Probing Molecular Shape 1: Conformational Studies of 5-Hydroxyhexahydropyrimidine and Related Compounds.

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Supporting Information

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General Methods.

Solvents that required the exclusion of moisture were dried according to standard procedures.[1] Melting points were measured on a capillary melting point apparatus and are uncorrected. Routine ^{1}H and ^{13}C NMR spectra were recorded at 298 K in $CDCl_3$ and referenced to the solvent or TMS unless otherwise stated. $CDCl_3$ was dried over $NaSO_4$, filtered and stored over 4A molecular sieves. NMR spectra recorded in D_2O were referenced to TSP (0.0 ppm). DMSO-d_6 was dried by vacuum distillation from CaH_2. Confirmation of peak assignments were made using a combination of techniques including D_2O exchange experiments, selective 1D ^{1}H NMR decoupling experiments, as well as DEPT and standard gradient 2D experiments (gCOSY, gHSQC and gHMBC). All 2D spectra were acquired on a spectrometer operating at 500 MHz with a sample concentration greater than 10 mg mL^{-1}. Routine ^{1}H NMR spectra were acquired with a sample concentration of ~ 0.5 mg mL^{-1} and therefore the hydroxyl proton may have a different appearance and/or chemical shift value in the 2D NMR spectra because higher sample concentrations (~ 10 mg mL^{-1}) were used to acquire this data.

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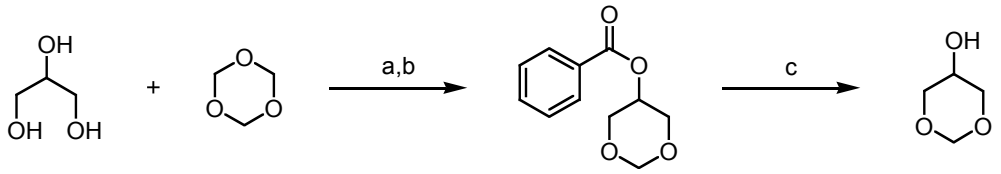
[1] Perrin, D.D.; Armarego, W.L.F. *Purification of Laboratory Chemicals*. 4th ed., Boston: Butterworth Heinemann, **1996** and Vogel, A.I.; Furniss. B.S. *Vogel's Textbook of Practical Organic Chemistry*. 5th ed., London: Longman Scientific & Technical, **1989**.

The Synthesis of 1,3-Dioxanol (4)



6 **4**

Scheme S1. *Reagents and Conditions:* (a) H_2SO_4, 100 °C, 20 h (b) benzoyl chloride (1 equiv), pyridine, rt, 48 h followed by fractional crystallization (c) Na, MeOH/$CHCl_3$.

*1,3-Dioxan-5-ol benzoate (**6**):* Glycerol (150 g, 0.9 mol) was mixed with paraformaldehyde (50 g, 0.3 mol) and conc HCl (4 mL) and the solution stirred at 100 °C for 1.5 h. The mixture was placed under vacuum at 50 °C and the vacuum maintained until the evolution of water ceased and then stirred at 100 °C for a further 18 h. The reaction mixture was distilled at reduced pressure yielding a fraction containing the mixed glycerol acetals, bp 75 - 110 °C/55 torr (63.9 g, 38%). An aliquot (50 g, 0.48 mol) of the mixed acetals was stirred with dry pyridine under nitrogen. Benzoyl chloride (67 g, 0.48 mol) was added dropwise to the stirred pyridine solution whilst maintaining the reaction mixture at a temperature less than 60 °C. The mixture was allowed to stand at room temperature for 48 h. The reaction mixture was dissolved in ether (200 mL) and the ether solution successively washed with water (2 × 200 mL), dilute sulfuric acid (2%, 200 mL) and $NaHCO_3$ solution (5%, 200 mL). The ether solution was dried over $CaCl_2$ and the solvent removed under reduced pressure to yield the mixed benzoates as a waxy semi-crystalline mass (81.4 g, 73%).

The mixed benzoates were separated via fractional crystallization from ether. The isolated semi-crystalline mass of mixed benzoates was dissolved in 100 mL of warm ether and the solution cooled to room temperature. The small crystals that formed were filtered off and the filtrate concentrated to 40 mL. After cooling the filtrate to 0 °C, a second crop of crystals was collected. Recrystallization of the

combined fractions from ligroin gave the 1,3-dioxan-5-ol benzoate (**6**) as colorless, needlelike crystals (26.7 g, 33%, based on the mass of mixed benzoates) mp 75.5 - 76.5 °C (lit.[2] 72 °C). The ^{1}H and ^{13}C NMR spectral data for **6** are given in the main paper.

*1,3-Dioxan-5-ol (**4**):* Dry methanol (30 mL) containing a trace of sodium was mixed with 1,3-dioxan-5-ol benzoate (18 g, 87 mmol) dissolved in dry $CHCl_3$. The mixture was kept at room temperature for 48 h and then neutralized with dry ice. The residue was taken up in water (100 mL) and the aqueous solution extracted with petroleum ether (100 mL) and then exhaustively extracted with ether. Removal of the ether and distillation at reduced pressure yielded **4** as a colorless liquid (5.7 g, 48%), bp 50 °C/55 torr (lit.[3] 80-85 °C/11 mm). The ^{1}H and ^{13}C NMR spectral data for **4** are given in the main paper.

[2] Main paper, reference 9

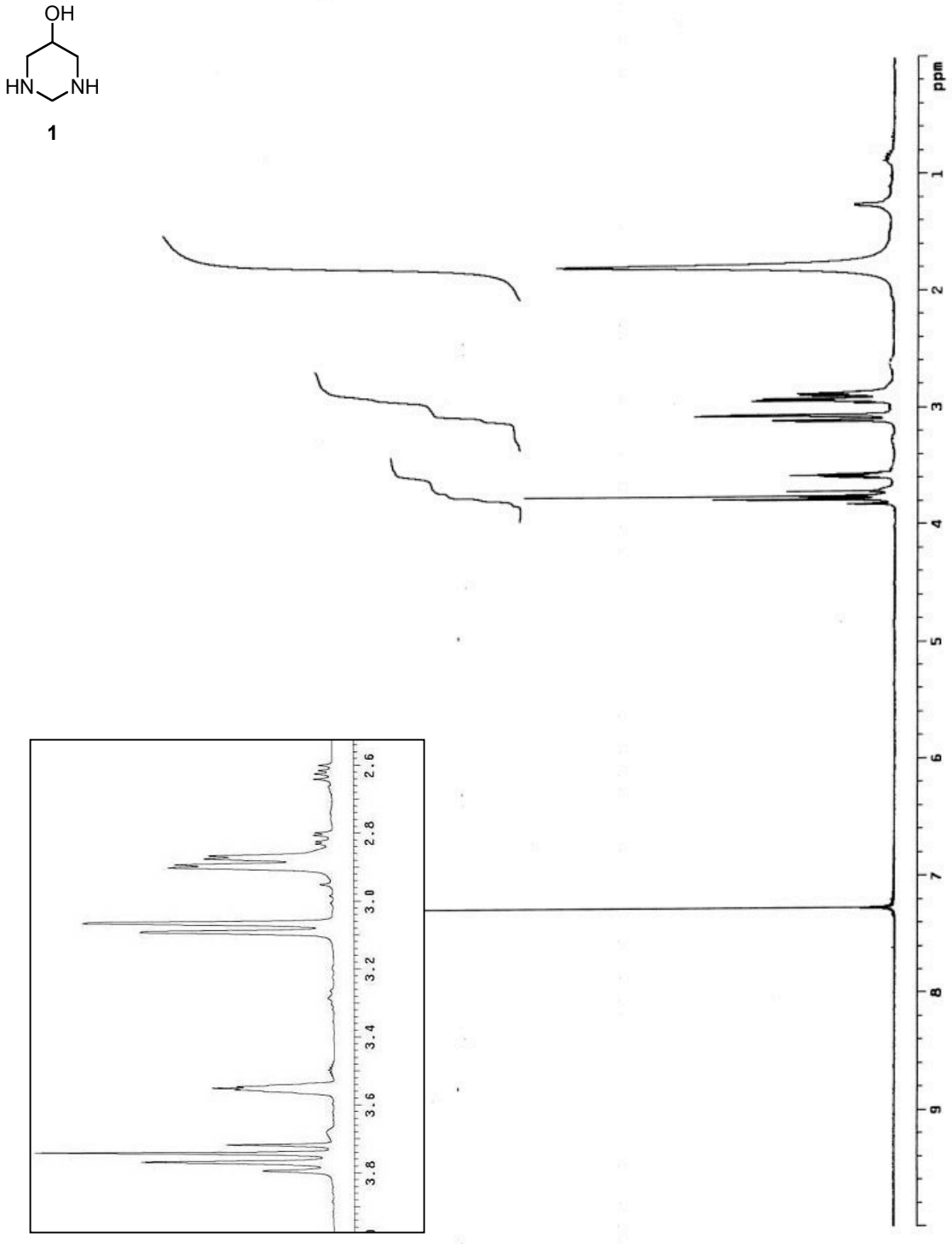
[3] Main paper, reference 10

Table S1: *A Summary of Coupling Constant Values for Compounds **1** and **4**.*

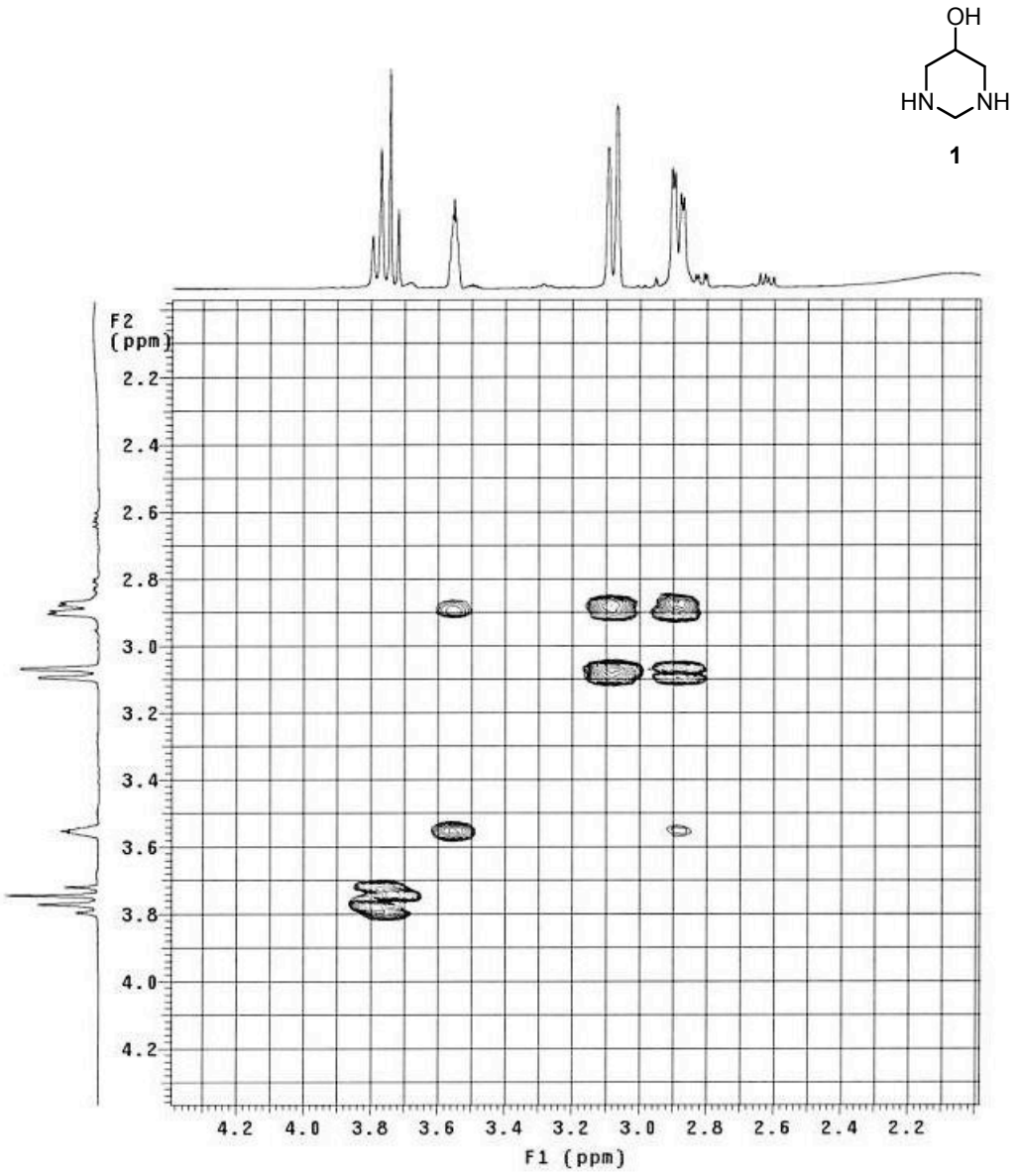
Compound	Solvent	(Geminal) ^2J (Hz)		(Vicinal) ^3J (Hz)			Long Range
		$J_{2e,2a}$	$J_{4e,4a}$	$J_{4a,5}$	$J_{4e,5}$	$J_{5,OH}$	$J_{4e,2e}$
1	$CDCl_3$ (300 MHz)	12.5	12.8	2.9	3.1	-	-
1	D_2O (300 MHz)	12.5	12.9	7.8	3.8	-	-
1	DMSO-*d6* (500 MHz)	12.6	12.9	7.9	3.1	-	-
4	$CDCl_3$ (300 MHz)	6.2	11.1	2.2	3.2	9.9	0.5 (^4J)
4	DMSO-*d6* (500 MHz)	5.9	11.3	7.6	4.3	4.7	-

Assorted 1D and 2D NMR Spectra for compounds 1, 2, 3, 4, and 1,3-dioxan-5-ol benzoate

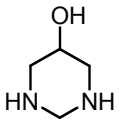
*The ^{1}H NMR Spectrum of 5-hydroxyhexahydropyrimidine (**1**) in $CDCl_3$ (300 MHz) at 298 K*



*5-Hydroxyhexahydropyrimidine (**1**) gCOSY (500 MHz) in $CDCl_3$ at 298 K, expanded*



*5-Hydroxyhexahydropyrimidine (**1**) gHSQC (500 MHz) in $CDCl_3$ at 298 K, expanded*



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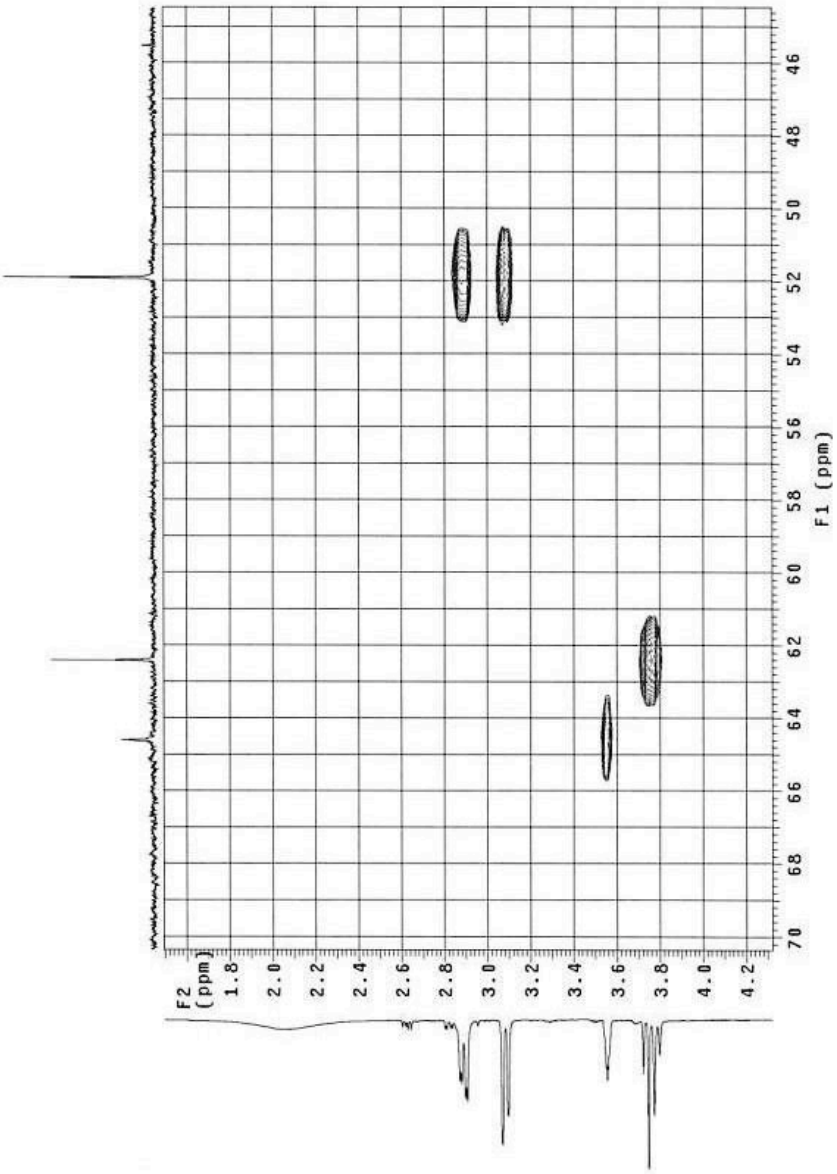
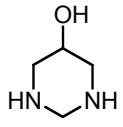


*[1]H NMR Spectrum of **1** in DMSO-d6 (500 MHz) at 298 K, with expansion*



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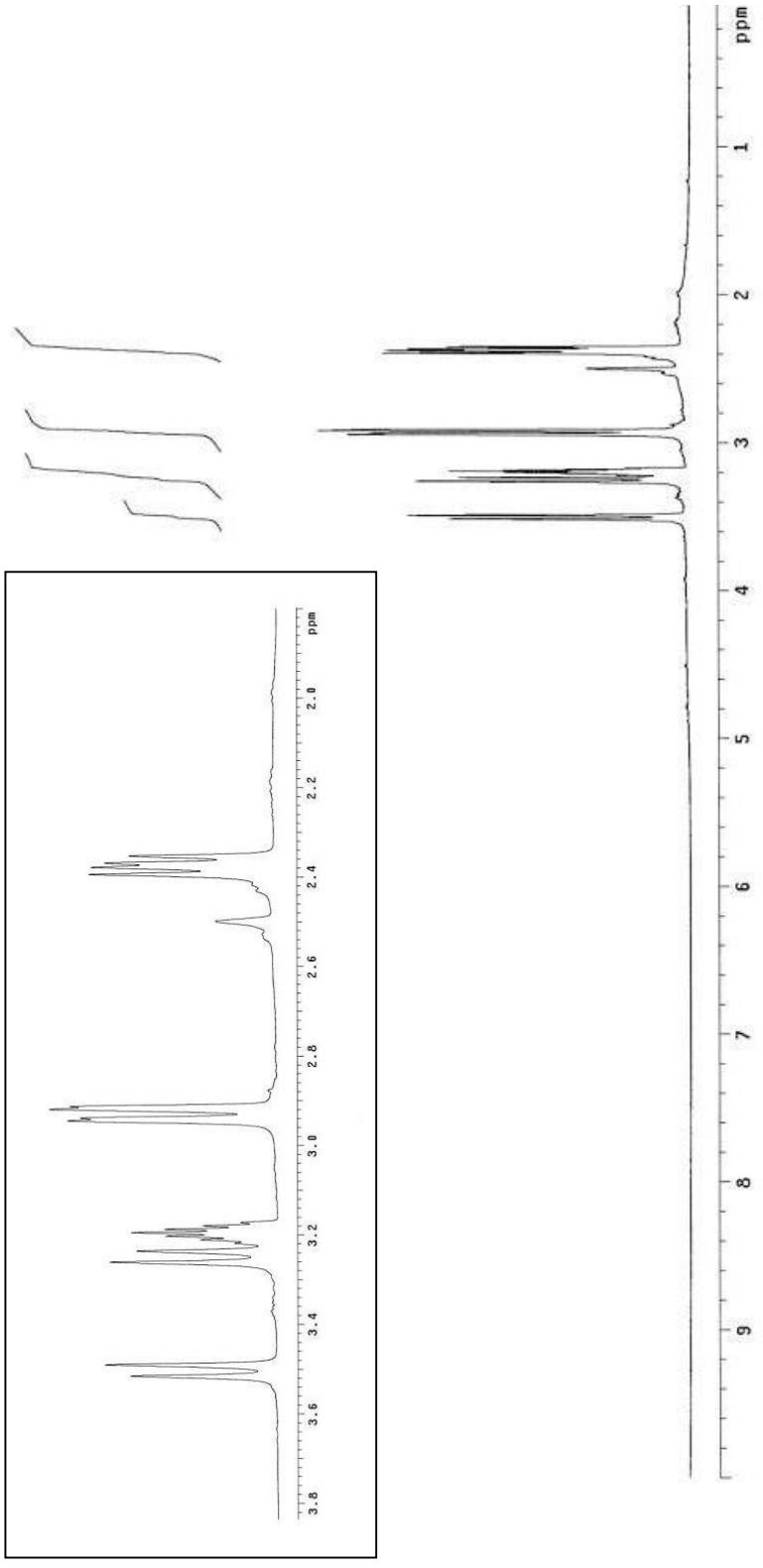
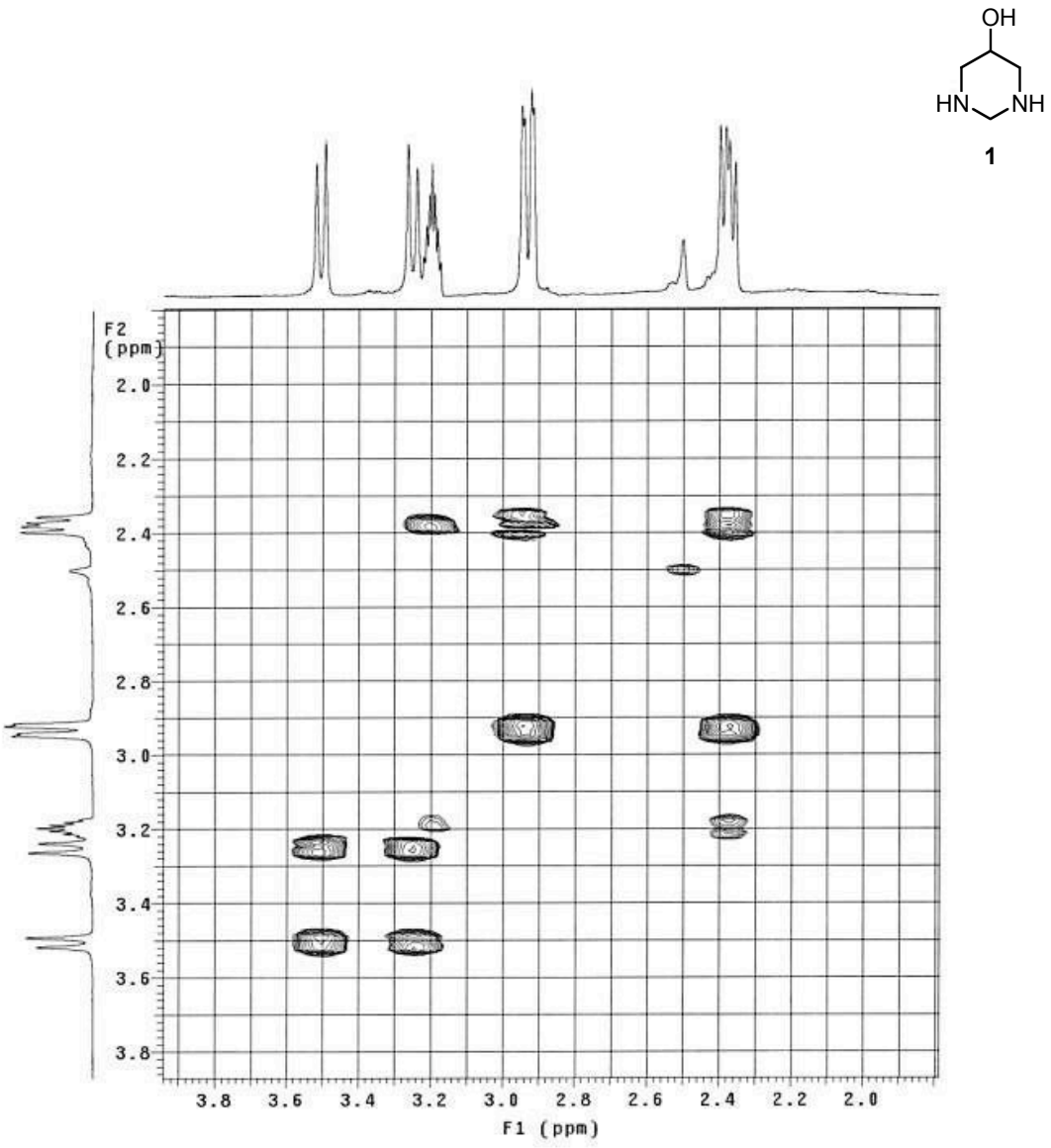
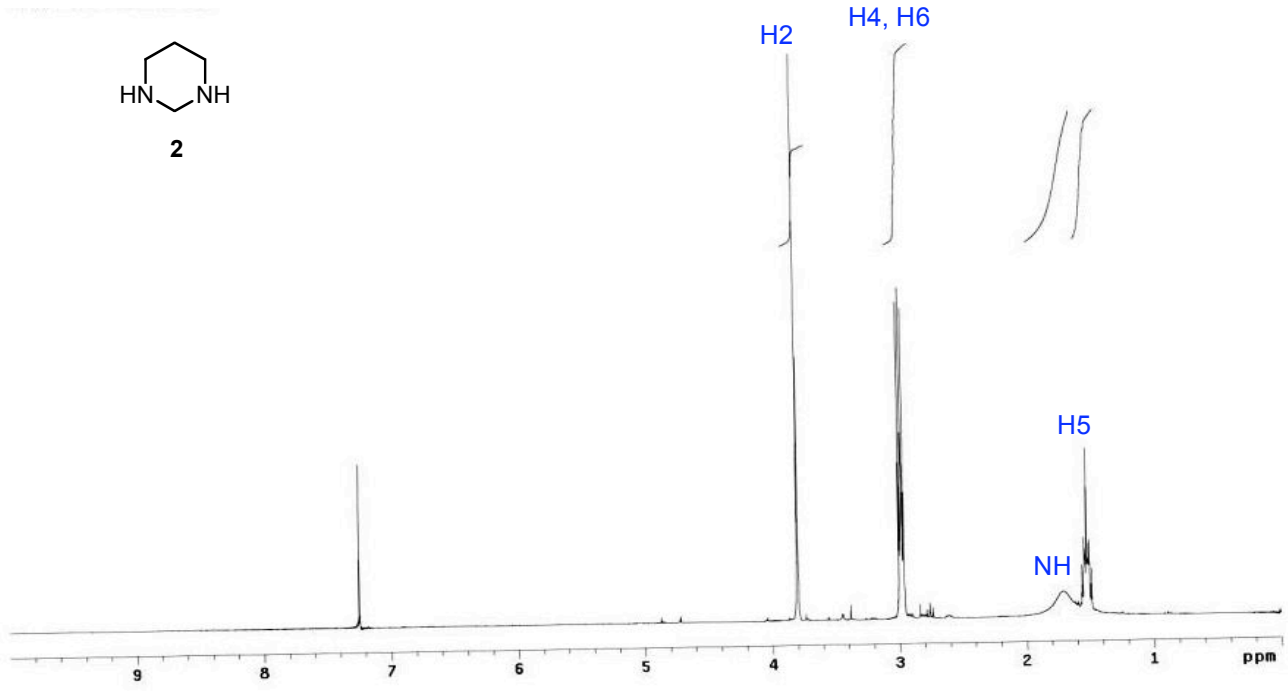


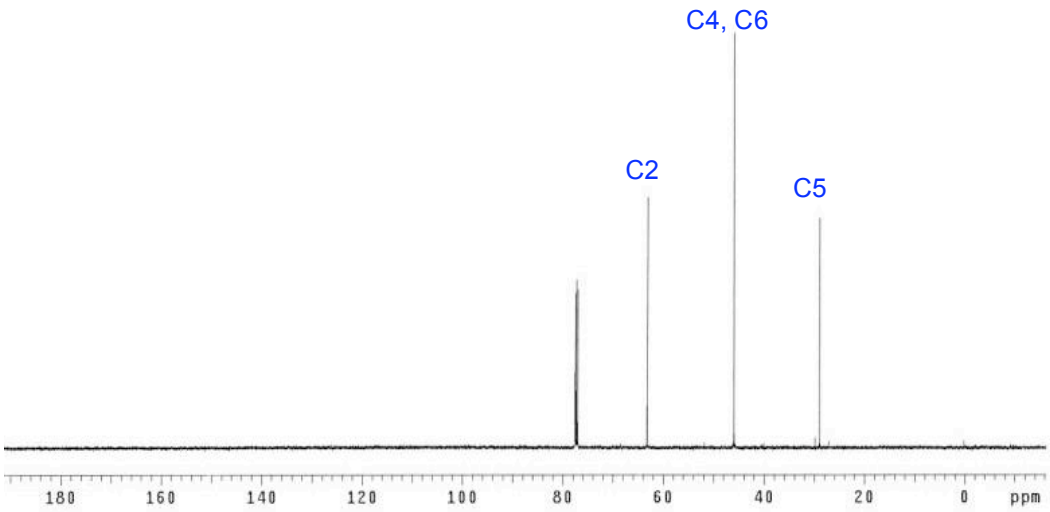
*5-Hydroxyhexahydropyrimidine (**1**) gCOSY (500 MHz) in DMSO-d6 at 298 K, expanded*



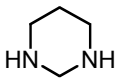
*The ^{1}H NMR Spectrum of **2** in $CDCl_3$ (300 MHz) at 298 K*



*The ^{13}C NMR Spectrum of **2** in $CDCl_3$ (126 MHz) at 298K*



*Hexahydropyrimidine (**2**) gHSQC (500 MHz) at 298 K, expanded*



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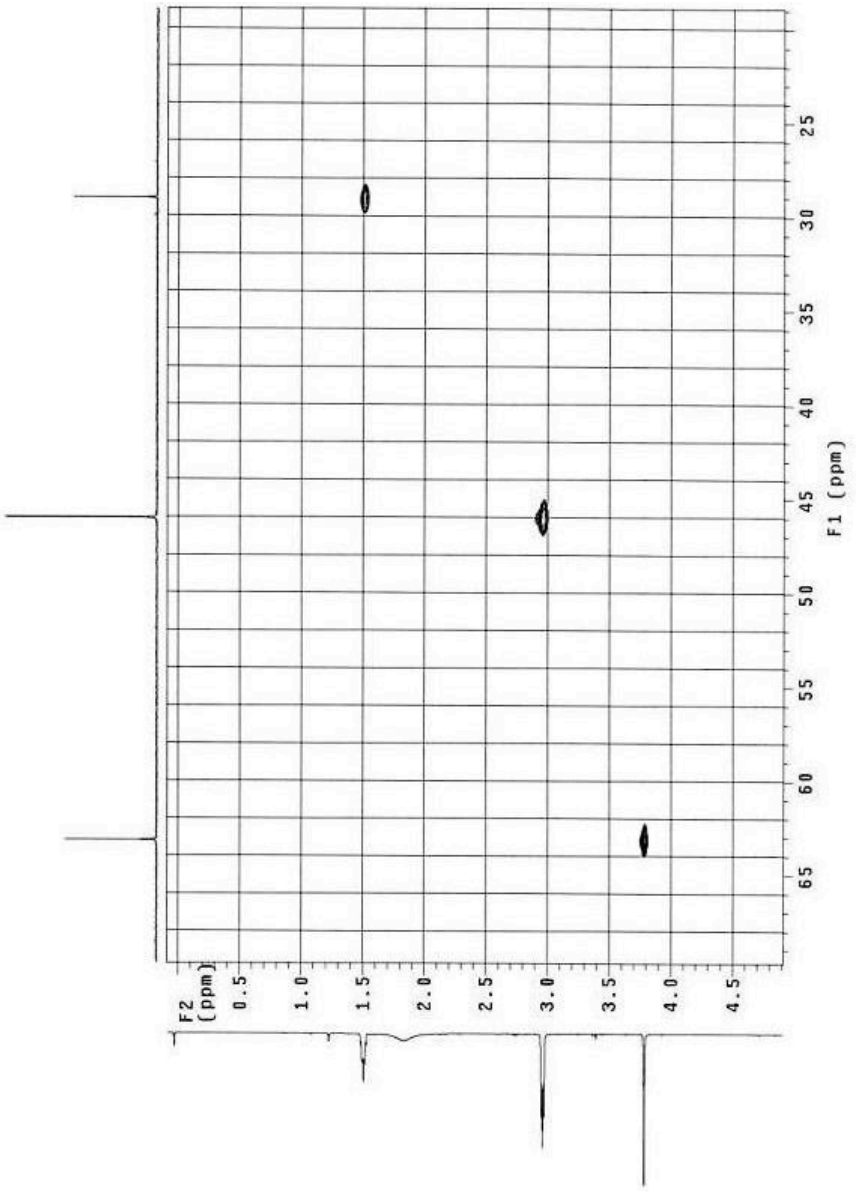
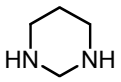


*Hexahydropyrimidine (**2**) gHMBC (500 MHz) at 298 K, expanded*



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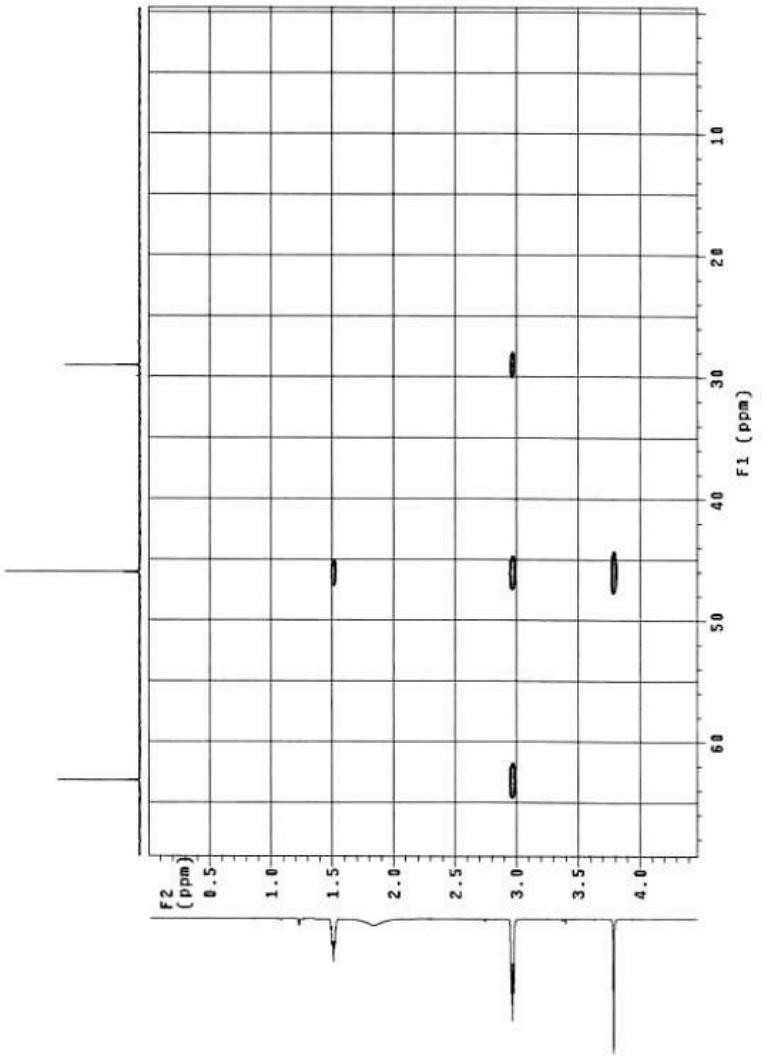
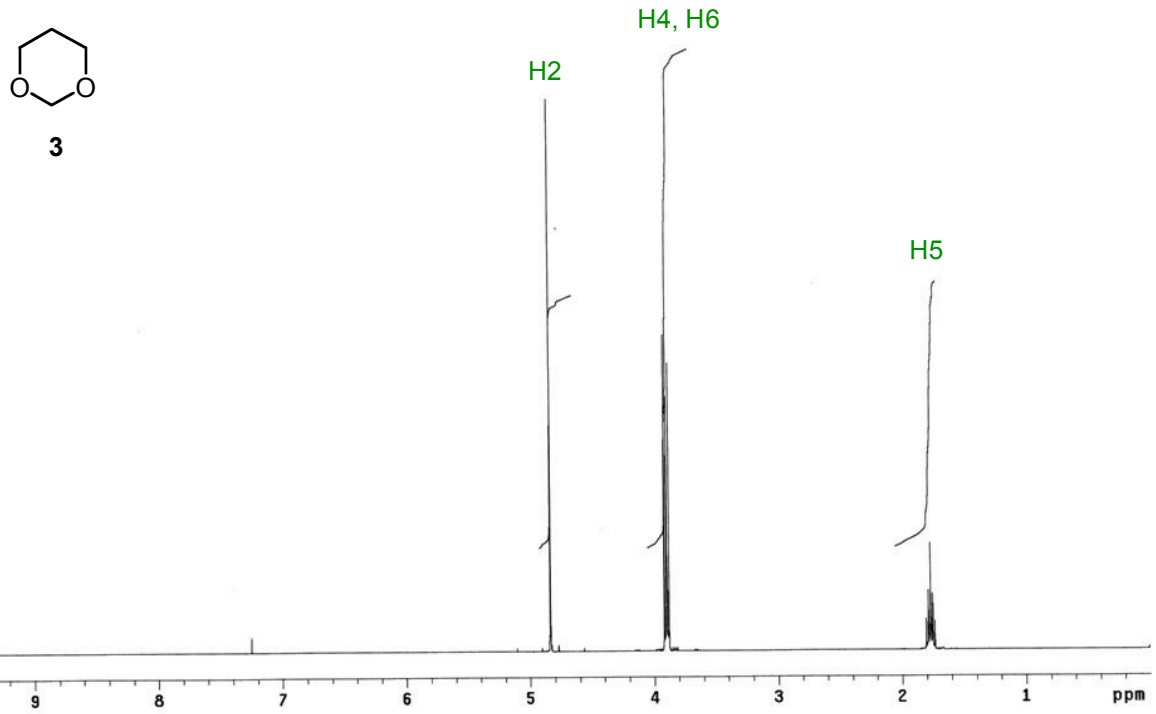
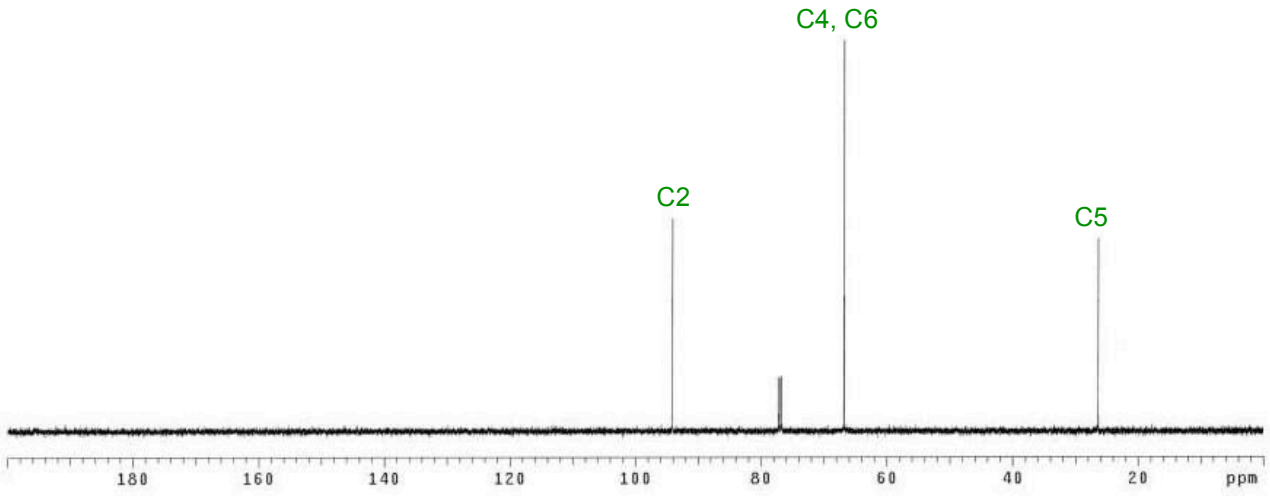


*The ^{1}H NMR Spectrum of 1,3-dioxane (**3**) in $CDCl_3$ (300 MHz) at 298 K*



*The ^{13}C NMR Spectrum of 1,3-dioxane (**3**) in $CDCl_3$ (75 MHz) at 298 K*



*The ^{1}H NMR Spectrum of 1,3-dioxan-5-ol (**4**) in $CDCl_3$ (300 MHz) at 298 K*

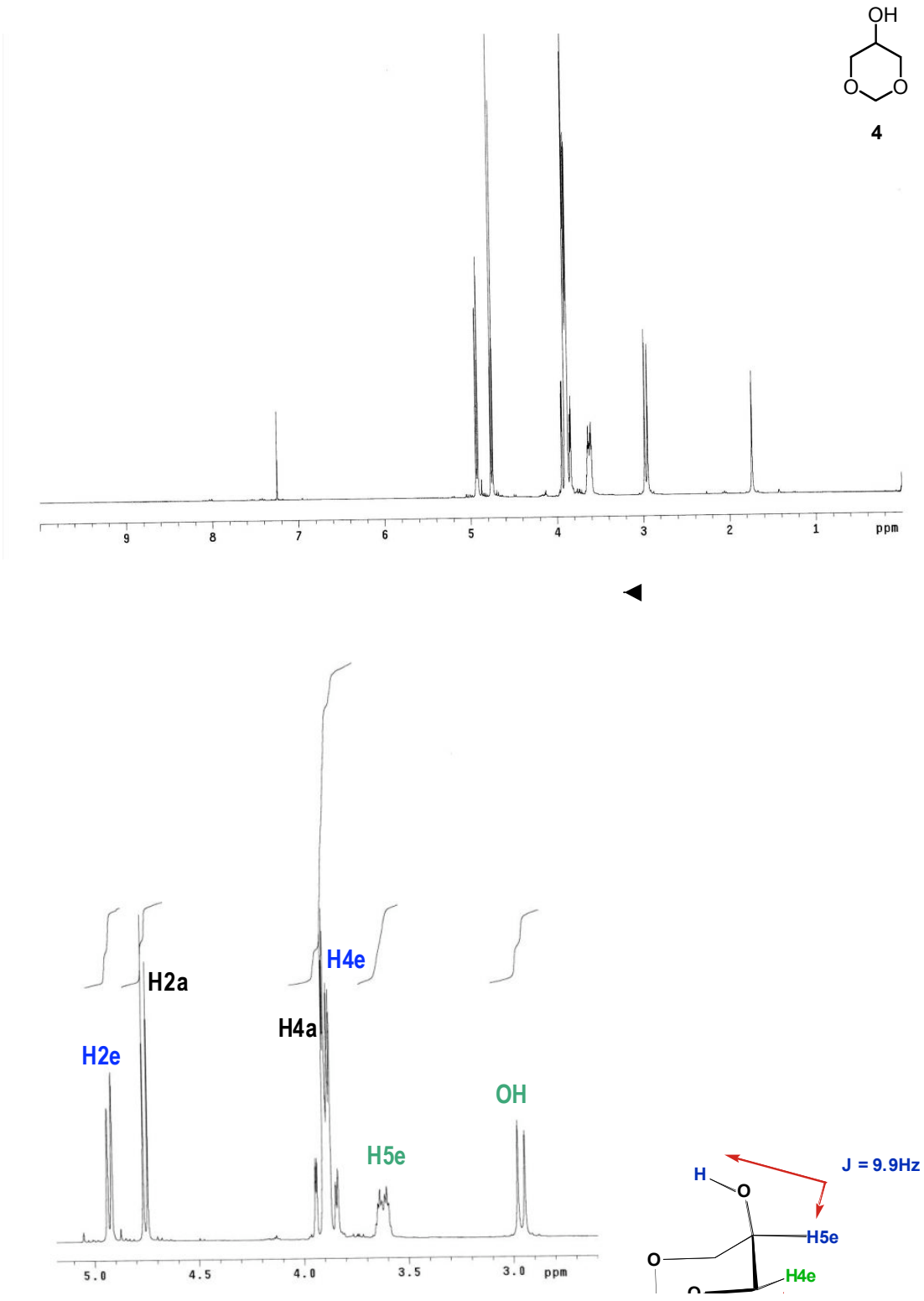
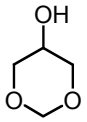


Figure S1. *The room temperature ^{1}H NMR spectrum of 1,3-dioxan-5-ol (**4**)*

*Arrayed selectively decoupled ^1H NMR Spectra of 1,3-dioxan-5-ol (**4**) in $CDCl_3$ (300 MHz) at 298 K*



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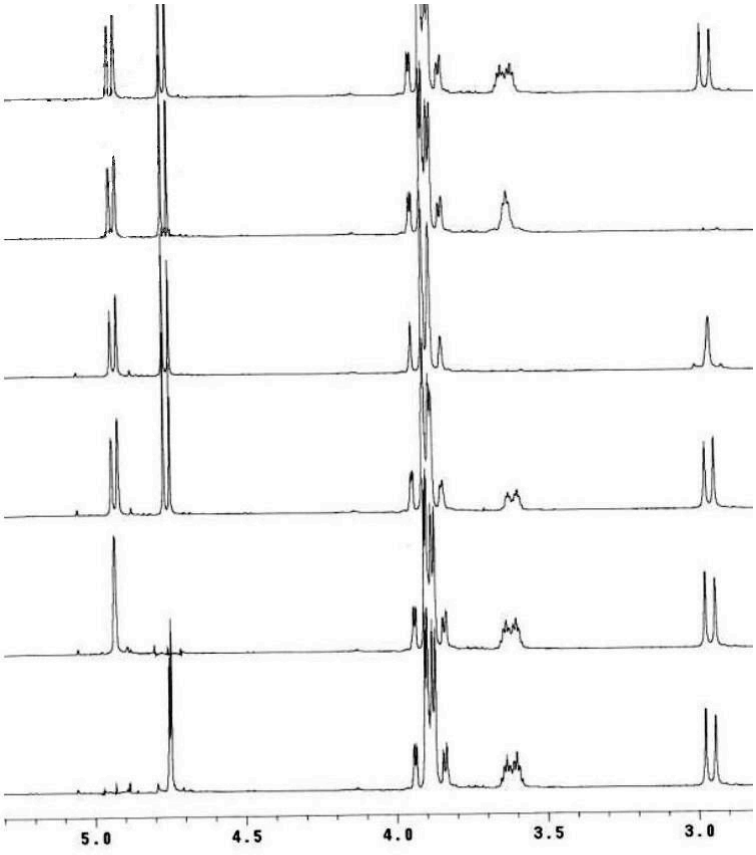
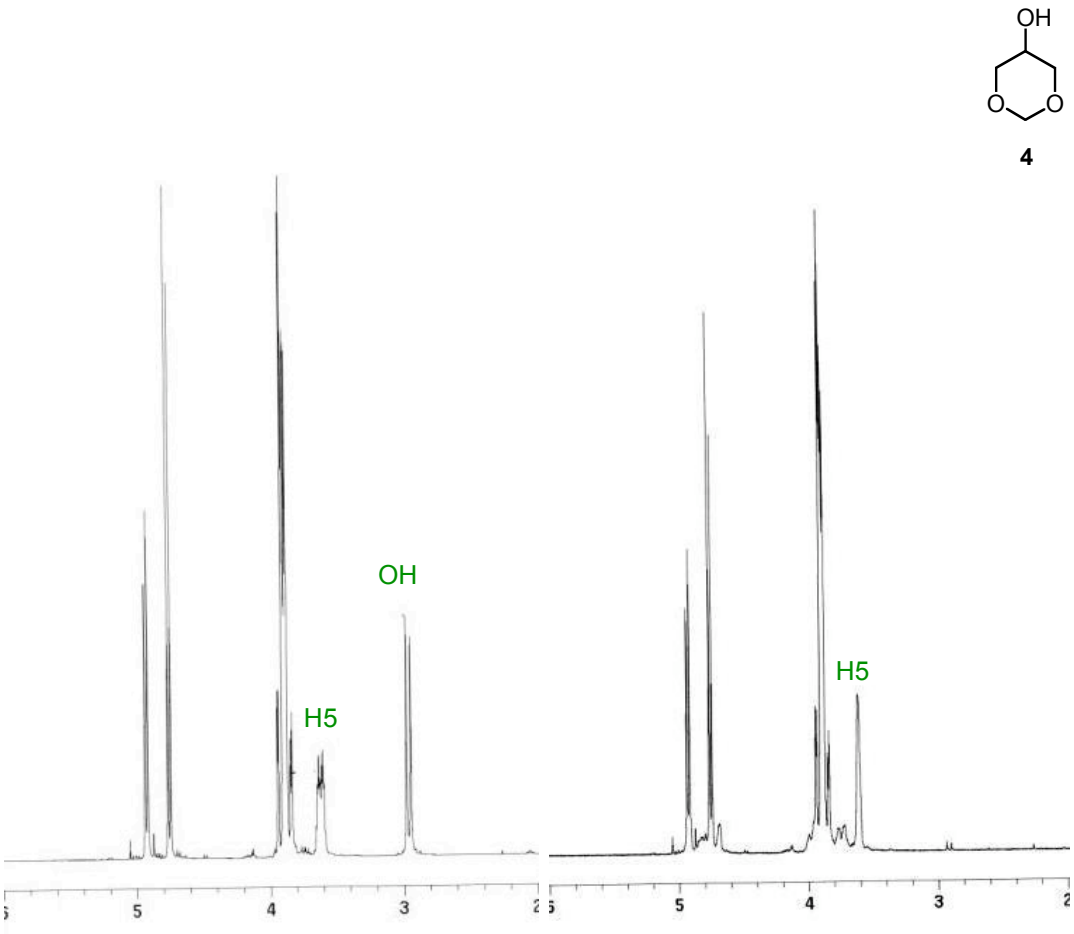


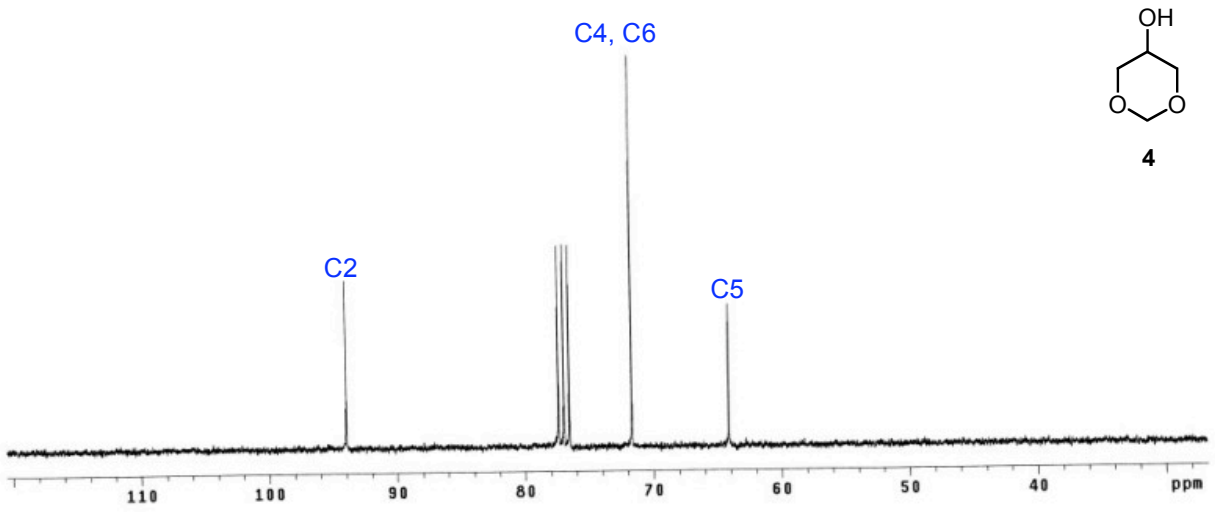
*The ^{1}H NMR Spectrum of 1,3-dioxan-5-ol (**4**) in $CDCl_3$ (300 MHz) at 298 K – D_2O exchange experiment*



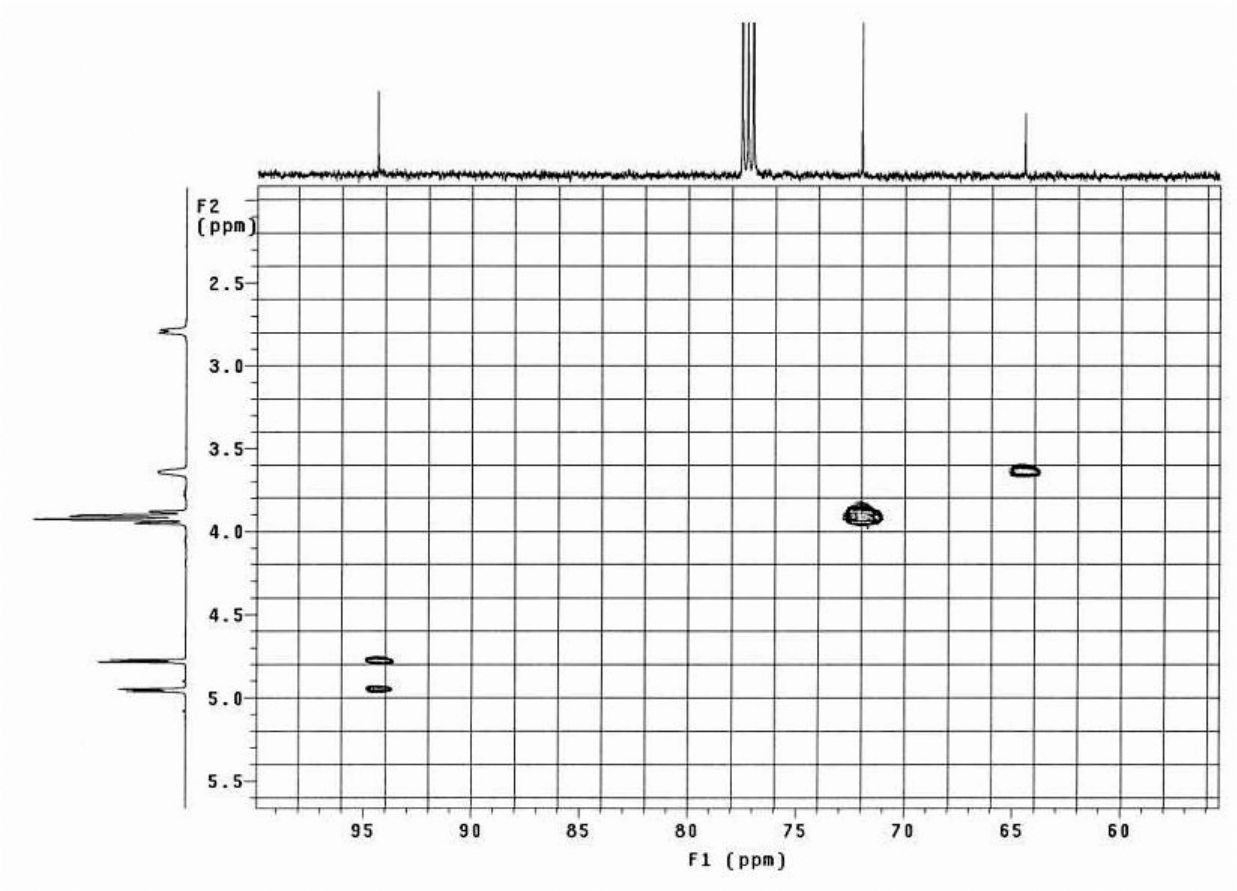
Before D_2O exchange

After D_2O exchange

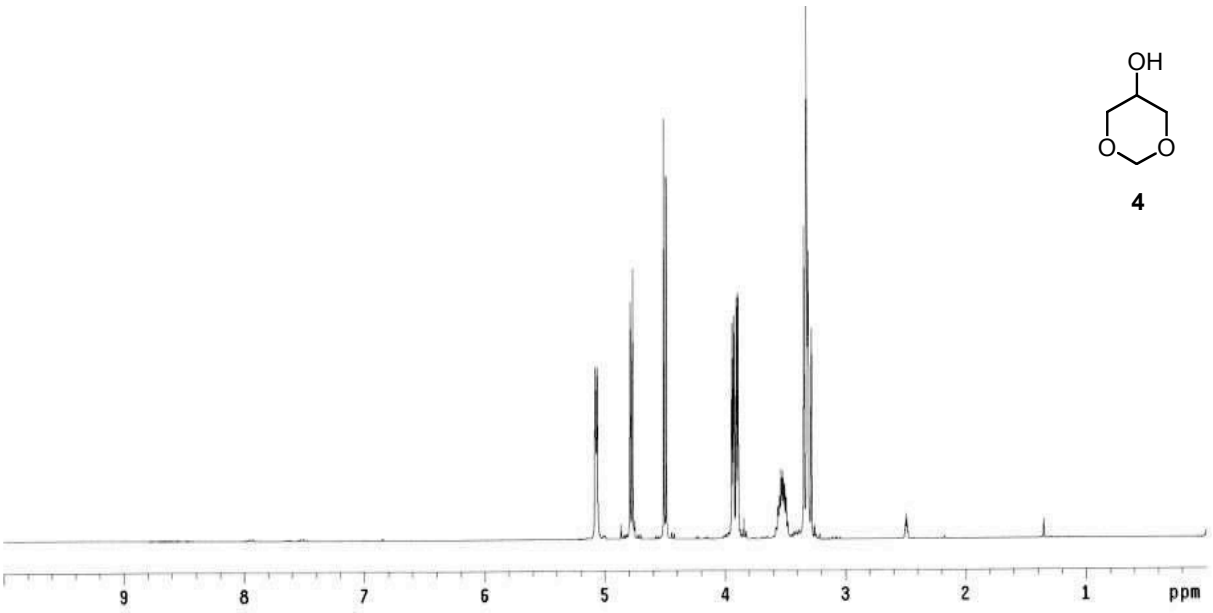
*The ^{13}C NMR Spectrum of 1,3-dioxan-5-ol (**4**) in $CDCl_3$ (75 MHz) at 298 K*

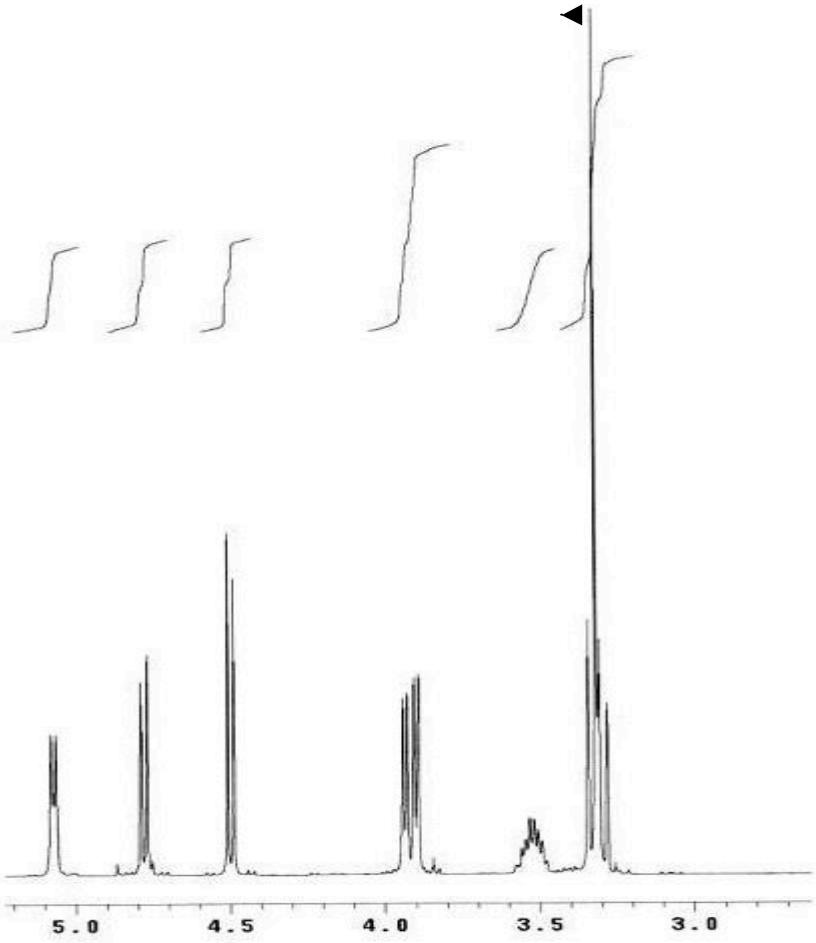


*1,3-dioxan-5-ol (**4**) gHSQC in $CDCl_3$ (500 MHz) at 298 K*

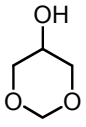


*The ^{1}H NMR Spectrum of 1,3-dioxan-5-ol (**4**) in DMSO-d6 (300 MHz) at 298 K*





*1,3-dioxan-5-ol (**4**) gHSQC in DMSO-d6 (500 MHz) at 298 K*



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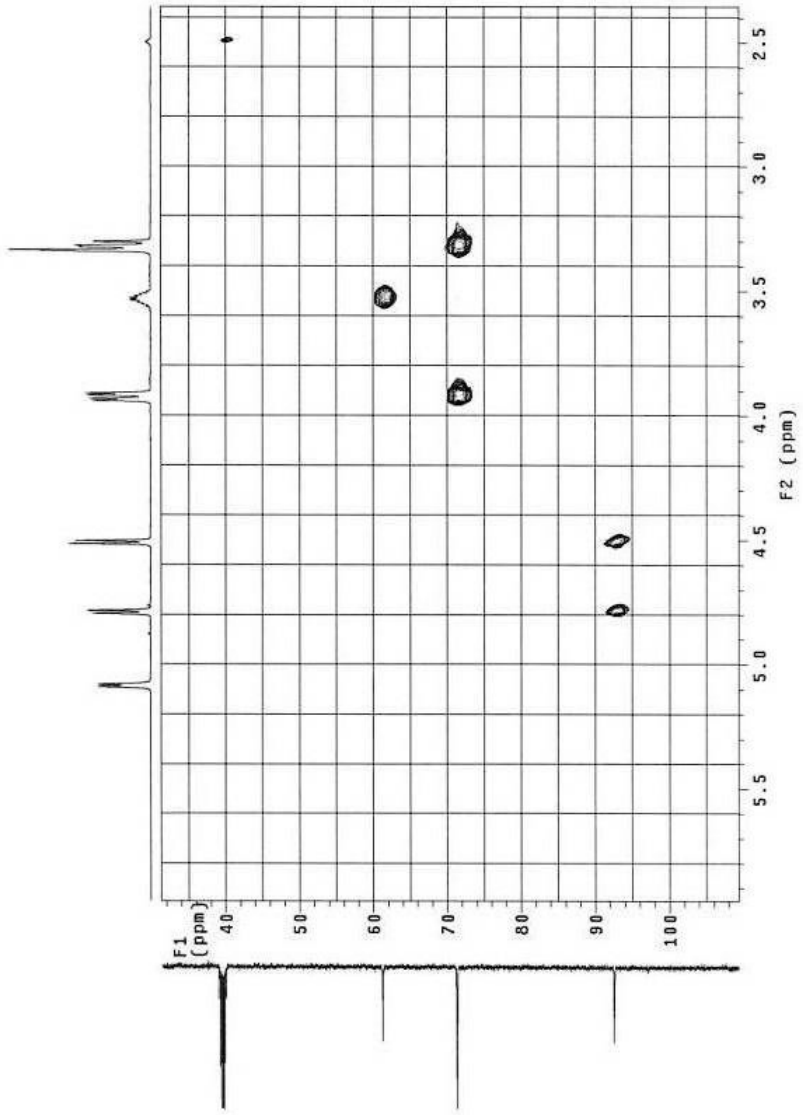
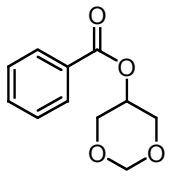


*The ^{1}H NMR Spectrum of 1,3-dioxanol benzoate (**6**) in $CDCl_3$ (300 MHz) at 298 K*



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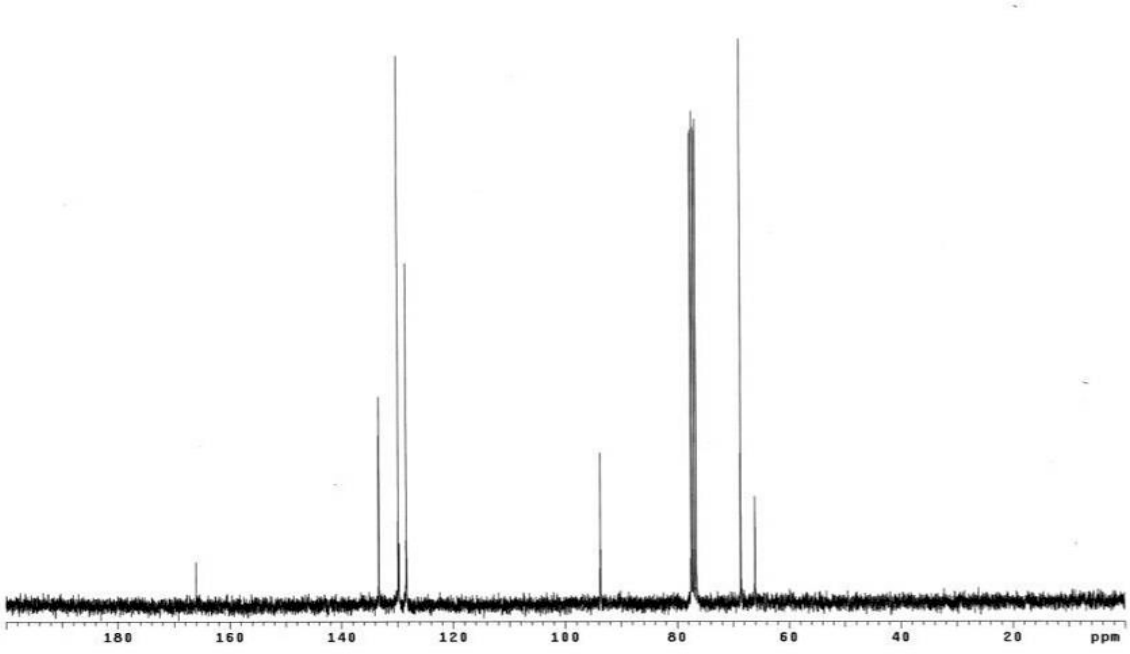
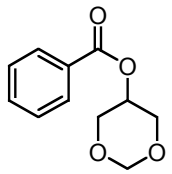
*The ^{13}C NMR Spectrum of **6** in $CDCl_3$ (75 MHz) at 298 K*



*1,3-dioxanol benzoate (**6**) DEPT in $CDCl_3$ (126 MHz) at 298 K*



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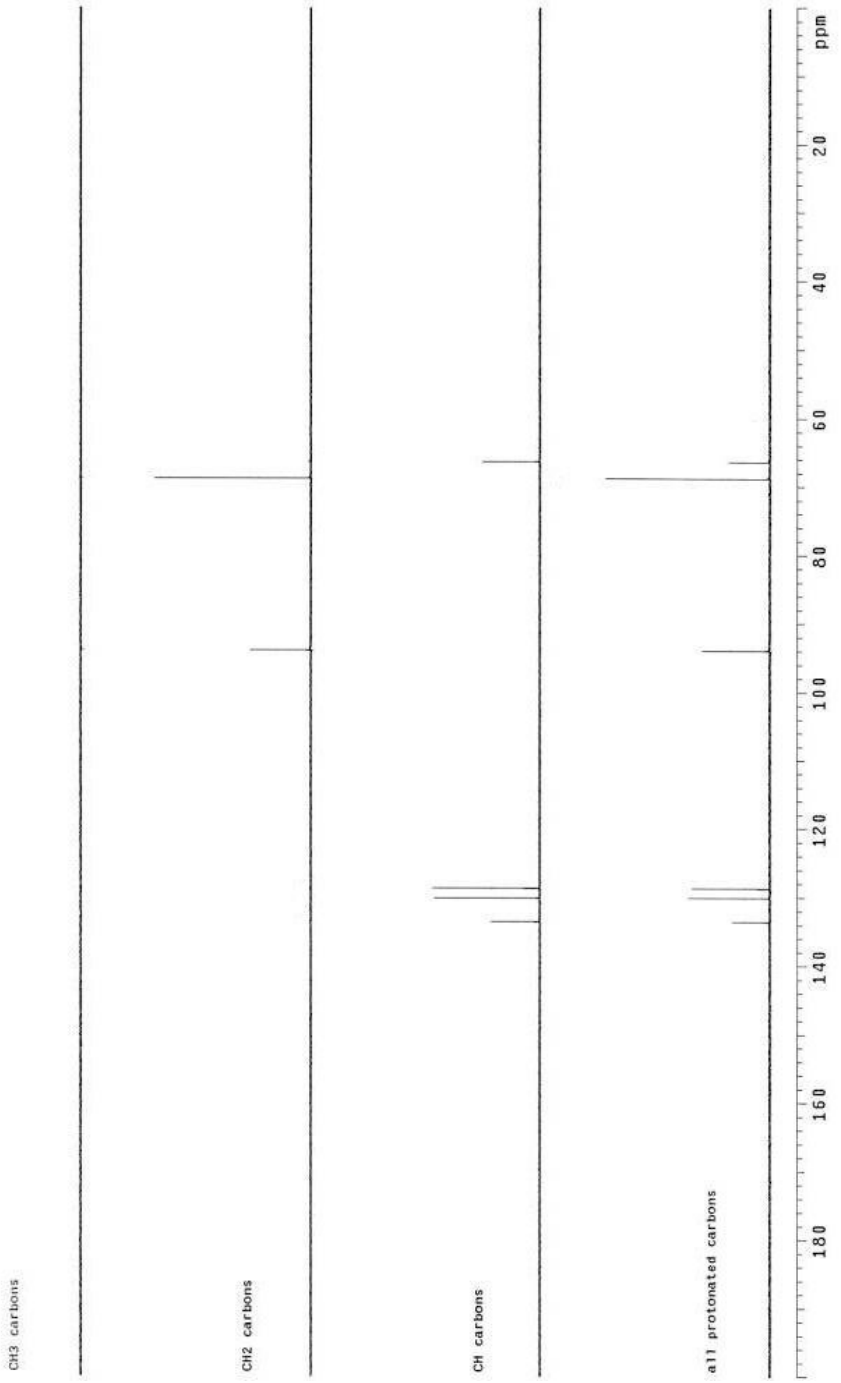
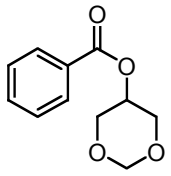


*1,3-dioxanol benzoate (**6**) gHSQC in $CDCl_3$ (500 MHz) at 298 K*



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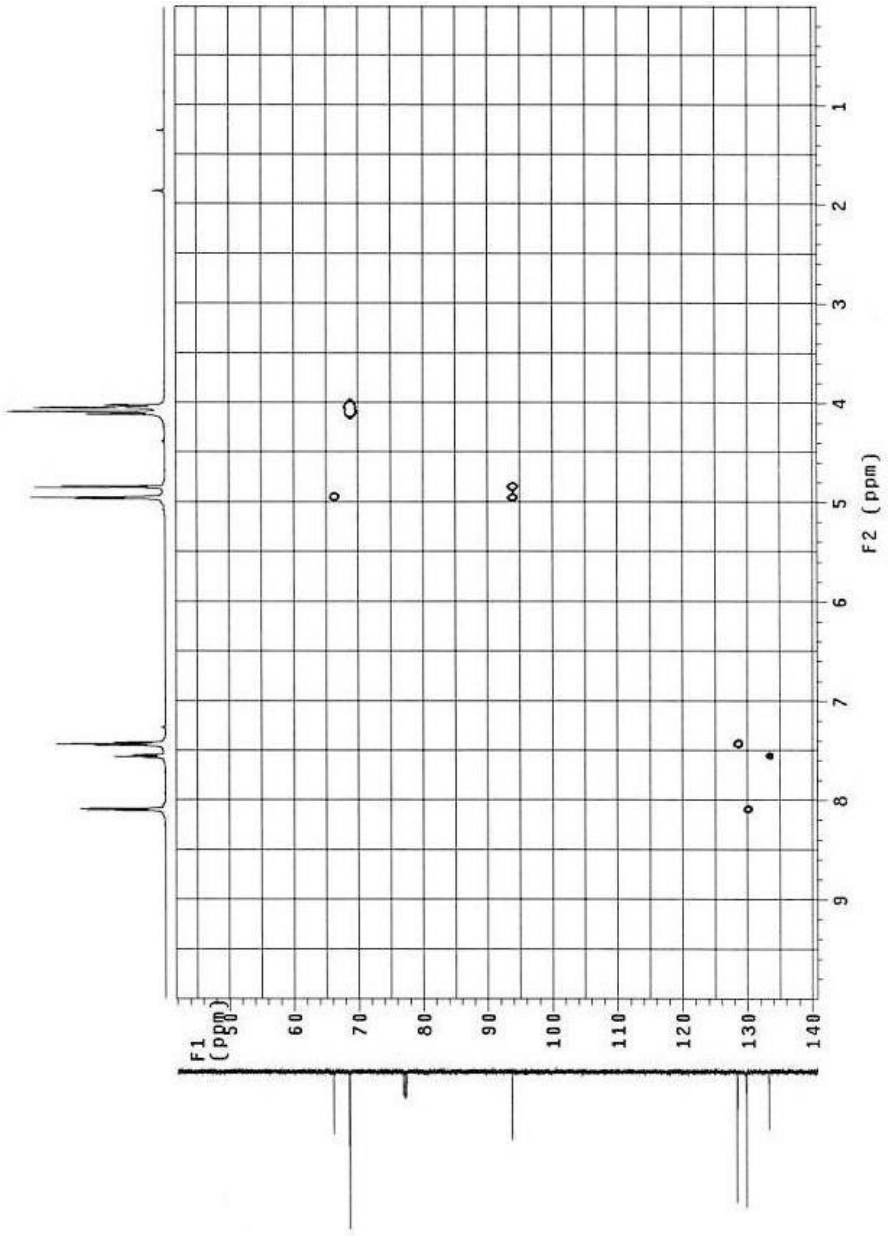

Acquisition and Analysis of Variable Temperature ^{1}H NMR Spectra.

General: The sample concentration used for all compounds was approximately 0.5 mg mL^{-1}. Spectral peaks of compounds in $CDCl_3$ or CD_2Cl_2were referenced to TMS. Copper stabilized $CDBr_3$ was stored over 4A molecular sieves and passed through a small plug of basic alumina before being used in sample preparation. Spectral peaks of compounds in $CDBr_3$ were referenced to the residual solvent signal occurring at 6.82 ppm.

Low Temperature VT ^{1}H NMR Spectroscopy. Low temperature ^{1}H NMR spectra of compounds **2** and **3** were recorded on a 400 MHz spectrometer. Spectra were acquired at 3 - 10 degree intervals, with the smaller temperature intervals employed in the proximity of the coalescence temperature, T_c. The temperature ranges were 298 K to 218 K ($CDCl_3$) for compound **2** and 298 K to 183 K (CD_2Cl_2) for compound **3**.

High Temperature VT ^{1}H NMR Spectroscopy. High temperature ^{1}H NMR spectra of compounds **1** and **4** were recorded on a 300 MHz spectrometer. Temperature accuracy of the probe between 198 K and 268 K was tested using a standard ethylene glycol solution. The ^{1}H NMR spectra were acquired at 10 degree intervals between 298 K and 388 K in $CDBr_3$.

Analysis of the Low Temperature ^{1}H NMR Spectral Data. The temperature dependence of the rate constants for compounds **2** and **3** was evaluated using lineshape analysis of the signals arising from the protons on C2. Computer simulation was conducted using the gNMR[4] program, which employs the Binsch[5] procedure for lineshape analysis. Lineshape analysis was carried out using spectra acquired in the region of the T_c. Chemical shifts and coupling constants used in the initial simulated spectrum were calculated from the slow exchange spectra. Spectra acquired at the fast exchange limits were deleted

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[4]Main paper, reference 29

[5] Binsch, G. "Bandshape Analysis" in. *Dynamic Nuclear Magnetic Resonance Spectroscopy,* Jackman, L.M.; Cotton, F.A. *eds*. Academic Press, London, **1975**.

from the analysis, as the errors calculated in the simulated lineshapes of these spectra were considerable and the rates calculated from them were deemed unreliable. The inaccuracy of rates calculated from fast exchange spectra is a commonly encountered problem in lineshape analysis.[6]

Determination of the activation parameters $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ (and therefore $\Delta G^{\ddagger}$) was achieved using the Eyring equation, which can take the form:

$$k = \kappa(k_B T/h)e^{-\Delta G^{\ddagger}/RT} \qquad \textit{equation (1)}$$

where

$$\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger} \qquad \textit{equation (2)}$$

then

$$k = \kappa(k_B T/h)e^{-(\Delta H^{\ddagger} - T\Delta S^{\ddagger})/RT} \qquad \textit{equation (3)}$$

where

k = the calculated rate constant, κ = the transmission coefficient, taken as unity, $k_B = 3.29986\times10^{-24}$ cal K^{-1}, 1.380662×10^{-23} J K^{-1}(Boltzmann constant), h = 1.058369×10^{-34} cal s, 6.626176×10^{-34} J s (Plancks constant), and R = 1.98719 cal mol^{-1} K^{-1}, 8.31441 J mol^{-1} K^{-1} (Universal Gas constant).

Rearrangement of ***equation (3)*** gives:

$$\ln(k/T) - \ln(k_B/h) = -\Delta H^{\ddagger}(1/RT) + \Delta S^{\ddagger}/R \qquad \textit{equation (4)}$$

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[6] See footnote 5 and (b) Sandström, J. *Dynamic NMR Spectroscopy*, Academic Press, London, **1982**. (c) Ōki, M. *Applications of Dynamic NMR Spectroscopy to Organic Chemistry,* VCH Publishers, Deerfield Beach (USA), **1985**.

The parameters were evaluated by plotting ln(k/T) - ln(k_B/h) against 1/T, which gives a straight line. $\Delta H^{\ddagger}$ was calculated from the slope of the line and extrapolation to the y axis to find the intercept allowed calculation of $\Delta S^{\ddagger}$.

Molecular Modelling Results:

Table S2: *Computed Total Energies for Compound **1** Conformers.*

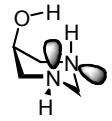
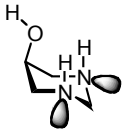
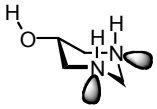
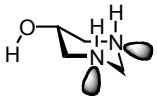
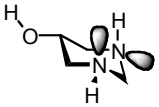
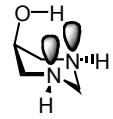
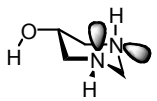
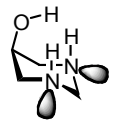
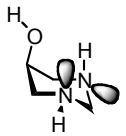
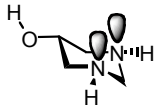
Conformer		DFT (B3LYP, 6-311+G**)		*ab initio* (HF 6-31G*)	
		Total Energy (hartree)	**Relative Energy (kcal mol^{-1})**	**Total Energy (hartree)**	**Relative Energy (kcal mol^{-1})**
	**1a**	-343.260377	0	-341.0265718	0
	**1b**	-343.258941	0.90	-341.0254897	0.68
	**1c**	-343.257660	1.71	-341.0233533	2.02
	**1d**	-343.257576	1.76	-341.0229498	2.27
	**1e**	-343.257367	1.89	-341.0238075	1.74
	**1f**	-343.257363	1.90	-341.0238044	1.74
	**1g**	-343.257236	1.97	-341.0232696	2.07
	**1h**	-343.256530	2.42	-341.0206627	3.71
	**1i**	-343.254415	3.75	-341.0208045	3.62
	**1j**	-343.252908	4.69	-341.0192903	4.57

Table S3: *Computed Total Energies for Compound **2** Conformers.*

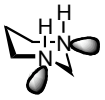
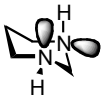
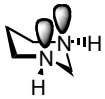
Conformer		DFT (B3LYP, 6-311+G**)		*ab initio* (HF 6-31G*)	
		Total Energy (hartree)	**Relative Energy (kcal mol^{-1})**	**Total Energy (hartree)**	**Relative Energy (kcal mol^{-1})**
	**2a**	-268.014980	0	-266.1716798	0.47
	**2b**	-268.014723	0.19	-266.1719281	0
	**2c**	-268.010725	2.70	-266.1672335	2.95

Table S4: *Computed Total Energies for Compound **4** Conformers.*

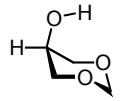
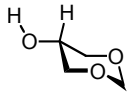
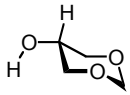
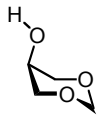
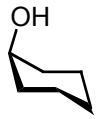
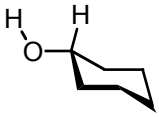
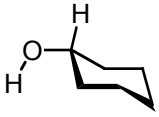
Conformer		DFT (B3LYP, 6-311+G**)		*ab initio* (HF 6-31G*)	
		Total Energy (hartree)	**Relative Energy (kcal mol^{-1})**	**Total Energy (hartree)**	**Relative Energy (kcal mol^{-1})**
	**4a**	-383.002916	0	-380.6876867	0
	**4b**	-383.000317	1.63	-380.6853400	1.47
	**4c**	-382.999830	1.94	-380.6841008	2.25
	**4d**	-382.997230	3.57	-380.6853400	4.14

Table S5: *Computed Total Energies for Cyclohexanol and Piperidine Conformers.*

Compound	Substituent Orientation*	DFT (B3LYP, 6-311+G**)		*ab initio* (HF 6-31G*)	
		Total Energy (hartree)	**Relative Energy (kcal mol^{-1})**	**Total Energy (hartree)**	**Relative Energy (kcal mol^{-1})**
Cyclohexanol 	**Axial**	-311.187486	0.77	-309.0598378	0.24
Cyclohexanol 	**Equatorial** (OH up)	-311.188711	0	-309.0602275	0
Cyclohexanol 	**Equatorial** (OH down)	-311.188537	0.11	-309.0599114	0.20
Piperidine	**Axial**	-251.977815	0.67	-250.1874085	0.82
Piperidine	**Equatorial**	-251.978866	0	-250.1887117	0

*This is the orientation of the hydroxyl group in cyclohexanol and the orientation of the N-H bond in piperidine.

Computational Data - ab initio method (HF/6-31G) - SPARTAN input files showing xyz coordinates*

Conformer 1a:

```
   OPT  HF 6-31G*

0 1
 1   1.355956769  -0.738632481   1.244755194
 7   0.487780890  -0.617991128  -1.331177190
 6   0.684469222   0.944279478   0.592268349
 1   1.848052948   0.965235656  -1.237095007
 6  -0.688187859   0.431207197   1.042278408
 6  -0.835492551  -0.994394792  -0.882610472
 6   0.818294093   0.758114660  -0.925631757
 8   1.700020560   0.177097631   1.255738453
 1  -1.765513615  -1.294918985   0.882785370
 1  -1.494452643   1.071545982   0.665806436
 1  -1.612716347  -0.360047937  -1.326195467
 1   0.165823532   1.461892242  -1.455819001
 1   1.150619135  -1.249684741  -0.884955156
 1   0.822432838   1.994097337   0.868225689
 7  -0.856554560  -0.955137845   0.568765964
 1  -0.741159455   0.425524997   2.136444981
 1  -1.039372957  -2.018187270  -1.213584793
ENDCART
ATOMLABELS
"H2"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1    8   13   13   13   13
   13   13    5   13   13
    7    4    1
    8    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1b:

```
   OPT  HF 6-31G*

0 1
 1   2.340889434   0.493123019   1.060067580
 1   1.060329999  -1.289714385  -0.715811070
 6   0.474947581   0.897534612   0.623939453
 1   1.717332703   0.944942441  -1.152897802
 6  -0.912153471   0.363278664   1.003492323
 6  -0.923579088  -1.081994079  -0.922353587
 6   0.683908140   0.700726657  -0.883475147
 8   1.473377118   0.165422959   1.353499963
 1  -0.372109570  -1.586541380   0.949096595
 1  -1.699925915   1.008559130   0.597149725
 1  -1.663035723  -0.467106018  -1.449697913
 1   0.029045654   1.367102672  -1.457303474
 7   0.434092394  -0.697513026  -1.260239238
 1   0.566134953   1.953912871   0.896805156
 7  -1.094455106  -1.012398628   0.514551019
 1  -1.023175542   0.353958400   2.093427220
 1  -1.091623560  -2.113293909  -1.250250803
ENDCART
ATOMLABELS
"H2"
"H7"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H9"
"H4"
"H5"
"H6"
"N1"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1    8   13   13   13   13
    5   13    5   13   13
    7    4    1
    8    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    2    1
   15    9    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    6    1
ENDHESS
```

Conformer 1c:

```
   OPT  HF 6-31G*

0 1
 1   0.812571972  -0.031180379   2.990043499
 7   0.165450865   1.229792422  -1.051806829
 6   0.386826929   0.000000000   1.098506404
 1   0.319301319   2.141531219   0.818370128
 6  -0.113259277  -1.252242449   0.374986799
 6  -0.282847727   0.000000000  -1.675841534
 6  -0.113259277   1.252242449   0.374986799
 1   1.472422942   0.000000000   1.089008572
 1   1.145422571  -1.364518833  -1.213434706
 1  -1.192627721  -1.326217460   0.505752318
 1  -1.367728134   0.000000000  -1.658496374
 1  -1.192627721   1.326217460   0.505752318
 1   1.145422571   1.364518833  -1.213434706
 8   0.029836548   0.000000000   2.455779583
 7   0.165450865  -1.229792422  -1.051806829
 1   0.319301319  -2.141531219   0.818370128
 1   0.027907803   0.000000000  -2.712348632
ENDCART
ATOMLABELS
"H8"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H7"
"H4"
"H5"
"H6"
"H13"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1   13   13   13   13   13
   13    8    5   13   13
    7    4    1
   14    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    9    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    6    1
ENDHESS
```

Conformer 1d:

```
   OPT  HF 6-31G*

0 1
 1  -0.914993714   0.000000000   2.535658677
 7   0.165450865   1.229792422  -1.051806829
 6   0.386826929   0.000000000   1.098506404
 1   0.319301319   2.141531219   0.818370128
 6  -0.113259277  -1.252242449   0.374986799
 6  -0.282847727   0.000000000  -1.675841534
 6  -0.113259277   1.252242449   0.374986799
 1   1.472422942   0.000000000   1.089008572
 1   1.145422571  -1.364518833  -1.213434706
 1  -1.192627721  -1.326217460   0.505752318
 1  -1.367728134   0.000000000  -1.658496374
 1  -1.192627721   1.326217460   0.505752318
 1   1.145422571   1.364518833  -1.213434706
 8   0.029836548   0.000000000   2.455779583
 7   0.165450865  -1.229792422  -1.051806829
 1   0.319301319  -2.141531219   0.818370128
 1   0.027907803   0.000000000  -2.712348632
ENDCART
ATOMLABELS
"H8"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H7"
"H4"
"H5"
"H6"
"H13"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1   13   13   13   13   13
   13    8    5   13   13
    7    4    1
   14    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    9    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    6    1
ENDHESS
```

Conformer 1e:

```
   OPT  HF 6-31G*

0 1
 1   1.625618362   2.091053934   1.663809631
 1   1.271670186  -1.482518744  -0.950539819
 6   0.724086777   0.707448386   0.646386464
 1   1.914409984   0.747903034  -1.154936331
 6  -0.649694827   0.204429532   1.082317496
 6  -0.716114827  -1.267992457  -0.820958281
 6   0.900542148   0.504811971  -0.859957904
 1   1.478293476   0.136349292   1.173315715
 1  -1.682024600  -1.546092353   0.952596202
 1  -1.413878634   0.878969020   0.675007280
 1  -1.465478443  -0.657339534  -1.329844123
 1   0.242167226   1.194065972  -1.388032771
 7   0.578506094  -0.845391189  -1.294214195
 8   0.930722502   2.044354802   1.020092284
 7  -0.817026918  -1.162874731   0.624969603
 1  -0.726515118   0.242421231   2.162449543
 1  -0.878621192  -2.299126660  -1.107688687
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1f:

```
   OPT  HF 6-31G*

0 1
 1   0.169986585   2.141794680   1.030541053
 6   0.404894477   1.250776865   0.438156761
 6   0.404894477  -1.250776865   0.438156761
 6  -0.324777446   0.000000000  -1.487376515
 1  -1.614633723   0.000000000   1.178838317
 1   1.047433092   0.000000000   2.105017549
 6   0.287037443   0.000000000   1.318263346
 1   1.425683176  -1.359539812   0.053159979
 1   0.677083220   0.000000000  -1.934222836
 7  -0.554434712  -1.176946040  -0.674631047
 7  -0.554434712   1.176946040  -0.674631047
 8  -1.001631991   0.000000000   1.946150490
 1   1.425683176   1.359539812   0.053159979
 1   0.169986585  -2.141794680   1.030541053
 1  -1.043447541   0.000000000  -2.313477608
 1  -0.459661053  -2.008426526  -1.253823118
 1  -0.459661053   2.008426526  -1.253823118
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"H6"
"H12"
"C6"
"H2"
"H3"
"N1"
"N2"
"O1"
"H7"
"H8"
"H9"
"H13"
"H4"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1   13   13    1   13   13    5    5    8
   13   13   13   13   13
    1    2    1
    2   13    1
    2   11    1
    2    7    1
    3    8    1
    3   14    1
    3   10    1
    3    7    1
    4    9    1
    4   15    1
   11    4    1
   10   16    1
    7    6    1
   12    5    1
    7   12    1
   10    4    1
   11   17    1
ENDHESS
```

Conformer 1g:

```
   OPT  HF 6-31G*

0 1
 1   0.214546813   3.885699228   2.126880055
 1   1.328982442  -0.075503175   0.720642345
 6   0.774952223   2.020623432   2.244444951
 1   1.929251438   2.148738966   0.460391655
 6  -0.632463808   1.588385449   2.685982092
 6  -0.774951810   0.038709448   0.714763983
 6   0.887803232   1.920930491   0.714763030
 1   1.556197827   1.440851913   2.749158903
 1  -1.826427325  -0.060502877   2.496141513
 1  -1.404322917   2.270245777   2.311127528
 1  -1.556197161   0.618480654   0.210049375
 1   0.216095006   2.624697612   0.210049494
 7   0.643439793   0.533280375   0.292205891
 8   0.900526991   3.386361547   2.571691471
 7  -0.876826225   0.200734860   2.263425916
 1  -0.632462719   1.588384481   3.781981929
 1  -0.872561651  -1.022885456   0.460392847
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1h:

```
   OPT  HF 6-31G*

0 1
 1  -1.562902102   0.000000000   1.248747389
 1  -1.374505597  -1.190677783  -0.534606348
 6   0.384759495   0.000000000   1.215984555
 1   0.223153157  -2.142699385   0.918609511
 6   0.490814398   1.253598851   0.337116509
 6  -0.139408898   0.000000000  -1.620595508
 6   0.490814398  -1.253598851   0.337116509
 8  -0.862785171   0.000000000   1.920598768
 1  -1.374505597   1.190677783  -0.534606348
 1   1.523079132   1.386930342  -0.008074201
 1   0.884344465   0.000000000  -2.014292772
 1   1.523079132  -1.386930342  -0.008074201
 7  -0.403280133  -1.179908412  -0.826569262
 1   1.178746558   0.000000000   1.969722325
 7  -0.403280133   1.179908412  -0.826569262
 1   0.223153157   2.142699385   0.918609511
 1  -0.801276264   0.000000000  -2.493116911
ENDCART
ATOMLABELS
"H2"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H7"
"H4"
"H5"
"H6"
"N1"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1    8   13   13   13   13
    5   13    5   13   13
    7    4    1
    8    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1i:

```
   OPT  HF 6-31G*

0 1
 1   1.546486456   0.248642703   2.186930279
 7   0.456975829  -0.578833760  -1.381984275
 6   0.687746535   0.902467453   0.600337248
 1   1.822689861   0.977817478  -1.227990785
 6  -0.705116143   0.454503195   1.036667703
 6  -0.815923530  -1.015534745  -0.867026230
 6   0.808973263   0.756532645  -0.918134328
 8   1.664598158   0.131072548   1.251864193
 1  -1.726274137  -1.312570878   0.937587995
 1  -1.457668740   1.128869483   0.620302100
 1  -1.589216065  -0.405825715  -1.338113205
 1   0.151701094   1.472318800  -1.406445917
 1   1.169697572  -1.225219854  -1.103655298
 1   0.857117175   1.934098976   0.887713833
 7  -0.874151708  -0.920458104   0.587523486
 1  -0.782532869   0.491153906   2.117217112
 1  -0.982201870  -2.045534233  -1.155704591
ENDCART
ATOMLABELS
"H2"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1    8   13   13   13   13
   13   13    5   13   13
    7    4    1
    8    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1j:

```
   OPT  HF 6-31G*

0 1
 1   1.732393395   2.046860089   1.671934665
 1   0.757499452  -1.026245663  -2.138465801
 6   0.767040941   0.671096184   0.704010903
 1   1.914953978   0.759009512  -1.109622089
 6  -0.600609351   0.169190931   1.156566991
 6  -0.688593059  -1.300697728  -0.748750247
 6   0.907640161   0.501666382  -0.805587534
 1   1.531979566   0.085431486   1.192963643
 1  -1.659243149  -1.560415382   1.008375612
 1  -1.366718570   0.855145143   0.771521802
 1  -1.471554456  -0.710212702  -1.250133731
 1   0.224681304   1.206236784  -1.298559587
 7   0.632393589  -0.877634488  -1.157328212
 8   0.981664279   2.001730210   1.094514238
 7  -0.786321673  -1.190737712   0.689493243
 1  -0.658163145   0.191828182   2.237986843
 1  -0.824394388  -2.337711672  -1.029006275
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1k:

```
   OPT  HF 6-31G*

0 1
 1   0.214546795   4.370247854   1.227004307
 1   0.766658191   0.943571513  -1.609391863
 6   0.774952205   2.505172058   1.344569202
 1   1.929251420   2.633287593  -0.439484093
 6  -0.632463826   2.072934075   1.786106344
 6  -0.774951828   0.523258074  -0.185111765
 6   0.887803214   2.405479117  -0.185112719
 1   1.556197809   1.925400539   1.849283155
 1  -1.769344867   0.374624410   1.725552098
 1  -1.404322935   2.754794403   1.411251780
 1  -1.556197179   1.103029280  -0.689826373
 1   0.216094988   3.109246238  -0.689826254
 7   0.643439775   1.017829001  -0.607669858
 8   0.900526972   3.870910173   1.671815723
 7  -0.876826244   0.685283486   1.363550167
 1  -0.632462737   2.072933108   2.882106181
 1  -0.872561669  -0.538336829  -0.439482901
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 2a:

```
   OPT  HF 6-31G*

0 1
 1  -0.932333474   0.000000000  -2.394155794
 1  -1.485293461  -1.141830204  -0.402005756
 6   0.251328958   0.000000000   1.281197037
 1   0.151308385  -2.136635079   1.010091068
 6   0.384772179   1.246519842   0.415940172
 6  -0.261420990   0.000000000  -1.528544506
 6   0.384772179  -1.246519842   0.415940172
 1  -0.724852966   0.000000000   1.783193973
 1  -1.485293461   1.141830204  -0.402005756
 1   1.417937280   1.363408913   0.066558247
 1   0.758907303   0.000000000  -1.931215485
 1   1.417937280  -1.363408913   0.066558247
 7  -0.523407889  -1.177830701  -0.727815542
 1   1.017738182   0.000000000   2.063988396
 7  -0.523407889   1.177830701  -0.727815542
 1   0.151308385   2.136635079   1.010091068
ENDCART
ATOMLABELS
"H11"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H1"
"H7"
"H4"
"H5"
"H6"
"N1"
"H8"
"N2"
"H10"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5   13    5   13
    7    4    1
   15    9    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6    1    1
ENDHESS
```

Conformer 2b:

```
   OPT  HF 6-31G*

0 1
 1  -0.955253008  -2.058762429  -1.148194582
 7   0.597999467  -0.683786230  -1.227956797
 6   0.783092725   0.875400912   0.661441756
 1   1.928072861   0.935906801  -1.163897873
 6  -0.561231406   0.344221027   1.141927190
 6  -0.739924514  -1.041192522  -0.805428550
 6   0.907768727   0.694686699  -0.846630502
 1   1.594877666   0.335438574   1.166043870
 1  -1.681398698  -1.345255840   0.953540768
 1  -1.375197307   1.000635101   0.810248552
 1  -1.502307414  -0.390499531  -1.251292602
 1   0.241315398   1.387973638  -1.374195124
 1   1.224538148  -1.307868631  -0.720341063
 1   0.886969558   1.933771436   0.924641915
 7  -0.768868843  -1.015694734   0.643112070
 1  -0.580453360   0.335025728   2.236980972
ENDCART
ATOMLABELS
"H11"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"H1"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"N2"
"H10"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1   13   13   13   13   13
   13   13    5   13
    7    4    1
   15    9    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6    1    1
ENDHESS
```

Conformer 2c:

```
   OPT  HF 6-31G*

0 1
 1   0.048447186   2.133744130   1.126057000
 6   0.270134619   1.247668422   0.521601314
 6   0.270134619  -1.247668422   0.521601314
 6  -0.437310771  -0.000000000  -1.405292197
 1  -0.558697430   2.008394150  -1.179999006
 1   0.919777802  -0.000000000   2.160445420
 6   0.145355480  -0.000000000   1.385405341
 1   1.297618418  -1.357688055   0.153375042
 1   0.564698475  -0.000000000  -1.852228354
 7  -0.663852282  -1.181213848  -0.598080320
 7  -0.663852282   1.181213848  -0.598080320
 1  -0.825215667  -0.000000000   1.898468781
 1   1.297618418   1.357688055   0.153375042
 1   0.048447186  -2.133744130   1.126057000
 1  -1.154606342  -0.000000000  -2.232707051
 1  -0.558697430  -2.008394150  -1.179999006
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"H4"
"H12"
"C6"
"H2"
"H3"
"N1"
"N2"
"H5"
"H7"
"H8"
"H9"
"H13"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1   13   13    1   13   13    5    5   13
   13   13   13   13
    1    2    1
    2   13    1
    2   11    1
    2    7    1
    3    8    1
    3   14    1
    3   10    1
    3    7    1
    4    9    1
    4   15    1
   11    4    1
   10   16    1
    7    6    1
   11    5    1
    7   12    1
   10    4    1
ENDHESS
```

Conformer 4a:

```
   OPT  HF 6-31G*

0 1
 1   0.126444999  -2.133761945   0.822792251
 8  -0.554556061  -1.171976685  -0.836169164
 6   0.201204779   0.000000000   1.136232614
 1   0.126444999   2.133761945   0.822792251
 6   0.380161835   1.245654827   0.269301742
 6  -0.383904018   0.000000000  -1.624026615
 6   0.380161835  -1.245654827   0.269301742
 8  -1.116455884   0.000000000   1.704153575
 8  -0.554556061   1.171976685  -0.836169164
 1   1.396506645   1.315014513  -0.104090170
 1   0.603152895   0.000000000  -2.075286747
 1   1.396506645  -1.315014513  -0.104090170
 1  -1.151723908   0.000000000  -2.373878503
 1   0.901684535   0.000000000   1.956471955
 1  -1.751073235   0.000000000   0.972664509
ENDCART
ATOMLABELS
"H12"
"O1"
"C2"
"H10"
"C4"
"C5"
"C6"
"O3"
"O2"
"H4"
"H5"
"H6"
"H11"
"H8"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    8    1   13    1    1    1    8    8   13   13   13
   13   13   13
    7   12    1
    7    1    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6   13    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
    8   15    1
ENDHESS
```

Conformer 4b:

```
   OPT  HF 6-31G*

0 1
 1  -0.490999968  -2.136379784   0.583816864
 1  -0.236586628   0.000000000  -2.788016322
 6  -0.516547587   0.000000000   0.935489754
 1  -0.490999968   2.136379784   0.583816864
 6  -0.033440562   1.240143182   0.190678015
 6   0.109039988   0.000000000  -1.768099248
 6  -0.033440562  -1.240143182   0.190678015
 1  -1.597711053   0.000000000   0.949705360
 8  -0.373569186   1.149342875  -1.165791079
 1   1.049745419   1.334993229   0.299859294
 1   1.200291319   0.000000000  -1.741652927
 1   1.049745419  -1.334993229   0.299859294
 8  -0.373569186  -1.149342875  -1.165791079
 8  -0.104489329  -0.000000000   2.273082408
 1  -0.849133946   0.139311225   2.843498760
ENDCART
ATOMLABELS
"H12"
"H11"
"C2"
"H10"
"C4"
"C5"
"C6"
"H2"
"O2"
"H4"
"H5"
"H6"
"O1"
"O3"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13    8   13   13   13
    8    8   13
    7   12    1
    7    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6    2    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
   14   15    1
ENDHESS
```

Conformer 4c:

```
   OPT  HF 6-31G*

0 1
 1  -0.514816849  -2.140397245   0.624542625
 1  -0.158546007   0.000000000  -2.836727058
 6  -0.533169628   0.000000000   0.942640784
 1  -0.514816849   2.140397245   0.624542625
 6  -0.052155342   1.244371965   0.196731531
 6   0.136079423   0.000000000  -1.783393201
 6  -0.052155342  -1.244371965   0.196731531
 1  -1.629582587   0.000000000   0.943439140
 8  -0.389114020   1.178409914  -1.184870008
 1   1.031794431   1.377401405   0.304224090
 1   1.232432398   0.000000000  -1.742482984
 1   1.031794431  -1.377401405   0.304224090
 8  -0.389114020  -1.178409914  -1.184870008
 8  -0.085573196   0.000000000   2.295454725
 1   0.886943157   0.000000000   2.299812117
ENDCART
ATOMLABELS
"H12"
"H11"
"C2"
"H10"
"C4"
"C5"
"C6"
"H2"
"O2"
"H4"
"H5"
"H6"
"O1"
"O3"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13    8   13   13   13
    8    8   13
    7   12    1
    7    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6    2    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
   14   15    1
ENDHESS
```

Conformer 4d:

```
   OPT  HF 6-31G*

0 1
 1   0.126444999  -2.133761945   0.822792251
 8  -0.554556061  -1.171976685  -0.836169164
 6   0.201204779   0.000000000   1.136232614
 1   0.126444999   2.133761945   0.822792251
 6   0.380161835   1.245654827   0.269301742
 6  -0.383904018   0.000000000  -1.624026615
 6   0.380161835  -1.245654827   0.269301742
 8  -1.116455884  -0.000000000   1.704153575
 8  -0.554556061   1.171976685  -0.836169164
 1   1.396506645   1.315014513  -0.104090170
 1   0.603152895   0.000000000  -2.075286747
 1   1.396506645  -1.315014513  -0.104090170
 1  -1.151723908   0.000000000  -2.373878503
 1   0.901684535   0.000000000   1.956471955
 1  -1.347582292  -0.917881455   1.908823199
ENDCART
ATOMLABELS
"H12"
"O1"
"C2"
"H10"
"C4"
"C5"
"C6"
"O3"
"O2"
"H4"
"H5"
"H6"
"H11"
"H8"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    8    1   13    1    1    1    8    8   13   13   13
   13   13   13
    7   12    1
    7    1    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6   13    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
    8   15    1
ENDHESS
```

Cyclohexanol axial:

```
   OPT  HF 6-31G*

0 1
 1   0.761827757  -0.549786111  -2.194951194
 6   0.712892397  -0.528953178  -1.099977220
 6   0.862633938   1.022494207   0.888412277
 6  -0.817799150  -0.865309000   0.885722187
 6  -0.511685701   0.555887581   1.359742209
 6  -0.657716029  -1.016028223  -0.627075987
 6   1.013969355   0.892517059  -0.624494061
 1   1.639201330   0.427369941   1.384580777
 1  -0.145496670  -1.566932860   1.394380225
 1  -1.279306121   1.243691934   0.984504777
 8  -1.685370693  -0.266743632  -1.272410545
 1   0.338148628   1.599102678  -1.121584023
 1   1.488842466  -1.206586210  -0.723496635
 1   1.020373171   2.065082847   1.186606551
 1  -1.843005180  -1.119093954   1.179975510
 1  -0.558430557   0.595575367   2.453956801
 1  -0.796465965  -2.066576979  -0.905262087
 1   2.033190294   1.169102371  -0.917290559
 1  -1.575803270  -0.384813839  -2.231339003
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"O1"
"H6"
"H7"
"H8"
"H9"
"H10"
"H11"
"H12"
"H5"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1    1    1    1   13   13   13    8   13
   13   13   13   13   13   13   13
    1    2    1
    2   13    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    7   12    1
    7   18    1
   11   19    1
ENDHESS
```

Cyclohexanol equatorial (OH up):

```
   OPT  HF 6-31G*

0 1
 1   0.632463252   0.862334523  -0.539220792
 6   0.632463252   0.862334523   0.556779164
 6   0.774952253   2.412009510   2.527999062
 6  -0.887802804   0.529788527   2.527999062
 6  -0.632463778   1.979771528   2.969536203
 6  -0.774951781   0.430095527   0.998318094
 6   0.887803262   2.312316570   0.998317141
 1   1.556197857   1.832237992   3.032713014
 1  -0.216094578  -0.173978534   3.032712657
 1  -1.404322887   2.661631855   2.594681639
 1  -1.556197132   1.009866732   0.493603486
 1   0.216095035   3.016083691   0.493603605
 1   1.404322301   0.180474195   0.931634027
 1   0.872562138   3.473604473   2.782369393
 8  -2.227622126   0.236713589   2.855246937
 1  -0.632462689   1.979770560   4.065536040
 1  -0.872561621  -0.631499377   0.743946958
 1   1.929251467   2.540125045   0.743945766
 1  -2.330321361  -0.709634241   2.963148150
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"H7"
"H8"
"O1"
"H10"
"H11"
"H12"
"H9"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1    1    1    1   13   13   13   13   13
   13   13    8   13   13   13   13
    1    2    1
    2   13    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    7   12    1
    7   18    1
   15   19    1
ENDHESS
```

Cyclohexanol equatorial (OH down):

```
   OPT  HF 6-31G*

0 1
 1   0.810110549  -0.528172277  -2.430750881
 6   0.757094224  -0.482357812  -1.337225704
 6   0.899313872   1.078980984   0.644768807
 6  -0.773798043  -0.813515799   0.643997749
 6  -0.475202687   0.610542159   1.110869723
 6  -0.617478545  -0.948597542  -0.869192009
 6   1.057923991   0.938678097  -0.867162124
 1   1.675346845   0.489921980   1.148849115
 1  -0.100118658  -1.519182144   1.144682986
 1  -1.249346492   1.292407700   0.735362383
 1  -1.400084969  -0.368345327  -1.375433078
 1   0.380417702   1.639425591  -1.370547674
 1   1.524510096  -1.164336296  -0.950859643
 1   1.051709740   2.124225517   0.936229911
 8  -2.107931530  -1.162945967   0.996232986
 1  -0.538612341   0.664066536   2.204377271
 1  -0.782755712  -1.991005112  -1.167250830
 1   2.077488285   1.215324215  -1.158255548
 1  -2.665524301  -0.381087576   0.843346350
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"H7"
"H8"
"O1"
"H10"
"H11"
"H12"
"H9"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1    1    1    1   13   13   13   13   13
   13   13    8   13   13   13   13
    1    2    1
    2   13    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    7   12    1
    7   18    1
   15   19    1
ENDHESS
```

Piperidine axial:

```
   OPT  HF 6-31G*

0 1
 1  -1.415463075   2.085667623  -0.135519658
 7  -1.566192756   0.000000000  -0.227213403
 6   0.571846941   1.255006683  -0.220815567
 6   0.571846941  -1.255006683  -0.220815567
 6   1.328808865   0.000000000   0.203723666
 6  -0.882705698  -1.206995285   0.244403763
 6  -0.882705698   1.206995285   0.244403763
 1   0.605794314   1.349258977  -1.313601764
 1   0.605794314  -1.349258977  -1.313601764
 1   1.451938624   0.000000000   1.293775254
 1  -0.934290840  -1.258683380   1.338758028
 1  -0.934290840   1.258683380   1.338758028
 1  -1.567696271   0.000000000  -1.247552616
 1   1.064821509   2.142132531   0.192311975
 1   1.064821509  -2.142132531   0.192311975
 1   2.333131334   0.000000000  -0.233794000
 1  -1.415463075  -2.085667623  -0.135519658
ENDCART
ATOMLABELS
"H12"
"N1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"H9"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1    1    1    1    1   13   13   13   13   13
   13   13   13   13   13
    7   12    1
    7    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    2    7    1
ENDHESS
```

Piperidine equatorial:

```
   OPT  HF 6-31G*

0 1
 1  -0.272237078  -2.085519816  -1.347350918
 1  -0.052865688   0.000000000  -2.465492284
 6  -0.278040703  -1.253750586   0.636772975
 6  -0.278040703   1.253750586   0.636772975
 6   0.175688017   0.000000000   1.377913799
 6   0.136831678   1.209360080  -0.832549816
 6   0.136831678  -1.209360080  -0.832549816
 1  -1.369404834  -1.344392100   0.708010348
 1  -1.369404834   1.344392100   0.708010348
 1   1.269557594   0.000000000   1.460109332
 1   1.228715141   1.266882522  -0.920223746
 1   1.228715141  -1.266882522  -0.920223746
 7  -0.356897378   0.000000000  -1.492268031
 1   0.148526310  -2.141914757   1.116321164
 1   0.148526310   2.141914757   1.116321164
 1  -0.224263492   0.000000000   2.397777087
 1  -0.272237078   2.085519816  -1.347350918
ENDCART
ATOMLABELS
"H12"
"H13"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"H8"
"H9"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1    1    1    1    1   13   13   13   13   13
    5   13   13   13   13
    7   12    1
    7    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   13    2    1
ENDHESS
```

*Computational Data – DFT method (B3LYP, 6-311+G**) - SPARTAN input files showing xyz coordinates*

Conformer 1a:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   1.313585470  -0.744857143   1.359840906
 7   0.456975829  -0.578833760  -1.381984275
 6   0.687746535   0.902467453   0.600337248
 1   1.822689861   0.977817478  -1.227990785
 6  -0.705116143   0.454503195   1.036667703
 6  -0.815923530  -1.015534745  -0.867026230
 6   0.808973263   0.756532645  -0.918134328
 8   1.664598158   0.131072548   1.251864193
 1  -1.726274137  -1.312570878   0.937587995
 1  -1.457668740   1.128869483   0.620302100
 1  -1.589216065  -0.405825715  -1.338113205
 1   0.151701094   1.472318800  -1.406445917
 1   1.169697572  -1.225219854  -1.103655298
 1   0.857117175   1.934098976   0.887713833
 7  -0.874151708  -0.920458104   0.587523486
 1  -0.782532869   0.491153906   2.117217112
 1  -0.982201870  -2.045534233  -1.155704591
ENDCART
ATOMLABELS
"H2"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1    8   13   13   13   13
   13   13    5   13   13
    7    4    1
    8    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1b:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   2.304020703   0.456101363   1.166896160
 1   1.130361393  -1.254731434  -0.970065296
 6   0.487086332   0.891919892   0.613166251
 1   1.700787161   0.981530450  -1.178438998
 6  -0.891674195   0.370193776   1.010198363
 6  -0.881241466  -1.109156149  -0.885015082
 6   0.687710603   0.710059187  -0.893149383
 8   1.430664084   0.131115041   1.338846222
 1  -0.560936827  -1.616741326   1.045521738
 1  -1.650550143   1.028088682   0.594203872
 1  -1.635036306  -0.535664327  -1.415183268
 1   0.021184870   1.383809248  -1.426009282
 7   0.420579335  -0.647991088  -1.334903269
 1   0.572464689   1.944638229   0.879589692
 7  -1.141660174  -0.979669916   0.535297925
 1  -0.994399406   0.393250717   2.088226824
 1  -0.999360601  -2.146752399  -1.169182312
ENDCART
ATOMLABELS
"H2"
"H7"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H9"
"H4"
"H5"
"H6"
"N1"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1    8   13   13   13   13
    5   13    5   13   13
    7    4    1
    8    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    2    1
   15    9    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    6    1
ENDHESS
```

Conformer 1c:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.343619818  -0.540010671   2.902705225
 7   0.043929808   1.231565271  -1.107771451
 6   0.364823950   0.072414679   1.059845614
 1   0.243913458   2.200242588   0.728140010
 6  -0.158293426  -1.203092890   0.395187982
 6  -0.406587995  -0.020289873  -1.683120791
 6  -0.187994822   1.291524811   0.326299529
 1   1.454836477   0.087028490   0.989181453
 1   1.057970262  -1.346663810  -1.225079887
 1  -1.228933461  -1.263822911   0.570044655
 1  -1.489859174  -0.035765609  -1.630161367
 1  -1.258436522   1.340313789   0.503909406
 1   1.015402557   1.375849841  -1.308185586
 8  -0.034763770   0.169363126   2.401504889
 7   0.080280316  -1.226118979  -1.038462937
 1   0.288201625  -2.086168378   0.844562709
 1  -0.128108891  -0.046369791  -2.728599454
ENDCART
ATOMLABELS
"H8"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H7"
"H4"
"H5"
"H6"
"H13"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1   13   13   13   13   13
   13    8    5   13   13
    7    4    1
   14    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    9    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    6    1
ENDHESS
```

Conformer 1d:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1  -0.914993714   0.000000000   2.535658677
 7   0.165450865   1.229792422  -1.051806829
 6   0.386826929   0.000000000   1.098506404
 1   0.319301319   2.141531219   0.818370128
 6  -0.113259277  -1.252242449   0.374986799
 6  -0.282847727   0.000000000  -1.675841534
 6  -0.113259277   1.252242449   0.374986799
 1   1.472422942   0.000000000   1.089008572
 1   1.145422571  -1.364518833  -1.213434706
 1  -1.192627721  -1.326217460   0.505752318
 1  -1.367728134   0.000000000  -1.658496374
 1  -1.192627721   1.326217460   0.505752318
 1   1.145422571   1.364518833  -1.213434706
 8   0.029836548   0.000000000   2.455779583
 7   0.165450865  -1.229792422  -1.051806829
 1   0.319301319  -2.141531219   0.818370128
 1   0.027907803   0.000000000  -2.712348632
ENDCART
ATOMLABELS
"H8"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H7"
"H4"
"H5"
"H6"
"H13"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1   13   13   13   13   13
   13    8    5   13   13
    7    4    1
   14    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    9    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    6    1
ENDHESS
```

Conformer 1e:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   1.021413798   2.182683111   1.777716145
 1   1.167480742  -1.485184528  -1.059940654
 6   0.731074192   0.696032233   0.562558438
 1   1.861685674   0.731287027  -1.272218520
 6  -0.652979484   0.245144747   1.024046720
 6  -0.809387186  -1.219370223  -0.875464491
 6   0.851708771   0.512502186  -0.947568595
 1   1.477519554   0.075224768   1.055379305
 1  -1.743650836  -1.470475729   0.917991503
 1  -1.389261520   0.950093511   0.628253994
 1  -1.556014850  -0.587907933  -1.361259736
 1   0.195968729   1.228804977  -1.433780461
 7   0.482577742  -0.826840563  -1.379239221
 8   0.955614259   2.053374047   0.841869567
 7  -0.871427927  -1.118292976   0.574616853
 1  -0.717864711   0.278267116   2.108074887
 1  -1.004456737  -2.245341508  -1.161036263
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1f:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.209208797   2.127812511   1.014990222
 6   0.421204823   1.245354096   0.424439472
 6   0.421204823  -1.245354096   0.424439472
 6  -0.320871864   0.000000000  -1.498527203
 1  -1.660730349   0.000000000   1.231763819
 1   0.986320510   0.000000000   2.082443076
 6   0.245225129   0.000000000   1.292132941
 1   1.458480921  -1.305457095   0.080897178
 1   0.680422510   0.000000000  -1.954922736
 7  -0.527496794  -1.172035159  -0.675428823
 7  -0.527496794   1.172035159  -0.675428823
 8  -1.003195337   0.000000000   1.917709775
 1   1.458480921   1.305457095   0.080897178
 1   0.209208797  -2.127812511   1.014990222
 1  -1.051479374   0.000000000  -2.297761859
 1  -0.499243332  -2.002908847  -1.231313383
 1  -0.499243332   2.002908847  -1.231313383
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"H6"
"H12"
"C6"
"H2"
"H3"
"N1"
"N2"
"O1"
"H7"
"H8"
"H9"
"H13"
"H4"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1   13   13    1   13   13    5    5    8
   13   13   13   13   13
    1    2    1
    2   13    1
    2   11    1
    2    7    1
    3    8    1
    3   14    1
    3   10    1
    3    7    1
    4    9    1
    4   15    1
   11    4    1
   10   16    1
    7    6    1
   12    5    1
    7   12    1
   10    4    1
   11   17    1
ENDHESS
```

Conformer 1g:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.308956115   2.600582587   0.569037631
 1   1.271670186  -1.482518744  -0.950539819
 6   0.724086777   0.707448386   0.646386464
 1   1.914409984   0.747903034  -1.154936331
 6  -0.649694827   0.204429532   1.082317496
 6  -0.716114827  -1.267992457  -0.820958281
 6   0.900542148   0.504811971  -0.859957904
 1   1.478293476   0.136349292   1.173315715
 1  -1.682024600  -1.546092353   0.952596202
 1  -1.413878634   0.878969020   0.675007280
 1  -1.465478443  -0.657339534  -1.329844123
 1   0.242167226   1.194065972  -1.388032771
 7   0.578506094  -0.845391189  -1.294214195
 8   0.930722502   2.044354802   1.020092284
 7  -0.817026918  -1.162874731   0.624969603
 1  -0.726515118   0.242421231   2.162449543
 1  -0.878621192  -2.299126660  -1.107688687
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1h:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1  -1.598322147   0.000000000   1.268905394
 1  -1.298141484  -1.406459728  -0.606959954
 6   0.347945683   0.000000000   1.212418104
 1   0.279696635  -2.136016345   0.926432885
 6   0.503970737   1.250708523   0.343585368
 6  -0.200605327   0.000000000  -1.596851617
 6   0.503970737  -1.250708523   0.343585368
 8  -0.887659909   0.000000000   1.894109475
 1  -1.298141484   1.406459728  -0.606959954
 1   1.537480681   1.329364424   0.015618508
 1   0.791822311   0.000000000  -2.035489231
 1   1.537480681  -1.329364424   0.015618508
 7  -0.340613668  -1.230966613  -0.842827272
 1   1.098791789   0.000000000   1.993479173
 7  -0.340613668   1.230966613  -0.842827272
 1   0.279696635   2.136016345   0.926432885
 1  -0.916758202   0.000000000  -2.408270420
ENDCART
ATOMLABELS
"H2"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H7"
"H4"
"H5"
"H6"
"N1"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1    8   13   13   13   13
    5   13    5   13   13
    7    4    1
    8    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1i:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   2.472577627   0.469536274   1.064462897
 7   0.400390747  -0.685979400  -1.346163685
 6   0.626076959   0.839445406   0.602530635
 1   1.745619217   0.894029193  -1.245828609
 6  -0.731587547   0.336998646   1.082135935
 6  -0.906219637  -1.071213293  -0.869221681
 6   0.738533580   0.658704917  -0.912850281
 8   1.622416963   0.107704980   1.274619820
 1  -1.861424736  -1.344262033   0.910604612
 1  -1.488562319   1.056878570   0.752221596
 1  -1.636406981  -0.421256153  -1.358916592
 1   0.071038183   1.357604338  -1.410524815
 1   1.071235413  -1.324464983  -0.961513051
 1   0.710066808   1.896598989   0.853781188
 7  -0.982476672  -0.999763464   0.577707459
 1  -0.740410837   0.317991076   2.164977370
 1  -1.110866926  -2.088552798  -1.178022535
ENDCART
ATOMLABELS
"H2"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"O1"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1    8   13   13   13   13
   13   13    5   13   13
    7    4    1
    8    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1j:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.335712428   0.487922273   2.971592143
 1   0.101678233   2.007480620  -1.443751325
 6   0.408426462  -0.066921819   1.113905568
 1   0.350975964   2.079222609   0.895395634
 6  -0.092830178  -1.285196645   0.354653322
 6  -0.149467331   0.013675263  -1.674595004
 6  -0.070981455   1.201647495   0.414330969
 1   1.494016866  -0.081716662   1.112248185
 1   0.060413997  -1.993133779  -1.544025281
 1  -1.180098921  -1.329734425   0.462075034
 1  -1.249378753   0.027699201  -1.713268177
 1  -1.157894432   1.256417975   0.522301649
 7   0.365850131   1.167527416  -0.968956775
 8  -0.095760815  -0.152039820   2.422541378
 7   0.340341724  -1.183444062  -1.027533469
 1   0.319230938  -2.184611063   0.795463527
 1   0.219765142   0.035205369  -2.692377430
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 1k:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.337744575   2.562320426   0.682020255
 1   0.757499452  -1.026245663  -2.138465801
 6   0.767040941   0.671096184   0.704010903
 1   1.914953978   0.759009512  -1.109622089
 6  -0.600609351   0.169190931   1.156566991
 6  -0.688593059  -1.300697728  -0.748750247
 6   0.907640161   0.501666382  -0.805587534
 1   1.531979566   0.085431486   1.192963643
 1  -1.659243149  -1.560415382   1.008375612
 1  -1.366718570   0.855145143   0.771521802
 1  -1.471554456  -0.710212702  -1.250133731
 1   0.224681304   1.206236784  -1.298559587
 7   0.632393589  -0.877634488  -1.157328212
 8   0.981664279   2.001730210   1.094514238
 7  -0.786321673  -1.190737712   0.689493243
 1  -0.658163145   0.191828182   2.237986843
 1  -0.824394388  -2.337711672  -1.029006275
ENDCART
ATOMLABELS
"H8"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"O1"
"N2"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5    8    5   13   13
    7    4    1
   14    1    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   15    9    1
ENDHESS
```

Conformer 2a:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   2.545387215   0.129361975   0.000000000
 1   0.937867275   1.191852951  -1.343194908
 6  -1.286077394   0.251936512   0.000000000
 1  -1.010249212   0.148238594  -2.166917105
 6  -0.533747347  -0.212824245   1.237498624
 6   1.500436788  -0.228422899   0.000000000
 6  -0.533747347  -0.212824245  -1.237498624
 1  -1.346160275   1.360228262   0.000000000
 1   0.937867275   1.191852951   1.343194908
 1  -0.565938858  -1.322511073   1.277582317
 1   1.529997766  -1.338711359   0.000000000
 1  -0.565938858  -1.322511073  -1.277582317
 7   0.863622370   0.171222267  -1.236144556
 1  -2.326692554  -0.126349478   0.000000000
 7   0.863622370   0.171222267   1.236144556
 1  -1.010249212   0.148238594   2.166917105
ENDCART
ATOMLABELS
"H11"
"H13"
"C2"
"H12"
"C4"
"C5"
"C6"
"H1"
"H7"
"H4"
"H5"
"H6"
"N1"
"H8"
"N2"
"H10"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13   13   13   13   13
    5   13    5   13
    7    4    1
   15    9    1
   13    2    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
   13    6    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6    1    1
ENDHESS
```

Conformer 2b:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   2.325439144   0.967173873   0.266964177
 7   0.310366101   1.501417715   0.196642260
 6  -1.249912356  -0.423417061   0.239708325
 1  -1.766420898   1.685952208   0.012273320
 6  -0.069156067  -1.321718095  -0.074912775
 6   1.362706775   0.572697745  -0.106046765
 6  -0.961492652   0.981521129  -0.265553953
 1  -1.391084487  -0.397378939   1.337492618
 1   1.939671596  -1.342172676   0.338253745
 1  -0.008662653  -1.439700301  -1.188999080
 1   1.424085195   0.528845489  -1.224840326
 1  -0.923278690   0.966865547  -1.375391222
 1   0.270927075   1.609632982   1.219599823
 1  -2.175679607  -0.829627850  -0.209105037
 7   1.127421427  -0.730843668   0.479751605
 1  -0.214929905  -2.329248098   0.354163284
ENDCART
ATOMLABELS
"H11"
"N1"
"C2"
"H12"
"C4"
"C5"
"C6"
"H1"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"N2"
"H10"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1   13    1    1    1   13   13   13   13   13
   13   13    5   13
    7    4    1
   15    9    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    7   12    1
    2    7    1
   15    6    1
   15    5    1
    5   10    1
    5   16    1
    6   11    1
    6    1    1
ENDHESS
```

Conformer 2c:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1  -1.084899263  -0.191742429  -2.153551876
 6  -0.568798950   0.131535990  -1.231959847
 6  -0.568798950   0.131535990   1.231959847
 6   1.448023803  -0.046701518   0.000000000
 1   1.282301673  -0.263244961  -2.012379930
 1  -2.346071278   0.206874844   0.000000000
 6  -1.350436827  -0.271720648   0.000000000
 1  -0.512715910   1.252866010   1.252350732
 1   1.566385664   1.082139448   0.000000000
 7   0.736170821  -0.483686491   1.173631145
 7   0.736170821  -0.483686491  -1.173631145
 1  -1.480822528  -1.368416476   0.000000000
 1  -0.512715910   1.252866010  -1.252350732
 1  -1.084899263  -0.191742429   2.153551876
 1   2.458804423  -0.493631888   0.000000000
 1   1.282301673  -0.263244961   2.012379930
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"H4"
"H12"
"C6"
"H2"
"H3"
"N1"
"N2"
"H5"
"H7"
"H8"
"H9"
"H13"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1   13   13    1   13   13    5    5   13
   13   13   13   13
    1    2    1
    2   13    1
    2   11    1
    2    7    1
    3    8    1
    3   14    1
    3   10    1
    3    7    1
    4    9    1
    4   15    1
   11    4    1
   10   16    1
    7    6    1
   11    5    1
    7   12    1
   10    4    1
ENDHESS
```

Conformer 4a:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.082008556  -2.130102049   0.790057717
 8  -0.544810045  -1.147697133  -0.847438364
 6   0.180010331   0.000000000   1.122245666
 1   0.082008556   2.130102049   0.790057717
 6   0.340747126   1.235154310   0.243908060
 6  -0.351671567   0.000000000  -1.599593231
 6   0.340747126  -1.235154310   0.243908060
 8  -1.068316418   0.000000000   1.753330864
 8  -0.544810045   1.147697133  -0.847438364
 1   1.365813465   1.323041708  -0.114308001
 1   0.653318316   0.000000000  -2.023735675
 1   1.365813465  -1.323041708  -0.114308001
 1  -1.086434019   0.000000000  -2.387317118
 1   0.925498200   0.000000000   1.908399113
 1  -1.739924158   0.000000000   1.082223461
ENDCART
ATOMLABELS
"H12"
"O1"
"C2"
"H10"
"C4"
"C5"
"C6"
"O3"
"O2"
"H4"
"H5"
"H6"
"H11"
"H8"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    8    1   13    1    1    1    8    8   13   13   13
   13   13   13
    7   12    1
    7    1    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6   13    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
    8   15    1
ENDHESS
```

Conformer 4b:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1  -0.386870533  -2.181325137   0.506729709
 1  -0.086454915   0.021492851  -2.818715323
 6  -0.467189532  -0.055474445   0.888911361
 1  -0.417002097   2.096943485   0.581451865
 6   0.042287136   1.199438497   0.186994677
 6   0.238135583   0.005927949  -1.791774374
 6   0.064582009  -1.269918557   0.143223198
 1  -1.552828673  -0.070655429   0.847627545
 8  -0.270972037   1.139608924  -1.178340888
 1   1.119192419   1.274222408   0.332024433
 1   1.327909716   0.018411664  -1.741013311
 1   1.141654829  -1.336377874   0.289109693
 8  -0.244812636  -1.158938499  -1.220704808
 8  -0.004229343  -0.132534135   2.209453024
 1  -0.503401925   0.449178190   2.765022830
ENDCART
ATOMLABELS
"H12"
"H11"
"C2"
"H10"
"C4"
"C5"
"C6"
"H2"
"O2"
"H4"
"H5"
"H6"
"O1"
"O3"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13    8   13   13   13
    8    8   13
    7   12    1
    7    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6    2    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
   14   15    1
ENDHESS
```

Conformer 4c:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.422876158  -2.229164802   0.305431856
 1  -2.782285032   0.221655927   0.588286574
 6   0.957987732  -0.119894071   0.295176278
 1   0.802542667   2.064986246   0.301926171
 6   0.260987581   1.195786410  -0.076756901
 6  -1.816460645   0.135071793   0.094851409
 6   0.038936162  -1.283758924  -0.077181065
 1   1.136530215  -0.142864457   1.376678658
 8  -1.044198991   1.242030176   0.498264215
 1   0.201666016   1.268936276  -1.173000118
 1  -1.932458087   0.146889560  -1.003015050
 1  -0.032290805  -1.350777525  -1.173140711
 8  -1.252405921  -1.089728610   0.496505069
 8   2.172484601  -0.292828599  -0.431197904
 1   2.002326022  -0.173049779  -1.370208932
ENDCART
ATOMLABELS
"H12"
"H11"
"C2"
"H10"
"C4"
"C5"
"C6"
"H2"
"O2"
"H4"
"H5"
"H6"
"O1"
"O3"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1   13    1    1    1   13    8   13   13   13
    8    8   13
    7   12    1
    7    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6    2    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
   14   15    1
ENDHESS
```

Conformer 4d:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.035983365  -2.096628995   0.687340391
 8  -0.559406076  -1.097610136  -0.943980456
 6   0.153006363   0.037257571   1.060352248
 1  -0.018462253   2.158965122   0.753066005
 6   0.276613066   1.283217998   0.195022242
 6  -0.363412158   0.063796392  -1.675808090
 6   0.293718880  -1.185727515   0.159973299
 8  -1.091392462   0.093993839   1.697525419
 8  -0.565456689   1.203191793  -0.921438457
 1   1.312033816   1.402225569  -0.124951343
 1   0.647521602   0.066540229  -2.089519763
 1   1.329583344  -1.273685452  -0.168732928
 1  -1.088191522   0.068502365  -2.472312615
 1   0.958259563   0.030970575   1.794791531
 1  -1.320398944  -0.755009249   2.048672624
ENDCART
ATOMLABELS
"H12"
"O1"
"C2"
"H10"
"C4"
"C5"
"C6"
"O3"
"O2"
"H4"
"H5"
"H6"
"H11"
"H8"
"H1"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    8    1   13    1    1    1    8    8   13   13   13
   13   13   13
    7   12    1
    7    1    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    6   11    1
    6   13    1
    9    6    1
    9    5    1
    5   10    1
    5    4    1
    8   15    1
ENDHESS
```

Cyclohexanol axial:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.788650846  -0.594732309  -2.180258051
 6   0.723563738  -0.529960378  -1.094866458
 6   0.866546372   1.026475008   0.890761364
 6  -0.816428842  -0.862244585   0.875430465
 6  -0.518870093   0.563015753   1.350063615
 6  -0.654079696  -1.011604387  -0.633851261
 6   1.020155997   0.897759151  -0.627388578
 1   1.630558038   0.424619656   1.382082490
 1  -0.137898987  -1.559612885   1.363353479
 1  -1.274915101   1.234888981   0.955602776
 8  -1.686892819  -0.260194601  -1.234665350
 1   0.335931402   1.585004714  -1.116987284
 1   1.477203212  -1.209938538  -0.701533137
 1   1.038188241   2.055109748   1.196759432
 1  -1.826015793  -1.151747774   1.149125436
 1  -0.588900722   0.609263410   2.433709558
 1  -0.773487431  -2.060977001  -0.900281898
 1   2.024296498   1.183058874  -0.930110403
 1  -1.627604805  -0.338182680  -2.176946406
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"O1"
"H6"
"H7"
"H8"
"H9"
"H10"
"H11"
"H12"
"H5"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1    1    1    1   13   13   13    8   13
   13   13   13   13   13   13   13
    1    2    1
    2   13    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    7   12    1
    7   18    1
   11   19    1
ENDHESS
```

Cyclohexanol equatorial (OH up):

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.834982696  -0.587389710  -2.356402318
 6   0.773288619  -0.517513124  -1.274304589
 6   0.947994636   1.047038889   0.703629790
 6  -0.766453607  -0.816367245   0.713615576
 6  -0.442030540   0.604414347   1.171861801
 6  -0.616177852  -0.955650349  -0.800329524
 6   1.099190524   0.906239217  -0.813818410
 1   1.703783628   0.438476904   1.197514938
 1  -0.077960192  -1.502631290   1.195670597
 1  -1.193225639   1.283289437   0.765608405
 1  -1.374299775  -0.339137157  -1.285496794
 1   0.428084127   1.606704844  -1.308579241
 1   1.520510020  -1.202854813  -0.877532039
 1   1.132186737   2.073405734   1.007399174
 8  -2.039806312  -1.224974157   1.149050504
 1  -0.522314984   0.657960629   2.253115650
 1  -0.817206097  -1.983428509  -1.086142654
 1   2.107366583   1.175674311  -1.116018361
 1  -2.697912624  -0.663258064   0.761157495
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"H7"
"H8"
"O1"
"H10"
"H11"
"H12"
"H9"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1    1    1    1   13   13   13   13   13
   13   13    8   13   13   13   13
    1    2    1
    2   13    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    7   12    1
    7   18    1
   15   19    1
ENDHESS
```

Cyclohexanol equatorial (OH down):

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1   0.834982696  -0.587389710  -2.356402318
 6   0.773288619  -0.517513124  -1.274304589
 6   0.947994636   1.047038889   0.703629790
 6  -0.766453607  -0.816367245   0.713615576
 6  -0.442030540   0.604414347   1.171861801
 6  -0.616177852  -0.955650349  -0.800329524
 6   1.099190524   0.906239217  -0.813818410
 1   1.703783628   0.438476904   1.197514938
 1  -0.077960192  -1.502631290   1.195670597
 1  -1.193225639   1.283289437   0.765608405
 1  -1.374299775  -0.339137157  -1.285496794
 1   0.428084127   1.606704844  -1.308579241
 1   1.520510020  -1.202854813  -0.877532039
 1   1.132186737   2.073405734   1.007399174
 8  -2.039806312  -1.224974157   1.149050504
 1  -0.522314984   0.657960629   2.253115650
 1  -0.817206097  -1.983428509  -1.086142654
 1   2.107366583   1.175674311  -1.116018361
 1  -2.697912624  -0.663258064   0.761157495
ENDCART
ATOMLABELS
"H1"
"C1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"H7"
"H8"
"O1"
"H10"
"H11"
"H12"
"H9"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    1    1    1    1    1    1   13   13   13   13   13
   13   13    8   13   13   13   13
    1    2    1
    2   13    1
    2    6    1
    2    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    7   12    1
    7   18    1
   15   19    1
ENDHESS
```

Piperidine axial:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1  -1.421435868   2.066984009  -0.155741204
 7  -1.570220666   0.000000000  -0.183728224
 6   0.589485728   1.260153702  -0.227298139
 6   0.589485728  -1.260153702  -0.227298139
 6   1.336997541   0.000000000   0.219682008
 6  -0.873807901  -1.210622817   0.224390627
 6  -0.873807901   1.210622817   0.224390627
 1   0.626153848   1.336395232  -1.313643785
 1   0.626153848  -1.336395232  -1.313643785
 1   1.420413973   0.000000000   1.305699564
 1  -0.918475647  -1.267265368   1.309869851
 1  -0.918475647   1.267265368   1.309869851
 1  -1.687759664   0.000000000  -1.179633827
 1   1.072708907   2.151344070   0.166408464
 1   1.072708907  -2.151344070   0.166408464
 1   2.351310786   0.000000000  -0.170006341
 1  -1.421435868  -2.066984009  -0.155741204
ENDCART
ATOMLABELS
"H12"
"N1"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"H13"
"H8"
"H9"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13    5    1    1    1    1    1   13   13   13   13   13
   13   13   13   13   13
    7   12    1
    7    1    1
    2    6    1
    2   13    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
    2    7    1
ENDHESS
```

Piperidine equatorial:

```
   OPT  B3LYP 6-311+G** CONVERGE NOSYMTRY

0 1
 1  -0.241845168  -2.066063664  -1.367189273
 1  -0.148689758   0.000000000  -2.429808463
 6  -0.280463042  -1.259658815   0.632601820
 6  -0.280463042   1.259658815   0.632601820
 6   0.174579808   0.000000000   1.374965003
 6   0.153793038   1.210551220  -0.830094050
 6   0.153793038  -1.210551220  -0.830094050
 1  -1.363781742  -1.334077806   0.670374069
 1  -1.363781742   1.334077806   0.670374069
 1   1.261136966   0.000000000   1.449494274
 1   1.246424463   1.272409712  -0.882074285
 1   1.246424463  -1.272409712  -0.882074285
 7  -0.356252813   0.000000000  -1.451058681
 1   0.124329771  -2.148806136   1.108675762
 1   0.124329771   2.148806136   1.108675762
 1  -0.207688841   0.000000000   2.391819675
 1  -0.241845168   2.066063664  -1.367189273
ENDCART
ATOMLABELS
"H12"
"H13"
"C2"
"C3"
"C4"
"C5"
"C6"
"H2"
"H3"
"H4"
"H5"
"H6"
"N1"
"H8"
"H9"
"H10"
"H11"
ENDATOMLABELS
ATOMCOLORS
ENDATOMCOLORS
FROZEN
ENDFROZEN
HESSIAN
   13   13    1    1    1    1    1   13   13   13   13   13
    5   13   13   13   13
    7   12    1
    7    1    1
   13    6    1
   13    7    1
    3    8    1
    3   14    1
    3    5    1
    3    7    1
    4    9    1
    4   15    1
    4    6    1
    4    5    1
    5   10    1
    5   16    1
    6   11    1
    6   17    1
   13    2    1
ENDHESS
```