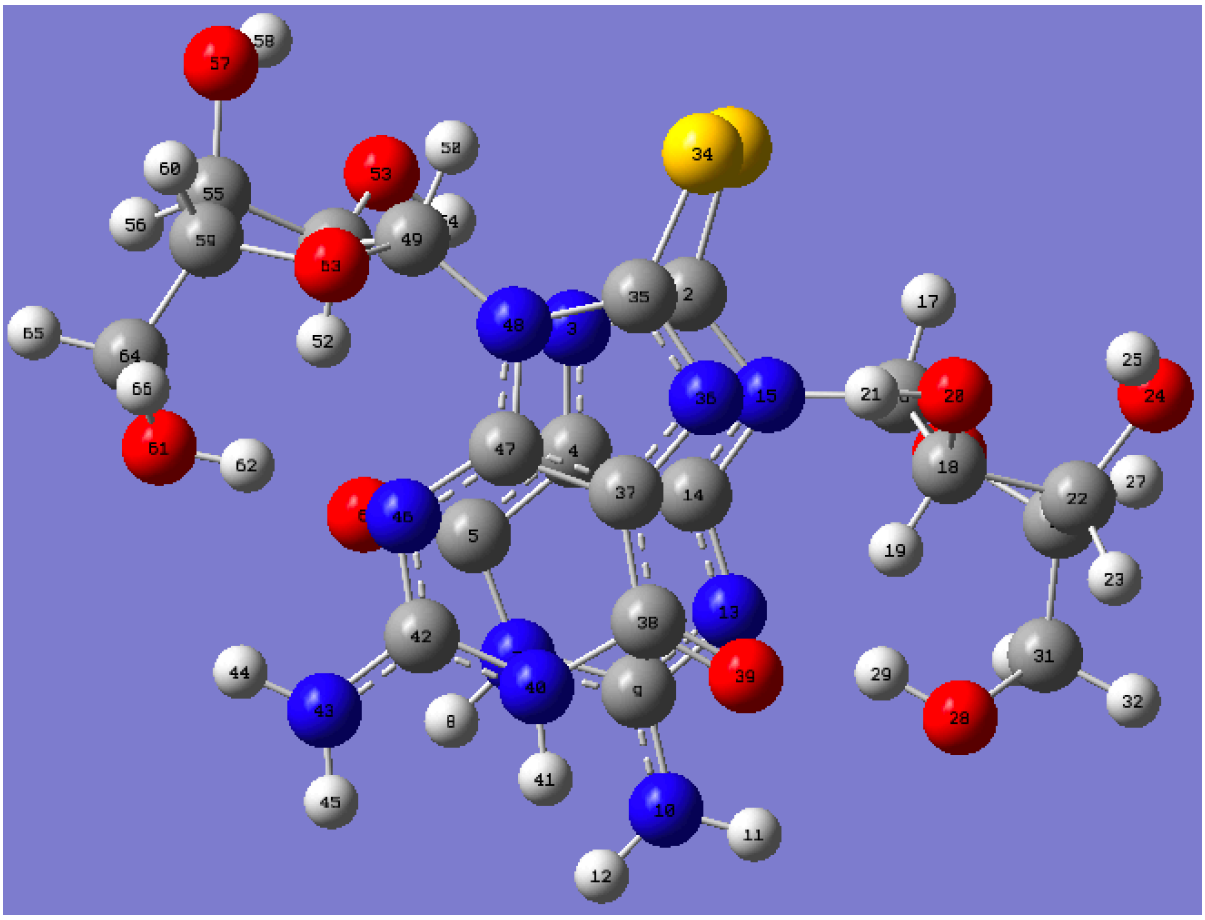


Figure S37. Conformational search on the on the dihedral angle of the disulfide C-S-S-C bonds with fully truncated model. The **Anti-Conf-270º** is lowest in energy.

π-π Stacking Interactions in Lowest-Energy Conformation of 8-ThioG Disulfide

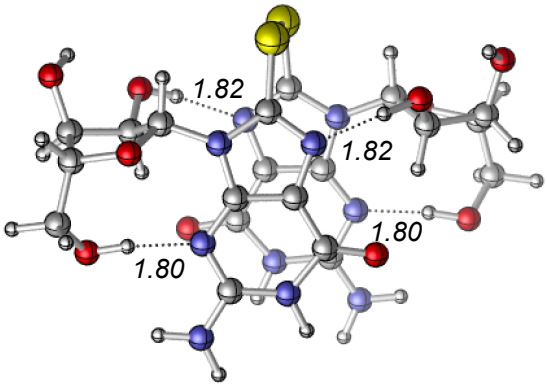


	APT charges				Mulliken charges		
Atom #	Charges	Atom #	Charges	Atom #	Charges	Atom #	Charges
35	-0.058511	2	-0.058474	35	0.250458	2	0.250672
36	-0.279003	15	-0.587174	36	-0.571944	15	-0.518936
37	-0.669007	14	0.930477	37	0.16219	14	0.59339
38	1.663634	13	-1.414717	38	0.632584	13	-0.670833
40	-0.657326	9	1.861668	40	-0.32975	9	0.823123
42	1.860597	7	-0.656988	42	0.824792	7	-0.329601
46	-1.415663	5	1.663807	46	-0.671389	5	0.632407
47	0.931909	4	-0.669185	47	0.593061	4	0.162329
48	-0.587604	3	-0.280381	48	-0.518902	3	-0.572236

Figure S38. Atomic polar tensor (APT) charges and Mulliken charges for selected atoms in the lowest energy conformation for disulfide **1**.

Energies and Coordinates for Calculated Structures

8-disulfideG **1**



Zero-point correction = 0.498025 (Hartree/Particle)

Thermal correction to Energy = 0.535558

Thermal correction to Enthalpy = 0.536502

Thermal correction to Gibbs Free Energy= 0.430068

Sum of electronic and zero-point Energies= -2872.385434

Sum of electronic and thermal Energies= -2872.347900

Sum of electronic and thermal Enthalpies= -2872.346956

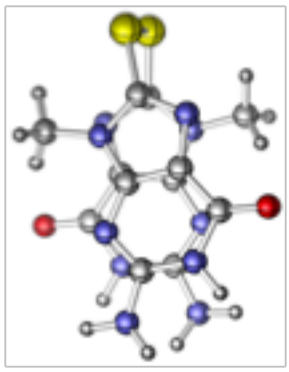
Sum of electronic and thermal Free Energies= -2872.453390

S	-2.03124200	0.75815300	7.35754100
C	-3.02324700	0.15836800	6.08253600
N	-2.54111200	-0.12836800	4.87456300
C	-3.61499000	-0.41456600	4.09411100
C	-3.67896300	-0.70487700	2.68355000
O	-2.76448200	-0.77301600	1.87257000
N	-5.02561900	-0.88243000	2.27391900
H	-5.14075500	-1.09043900	1.28667000
C	-6.13385200	-0.79314700	3.08542600
N	-7.34454700	-1.00466500	2.54934200
H	-8.15504200	-0.88184300	3.14358000
H	-7.49258400	-1.12635000	1.55809300
N	-6.05211900	-0.51045000	4.38240800
C	-4.80185200	-0.31222900	4.83525900
N	-4.42698800	0.05983500	6.09662700
C	-5.32599600	0.34350900	7.21397700

H	-4.68827300	0.52419500	8.08480000
C	-6.24905400	1.56595400	7.00173700
H	-6.61507900	1.58877500	5.97037000
O	-5.65701100	2.78642800	7.37232600
H	-5.07736400	3.05525200	6.61827500
C	-7.39243400	1.21639800	7.96267400
H	-8.33168300	1.70634700	7.67594000
O	-7.01717900	1.55660600	9.29495900
H	-6.54585100	2.40663800	9.22324100
C	-7.48741500	-0.31092400	7.85745400
H	-7.66336300	-0.73842900	8.85137600
O	-8.51714400	-0.15543800	5.63286600
H	-7.61306700	-0.29407600	5.26486500
O	-6.17974600	-0.76628100	7.39883300
C	-8.55290200	-0.81718700	6.88858900
H	-9.54112500	-0.63426900	7.32540200
H	-8.42946900	-1.90594800	6.77904700
S	-1.87059400	3.02467800	6.76760400
C	-2.68221700	3.02474900	5.24741700
N	-4.01008600	3.02792700	5.14450800
C	-4.29050700	2.86138100	3.82615900
C	-5.56236400	2.70086600	3.16647100
O	-6.68466700	2.69699000	3.65533300
N	-5.37677100	2.48776100	1.77615600
H	-6.23614600	2.36098800	1.25033900
C	-4.16653600	2.43770100	1.12256000
N	-4.15866300	2.24197200	-0.20345600
H	-3.26349300	2.17022900	-0.67096400
H	-4.99686500	2.07081500	-0.73941100
N	-3.00404000	2.57465600	1.75382600
C	-3.10577700	2.75950500	3.08156100
N	-2.08369600	2.85526600	3.98496100
C	-0.65682100	2.74764200	3.68505100
H	-0.12825900	2.95530600	4.62058600
C	-0.21630900	1.36426600	3.15247800
H	-0.96619900	0.96971900	2.45947100
O	0.08801900	0.44341500	4.17085800

H	-0.77554000	0.07829700	4.48357500
C	1.05655200	1.75521400	2.39085600
H	1.29727900	1.03378600	1.59957000
O	2.13774200	1.89645000	3.30870300
H	2.03325700	1.16806100	3.94775100
C	0.71681500	3.13839700	1.82103100
H	1.58980500	3.79586700	1.90615400
O	-0.77494700	2.14882000	0.13947500
H	-1.51394700	2.34105000	0.76315100
O	-0.33651300	3.67905000	2.67302800
C	0.22475300	3.12883300	0.37610300
H	1.07000500	2.89790200	-0.28200900
H	-0.12969200	4.14107600	0.12630500

N-methylguanine disulfide (**MGD**)



Zero-point correction= 0.272970 (Hartree/Particle)

Thermal correction to Energy= 0.296416

Thermal correction to Enthalpy= 0.297361

Thermal correction to Gibbs Free Energy= 0.220502

Sum of electronic and zero-point Energies= -1958.728385

Sum of electronic and thermal Energies= -1958.704939

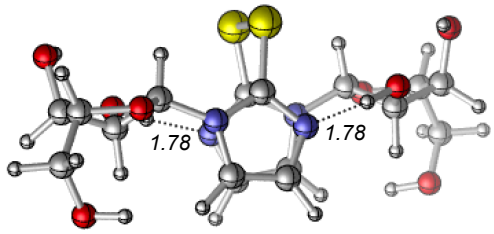
Sum of electronic and thermal Enthalpies= -1958.703995

Sum of electronic and thermal Free Energies= -1958.780854

S	-2.12554700	0.86168200	7.52101900
C	-2.88020900	0.16047100	6.13117700
N	-2.22190800	-0.36247900	5.09827000
C	-3.17361900	-0.60999900	4.15797400
C	-3.02913800	-1.04757200	2.79261300
O	-2.00873800	-1.34783900	2.18137100
N	-4.29022300	-1.07719900	2.14900900
H	-4.26172600	-1.36945200	1.17756200
C	-5.49080100	-0.68133200	2.69816000
N	-6.58989800	-0.77265600	1.90372000
H	-7.41559300	-0.31698700	2.27154900
H	-6.46948100	-0.67803300	0.90273400
N	-5.61783500	-0.25710300	3.94340900
C	-4.44662900	-0.22736500	4.61569100
N	-4.25748600	0.25691800	5.87336200
C	-5.31607500	0.78332400	6.72781400
S	-1.66703800	2.99436000	6.71824300

C	-2.71951400	3.04891300	5.34566000
N	-4.01322800	3.36136300	5.39724500
C	-4.49015800	3.10837700	4.14825200
C	-5.84042500	3.15859100	3.64772700
O	-6.87025400	3.47867100	4.23134000
N	-5.88092700	2.73767300	2.29439800
H	-6.81175400	2.71432200	1.89042200
C	-4.81218800	2.27204700	1.55896200
N	-5.08152300	1.78235900	0.31841900
H	-4.26944700	1.61927600	-0.26336200
H	-5.90264200	2.10542700	-0.17696700
N	-3.57759200	2.21290000	2.02482800
C	-3.47372100	2.61988500	3.30914400
N	-2.34677200	2.59073900	4.07150100
C	-1.03682700	2.15224600	3.60205400
H	-4.86800600	1.41437500	7.49307100
H	-5.99334200	1.38122200	6.11611100
H	-5.86468800	-0.03860200	7.19576800
H	-0.42674900	1.88548300	4.46290700
H	-1.16873900	1.27530700	2.96677200
H	-0.55437100	2.95361200	3.03576700

N-ribofuranosyl imidazole disulfide (**RID**)



Zero-point correction= 0.406345 (Hartree/Particle)

Thermal correction to Energy= 0.434749

Thermal correction to Enthalpy= 0.435693

Thermal correction to Gibbs Free Energy= 0.345887

Sum of electronic and zero-point Energies= -2239.732096

Sum of electronic and thermal Energies= -2239.703692

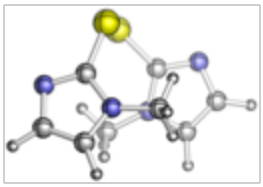
Sum of electronic and thermal Enthalpies= -2239.702747

Sum of electronic and thermal Free Energies= -2239.792554

S	-2.08117600	0.70292900	6.91960200
C	-3.22787800	0.09966000	5.76227200
N	-2.88920300	-0.29706200	4.53424000
C	-4.04666700	-0.66167300	3.91030400
C	-5.11474300	-0.47074900	4.75958200
N	-4.59579900	0.01794700	5.92970900
C	-5.36255600	0.41914100	7.09677800
H	-4.64735100	0.78609200	7.83960800
C	-6.42512300	1.50648000	6.82568600
H	-6.97693600	1.24974900	5.91165400
O	-5.93747400	2.81992300	6.81802800
H	-5.35295900	2.94982500	6.02329900
C	-7.33419700	1.29632700	8.04307500
H	-8.35874700	1.64254000	7.85388400
O	-6.77208000	1.95361100	9.17445100
H	-6.38466400	2.77803400	8.82540400
C	-7.27218100	-0.22277200	8.27582800
H	-7.14516400	-0.41427700	9.34822100
O	-8.67395500	-0.80699800	6.35621300
H	-7.97876800	-1.31443500	5.90962400

O	-6.09265400	-0.69927000	7.56778500
C	-8.47189000	-1.00292300	7.75437700
H	-9.37661300	-0.65191900	8.26084700
H	-8.34184700	-2.06807900	7.98960900
S	-2.23405500	2.91406600	6.55813600
C	-2.87790100	2.94090800	4.94474200
N	-4.18250300	3.02522000	4.67794600
C	-4.30571400	2.97739500	3.31986200
C	-3.06150400	2.84470200	2.74291200
N	-2.15879300	2.81475400	3.77311900
C	-0.72395500	2.62999100	3.63895900
H	-0.30429600	2.63193700	4.64984000
C	-0.30843900	1.33242600	2.91212100
H	-0.92994600	1.20808200	2.01544300
O	-0.27976800	0.18718200	3.71872600
H	-1.20916500	-0.05660100	3.97710900
C	1.11781500	1.70980600	2.49266300
H	1.45152400	1.13928200	1.61603100
O	2.00208300	1.52188300	3.59302300
H	1.68157200	0.71938400	4.04557300
C	1.01508600	3.21554500	2.19621000
H	1.87474800	3.72676100	2.64613600
O	-0.19491000	2.95320900	0.08436600
H	-0.98091300	3.43334200	0.38769700
O	-0.20300600	3.67996200	2.84422300
C	0.92032400	3.57559500	0.71930000
H	1.81975300	3.22221800	0.20505600
H	0.87564700	4.66819500	0.61463800
H	-5.26749100	3.04001900	2.83158000
H	-2.75594200	2.76707400	1.71233000
H	-4.05505500	-1.03757700	2.89738900
H	-6.17162000	-0.63429300	4.62645100

N-methyl imidazole disulfide (**MTID**)



Zero-point correction= 0.182288 (Hartree/Particle)

Thermal correction to Energy= 0.196235

Thermal correction to Enthalpy= 0.197179

Thermal correction to Gibbs Free Energy= 0.139740

Sum of electronic and zero-point Energies= -1326.098346

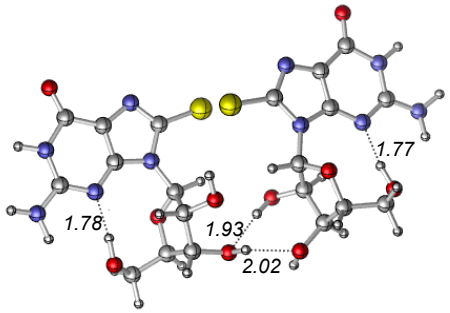
Sum of electronic and thermal Energies= -1326.084398

Sum of electronic and thermal Enthalpies= -1326.083454

Sum of electronic and thermal Free Energies= -1326.140893

S	-0.80751200	2.25269800	3.07427800
N	-2.56615000	0.73558800	4.54127100
N	-0.84157800	-0.43134500	3.71196700
C	-1.44273500	0.80831900	3.82891800
C	-2.68334200	-0.57557900	4.90358900
H	-3.51307600	-0.92877000	5.50133000
C	-1.62739200	-1.31240000	4.40315700
H	-1.37025900	-2.35858400	4.48054300
S	-1.81470400	2.26738600	1.14223100
N	-0.07120600	0.74423100	-0.33634400
N	-1.80945700	-0.41114600	0.48055100
C	-1.19501200	0.82303400	0.37476700
C	0.03285800	-0.56520600	-0.70894800
H	0.85972600	-0.92220900	-1.30839400
C	-1.03156500	-1.29485900	-0.21615100
H	-1.29944900	-2.33764700	-0.30225800
C	0.39854200	-0.78230600	3.02383900
H	0.21363300	-1.62250700	2.35138300
H	0.73599500	0.07067400	2.43705900
H	1.16685000	-1.05389300	3.75195800
C	-3.05314600	-0.75512100	1.16567000
H	-2.87186200	-1.58585200	1.85089100
H	-3.39560400	0.10545700	1.73828000
H	-3.81595500	-1.03760800	0.43601400

8-disulfideG **1**-anti-conf-180º



Zero-point correction= 0.498280 (Hartree/Particle)

Thermal correction to Energy= 0.535948

Thermal correction to Enthalpy= 0.536893

Thermal correction to Gibbs Free Energy= 0.428832

Sum of electronic and zero-point Energies= -2872.358557

Sum of electronic and thermal Energies= -2872.320888

Sum of electronic and thermal Enthalpies= -2872.319944

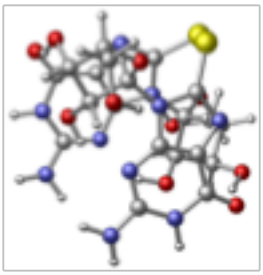
Sum of electronic and thermal Free Energies= -2872.428004

S	-1.69943500	0.71185700	6.94484000
C	-2.83434000	0.22784900	5.71678500
N	-2.48394100	-0.20190300	4.51710800
C	-3.66093300	-0.49355800	3.88469800
C	-3.89124300	-1.01587800	2.56116100
O	-3.08033500	-1.31871900	1.69561700
N	-5.28572600	-1.16953000	2.32085700
H	-5.51341300	-1.55542800	1.40984900
C	-6.29448100	-0.87546100	3.20388200
N	-7.56651700	-1.12967600	2.84351800
H	-8.29937700	-0.83862300	3.47873800
H	-7.82578700	-1.33488800	1.88959200
N	-6.06202200	-0.38187100	4.41490200
C	-4.75678000	-0.21686200	4.70891900
N	-4.23112100	0.25364600	5.88393600
C	-4.97728500	0.64475300	7.07424600
H	-4.23714800	0.83635600	7.85930900

C	-5.86572500	1.89603400	6.89358200
H	-6.31613400	1.89118200	5.89547500
O	-5.21172900	3.11879900	7.16899700
H	-4.55651200	3.29624100	6.47454300
C	-6.95236000	1.64600100	7.94821100
H	-7.89223900	2.14552700	7.69242700
O	-6.50141900	2.05467000	9.23690700
H	-6.36376800	3.02149100	9.23637600
C	-7.09452000	0.11903100	7.96163000
H	-7.18680700	-0.22868400	8.99692200
O	-8.34960300	0.19959400	5.85588700
H	-7.49848400	0.00011500	5.39495700
O	-5.85375500	-0.40922200	7.41786900
C	-8.26699400	-0.40596200	7.13656600
H	-9.19862300	-0.17889800	7.66701400
H	-8.17609200	-1.50087600	7.06718300
S	-1.70926100	2.91539000	6.63153600
C	-0.82720300	3.39745700	8.05571800
N	0.49335000	3.37635600	8.11255000
C	0.80398100	3.80428800	9.37232600
C	2.09397900	4.00725600	9.98230000
O	3.20992100	3.80920800	9.51942900
N	1.94582900	4.51323100	11.30338700
H	2.82101900	4.67906900	11.79014300
C	0.75840400	4.79015300	11.93214300
N	0.79062800	5.26649500	13.19605400
H	-0.08020100	5.63833600	13.55933600
H	1.63949300	5.66253700	13.57600900
N	-0.41966200	4.57718000	11.35930300
C	-0.35301700	4.09285700	10.10163000
N	-1.40692400	3.81086400	9.26957600
C	-2.81908400	4.05496000	9.57073900
H	-3.38335700	3.81933400	8.66258900
C	-3.37026200	3.22593300	10.75808000

H	-2.56387000	3.07037400	11.47920400
O	-3.84518300	1.95102900	10.40165300
H	-4.69218200	2.03588100	9.91530100
C	-4.41240500	4.18529100	11.39722400
H	-4.40758100	4.08579000	12.48564000
O	-5.73362100	3.97554000	10.89576000
H	-6.11894500	3.22638300	11.37954300
C	-3.95122400	5.58676100	10.96851800
H	-4.79930500	6.12851200	10.53293400
O	-2.44661200	5.63069500	12.89639600
H	-1.79014500	5.23636800	12.27140300
O	-2.94336000	5.41397900	9.94032700
C	-3.34528700	6.39938300	12.11105300
H	-4.15176200	6.73625400	12.77185600
H	-2.86018000	7.29127000	11.68521200

8-disulfideG **1**-anti-conf-270º



Zero-point correction= 0.497312 (Hartree/Particle)

Thermal correction to Energy= 0.535237

Thermal correction to Enthalpy= 0.536181

Thermal correction to Gibbs Free Energy= 0.428695

Sum of electronic and zero-point Energies= -2872.355184

Sum of electronic and thermal Energies= -2872.317259

Sum of electronic and thermal Enthalpies= -2872.316315

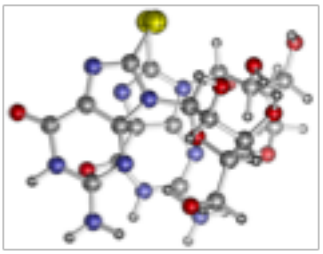
Sum of electronic and thermal Free Energies= -2872.423800

S	-1.96963600	0.62434700	7.16296200
C	-3.39238700	0.32982400	6.17711100
N	-3.45675100	0.41128100	4.86306900

C	-4.79134400	0.30885600	4.56443600
C	-5.45826000	0.45568200	3.30047200
O	-4.97654100	0.67207800	2.18969100
N	-6.85728400	0.32308900	3.45346400
H	-7.38306700	0.43520000	2.59274200
C	-7.53008600	0.24873500	4.64766300
N	-8.87950500	0.22863700	4.60884800
H	-9.36439900	0.30881600	5.49235800
H	-9.37828400	0.55729000	3.79340600
N	-6.91013500	0.15992700	5.81722400
C	-5.56023700	0.16902100	5.72579000
N	-4.65899400	0.15538300	6.76296900
C	-4.89042300	-0.00080800	8.19184800
H	-4.49114600	0.88435600	8.69315800
C	-6.34499200	-0.24238800	8.62132700
H	-6.73203000	-1.10349900	8.06720800
O	-7.20138900	0.86684200	8.52387500
H	-7.46192100	0.88410600	7.57851800
C	-6.09639800	-0.67800800	10.06621000
H	-6.94933400	-1.23606800	10.47391100
O	-5.75299600	0.42439100	10.89715400
H	-6.31433300	1.19112100	10.67253800
C	-4.83950000	-1.56094600	9.91572000
H	-4.14703400	-1.33638500	10.73547800
O	-5.93333400	-3.41300000	8.74927800
H	-5.46661700	-3.11626000	7.94943500
O	-4.22512300	-1.17345600	8.64833500
C	-5.08911100	-3.06236600	9.84137400
H	-5.59045300	-3.39675900	10.75482100
H	-4.12061900	-3.57944100	9.77451400
S	-1.79474500	2.80255300	7.00526600
C	-3.42966700	3.30299000	7.40490100
N	-3.98447300	3.26128300	8.59981100
C	-5.30832800	3.55088300	8.38869400

C	-6.40795300	3.52279400	9.31261000
O	-6.40427900	3.26501000	10.51528400
N	-7.62048800	3.84211000	8.65962700
H	-8.43684300	3.81422300	9.26208700
C	-7.78678400	3.99558700	7.30525900
N	-9.03488100	4.21772300	6.84456500
H	-9.16788900	4.20439500	5.84271500
H	-9.84651000	4.01838500	7.41218300
N	-6.77303700	3.96883800	6.44920200
C	-5.56811000	3.76915300	7.03056300
N	-4.35519800	3.63414900	6.39885000
C	-4.02089700	3.78161600	4.98994500
H	-3.58422300	2.83893800	4.65072200
C	-5.16899700	4.19786200	4.05892800
H	-5.61698000	5.11717600	4.44880300
O	-6.13816300	3.21202100	3.80931000
H	-6.73045400	3.25603600	4.58945600
C	-4.34997500	4.55673800	2.81813000
H	-4.91151900	5.20863100	2.13633100
O	-3.87005200	3.39669400	2.14895800
H	-4.57139400	2.71784800	2.12712700
C	-3.13433800	5.27404600	3.44240900
H	-2.22348800	4.94021900	2.93175300
O	-4.33162200	7.28273200	4.16332900
H	-4.23546400	6.95085000	5.07229800
O	-3.08696200	4.84515500	4.83808100
C	-3.19717500	6.79661400	3.45262900
H	-3.27847100	7.16741800	2.42626000
H	-2.26357300	7.18677500	3.88381500

8-disulfideG **1**-syn-conf-0º



Zero-point correction= 0.498329 (Hartree/Particle)

Thermal correction to Energy= 0.535917

Thermal correction to Enthalpy= 0.536861

Thermal correction to Gibbs Free Energy= 0.430715

Sum of electronic and zero-point Energies= -2872.375427

Sum of electronic and thermal Energies= -2872.337839

Sum of electronic and thermal Enthalpies= -2872.336895

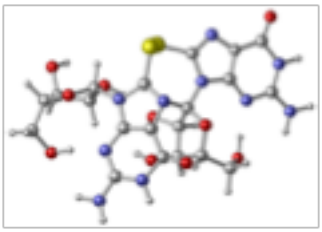
Sum of electronic and thermal Free Energies= -2872.443041

S	-2.07690900	0.78989700	6.94395700
C	-3.37412300	0.49363200	5.82398400
N	-3.18542500	0.47723800	4.51389000
C	-4.43254000	0.37457900	3.96929000
C	-4.83763700	0.45758600	2.59123800
O	-4.15045800	0.60032400	1.58626800
N	-6.25359000	0.38595900	2.48507600
H	-6.60890000	0.46747400	1.53794800
C	-7.13439900	0.26320800	3.53023500
N	-8.45778100	0.24875800	3.25604100
H	-9.07801400	0.02397100	4.02476100
H	-8.79444100	0.03736200	2.32679000
N	-6.74293700	0.21003000	4.79538600
C	-5.41005500	0.31292300	4.96820000
N	-4.74022100	0.40486500	6.15771000
C	-5.33507600	0.39173600	7.48753700
H	-4.50460100	0.44550800	8.19911800
C	-6.31739100	1.54132300	7.77272200
H	-6.92194800	1.74143800	6.88828900
O	-5.62486700	2.69176700	8.21396800

H	-6.12050700	3.48814000	7.91443800
C	-7.18379200	0.91537600	8.88173800
H	-8.18073700	1.37244400	8.92982400
O	-6.49961700	1.03023200	10.12389600
H	-6.05670700	1.89980700	10.08458000
C	-7.25008400	-0.56077300	8.47684300
H	-7.16300200	-1.19609800	9.36595500
O	-8.80057900	-0.02421200	6.65081600
H	-8.01932100	-0.00827600	6.04770100
O	-6.08260400	-0.80012500	7.63711500
C	-8.50506300	-0.94025500	7.69473700
H	-9.36019400	-0.93984100	8.38016500
H	-8.37879700	-1.96578500	7.31406600
S	-1.89650900	3.02834800	6.81111000
C	-2.20893800	3.29232500	5.11865900
N	-1.34238400	3.10701200	4.13802600
C	-2.05200400	3.30336700	2.98778100
C	-1.63771700	3.16882300	1.61380000
O	-0.53829200	2.87242400	1.16223000
N	-2.72457600	3.42775600	0.73564700
H	-2.50501200	3.30882600	-0.24796600
C	-4.00673000	3.74009800	1.10855500
N	-4.94082500	3.89618200	0.14848900
H	-5.84426500	4.24793400	0.44024500
H	-4.68812700	4.02347600	-0.82110900
N	-4.37008200	3.87192200	2.37767600
C	-3.38517800	3.62633900	3.26565300
N	-3.49102100	3.62614500	4.62849200
C	-4.68516600	3.89755100	5.41215600
H	-4.44879500	3.61346600	6.43881100
C	-5.17104500	5.36086700	5.38944500
H	-5.07957100	5.77840000	4.38184400
O	-4.55834800	6.17370100	6.36907400
H	-3.68879600	6.45700000	6.04682300

C	-6.65442100	5.17586200	5.73094600
H	-7.26972700	6.01546700	5.39323900
O	-6.81173000	4.98959000	7.14750500
H	-6.31362400	5.70890300	7.57808600
C	-7.01420800	3.86283700	5.03116900
H	-7.69335600	3.27883500	5.66317000
O	-6.90632100	4.89496100	2.80639900
H	-6.00640800	4.49758200	2.70105900
O	-5.76579300	3.12872100	4.90830800
C	-7.64109500	4.02354600	3.64845400
H	-8.64509200	4.44637700	3.76770500
H	-7.75131000	3.02262200	3.20594000

8-disulfideG **1**-syn-conf-90º



Zero-point correction= 0.497582 (Hartree/Particle)

Thermal correction to Energy= 0.535399

Thermal correction to Enthalpy= 0.536343

Thermal correction to Gibbs Free Energy= 0.428947

Sum of electronic and zero-point Energies= -2872.369842

Sum of electronic and thermal Energies= -2872.332025

Sum of electronic and thermal Enthalpies= -2872.331081

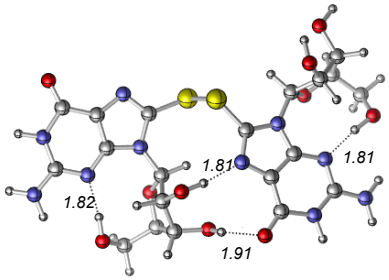
Sum of electronic and thermal Free Energies= -2872.438477

S	-2.25245200	1.03409400	7.14670200
C	-3.35298900	0.47527100	5.90298000
N	-4.58523200	0.07548900	6.14962600
C	-5.02849900	-0.46705800	4.97222900
C	-6.29852300	-1.06772700	4.65510300
O	-7.28269400	-1.22555000	5.36635800
N	-6.31590100	-1.51028700	3.30176300

H	-7.18135100	-1.95844800	3.01806000
C	-5.28290300	-1.40720600	2.40527300
N	-5.44321600	-1.92454800	1.17003500
H	-4.71897900	-1.72306600	0.49131900
H	-6.35711200	-2.16227000	0.81109900
N	-4.11962500	-0.84907500	2.71718400
C	-4.03960000	-0.40019400	3.98654800
N	-2.96223500	0.20930400	4.57673600
C	-1.72221200	0.60269100	3.91412400
H	-1.18849500	1.24749000	4.61469000
C	-0.78977400	-0.54845100	3.51564300
H	-1.36256200	-1.41275000	3.17202700
O	0.03952900	-0.88149500	4.62521500
H	0.33657900	-1.80146400	4.54344700
C	-0.00886700	0.08445900	2.34545000
H	0.37557400	-0.67338200	1.65195900
O	1.03682300	0.90914200	2.84567100
H	1.49298700	0.39506200	3.53427400
C	-1.05514300	0.99078600	1.68760800
H	-0.59573300	1.93811400	1.39136100
O	-2.20882500	-0.95092000	0.72333700
H	-2.85630200	-0.89603500	1.46809900
O	-2.03933300	1.28225900	2.72179200
C	-1.76000900	0.37397200	0.48387600
H	-1.05238900	0.33439800	-0.35202300
H	-2.58761400	1.03896400	0.19302900
S	-2.16559600	3.18609100	6.99794100
C	-0.99312300	3.45154100	5.72023100
N	-1.32474000	3.88747700	4.52036600
C	-0.14645300	3.93701700	3.82005200
C	0.09423800	4.27427900	2.44360000
O	-0.70201200	4.61899300	1.57658000
N	1.47376600	4.13760900	2.12871600
H	1.70321000	4.33625200	1.16018300

C	2.45631400	3.70792200	2.98267000
N	3.71484600	3.57827200	2.50850500
H	4.44162300	3.41621500	3.19557600
H	3.99735300	4.03916300	1.65482100
N	2.21407600	3.39000800	4.24668800
C	0.92001500	3.49747400	4.60632500
N	0.38233800	3.18131100	5.82897500
C	1.11866600	2.68017700	6.98294300
H	0.40244400	2.60134700	7.80693700
C	1.80259500	1.30632600	6.77797600
H	2.23039600	1.25125000	5.77291800
O	0.97203900	0.20694500	7.06516200
H	0.53151400	-0.09772200	6.24698700
C	2.92788700	1.39239400	7.82069300
H	3.77431800	0.74528600	7.55820100
O	2.40950400	1.07195500	9.10811500
H	1.84223700	0.29078100	8.97647100
C	3.31389200	2.87580300	7.80820600
H	3.48526500	3.22026100	8.83480300
O	4.46920200	2.60626900	5.66112700
H	3.63410800	2.92064600	5.23728400
O	2.16014700	3.59003800	7.27867600
C	4.53057900	3.20403200	6.94703500
H	5.42846700	2.81946600	7.44406200
H	4.62320000	4.29959900	6.88430200

8-disulfideG **1**-syn-conf-180°



Zero-point correction= 0.498059 (Hartree/Particle)

Thermal correction to Energy= 0.535675

Thermal correction to Enthalpy= 0.536619

Thermal correction to Gibbs Free Energy= 0.428382

Sum of electronic and zero-point Energies= -2872.368633

Sum of electronic and thermal Energies= -2872.331017

Sum of electronic and thermal Enthalpies= -2872.330072

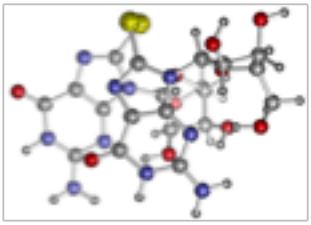
Sum of electronic and thermal Free Energies= -2872.438310

S	-1.10480900	0.70320400	4.95159400
C	-2.73913100	0.46329600	4.36899500
N	-3.00335600	0.16167800	3.10998300
C	-4.34906700	-0.08935900	3.07945700
C	-5.18854400	-0.49520500	1.98106200
O	-4.89365900	-0.69109500	0.80879200
N	-6.53203400	-0.66935600	2.41931100
H	-7.17762300	-0.95301200	1.68882900
C	-6.99282900	-0.49738000	3.70074200
N	-8.30709400	-0.68686000	3.94688500
H	-8.58692700	-0.70908100	4.92023300
H	-8.89235100	-1.19237000	3.29664600
N	-6.20514000	-0.11916800	4.69867800
C	-4.91690700	0.07423500	4.34638600
N	-3.88969000	0.44666400	5.17315300
C	-3.98921200	0.71422500	6.59962100
H	-2.97680900	0.94990300	6.94444500
C	-4.95209500	1.86117700	6.98418800
H	-5.87749100	1.75615700	6.41474100
O	-4.46946900	3.15440900	6.75124400
H	-3.55260500	3.24227600	7.10740100
C	-5.23834100	1.48285300	8.45220500
H	-6.18021100	1.91926100	8.80886100
O	-4.14473200	1.82950700	9.29017900
H	-4.07249300	2.80258800	9.36127600
C	-5.29841800	-0.04974800	8.39582400

H	-4.82386200	-0.46523100	9.29254000
O	-7.45265600	-0.04535000	7.20437300
H	-6.92757000	-0.12766900	6.37354700
O	-4.49688900	-0.44046400	7.24148000
C	-6.69491900	-0.64721000	8.24302400
H	-7.24708000	-0.49721100	9.17786000
H	-6.58571000	-1.73237800	8.08819700
S	-0.85272700	2.85591100	5.02533700
C	-0.76220900	3.21102400	6.74101500
N	-1.80249900	3.46848700	7.51242700
C	-1.28866200	3.76061700	8.74688100
C	-1.95528700	4.15360900	9.95417600
O	-3.16332800	4.28147400	10.16248500
N	-1.02407000	4.41040700	10.98446300
H	-1.43706500	4.70356000	11.86456800
C	0.34391000	4.31188800	10.87359300
N	1.10006700	4.62502500	11.94230800
H	2.09276500	4.43549700	11.87781800
H	0.70513900	4.71428800	12.86775900
N	0.94517800	3.94990500	9.74667800
C	0.10517200	3.69446400	8.72456800
N	0.44310700	3.33093300	7.44488500
C	1.79582900	3.13345400	6.93359900
H	1.68980400	2.72388200	5.92419600
C	2.64488000	4.42295600	6.87432400
H	2.46718200	5.02287300	7.76900000
O	2.37959800	5.21580100	5.74512000
H	2.92102700	4.83215000	5.02920900
C	4.06108900	3.82585500	6.92056700
H	4.79999400	4.53422700	7.30695800
O	4.34718700	3.45394300	5.56985800
H	5.30408300	3.33388200	5.47257500
C	3.89714300	2.59551800	7.83290900
H	4.46493000	1.75206400	7.42261000

O	3.73465700	4.01161200	9.82779500
H	2.75515900	3.92485900	9.74997600
O	2.48241000	2.24724400	7.79109900
C	4.29761100	2.82597700	9.28738900
H	5.38747000	2.92626100	9.34229600
H	4.01138500	1.93611900	9.86911400

8-disulfideG 1-syn-conf-270°



Zero-point correction= 0.497039 (Hartree/Particle)

Thermal correction to Energy= 0.535346

Thermal correction to Enthalpy= 0.536290

Thermal correction to Gibbs Free Energy= 0.426896

Sum of electronic and zero-point Energies= -2872.357448

Sum of electronic and thermal Energies= -2872.319141

Sum of electronic and thermal Enthalpies= -2872.318197

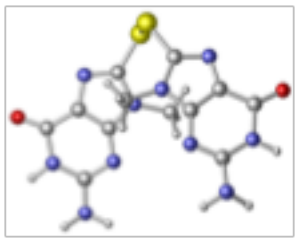
Sum of electronic and thermal Free Energies= -2872.427591

S	-2.04102000	-0.01904400	7.08634400
C	-3.57500200	-0.03988700	6.23606500
N	-3.70851900	-0.03455400	4.92518100
C	-5.02960300	0.24219700	4.70294200
C	-5.71873400	0.45721100	3.45814500
O	-5.29732900	0.36329300	2.31112200
N	-7.06677400	0.83585200	3.69626400
H	-7.61011700	1.00209500	2.85515800
C	-7.65335500	1.00838600	4.92422100
N	-8.95766500	1.37068100	4.95459700
H	-9.31256700	1.66733800	5.85416800
H	-9.36448200	1.84236700	4.15778700
N	-7.01454100	0.78203400	6.06210500

C	-5.72293600	0.40622600	5.90720300
N	-4.79545900	0.19202300	6.89733800
C	-4.98595300	0.19415400	8.34452600
H	-4.45287100	1.04754900	8.77374600
C	-6.45382200	0.19049300	8.80545300
H	-6.99057000	-0.58257000	8.24530500
O	-7.10214100	1.43632700	8.74377900
H	-7.36116700	1.52322900	7.79964800
C	-6.29359900	-0.28275600	10.25108000
H	-7.20354200	-0.77893300	10.61130700
O	-5.94221700	0.80472800	11.09795700
H	-6.45402200	1.57378000	10.79151700
C	-5.10518900	-1.25983800	10.16235600
H	-4.39017100	-1.03492600	10.96257100
O	-6.40216400	-3.04780900	9.13648800
H	-5.93857800	-2.82990000	8.30988500
O	-4.47463900	-1.02245100	8.86984900
C	-5.49083700	-2.73283300	10.18477600
H	-5.99202500	-2.96871200	11.12847600
H	-4.57902600	-3.34405900	10.11787500
S	-1.35663500	2.00759500	6.56222000
C	-2.79241800	2.90285900	7.00400400
N	-3.78609400	3.12151800	6.16205200
C	-4.80053500	3.63239900	6.92754900
C	-6.14991400	3.97002500	6.55839400
O	-6.68707000	3.93300400	5.45745700
N	-6.89087600	4.37439000	7.70295800
H	-7.85829300	4.61376400	7.51125600
C	-6.42665100	4.41504500	8.99379700
N	-7.26552400	4.82236700	9.96948100
H	-6.94383500	4.70270300	10.92260600
H	-8.26600200	4.83170100	9.82742400
N	-5.17553000	4.11038800	9.31428200
C	-4.41817400	3.71997400	8.27047100

N	-3.12224700	3.27185600	8.31888900
C	-2.29155700	3.13686000	9.50433300
H	-1.34479400	2.70075100	9.16946500
C	-2.00544000	4.45913200	10.25010100
H	-2.90860000	5.07087600	10.28052300
O	-0.97116700	5.21697700	9.67387800
H	-0.14635100	4.84038800	10.03523900
C	-1.69394700	3.92228800	11.65663800
H	-1.86749900	4.66989200	12.43663200
O	-0.31869500	3.53159700	11.60452600
H	0.01522900	3.43906600	12.50967300
C	-2.63219400	2.70911800	11.79194300
H	-2.10015700	1.88213200	12.27724800
O	-4.59740100	4.15134500	12.05255800
H	-4.75179800	4.02020300	11.08774000
O	-2.95504800	2.29922500	10.43100400
C	-3.93107700	2.99250400	12.53960400
H	-3.69535400	3.17367900	13.59477000
H	-4.56680100	2.10113900	12.47312100

MGD-anti-conf-270°



Zero-point correction= 0.272628 (Hartree/Particle)

Thermal correction to Energy= 0.296217

Thermal correction to Enthalpy= 0.297161

Thermal correction to Gibbs Free Energy= 0.218972

Sum of electronic and zero-point Energies= -1958.724031

Sum of electronic and thermal Energies= -1958.700442

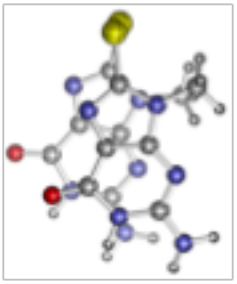
Sum of electronic and thermal Enthalpies= -1958.699498

Sum of electronic and thermal Free Energies= -1958.777687

S	-1.50718700	0.79458900	7.21151400
C	-2.76138200	0.40030000	6.05703300
N	-2.57772300	0.24115600	4.75588800
C	-3.83192600	0.03777000	4.24654500
C	-4.25819100	-0.18487100	2.89013500
O	-3.58984200	-0.26354100	1.86468500
N	-5.67127100	-0.31990700	2.83658300
H	-6.03857700	-0.49879000	1.90764200
C	-6.53765000	-0.25025800	3.90549600
N	-7.85534200	-0.44961600	3.65091200
H	-8.48732200	-0.21931000	4.40624800
H	-8.21970400	-0.30681600	2.71853300
N	-6.13895900	-0.04788900	5.15058000
C	-4.79943100	0.08287200	5.26037300
N	-4.11307300	0.31993700	6.41690800
C	-4.72180300	0.40123900	7.74064800
S	-1.43318600	2.97288700	7.07869400
C	-2.99271300	3.43073100	7.72639100
N	-3.26882100	3.58839800	9.01134100
C	-4.61206800	3.84967100	9.05250600
C	-5.47703500	4.09294300	10.17690200
O	-5.20737900	4.14292900	11.37239500
N	-6.81299000	4.28942500	9.73476600
H	-7.47507100	4.48305500	10.47965300
C	-7.25092000	4.25829800	8.42862200
N	-8.56314900	4.52038200	8.20541800
H	-8.89798400	4.31659200	7.27307700
H	-9.23879900	4.39994200	8.94761300
N	-6.45031500	4.03429400	7.39959000
C	-5.16451200	3.84278000	7.76395700
N	-4.12847500	3.56904100	6.91770200
C	-4.24136600	3.50289700	5.46429800
H	-4.06224800	0.95189800	8.40968500

H	-5.67501700	0.92449300	7.65114900
H	-4.89413900	-0.60143000	8.14121400
H	-3.40642300	2.93111700	5.06201600
H	-5.18062700	3.00805300	5.21229600
H	-4.23493000	4.50930400	5.03711900

MGD-syn-conf-0º



Zero-point correction= 0.272728 (Hartree/Particle)

Thermal correction to Energy= 0.296182

Thermal correction to Enthalpy= 0.297126

Thermal correction to Gibbs Free Energy= 0.220747

Sum of electronic and zero-point Energies= -1958.725318

Sum of electronic and thermal Energies= -1958.701865

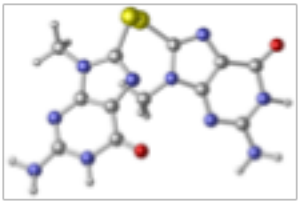
Sum of electronic and thermal Enthalpies= -1958.700920

Sum of electronic and thermal Free Energies= -1958.777299

S	-2.36635200	0.84729600	7.50139200
C	-3.05204200	0.33177300	6.00509400
N	-2.37934300	-0.24775900	5.00880600
C	-3.27266200	-0.36409700	3.99255100
C	-3.09934800	-0.87645200	2.65557200
O	-2.10501500	-1.36531200	2.13355700
N	-4.30801100	-0.75348500	1.92164000
H	-4.25223600	-1.09068600	0.96620400
C	-5.49003500	-0.21674900	2.38192400
N	-6.54241500	-0.21017500	1.52964400
H	-7.34474900	0.33400100	1.81701800
H	-6.39726200	-0.29523200	0.53287100
N	-5.64725700	0.25157100	3.61042300

C	-4.52562000	0.16420200	4.35556600
N	-4.38372800	0.60047900	5.63563400
C	-5.46565200	1.16420200	6.43213300
S	-1.50873600	2.96660700	6.92156500
C	-2.41548600	3.25084700	5.48434100
N	-2.07574700	2.77961700	4.28505400
C	-3.16076400	2.99908300	3.49527600
C	-3.39124600	2.63730600	2.12031800
O	-2.63648000	2.09487000	1.32057500
N	-4.71435000	2.97901000	1.73738200
H	-4.94513200	2.74980200	0.77593600
C	-5.66697900	3.56615000	2.54141800
N	-6.87202800	3.82381600	1.98483800
H	-7.60993500	4.10003300	2.61843200
H	-7.16148400	3.35300700	1.13867700
N	-5.44309600	3.91768200	3.79893000
C	-4.20089700	3.61193900	4.22168500
N	-3.71586900	3.78235200	5.48304900
C	-4.40185400	4.45144900	6.58131900
H	-5.04899400	1.58085500	7.34754300
H	-5.96338500	1.94577700	5.85463600
H	-6.18989900	0.38501500	6.68409000
H	-4.00683900	5.46214500	6.71395200
H	-5.46284200	4.50388300	6.33619200
H	-4.25951500	3.88599700	7.50291900

MGD-syn-conf-90º



Zero-point correction= 0.272398 (Hartree/Particle)

Thermal correction to Energy= 0.296242

Thermal correction to Enthalpy= 0.297186

Thermal correction to Gibbs Free Energy= 0.216464

Sum of electronic and zero-point Energies= -1958.722834

Sum of electronic and thermal Energies= -1958.698991

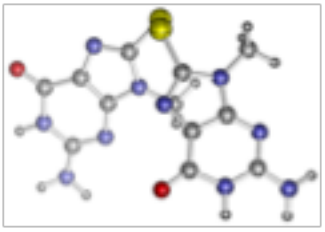
Sum of electronic and thermal Enthalpies= -1958.698046

Sum of electronic and thermal Free Energies= -1958.778768

S	-2.19383900	0.88129200	7.46079600
C	-3.19925600	0.34516400	6.13239900
N	-4.51128600	0.18581700	6.19772000
C	-4.87528900	-0.22591100	4.94414200
C	-6.17068000	-0.56444300	4.41763200
O	-7.26453300	-0.56547400	4.97363500
N	-6.06203800	-0.93878700	3.05144300
H	-6.94076400	-1.20882200	2.62127900
C	-4.90177200	-0.98653800	2.30985700
N	-5.00202600	-1.42641500	1.02846400
H	-4.18364000	-1.27676900	0.45305100
H	-5.88741100	-1.36583700	0.54356500
N	-3.71395500	-0.67490200	2.79952000
C	-3.75934200	-0.31234800	4.10000600
N	-2.68803400	0.05202800	4.86298000
S	-2.17141600	3.04043000	7.21935900
C	-1.16224200	3.25441800	5.80574000
N	-1.62672200	3.54328100	4.60079900
C	-0.51096700	3.61126800	3.80693100
C	-0.38990400	3.88696600	2.40048900
O	-1.26291600	4.13957000	1.57627500
N	0.97361700	3.82787500	2.00438500
H	1.12765900	3.98776700	1.01392500
C	2.04716700	3.55462500	2.82321200
N	3.27369900	3.49499500	2.24361700
H	4.05607000	3.47389300	2.88444500
H	3.44341300	3.97437200	1.36954700
N	1.92811900	3.30361300	4.11602300
C	0.64978500	3.33918300	4.54665300

N	0.22528400	3.11769000	5.82715800
C	1.06705500	2.78052800	6.96881900
H	0.87136100	3.47189100	7.79078600
H	0.86402600	1.75835100	7.29826900
H	2.10680200	2.86466900	6.65251300
C	-1.31130400	0.10284600	4.38503200
H	-1.17687200	0.95783200	3.71844900
H	-0.64224700	0.19877000	5.23918500
H	-1.08701300	-0.81864800	3.84446000

MGD-syn-conf-270°



Zero-point correction= 0.272283 (Hartree/Particle)

Thermal correction to Energy= 0.296150

Thermal correction to Enthalpy= 0.297094

Thermal correction to Gibbs Free Energy= 0.216601

Sum of electronic and zero-point Energies= -1958.722907

Sum of electronic and thermal Energies= -1958.699041

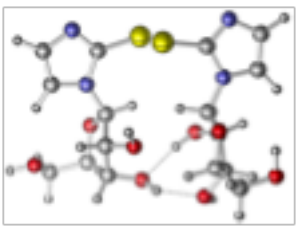
Sum of electronic and thermal Enthalpies= -1958.698096

Sum of electronic and thermal Free Energies= -1958.778590

S	-1.48555700	1.30311300	7.07076000
C	-2.69284300	0.69127000	5.96163600
N	-2.43632600	0.21351200	4.75454100
C	-3.66049800	-0.13054900	4.24824000
C	-4.01079700	-0.70949500	2.97845500
O	-3.28820200	-1.03346600	2.04113600
N	-5.41696500	-0.89391500	2.89507400
H	-5.73247700	-1.31813200	2.02868600
C	-6.33866500	-0.58155100	3.87056500
N	-7.63659200	-0.89383100	3.61984800

H	-8.31215800	-0.49129100	4.25600800
H	-7.95238100	-1.00416800	2.66559900
N	-6.01101800	-0.04705400	5.03442500
C	-4.68118100	0.14908700	5.16784000
N	-4.05951900	0.67403100	6.26348900
C	-4.74540300	1.11295300	7.47313900
S	-1.37009500	3.41221400	6.55519900
C	-2.90434100	4.02729300	7.12865700
N	-3.92433800	4.32144300	6.33846400
C	-4.90827500	4.75333900	7.18979600
C	-6.24277700	5.20998500	6.90789700
O	-6.81351900	5.33626600	5.82926300
N	-6.91521400	5.53588800	8.11645100
H	-7.85924300	5.88532000	7.98733100
C	-6.39483400	5.44029200	9.38828200
N	-7.18294100	5.84934800	10.41515800
H	-6.85675800	5.60284200	11.34032700
H	-8.18746700	5.87720700	10.30226600
N	-5.16671900	5.01930700	9.63991400
C	-4.47768900	4.70033700	8.52432700
N	-3.19116300	4.24047000	8.47651200
C	-2.31821300	3.99909700	9.61890900
H	-4.01517800	1.23588300	8.27190700
H	-5.25423300	2.06305900	7.29320300
H	-5.47922800	0.35724800	7.75910600
H	-1.37342100	4.52880500	9.48204800
H	-2.82562700	4.36901700	10.50992000
H	-2.12228200	2.92896200	9.72402500

RID-anti-conf-180º



Zero-point correction= 0.407118 (Hartree/Particle)

Thermal correction to Energy= 0.435637

Thermal correction to Enthalpy= 0.436581

Thermal correction to Gibbs Free Energy= 0.347612

Sum of electronic and zero-point Energies= -2239.718158

Sum of electronic and thermal Energies= -2239.689639

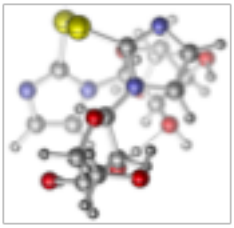
Sum of electronic and thermal Enthalpies= -2239.688695

Sum of electronic and thermal Free Energies= -2239.777663

S	-1.59949100	0.61406400	6.88208200
C	-2.87625500	0.50482400	5.69574600
N	-2.66666200	0.29685400	4.39869700
C	-3.90888400	0.24101700	3.82855200
C	-4.89009600	0.42349200	4.77887600
N	-4.23094900	0.60607400	5.96816200
C	-4.88815100	0.78711500	7.25429100
H	-4.10070700	0.84936800	8.01168000
C	-5.78845500	2.04419800	7.32486100
H	-6.24769500	2.22595400	6.34963400
O	-5.12063600	3.19504500	7.80910200
H	-4.66722100	3.62754900	7.06803200
C	-6.87195400	1.59839700	8.31277300
H	-7.80589900	2.15337300	8.17742400
O	-6.41382200	1.69837500	9.65848900
H	-6.36626300	2.63590800	9.93786700
C	-7.02448200	0.10800900	7.98865600
H	-7.22580800	-0.44460400	8.91233300
O	-7.98379900	0.62843600	5.84570300
H	-8.65708200	0.37395900	5.19571300
O	-5.73623500	-0.32322000	7.48692000
C	-8.11868900	-0.22093200	6.98517300
H	-9.09381400	-0.07553200	7.47247200
H	-8.02598200	-1.27969400	6.70757800
S	-1.12521200	2.76973000	6.76429100
C	-0.41059400	3.06235400	8.33217100

N	0.89760500	3.06130800	8.56462600
C	1.03945000	3.42476600	9.87639000
C	-0.19152900	3.63844700	10.45558400
N	-1.11999900	3.39162900	9.47562600
C	-2.55174000	3.56253600	9.59409000
H	-3.00954800	3.13026200	8.70375700
C	-3.19322000	2.91289200	10.85190800
H	-2.42886600	2.75909400	11.61713100
O	-3.74461500	1.64091100	10.60977700
H	-4.60763800	1.72268400	10.15003100
C	-4.19712500	4.01120300	11.34141800
H	-3.87499300	4.39195400	12.31570600
O	-5.55301600	3.58183900	11.40755400
H	-5.62714400	2.92244200	12.11757200
C	-4.10105200	5.13030600	10.29514000
H	-4.90138800	4.99394600	9.55553800
O	-3.08626500	6.74639900	11.80991700
H	-2.26460800	6.48916100	11.35753200
O	-2.81637400	4.95770600	9.67460600
C	-4.13110800	6.54023300	10.86644300
H	-5.07808300	6.69438300	11.39290900
H	-4.07397800	7.26518500	10.04086700
H	-4.03838600	0.06727200	2.76862900
H	-5.97028300	0.41471500	4.74002200
H	2.01316100	3.51461000	10.33873300
H	-0.47567000	3.94850400	11.44955300

RID-anti-conf-270º



Zero-point correction= 0.407452 (Hartree/Particle)

Thermal correction to Energy= 0.435671

Thermal correction to Enthalpy= 0.436615

Thermal correction to Gibbs Free Energy= 0.348293

Sum of electronic and zero-point Energies= -2239.720347

Sum of electronic and thermal Energies= -2239.692128

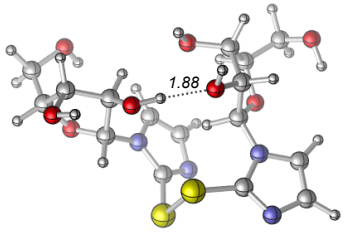
Sum of electronic and thermal Enthalpies= -2239.691183

Sum of electronic and thermal Free Energies= -2239.779506

S	-1.52078300	0.62405500	7.24538600
C	-2.74301100	0.20881800	6.05496200
N	-2.54306400	0.02470600	4.75862900
C	-3.77049500	-0.29855500	4.23956900
C	-4.72710000	-0.31765800	5.22957300
N	-4.07726300	0.02698300	6.39119500
C	-4.61503700	0.10741100	7.73554600
H	-4.11716600	0.94243900	8.23858000
C	-6.13669200	0.29254400	7.85967400
H	-6.65836000	-0.44558900	7.23833600
O	-6.60796600	1.60093800	7.66373100
H	-6.39267100	1.90142700	6.75479600
C	-6.30987300	-0.09155900	9.33603200
H	-7.33606100	-0.41119400	9.55724600
O	-5.92402700	1.00375800	10.16109200
H	-6.20425200	1.80734800	9.68400700
C	-5.29260000	-1.23160300	9.51986500
H	-4.75697400	-1.08676000	10.46558700
O	-6.56454000	-2.87453900	8.23450800
H	-5.89022300	-2.81336000	7.53748500
O	-4.35373400	-1.11484700	8.41272400
C	-5.88070000	-2.63579500	9.46117200
H	-6.61297800	-2.75953000	10.26497900
H	-5.07534500	-3.36815100	9.61635300
S	-1.34937000	2.76193800	7.04523100
C	-2.83957000	3.36173300	7.75454900
N	-3.06660300	3.57074900	9.04229500
C	-4.34022900	4.07277000	9.11600500

C	-4.89421200	4.17933100	7.86044100
N	-3.94304900	3.70964500	6.98635800
C	-4.00407400	3.62170600	5.54154900
H	-3.54289500	2.67304600	5.24924200
C	-5.39256100	3.71731400	4.90807200
H	-5.94050600	4.57957600	5.29722500
O	-6.11493100	2.50182800	5.08020700
H	-7.02748200	2.63738200	4.77035600
C	-4.98975300	3.98429100	3.44824500
H	-5.80379800	4.44488000	2.87433100
O	-4.53998100	2.78084600	2.83783300
H	-5.11392600	2.06370200	3.16271900
C	-3.78318900	4.92498300	3.61338100
H	-3.00076800	4.63500200	2.90281900
O	-5.09587000	6.82769300	4.40279700
H	-4.69723200	6.73739100	5.28437900
O	-3.29974500	4.71589100	4.97235300
C	-4.10040000	6.40856400	3.47351500
H	-4.49411500	6.60546700	2.47165500
H	-3.17319500	6.98570300	3.59636900
H	-5.78458700	-0.52335000	5.19567200
H	-3.90491400	-0.50293000	3.18599800
H	-5.86456900	4.51848400	7.53597200
H	-4.79433100	4.33276200	10.06254100

RID-syn-conf-90º



Zero-point correction= 0.406303 (Hartree/Particle)

Thermal correction to Energy= 0.435170

Thermal correction to Enthalpy= 0.436114

Thermal correction to Gibbs Free Energy= 0.346072

Sum of electronic and zero-point Energies= -2239.721075

Sum of electronic and thermal Energies= -2239.692208

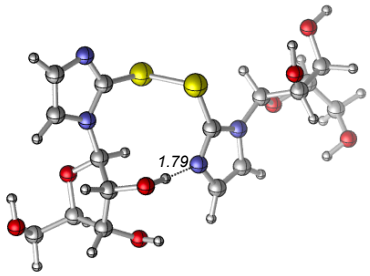
Sum of electronic and thermal Enthalpies= -2239.691264

Sum of electronic and thermal Free Energies= -2239.781306

S	-2.30815000	0.68203900	7.24500700
C	-3.44183700	0.44674500	5.92908500
N	-4.74757600	0.24926300	6.06622500
C	-5.22720100	0.05780900	4.79924500
C	-4.20684500	0.13578700	3.87627200
N	-3.06758400	0.38868700	4.59630600
C	-1.72885000	0.51914000	4.04887700
H	-1.14398500	1.12072100	4.74796300
C	-0.98827200	-0.79497700	3.78563500
H	-1.66186000	-1.50121300	3.28861200
O	-0.49552300	-1.31013700	5.00986000
H	-0.24518700	-2.24098500	4.89476600
C	0.10566100	-0.31991300	2.80363900
H	0.41115400	-1.11701500	2.11748200
O	1.22850100	0.20656800	3.50571400
H	1.67301000	-0.53862500	3.94229500
C	-0.58179800	0.84384500	2.06099200
H	0.06352100	1.72870400	2.10753100
O	-1.70557000	-0.67998600	0.52358100
H	-2.57345200	-0.50117200	0.91827400
O	-1.81416200	1.12558800	2.77848100
C	-0.95360300	0.52586500	0.62158700
H	-0.03811200	0.37651700	0.04115600
H	-1.49833100	1.37705900	0.19006400
S	-2.18474800	2.82579300	7.47260500
C	-1.23888000	3.28256500	6.06603600
N	-1.77180400	3.76236500	4.94878400
C	-0.72806600	3.89997000	4.07072500
C	0.44598800	3.47722100	4.64857000
N	0.12365300	3.08356800	5.92674500

C	1.06657700	2.59303600	6.91629200
H	0.50655300	2.41539300	7.83971500
C	1.81317700	1.30356900	6.51551400
H	2.09538500	1.35830300	5.46055100
O	1.11319300	0.12320700	6.83061500
H	0.59041400	-0.20697000	6.07204200
C	3.06240900	1.40964800	7.40123900
H	3.91564400	0.87305200	6.96548500
O	2.76869500	0.92700900	8.70839200
H	2.23563600	0.12203600	8.57397600
C	3.31566300	2.92186700	7.48803700
H	3.54003600	3.18712600	8.52853000
O	4.18121000	3.12940000	5.20781100
H	3.51514900	3.76420500	4.90326400
O	2.07817200	3.57194700	7.09098100
C	4.42542600	3.43595200	6.58017500
H	5.36787800	2.95104600	6.85445500
H	4.54414300	4.51777800	6.72754900
H	-0.87534000	4.27876300	3.06887200
H	1.45245200	3.41021400	4.27068900
H	-4.19454800	0.06174500	2.80109800
H	-6.27680400	-0.12246300	4.60976500

RID-syn-conf-180°



Zero-point correction= 0.405797 (Hartree/Particle)

Thermal correction to Energy= 0.433959

Thermal correction to Enthalpy= 0.434904

Thermal correction to Gibbs Free Energy= 0.345581

Sum of electronic and zero-point Energies= -2239.719381

Sum of electronic and thermal Energies= -2239.691218

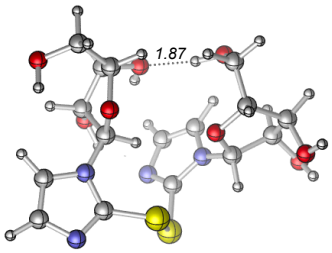
Sum of electronic and thermal Enthalpies= -2239.690274

Sum of electronic and thermal Free Energies= -2239.779597

S	-1.13570400	0.50429200	4.92745800
C	-2.77254000	0.47506100	4.29892600
N	-3.04937300	0.28406000	3.01425600
C	-4.41436500	0.21742100	2.93641200
C	-4.97703500	0.38352600	4.18098800
N	-3.93029600	0.54992600	5.05446400
C	-4.05493300	0.78023800	6.47980100
H	-3.04315700	0.90110700	6.87900600
C	-4.92906900	1.99642700	6.84905900
H	-5.82608400	1.98360700	6.22092800
O	-4.30892400	3.24333700	6.69481000
H	-3.37557600	3.17227700	7.03169900
C	-5.34839000	1.64761800	8.29568000
H	-6.35702200	2.02002700	8.51372500
O	-4.41018600	2.16157700	9.23594900
H	-4.34749300	3.11512100	9.05263400
C	-5.29711000	0.10831400	8.33159600
H	-4.65021700	-0.20997500	9.15909000
O	-7.51871300	-0.15991800	7.37290400
H	-7.11242100	-0.50276200	6.56044700
O	-4.71515700	-0.32596800	7.07209500
C	-6.65985600	-0.56131300	8.43642100
H	-7.14320500	-0.25901600	9.37040100
H	-6.53025600	-1.65291200	8.45420500
S	-0.62545500	2.59931000	5.11421200
C	-0.62190700	2.82789400	6.85434400
N	-1.70090500	2.97638000	7.61903100
C	-1.25428700	3.04803000	8.90970100
C	0.11924200	2.96393500	8.93623100
N	0.51480200	2.80852000	7.63062400
C	1.88630200	2.80321700	7.14374600

H	1.91608900	2.17839700	6.24400700
C	2.43293700	4.21249700	6.82875000
H	2.17687900	4.87484800	7.66039700
O	1.94544700	4.77602600	5.64029600
H	2.47848200	4.38126500	4.92453300
C	3.94022700	3.92113400	6.84029300
H	4.53732500	4.81181500	7.05775100
O	4.22877100	3.40196500	5.54123800
H	5.18348600	3.45860200	5.38342700
C	4.07354700	2.84477300	7.94074000
H	4.71574600	2.03132700	7.58296200
O	3.84886900	4.49707300	9.73077100
H	2.97769400	4.16995400	10.00406600
O	2.73200400	2.31274700	8.15945800
C	4.59060300	3.37003000	9.27217900
H	5.62492200	3.70465500	9.14476700
H	4.58351000	2.55649800	10.01067900
H	-4.92287800	0.05456000	1.99577700
H	-6.00415200	0.39439700	4.50992500
H	-1.93797600	3.13779100	9.74080200
H	0.83042100	2.97406800	9.74540500

RID-syn-conf-270°



Zero-point correction= 0.406805 (Hartree/Particle)

Thermal correction to Energy= 0.435281

Thermal correction to Enthalpy= 0.436225

Thermal correction to Gibbs Free Energy= 0.347639

Sum of electronic and zero-point Energies= -2239.723379

Sum of electronic and thermal Energies= -2239.694903

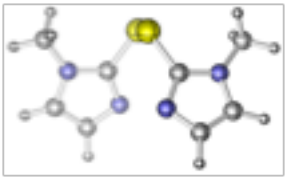
Sum of electronic and thermal Enthalpies= -2239.693959

Sum of electronic and thermal Free Energies= -2239.782545

S	-2.01443800	1.06137200	6.83701900
C	-3.22895500	-0.01823700	6.17800200
N	-3.09920600	-0.70204700	5.05136800
C	-4.21917400	-1.48734600	4.96627600
C	-5.04343500	-1.27513000	6.04624600
N	-4.41900000	-0.32436900	6.82115400
C	-4.86514000	0.17695300	8.10472900
H	-4.31443700	1.09973000	8.30981600
C	-6.37919200	0.42492800	8.20545200
H	-6.92196000	-0.43661200	7.80459200
O	-6.86200500	1.61775500	7.62608400
H	-6.17014900	2.07870200	7.11415400
C	-6.55452200	0.43002600	9.73208400
H	-7.57920800	0.18301500	10.03189600
O	-6.18582800	1.71110400	10.24360100
H	-6.50852400	2.36338100	9.59181800
C	-5.54248800	-0.62663500	10.19803100
H	-5.01712200	-0.26452500	11.08830100
O	-6.78198200	-2.53895100	9.32098500
H	-6.07401600	-2.71279800	8.67888900
O	-4.58986200	-0.78660700	9.11119400
C	-6.14093300	-2.00179100	10.47456700
H	-6.90126800	-1.92111100	11.25724300
H	-5.34736800	-2.67076400	10.83520000
S	-2.58636600	3.02343900	6.18696700
C	-3.80628400	3.57085100	7.33339000
N	-5.05052300	3.86111100	6.96829800
C	-5.64867800	4.39418000	8.08783900
C	-4.77375900	4.38988300	9.14530500
N	-3.58695400	3.88408000	8.66021800
C	-2.40940800	3.52805600	9.43729700
H	-1.56603800	3.51680700	8.73992600

C	-2.08924400	4.48908500	10.60389300
H	-3.00706800	4.83193000	11.08170500
O	-1.34057800	5.61409200	10.21602500
H	-0.41274900	5.31273800	10.19803600
C	-1.36273900	3.53808700	11.56278200
H	-1.38493900	3.88815600	12.60026800
O	-0.02340200	3.46739200	11.06799100
H	0.54280600	3.07518500	11.75025600
C	-2.11279200	2.21267300	11.36739400
H	-1.40858600	1.37770100	11.46233800
O	-4.36125800	2.89841100	12.07650600
H	-4.92358800	2.50207200	11.38025700
O	-2.60247300	2.24035600	10.00352800
C	-3.29889500	1.98582300	12.30956000
H	-2.96241400	2.10687900	13.34632500
H	-3.63922000	0.94812100	12.19583600
H	-4.37853100	-2.16077900	4.13512500
H	-5.99708900	-1.70392100	6.31062400
H	-6.67687200	4.72751100	8.07373800
H	-4.89984000	4.66675200	10.17914400

MTID-anti-conf-90º



Zero-point correction= 0.181913 (Hartree/Particle)

Thermal correction to Energy= 0.196151

Thermal correction to Enthalpy= 0.197095

Thermal correction to Gibbs Free Energy= 0.137395

Sum of electronic and zero-point Energies= -1326.094879

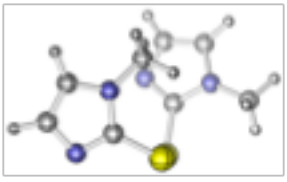
Sum of electronic and thermal Energies= -1326.080641

Sum of electronic and thermal Enthalpies= -1326.079697

Sum of electronic and thermal Free Energies= -1326.139397

S	-0.43659300	0.17397900	2.71370300
N	-0.07488800	2.74562600	3.57548000
N	-1.50424500	1.57722100	4.84327700
C	-0.67123400	1.56745700	3.74749700
C	-0.53355700	3.53298300	4.59513800
H	-0.20395800	4.55630900	4.71608300
C	-1.42473100	2.83271300	5.38325000
S	-2.21692200	0.17603100	1.47996500
N	-2.57279900	2.74868400	0.61873700
N	-1.14633300	1.57720200	-0.64947400
C	-1.97921600	1.56916300	0.44641200
C	-2.11245300	3.53516000	-0.40084100
H	-2.43966500	4.55928200	-0.52153500
C	-1.22303000	2.83296300	-1.18921900
C	-2.36242900	0.48926000	5.30101900
H	-3.19085900	0.34297800	4.60261100
H	-1.78367000	-0.43376200	5.36872200
H	-2.75555200	0.74473300	6.28536500
C	-0.29093700	0.48722900	-1.10765200
H	0.53649500	0.33785600	-0.40872100
H	-0.87228400	-0.43406400	-1.17679500
H	0.10373300	0.74260900	-2.09140100
H	-1.99311900	3.10906900	6.25903900
H	-0.65415200	3.10814500	-2.06505900

MTID-syn-conf-90º



Zero-point correction= 0.182184 (Hartree/Particle)

Thermal correction to Energy= 0.196211

Thermal correction to Enthalpy= 0.197155

Thermal correction to Gibbs Free Energy= 0.138931

Sum of electronic and zero-point Energies= -1326.097045

Sum of electronic and thermal Energies= -1326.083018

Sum of electronic and thermal Enthalpies= -1326.082074

Sum of electronic and thermal Free Energies= -1326.140298

S	-0.78606100	0.20300700	2.74109900
N	-1.70608400	1.60520900	4.91263000
N	-0.46116500	2.83511100	3.51213000
C	-1.00478000	1.59442000	3.78045900
C	-1.61024600	2.88271200	5.38546500
H	-2.08189700	3.18368100	6.31157500
C	-0.84743800	3.65769900	4.53427000
H	-0.54731900	4.69466500	4.57011300
S	-2.46371900	0.31396500	1.37374300
N	-2.65923500	2.89332100	0.49151300
N	-1.11648000	1.70057200	-0.60950500
C	-2.07522700	1.70183200	0.37858400
C	-2.06376600	3.67836100	-0.45787000
H	-2.35412900	4.70963300	-0.60732800
C	-1.09875600	2.96272600	-1.13938100
H	-0.42041000	3.23308300	-1.93500600
C	0.33712500	3.24484100	2.35900600
H	0.82138600	2.36904000	1.92775700
H	-0.29831800	3.71446100	1.60415900
H	1.10050200	3.95141700	2.68937600
C	-0.23587200	0.59541400	-0.97504900
H	-0.82026700	-0.32109500	-1.07316900
H	0.24004900	0.82749500	-1.92805300
H	0.52970000	0.45181900	-0.20775800

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