Supporting Information

Characterization by Empirical and Computational Methods of Dictyospiromide, an Intriguing Antioxidant Alkaloid from the Marine Alga *Dictyota coriacea*

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Supporting Information

Experimental Details

General Procedures. NMR spectra were recorded on a Bruker Avance III NMR spectrometer operating at 600 MHz for ^{1}H and 150 MHz for ^{13}C. TMS was used as an internal standard. UV, IR spectra and optical rotations were measured with a TU 1901 spectrometer, a Bruker Equinox 55 spectrometer, and a PoLAAR 3005 digital polarimeter, respectively. ECD spectra were acquired with a Chirascan circular dichroism spectrometer. (+) HRESIMS data were recorded on a Thermo Scientific Q Exactive hybrid quadrupole-Orbitrap mass spectrometer. Column chromatography was performed using Silica gel (200–300 mesh, Qingdao Marine Chemistry Co. Ltd.), ODS (50 μm, YMC), and Sephadex LH-20 (GE Healthcare Bio-sciences AB). HPLC separation was run on an Agilent 1100 series instrument using a YMC-Pack C_{18} column (10 μm, 250 × 10 mm) and a VWD G1314A detector.

Plant Material. Specimens of the brown alga *Dictyota coriacea* were collected from the coast of Nanji Island, Wenzhou, Zhejiang Province, China, in June 2015. The identification was carried out by one of the authors (Z.S.). A voucher specimen of the alga (ZN201501) was deposited at the Laboratory of Marine Natural Products Chemistry, Wenzhou Medical University, China.

Extraction and Isolation. The air-dried algal material (700 g) was extracted with 95% EtOH at room temperature. The concentrated extract was partitioned between H_2O and EtOAc. Evaporation of EtOAc *in vacuo* afforded a dark residue of 25.0 g. The EtOAc fraction was separated by silica gel vacuum column chromatography, eluting with a gradient of EtOAc/petroleum ether (1:20, 1:10, 1:5, 1:3, 1:2, and 1:1), to obtain six fractions (A–F). Fraction C (4.9 g) was separated on a Sephadex LH-20 column, eluting with petroleum ether/CH_2Cl_2/MeOH (5:5:1), to obtain three fractions (C1–C3). Fraction C2 (345.0 mg) was subjected to an ODS column, eluting with a gradient of MeOH/H_2O (75:25, 80:20, 85:15, and 90:10), to afford four fractions (C2a–C2d). Fraction C2a (5.5 mg) was purified by C_{18} HPLC (MeOH/H_2O, 85:15) to yield dictyospiromide (**1**, 4.0 mg).

*Dictyospiromide (**1**):* colorless oil; $[\alpha]_D^{25}$ −80 (*c* 0.05, MeOH); UV (MeOH) λ_{max} (log ε) 209 (3.63), 262 (3.82) nm; IR (KBr) ν_{max} 3446, 2966, 2919, 1701, 1652, 1458, 1225, 1101 cm^{-1}; ^{1}H and ^{13}C NMR data, Table 1; HRESIMS *m/z* 398.2298 $[M + Na]^+$ (Calcd for $C_{22}H_{33}NO_4Na$, 398.2307).

ECD Calculations. Structures for the four isomers of **1** [(1*E*, 2*S*), (1*Z*, 2*S*), (1*E*, 2*R*), and (1*Z*, 2*R*)] were fully optimized at the CAM-B3LYP/6-311G (2*d*, *p*) level. Then the ECD calculations were performed at the B3LYP/Def2-TZVP level. The solvent effects were taken into account in

all calculations by using the Polarizable Continuum Model (PCM, methanol as the solvent). All quantum mechanical calculations were carried out using the Gaussian 09 program package.

Cell Culture. The rat pheochromocytoma PC12 cell line was provided by the Cell Storage Center of Wuhan University. Cells were cultured in Dulbecco's modified Eagle's medium (DMEM; Gibco) containing 100 μg/mL streptomycin, 100 U/mL penicillin, and 10% fetal bovine serum (FBS; Gibco), at 37 °C with 5% CO_2.

MTT Assay. Cell viability was detected by the 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2*H*-tetrazolium bromide (MTT; 0.5 mg/mL; Sigma) assay. PC12 cells were cultured at a density of 5×10^3 per well for 24 h in 96-well plates (NEST Biotechnology Co. LTD) then treated with **1** and TBHQ for 18 h. H_2O_2 (450 μM; Sinopharm Chemical) was added for an additional 24 h. The cells were cultured with 20 μL MTT solution at 37 °C for 4 h. The crystals were dissolved in 120 μL dimethyl sulfoxide (DMSO; Sigma) and the UV absorbance at 490 nm was determined with a microplate reader (Thermo Fisher Scientific). The cell viability was calculated by the formula: cell viability (%) = [OD_{490} (experiment group)/OD_{490} (DMSO group)] × 100%.

LDH Assay. PC12 cells were seeded in 96-well plates (NEST Biotechnology Co. LTD) at a density of 5×10^3 per well for 24 h. The cell treatments with compound and H_2O_2 were the same as those described in the MTT assay. The next procedures were exactly followed according to the manufacturer's protocols from the lactate dehydrogenase (LDH) release cytotoxicity detection kit (Beyotime Biotech). Absorbance was measured at 490 nm using a microplate reader (Thermo Fisher Scientific).

Immunostaining of Nrf2. PC12 cells were cultured in 6-well plate (NEST Biotechnology Co. LTD) at a density of 3×10^5 per well for 24 h and then treated with **1** and TBHQ for 6 h. For immunofluorescence staining, PC12 cells were fixed with 4% paraformaldehyde at 37 °C for 20 min, followed by a 15 min permeabilization with 1% Triton X-100 (Sigma-Aldrich). Then, cells were rinsed three times with PBS buffer and blocked with 1% bovine serum albumin (BSA) at 37 °C for 1 h. After removing blocking buffer, cells were cultured with a 1:200 dilution of primary antibody for Nrf2 (sc-13032, Santa Cruz Biotechnology) at 4 °C overnight. After washing with PBS, cells were incubated with secondary antibody (sc-13032, goat anti-rabbit IgG-PE, Santa Cruz Biotechnology, 1:300) for 1 h at 37 °C and treated with DAPI (Beyotime Biotech) for 8 min. Then, cells were photographed with a fluorescence microscope (Nikon).

Western Blot Analysis. PC12 cells were seeded in 6-well plate at a density of 5×10^5 per well for 24 h, then treated with **1** and TBHQ for 18 h and lysed with ice-cold radio-immunoprecipitation assay (RIPA) lysis buffer, followed by centrifugation at 1.2×10^4 rpm for 10 min at 4 °C. Total

protein content in cells was determined by Bradford's method. Equal amounts of total protein were separated by 10% sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) and then transferred onto a PVDF membrane (Millipore). The membrane was blocked with 5% non-fat milk in Tris-buffered saline containing 0.1% Tween 20 (TBST) at 37 °C for 2 h, and cultured with the primary antibodies against HO-1 (sc-10789, Santa Cruz Biotech Co. Ltd., 1:500) and β-actin (AP0060, Bioworld Technology, 1:3000) at 4 °C overnight, and followed by incubation with horseradish peroxidase labeled secondary antibodies (1:5000) at 37 °C for 1 h. After washing with TBST, antibody-bound proteins were detected using a ChemiDoc XRS + system (Bio-Rad) and immunoreactive labeling was analyzed with Image J software (NIH).

Transfection Assay. Nrf2 siRNA and control siRNA were purchased from GenePharma. The transfection of Nrf2 siRNA or control siRNA was performed using Lipofectamine 2000 reagent (Invitrogen) following the manufacturer's instructions. After a 10 h transfection, cells were collected and seeded into 96-well plates at a density of 5×10^3 per well. After that, cells were incubated with 2 μM **1** for 18 h and treated with 450 μM H_2O_2 for another 24 h. Cell viability was determined by MTT assay.

Structure Elucidation

Dictyospiromide (**1**) had a molecular formula of $C_{22}H_{33}NO_4$ according to its HRESIMS data, which implied seven degrees of unsaturation. The ^{13}C NMR spectrum (in acetone-d_6) displayed 22 carbon signals including two carbonyls (δ_C 182.0, C-18; 171.8, C-19) and six additional sp^2 carbons (Table S1), which indicated that **1** was bicyclic. The presence of a monosubstituted olefinic double bond was revealed by ^1H NMR signals (in acetone-d_6) at δ_H 5.93 (dd, J = 16.8, 10.2 Hz, H-7), 4.97 (d, J = 16.8 Hz, H-8a), and 4.95 (d, J = 10.2 Hz, H-8b) and ^{13}C NMR signals at δ_C 145.9 (CH, C-7) and 111.8 (CH_2, C-8), as well as COSY correlations between H-7 and H_2-8 (Figure S1). An exocyclic double bond with an ethoxy substituent was established by ^1H NMR signals for an olefinic proton (δ_H 7.33, s, H-9), an oxymethylene (δ_H 4.19, q, J = 7.2 Hz), and a methyl triplet (δ_H 1.34, t, J = 7.2 Hz) and ^{13}C NMR signals at δ_C 155.4 (CH, C-9), 109.6 (C, C-1), 72.0 (CH_2, OEt), and 15.7 (CH_3, OEt), in combination with a COSY correlation between the oxymethylene and methyl triplet and HMBC correlations from the olefinic proton H-9 to an olefinic nonprotonated carbon C-1 and from the oxymethylene protons to the olefinic methine carbon C-9. A 6-methylhept-5-en-2-yl side chain was established based on COSY correlations between H-13 (δ_H 4.99, t, J = 7.2 Hz)/H_2-12 (δ_H 1.99, m; 1.83, m), H_2-12/H_2-11 (δ_H 1.38, m; 1.12, m), H_2-11/H-10 (δ_H 1.84, m), and H-10/H_3-17 (δ_H 0.97, d, J = 6.0 Hz), as well as HMBC correlations from two olefinic methyls H_3-15 (δ_H 1.55, s) and H_3-16 (δ_H 1.62, s) to two olefinic carbons C-13 (δ_C 125.3, CH) and C-14 (δ_C 131.8, C) and from H_3-17 to an aliphatic methine carbon C-10 (δ_C 31.7, CH) and an aliphatic methylene carbon C-11 (δ_C 34.6, CH_2). COSY correlations between H-3 (δ_H 2.78, dd, J = 10.2, 7.2 Hz)/H-4 (δ_H 4.28, m), and H-4/H_2-5 (δ_H 2.51, dd, J = 14.4, 7.8 Hz; 1.71, dd, J = 14.4, 4.2 Hz) and HMBC correlations from both a methyl singlet H_3-20 (δ_H 1.00, s) and H-3 to two nonprotonated carbons C-2 (δ_C 65.4, C) and C-6 (δ_C 53.2, C) and from H_3-20 to a methylene carbon C-5 (δ_C 46.9, CH_2) led to the establishment of a cyclopentane ring and revealed that C-4 (δ_C 72.1, CH) was hydroxylated and C-6 was substituted by a methyl group. An HMBC correlation from H_3-20 to an olefinic carbon C-7 indicated that C-6 was joined to the monosubstituted olefin residue established above, while an HMBC correlation from H_3-17 to a methine carbon C-3 (δ_C 51.1, CH) and a COSY correlation between H-3 and H-10 (δ_H 1.84, m) revealed that the 6-methylhept-5-en-2-yl side chain was attached to C-3. HMBC correlations from H-3 to C-1 and the C-18 carbonyl carbon, and from H-9 to C-2 suggested that C-2 was connected to both C-18 and the exocyclic double bond. In addition, an HMBC correlation from H-9 to the C-19 carbonyl carbon revealed that the ethoxy substituted exocyclic double bond was conjugated to C-19. An NH group remained to be assigned according to the HRESIMS data, and it was

positioned between the two carbonyl carbons to form a succinimide moiety based on the chemical shifts of C-18 (δ_C 182.0), C-19 (δ_C 171.8), and the NH proton (δ_H 10.13, br s). This was confirmed by HMBC correlations (in $CDCl_3$) from the NH proton (δ_H 8.15, br s) to C-1 (δ_C 108.4, C) and C-2 (δ_C 64.8, C).

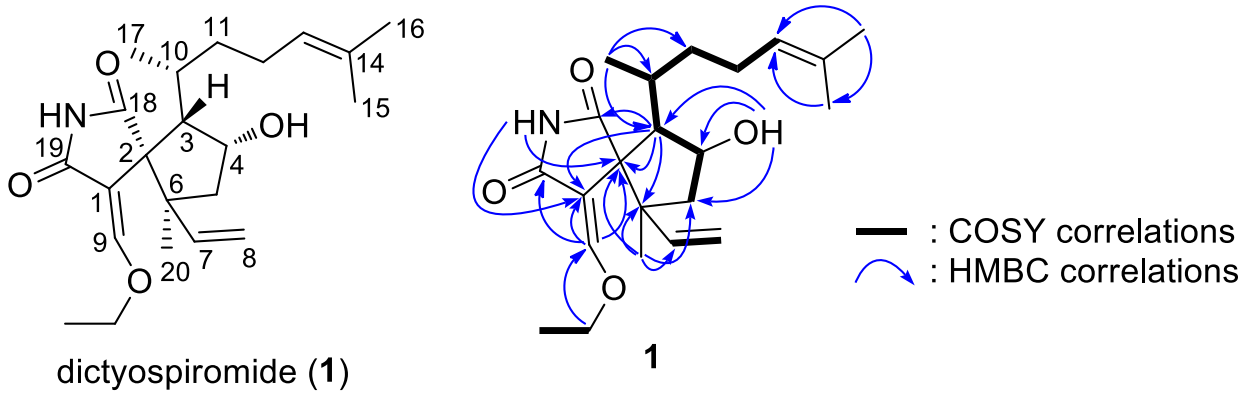


Figure S1. Structure of dictyosporomide (**1**) and COSY and key HMBC correlations

The relative configurations at C-3, C-4, C-6, and C-10 in **1** were determined by NOESY analysis (in acetone-d_6). NOESY correlations between H-3/H_3-17, H-4/H_3-17, and 4-OH (δ_H 3.79, d, J = 12.0 Hz)/H-10 suggested the assignment of a 3*S**,4*R**,10*R** configuration, while a NOESY correlation between H-7 and H-3 was indicative of 6*S** (Figure 2). The rare large proton-proton coupling (12.0 Hz) between 4-OH and H-4 implied that the rotation around C-4/O bond was restricted probably because 4-OH and a carbonyl had an inclination to form a hydrogen bridge in the dominant conformation; thus the relative configuration at C-2 was tentatively assigned as *R**, in this case, the 4-OH could be adjacent to C-18 carbonyl in the space. In addition, the geometry of the exocyclic double bond was suggested to be *E* based on the chemical shift of H-9 (δ_H 7.33, s) and the absence of NOE correlation between H-9/H-3 or H-9/H-7. The absolute configuration at C-4 was determined by an *in situ* $Rh_2(OCOCF_3)_4$ CD method, according to which the sign of the E band (350 nm) in the induced CD (ICD) spectrum reflected the absolute configuration of secondary alcohol by applying the bulkiness rule.[1S,2S] A metal complex as an auxiliary chromophore was generated after addition of $Rh_2(OCOCF_3)_4$ into a $CHCl_3$ solution of **1** and the ICD spectrum was acquired. The negative CD effect (Figure 3) observed at 350 nm was in agreement with a 4*R* configuration. Therefore, the absolute configurations at C-2, C-3, C-6, and C-10 were defined as *R*, *S*, *S*, and *R*, respectively. In order to support this assignment, the ECD data calculations were carried out for four possible isomers of **1** [**1a** (1*E*,2*S*), **1b** (1*Z*,2*S*), **1c**

(1*E*,2*R*), and **1d** (1*Z*,2*R*)] at the B3LYP/def2-TZVP level (Figure 4) and the measured ECD spectrum of **1** was similar to the calculated ECD spectrum for the isomer **1c** (1*E*,2*R*).

References

1S M. Gerards, G. Snatzke, *Tetrahedron: Asymmetry* 1990, **1**, 221.

2S Frelek, W. J. Szczepek, *Tetrahedron: Asymmetry* 1999, **10**, 1507.

Table S1. ^{1}H and ^{13}C NMR Spectroscopic Data for Dictyospiromide (**1**)[a]

Pos.	$(CD_3)_2CO$		$CDCl_3$	
	δ_H mult. (*J* in Hz)	δ_C, type	δ_H mult. (*J* in Hz)	δ_C, type
1		109.6, C		108.4, C
2		65.4, C		64.8, C
3	2.78, dd (10.2, 7.2)	51.1, CH	2.73, dd (10.2, 7.1)	50.5, CH
4	4.28, m	72.1, CH	4.38, dtd (12.0, 7.8, 4.2)	71.8, CH
5	2.51, dd (14.4, 7.8)	46.9, CH_2	2.58, dd (14.9, 7.9)	45.8, CH_2
	1.71, dd (14.4, 4.2)		1.81, m	
6		53.2, C		52.9, C
7	5.93, dd (16.8, 10.2)	145.9, CH	5.84, dd (17.2, 10.7)	144.3, CH
8	4.97, d (16.8)	111.8, CH_2	4.95, m	111.9, CH_2
	4.95, d (10.2)			
9	7.33, s	155.4, CH	7.35, s	155.1, CH
10	1.84, m	31.7, CH	1.85, m	30.8, CH
11	1.38, m	34.6, CH_2	1.29, m	33.9, CH_2
	1.12, m		1.07, m	
12	1.99, m	26.3, CH_2	1.99, m	25.5, CH_2
	1.83, m		1.83, m	
13	4.99, t (7.2)	125.3, CH	4.96, m	124.3, CH
14		131.8, C		131.5, C
15	1.55, s	17.7, CH_3	1.56, s	17.7, CH_3
16	1.62, s	25.8, CH_3	1.66, s	25.7, CH_3
17	0.97, d (6.0)	18.5, CH_3	1.00, d (6.3)	18.2, CH_3
18		182.0, C		180.4, C
19		171.8, C		171.2, C
20	1.00, s	22.1, CH_3	1.05, s	21.5, CH_3
OEt	4.19, q (7.2)	72.0, CH_2	4.09, q (7.1)	71.6, CH_2
	1.34, t (7.2)	15.7, CH_3	1.35, t (7.1)	15.3, CH_3
NH	10.13, br s		8.15, br s	
OH	3.79, d (12.0)		3.78, d (12.0)	

[a] 600 MHz for ^{1}H and 150 MHz for ^{13}C.

Figure S2. ^{1}H NMR spectrum (600 MHz) of dictyospiromide (**1**) in $(CD_3)_2CO$.

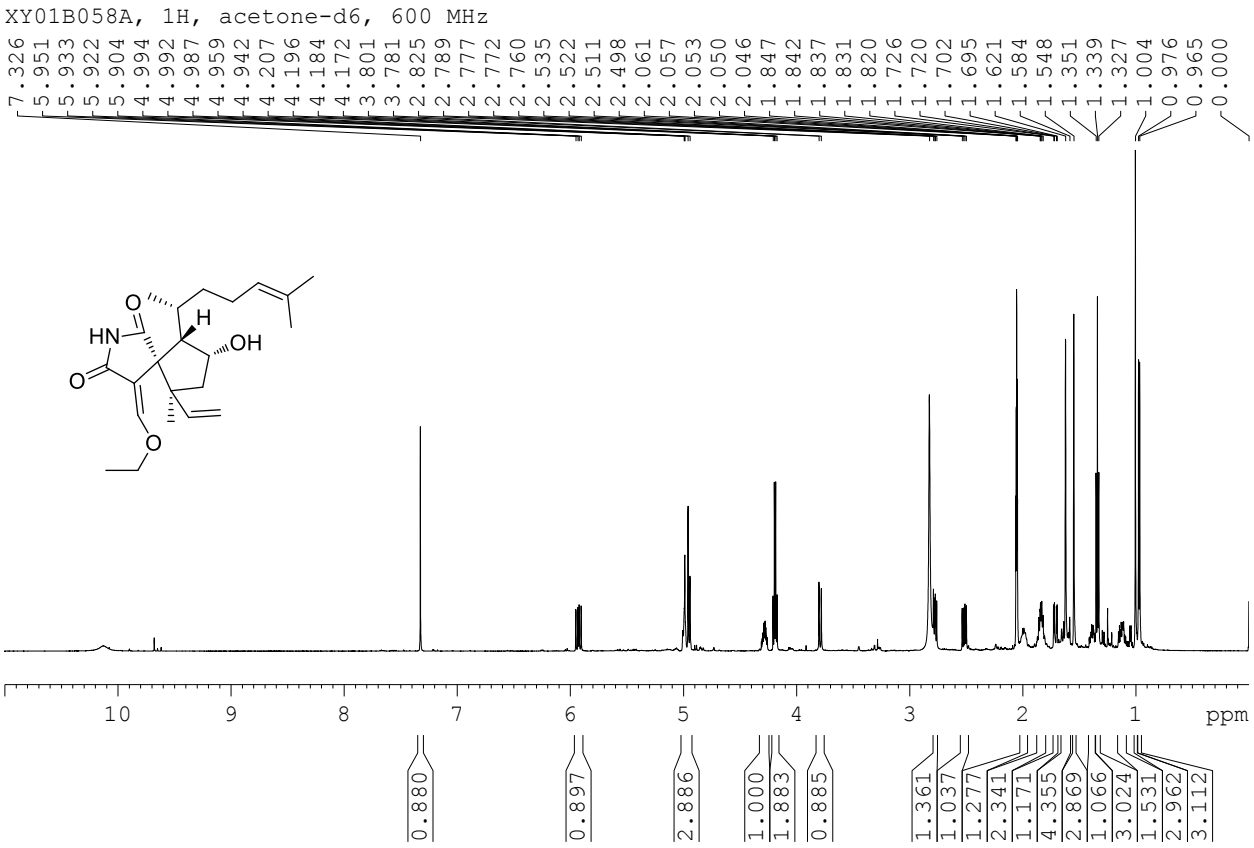


Figure S3. Enlarged ^{1}H NMR spectrum (600 MHz) of dictyospiromide (**1**) in $(CD_3)_2CO$.

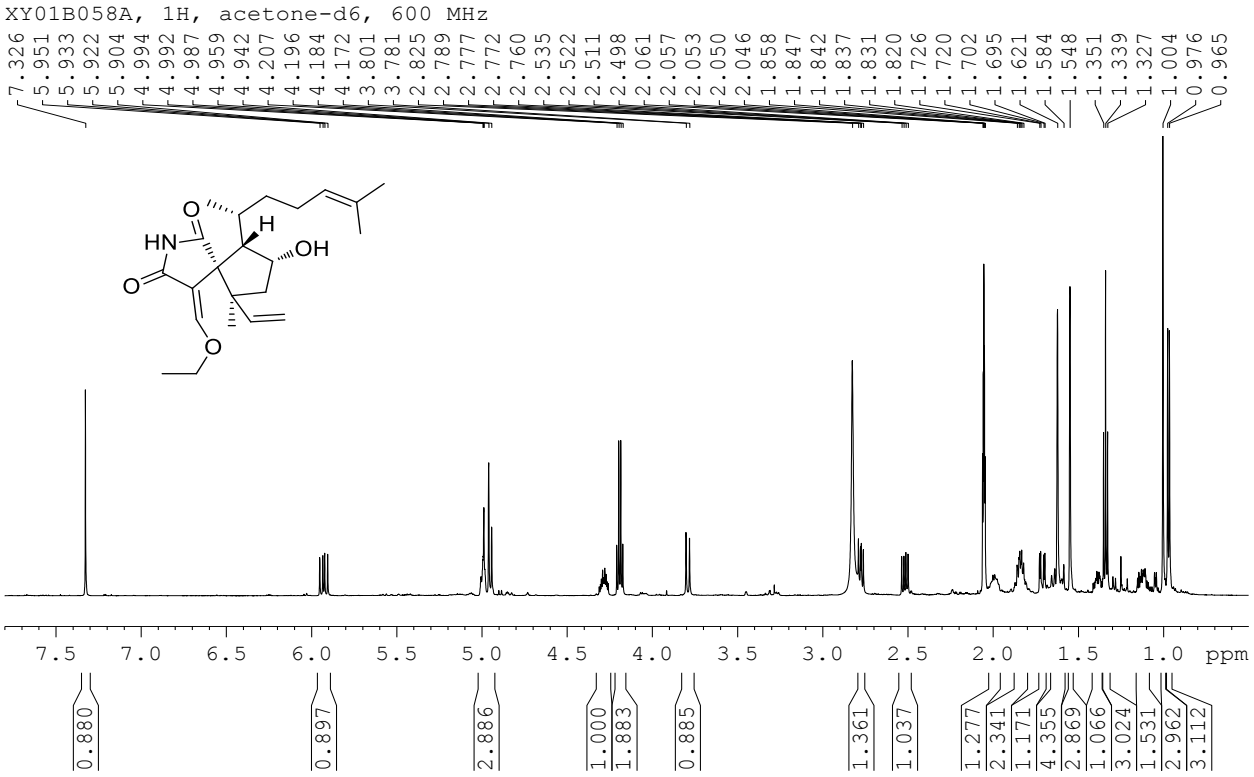


Figure S4. ^{13}C NMR spectrum (150 MHz) of dictyospiromide (**1**) in $(CD_3)_2CO$.

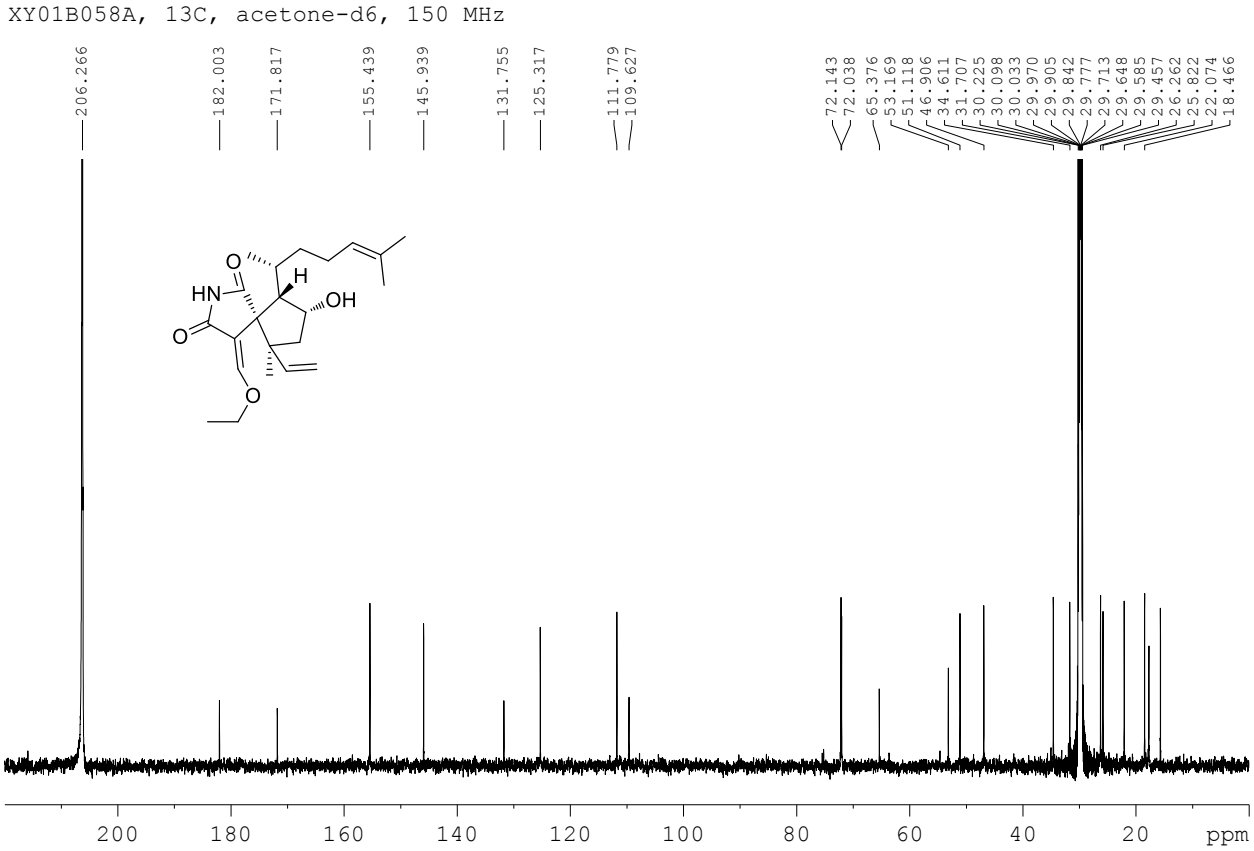


Figure S5. HMQC spectrum of dictyospiromide (**1**) in $(CD_3)_2CO$.

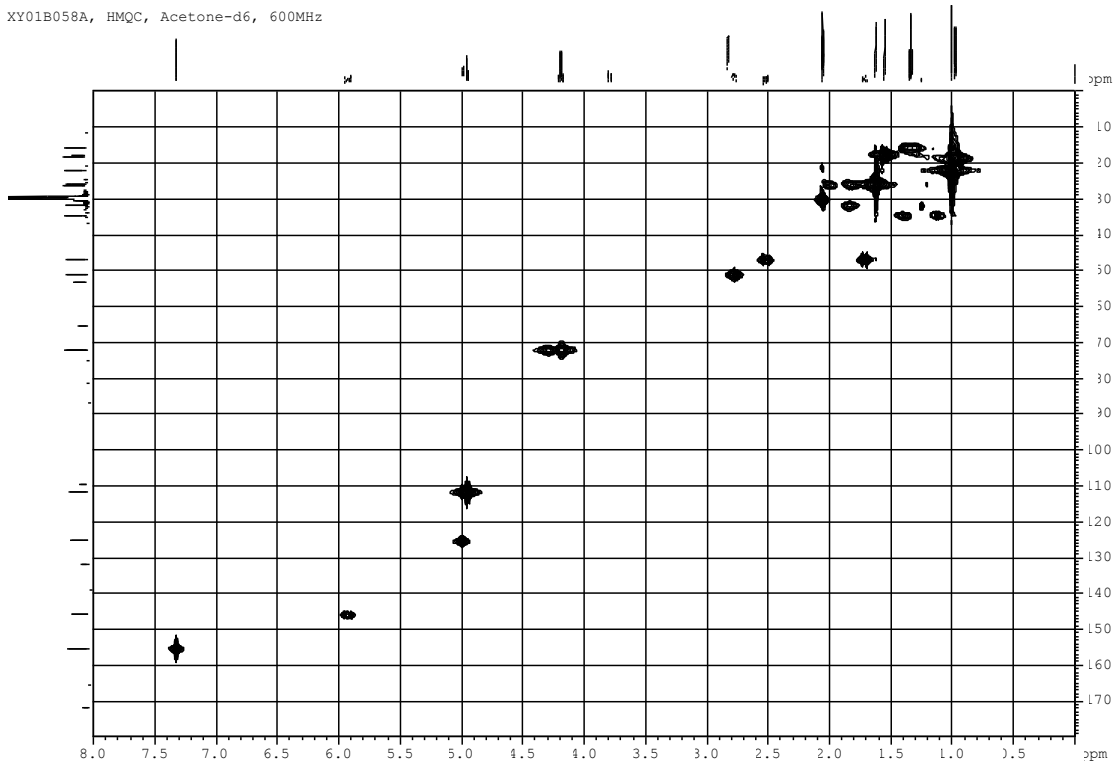


Figure S6. HMBC spectrum of dictyospiromide (**1**) in $(CD_3)_2CO$.

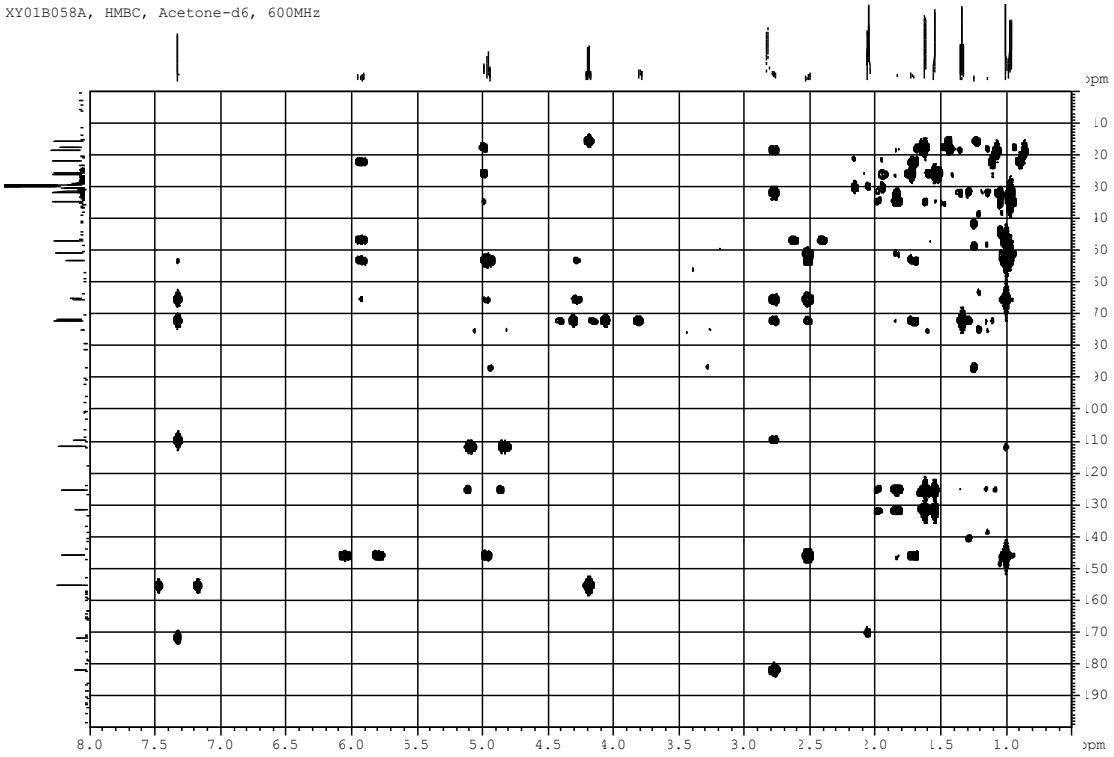


Figure S7. COSY spectrum of dictyospiromide (**1**) in $(CD_3)_2CO$.

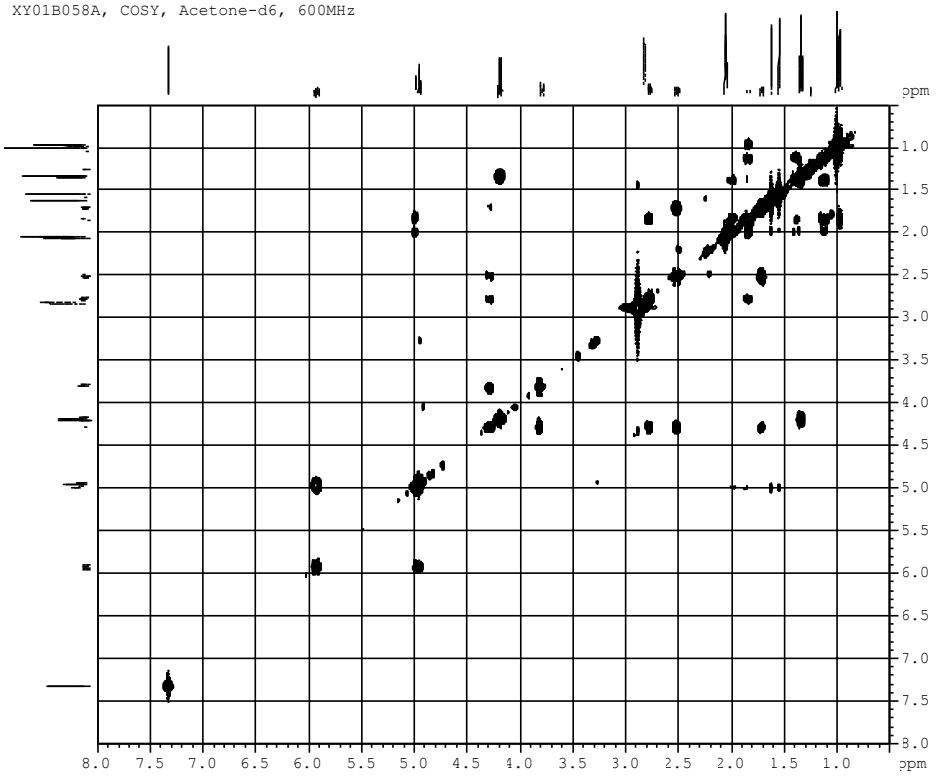


Figure S8. NOESY spectrum of dictyospiromide (**1**) in $(CD_3)_2CO$.

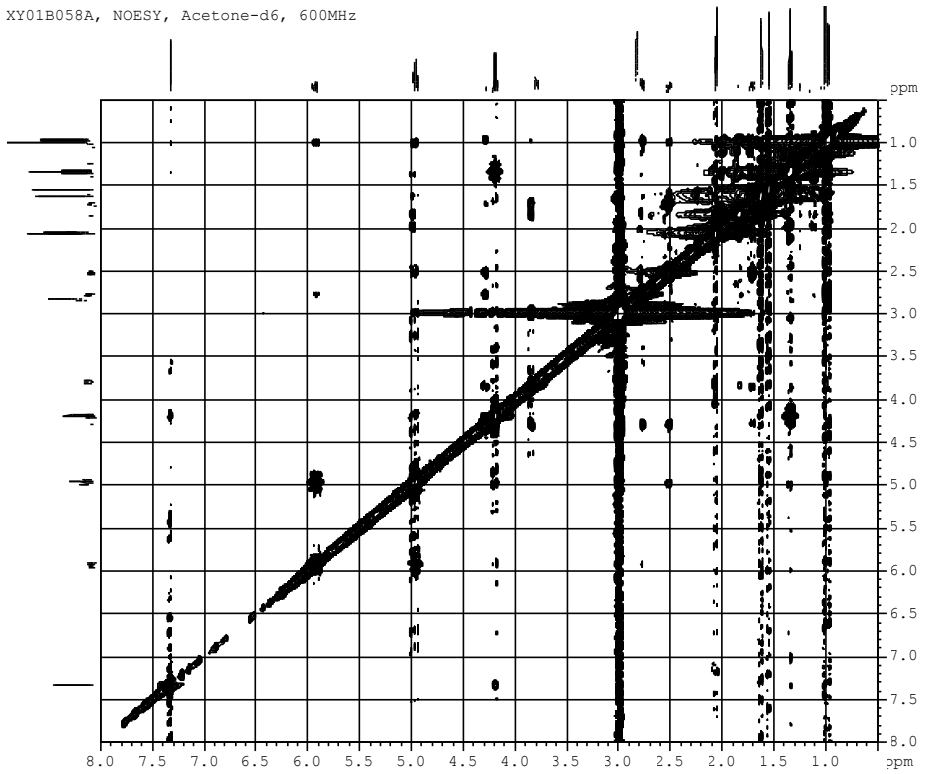


Figure S9. ^1H NMR spectrum (600 MHz) of dictyospiromide (**1**) in $CDCl_3$.

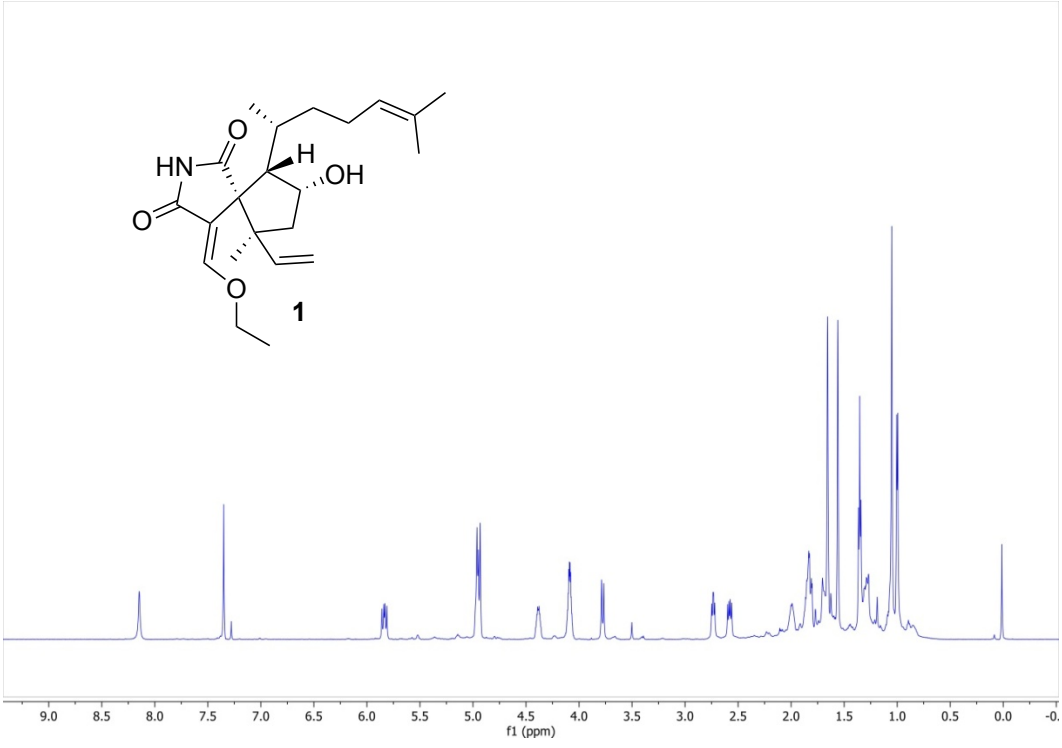


Figure S10. ^{13}C NMR spectrum (150 MHz) of dictyospiromide (**1**) in $CDCl_3$.

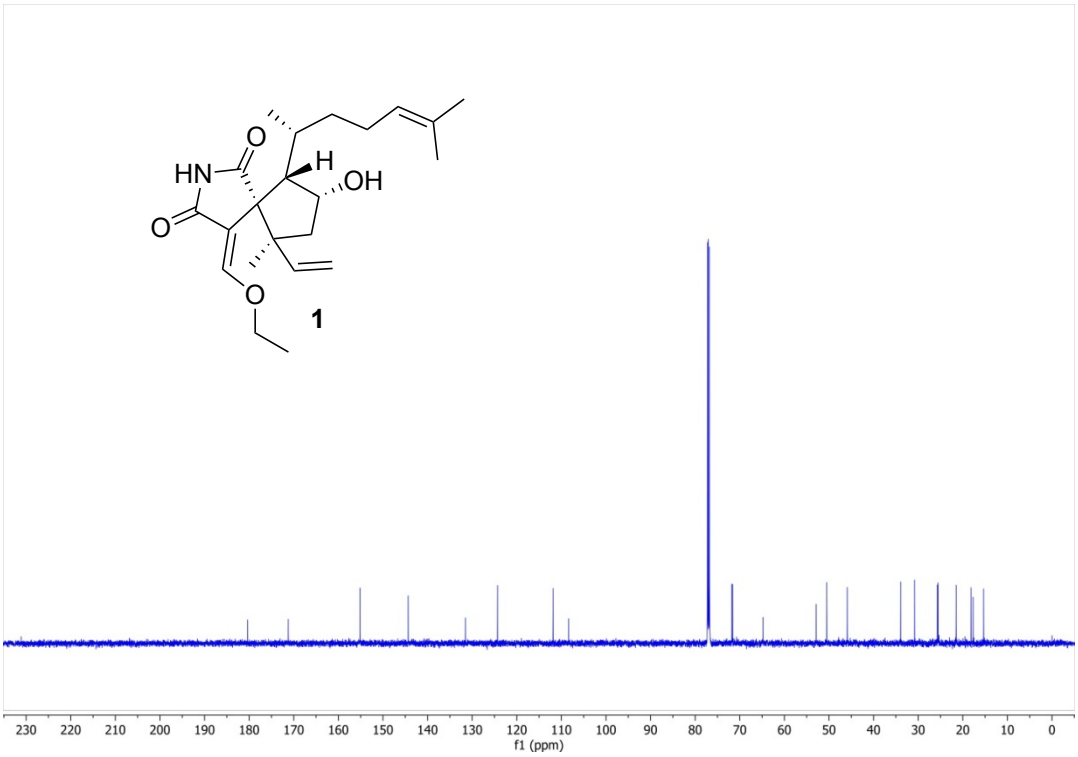


Figure S11. ^{1}H-^{13}C ps-HSQC spectrum of dictyospiromide (**1**) in $CDCl_3$.

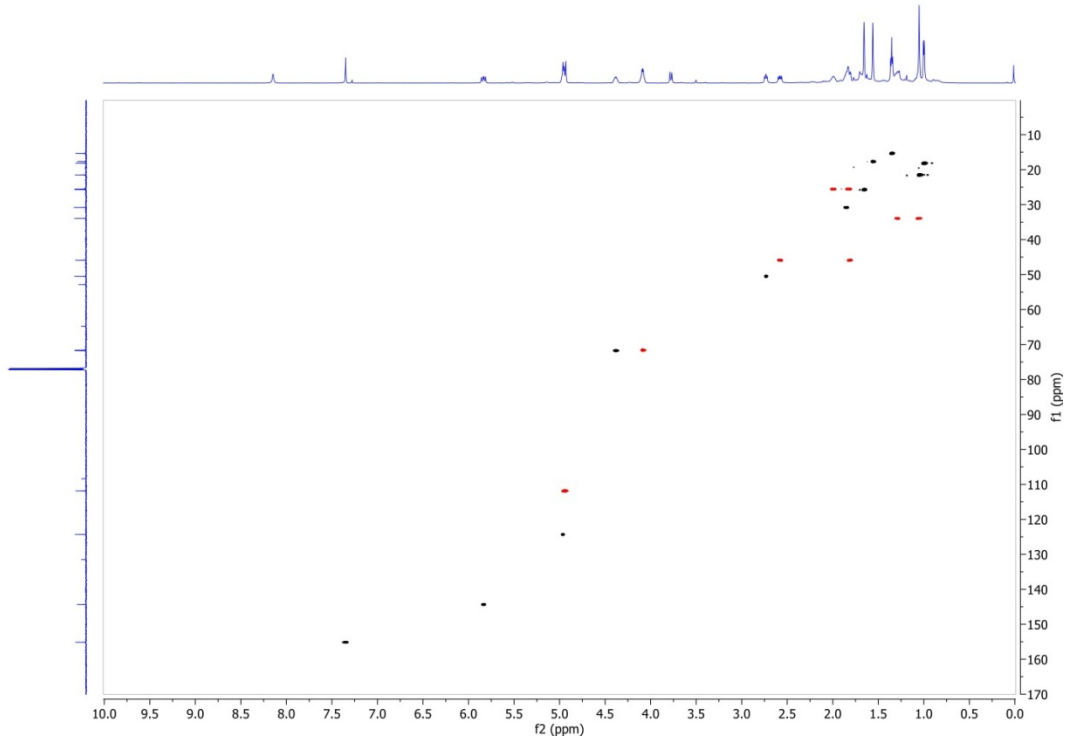


Figure S12. HMBC spectrum of dictyospiromide (**1**) in $CDCl_3$.

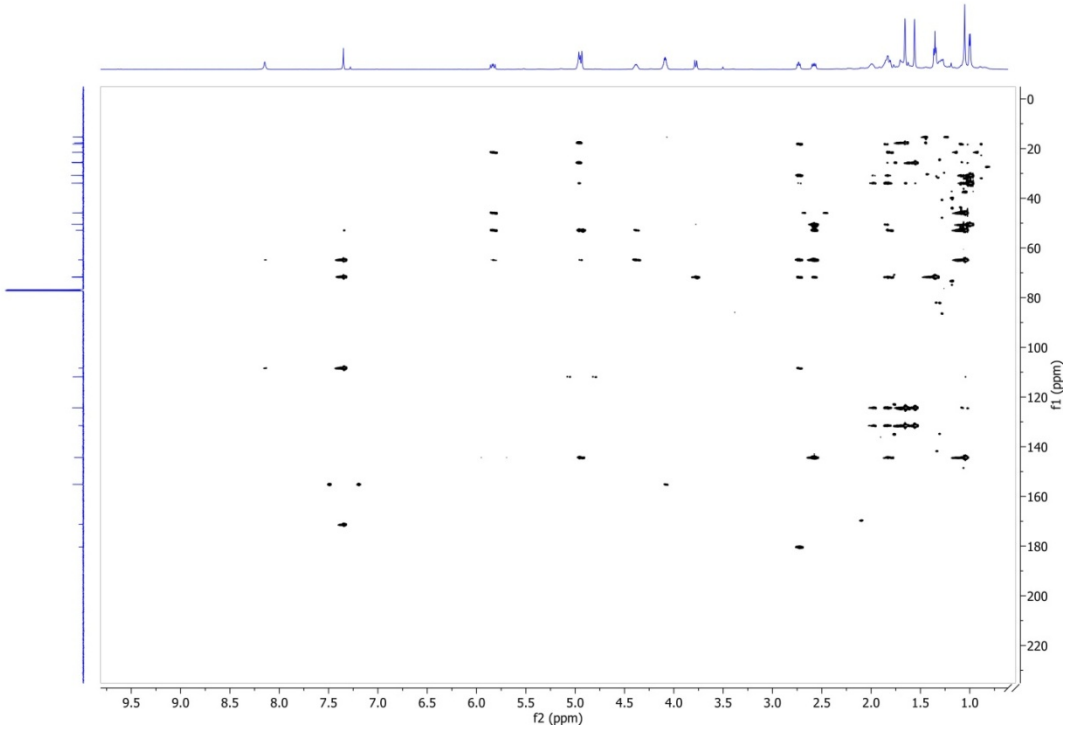


Figure S13. COSY spectrum of dictyospiromide (**1**) in $CDCl_3$.

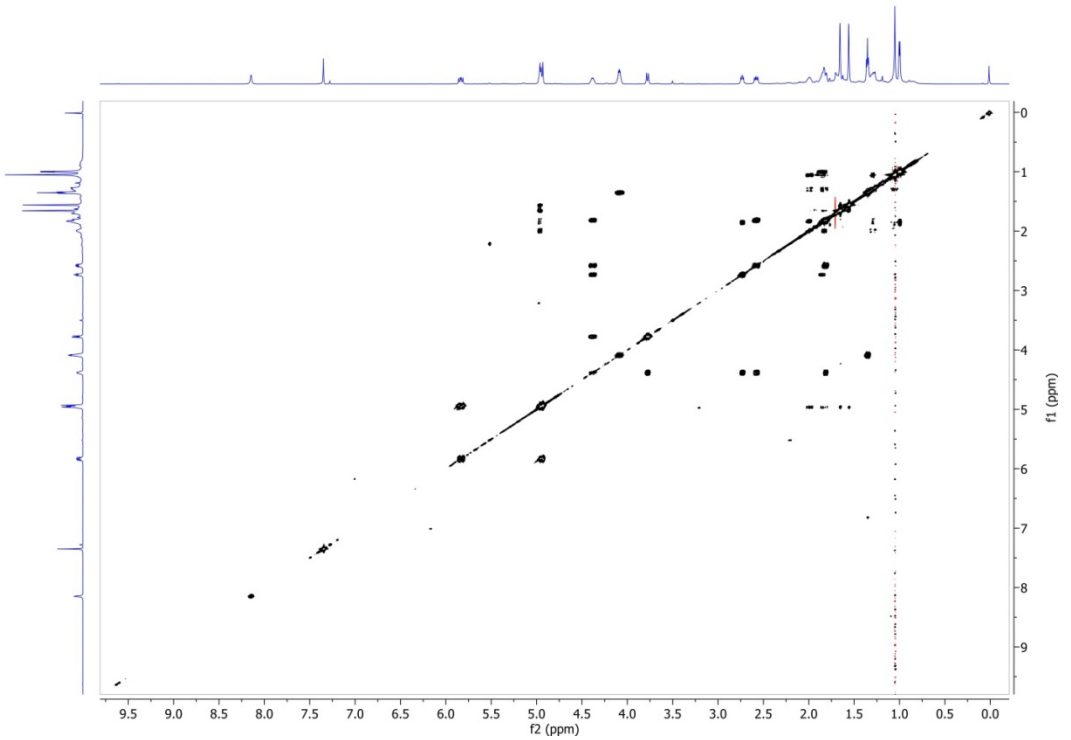


Figure S14. ROESY spectrum of dictyospiromide (**1**) in $CDCl_3$.

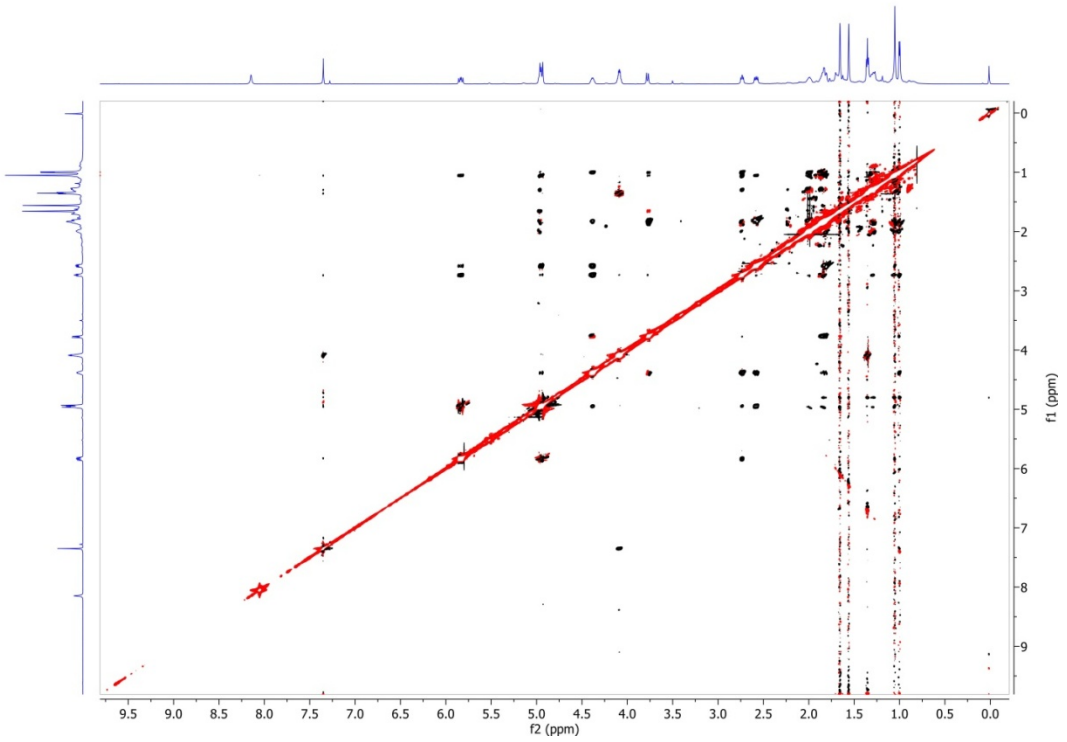


Figure S15. HRESIMS spectrum of dictyospiromide (**1**).

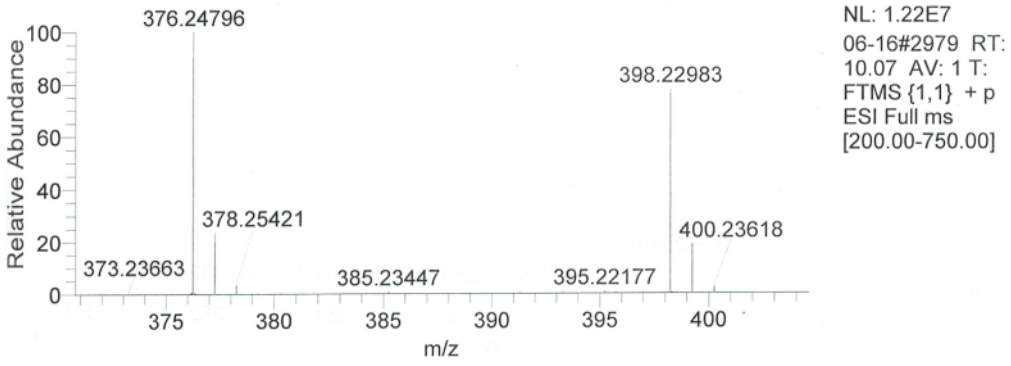
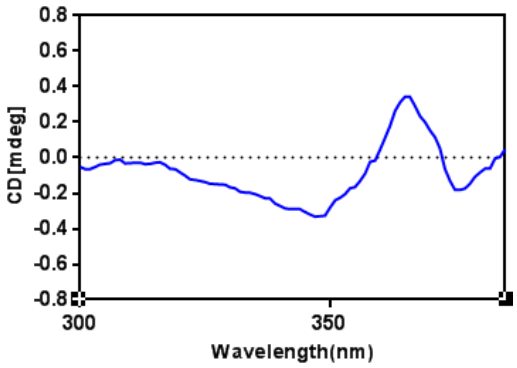


Figure S16. CD spectrum for $Rh_2(OCOCF_3)_4$ complex of dictyospiromide (**1**).



Biological Characterization

Dictyospiromide (**1**) was evaluated for its cytoprotective effect against H_2O_2-induced oxidative damage in neuron-like PC12 cells by the MTT method. Compared with the control group, the cell survival rate of PC12 cells treated with H_2O_2 was around 54%, and it was increased by **1** in a dose-dependent manner. The cytoprotective effect of 5 μM **1** was comparable to that of the positive control *tert*-butylhydroquinone (TBHQ, 2 μM). The cytoprotection of **1** was further evaluated in a lactate dehydrogenase (LDH) assay that uses release of this cytosolic enzyme as an index of cell injury. Compound **1** inhibited the H_2O_2-induced LDH production in PC12 cells in a dose-dependent manner. The inhibitory effect of **1** was observed even at a low concentration of 0.5 μM. Thus, **1** is a potent cytoprotectant with antioxidant properties in PC12 neuronal cells.

Dictyospiromide (**1**) was also investigated for activation of the Nrf2 (nuclear erythroid 2-related factor 2)/ARE (antioxidant response element) signaling pathway, which regulates the expression of genes involved with cellular response to oxidative stress and is a key pathway associated with neuroprotection. First, the promotion effect of **1** on the nuclear translocation of Nrf2 was determined using an immunofluorescence assay. Both **1** and the positive control TBHQ significantly promoted the delivery and accumulation of Nrf2 in the nucleus as indicated by the strong red fluorescence observed in the nucleus, suggesting that **1** is a potent Nrf2 activator. Second, compound **1** was evaluated for its up-regulation effect on the expression of heme oxygenase-1 (HO-1), an antioxidant protein regulated by Nrf2, in PC12 cells based on a Western blot assay. This showed that **1** promoted HO-1 production in a dose-dependent manner, and the promotion effect of 2 μM **1** was comparable to that of the positive control TBHQ. These findings confirmed the potent induction of Nrf2-ARE signaling by treatment with **1**. Nrf2 siRNA was applied to investigate whether the antioxidant effect of **1** in PC12 cells is dependent on the role of Nrf2. Cellular viability in the control siRNA (si Con) group was increased by **1**, while the cytoprotective activity of **1** was reversed by knockdown of Nrf2. This established that Nrf2 is a key mediator of the antioxidant effect of **1**. Furthermore, the role of HO-1 in the cytoprotective effect of **1** was investigated by using the HO-1 inhibitor zinc protoporphyrin (ZnPP). The result showed that the cytoprotective effect of **1** was partially suppressed when **1** and the maximum non-cytotoxic concentration (10 μM) of ZnPP were applied together, implying that HO-1 contributes in part to the antioxidant effect of **1** in PC12 cells. Overall, dictyospiromide (**1**) exerted an antioxidant effect in PC12 cells that is mediated by activation of the Nrf2/ARE signaling pathway and enhancement of HO-1 expression.

Anisotropic Data: Sample Preparation and Acquisition of ^{13}C Spectra

Residual Chemical Shift Anisotropy (RCSA) data were obtained using Eq. 1 shown below:

$$RCSA_i = \left(\delta_{A1}^{i} - \delta_{A1}^{TMS}\right) - \left(\delta_{I0}^{i} - \delta_{I0}^{TMS}\right) - \frac{[PBLG]_{A1}}{[PBLG]_{I1}}\left[\left(\delta_{I1}^{i} - \delta_{I1}^{TMS}\right) - \left(\delta_{I0}^{i} - \delta_{I0}^{TMS}\right)\right]$$

Eq. 1

Parameters I_0, I_1, and A_1 were determined from three different ^{13}C NMR experiments acquired in a 5 mm NMR tube on a Bruker Avance III 600 MHz spectrometer equipped with a 5 mm TXI CryoProbe™ at 25 ºC.

The first ^{13}C experiment was acquired in isotropic conditions with no poly-γ-(benzyl-L-glutamate) (PBLG) added by just dissolving approximately 3 mg of **1** in 500 μL of $CDCl_3$ in a 5 mm tube. TMS - 4% (v/v), was added for RCSA referencing purposes. This experiment is referred to as I_0.

A second ^{13}C spectrum was acquired following addition of 27.1 mg of PBLG, which still corresponds to isotropic conditions where the amount of PBLG is below the critical concentration required to produce a pure anisotropic liquid crystalline solution. This experiment is referred to as I_1.

A final third ^{13}C spectrum was acquired following addition of 33.5 mg of PBLG (60.6 mg total PBLG), which corresponds to the full anisotropic liquid crystalline medium, is referred to as A_1.

Further details about the sample preparation can be found in the original research article.[1]

All ^{13}C spectra were acquired using a spectral width of 36231.88 Hz, with 64K points acquired and a relaxation delay of 1 s. 4096 scans were acquired for I_0 and I_1 experiments, while 12228 scans were acquired for A_1 to compensate for decreased signal-to-noise ratio due to line-broadening in anisotropic conditions.

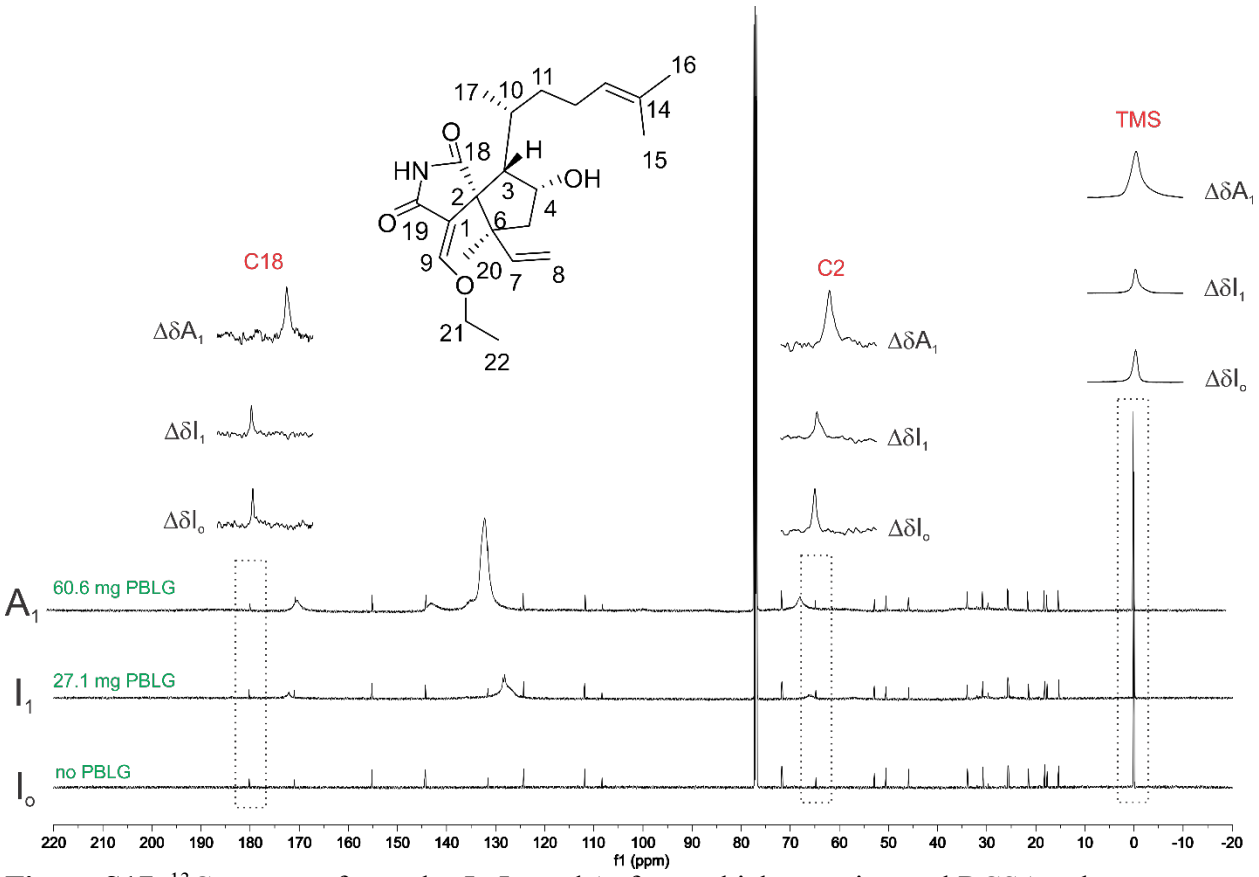


Figure S17. ^{13}C spectra of samples I_0, I_1, and A_1 from which experimental RCSA values are obtained. Spectra are all referenced against TMS signal.

Table S2. Residual chemical shift anisotropy (RCSA) values derived from Eq. 1.

Carbon atom	I_0 (Hz)	I_1 (27.1 mg PBLG) (Hz)	A_1 (60.6) mg PBLG) (Hz)	Experimental RCSA (Hz)
C18	27178.9	27180.3	27147.5	-34.61
C19	25790.8	25790.8	25747.5	-43.28
C9	23402.0	23404.9	23381.0	-27.45
C7	21765.5	21766.1	21729.7	-37.05
C8	16876.4	16874.5	16838.5	-33.69
C1	16341.5	16341.5	16312.0	-29.50
C2	9772.8	9771.8	9766.2	-4.32
C6	7977.7	7976.1	7956.1	-18.04
C3	7616.8	7615.5	7596.7	-17.13
C5	6920.9	6920.9	6908.0	-12.91
C11	5115.9	5115.9	5107.8	-8.07
C10	4645.8	4645.8	4637.3	-8.50
C20	3241.7	3241.7	3252.1	10.38
C17	2740.0	2740.0	2749.8	9.79

Procedure for DFT Geometry Optimization and Chemical Shift Calculation

Conformational search was performed using OPLS3e force field in Maestro.[2] Structures having relative energy under 40 kJ/mol were saved and submitted to further DFT calculations. DFT calculation was performed using Gaussian'16 software package.[3] For chemical shift calculation, geometry optimization was calculated using M06-2X/6-31+G(d,p) level of theory with chloroform as solvent using SMD model. Frequency calculation was carried out to ensure no imaginary frequency. Energy was calculated using M06-2X/6-311+G(d,p) level of theory with chloroform as solvent using SMD model, and Gibbs free energy was calculated for 298 K. NMR chemical shielding was calculated using mPW1PW91/6-311+G(2d,p) level of theory with chloroform as solvent using PCM model, and the chemical shifts were then converted from the shielding with scaling factors: ^{1}H slope = -1.0719, ^{1}H intercept = 31.8733; ^{13}C slope = -1.0420, ^{13}C intercept = 186.3567. For RCSA tensor calculation, geometry optimization was obtained using B3LYP/6-31+G(d,p) level of theory without employing solvent model. The chemical shielding tensors and Gibbs free energy were calculated using the same level of theory as the chemical shift calculation mentioned above.

Summary of DFT Chemical Shift RMSD and MAE Values Obtained for 1a, 1b, 1c and 1d and DP4+ Probabilities for the Isomers

	1a: 1*E*2*S*	**1b**: 1*Z*2*S*	**1c**: 1*E*2*R*	**1d**: 1*Z*2*R*
^{1}H RMSD, ppm	0.16	0.16	0.16	0.33
^{1}H MAE, ppm	0.12	0.13	0.12	0.21
^{13}C RMSD, ppm	2.29	2.44	1.91	2.65
^{13}C MAE, ppm	1.74	1.74	1.34	1.93
DP4+ (^{1}H)	43.03%	4.01%	52.96%	0%
DP4+ (^{13}C)	0.06%	0.06%	99.88%	0%
DP4+ (^{1}H+^{13}C)	0.05%	0%	99.95%	0%

Superposition of Low Energy Conformers

As described in the main manuscript, superposition of the lowest energy conformers with > 2% Boltzmann population for each isomer led to the realization that the core of the structure was very rigid from the conformational point of view, showing an excellent alignment between all conformers when the flexible side chains were not considered.

Figures S18-S21 illustrate the superposition of the low energy conformers for **1a**, **1b**, **1c** and **1d**, respectively.

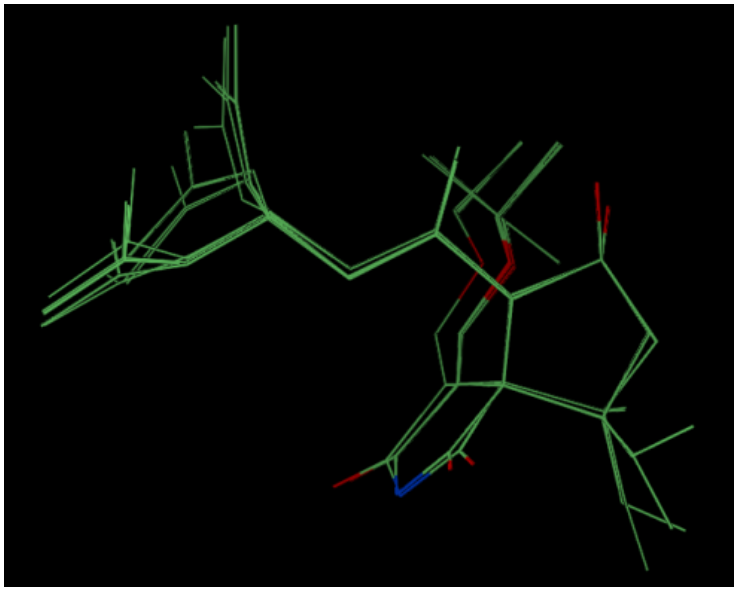


Figure S18. Superposition of 20 conformers (above 2% Boltzmann population) **1a** (1E2R).

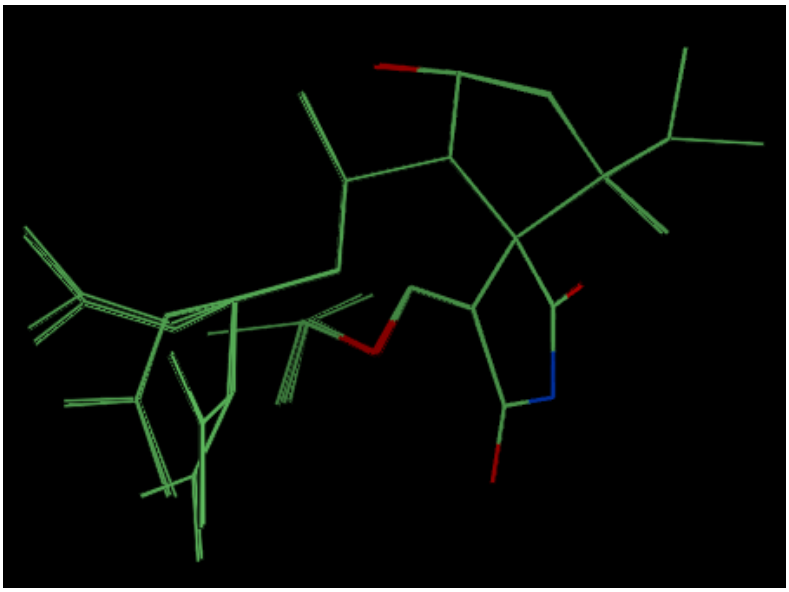


Figure S19. Superposition of 14 conformers (above 2% Boltzmann population) **1b** (1Z2R).

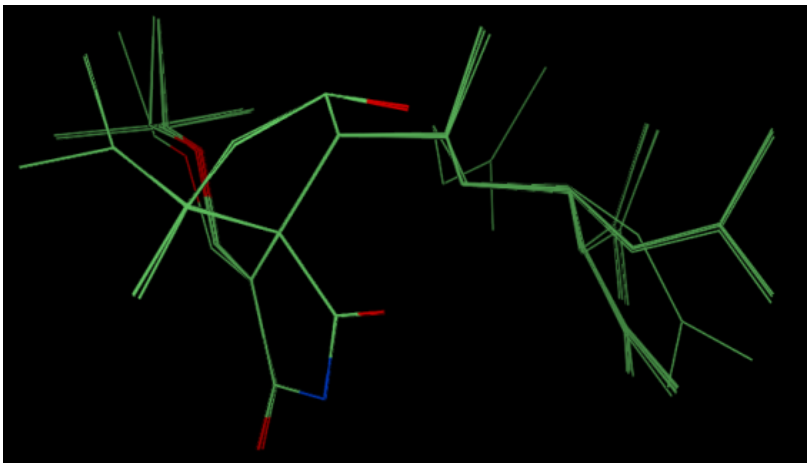


Figure S20. Superposition of 18 conformers (above 2% Boltzmann population) **1c** (1E2S).

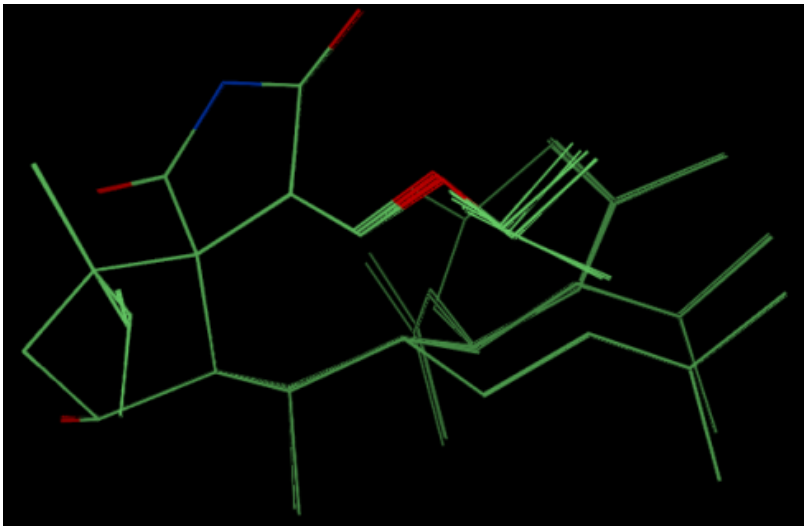


Figure 21. Superposition of 19 conformers (above 2% Boltzmann population) **1d** (1Z2S).

The completed lists of conformers obtained from DFT calculations for each isomer **1a**, **1b**, **1c** and **1d** are listed below in Table S3-S6, respectively.

Table S3. List of conformers obtained from DFT calculations for **1a**.

1E2S (1a)		
Conformer #	Gibbs Free Energy (Hartree)	Boltzmann Distribution
11	-1213.23606692	0.078
3	-1213.23570489	0.053
30	-1213.23568788	0.052
32	-1213.23567213	0.051
43	-1213.23567048	0.051
22	-1213.23559233	0.047
9	-1213.23557204	0.046
19	-1213.23524718	0.033
35	-1213.23524649	0.033

13	-1213.23517954	0.03
20	-1213.23514515	0.029
31	-1213.23513285	0.029
1	-1213.23511591	0.028
5	-1213.23506744	0.027
6	-1213.23501603	0.026
2	-1213.23491939	0.023
12	-1213.23491166	0.023
53	-1213.23489334	0.022
37	-1213.23488269	0.022
24	-1213.23482089	0.021
57	-1213.23479574	0.02
23	-1213.23472956	0.019
47	-1213.23468543	0.018
15	-1213.23466221	0.018
45	-1213.23464822	0.017
16	-1213.23461115	0.017
48	-1213.23452647	0.015
49	-1213.23448436	0.015
26	-1213.23447078	0.014
14	-1213.23433349	0.012
33	-1213.23430447	0.012
18	-1213.23422217	0.011
44	-1213.23388295	0.008
27	-1213.23373638	0.007
39	-1213.23361157	0.006
29	-1213.23359637	0.006
25	-1213.23357825	0.006
58	-1213.23357749	0.006
40	-1213.23350749	0.005
42	-1213.23344679	0.005
38	-1213.23344285	0.005
50	-1213.23342947	0.005
21	-1213.23323702	0.004
7	-1213.23321142	0.004
66	-1213.23319078	0.004
28	-1213.23311382	0.003
54	-1213.23274548	0.002
17	-1213.23273108	0.002
52	-1213.23270535	0.002
56	-1213.23254734	0.002
41	-1213.23251851	0.002
34	-1213.23231829	0.001
51	-1213.23225051	0.001
46	-1213.23219494	0.001

Table S4. List of conformers obtained from DFT calculations for **1b**.

1Z2S (1b)		
Conformer #	Gibbs Free Energy (Hartree)	Boltzmann Distribution
2	-1213.23208299	0.133
3	-1213.23144457	0.068
6	-1213.23137958	0.063
18	-1213.23137353	0.063
1	-1213.23136323	0.062
9	-1213.23115865	0.05
21	-1213.23072586	0.032
19	-1213.23071752	0.031
26	-1213.23065365	0.029
23	-1213.23063234	0.029
4	-1213.23057047	0.027
30	-1213.23056989	0.027
7	-1213.23051914	0.025
8	-1213.23046174	0.024
68	-1213.23023828	0.019
50	-1213.23022390	0.019
20	-1213.23016728	0.018
12	-1213.23015172	0.017
5	-1213.23010998	0.016
29	-1213.22991841	0.013
15	-1213.22979725	0.012
35	-1213.22976812	0.011
56	-1213.22973648	0.011
16	-1213.22969518	0.011
76	-1213.22969326	0.011
77	-1213.22968658	0.011
67	-1213.22967522	0.01
41	-1213.22964411	0.01
45	-1213.22961102	0.01
51	-1213.22959465	0.01
24	-1213.22952900	0.009
39	-1213.22945522	0.008
25	-1213.22944639	0.008
36	-1213.22939055	0.008

55	-1213.22934187	0.007
28	-1213.22932510	0.007
88	-1213.22928285	0.007
32	-1213.22924511	0.007
71	-1213.22918380	0.006
37	-1213.22913962	0.006
65	-1213.22913083	0.006
47	-1213.22911680	0.006
34	-1213.22908539	0.006
46	-1213.22904590	0.005
81	-1213.22897957	0.005
22	-1213.22889059	0.005
53	-1213.22888757	0.005
49	-1213.22880052	0.004
44	-1213.22879895	0.004
52	-1213.22849731	0.003
42	-1213.22833287	0.003
43	-1213.22816362	0.002
33	-1213.22812894	0.002

Table S5. List of conformers obtained from DFT calculations for **1c**.

1E2R (1c)		
Conformer #	Gibbs Free Energy (Hartree)	Boltzmann Distribution
14	-1213.23921448	0.11
182	-1213.23909228	0.096
27	-1213.23902993	0.09
342	-1213.23863584	0.059
34	-1213.23857661	0.056
16	-1213.23844416	0.049
22	-1213.23832810	0.043
323	-1213.23832135	0.043
15	-1213.23831382	0.042
30	-1213.23827870	0.041
341	-1213.23826876	0.04
18	-1213.23826807	0.04
6	-1213.23815863	0.036
39	-1213.23796964	0.029
47	-1213.23781424	0.025
42	-1213.23775648	0.023
56	-1213.23770519	0.022
53	-1213.23760449	0.02

62	-1213.23753238	0.018
11	-1213.23751979	0.018
8	-1213.23736639	0.015
59	-1213.23719004	0.013
105	-1213.23716989	0.013
25	-1213.23695056	0.01
70	-1213.23645255	0.006
124	-1213.23603205	0.004
153	-1213.23601315	0.004
110	-1213.23593679	0.003
79	-1213.23592023	0.003
143	-1213.23588111	0.003
128	-1213.23586397	0.003
100	-1213.23569806	0.003
209	-1213.23566307	0.003
116	-1213.23547210	0.002
221	-1213.23545519	0.002
123	-1213.23541083	0.002
134	-1213.23540726	0.002
144	-1213.23539548	0.002
180	-1213.23539159	0.002
129	-1213.23535576	0.002
84	-1213.23523471	0.002

Table S6. List of conformers obtained from DFT calculations for **1d**.

1Z2R (1d)		
Conformer #	Gibbs Free Energy (Hartree)	Boltzmann Distribution
9	-1213.23457416	0.107
16	-1213.23448104	0.097
266	-1213.23418726	0.071
290	-1213.23394843	0.055
1	-1213.23392734	0.054
27	-1213.23389782	0.052
21	-1213.23387882	0.051
39	-1213.23375459	0.045
11	-1213.23372922	0.044
17	-1213.23371646	0.043
267	-1213.23364976	0.04
12	-1213.23360681	0.038
30	-1213.23325485	0.026

31	-1213.23325101	0.026
19	-1213.23324981	0.026
33	-1213.23323102	0.026
41	-1213.23319065	0.025
301	-1213.23309680	0.022
7	-1213.23297914	0.02
35	-1213.23295751	0.019
32	-1213.23295637	0.019
44	-1213.23286009	0.017
3	-1213.23277050	0.016
25	-1213.23225012	0.009
20	-1213.23217999	0.008
42	-1213.23174270	0.005
147	-1213.23159239	0.005
146	-1213.23133980	0.003
62	-1213.23124275	0.003
46	-1213.23123340	0.003
54	-1213.23117881	0.003
111	-1213.23115574	0.003
59	-1213.23112168	0.003
110	-1213.23104511	0.003
64	-1213.23100331	0.002
115	-1213.23098351	0.002
65	-1213.23089431	0.002
53	-1213.23088367	0.002
61	-1213.23086481	0.002

Standard Q factors and CSA weighted Q factors

Q factors were obtained by using the single tensor approach with RCSA fitting against the lowest energy conformer of each isomer.
However, it is known[4] that sp^2 carbons exhibit much larger RCSA than the sp^3 carbons. Since most of the carbon atoms used in the RCSA analysis are sp^3, but there are also a few sp^2 carbons, we decided to calculate a CSA-weighted Q factor, $Q_{(CSA)}$[4]. This was done in order to ensure that a few sp^2 carbons do not contribute disproportionally to the conventional RCSA analysis. $Q_{(CSA)}$ values are compensated for the difference in CSA between sp^2 and sp^3 carbons as illustrated by Eq.2 below.

$$Q_{(CSA)} = \sqrt{\frac{\Sigma\left(\left(\Delta RCSA_{i,ax}^{exp} - \Delta RCSA_{i}^{theo}\right)/CSA_{i,ax}\right)^2}{\Sigma\left(\Delta RCSA_{i,}^{exp}/CSA_{i,ax}\right)^2}} \qquad \textbf{Eq. 2}$$

A comparison of standard Q factors and $Q_{(CSA)}$ factors is summarized in Table S6.

Table S7. Measured Q and $Q_{(CSA)}$ factors using single tensor fitting.

	1a: 1E2S	1b: 1Z2S	1c: 1E2R	1d: 1Z2R
Q	0.196	0.138	0.097	0.234
Q(csa)	0.344	0.286	0.195	0.430

As evident from these results, $Q_{(CSA)}$ were also strongly indicating **1c** as the correct isomer with a $Q_{(CSA)}$ ratio between the lowest Q and the second best Q of 1.467, just slightly better than the corresponding ratio for standard Q, which is 1.423.

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Cartesian Coordinates of Conformers (>2% population) of 1a

Conf 11

C	0.918531	2.793860	2.086590
C	0.206318	2.322360	3.351590
C	1.012190	2.719620	4.537920
N	2.068610	3.483020	4.048080
C	2.013330	3.706320	2.678240
C	1.619480	1.586790	1.261820
C	0.081660	3.527840	0.986034
C	-0.941591	1.677550	3.628740
O	0.823752	2.476180	5.720410
O	2.732300	4.482990	2.081750
H	2.721300	3.964280	4.654530
H	-1.179400	1.498320	4.676620
O	-1.837100	1.211990	2.731630
C	-3.028980	0.601816	3.298770
H	-2.712650	-0.202973	3.972440
C	-3.885170	0.070082	2.166730
H	-3.560520	1.363330	3.880770
H	-4.779250	-0.404573	2.583150
H	-3.342430	-0.675926	1.579180

H	-4.207520	0.874150	1.498650
C	2.756860	2.110030	0.396977
C	2.081050	0.423989	2.149800
C	0.460491	1.156960	0.325319
C	-0.373298	2.409670	-0.022870
H	0.824643	4.137430	0.456332
C	-1.040430	4.507510	1.416240
H	-0.171347	2.747870	-1.042590
O	-1.769250	2.121880	-0.028022
H	-0.187415	0.452775	0.857615
H	0.835125	0.640506	-0.563463
H	2.463740	-0.390887	1.527630
H	2.879390	0.720342	2.838280
H	1.253510	0.026479	2.740700
C	3.998230	1.622350	0.318775
H	-1.996420	1.785270	0.851765
C	-0.558945	5.544850	2.454450
C	-1.599990	5.213340	0.164756
H	-1.857010	3.933060	1.870190
H	-2.443710	5.860800	0.418989
H	-1.956940	4.490590	-0.570956
H	-0.828608	5.840140	-0.301803
H	-0.123021	5.031100	3.318350
H	0.246592	6.147720	2.015540
C	-1.649170	6.495320	3.001470
C	-2.721100	5.789090	3.791230
H	-1.144870	7.213030	3.665830
H	-2.077300	7.091910	2.191630
C	-4.057790	5.880110	3.675260
C	-4.969850	5.103610	4.598120
C	-4.783240	6.743160	2.670530
H	-5.462300	6.135720	2.057380
H	-5.408420	7.486440	3.183510
H	-4.112810	7.280870	1.997810
H	-5.622020	5.779190	5.168120
H	-5.634770	4.438640	4.029520
H	-4.406090	4.497130	5.313480
H	-2.337130	5.132690	4.575610
H	4.716700	2.058050	-0.368937
H	4.352960	0.795527	0.925814
H	2.507680	2.948110	-0.249625

Conf 3

C	0.951519	2.874900	1.851100
C	0.399673	2.528100	3.228740
C	1.300900	3.071930	4.275950
N	2.261930	3.821490	3.600120
C	2.067220	3.878670	2.230860
C	1.623130	1.589020	1.063230
C	-0.002454	3.554020	0.789600
C	-0.704230	1.897970	3.669030
O	1.245110	2.949510	5.490070
O	2.684830	4.609340	1.479030
H	2.963980	4.372580	4.077990
H	-0.864877	1.817040	4.743090
O	-1.638610	1.331660	2.878600

C	-2.857280	0.886412	3.532060
H	-2.577350	0.275943	4.398720
C	-3.672460	0.091953	2.531140
H	-3.398620	1.772710	3.881280
H	-4.602760	-0.239519	3.003240
H	-3.124860	-0.791712	2.191030
H	-3.927080	0.700607	1.658890
C	3.139230	1.685740	0.994750
C	1.199430	0.243959	1.681050
C	1.037860	1.723790	-0.372869
C	-0.293973	2.472280	-0.272355
H	0.652046	4.269930	0.272470
C	-1.223030	4.360610	1.302530
H	-0.537702	2.935140	-1.233320
O	-1.407450	1.625450	0.015473
H	0.917776	0.747266	-0.851149
H	1.718730	2.315820	-0.996315
H	1.632190	-0.567462	1.088190
H	1.545660	0.132246	2.711920
H	0.118022	0.113393	1.670350
C	4.032160	0.847253	1.530920
H	-1.479280	1.484070	0.971623
C	-0.779882	5.566400	2.161930
C	-2.084980	4.824250	0.112344
H	-1.845990	3.709850	1.926650
H	-2.947170	5.404180	0.453031
H	-2.468940	3.973140	-0.454790
H	-1.505220	5.461980	-0.567556
H	-0.095483	5.230590	2.948990
H	-0.202615	6.256040	1.531200
C	-1.914580	6.358270	2.850940
C	-2.652680	5.570840	3.903090
H	-1.449240	7.228950	3.336850
H	-2.600980	6.768420	2.105320
C	-3.978350	5.409540	4.064060
C	-4.525810	4.614940	5.228480
C	-5.038360	5.996730	3.162660
H	-4.628650	6.540290	2.309540
H	-5.698220	5.208520	2.776120
H	-5.679070	6.690040	3.724160
H	-5.170830	5.239110	5.861650
H	-5.151650	3.780600	4.881390
H	-3.728060	4.209850	5.858310
H	-2.003740	5.099060	4.644280
H	5.096000	1.015760	1.391420
H	3.755170	-0.023573	2.116800
H	3.514730	2.532120	0.423991

Conf 30

C	0.770960	2.672740	2.105250
C	-0.116381	2.027410	3.169480
C	0.354194	2.453560	4.516550
N	1.360500	3.388850	4.294630
C	1.568020	3.686070	2.954600
C	1.785410	1.624240	1.399700
C	0.095376	3.345180	0.864515

C	-1.198070	1.226240	3.181770
O	-0.037065	2.106950	5.620720
O	2.286250	4.584300	2.560600
H	1.783220	3.923100	5.043900
H	-1.609110	0.956156	4.153880
O	-1.836790	0.711005	2.109340
C	-2.997300	-0.111881	2.409820
H	-2.672380	-0.938279	3.052440
C	-3.579120	-0.620521	1.106000
H	-3.720490	0.500994	2.960360
H	-4.446140	-1.253250	1.320300
H	-2.847160	-1.216750	0.553767
H	-3.909610	0.204704	0.468335
C	3.018900	2.329720	0.849668
C	2.290850	0.522877	2.352300
C	0.883973	1.061020	0.287874
C	-0.003552	2.214620	-0.227017
H	0.861130	4.045170	0.507663
C	-1.202040	4.168630	1.060110
H	0.368657	2.608350	-1.175750
O	-1.322140	1.769420	-0.534782
H	0.232713	0.292604	0.715636
H	1.457380	0.575432	-0.506509
H	2.917740	-0.180611	1.795120
H	2.902640	0.935152	3.162560
H	1.464430	-0.036603	2.798930
C	3.394740	2.440030	-0.427391
H	-1.685360	1.365950	0.267555
C	-1.094950	5.191190	2.212590
C	-1.559740	4.866960	-0.267351
H	-2.020280	3.478040	1.305830
H	-2.517030	5.391370	-0.196899
H	-1.644490	4.146000	-1.082530
H	-0.793172	5.607370	-0.530511
H	-0.820654	4.678130	3.140010
H	-0.283376	5.899790	1.999180
C	-2.393820	5.974290	2.505680
C	-2.242100	6.896060	3.687800
H	-2.664290	6.576860	1.628980
H	-3.215870	5.265440	2.657250
C	-2.884030	6.865240	4.869000
C	-2.578650	7.884480	5.942920
C	-3.943030	5.859040	5.253010
H	-3.640980	5.308180	6.153710
H	-4.885580	6.366360	5.499250
H	-4.151290	5.129390	4.468080
H	-3.477450	8.456380	6.211080
H	-2.234070	7.394640	6.863810
H	-1.807750	8.592650	5.625420
H	-1.495190	7.680560	3.550680
H	4.327830	2.932260	-0.684763
H	2.806020	2.063690	-1.258590
H	3.680680	2.746640	1.605520

Conf 32

C	0.706019	2.634220	2.107080

C	-0.135753	1.822330	3.088040
C	0.326228	2.108430	4.474210
N	1.286340	3.109940	4.361580
C	1.459900	3.579670	3.066020
C	1.779890	1.733800	1.292110
C	-0.022531	3.422860	0.968419
C	-1.165470	0.961674	2.993740
O	-0.039851	1.614640	5.530120
O	2.115050	4.560130	2.774800
H	1.694870	3.567070	5.167520
H	-1.563890	0.547762	3.919310
O	-1.761060	0.544695	1.854950
C	-2.873730	-0.374025	2.033640
H	-2.508950	-1.249070	2.583860
C	-3.404850	-0.761632	0.668029
H	-3.640880	0.127353	2.635180
H	-4.234930	-1.464560	0.789948
H	-2.630370	-1.246450	0.066838
H	-3.775920	0.110822	0.122131
C	2.941560	2.586260	0.802953
C	2.274700	0.510339	2.074450
C	0.937917	1.313160	0.059453
C	-0.038684	2.461450	-0.276848
H	0.675110	4.233760	0.724142
C	-1.378400	4.109300	1.273150
H	0.292407	3.016250	-1.158590
O	-1.321810	1.963630	-0.647797
H	0.347810	0.426766	0.314746
H	1.575860	1.041990	-0.786995
H	2.925740	-0.099148	1.440230
H	2.846190	0.791720	2.965150
H	1.440660	-0.118900	2.391250
C	4.244670	2.325170	0.939776
H	-1.647810	1.428850	0.091567
C	-1.341010	4.973050	2.552930
C	-1.803310	4.953370	0.054478
H	-2.138540	3.330810	1.422620
H	-2.797210	5.386650	0.199121
H	-1.099680	5.781170	-0.103554
H	-1.842230	4.348150	-0.852959
H	-1.026310	4.357900	3.402790
H	-0.585739	5.762630	2.447670
C	-2.693800	5.614520	2.933940
C	-2.667560	6.220780	4.313030
H	-2.983330	6.358260	2.187640
H	-3.469020	4.832640	2.906080
C	-2.808440	7.510260	4.667530
C	-2.743700	7.924840	6.119760
C	-3.039190	8.651920	3.706150
H	-3.062940	8.340460	2.660220
H	-3.988240	9.158060	3.928850
H	-2.250760	9.408690	3.813580
H	-1.933450	8.647420	6.287160
H	-3.673400	8.421360	6.429510
H	-2.578630	7.069450	6.781320
H	-2.498760	5.502300	5.117860

H	4.986000	2.992780	0.511190
H	4.626540	1.464050	1.478830
H	2.666990	3.482740	0.252102

Conf 43

C	0.733188	2.601530	2.200330
C	-0.139667	1.779510	3.148280
C	0.266635	2.065190	4.552030
N	1.218530	3.077680	4.478840
C	1.443640	3.547690	3.192000
C	1.828610	1.709320	1.406360
C	0.048549	3.381580	1.029630
C	-1.169530	0.921089	3.026680
O	-0.133256	1.565660	5.592830
O	2.115950	4.526940	2.933800
H	1.589200	3.538670	5.300820
H	-1.589740	0.511091	3.944420
O	-1.744370	0.503300	1.878600
C	-2.868270	-0.405524	2.038280
H	-2.523530	-1.278140	2.604960
C	-3.368560	-0.801136	0.663382
H	-3.645690	0.107321	2.616440
H	-4.206710	-1.496800	0.770932
H	-2.583050	-1.296630	0.085717
H	-3.719330	0.069236	0.101026
C	3.030450	2.547700	0.988684
C	2.375330	0.529336	2.233770
C	0.993475	1.237150	0.204084
C	0.049966	2.391980	-0.195352
H	0.776821	4.165640	0.787684
C	-1.303900	4.093090	1.281150
H	0.422312	2.922050	-1.075170
O	-1.229450	1.912010	-0.600758
H	0.380175	0.384814	0.512207
H	1.616720	0.888485	-0.623968
H	3.058280	-0.062684	1.616170
H	2.939480	0.872497	3.108280
H	1.573150	-0.127492	2.580940
C	3.430900	2.839060	-0.251880
H	-1.587410	1.389510	0.132238
C	-1.300930	4.964620	2.555930
C	-1.669620	4.933250	0.040877
H	-2.082760	3.328780	1.407800
H	-2.662060	5.381810	0.143123
H	-0.947705	5.748650	-0.097025
H	-1.682300	4.320440	-0.862350
H	-1.034420	4.347550	3.421260
H	-0.525926	5.737890	2.477690
C	-2.654710	5.635940	2.877370
C	-2.673120	6.251240	4.252540
H	-2.897720	6.380230	2.115170
H	-3.444220	4.869970	2.822070
C	-2.800810	7.545910	4.592870
C	-2.788180	7.969450	6.043920
C	-2.966240	8.685380	3.615540
H	-2.950840	8.367260	2.571480

H	-3.913540	9.212060	3.793650
H	-2.167880	9.426790	3.752600
H	-1.969770	8.675160	6.241000
H	-3.718770	8.488620	6.310960
H	-2.670410	7.115410	6.717280
H	-2.553820	5.535150	5.068350
H	4.338400	3.412450	-0.415760
H	2.887080	2.537190	-1.141930
H	3.646280	2.903500	1.811630

Conf 22

C	0.975189	2.743320	2.151270
C	0.216806	2.181640	3.354290
C	0.928668	2.566600	4.602170
N	1.974900	3.395970	4.208510
C	1.998670	3.666440	2.847050
C	1.748390	1.606930	1.292730
C	0.170797	3.490060	1.034720
C	-0.907058	1.465600	3.547280
O	0.682111	2.268050	5.761370
O	2.735730	4.483930	2.330510
H	2.566940	3.880570	4.871930
H	-1.181510	1.228450	4.574610
O	-1.728330	0.985689	2.591040
C	-2.911710	0.276408	3.047390
H	-3.183330	-0.365548	2.206380
C	-4.039490	1.228700	3.409660
H	-2.627130	-0.362073	3.891420
H	-4.922990	0.652198	3.704500
H	-4.307990	1.858750	2.556960
H	-3.763140	1.877740	4.246010
C	2.938470	2.191810	0.541786
C	2.292380	0.451076	2.155330
C	0.625225	1.145990	0.347166
C	-0.228433	2.382400	-0.009780
H	0.934906	4.105520	0.543240
C	-0.979043	4.448380	1.435090
H	0.002363	2.747520	-1.013400
O	-1.617330	2.066340	-0.072204
H	-0.011942	0.430427	0.875225
H	1.012390	0.625863	-0.533211
H	2.745980	-0.305039	1.506540
H	3.067290	0.792469	2.850970
H	1.499770	-0.028903	2.735600
C	3.103920	2.286010	-0.780345
H	-1.864200	1.685840	0.783961
C	-0.547369	5.470480	2.509910
C	-1.496240	5.167920	0.173489
H	-1.807500	3.857350	1.845030
H	-2.364800	5.791770	0.401676
H	-1.804250	4.452210	-0.590742
H	-0.718071	5.818720	-0.246451
H	-0.189941	4.939360	3.399770
H	0.305024	6.049840	2.132750
C	-1.639700	6.456690	2.982800
C	-2.794930	5.793610	3.687610

H	-1.157900	7.151470	3.687350
H	-1.982440	7.073720	2.148050
C	-4.114700	5.964310	3.493820
C	-5.124940	5.229250	4.345310
C	-4.726350	6.885420	2.465130
H	-3.986410	7.387870	1.839650
H	-5.407080	6.330960	1.805450
H	-5.331020	7.660590	2.955060
H	-5.771380	5.934110	4.885640
H	-5.789780	4.610950	3.726440
H	-4.642310	4.581550	5.083400
H	-2.497310	5.103290	4.480430
H	4.026570	2.684900	-1.191260
H	2.348130	1.987160	-1.500480
H	3.757530	2.525420	1.174900

Conf 9

C	0.893750	2.746060	2.116000
C	0.051640	2.289040	3.306980
C	0.706396	2.739330	4.565320
N	1.787740	3.525220	4.176430
C	1.889040	3.704960	2.803850
C	1.698840	1.534570	1.402050
C	0.176367	3.413980	0.896149
C	-1.114110	1.639510	3.483810
O	0.394753	2.519230	5.726020
O	2.664430	4.478090	2.275190
H	2.351430	4.044200	4.838530
H	-1.453870	1.492620	4.508320
O	-1.917650	1.140470	2.520860
C	-3.147960	0.524946	2.992120
H	-2.882480	-0.273294	3.694870
C	-3.904020	-0.019974	1.796790
H	-3.730760	1.285890	3.523630
H	-4.826400	-0.498364	2.140910
H	-3.309720	-0.765649	1.261020
H	-4.174950	0.777691	1.098840
C	2.942470	2.041450	0.682182
C	2.167690	0.444969	2.386410
C	0.626127	1.015220	0.429918
C	-0.166956	2.234040	-0.088837
H	0.977627	3.988260	0.414391
C	-0.989400	4.402040	1.149690
H	0.150005	2.513920	-1.096260
O	-1.553350	1.937660	-0.235702
H	-0.063516	0.366071	0.978252
H	1.051800	0.408247	-0.373844
H	2.644330	-0.367991	1.829410
H	2.906100	0.830382	3.098460
H	1.332230	0.025954	2.953770
C	3.193400	2.016510	-0.629561
H	-1.876920	1.637690	0.626764
C	-0.636165	5.480220	2.197990
C	-1.400660	5.049860	-0.187533
H	-1.848680	3.834210	1.526580
H	-2.275430	5.695780	-0.066011

H	-0.584851	5.668790	-0.583101
H	-1.657580	4.292740	-0.930588
H	-0.370556	4.996660	3.144140
H	0.253169	6.029620	1.862050
C	-1.751080	6.506800	2.518550
C	-3.038880	5.899730	3.015640
H	-1.349240	7.211780	3.253450
H	-1.964550	7.103040	1.622350
C	-3.517620	5.879710	4.272940
C	-4.845920	5.229640	4.587110
C	-2.822570	6.480530	5.471560
H	-1.874120	6.961250	5.225050
H	-3.465070	7.227910	5.956170
H	-2.619440	5.708140	6.225180
H	-4.728400	4.428400	5.329800
H	-5.545840	5.955200	5.023430
H	-5.313640	4.804560	3.693800
H	-3.651400	5.420460	2.250520
H	4.145840	2.369630	-1.013460
H	2.481030	1.660590	-1.367730
H	3.723780	2.423190	1.335570

Conf 19

C	0.744944	2.696930	2.011550
C	-0.111163	2.057810	3.101860
C	0.408178	2.477390	4.432840
N	1.418230	3.400820	4.178770
C	1.577920	3.703670	2.832850
C	1.742780	1.644460	1.286820
C	0.028584	3.385380	0.802331
C	-1.189230	1.253850	3.136000
O	0.048724	2.132160	5.548220
O	2.276490	4.603550	2.411120
H	1.873600	3.926710	4.914620
H	-1.581210	0.976619	4.113860
O	-1.841460	0.739532	2.070170
C	-3.000480	-0.079932	2.384270
H	-2.673520	-0.898842	3.035430
C	-3.587400	-0.604316	1.088940
H	-3.721940	0.539204	2.930150
H	-4.453800	-1.234080	1.314240
H	-2.857790	-1.207800	0.541429
H	-3.920370	0.212867	0.442245
C	2.933800	2.363830	0.670671
C	2.193570	0.497042	2.199960
C	0.841928	1.129040	0.134414
C	-0.079568	2.283980	-0.315724
H	0.763886	4.117280	0.445104
C	-1.275580	4.185520	1.052060
H	0.254315	2.708280	-1.266190
O	-1.399250	1.821560	-0.592128
H	0.211956	0.315484	0.509043
H	1.438040	0.721727	-0.687614
H	2.790350	-0.220980	1.629110
H	2.806890	0.849628	3.035790
H	1.336490	-0.040022	2.610950

C	4.224260	2.045690	0.806586
H	-1.730830	1.399150	0.214445
C	-1.142200	5.196020	2.212750
C	-1.689730	4.896380	-0.252226
H	-2.073380	3.478860	1.317070
H	-2.650750	5.406250	-0.139741
H	-1.793960	4.186110	-1.074330
H	-0.943948	5.652120	-0.531460
H	-0.823059	4.678270	3.122620
H	-0.352051	5.921650	1.976710
C	-2.442440	5.952170	2.564720
C	-2.261230	6.864150	3.750330
H	-2.758110	6.558730	1.706090
H	-3.244830	5.226580	2.740530
C	-2.855390	6.808380	4.955340
C	-2.526830	7.821630	6.028060
C	-3.878950	5.777740	5.369300
H	-3.529730	5.221820	6.249570
H	-4.819700	6.264140	5.660460
H	-4.105840	5.053840	4.584220
H	-3.424850	8.373260	6.337990
H	-2.136950	7.328500	6.928870
H	-1.782460	8.547760	5.688610
H	-1.535060	7.664140	3.592980
H	4.987480	2.613450	0.283049
H	4.574800	1.234060	1.436100
H	2.691750	3.202850	0.022596

Conf 35

C	0.969321	2.733640	2.148370
C	0.209811	2.242480	3.380670
C	0.959359	2.636450	4.603420
N	2.025490	3.417540	4.166170
C	2.031260	3.647500	2.796810
C	1.694780	1.540750	1.326280
C	0.173351	3.462840	1.014680
C	-0.949646	1.599390	3.614090
O	0.725699	2.379060	5.775020
O	2.782030	4.426620	2.242270
H	2.645250	3.901860	4.804020
H	-1.221380	1.414050	4.652710
O	-1.830110	1.168100	2.687770
C	-2.992410	0.452449	3.183910
H	-3.357100	0.962283	4.082800
C	-2.681380	-1.012170	3.447360
H	-3.740990	0.566315	2.396740
H	-3.591130	-1.526120	3.775820
H	-1.926480	-1.126840	4.231620
H	-2.318880	-1.501920	2.538930
C	2.889180	2.057840	0.533863
C	2.217700	0.404534	2.227120
C	0.541959	1.078760	0.418812
C	-0.266175	2.330000	0.012323
H	0.947126	4.042340	0.495567
C	-0.949921	4.459840	1.394800
H	-0.020834	2.646650	-1.004150

O	-1.664900	2.061290	-0.042270
H	-0.116343	0.417693	0.990482
H	0.894562	0.500227	-0.439469
H	2.633990	-0.392638	1.602950
H	3.016530	0.748623	2.893720
H	1.421090	-0.023731	2.841460
C	3.040110	2.081890	-0.793153
H	-1.933270	1.751130	0.835518
C	-0.496608	5.498330	2.444190
C	-1.452290	5.161420	0.117038
H	-1.791310	3.899760	1.821180
H	-2.300910	5.816680	0.332013
H	-0.657112	5.777850	-0.322352
H	-1.784670	4.435530	-0.627185
H	-0.113056	4.983560	3.332430
H	0.340971	6.080320	2.038600
C	-1.590950	6.476310	2.930900
C	-2.717130	5.799530	3.669110
H	-1.104350	7.187130	3.615640
H	-1.963910	7.076730	2.096970
C	-4.043840	5.921250	3.486480
C	-5.018850	5.169140	4.363970
C	-4.697570	6.796450	2.443760
H	-5.330100	7.556420	2.922170
H	-3.981840	7.315280	1.803640
H	-5.358970	6.201930	1.799470
H	-4.505850	4.553780	5.109280
H	-5.684690	5.861400	4.897020
H	-5.667220	4.515450	3.764210
H	-2.388350	5.136860	4.473100
H	3.967210	2.435930	-1.234040
H	2.268070	1.766900	-1.488740
H	3.724370	2.401240	1.140130

Conf 13

C	0.934682	2.767310	2.062750
C	0.207489	2.215540	3.286720
C	0.960734	2.593510	4.511970
N	2.008400	3.405160	4.085490
C	1.989750	3.679490	2.724080
C	1.684990	1.623290	1.192930
C	0.102649	3.534440	0.980114
C	-0.909644	1.496090	3.498610
O	0.742843	2.299560	5.678110
O	2.706820	4.496420	2.181390
H	2.628350	3.880060	4.730060
H	-1.169370	1.252970	4.528250
O	-1.738240	1.015240	2.547930
C	-2.911970	0.296130	3.013370
H	-3.191400	-0.340084	2.170550
C	-4.040250	1.238780	3.398760
H	-2.613250	-0.348274	3.848010
H	-3.757040	1.881640	4.237560
H	-4.916790	0.654660	3.699340
H	-4.322990	1.875230	2.555440
C	2.831550	2.218290	0.388249

C	2.153080	0.425661	2.029960
C	0.563526	1.215160	0.200485
C	-0.310835	2.456300	-0.086610
H	0.844124	4.179650	0.491802
C	-1.043420	4.477120	1.430160
H	-0.116578	2.853900	-1.086150
O	-1.697480	2.125300	-0.114608
H	-0.068112	0.451874	0.666121
H	0.979677	0.775107	-0.710622
H	2.574350	-0.344088	1.376070
H	2.923990	0.704223	2.756160
H	1.320850	-0.024429	2.574510
C	4.086980	1.766330	0.320738
H	-1.914110	1.726360	0.741682
C	-0.584365	5.485900	2.506580
C	-1.604430	5.213590	0.197379
H	-1.853760	3.873070	1.856290
H	-2.468120	5.828700	0.464044
H	-0.843998	5.876550	-0.236123
H	-1.933280	4.509130	-0.568455
H	-0.195492	4.944830	3.376680
H	0.252159	6.076450	2.111310
C	-1.667300	6.458300	3.027310
C	-2.799080	5.777590	3.753050
H	-1.168510	7.143110	3.729730
H	-2.036560	7.088030	2.213630
C	-4.124530	5.944260	3.598110
C	-5.107320	5.189980	4.464790
C	-4.768990	6.878140	2.601420
H	-4.049460	7.394340	1.963380
H	-5.465270	6.330450	1.952410
H	-5.363450	7.642360	3.120180
H	-5.742980	5.882410	5.033230
H	-5.784990	4.577340	3.854300
H	-4.601360	4.533910	5.179460
H	-2.476230	5.076370	4.526090
H	4.811830	2.254040	-0.324002
H	4.447080	0.919081	0.895579
H	2.577730	3.081240	-0.222877

Conf 20

C	0.932658	2.756160	2.054940
C	0.207974	2.275400	3.309500
C	1.003180	2.658030	4.506540
N	2.068600	3.419790	4.033850
C	2.027820	3.655850	2.665440
C	1.632470	1.554910	1.221630
C	0.107449	3.506720	0.956131
C	-0.946652	1.634450	3.566390
O	0.802402	2.403660	5.684930
O	2.757300	4.433380	2.083030
H	2.718440	3.891490	4.650770
H	-1.200740	1.444280	4.608490
O	-1.840730	1.206870	2.650180
C	-2.996540	0.490667	3.160150
H	-3.348870	0.998267	4.065210

C	-2.683320	-0.974940	3.415690
H	-3.756030	0.606864	2.383770
H	-3.589050	-1.489020	3.754900
H	-1.918150	-1.092350	4.189510
H	-2.333360	-1.462690	2.501270
C	2.777430	2.081440	0.368636
C	2.084030	0.381100	2.100150
C	0.477134	1.140410	0.273537
C	-0.347117	2.401380	-0.067787
H	0.857691	4.117190	0.437791
C	-1.011910	4.489060	1.387730
H	-0.134453	2.748640	-1.082260
O	-1.744870	2.122910	-0.088617
H	-0.178734	0.434920	0.794018
H	0.854863	0.630875	-0.617931
H	2.464660	-0.430138	1.471970
H	2.881170	0.666529	2.794630
H	1.251840	-0.016653	2.684160
C	4.016680	1.588100	0.292199
H	-1.985430	1.795630	0.791294
C	-0.532208	5.511860	2.441130
C	-1.556190	5.211870	0.139212
H	-1.836130	3.915660	1.828830
H	-2.399310	5.860160	0.393097
H	-0.777443	5.840260	-0.312760
H	-1.909610	4.499210	-0.607951
H	-0.111519	4.985350	3.304900
H	0.284182	6.111040	2.017430
C	-1.619210	6.468050	2.984700
C	-2.711960	5.763960	3.747260
H	-1.116500	7.170160	3.666690
H	-2.027040	7.081110	2.176700
C	-4.045370	5.869240	3.608300
C	-4.981260	5.088800	4.503430
C	-4.744190	6.751460	2.601380
H	-5.417560	6.158010	1.968610
H	-5.371580	7.494450	3.112110
H	-4.056520	7.290830	1.947630
H	-5.640760	5.762290	5.067430
H	-5.637810	4.434280	3.913510
H	-4.436180	4.470300	5.222900
H	-2.348590	5.093720	4.529770
H	4.741260	2.027210	-0.386868
H	4.363780	0.753116	0.892446
H	2.536370	2.927540	-0.270536

Conf 31

C	0.692070	2.732860	1.936640
C	-0.002412	2.001220	3.079420
C	0.633408	2.378170	4.368410
N	1.555140	3.376520	4.061290
C	1.563830	3.740080	2.725680
C	1.671560	1.762100	1.028620
C	-0.180318	3.531150	0.888082
C	-1.042190	1.151860	3.161940
O	0.415232	1.957560	5.494100

O	2.165340	4.697980	2.277830
H	2.078340	3.876790	4.769050
H	-1.342280	0.790506	4.144490
O	-1.751610	0.691984	2.110080
C	-2.913160	-0.122580	2.420880
H	-2.592770	-0.940007	3.077380
C	-3.490850	-0.645801	1.120990
H	-3.635390	0.501734	2.959870
H	-4.375190	-1.253810	1.336210
H	-2.765030	-1.269120	0.590948
H	-3.789160	0.175520	0.463367
C	3.145590	2.047960	1.269520
C	1.373040	0.267519	1.246800
C	1.303600	2.171090	-0.427490
C	-0.128607	2.711810	-0.418930
H	0.423454	4.423980	0.673060
C	-1.578400	4.036120	1.325240
H	-0.289969	3.360490	-1.285070
O	-1.126610	1.696400	-0.535485
H	1.415360	1.332330	-1.120870
H	1.971110	2.972180	-0.767225
H	2.015000	-0.319915	0.583516
H	1.567230	-0.049946	2.274650
H	0.340644	0.018965	1.003680
C	4.064590	1.214050	1.767350
H	-1.323140	1.320340	0.335738
C	-1.486100	5.014110	2.518020
C	-2.301660	4.688630	0.130887
H	-2.180560	3.176030	1.644370
H	-3.290400	5.054840	0.421746
H	-1.731160	5.544860	-0.251489
H	-2.444920	3.976380	-0.685073
H	-0.898078	4.560600	3.323140
H	-0.936872	5.914550	2.211110
C	-2.845200	5.429880	3.122050
C	-2.687200	6.193030	4.411540
H	-3.422000	6.008360	2.396070
H	-3.428580	4.517160	3.321320
C	-3.037130	7.462130	4.685700
C	-2.787990	8.054710	6.053810
C	-3.693560	8.409380	3.709580
H	-3.845290	7.976060	2.719210
H	-4.671520	8.736440	4.087780
H	-3.087450	9.317200	3.589950
H	-2.140190	8.939320	5.987770
H	-3.727200	8.389550	6.514850
H	-2.314980	7.336370	6.729640
H	-2.213920	5.625550	5.215370
H	5.097370	1.533930	1.870450
H	3.840250	0.200897	2.085920
H	3.467870	3.045250	0.978564

Conf 1

C	0.812863	2.873830	1.865730
C	0.077494	2.494000	3.145760
C	0.848977	2.970920	4.321410

N	1.907610	3.716250	3.805780
C	1.893800	3.829870	2.426650
C	1.549060	1.596190	1.122880
C	0.026025	3.618760	0.715125
C	-1.088880	1.881460	3.416310
O	0.635168	2.803440	5.512410
O	2.621760	4.569120	1.790780
H	2.555500	4.227710	4.391870
H	-1.386560	1.765620	4.457220
O	-1.932540	1.379070	2.491290
C	-3.208950	0.888318	2.980870
H	-3.013620	0.173016	3.788460
C	-3.944280	0.237021	1.826540
H	-3.768020	1.738530	3.387760
H	-4.915120	-0.128806	2.175470
H	-3.379420	-0.610983	1.428840
H	-4.116190	0.950567	1.015740
C	3.062870	1.648780	1.256670
C	1.012740	0.243908	1.626970
C	1.161680	1.798890	-0.371036
C	-0.151652	2.584410	-0.416477
H	0.761720	4.331560	0.316626
C	-1.230060	4.444190	1.093990
H	-0.254449	3.087430	-1.382640
O	-1.315740	1.763730	-0.309144
H	1.080290	0.843837	-0.898306
H	1.933820	2.391090	-0.876868
H	1.497580	-0.559127	1.063730
H	1.217930	0.084812	2.688840
H	-0.061162	0.148158	1.470590
C	3.856110	0.763062	1.868330
H	-1.517430	1.591540	0.623025
C	-0.874508	5.586950	2.072350
C	-1.903800	4.993360	-0.178145
H	-1.948730	3.782010	1.589630
H	-2.794480	5.578890	0.067936
H	-1.221150	5.650420	-0.732440
H	-2.218880	4.184160	-0.841024
H	-0.390926	5.169220	2.961530
H	-0.134615	6.243490	1.593500
C	-2.054000	6.460920	2.565580
C	-3.158580	5.699060	3.254700
H	-1.641700	7.225690	3.231780
H	-2.481510	7.008630	1.716170
C	-3.410220	5.613560	4.573730
C	-4.581490	4.809250	5.090130
C	-2.592780	6.282260	5.653020
H	-1.770510	6.883790	5.261280
H	-3.226230	6.934130	6.269280
H	-2.163670	5.531810	6.329890
H	-4.247990	4.023660	5.782150
H	-5.275840	5.444710	5.656280
H	-5.143480	4.338120	4.277570
H	-3.833030	5.156840	2.590030
H	4.933000	0.903946	1.875530
H	3.482600	-0.120853	2.375780

H	3.531420	2.504640	0.775891

Conf 5

C	0.855338	2.769340	2.025910
C	0.044604	2.317900	3.238010
C	0.743498	2.754070	4.477330
N	1.825910	3.523510	4.058770
C	1.883230	3.713340	2.684350
C	1.640480	1.552830	1.296260
C	0.106522	3.461290	0.838281
C	-1.116240	1.667130	3.434790
O	0.462141	2.533140	5.645650
O	2.639360	4.486680	2.130880
H	2.419570	4.027940	4.705620
H	-1.439210	1.511590	4.463360
O	-1.930980	1.171220	2.478410
C	-3.157160	0.556885	2.961490
H	-2.886120	-0.235747	3.668490
C	-3.919810	0.001545	1.775160
H	-3.738180	1.320620	3.491010
H	-4.839200	-0.475678	2.128770
H	-3.327720	-0.747458	1.241530
H	-4.196770	0.793158	1.072670
C	2.839010	2.071900	0.515590
C	2.042170	0.421147	2.251070
C	0.570424	1.079890	0.278307
C	-0.246339	2.310100	-0.174368
H	0.883712	4.068610	0.357424
C	-1.061180	4.434080	1.144700
H	0.037766	2.623940	-1.182200
O	-1.633220	2.001910	-0.289699
H	-0.111344	0.380966	0.774137
H	1.025290	0.544875	-0.560649
H	2.484820	-0.404385	1.685240
H	2.777590	0.747404	2.993960
H	1.173990	0.027629	2.783380
C	4.089190	1.602260	0.554126
H	-1.928580	1.681050	0.575662
C	-0.682596	5.496540	2.200580
C	-1.518410	5.103800	-0.166569
H	-1.903180	3.851750	1.537440
H	-2.393200	5.740560	-0.004615
H	-0.720344	5.737620	-0.574894
H	-1.793160	4.359560	-0.916037
H	-0.382037	4.999290	3.128660
H	0.191111	6.059110	1.845520
C	-1.794400	6.508320	2.574400
C	-3.062100	5.882820	3.099610
H	-1.374810	7.202470	3.309660
H	-2.039800	7.119670	1.696740
C	-3.500660	5.835080	4.370750
C	-4.814960	5.171160	4.713470
C	-2.771080	6.415880	5.558600
H	-1.833110	6.906360	5.292100
H	-3.401600	7.149980	6.077950
H	-2.540480	5.629740	6.289690

H	-4.669950	4.356590	5.436510
H	-5.504660	5.884060	5.185430
H	-5.308250	4.760680	3.827090
H	-3.696070	5.415280	2.344750
H	4.856650	2.031900	-0.082570
H	4.403210	0.796662	1.210160
H	2.633550	2.889440	-0.171445

Conf 6

C	0.956428	2.830980	1.936310
C	0.368856	2.524860	3.308710
C	1.253080	3.081540	4.363100
N	2.250410	3.787980	3.691740
C	2.083190	3.822410	2.313780
C	1.618250	1.530480	1.181390
C	0.038026	3.510120	0.841534
C	-0.754838	1.919590	3.734020
O	1.163710	2.995740	5.578650
O	2.729880	4.523240	1.561530
H	2.936970	4.355070	4.173830
H	-0.944092	1.862710	4.804960
O	-1.678360	1.354550	2.930280
C	-2.913200	0.925592	3.563930
H	-2.655610	0.310416	4.434180
C	-3.722950	0.143196	2.549210
H	-3.448160	1.818750	3.905410
H	-4.664600	-0.177147	3.006230
H	-3.181540	-0.746841	2.215890
H	-3.956310	0.756458	1.674240
C	3.132080	1.493340	1.306260
C	1.137920	0.188108	1.791100
C	1.108600	1.672020	-0.272123
C	-0.226564	2.419690	-0.217318
H	0.713631	4.214920	0.337140
C	-1.188460	4.332610	1.311580
H	-0.443628	2.872520	-1.189360
O	-1.348950	1.576350	0.050297
H	1.007770	0.703601	-0.770809
H	1.807750	2.281480	-0.855319
H	1.577190	-0.628177	1.209810
H	1.468800	0.074176	2.827690
H	0.054292	0.075075	1.759020
C	4.026470	1.366640	0.323743
H	-1.460550	1.464810	1.006370
C	-0.754601	5.549090	2.160760
C	-2.017840	4.783230	0.093634
H	-1.831550	3.697910	1.931550
H	-2.883860	5.374340	0.404209
H	-2.393640	3.925700	-0.469379
H	-1.417280	5.406040	-0.581959
H	-0.089444	5.221210	2.967590
H	-0.158624	6.223690	1.531120
C	-1.897540	6.360950	2.811750
C	-2.664320	5.597360	3.860980
H	-1.436170	7.236420	3.292800
H	-2.564510	6.763290	2.044490

C	-3.994320	5.446750	3.994320
C	-4.573300	4.677690	5.160670
C	-5.029680	6.023020	3.057870
H	-5.677840	6.731620	3.591000
H	-4.597090	6.546700	2.203590
H	-5.686330	5.231720	2.672170
H	-5.228730	5.317590	5.766880
H	-5.196280	3.840520	4.815240
H	-3.792750	4.280110	5.816330
H	-2.035410	5.136140	4.625700
H	5.086690	1.292000	0.546146
H	3.749690	1.338890	-0.725709
H	3.501860	1.492780	2.333230

Conf 2

C	0.803933	2.825890	1.951240
C	0.026351	2.486140	3.217370
C	0.771293	2.976190	4.404200
N	1.867640	3.677930	3.904240
C	1.891510	3.769330	2.519290
C	1.530920	1.534190	1.242120
C	0.064358	3.572270	0.768577
C	-1.158260	1.898120	3.462670
O	0.516166	2.845790	5.592020
O	2.651750	4.478820	1.891550
H	2.495360	4.205780	4.498070
H	-1.490600	1.805720	4.495410
O	-1.982160	1.397450	2.519370
C	-3.275440	0.922135	2.978860
H	-3.107880	0.204617	3.790720
C	-3.990920	0.279199	1.807510
H	-3.834050	1.778870	3.372500
H	-4.973440	-0.076319	2.133670
H	-3.426190	-0.574672	1.422400
H	-4.136480	0.994831	0.993402
C	3.011470	1.446930	1.571810
C	0.937777	0.185429	1.725510
C	1.229970	1.743390	-0.260619
C	-0.080255	2.529690	-0.359070
H	0.821509	4.273230	0.390647
C	-1.193460	4.415130	1.098070
H	-0.149432	3.023660	-1.332850
O	-1.250830	1.713250	-0.281279
H	1.173920	0.797079	-0.806582
H	2.018060	2.351480	-0.718351
H	1.431430	-0.621775	1.176050
H	1.120780	0.022777	2.791810
H	-0.133881	0.107409	1.542000
C	4.030220	1.331260	0.717359
H	-1.496560	1.570520	0.645068
C	-0.851182	5.570140	2.066880
C	-1.824950	4.951130	-0.201018
H	-1.933500	3.769860	1.584300
H	-2.715820	5.549620	0.010898
H	-1.119920	5.592270	-0.745797
H	-2.129640	4.134900	-0.860226

H	-0.390289	5.162790	2.972870
H	-0.095661	6.213450	1.594400
C	-2.034530	6.460170	2.520360
C	-3.157920	5.717440	3.200310
H	-1.630690	7.233710	3.181730
H	-2.440970	6.995840	1.653240
C	-3.422080	5.639290	4.517330
C	-4.609370	4.853890	5.026100
C	-2.603100	6.298490	5.601270
H	-1.774010	6.893390	5.213710
H	-3.233090	6.954860	6.216240
H	-2.183060	5.542940	6.278140
H	-4.293360	4.065700	5.723380
H	-5.299050	5.501220	5.584440
H	-5.171370	4.388580	4.210180
H	-3.834200	5.183400	2.530910
H	5.047170	1.216660	1.080400
H	3.901400	1.351860	-0.360483
H	3.235100	1.396290	2.638980

Conf 12

C	0.688805	2.774720	1.869940
C	-0.100847	2.183280	3.031840
C	0.506030	2.618880	4.316500
N	1.506380	3.526860	3.976940
C	1.595100	3.781810	2.619390
C	1.635180	1.672990	1.084650
C	-0.083052	3.542660	0.724368
C	-1.198220	1.411870	3.130920
O	0.214148	2.302730	5.459470
O	2.279510	4.659370	2.127840
H	2.031230	4.048310	4.668000
H	-1.561230	1.148460	4.123300
O	-1.894920	0.918336	2.085580
C	-3.112490	0.194178	2.404780
H	-2.863500	-0.595252	3.123560
C	-3.677030	-0.379619	1.120540
H	-3.813870	0.892912	2.875750
H	-4.602430	-0.920839	1.341340
H	-2.972260	-1.076710	0.658346
H	-3.904120	0.412361	0.401365
C	3.114460	1.879720	1.370230
C	1.225820	0.223224	1.402430
C	1.355770	1.988500	-0.413793
C	-0.035250	2.620250	-0.512187
H	0.589443	4.373670	0.469127
C	-1.458850	4.173550	1.057200
H	-0.116869	3.207200	-1.431870
O	-1.094710	1.665710	-0.596014
H	1.438090	1.092060	-1.035410
H	2.089940	2.715040	-0.782431
H	1.851820	-0.455786	0.815759
H	1.356240	-0.023869	2.459280
H	0.189328	0.024698	1.132320
C	3.952790	1.029090	1.971450
H	-1.352220	1.374210	0.291553

C	-1.339610	5.243050	2.166720
C	-2.088310	4.767490	-0.218102
H	-2.130200	3.385250	1.420350
H	-3.054630	5.231980	-0.002187
H	-1.439870	5.540430	-0.650372
H	-2.258190	3.996730	-0.973589
H	-0.787695	4.838910	3.021040
H	-0.741668	6.084880	1.789760
C	-2.684520	5.771820	2.710680
C	-2.491800	6.800050	3.795050
H	-3.256330	6.231620	1.893870
H	-3.283820	4.926690	3.067810
C	-2.852820	6.738130	5.088900
C	-2.555500	7.882760	6.030510
C	-3.567810	5.574830	5.734260
H	-3.781860	4.759560	5.040500
H	-2.969400	5.165400	6.558760
H	-4.520070	5.903180	6.172060
H	-3.479940	8.283700	6.467990
H	-1.931840	7.548750	6.870760
H	-2.035440	8.701910	5.525430
H	-1.974950	7.704390	3.467830
H	5.000140	1.287580	2.097140
H	3.646220	0.061186	2.355530
H	3.516200	2.827720	1.019520

Conf 53

C	0.729068	2.593530	2.176430
C	-0.160371	1.742500	3.082570
C	0.198358	2.006360	4.502370
N	1.138950	3.031890	4.477470
C	1.397400	3.528890	3.207030
C	1.859040	1.730940	1.398050
C	0.070073	3.387410	1.000190
C	-1.170710	0.869615	2.910710
O	-0.227866	1.482990	5.521060
O	2.064910	4.520940	2.988160
H	1.478190	3.481960	5.318830
H	-1.613170	0.430879	3.804440
O	-1.688110	0.459092	1.733830
C	-2.833670	-0.431686	1.807460
H	-2.836030	-0.949944	0.845971
C	-4.130810	0.328092	2.034730
H	-2.647440	-1.168910	2.596740
H	-4.970110	-0.375659	2.038580
H	-4.299750	1.059170	1.238770
H	-4.125100	0.852703	2.995260
C	3.062060	2.592430	1.034180
C	2.395770	0.541141	2.217930
C	1.067410	1.272350	0.161134
C	0.116560	2.420090	-0.241478
H	0.797493	4.182120	0.792728
C	-1.295590	4.082120	1.224490
H	0.501868	2.971450	-1.102400
O	-1.145690	1.928910	-0.686996
H	0.460355	0.402920	0.431495

H	1.721040	0.952633	-0.655012
H	3.105130	-0.029321	1.609870
H	2.928240	0.873290	3.116240
H	1.592110	-0.132887	2.526530
C	3.496270	2.914950	-0.187172
H	-1.507850	1.381740	0.025872
C	-1.336370	4.933670	2.512080
C	-1.635350	4.937480	-0.012746
H	-2.069790	3.308510	1.317710
H	-2.633710	5.376950	0.069631
H	-0.916701	5.760350	-0.119910
H	-1.619270	4.337780	-0.924690
H	-1.090280	4.305000	3.375120
H	-0.565242	5.713460	2.468550
C	-2.703660	5.590740	2.804700
C	-2.767050	6.181260	4.189350
H	-2.928780	6.346920	2.048740
H	-3.486200	4.821180	2.712350
C	-2.914890	7.468610	4.548800
C	-2.948070	7.865920	6.006910
C	-3.060510	8.624230	3.587460
H	-4.015830	9.141900	3.748270
H	-2.271140	9.367890	3.759850
H	-3.013930	8.324810	2.538800
H	-2.142140	8.574890	6.240320
H	-3.890670	8.372230	6.255930
H	-2.842150	7.000890	6.668090
H	-2.665750	5.451590	4.995530
H	4.400880	3.502820	-0.310880
H	2.984230	2.625340	-1.099890
H	3.648160	2.938360	1.882660

Conf 37

C	0.779161	2.646860	2.086550
C	-0.130518	1.970380	3.111950
C	0.289826	2.379890	4.479540
N	1.289870	3.332110	4.305770
C	1.536490	3.654530	2.978230
C	1.828340	1.625460	1.391780
C	0.132468	3.333410	0.837965
C	-1.195150	1.147480	3.074490
O	-0.132861	2.010220	5.564750
O	2.255760	4.567970	2.622870
H	1.681070	3.859150	5.076940
H	-1.632700	0.848696	4.026450
O	-1.774320	0.629929	1.970630
C	-2.963060	-0.177821	2.183100
H	-3.026660	-0.806011	1.291810
C	-4.208590	0.677404	2.352580
H	-2.790130	-0.825241	3.050320
H	-5.084210	0.029044	2.464910
H	-4.364900	1.316860	1.478920
H	-4.140970	1.311400	3.242140
C	3.068550	2.357680	0.894102
C	2.319280	0.511907	2.337790
C	0.969980	1.072000	0.241111

C	0.076695	2.220850	-0.274691
H	0.901547	4.046230	0.515068
C	-1.177640	4.141950	1.008450
H	0.464456	2.636960	-1.207530
O	-1.227870	1.761460	-0.621245
H	0.321331	0.281792	0.631326
H	1.575900	0.615368	-0.546218
H	2.972580	-0.171981	1.786560
H	2.900170	0.915776	3.174610
H	1.487320	-0.067359	2.747320
C	3.480110	2.501900	-0.368474
H	-1.597340	1.329380	0.163349
C	-1.110640	5.150140	2.176590
C	-1.506020	4.853840	-0.319377
H	-1.995410	3.440660	1.222920
H	-2.470230	5.367750	-0.268754
H	-0.740262	5.605180	-0.552112
H	-1.561110	4.142650	-1.145600
H	-0.867650	4.624890	3.106020
H	-0.292348	5.861000	1.999760
C	-2.417970	5.931080	2.435560
C	-2.305330	6.836450	3.634590
H	-2.656940	6.546180	1.558380
H	-3.246070	5.222130	2.548940
C	-2.997570	6.800940	4.786870
C	-2.725820	7.804260	5.884550
C	-4.084770	5.804660	5.113550
H	-3.828380	5.239460	6.019560
H	-5.030330	6.321630	5.325790
H	-4.268980	5.087370	4.311400
H	-3.627860	8.385400	6.120050
H	-2.427920	7.300020	6.813920
H	-1.932710	8.505310	5.608720
H	-1.543800	7.612970	3.538650
H	4.413970	3.011230	-0.586942
H	2.920790	2.137840	-1.225050
H	3.702590	2.765120	1.678370

Conf 24

C	0.829502	2.737850	2.111160
C	-0.076486	2.285570	3.256310
C	0.542858	2.677520	4.550410
N	1.671100	3.425900	4.225760
C	1.835470	3.635470	2.863340
C	1.611200	1.514030	1.392540
C	0.186528	3.467480	0.884657
C	-1.273800	1.680400	3.366410
O	0.175064	2.441700	5.691690
O	2.663540	4.387570	2.386820
H	2.228650	3.903720	4.923080
H	-1.665790	1.520760	4.370160
O	-2.058770	1.260200	2.352840
C	-3.291380	0.588698	2.726110
H	-3.738800	1.127160	3.569190
C	-3.058210	-0.878820	3.047520
H	-3.942510	0.708271	1.857310

H	-2.611130	-1.397270	2.194360
H	-4.014910	-1.359120	3.279270
H	-2.400590	-0.999797	3.914100
C	2.899660	1.988580	0.731858
C	2.000170	0.380708	2.362130
C	0.555221	1.065210	0.368236
C	-0.167661	2.329230	-0.145067
H	1.028570	4.019520	0.448612
C	-0.946031	4.497500	1.122430
H	0.199051	2.622010	-1.131720
O	-1.558380	2.095470	-0.353036
H	-0.180553	0.431594	0.872671
H	0.985662	0.462406	-0.436142
H	2.462530	-0.436858	1.799830
H	2.728250	0.716416	3.109160
H	1.128920	-0.017344	2.889290
C	3.198900	1.984930	-0.569977
H	-1.929750	1.800260	0.491824
C	-0.587469	5.533060	2.211180
C	-1.279860	5.196100	-0.210855
H	-1.842010	3.957990	1.452500
H	-0.424805	5.789580	-0.559852
H	-1.540330	4.469660	-0.982719
H	-2.130940	5.875280	-0.103503
H	-0.370438	5.015210	3.151540
H	0.332054	6.057090	1.918620
C	-1.673920	6.591740	2.524860
C	-2.996360	6.019590	2.969470
H	-1.269310	7.264040	3.288280
H	-1.839460	7.216420	1.637910
C	-3.515320	5.992400	4.210560
C	-4.873810	5.381770	4.469990
C	-2.839620	6.547210	5.441990
H	-1.867010	6.997470	5.235330
H	-3.470910	7.308920	5.918990
H	-2.689330	5.755200	6.187590
H	-4.806740	4.563870	5.200680
H	-5.563200	6.122520	4.897530
H	-5.325890	4.988330	3.554470
H	-3.599680	5.575370	2.176450
H	4.178150	2.309210	-0.909311
H	2.501970	1.675150	-1.342910
H	3.669940	2.323420	1.422930
Conf 57			
C	0.691507	2.610450	2.168600
C	-0.238818	1.786240	3.058390
C	0.127174	2.009530	4.483280
N	1.115590	2.989300	4.477760
C	1.400120	3.495620	3.216510
C	1.781570	1.711450	1.375930
C	0.069869	3.454510	1.006480
C	-1.293030	0.970795	2.869250
O	-0.325405	1.488620	5.491800
O	2.114050	4.458810	3.016060
H	1.473340	3.408530	5.327340
H	-1.762880	0.542998	3.754230

O	-1.847830	0.635014	1.685750
C	-2.950140	-0.309736	1.734080
H	-3.598370	-0.044683	2.577200
C	-2.458570	-1.745440	1.824860
H	-3.501860	-0.134552	0.807812
H	-3.315890	-2.427010	1.813980
H	-1.899740	-1.920090	2.749660
H	-1.814240	-1.990110	0.975460
C	3.022000	2.523660	1.024400
C	2.265030	0.486171	2.176460
C	0.969406	1.309550	0.132918
C	0.077211	2.508960	-0.253233
H	0.831062	4.221050	0.814932
C	-1.265300	4.203020	1.242660
H	0.495109	3.056750	-1.101110
O	-1.203550	2.088130	-0.716578
H	0.318765	0.468660	0.391529
H	1.606400	0.968915	-0.687977
H	2.946960	-0.106617	1.558460
H	2.813230	0.780226	3.078570
H	1.432030	-0.155086	2.476980
C	3.472790	2.840190	-0.192518
H	-1.608110	1.564540	-0.008821
C	-1.271580	5.030110	2.546650
C	-1.564490	5.097240	0.022483
H	-2.072970	3.462450	1.319760
H	-0.811212	5.890890	-0.065789
H	-1.571090	4.516260	-0.901605
H	-2.543610	5.576740	0.111853
H	-1.051620	4.375470	3.397240
H	-0.469294	5.778600	2.517710
C	-2.611360	5.735880	2.852860
C	-2.649820	6.303600	4.247900
H	-2.806830	6.513780	2.110800
H	-3.423740	4.999590	2.748210
C	-2.744480	7.589280	4.630490
C	-2.760840	7.961480	6.095510
C	-2.842830	8.766980	3.690160
H	-2.808590	8.484760	2.636280
H	-3.776220	9.320260	3.860970
H	-2.023750	9.474610	3.875230
H	-1.926270	8.632330	6.340740
H	-3.681680	8.501700	6.354530
H	-2.690540	7.081100	6.741000
H	-2.578670	5.556000	5.040750
H	4.402790	3.388800	-0.308041
H	2.950470	2.583730	-1.109300
H	3.620860	2.833790	1.877730

Cartesian Coordinates of Conformers (>2% population) of 1b

Conf 2

C	1.181460	2.582350	0.382043
C	1.589550	1.135190	0.662204
C	1.375440	0.842703	2.094690
N	0.720509	1.974990	2.616630
C	0.439421	2.951400	1.681220
C	2.449010	3.570010	0.174308
C	0.354292	2.881690	-0.907587
C	2.011630	0.221744	-0.241957
O	1.641720	-0.142830	2.760460
O	-0.249763	3.934650	1.891450
H	0.356996	1.999890	3.561460
H	2.075010	0.476358	-1.299130
O	2.355520	-1.031170	0.088789
C	2.706130	-1.903080	-1.007580
H	3.510710	-1.436840	-1.590590
C	3.146370	-3.230770	-0.422361
H	1.830830	-2.024420	-1.658330
H	3.415630	-3.920110	-1.229340
H	4.015490	-3.097710	0.228049
H	2.341650	-3.679610	0.166633
C	2.076330	5.019990	0.455429
C	3.649630	3.232670	1.080000
C	2.761200	3.320280	-1.312360
C	1.424550	3.088710	-2.034950
H	-0.077017	3.872880	-0.718060
C	-0.817375	1.949890	-1.305110
H	1.145580	3.948150	-2.655070
O	1.620720	1.953470	-2.900480
H	3.353520	2.405320	-1.410460
H	3.357320	4.122390	-1.754600
H	4.492240	3.884290	0.826937
H	3.416090	3.395520	2.137770
H	3.969130	2.194530	0.956987
C	2.074520	6.046930	-0.399563
H	0.857278	1.861750	-3.485010
C	-1.759070	1.625320	-0.126487
C	-1.609990	2.592850	-2.463560
H	-0.403328	0.998726	-1.661330
H	-2.352770	1.902560	-2.871720
H	-2.137000	3.490940	-2.118460
H	-0.970880	2.903950	-3.298150
H	-1.176960	1.167350	0.680693
H	-2.171860	2.557910	0.277705
C	-2.924030	0.662841	-0.452079
C	-2.467920	-0.704332	-0.893567
H	-3.514970	0.554065	0.469628
H	-3.600200	1.114300	-1.183740
C	-2.879220	-1.434200	-1.945650
C	-2.313240	-2.812820	-2.200770
C	-3.926530	-1.000130	-2.943830
H	-3.528370	-1.041020	-3.966650
H	-4.786060	-1.683540	-2.919170
H	-4.302540	0.009378	-2.766760
H	-3.106170	-3.572880	-2.187140

H	-1.844880	-2.870850	-3.193030
H	-1.565720	-3.091260	-1.452180
H	-1.713970	-1.154480	-0.244095
H	1.827870	7.047300	-0.056410
H	2.307120	5.947380	-1.455860
H	1.823760	5.230300	1.492100

Conf 3

C	1.161600	2.540000	0.337749
C	1.514120	1.095350	0.696745
C	1.264310	0.881905	2.136890
N	0.639625	2.060250	2.589900
C	0.408996	2.997620	1.602420
C	2.464870	3.474410	0.107372
C	0.368535	2.801810	-0.980963
C	1.912710	0.122245	-0.154493
O	1.486200	-0.076797	2.856110
O	-0.249740	4.012640	1.750110
H	0.261511	2.144640	3.525500
H	2.014120	0.324565	-1.220160
O	2.159720	-1.136160	0.234662
C	2.652710	-2.042740	-0.773253
H	2.175790	-1.811140	-1.734010
C	4.170120	-1.989980	-0.875695
H	2.314000	-3.029360	-0.448133
H	4.520180	-2.735500	-1.598230
H	4.511970	-1.005550	-1.211610
H	4.627540	-2.204840	0.094409
C	2.136430	4.948120	0.309238
C	3.636590	3.143610	1.052370
C	2.795810	3.141210	-1.358780
C	1.465560	2.918270	-2.095730
H	-0.033098	3.814540	-0.848807
C	-0.825432	1.889210	-1.355810
H	1.227100	3.755020	-2.762100
O	1.639450	1.736440	-2.901780
H	3.358120	2.203270	-1.399680
H	3.426990	3.900110	-1.827860
H	4.505750	3.752800	0.783772
H	3.389660	3.367710	2.095790
H	3.921680	2.090280	0.988124
C	2.182850	5.930130	-0.595803
H	0.882937	1.640470	-3.494600
C	-1.798410	1.651960	-0.181817
C	-1.575920	2.499510	-2.559140
H	-0.436287	0.909124	-1.657450
H	-2.334320	1.814600	-2.947160
H	-2.078420	3.430270	-2.268360
H	-0.912527	2.748080	-3.395830
H	-1.245280	1.221460	0.660025
H	-2.193180	2.615060	0.164843
C	-2.981950	0.703930	-0.481708
C	-2.552650	-0.695727	-0.840907
H	-3.594020	0.659085	0.431499
H	-3.631130	1.132870	-1.250460
C	-2.962390	-1.470350	-1.861120

C	-2.426990	-2.874090	-2.030980
C	-3.978930	-1.064510	-2.902060
H	-3.562300	-1.169370	-3.912920
H	-4.855930	-1.724430	-2.859290
H	-4.332420	-0.038107	-2.786120
H	-3.239190	-3.612690	-1.992080
H	-1.942400	-2.996970	-3.009440
H	-1.700230	-3.129520	-1.254370
H	-1.822630	-1.128930	-0.153725
H	1.964180	6.954070	-0.307618
H	2.428890	5.769650	-1.641500
H	1.874170	5.218390	1.329460

Conf 6

C	1.149000	2.576570	0.371434
C	1.575520	1.131050	0.627169
C	1.410880	0.826593	2.063820
N	0.758316	1.947100	2.612960
C	0.439924	2.928200	1.693930
C	2.402150	3.578830	0.147144
C	0.286718	2.876160	-0.896379
C	1.952010	0.223042	-0.301543
O	1.710820	-0.159594	2.713990
O	-0.248199	3.905110	1.933260
H	0.422796	1.961290	3.568290
H	1.963420	0.484088	-1.359090
O	2.307950	-1.033140	0.003691
C	2.570370	-1.907760	-1.114420
H	3.340450	-1.451760	-1.750480
C	3.031950	-3.242220	-0.561830
H	1.651440	-2.015670	-1.704060
H	3.235560	-3.933990	-1.385790
H	3.945240	-3.122270	0.027822
H	2.263170	-3.680810	0.080386
C	2.024360	5.022550	0.451379
C	3.626800	3.241330	1.019950
C	2.679970	3.348350	-1.350240
C	1.320040	3.115760	-2.042340
H	-0.153703	3.858360	-0.684238
C	-0.885015	1.933580	-1.274290
H	1.011490	3.985040	-2.634380
O	1.374740	1.972480	-2.922140
H	3.275190	2.436140	-1.463490
H	3.262490	4.162520	-1.791930
H	4.458000	3.903390	0.756131
H	3.416460	3.388970	2.084730
H	3.951400	2.207240	0.877044
C	1.983180	6.056190	-0.394360
H	1.913270	2.205450	-3.689100
C	-1.804990	1.626330	-0.074027
C	-1.683200	2.561250	-2.433870
H	-0.472203	0.985363	-1.633650
H	-2.467950	1.885980	-2.785300
H	-2.162670	3.496460	-2.116620
H	-1.039820	2.775840	-3.290550
H	-1.209720	1.193290	0.737935

H	-2.223870	2.563050	0.314902
C	-2.963260	0.642827	-0.358576
C	-2.497510	-0.736918	-0.747172
H	-3.550930	0.564339	0.568441
H	-3.644190	1.060050	-1.105630
C	-2.891300	-1.503800	-1.779170
C	-2.314150	-2.886650	-1.980930
C	-3.923690	-1.107600	-2.807860
H	-4.776110	-1.799970	-2.782890
H	-4.312810	-0.097911	-2.664030
H	-3.503820	-1.168510	-3.820930
H	-3.102790	-3.651020	-1.955590
H	-1.829680	-2.972900	-2.963440
H	-1.577060	-3.136430	-1.212010
H	-1.749160	-1.160970	-0.073911
H	1.735640	7.050770	-0.035593
H	2.181020	5.967840	-1.458760
H	1.802670	5.221530	1.497210

Conf 18

C	1.243540	2.446720	0.220001
C	1.883410	1.063950	0.351719
C	1.543370	0.500192	1.675290
N	0.618313	1.398290	2.241040
C	0.278961	2.457080	1.421800
C	2.311910	3.656190	0.361647
C	0.550085	2.815970	-1.128700
C	2.588120	0.402040	-0.594391
O	1.906830	-0.523682	2.227350
O	-0.608672	3.258730	1.655960
H	0.132624	1.197820	3.106720
H	2.739460	0.838859	-1.580780
O	3.121810	-0.811654	-0.394716
C	3.757890	-1.421620	-1.538250
H	4.517140	-0.734383	-1.933200
C	4.377950	-2.728210	-1.082960
H	3.002530	-1.589480	-2.316760
H	4.865610	-3.221680	-1.930050
H	5.125180	-2.551190	-0.304230
H	3.613670	-3.398870	-0.680495
C	1.632000	4.952670	0.782586
C	3.425120	3.379320	1.391000
C	2.858960	3.718720	-1.075690
C	1.697160	3.395240	-2.028380
H	-0.089154	3.669450	-0.869727
C	-0.352796	1.777240	-1.838750
H	1.340700	4.290670	-2.549890
O	2.218270	2.478900	-3.011050
H	3.621140	2.944650	-1.208180
H	3.345550	4.671910	-1.297130
H	4.151870	4.197910	1.371850
H	3.027170	3.318650	2.409760
H	3.952440	2.446560	1.174500
C	1.546080	6.094360	0.093553
H	1.579730	2.383680	-3.729370
C	-1.346630	1.077670	-0.887903

C	-1.105840	2.464700	-2.998590
H	0.289222	0.994041	-2.263790
H	-0.442217	3.026750	-3.666120
H	-1.641070	1.739150	-3.617300
H	-1.840230	3.179900	-2.608320
H	-0.786897	0.592744	-0.081145
H	-1.996160	1.822330	-0.411213
C	-2.219800	-0.006508	-1.557860
C	-2.965510	-0.838424	-0.546842
H	-2.911550	0.449944	-2.270800
H	-1.563640	-0.668845	-2.144270
C	-4.292530	-0.935240	-0.352926
C	-4.852470	-1.827970	0.730718
C	-5.340720	-0.200042	-1.153970
H	-6.016970	-0.910211	-1.648680
H	-5.965590	0.415447	-0.493256
H	-4.921740	0.453805	-1.921260
H	-4.061890	-2.342580	1.284400
H	-5.450200	-1.248970	1.447650
H	-5.522970	-2.588150	0.307251
H	-2.323800	-1.422980	0.115210
H	1.067600	6.965650	0.530839
H	1.932440	6.216160	-0.914272
H	1.207690	4.937790	1.783760

Conf 1

C	1.154450	2.581610	0.278612
C	1.512700	1.104020	0.443427
C	1.234400	0.692941	1.834970
N	0.588047	1.793350	2.430610
C	0.370789	2.856550	1.576620
C	2.456030	3.544390	0.209302
C	0.389856	3.020170	-1.009960
C	1.945700	0.261356	-0.522039
O	1.448200	-0.354611	2.420270
O	-0.299201	3.838070	1.848420
H	0.188990	1.746210	3.360090
H	2.051470	0.603714	-1.550690
O	2.257170	-1.021290	-0.288677
C	2.576420	-1.819430	-1.448410
H	3.336690	-1.297570	-2.043750
C	3.081550	-3.164330	-0.963098
H	1.671840	-1.930740	-2.059630
H	3.321470	-3.801400	-1.820720
H	3.982490	-3.043300	-0.354899
H	2.322270	-3.666170	-0.356874
C	2.111400	4.975230	0.602069
C	3.608140	3.092670	1.128030
C	2.823030	3.415410	-1.280040
C	1.511310	3.294320	-2.071760
H	-0.022214	4.003030	-0.748171
C	-0.789384	2.163710	-1.534560
H	1.283060	4.215620	-2.619590
O	1.709750	2.237330	-3.031020
H	3.390250	2.492550	-1.435720
H	3.461640	4.232200	-1.625570

H	4.478470	3.736720	0.965553
H	3.335840	3.171350	2.186150
H	3.903060	2.059390	0.927373
C	2.174360	6.072050	-0.158602
H	0.976959	2.235320	-3.660160
C	-1.784100	1.766380	-0.423172
C	-1.515990	2.932150	-2.659510
H	-0.381770	1.237120	-1.956430
H	-0.835733	3.292580	-3.439890
H	-2.267100	2.310010	-3.154330
H	-2.027440	3.814240	-2.255140
H	-1.250400	1.194580	0.342864
H	-2.162750	2.674450	0.063263
C	-2.992060	0.906844	-0.871724
C	-2.625030	-0.391387	-1.547260
H	-3.605910	0.717469	0.014857
H	-3.627060	1.492080	-1.549160
C	-2.610650	-1.626430	-1.013900
C	-2.216300	-2.826310	-1.843990
C	-2.967830	-1.950480	0.416901
H	-2.107300	-2.393450	0.935158
H	-3.286890	-1.078420	0.990717
H	-3.773930	-2.695240	0.454715
H	-1.958830	-2.546600	-2.870100
H	-1.354910	-3.345050	-1.401770
H	-3.032250	-3.560430	-1.886440
H	-2.333170	-0.307290	-2.595370
H	1.940840	7.046130	0.260886
H	2.449150	6.057120	-1.209340
H	1.820580	5.102340	1.642230

Conf 9

C	1.210150	2.506860	0.181362
C	1.717010	1.066080	0.259900
C	1.373550	0.506481	1.584440
N	0.561777	1.475760	2.204000
C	0.295905	2.580890	1.419800
C	2.396000	3.603470	0.307019
C	0.507834	2.975080	-1.131530
C	2.320830	0.362892	-0.725218
O	1.657600	-0.559774	2.101580
O	-0.501395	3.457890	1.704090
H	0.089412	1.301100	3.082540
H	2.477510	0.806438	-1.707730
O	2.743710	-0.900204	-0.569929
C	3.283530	-1.538350	-1.746800
H	4.088300	-0.913353	-2.154780
C	3.797800	-2.905340	-1.339410
H	2.490730	-1.619970	-2.501610
H	4.210140	-3.421400	-2.212640
H	4.583660	-2.813610	-0.584345
H	2.990000	-3.513620	-0.923038
C	1.861430	4.948670	0.781616
C	3.514020	3.195300	1.286270
C	2.893950	3.648700	-1.148860
C	1.672740	3.460560	-2.062890

H	-0.033323	3.881030	-0.830586
C	-0.520096	2.048120	-1.826840
H	1.386780	4.397770	-2.553490
O	2.066080	2.520380	-3.081900
H	3.573130	2.809210	-1.326610
H	3.461350	4.556470	-1.368830
H	4.315300	3.940760	1.256580
H	3.149540	3.147360	2.318130
H	3.940550	2.222150	1.029430
C	1.860300	6.109950	0.120563
H	1.395530	2.503690	-3.776800
C	-1.545920	1.436570	-0.849146
C	-1.237480	2.833080	-2.946780
H	0.024238	1.212950	-2.287680
H	-1.862370	2.179790	-3.561690
H	-1.883710	3.608780	-2.518050
H	-0.542406	3.341560	-3.625090
H	-1.015360	0.892532	-0.061790
H	-2.103050	2.240630	-0.350813
C	-2.538500	0.443053	-1.492280
C	-3.460050	-0.172733	-0.471312
H	-3.151000	0.964967	-2.239530
H	-1.977620	-0.326268	-2.035300
C	-3.558170	-1.459660	-0.094233
C	-4.547490	-1.880590	0.968413
C	-2.732800	-2.592660	-0.656225
H	-3.382580	-3.361650	-1.095270
H	-2.024600	-2.274180	-1.423490
H	-2.162640	-3.084470	0.142881
H	-5.255200	-2.623460	0.575957
H	-4.035130	-2.354820	1.816360
H	-5.122340	-1.031700	1.349820
H	-4.117090	0.541902	0.028083
H	1.485340	7.012070	0.594795
H	2.217910	6.218940	-0.899251
H	1.476050	4.950050	1.798550

Conf 21

C	1.260160	2.463120	0.228998
C	1.932440	1.101300	0.410382
C	1.579070	0.562914	1.740160
N	0.622507	1.453000	2.265520
C	0.273742	2.481590	1.412900
C	2.294790	3.702960	0.355670
C	0.582082	2.778200	-1.141000
C	2.679980	0.436776	-0.500764
O	1.953220	-0.439081	2.324620
O	-0.636895	3.267530	1.609560
H	0.124651	1.262460	3.126500
H	2.837480	0.848274	-1.497360
O	3.265510	-0.742154	-0.249256
C	3.889390	-1.409800	-1.365220
H	4.687150	-2.008380	-0.919076
C	2.898250	-2.287450	-2.115540
H	4.345050	-0.661182	-2.025940
H	3.413020	-2.829480	-2.916580

H	2.442770	-3.016780	-1.439500
H	2.101100	-1.688530	-2.568040
C	1.575240	4.993160	0.727581
C	3.395470	3.483470	1.412020
C	2.866540	3.739760	-1.073040
C	1.730630	3.360910	-2.036510
H	-0.082088	3.622500	-0.917035
C	-0.282709	1.698480	-1.836960
H	1.361810	4.232310	-2.589100
O	2.291220	2.430950	-2.984470
H	3.650110	2.982030	-1.170160
H	3.333280	4.698460	-1.312610
H	4.101160	4.320010	1.383150
H	2.980220	3.440290	2.424740
H	3.950560	2.559300	1.231190
C	1.475490	6.113410	0.005952
H	1.670770	2.305940	-3.713980
C	-1.277320	1.002550	-0.884099
C	-1.030380	2.334080	-3.029340
H	0.385804	0.919457	-2.227620
H	-1.535640	1.578430	-3.637120
H	-1.789570	3.040980	-2.672920
H	-0.368182	2.894000	-3.699940
H	-0.721253	0.553414	-0.054488
H	-1.951840	1.745070	-0.439923
C	-2.113850	-0.119633	-1.537850
C	-2.861170	-0.937382	-0.516575
H	-2.801310	0.300169	-2.276950
H	-1.432370	-0.784379	-2.091910
C	-4.189390	-1.067780	-0.352883
C	-4.750730	-1.937860	0.748343
C	-5.237670	-0.394564	-1.206560
H	-5.877360	-1.142830	-1.693680
H	-5.899510	0.222661	-0.584646
H	-4.818520	0.245663	-1.985170
H	-5.383860	-1.352030	1.428390
H	-5.387150	-2.732890	0.336445
H	-3.959950	-2.407780	1.340150
H	-2.220210	-1.478430	0.182205
H	0.967540	6.984100	0.409928
H	1.878800	6.217630	-0.997208
H	1.131580	4.994900	1.720440

Conf 19

C	1.113220	2.624490	0.179555
C	1.458840	1.152120	0.395197
C	1.183720	0.796827	1.803380
N	0.556338	1.926620	2.362840
C	0.336737	2.956040	1.467390
C	2.424430	3.573900	0.092739
C	0.333609	3.015930	-1.115690
C	1.898820	0.282281	-0.541527
O	1.389540	-0.232043	2.423980
O	-0.334528	3.946860	1.692920
H	0.164254	1.918330	3.296370
H	2.015750	0.598564	-1.577710

O	2.209910	-0.993485	-0.270928
C	2.542560	-1.821220	-1.405680
H	3.309470	-1.314640	-2.005760
C	3.042870	-3.152740	-0.880124
H	1.645090	-1.949020	-2.024200
H	3.293140	-3.811470	-1.718200
H	3.936570	-3.015250	-0.264807
H	2.277000	-3.639650	-0.270001
C	2.076680	5.020620	0.413977
C	3.600280	3.081600	0.946897
C	2.754760	3.477990	-1.421880
C	1.437050	3.292670	-2.192190
H	-0.114177	3.989200	-0.877959
C	-0.831741	2.120410	-1.609500
H	1.177820	4.188060	-2.769330
O	1.658730	2.209940	-3.116840
H	3.371420	2.592440	-1.608020
H	3.327510	4.344900	-1.763000
H	4.480900	3.705550	0.764718
H	3.376740	3.125320	2.017590
H	3.865660	2.052540	0.698573
C	2.715200	5.833250	1.260740
H	0.921471	2.165190	-3.739320
C	-1.816080	1.743890	-0.481885
C	-1.576350	2.837030	-2.756730
H	-0.408641	1.187810	-2.001010
H	-2.319370	2.184990	-3.224350
H	-2.101640	3.723720	-2.380870
H	-0.907386	3.180940	-3.554080
H	-1.269620	1.211500	0.302857
H	-2.212540	2.661080	-0.027515
C	-3.006050	0.843409	-0.896819
C	-2.611490	-0.468192	-1.530620
H	-3.611590	0.669242	-0.001306
H	-3.657360	1.390890	-1.589870
C	-2.530130	-1.676420	-0.944554
C	-2.115920	-2.896660	-1.734140
C	-2.825420	-1.947190	0.511154
H	-3.592040	-2.726950	0.611467
H	-1.927900	-2.321770	1.020470
H	-3.168820	-1.064180	1.053420
H	-1.220990	-3.361820	-1.298960
H	-2.903180	-3.662390	-1.716320
H	-1.903050	-2.654170	-2.779770
H	-2.357780	-0.419241	-2.590820
H	2.392310	6.862840	1.382140
H	3.558610	5.518340	1.866710
H	1.236500	5.438240	-0.136015

Conf 26

C	1.229500	2.360810	0.184630
C	1.821980	0.958133	0.329675
C	1.478270	0.426084	1.664660
N	0.592420	1.364670	2.228200
C	0.280059	2.422260	1.397080
C	2.339820	3.534770	0.296856

C	0.533683	2.734140	-1.161580
C	2.485670	0.255358	-0.616966
O	1.813460	-0.600996	2.228770
O	-0.576170	3.258060	1.629110
H	0.110715	1.194000	3.102440
H	2.650540	0.676749	-1.608110
O	2.935570	-0.992075	-0.422929
C	3.686150	-1.587880	-1.501080
H	3.264330	-1.261780	-2.460320
C	5.167340	-1.253980	-1.400180
H	3.515980	-2.662080	-1.396370
H	5.720560	-1.774060	-2.190030
H	5.341570	-0.179179	-1.515500
H	5.566120	-1.569120	-0.431597
C	1.710000	4.860600	0.704526
C	3.454010	3.235420	1.318780
C	2.872840	3.556750	-1.146880
C	1.689680	3.261060	-2.082060
H	-0.073372	3.612620	-0.908870
C	-0.411312	1.716080	-1.846430
H	1.358540	4.161310	-2.611860
O	2.167500	2.314320	-3.058150
H	3.605040	2.753600	-1.275220
H	3.390910	4.488310	-1.388090
H	3.944850	2.280730	1.112430
H	4.209210	4.027050	1.278240
H	3.065590	3.205580	2.342550
C	1.657620	5.994360	-0.000790
H	1.515670	2.229480	-3.765810
C	-1.417570	1.064130	-0.875040
C	-1.153690	2.411290	-3.008560
H	0.199357	0.905500	-2.266240
H	-0.479134	2.942130	-3.690580
H	-1.718490	1.694870	-3.611380
H	-1.860480	3.155400	-2.621410
H	-0.865751	0.574612	-0.065680
H	-2.038470	1.836830	-0.404813
C	-2.330640	-0.002689	-1.519100
C	-3.094890	-0.791599	-0.487737
H	-3.012790	0.463125	-2.235220
H	-1.700550	-0.696384	-2.097840
C	-4.423600	-0.852686	-0.290889
C	-5.002820	-1.705920	0.814251
C	-5.455500	-0.113445	-1.109180
H	-6.066830	0.530784	-0.463359
H	-5.022400	0.512848	-1.891470
H	-6.147070	-0.820070	-1.587560
H	-5.690660	-2.460840	0.409586
H	-4.223600	-2.224640	1.380060
H	-5.586740	-1.096290	1.517050
H	-2.466400	-1.375530	0.187403
H	1.214310	6.888310	0.427740
H	2.038110	6.087690	-1.013880
H	1.295140	4.875530	1.709650

Conf 23

C	1.206180	2.406990	0.186496
C	1.861740	1.031210	0.305579
C	1.571030	0.473133	1.643400
N	0.651769	1.363210	2.230380
C	0.275883	2.413500	1.415410
C	2.264640	3.627830	0.300927
C	0.473351	2.761620	-1.146550
C	2.521920	0.362547	-0.666810
O	1.965810	-0.541351	2.191140
O	-0.610388	3.208870	1.673120
H	0.193635	1.162310	3.110830
H	2.623810	0.790976	-1.663240
O	3.065010	-0.849890	-0.483635
C	3.625690	-1.478050	-1.655910
H	4.376920	-0.808165	-2.094660
C	4.244110	-2.794300	-1.226840
H	2.826900	-1.634040	-2.392070
H	4.676820	-3.301070	-2.095660
H	5.034450	-2.628510	-0.489240
H	3.489190	-3.448010	-0.781253
C	1.583890	4.918100	0.738530
C	3.408290	3.362270	1.299510
C	2.771530	3.695890	-1.151960
C	1.580560	3.356670	-2.073220
H	-0.170280	3.606270	-0.871472
C	-0.437525	1.710020	-1.830390
H	1.191810	4.247560	-2.579610
O	1.962540	2.398980	-3.083880
H	3.537870	2.926990	-1.296230
H	3.241690	4.657190	-1.380310
H	4.125810	4.188440	1.262340
H	3.038260	3.296410	2.328350
H	3.938600	2.434680	1.068250
C	1.458430	6.055290	0.048295
H	2.539170	2.842030	-3.719260
C	-1.411350	1.029800	-0.845568
C	-1.198280	2.380530	-2.991740
H	0.197769	0.927020	-2.260620
H	-1.783060	1.650100	-3.557980
H	-1.891430	3.142880	-2.613290
H	-0.512477	2.857060	-3.696570
H	-0.838271	0.562160	-0.037241
H	-2.056110	1.781470	-0.372878
C	-2.292210	-0.071110	-1.476970
C	-3.019950	-0.882960	-0.437145
H	-2.995410	0.368421	-2.188950
H	-1.643260	-0.743681	-2.059500
C	-4.343860	-0.986064	-0.225621
C	-4.884360	-1.856380	0.885891
C	-5.407040	-0.279722	-1.032940
H	-6.082020	-1.007550	-1.503300
H	-6.030620	0.346308	-0.380849
H	-5.001410	0.358651	-1.820070
H	-5.479650	-1.265150	1.594950
H	-5.552530	-2.632870	0.488930
H	-4.083230	-2.350170	1.443490

H	-2.366490	-1.446230	0.232086
H	0.982473	6.921650	0.497810
H	1.806530	6.178030	-0.973324
H	1.194130	4.902200	1.753560

Conf 4

C	1.120750	2.570890	0.267328
C	1.503370	1.098870	0.419644
C	1.272900	0.682986	1.818700
N	0.622361	1.771170	2.431660
C	0.365003	2.831720	1.585030
C	2.405660	3.553970	0.177088
C	0.320264	2.998330	-1.004490
C	1.898010	0.259470	-0.564254
O	1.524020	-0.359711	2.397550
O	-0.309762	3.803750	1.876960
H	0.247767	1.716350	3.370830
H	1.954120	0.602652	-1.596680
O	2.226170	-1.021970	-0.346282
C	2.465680	-1.825720	-1.520730
H	3.196840	-1.314580	-2.160900
C	2.982030	-3.176060	-1.063110
H	1.525790	-1.925970	-2.077700
H	3.163550	-3.817350	-1.931880
H	3.918180	-3.065640	-0.508357
H	2.252910	-3.667360	-0.412909
C	2.049490	4.977780	0.583883
C	3.584260	3.113760	1.067400
C	2.741010	3.438800	-1.321860
C	1.406170	3.302330	-2.084580
H	-0.104158	3.971490	-0.728045
C	-0.857646	2.123820	-1.506190
H	1.144260	4.225640	-2.613990
O	1.468900	2.234190	-3.053970
H	3.317400	2.522270	-1.486180
H	3.361810	4.269600	-1.670680
H	4.441530	3.771710	0.891356
H	3.333380	3.181200	2.131500
H	3.889190	2.085910	0.853766
C	2.069370	6.077820	-0.174346
H	2.046830	2.513220	-3.775550
C	-1.828850	1.741030	-0.369203
C	-1.592900	2.869090	-2.637590
H	-0.447766	1.200250	-1.927270
H	-2.381960	2.251060	-3.075780
H	-2.061760	3.786930	-2.259910
H	-0.910398	3.137770	-3.447470
H	-1.280530	1.185360	0.399176
H	-2.205960	2.654690	0.108390
C	-3.039930	0.867195	-0.779942
C	-2.676870	-0.440952	-1.436950
H	-3.639130	0.692224	0.119505
H	-3.686810	1.436910	-1.459380
C	-2.689410	-1.672560	-0.895680
C	-2.295170	-2.882650	-1.711280
C	-3.078660	-1.984800	0.529547

H	-3.902320	-2.710830	0.555341
H	-2.237730	-2.446470	1.063690
H	-3.387650	-1.104220	1.095810
H	-1.448620	-3.409820	-1.250410
H	-3.119430	-3.606880	-1.765000
H	-2.015390	-2.611910	-2.733950
H	-2.362680	-0.366896	-2.479130
H	1.830300	7.046110	0.255106
H	2.310730	6.071470	-1.233410
H	1.787760	5.096640	1.632640

Conf 30

C	1.093020	2.637860	0.253777
C	1.503160	1.211340	0.612868
C	1.301380	1.005360	2.062980
N	0.647697	2.165140	2.521510
C	0.350713	3.080330	1.528950
C	2.359320	3.621600	0.019970
C	0.252709	2.852220	-1.046140
C	1.915110	0.253210	-0.246829
O	1.578510	0.061639	2.782830
O	-0.349580	4.065690	1.673880
H	0.291477	2.245190	3.465970
H	1.966800	0.455931	-1.316230
O	2.264650	-0.981919	0.141785
C	2.571000	-1.916640	-0.914550
H	3.360360	-1.491880	-1.548690
C	3.020450	-3.214010	-0.271031
H	1.673910	-2.065060	-1.528600
H	3.256360	-3.950100	-1.046550
H	3.912000	-3.053850	0.341885
H	2.232240	-3.621030	0.368418
C	1.963870	5.080350	0.200622
C	3.583430	3.265730	0.874048
C	2.640090	3.380770	-1.489900
C	1.298210	3.061800	-2.183790
H	-0.229955	3.825820	-0.895321
C	-0.890471	1.862510	-1.395790
H	0.973604	3.882520	-2.834530
O	1.405270	1.869120	-2.989510
H	3.289840	2.504770	-1.597300
H	3.163310	4.232830	-1.935790
H	4.432100	3.897690	0.593824
H	3.395600	3.415160	1.942000
H	3.879490	2.225670	0.725666
C	2.600720	6.002460	0.928131
H	1.965520	2.066650	-3.750990
C	-1.834990	1.611200	-0.201455
C	-1.671380	2.400560	-2.610850
H	-0.449345	0.903677	-1.685630
H	-2.435670	1.689430	-2.935390
H	-2.175720	3.344290	-2.364960
H	-1.012230	2.572240	-3.465110
H	-1.252590	1.245480	0.651527
H	-2.284250	2.561060	0.115291
C	-2.963890	0.585073	-0.451229

C	-2.458330	-0.805276	-0.739213
H	-3.573490	0.551899	0.464249
H	-3.634240	0.937921	-1.239870
C	-2.810000	-1.645330	-1.728610
C	-2.198840	-3.024770	-1.826990
C	-3.825240	-1.339820	-2.804260
H	-3.380040	-1.457490	-3.801370
H	-4.663670	-2.047660	-2.753140
H	-4.238450	-0.331746	-2.736030
H	-2.971480	-3.803610	-1.769820
H	-1.689250	-3.163270	-2.790630
H	-1.475460	-3.207600	-1.026850
H	-1.717970	-1.167850	-0.022681
H	2.239220	7.026000	0.954827
H	3.479630	5.786250	1.526910
H	1.084770	5.403280	-0.352193

Conf 7

C	1.129380	2.542130	0.333422
C	1.501080	1.098680	0.673563
C	1.292290	0.874601	2.118560
N	0.664746	2.042680	2.593460
C	0.400136	2.983810	1.617530
C	2.419190	3.492290	0.091478
C	0.308295	2.802860	-0.969673
C	1.860980	0.130082	-0.199119
O	1.545100	-0.085013	2.826230
O	-0.261404	3.992970	1.788490
H	0.307046	2.116890	3.537890
H	1.916110	0.338518	-1.267080
O	2.120400	-1.131530	0.171424
C	2.536470	-2.041870	-0.866688
H	2.012050	-1.794360	-1.798090
C	4.047160	-2.021790	-1.050480
H	2.194860	-3.023380	-0.529305
H	4.341840	-2.768550	-1.796140
H	4.551210	-2.254620	-0.108044
H	4.393120	-1.041770	-1.395640
C	2.081430	4.960970	0.312095
C	3.610710	3.162290	1.011600
C	2.725850	3.176930	-1.384650
C	1.376410	2.951630	-2.099220
H	-0.105203	3.807810	-0.818790
C	-0.882975	1.878160	-1.329970
H	1.110430	3.798580	-2.742010
O	1.416790	1.763980	-2.919450
H	3.293320	2.241760	-1.436320
H	3.345310	3.948620	-1.851660
H	4.469780	3.782220	0.734925
H	3.380160	3.372590	2.061540
H	3.903110	2.111990	0.931093
C	2.093410	5.950210	-0.586037
H	1.971400	1.945660	-3.688770
C	-1.840800	1.657900	-0.140272
C	-1.633600	2.470330	-2.538950
H	-0.491392	0.901223	-1.631430

H	-2.431240	1.802630	-2.875550
H	-2.090220	3.434680	-2.280820
H	-0.964083	2.621490	-3.389180
H	-1.277840	1.255380	0.709470
H	-2.246560	2.623650	0.186692
C	-3.014280	0.686632	-0.403865
C	-2.570120	-0.721759	-0.705415
H	-3.627870	0.671328	0.509475
H	-3.665330	1.077780	-1.190650
C	-2.957890	-1.536300	-1.702580
C	-2.406200	-2.939520	-1.814740
C	-3.959220	-1.176570	-2.774470
H	-3.520310	-1.305040	-3.773050
H	-4.828300	-1.846860	-2.728740
H	-4.327080	-0.151720	-2.696850
H	-1.691310	-3.160780	-1.016780
H	-3.211450	-3.685210	-1.765730
H	-1.902200	-3.089570	-2.779610
H	-1.845570	-1.123100	0.006606
H	1.869690	6.969240	-0.284833
H	2.312920	5.800740	-1.639310
H	1.841820	5.220620	1.340520

Conf 8

C	1.185200	2.476340	0.155171
C	1.714320	1.043180	0.209585
C	1.432770	0.476045	1.545630
N	0.627628	1.429760	2.196750
C	0.315001	2.532750	1.426220
C	2.357350	3.590520	0.250910
C	0.431501	2.936320	-1.133310
C	2.268280	0.345828	-0.807776
O	1.756630	-0.585088	2.049590
O	-0.481347	3.398400	1.744510
H	0.190503	1.245290	3.091360
H	2.365800	0.791558	-1.797020
O	2.706830	-0.915168	-0.678851
C	3.159940	-1.556660	-1.889470
H	3.944480	-0.940308	-2.348000
C	3.684210	-2.930410	-1.519120
H	2.318940	-1.626640	-2.591080
H	4.033070	-3.448860	-2.418240
H	4.518180	-2.849820	-0.816150
H	2.897940	-3.530440	-1.052690
C	1.820060	4.924580	0.752331
C	3.514220	3.191680	1.188030
C	2.804260	3.654360	-1.221860
C	1.548120	3.451280	-2.095500
H	-0.115625	3.829840	-0.808245
C	-0.606256	1.995730	-1.798630
H	1.222550	4.387490	-2.563230
O	1.795140	2.490090	-3.144240
H	3.489620	2.823590	-1.420230
H	3.350330	4.575260	-1.447730
H	4.302840	3.949610	1.138840
H	3.185280	3.129060	2.230920

H	3.945760	2.226950	0.908478
C	1.768820	6.087910	0.097040
H	2.382340	2.895290	-3.795030
C	-1.600540	1.395660	-0.782155
C	-1.342520	2.765740	-2.913100
H	-0.069611	1.164170	-2.270100
H	-2.021320	2.112070	-3.467890
H	-1.938760	3.584950	-2.490880
H	-0.641190	3.186880	-3.637570
H	-1.047960	0.865883	0.000493
H	-2.149960	2.203640	-0.281041
C	-2.604390	0.386534	-1.381860
C	-3.493380	-0.219272	-0.326865
H	-3.239920	0.894403	-2.119220
H	-2.054170	-0.386806	-1.929790
C	-3.585180	-1.503230	0.061892
C	-4.541580	-1.913020	1.158630
C	-2.784140	-2.643810	-0.519851
H	-2.193610	-3.136790	0.263733
H	-3.451470	-3.410220	-0.936764
H	-2.097360	-2.332180	-1.309050
H	-5.265430	-2.654670	0.794051
H	-4.004640	-2.384770	1.992770
H	-5.099700	-1.058880	1.553090
H	-4.131130	0.501225	0.189110
H	1.396370	6.980830	0.590139
H	2.079230	6.207660	-0.936987
H	1.477700	4.915220	1.784420

Cartesian Coordinates of Conformers (>2% population) of 1c

Conf 14

C	2.046990	1.489720	2.866520
C	1.961950	0.746950	1.540900
C	2.240880	-0.688072	1.760450
N	2.630660	-0.796511	3.102950
C	2.638900	0.401328	3.785730
C	0.607143	1.921520	3.457540
C	2.852210	2.830220	2.955990
C	1.786830	1.144010	0.264169
O	2.197950	-1.628940	0.983458
O	3.039110	0.526198	4.935590
H	2.949890	-1.666090	3.512710
H	1.796050	0.383601	-0.517142
O	1.634100	2.416380	-0.127279
C	1.446160	2.628550	-1.546580
H	0.505932	2.151210	-1.849680
C	1.413260	4.122680	-1.800020
H	2.271820	2.149380	-2.087020
H	1.262390	4.311020	-2.867780
H	0.596212	4.593390	-1.246210
H	2.353900	4.590450	-1.495700
C	-0.191036	2.647510	2.386740
C	-0.250832	0.721390	3.911780
C	1.005900	2.828250	4.636090
C	2.361810	3.492740	4.296890
H	2.453750	3.445070	2.140310
C	4.398920	2.820940	2.819520
H	2.250420	4.569100	4.142520
O	3.276980	3.383980	5.381090
H	1.147220	2.217470	5.531600
H	0.224998	3.553590	4.878780
H	-1.199480	1.085050	4.319070
H	-0.485771	0.052330	3.076450
H	0.245513	0.140117	4.694980
C	-0.607469	3.916540	2.390760
H	3.379790	2.435300	5.569880
C	4.915040	2.047380	1.587750
C	4.901910	4.277760	2.806450
H	4.818450	2.341190	3.710440
H	5.993910	4.320240	2.780770
H	4.525020	4.813490	1.924640
H	4.582430	4.813030	3.702860
H	4.530030	1.022340	1.607180
H	4.515100	2.506200	0.672985
C	6.453680	1.951750	1.460520
C	7.099780	1.208600	2.601390
H	6.665530	1.412200	0.524738
H	6.890190	2.946290	1.334920
C	8.147540	1.569560	3.362610
C	8.651080	0.666150	4.464960
C	8.921100	2.858150	3.215440
H	8.536830	3.507270	2.426300
H	8.909070	3.424360	4.156210
H	9.975860	2.648850	2.991450
H	9.702440	0.392545	4.301860

H	8.607110	1.172870	5.438470
H	8.066430	-0.255605	4.535890
H	6.642380	0.240964	2.820070
H	-1.213730	4.301130	1.575670
H	-0.370921	4.618460	3.184540
H	-0.483847	2.018840	1.547540

Conf 182

C	2.007720	1.596950	2.987660
C	2.247010	0.819167	1.701640
C	2.610270	-0.575667	2.029300
N	2.751590	-0.611442	3.424570
C	2.519510	0.596859	4.045060
C	0.446700	1.889130	3.282100
C	2.644580	3.016110	3.169830
C	2.285510	1.168150	0.399797
O	2.797330	-1.536020	1.299440
O	2.686150	0.790649	5.242450
H	3.069750	-1.434180	3.922390
H	2.518040	0.395510	-0.333383
O	2.089980	2.409470	-0.065578
C	2.181420	2.572750	-1.500910
H	3.155320	2.195880	-1.836590
C	2.019180	4.045790	-1.819570
H	1.392650	1.973030	-1.972000
H	1.051230	4.415480	-1.469890
H	2.808350	4.636410	-1.345670
H	2.077320	4.195990	-2.902340
C	-0.200261	2.503870	2.051500
C	-0.360029	0.616774	3.618250
C	0.523192	2.858730	4.475580
C	1.847350	3.652490	4.368540
H	2.349590	3.568460	2.269960
C	4.182440	3.165570	3.323300
H	1.662990	4.708260	4.153940
O	2.547620	3.660240	5.607440
H	0.549828	2.286490	5.406650
H	-0.356540	3.504550	4.537080
H	-1.399570	0.888955	3.826360
H	-0.365982	-0.091847	2.782570
H	0.033438	0.108000	4.503710
C	-0.734024	3.721630	1.925160
H	2.699640	2.730640	5.850750
C	4.996770	2.416460	2.246880
C	4.532940	4.666730	3.344950
H	4.467100	2.750690	4.297820
H	5.599360	4.825470	3.526730
H	4.284210	5.138230	2.384660
H	3.992910	5.186460	4.138880
H	4.718950	1.358440	2.238120
H	4.740870	2.807110	1.251500
C	6.528800	2.478360	2.438410
C	7.262750	1.673050	1.397760
H	6.867600	3.520040	2.370550
H	6.776770	2.140510	3.450720
C	8.013420	0.569290	1.560550

C	8.666790	-0.105164	0.375921
C	8.287700	-0.101902	2.885410
H	9.366650	-0.126875	3.089140
H	7.799160	0.388611	3.729360
H	7.951810	-1.147230	2.862140
H	9.757960	-0.143884	0.496680
H	8.326050	-1.144760	0.277690
H	8.447420	0.414498	-0.561506
H	7.147820	2.045740	0.377510
H	-1.207970	4.022710	0.995357
H	-0.725266	4.461310	2.719890
H	-0.262349	1.830300	1.198510

Conf 27

C	1.965930	1.645260	3.235370
C	2.224770	0.628504	2.132990
C	2.477260	-0.697686	2.734420
N	2.534270	-0.480354	4.119080
C	2.347190	0.833478	4.490750
C	0.415186	2.076990	3.364310
C	2.688330	3.034470	3.197470
C	2.360670	0.724904	0.794782
O	2.646380	-1.785630	2.206950
O	2.456630	1.237520	5.641220
H	2.767600	-1.211770	4.779840
H	2.584300	-0.182868	0.233931
O	2.272450	1.864880	0.096713
C	2.473660	1.752760	-1.332610
H	1.688220	1.108190	-1.746550
C	2.415390	3.145650	-1.927570
H	3.446810	1.280710	-1.514580
H	2.558460	3.088390	-3.011360
H	1.446850	3.613440	-1.730060
H	3.200370	3.781380	-1.508240
C	-0.117043	2.487810	2.000930
C	-0.495759	0.938536	3.871010
C	0.491732	3.246110	4.363240
C	1.871520	3.928440	4.202790
H	2.482560	3.424970	2.193920
C	4.221950	3.119230	3.423080
H	1.772700	4.934200	3.786360
O	2.500470	4.127770	5.463700
H	0.426907	2.856830	5.382680
H	-0.343385	3.941580	4.246130
H	-1.523930	1.304530	3.954470
H	-0.503873	0.088213	3.180040
H	-0.189347	0.581688	4.859190
C	-0.555125	3.689970	1.617930
H	2.573520	3.253290	5.883560
C	5.039390	2.144770	2.548790
C	4.675590	4.576390	3.204050
H	4.425600	2.869080	4.471470
H	5.739200	4.699790	3.426020
H	4.514260	4.881500	2.161340
H	4.131150	5.261790	3.856530
H	4.697730	1.119240	2.722880

H	4.854310	2.350490	1.485560
C	6.562170	2.170180	2.806140
C	7.273380	1.045070	2.100300
H	6.981480	3.136640	2.516570
H	6.731510	2.073430	3.889850
C	8.236460	1.112630	1.163920
C	8.830740	-0.145590	0.572814
C	8.826160	2.392100	0.619030
H	8.721230	2.429520	-0.473642
H	8.366200	3.292030	1.031520
H	9.903390	2.439640	0.828314
H	8.696500	-0.171712	-0.517287
H	9.913220	-0.192512	0.754077
H	8.376800	-1.047680	0.993109
H	6.944400	0.047311	2.398360
H	-0.953580	3.839580	0.618622
H	-0.538122	4.563260	2.262780
H	-0.178676	1.671490	1.283320

Conf 342

C	1.823830	1.866600	3.403160
C	2.129370	0.790528	2.375120
C	2.299500	-0.508467	3.055130
N	2.260850	-0.222786	4.430400
C	2.079200	1.110180	4.722800
C	0.275130	2.330170	3.381370
C	2.601240	3.226330	3.357510
C	2.325710	0.822433	1.042200
O	2.473930	-1.626560	2.597470
O	2.100400	1.570480	5.857620
H	2.415170	-0.927468	5.141440
H	2.532570	-0.115527	0.526782
O	2.337580	1.938240	0.299548
C	2.445390	1.750630	-1.130650
H	1.518470	1.286880	-1.489550
C	2.669020	3.106050	-1.771820
H	3.280910	1.069710	-1.334990
H	2.745530	2.990840	-2.857740
H	1.836610	3.782120	-1.556080
H	3.593310	3.563040	-1.406710
C	-0.123091	2.724250	1.969940
C	-0.681481	1.274520	3.956120
C	0.302976	3.616550	4.254670
C	1.735330	4.206360	4.227550
H	2.521100	3.567380	2.318470
C	4.110890	3.262880	3.722140
H	1.745390	5.198930	3.769840
O	2.233640	4.419440	5.542830
H	0.058648	3.368380	5.291440
H	-0.449372	4.335110	3.915060
H	-1.706490	1.657590	3.949220
H	-0.667862	0.346104	3.375670
H	-0.433208	1.037120	4.993710
C	-1.139540	2.239480	1.250480
H	2.226260	3.555500	5.991680
C	4.960440	2.228530	2.953150

C	4.643160	4.692860	3.502090
H	4.207610	3.040440	4.791700
H	5.689240	4.778260	3.808670
H	4.583140	4.972550	2.441530
H	4.077620	5.419800	4.088200
H	4.561680	1.223690	3.125010
H	4.877470	2.405920	1.872010
C	6.454320	2.201880	3.344860
C	7.176360	1.026200	2.739550
H	6.938750	3.140480	3.065310
H	6.523030	2.134840	4.441810
C	8.220450	1.024080	1.891840
C	8.810180	-0.275863	1.393860
C	8.909750	2.260030	1.363780
H	9.965610	2.271350	1.666310
H	8.902230	2.265120	0.265497
H	8.454440	3.190940	1.706870
H	8.771040	-0.332979	0.297413
H	9.869600	-0.359742	1.672150
H	8.283010	-1.144590	1.798650
H	6.779820	0.052954	3.036270
H	-1.356230	2.637630	0.263231
H	-1.791470	1.446730	1.602910
H	0.472268	3.520250	1.527420

Conf 34

C	2.058960	1.754220	3.145760
C	2.283710	0.875414	1.927040
C	2.656100	-0.485491	2.361420
N	2.811790	-0.407206	3.755820
C	2.575860	0.844161	4.278550
C	0.493288	2.054580	3.416860
C	2.708630	3.178520	3.207140
C	2.264750	1.120150	0.602117
O	2.838330	-1.503060	1.712680
O	2.738920	1.135370	5.457130
H	3.129860	-1.188450	4.316500
H	2.458470	0.292643	-0.080489
O	2.075750	2.328490	0.052523
C	1.951040	2.361110	-1.387880
H	1.003690	1.882090	-1.663870
C	1.988790	3.809080	-1.835530
H	2.775810	1.785920	-1.826800
H	1.887150	3.860150	-2.924280
H	1.169040	4.377810	-1.387140
H	2.934900	4.280410	-1.554050
C	-0.149550	2.606770	2.156760
C	-0.274914	0.833919	3.945670
C	0.553459	3.196320	4.470600
C	1.911900	3.928540	4.334480
H	2.442040	3.655950	2.256770
C	4.248590	3.318660	3.359430
H	1.770800	4.972420	4.042630
O	2.589650	3.999960	5.583190
H	0.494947	2.776340	5.478770
H	-0.297996	3.874920	4.360030

H	-1.316030	1.106250	4.144030
H	-0.276715	0.005725	3.229350
H	0.149437	0.475584	4.887000
C	-1.222350	2.128940	1.519100
H	2.722500	3.084070	5.885680
C	5.053170	2.485620	2.338530
C	4.621480	4.812310	3.280080
H	4.522310	2.967300	4.361430
H	5.691120	4.965430	3.446530
H	4.376480	5.223410	2.291370
H	4.093720	5.391860	4.040070
H	4.758520	1.434060	2.399790
H	4.804800	2.811410	1.318160
C	6.585530	2.536360	2.530230
C	7.308110	1.646940	1.551940
H	6.941580	3.564980	2.389510
H	6.825880	2.267370	3.564780
C	8.047890	0.550984	1.796450
C	8.690120	-0.218493	0.664826
C	8.319600	-0.020712	3.167700
H	7.837730	0.536482	3.973220
H	7.974430	-1.061740	3.224040
H	9.398830	-0.039898	3.370680
H	9.781110	-0.260888	0.786005
H	8.336920	-1.258400	0.646084
H	8.473940	0.231456	-0.308672
H	7.193720	1.942470	0.506729
H	-1.621400	2.642500	0.648940
H	-1.744970	1.229470	1.828120
H	0.302970	3.516800	1.768130

Conf 16

C	2.030140	1.544970	2.884070
C	1.909210	0.841732	1.539470
C	2.195530	-0.597966	1.708020
N	2.617350	-0.747454	3.036960
C	2.641740	0.428769	3.755740
C	0.607655	1.963830	3.524090
C	2.843650	2.879200	2.993120
C	1.687170	1.272420	0.280661
O	2.136020	-1.514890	0.903456
O	3.068480	0.518646	4.899390
H	2.946410	-1.628930	3.411950
H	1.674130	0.532537	-0.520317
O	1.487840	2.549670	-0.069014
C	1.332180	2.823190	-1.480990
H	0.743136	3.742400	-1.518700
C	2.674140	2.997960	-2.175550
H	0.743562	2.017090	-1.935960
H	2.513230	3.252830	-3.228720
H	3.249410	3.803430	-1.710090
H	3.267700	2.079070	-2.136000
C	-0.214085	2.723940	2.495590
C	-0.242845	0.753763	3.965270
C	1.039120	2.835000	4.717900
C	2.388460	3.504920	4.364080

H	2.428990	3.518970	2.204950
C	4.386800	2.867010	2.821650
H	2.277360	4.585590	4.243090
O	3.329740	3.362670	5.421840
H	1.200440	2.198520	5.591870
H	0.266915	3.555380	5.000040
H	-1.179710	1.108340	4.406500
H	-0.501065	0.109656	3.117300
H	0.270679	0.148818	4.718900
C	-0.610392	3.998680	2.539530
H	3.432510	2.408700	5.581800
C	4.873370	2.122280	1.560640
C	4.896210	4.321650	2.833470
H	4.823480	2.363710	3.690990
H	5.987580	4.360700	2.783680
H	4.501530	4.881030	1.974390
H	4.599820	4.835660	3.750060
H	4.479180	1.100610	1.558940
H	4.462050	2.608980	0.665826
C	6.408640	2.016840	1.403620
C	7.067550	1.237100	2.512280
H	6.599420	1.501460	0.449800
H	6.852090	3.010630	1.297870
C	8.133790	1.566650	3.261960
C	8.647840	0.629793	4.331010
C	8.919220	2.850030	3.132890
H	9.967200	2.634890	2.884010
H	8.528060	3.523320	2.367740
H	8.931010	3.392170	4.087730
H	9.692820	0.349309	4.140910
H	8.627860	1.111800	5.317750
H	8.054400	-0.287185	4.389640
H	6.603110	0.269335	2.714850
H	-1.233960	4.410270	1.751170
H	-0.338845	4.679340	3.340680
H	-0.541232	2.118770	1.652010

Conf 22

C	2.063850	1.731970	3.112350
C	2.322520	0.904111	1.861660
C	2.670130	-0.478774	2.248540
N	2.780990	-0.463831	3.647020
C	2.545730	0.768489	4.216930
C	0.500976	2.049700	3.364730
C	2.711290	3.151430	3.253400
C	2.393740	1.203440	0.548647
O	2.866460	-1.466960	1.558940
O	2.689320	1.005970	5.409450
H	3.083580	-1.269150	4.181630
H	2.641950	0.402471	-0.148402
O	2.227320	2.428190	0.032682
C	2.318670	2.545800	-1.406110
H	3.129390	1.899850	-1.764690
C	0.997761	2.217270	-2.085730
H	2.605750	3.585410	-1.578550
H	1.092740	2.364980	-3.166960

H	0.705992	1.176530	-1.911430
H	0.200197	2.869120	-1.717870
C	-0.114127	2.624940	2.099340
C	-0.325390	0.798658	3.731240
C	0.563789	3.062430	4.522500
C	1.896860	3.840330	4.410930
H	2.439220	3.671720	2.327550
C	4.247230	3.293330	3.431610
H	1.726220	4.888450	4.152090
O	2.573030	3.890340	5.662180
H	0.567983	2.525030	5.474440
H	-0.311118	3.717380	4.543140
H	-1.366180	1.088100	3.907480
H	-0.321212	0.059290	2.922620
H	0.044778	0.319749	4.643000
C	-0.623737	3.845600	1.914600
H	2.711320	2.969680	5.944290
C	5.075810	2.496570	2.401230
C	4.611110	4.791210	3.402520
H	4.508740	2.913820	4.426830
H	5.675400	4.947680	3.598320
H	4.384730	5.227430	2.420290
H	4.061200	5.345590	4.165660
H	4.787570	1.441630	2.426390
H	4.844900	2.851880	1.386760
C	6.604100	2.550880	2.622930
C	7.350920	1.698530	1.629970
H	6.955380	3.585700	2.522110
H	6.827330	2.250130	3.652580
C	8.080320	0.590553	1.850670
C	8.751580	-0.135898	0.707538
C	8.311780	-0.036243	3.205130
H	7.810300	0.491559	4.018410
H	7.960370	-1.076710	3.210930
H	9.384910	-0.069628	3.436630
H	9.838750	-0.186549	0.856694
H	8.396870	-1.173150	0.638046
H	8.563360	0.352850	-0.253000
H	7.266100	2.035690	0.594563
H	-1.074490	4.118290	0.964709
H	-0.616350	4.616090	2.679500
H	-0.171438	1.918850	1.272860

Conf 323

C	1.878220	1.815650	3.293890
C	2.161720	0.876433	2.130220
C	2.487630	-0.467855	2.649370
N	2.562870	-0.327116	4.043200
C	2.323680	0.953155	4.493130
C	0.311973	2.164190	3.475590
C	2.533550	3.238110	3.323070
C	2.269040	1.055340	0.797880
O	2.693150	-1.515580	2.057180
O	2.438950	1.296710	5.662680
H	2.845080	-1.082560	4.656040
H	2.528200	0.193122	0.182705

O	2.126120	2.229410	0.169306
C	2.255880	2.215940	-1.271320
H	3.070490	1.535680	-1.548370
C	0.950528	1.834770	-1.953490
H	2.555680	3.234080	-1.529100
H	1.074750	1.883710	-3.040710
H	0.646003	0.815685	-1.693930
H	0.148914	2.521660	-1.667210
C	-0.265811	2.626040	2.147690
C	-0.533711	0.956390	3.931970
C	0.353650	3.277240	4.538280
C	1.695610	4.033800	4.391900
H	2.289590	3.674090	2.347200
C	4.065610	3.386370	3.527910
H	1.540470	5.055240	4.035160
O	2.339940	4.192700	5.650840
H	0.328981	2.828330	5.534720
H	-0.515980	3.936640	4.476630
H	-1.576250	1.266720	4.054080
H	-0.515034	0.146806	3.193880
H	-0.190843	0.559847	4.892630
C	-0.760246	3.828020	1.840030
H	2.463430	3.300500	6.018370
C	4.913610	2.494520	2.596020
C	4.442560	4.873240	3.372890
H	4.298360	3.097150	4.559930
H	5.502790	5.040500	3.581400
H	4.244910	5.219900	2.349620
H	3.878010	5.497830	4.068090
H	4.711980	2.757940	1.547830
H	4.615840	1.447970	2.708670
C	6.436080	2.559200	2.852310
C	7.200960	1.615890	1.960470
H	6.798730	3.578460	2.667870
H	6.630020	2.351410	3.910450
C	7.915020	0.528015	2.299530
C	8.609180	-0.303125	1.244800
C	8.106340	0.025048	3.710720
H	7.746580	-1.008630	3.801150
H	9.172820	0.006710	3.972620
H	7.588230	0.627103	4.459450
H	9.691600	-0.347353	1.426860
H	8.247010	-1.340030	1.259610
H	8.450370	0.098137	0.239457
H	7.145640	1.858470	0.896962
H	-1.184310	4.016240	0.857910
H	-0.765889	4.664560	2.532080
H	-0.307964	1.848280	1.387270

Conf 15

C	1.940900	1.667620	3.237540
C	2.178110	0.676934	2.106490
C	2.477080	-0.654726	2.671540
N	2.573570	-0.465137	4.058260
C	2.374100	0.836819	4.463340
C	0.389773	2.075980	3.424990

C	2.645520	3.066230	3.206440
C	2.251770	0.797058	0.764881
O	2.652050	-1.728240	2.116350
O	2.511760	1.219260	5.618230
H	2.841650	-1.205370	4.695560
H	2.468920	-0.097614	0.180450
O	2.085560	1.939380	0.086978
C	2.283630	1.884170	-1.345360
H	1.664220	2.693130	-1.739580
C	3.745330	2.072770	-1.720930
H	1.888890	0.932325	-1.721380
H	3.848030	2.070020	-2.811620
H	4.122830	3.026730	-1.341760
H	4.369230	1.268830	-1.318040
C	-0.192316	2.506130	2.088190
C	-0.488434	0.915462	3.938980
C	0.483219	3.226740	4.443410
C	1.847800	3.930870	4.252590
H	2.406990	3.473760	2.216890
C	4.183590	3.165090	3.393110
H	1.722900	4.942490	3.857920
O	2.512780	4.116260	5.497140
H	0.456582	2.817310	5.456620
H	-0.364359	3.912660	4.366340
H	-1.518520	1.264630	4.061910
H	-0.506541	0.077921	3.232760
H	-0.145454	0.545267	4.910070
C	-0.645130	3.713220	1.739130
H	2.608460	3.235640	5.899160
C	4.991120	2.211570	2.487350
C	4.615290	4.630120	3.182480
H	4.416120	2.903850	4.432630
H	5.683000	4.762790	3.377880
H	4.422700	4.947920	2.148890
H	4.080790	5.300160	3.858720
H	4.658040	1.180980	2.647390
H	4.787870	2.435710	1.431450
C	6.517410	2.241350	2.722100
C	7.226220	1.137420	1.981250
H	6.926320	3.216940	2.448750
H	6.702760	2.121520	3.800960
C	8.196930	1.231380	1.055010
C	8.789950	-0.009547	0.427089
C	8.798700	2.525090	0.559199
H	8.706540	2.599220	-0.532732
H	8.338670	3.413280	0.996342
H	9.873650	2.560020	0.782164
H	9.870400	-0.068627	0.616658
H	8.327420	-0.922781	0.812537
H	8.666030	0.001918	-0.664490
H	6.890860	0.131808	2.243830
H	-1.077480	3.877470	0.756366
H	-0.607211	4.576510	2.396550
H	-0.277498	1.701300	1.360330

Conf 30

C	1.987480	1.716560	3.206370
C	2.242220	0.752141	2.056660
C	2.432140	-0.612402	2.589660
N	2.453140	-0.474210	3.985510
C	2.300720	0.823054	4.424760
C	0.451761	2.201960	3.316510
C	2.763540	3.076150	3.266240
C	2.424450	0.916070	0.730320
O	2.580730	-1.675230	2.007050
O	2.388530	1.158710	5.598860
H	2.640990	-1.248780	4.610600
H	2.638920	0.032563	0.128298
O	2.407700	2.094660	0.095105
C	2.609350	2.064440	-1.337190
H	3.380830	1.320950	-1.571510
C	1.314210	1.784730	-2.084780
H	3.001610	3.054510	-1.579550
H	1.497230	1.817640	-3.164280
H	0.916470	0.794576	-1.839760
H	0.556313	2.534760	-1.841020
C	-0.022364	2.707240	1.963620
C	-0.516404	1.074570	3.733710
C	0.542552	3.311520	4.380170
C	1.952080	3.945270	4.297240
H	2.602740	3.529240	2.280900
C	4.291990	3.088110	3.537630
H	1.905060	4.975750	3.935840
O	2.549880	4.048730	5.584570
H	0.431133	2.870930	5.374360
H	-0.261006	4.045400	4.277310
H	-1.532330	1.475170	3.807850
H	-0.534889	0.263451	2.997270
H	-0.253770	0.653521	4.709120
C	-0.395329	3.946490	1.633570
H	2.576350	3.149980	5.955910
C	5.097510	2.132960	2.631400
C	4.805910	4.536420	3.413730
H	4.455670	2.772330	4.575290
H	5.866360	4.605700	3.671370
H	4.686950	4.904820	2.385860
H	4.268530	5.205220	4.088890
H	4.714800	1.112860	2.739660
H	4.948880	2.403330	1.577050
C	6.612650	2.087690	2.928390
C	7.302370	0.976293	2.180750
H	7.074060	3.051950	2.702540
H	6.748790	1.926930	4.009170
C	8.288710	1.058620	1.270150
C	8.854460	-0.187273	0.627244
C	8.932750	2.343370	0.805120
H	10.006300	2.342320	1.037360
H	8.852070	2.441380	-0.285857
H	8.494800	3.236070	1.255520
H	8.744960	-0.152629	-0.465388
H	9.930240	-0.280754	0.829252
H	8.360990	-1.093610	0.989921

H	6.933440	-0.023497	2.419310
H	-0.755919	4.167020	0.633001
H	-0.359376	4.783120	2.324600
H	-0.097623	1.933140	1.202040

Conf 341

C	1.893400	1.796880	3.383510
C	2.195140	0.794383	2.278570
C	2.662030	-0.473188	2.876820
N	2.794900	-0.217469	4.249920
C	2.468820	1.070120	4.616650
C	0.313952	2.032470	3.625920
C	2.429300	3.264210	3.271440
C	2.199680	0.868486	0.931864
O	2.928290	-1.543680	2.353450
O	2.611570	1.512940	5.749240
H	3.171140	-0.896965	4.900010
H	2.489610	-0.019564	0.369409
O	1.881020	1.959310	0.223388
C	2.010500	1.865200	-1.214440
H	1.687910	0.867105	-1.535290
C	3.426920	2.171740	-1.676350
H	1.298970	2.597760	-1.602380
H	3.733660	3.169360	-1.349170
H	4.141950	1.441960	-1.283680
H	3.472800	2.138100	-2.770350
C	-0.367660	2.339970	2.302400
C	-0.402537	0.800764	4.218990
C	0.314705	3.225970	4.598140
C	1.578680	4.074030	4.320230
H	2.106100	3.601170	2.279430
C	3.951470	3.547990	3.388260
H	1.320600	5.047310	3.895000
O	2.267000	4.386060	5.526190
H	0.378191	2.856990	5.625220
H	-0.609558	3.806250	4.536380
H	-1.460300	1.034770	4.375440
H	-0.352031	-0.060991	3.544180
H	0.019787	0.511207	5.186200
C	-0.970561	3.472850	1.932150
H	2.480900	3.539560	5.955120
C	4.833020	2.646580	2.497850
C	4.199190	5.040410	3.091370
H	4.248450	3.369880	4.428760
H	5.250120	5.307320	3.232380
H	3.929940	5.280760	2.054030
H	3.615590	5.677320	3.759190
H	4.617370	1.593760	2.701830
H	4.580960	2.809480	1.440360
C	6.353500	2.841170	2.694260
C	7.162130	1.890300	1.850320
H	6.632810	3.866880	2.421710
H	6.592850	2.730670	3.757680
C	7.961370	0.883777	2.245910
C	8.688700	0.027941	1.234170
C	8.222830	0.501827	3.683520

H	9.293760	0.579153	3.914590
H	7.680090	1.119120	4.401750
H	7.942130	-0.545341	3.858680
H	9.775490	0.074391	1.387170
H	8.403750	-1.028100	1.334680
H	8.477040	0.341080	0.207472
H	7.064310	2.049010	0.774144
H	-1.458630	3.547560	0.964707
H	-1.005670	4.360380	2.556590
H	-0.388908	1.502230	1.607720

Conf 18

C	2.009280	1.687300	3.131570
C	2.244610	0.847935	1.883820
C	2.670750	-0.510971	2.276780
N	2.844060	-0.465834	3.668310
C	2.580350	0.765122	4.228560
C	0.446830	1.944980	3.449510
C	2.603820	3.133500	3.220840
C	2.222990	1.119570	0.562872
O	2.880450	-1.501970	1.595070
O	2.766080	1.030270	5.409430
H	3.205420	-1.247680	4.201250
H	2.463150	0.313715	-0.131367
O	1.934990	2.314300	0.030850
C	2.029460	2.428370	-1.408240
H	1.341300	3.237030	-1.664980
C	3.447280	2.744840	-1.859030
H	1.658230	1.501720	-1.862890
H	3.468180	2.871100	-2.947010
H	3.802780	3.670760	-1.397850
H	4.139190	1.938130	-1.597240
C	-0.249935	2.470230	2.204730
C	-0.307767	0.667706	3.875410
C	0.518834	2.981150	4.585670
C	1.810940	3.811860	4.400040
H	2.273610	3.625200	2.298190
C	4.138730	3.338360	3.335800
H	1.584660	4.846330	4.129180
O	2.537860	3.916120	5.619170
H	0.589071	2.462550	5.545450
H	-0.381390	3.599170	4.635180
H	-1.351110	0.916537	4.093600
H	-0.308163	-0.086456	3.080560
H	0.122877	0.222723	4.777760
C	-0.812835	3.667520	2.021360
H	2.725200	3.008050	5.913480
C	4.962010	2.545030	2.298810
C	4.442450	4.847620	3.254130
H	4.450560	2.997410	4.330320
H	5.506460	5.050250	3.403830
H	4.161240	5.248600	2.271040
H	3.900680	5.400950	4.023900
H	4.707090	1.482640	2.352570
H	4.693710	2.871400	1.284010
C	6.493250	2.650540	2.478930

C	7.242580	1.804270	1.482650
H	6.809030	3.693830	2.351580
H	6.751260	2.375620	3.507610
C	8.007420	0.720582	1.704120
C	8.675850	-0.003851	0.558063
C	8.284060	0.121015	3.062400
H	9.362200	0.121224	3.271870
H	7.784520	0.646622	3.878290
H	7.962440	-0.928661	3.090370
H	8.349750	-1.051680	0.511123
H	8.454440	0.464723	-0.405464
H	9.766790	-0.021377	0.685507
H	7.127900	2.123520	0.444461
H	-1.318240	3.902760	1.089180
H	-0.797251	4.453880	2.769900
H	-0.321248	1.745670	1.395560

Conf 6

C	2.077630	1.578530	2.932870
C	2.137400	0.814210	1.618250
C	2.560510	-0.578653	1.875970
N	2.890620	-0.628212	3.237560
C	2.735490	0.571121	3.898830
C	0.573693	1.863670	3.447500
C	2.732460	2.997600	3.036440
C	1.981050	1.173260	0.327970
O	2.660080	-1.527410	1.113820
O	3.059780	0.752056	5.065120
H	3.286920	-1.450730	3.676090
H	2.110030	0.408475	-0.438328
O	1.710720	2.416470	-0.092976
C	1.561460	2.587760	-1.522240
H	0.687232	2.013500	-1.853480
C	1.389250	4.067110	-1.804500
H	2.452640	2.186630	-2.020560
H	1.263030	4.223790	-2.880540
H	0.507692	4.460960	-1.291100
H	2.265350	4.631740	-1.473030
C	-0.243290	2.486640	2.327150
C	-0.174784	0.585853	3.883250
C	0.816767	2.823440	4.626870
C	2.112690	3.620210	4.342290
H	2.311780	3.557770	2.192980
C	4.276600	3.146550	2.971410
H	1.899980	4.677930	4.166840
O	2.980970	3.616270	5.469930
H	0.973932	2.243410	5.540000
H	-0.045935	3.467300	4.816550
H	-1.174660	0.852894	4.239630
H	-0.298255	-0.115155	3.050230
H	0.341584	0.070368	4.698870
C	-0.790073	3.704560	2.287590
H	3.165120	2.684410	5.680280
C	4.921330	2.419610	1.771250
C	4.629540	4.647030	2.966600
H	4.693010	2.715230	3.887810

H	5.711780	4.803350	2.991990
H	4.245220	5.135760	2.061170
H	4.212670	5.152700	3.839770
H	4.677620	1.353540	1.812970
H	4.483430	2.803840	0.839192
C	6.463310	2.525870	1.663390
C	7.207160	2.003890	2.866140
H	6.769300	1.990190	0.758835
H	6.746450	3.573580	1.497820
C	7.939700	0.880169	2.969940
C	8.621010	0.517913	4.269800
C	8.167000	-0.111759	1.853730
H	7.667080	0.160026	0.922119
H	9.239970	-0.216556	1.643560
H	7.809930	-1.108160	2.146480
H	8.277690	-0.459119	4.636150
H	9.708190	0.435755	4.134860
H	8.429840	1.259300	5.050880
H	7.131360	2.622050	3.761350
H	-1.392980	4.011620	1.437850
H	-0.667188	4.438590	3.078060
H	-0.427419	1.818980	1.487230

Conf 39

C	2.059970	1.632630	2.898460
C	1.917050	0.949964	1.548280
C	2.167650	-0.496575	1.697620
N	2.594740	-0.671546	3.024350
C	2.644530	0.493336	3.757490
C	0.637319	2.061370	3.535980
C	2.912750	2.941690	3.018380
C	1.677880	1.409180	0.303567
O	2.081150	-1.404320	0.885374
O	3.066000	0.561884	4.905150
H	2.896500	-1.566730	3.389630
H	1.620040	0.686036	-0.510140
O	1.526260	2.700550	-0.020081
C	1.309340	2.999010	-1.418760
H	0.766109	3.946870	-1.417060
C	2.619800	3.114760	-2.182740
H	0.656286	2.229890	-1.848140
H	2.416600	3.388810	-3.223720
H	3.259010	3.885400	-1.742180
H	3.167900	2.167240	-2.182580
C	-0.149805	2.882710	2.530040
C	-0.184191	0.866599	4.043820
C	1.065700	2.998930	4.700120
C	2.464880	3.582130	4.381370
H	2.542320	3.598020	2.221590
C	4.457120	2.875320	2.861300
H	2.424720	4.669050	4.272520
O	3.372330	3.368780	5.455960
H	1.141410	2.427760	5.629750
H	0.317403	3.779760	4.867570
H	-1.115140	1.220610	4.497080
H	-0.447607	0.174535	3.237100

H	0.357528	0.311034	4.813470
C	-1.389010	2.649530	2.087930
H	3.428900	2.406500	5.592320
C	4.921500	2.142860	1.584470
C	5.023390	4.307760	2.911530
H	4.865590	2.334650	3.721680
H	6.115360	4.303710	2.862610
H	4.653500	4.905070	2.066900
H	4.747250	4.809110	3.841270
H	4.531210	2.665500	0.700329
H	4.489480	1.137160	1.556780
C	6.452330	1.985040	1.428750
C	7.079660	1.159020	2.522090
H	6.626630	1.483090	0.464737
H	6.931860	2.963950	1.344390
C	8.154060	1.435110	3.281690
C	8.631990	0.457750	4.331040
C	8.983740	2.693100	3.182890
H	8.617280	3.397150	2.433340
H	10.024000	2.447580	2.929760
H	9.013010	3.212210	4.150070
H	9.667370	0.145842	4.137470
H	8.625140	0.918142	5.328210
H	8.007290	-0.439390	4.367590
H	6.581360	0.203743	2.702090
H	-1.867320	3.338930	1.398050
H	-1.972930	1.784740	2.386030
H	0.352101	3.778850	2.170820

Conf 47

C	2.042400	1.789700	3.143170
C	2.242870	0.954378	1.889590
C	2.624250	-0.419792	2.268380
N	2.809650	-0.390174	3.661230
C	2.583980	0.841831	4.232150
C	0.482537	2.076620	3.458010
C	2.692530	3.211880	3.240680
C	2.198410	1.241970	0.573364
O	2.795410	-1.413920	1.580780
O	2.771620	1.092540	5.416460
H	3.140110	-1.190100	4.187290
H	2.384850	0.436134	-0.136675
O	1.962310	2.458260	0.063149
C	1.992480	2.575390	-1.378420
H	1.348800	3.430170	-1.598930
C	3.404680	2.797990	-1.898250
H	1.535810	1.679750	-1.816220
H	3.380880	2.928630	-2.985650
H	3.844860	3.695030	-1.453110
H	4.052510	1.945040	-1.672800
C	-0.188876	2.664310	2.229190
C	-0.271338	0.838297	3.966330
C	0.561955	3.185090	4.545460
C	1.916570	3.923140	4.407200
H	2.409150	3.721200	2.311780
C	4.234790	3.348330	3.373030

H	1.769250	4.975960	4.153100
O	2.618360	3.953590	5.644450
H	0.522618	2.734090	5.541120
H	-0.292041	3.865450	4.471810
H	-1.307600	1.102510	4.198260
H	-0.289966	0.033119	3.224460
H	0.175674	0.451478	4.885620
C	-1.282570	2.210760	1.609910
H	2.756890	3.028250	5.913760
C	5.026930	2.547500	2.317370
C	4.606030	4.844020	3.333060
H	4.523100	2.967540	4.359950
H	5.678670	4.992890	3.483440
H	4.341730	5.285580	2.362580
H	4.093030	5.399530	4.120640
H	4.721690	1.497450	2.337180
H	4.779570	2.916130	1.311510
C	6.560360	2.575610	2.507060
C	7.274720	1.730610	1.484360
H	6.925190	3.606780	2.417450
H	6.799930	2.253270	3.526400
C	7.990110	0.607312	1.670720
C	8.629420	-0.107085	0.501988
C	8.235470	-0.049221	3.008490
H	9.311920	-0.105074	3.219180
H	7.758160	0.471133	3.840900
H	7.866360	-1.083500	3.000970
H	8.257170	-1.137150	0.419127
H	8.432130	0.403118	-0.445492
H	9.718090	-0.177376	0.630654
H	7.177470	2.089240	0.457339
H	-1.697820	2.746400	0.761023
H	-1.805180	1.308960	1.912100
H	0.262032	3.578590	1.848620

Conf 42

C	1.972510	1.769210	3.241810
C	2.173700	0.786475	2.100210
C	2.429560	-0.559604	2.647150
N	2.540270	-0.388187	4.037620
C	2.379440	0.912808	4.457950
C	0.426369	2.203240	3.428470
C	2.727770	3.141820	3.224610
C	2.223420	0.927586	0.760311
O	2.565360	-1.633330	2.081840
O	2.521670	1.279770	5.617910
H	2.779270	-1.145660	4.666140
H	2.387020	0.036360	0.154245
O	2.108410	2.091980	0.108242
C	2.239320	2.046380	-1.332040
H	1.752610	1.136440	-1.702920
C	3.693960	2.124960	-1.769840
H	1.669940	2.908250	-1.687870
H	3.749140	2.133320	-2.863930
H	4.163440	3.038730	-1.394210
H	4.268220	1.266850	-1.406840

C	-0.130788	2.696450	2.104650
C	-0.448996	1.088130	4.020400
C	0.536954	3.418220	4.392710
C	1.952050	4.033850	4.259310
H	2.533480	3.563820	2.231250
C	4.267080	3.176680	3.431980
H	1.903310	5.059900	3.885690
O	2.588690	4.149560	5.526320
H	0.408645	3.086300	5.426960
H	-0.254436	4.147320	4.193350
H	-1.472080	1.451160	4.157890
H	-0.491297	0.208183	3.370030
H	-0.083656	0.775706	5.001960
C	-1.222870	2.257150	1.472390
H	2.638030	3.252240	5.901000
C	5.044170	2.213340	2.509800
C	4.760250	4.627390	3.262220
H	4.475680	2.881260	4.467210
H	5.831930	4.708900	3.463370
H	4.585890	4.981320	2.237040
H	4.252680	5.301020	3.955410
H	4.666850	1.193960	2.639220
H	4.860880	2.472220	1.457970
C	6.567810	2.173620	2.759730
C	7.237290	1.057520	2.000740
H	7.020460	3.136830	2.512590
H	6.736630	2.021790	3.837280
C	8.220550	1.131130	1.086050
C	8.767470	-0.119433	0.435836
C	8.880780	2.409020	0.624802
H	8.454410	3.305960	1.077920
H	9.954110	2.393590	0.857578
H	8.802020	2.511180	-0.465909
H	8.655450	-0.078437	-0.656306
H	9.842450	-0.228231	0.634276
H	8.262990	-1.020660	0.796059
H	6.857260	0.061449	2.237390
H	-1.548890	2.722650	0.546662
H	-1.830580	1.435670	1.837810
H	0.410663	3.526590	1.655530

Conf 56

C	2.031030	1.630160	3.322350
C	2.384480	0.640606	2.218450
C	2.432310	-0.727808	2.778470
N	2.243430	-0.581999	4.158910
C	2.083240	0.722088	4.570920
C	0.542210	2.241730	3.201490
C	2.904260	2.918600	3.524760
C	2.696790	0.755860	0.910252
O	2.619060	-1.800170	2.225160
O	1.988340	1.054770	5.745390
H	2.291010	-1.360980	4.804640
H	2.928780	-0.158176	0.362923
O	2.756030	1.903020	0.222335
C	3.240960	1.801510	-1.140600

H	2.649450	1.041620	-1.666020
C	3.100290	3.161760	-1.794200
H	4.288060	1.478030	-1.111830
H	3.468340	3.112470	-2.823990
H	2.054330	3.480530	-1.814650
H	3.683000	3.914590	-1.255920
C	0.315876	2.783080	1.799530
C	-0.564221	1.196150	3.457240
C	0.558371	3.344230	4.275970
C	2.011710	3.853900	4.426910
H	2.945030	3.389760	2.535850
C	4.353830	2.784170	4.066590
H	2.114980	4.884740	4.077890
O	2.394990	3.904280	5.796870
H	0.251395	2.920900	5.235720
H	-0.151835	4.144240	4.052240
H	-1.545070	1.675810	3.379900
H	-0.533921	0.387265	2.718660
H	-0.486803	0.758640	4.457310
C	0.115880	4.051180	1.431060
H	2.272740	3.008710	6.156380
C	5.282980	1.802310	3.313040
C	5.008580	4.177370	4.166090
H	4.279450	2.400500	5.090380
H	6.053300	4.083960	4.485120
H	5.003250	4.697550	3.200580
H	4.490890	4.800890	4.897140
H	6.176920	1.656760	3.934400
H	4.813330	0.814937	3.242300
C	5.745540	2.238840	1.906570
C	6.467120	1.132210	1.181370
H	4.868060	2.541280	1.320580
H	6.376920	3.127630	1.988040
C	7.695630	1.140370	0.632841
C	8.250230	-0.092913	-0.043322
C	8.633060	2.324530	0.627572
H	8.875140	2.620430	-0.402241
H	8.229570	3.199380	1.140650
H	9.586010	2.061850	1.105880
H	8.502840	0.110971	-1.092950
H	9.179510	-0.421779	0.441248
H	7.541950	-0.926221	-0.018229
H	5.908180	0.195739	1.117990
H	-0.074796	4.299770	0.391131
H	0.134190	4.884400	2.126860
H	0.274218	2.017770	1.027220

Conf 53

C	2.096970	1.827050	3.116830
C	2.325190	1.002930	1.860310
C	2.640400	-0.389434	2.234580
N	2.766210	-0.385228	3.634260
C	2.560390	0.846469	4.213160
C	0.536734	2.162190	3.371780
C	2.789360	3.225490	3.261590
C	2.375720	1.313990	0.549763

O	2.805240	-1.379640	1.539970
O	2.707170	1.074660	5.407700
H	3.046150	-1.203220	4.161870
H	2.584270	0.514335	-0.161195
O	2.243970	2.550610	0.049547
C	2.329960	2.679030	-1.389240
H	3.125250	2.018730	-1.756130
C	1.000800	2.385940	-2.068320
H	2.640680	3.713290	-1.553850
H	1.100150	2.535820	-3.148940
H	0.682673	1.353060	-1.895780
H	0.219018	3.053990	-1.696590
C	-0.062238	2.787740	2.124510
C	-0.279267	0.944409	3.831340
C	0.607527	3.253910	4.477220
C	1.991450	3.945730	4.407060
H	2.559700	3.757110	2.330460
C	4.329090	3.309910	3.454140
H	1.891100	5.006790	4.164640
O	2.642280	3.932900	5.672090
H	0.509815	2.791980	5.463820
H	-0.218570	3.964560	4.376700
H	-1.314100	1.241470	4.027040
H	-0.296304	0.150894	3.076920
H	0.117074	0.529483	4.761530
C	-1.158480	2.394130	1.469880
H	2.739490	2.999260	5.930740
C	5.133700	2.502020	2.413290
C	4.748390	4.793400	3.454790
H	4.568150	2.903280	4.444020
H	5.818250	4.905050	3.650290
H	4.537690	5.258480	2.482200
H	4.221960	5.352530	4.230830
H	4.803840	1.459230	2.413650
H	4.924070	2.886810	1.404800
C	6.661160	2.492030	2.646450
C	7.381670	1.631800	1.640950
H	7.053430	3.514180	2.569860
H	6.864430	2.161390	3.671020
C	8.076940	0.499028	1.845000
C	8.726100	-0.230117	0.690856
C	8.289220	-0.154991	3.189690
H	7.805730	0.376257	4.011590
H	7.904890	-1.183720	3.180370
H	9.360940	-0.225893	3.419160
H	9.811240	-0.315636	0.838816
H	8.340360	-1.255070	0.606135
H	8.552580	0.278282	-0.262209
H	7.308020	1.987230	0.610812
H	-1.520100	2.954270	0.612379
H	-1.736400	1.519640	1.750740
H	0.447305	3.678770	1.763180

Cartesian Coordinates of Conformers (>2% population) of 1d

Conf 9

C	-0.293099	-1.816240	-1.458090
C	0.663116	-0.651326	-1.215110
C	-0.108303	0.596564	-1.061280
N	-1.448730	0.241602	-1.326880
C	-1.637210	-1.082710	-1.635760
C	-0.421222	-2.828810	-0.206841
C	-0.012085	-2.795130	-2.649050
C	2.012280	-0.715982	-1.212240
O	0.241791	1.731730	-0.794495
O	-2.712970	-1.563620	-1.973320
H	-2.195670	0.925250	-1.353460
H	2.517570	-1.663630	-1.394990
O	2.805430	0.342550	-1.005470
C	4.227080	0.109257	-1.110460
H	4.454850	-0.240226	-2.125620
C	4.935930	1.414160	-0.805587
H	4.511620	-0.675744	-0.397637
H	4.636470	2.190990	-1.514470
H	4.696090	1.757860	0.204475
H	6.019020	1.272250	-0.879010
C	0.964078	-3.215920	0.288417
C	-1.165310	-2.215310	0.997338
C	-1.193360	-4.014140	-0.821592
C	-0.898103	-4.056970	-2.340710
H	1.030160	-3.114790	-2.511150
C	-0.152051	-2.302000	-4.115040
H	-0.344134	-4.959320	-2.613500
O	-2.096920	-4.134800	-3.101470
H	-2.266880	-3.851060	-0.696205
H	-0.961508	-4.955990	-0.316887
H	-1.222160	-2.949250	1.807970
H	-0.644307	-1.333250	1.386530
H	-2.188610	-1.929110	0.737481
C	1.612950	-4.369960	0.103289
H	-2.632480	-3.357230	-2.864070
C	0.625837	-1.004310	-4.423420
C	0.279990	-3.437570	-5.063860
H	-1.212560	-2.105170	-4.306300
H	0.145423	-3.151440	-6.110070
H	1.340800	-3.685180	-4.920320
H	-0.314913	-4.337940	-4.899510
H	0.341343	-0.220136	-3.714930
H	1.701190	-1.173860	-4.267420
C	0.420342	-0.431993	-5.845950
C	-1.003310	-0.020381	-6.119880
H	1.065170	0.455891	-5.929770
H	0.783893	-1.135630	-6.599610
C	-1.789590	-0.333383	-7.164590
C	-3.202730	0.195402	-7.255370
C	-1.378200	-1.204710	-8.327370
H	-0.360509	-1.590420	-8.242110
H	-2.058220	-2.061160	-8.426530
H	-1.444650	-0.643637	-9.269290
H	-3.459250	0.823215	-6.397180

H	-3.343750	0.789987	-8.168240
H	-3.927630	-0.628355	-7.303450
H	-1.435540	0.628278	-5.354640
H	2.591440	-4.534030	0.546120
H	1.205230	-5.191930	-0.478000
H	1.450460	-2.453530	0.895884

Conf 16

C	-0.514204	-2.090220	-1.331260
C	0.252517	-0.770364	-1.336640
C	-0.680201	0.343136	-1.081320
N	-1.964660	-0.243975	-1.059640
C	-1.974600	-1.600090	-1.269250
C	-0.224336	-3.008260	-0.034745
C	-0.298111	-3.103170	-2.507330
C	1.566410	-0.613392	-1.608140
O	-0.489581	1.536680	-0.935850
O	-2.994650	-2.273390	-1.366970
H	-2.810480	0.305310	-0.965052
H	2.183280	-1.476030	-1.857670
O	2.188870	0.571082	-1.600130
C	3.563350	0.577678	-2.044900
H	3.593610	0.279429	-3.100420
C	4.107160	1.979760	-1.853710
H	4.131010	-0.155258	-1.456540
H	4.067950	2.270350	-0.800122
H	5.148390	2.021090	-2.189540
H	3.524470	2.701270	-2.432860
C	1.275860	-3.125810	0.188073
C	-0.820334	-2.429360	1.265070
C	-0.881965	-4.347370	-0.426845
C	-0.879377	-4.461720	-1.970830
H	0.790382	-3.240790	-2.565880
C	-0.793944	-2.753200	-3.936660
H	-0.241449	-5.283040	-2.308360
O	-2.170050	-4.787740	-2.470830
H	-1.923390	-4.350510	-0.094768
H	-0.397925	-5.196840	0.062674
H	-0.592858	-3.096080	2.103350
H	-0.396344	-1.446640	1.500320
H	-1.908350	-2.333790	1.203810
C	2.067780	-4.172160	-0.067129
H	-2.775800	-4.091190	-2.161200
C	-0.316265	-1.378400	-4.452070
C	-0.372976	-3.880580	-4.900890
H	-1.890510	-2.734290	-3.916770
H	-0.757002	-3.704080	-5.909200
H	0.721515	-3.946570	-4.969070
H	-0.762342	-4.846670	-4.574610
H	0.782305	-1.355010	-4.496620
H	-0.601751	-0.595524	-3.742860
C	-0.879614	-0.977833	-5.833300
C	-0.560639	0.453543	-6.179000
H	-0.511995	-1.655240	-6.607670
H	-1.973340	-1.103110	-5.808710
C	0.135605	0.931994	-7.225420

C	0.346718	2.418940	-7.398870
C	0.754992	0.086888	-8.313450
H	1.832350	0.286435	-8.389330
H	0.622381	-0.985582	-8.158910
H	0.323499	0.340782	-9.291100
H	1.417040	2.665460	-7.424170
H	-0.075530	2.768070	-8.351040
H	-0.115622	2.993560	-6.591150
H	-0.950533	1.185800	-5.469070
H	3.126200	-4.139500	0.175990
H	1.705840	-5.094580	-0.512058
H	1.729560	-2.247590	0.645931

Conf 266

C	-0.498176	-2.252090	-1.278990
C	0.154420	-0.872341	-1.305120
C	-0.890026	0.168050	-1.253700
N	-2.115280	-0.529762	-1.338150
C	-1.989000	-1.892680	-1.435360
C	-0.301753	-3.038080	0.118278
C	-0.053554	-3.327500	-2.328000
C	1.475090	-0.618115	-1.429210
O	-0.816205	1.380820	-1.180960
O	-2.930140	-2.661110	-1.600730
H	-3.007680	-0.053640	-1.392150
H	2.185820	-1.437890	-1.528050
O	1.994260	0.615377	-1.449200
C	3.414630	0.710403	-1.693570
H	3.630380	0.301465	-2.688850
C	3.804900	2.172510	-1.603290
H	3.945330	0.108063	-0.944543
H	4.878360	2.280660	-1.789350
H	3.260360	2.763380	-2.344850
H	3.580160	2.572570	-0.610618
C	1.162810	-3.002430	0.528263
C	-1.102130	-2.417900	1.282130
C	-0.794248	-4.457110	-0.231385
C	-0.582559	-4.689670	-1.747020
H	1.041350	-3.366540	-2.246250
C	-0.395289	-3.140120	-3.831390
H	0.160194	-5.470750	-1.930430
O	-1.766140	-5.174180	-2.368910
H	-1.866420	-4.527760	-0.030596
H	-0.311868	-5.219050	0.386909
H	-0.928977	-2.994650	2.196660
H	-0.792437	-1.385400	1.479270
H	-2.177870	-2.427010	1.083660
C	2.062360	-3.988800	0.457605
H	-2.463040	-4.516090	-2.198220
C	-0.000994	-1.761780	-4.405110
C	0.257334	-4.283540	-4.634120
H	-1.481450	-3.243210	-3.942390
H	-0.007427	-4.228610	-5.693330
H	1.352480	-4.234130	-4.562680
H	-0.072821	-5.259160	-4.272350
H	-0.436661	-0.962530	-3.799280

H	1.089310	-1.628840	-4.337660
C	-0.449763	-1.522380	-5.864320
C	-0.095153	-0.139636	-6.346330
H	0.033810	-2.253110	-6.525100
H	-1.527170	-1.706070	-5.940390
C	-0.915480	0.867837	-6.692720
C	-0.359518	2.198830	-7.144560
C	-2.424080	0.799573	-6.675760
H	-2.835070	1.578440	-6.019700
H	-2.830150	0.991248	-7.678080
H	-2.811190	-0.163112	-6.336700
H	-0.705428	2.447480	-8.157090
H	-0.701746	3.010530	-6.488520
H	0.734477	2.203650	-7.148650
H	0.977939	0.055386	-6.402950
H	3.075560	-3.843330	0.821880
H	1.834720	-4.969880	0.050825
H	1.482540	-2.055650	0.961993

Conf 290

C	-0.463577	-2.352930	-1.355190
C	0.138831	-0.952286	-1.349430
C	-0.939044	0.050667	-1.283680
N	-2.141750	-0.686931	-1.368090
C	-1.970450	-2.042120	-1.479560
C	-0.214764	-3.163320	0.018727
C	-0.017485	-3.386720	-2.447270
C	1.453130	-0.648077	-1.416410
O	-0.907872	1.264420	-1.196240
O	-2.887290	-2.841330	-1.638550
H	-3.050460	-0.241011	-1.403540
H	2.199310	-1.435620	-1.504210
O	1.925260	0.603548	-1.400300
C	3.358210	0.749982	-1.502100
H	3.696220	0.291346	-2.440450
C	3.677340	2.231650	-1.468110
H	3.828190	0.220864	-0.663083
H	4.759690	2.378540	-1.543130
H	3.195480	2.749800	-2.301810
H	3.327550	2.680630	-0.534365
C	1.271340	-3.227420	0.328899
C	-1.008890	-2.590160	1.201060
C	-0.674238	-4.597530	-0.358506
C	-0.490889	-4.779850	-1.887160
H	1.081010	-3.392000	-2.413830
C	-0.408086	-3.164750	-3.934220
H	0.270159	-5.533130	-2.107520
O	-1.673660	-5.283640	-2.493160
H	-1.735490	-4.720670	-0.126476
H	-0.132096	-5.352620	0.219273
H	-0.826715	-3.184820	2.101540
H	-0.727754	-1.554630	1.419910
H	-2.083770	-2.619410	1.004190
C	1.898740	-2.766280	1.415400
H	-2.385020	-4.651350	-2.286940
C	-0.037828	-1.766990	-4.476700

C	0.231364	-4.278170	-4.788160
H	-1.496120	-3.274360	-4.016010
H	-0.064744	-4.194430	-5.837100
H	1.327720	-4.218820	-4.748010
H	-0.078869	-5.267030	-4.445630
H	-0.458861	-0.988559	-3.834940
H	1.053460	-1.630920	-4.434780
C	-0.527904	-1.485560	-5.914930
C	-0.187118	-0.088878	-6.365890
H	-0.063326	-2.196020	-6.610520
H	-1.607100	-1.667650	-5.965800
C	-1.016910	0.929324	-6.653190
C	-0.473977	2.273360	-7.081650
C	-2.524130	0.861940	-6.586560
H	-2.964230	1.087470	-7.567210
H	-2.901120	-0.111243	-6.266550
H	-2.910380	1.618670	-5.890780
H	-0.792032	3.064170	-6.388970
H	0.619239	2.277160	-7.122870
H	-0.853684	2.554190	-8.073460
H	0.883817	0.107088	-6.451810
H	2.964990	-2.926390	1.549080
H	1.388990	-2.226630	2.207080
H	1.873390	-3.767660	-0.402304

Conf 1

C	-0.327721	-1.923340	-1.451860
C	0.600754	-0.717869	-1.328040
C	-0.199129	0.521482	-1.309360
N	-1.530350	0.110076	-1.535140
C	-1.687960	-1.242600	-1.704660
C	-0.436560	-2.808120	-0.105856
C	-0.021372	-3.010510	-2.538430
C	1.950890	-0.751244	-1.312120
O	0.124908	1.686300	-1.165500
O	-2.751970	-1.780520	-1.989800
H	-2.291190	0.770211	-1.641320
H	2.478290	-1.701130	-1.391220
O	2.719220	0.341027	-1.215490
C	4.146530	0.128638	-1.278190
H	4.438400	-0.561484	-0.475801
C	4.824310	1.475450	-1.120280
H	4.394600	-0.331563	-2.243250
H	5.910970	1.349810	-1.165030
H	4.564140	1.929130	-0.159890
H	4.518320	2.157710	-1.918150
C	0.955527	-3.113190	0.426464
C	-1.197130	-2.093630	1.030340
C	-1.180480	-4.066300	-0.599159
C	-0.882211	-4.253150	-2.106880
H	1.027010	-3.292350	-2.368460
C	-0.166837	-2.666130	-4.045680
H	-0.309983	-5.166760	-2.289750
O	-2.078330	-4.429160	-2.855780
H	-2.257610	-3.916420	-0.489410
H	-0.927481	-4.947770	-0.003731

H	-1.238300	-2.742740	1.911240
H	-0.697464	-1.164700	1.327550
H	-2.226320	-1.859200	0.743352
C	1.630150	-4.265250	0.357362
H	-2.631360	-3.645050	-2.690410
C	0.597794	-1.394040	-4.473360
C	0.278025	-3.883360	-4.880780
H	-1.230870	-2.502050	-4.246510
H	0.138341	-3.704750	-5.950590
H	1.342770	-4.100500	-4.719100
H	-0.302954	-4.771480	-4.625720
H	0.266001	-0.541733	-3.873690
H	1.668370	-1.524250	-4.255490
C	0.454252	-0.986882	-5.961370
C	-0.966065	-0.740775	-6.403030
H	1.066780	-0.093262	-6.118710
H	0.894660	-1.764610	-6.598700
C	-1.559500	0.434589	-6.679810
C	-3.005640	0.487177	-7.116670
C	-0.886929	1.784450	-6.597580
H	-1.420070	2.437040	-5.893550
H	0.155216	1.732330	-6.277060
H	-0.916647	2.289860	-7.572310
H	-3.603420	1.100490	-6.428850
H	-3.100250	0.949527	-8.108710
H	-3.455020	-0.509031	-7.160930
H	-1.581730	-1.635190	-6.504340
H	2.610700	-4.362940	0.815000
H	1.242130	-5.149630	-0.139713
H	1.423090	-2.283730	0.955831

Conf 27

C	-0.458608	-2.029520	-1.389760
C	0.263781	-0.684761	-1.425380
C	-0.700530	0.400322	-1.168400
N	-1.964270	-0.228539	-1.113480
C	-1.933140	-1.586670	-1.305780
C	-0.115543	-2.923080	-0.090028
C	-0.231735	-3.047340	-2.559520
C	1.565200	-0.486891	-1.729970
O	-0.547253	1.601430	-1.040980
O	-2.931890	-2.294650	-1.375350
H	-2.825980	0.293847	-1.010340
H	2.211010	-1.332800	-1.964390
O	2.132670	0.721643	-1.806320
C	3.548280	0.771279	-2.080020
H	3.694700	1.714910	-2.610470
C	4.364640	0.728355	-0.796843
H	3.814610	-0.049920	-2.757960
H	4.226230	-0.220092	-0.267334
H	5.429680	0.834992	-1.030270
H	4.072400	1.543990	-0.129333
C	1.391540	-2.989280	0.105666
C	-0.705770	-2.349590	1.214850
C	-0.735707	-4.287250	-0.455521
C	-0.757400	-4.418520	-1.998040

H	0.859409	-3.149390	-2.637910
C	-0.765906	-2.729530	-3.982510
H	-0.098697	-5.221890	-2.338850
O	-2.045500	-4.792910	-2.470130
H	-1.770300	-4.320380	-0.104417
H	-0.215379	-5.115020	0.034020
H	-0.440571	-2.998800	2.055810
H	-0.310476	-1.350650	1.431110
H	-1.797300	-2.290690	1.173410
C	2.212410	-4.012200	-0.153062
H	-2.668320	-4.113150	-2.157100
C	-0.341939	-1.346630	-4.523010
C	-0.327876	-3.854400	-4.942240
H	-1.861940	-2.745140	-3.941120
H	-0.735500	-3.701390	-5.945060
H	0.766721	-3.887100	-5.030140
H	-0.680954	-4.828270	-4.598320
H	0.754062	-1.290580	-4.593470
H	-0.634618	-0.564387	-3.816070
C	-0.949258	-0.979315	-5.894800
C	-0.673984	0.454107	-6.268250
H	-0.584662	-1.658480	-6.668990
H	-2.038630	-1.130900	-5.840640
C	-0.024545	0.933997	-7.343670
C	0.148582	2.422770	-7.541460
C	0.575650	0.088789	-8.442330
H	0.472770	-0.984303	-8.270350
H	0.104747	0.320346	-9.407280
H	1.644940	0.311185	-8.558180
H	1.212000	2.691410	-7.604300
H	-0.311678	2.751090	-8.483390
H	-0.299497	2.997320	-6.725720
H	-1.055230	1.186760	-5.554090
H	3.273590	-3.943190	0.069603
H	1.872250	-4.950630	-0.581348
H	1.824010	-2.091120	0.545155

Conf 21

C	-0.254786	-1.803510	-1.325520
C	0.824371	-0.738924	-1.161710
C	0.195401	0.583144	-0.992081
N	-1.190380	0.361964	-1.153870
C	-1.531970	-0.940865	-1.411140
C	-0.383041	-2.791300	-0.055337
C	-0.178505	-2.803990	-2.531280
C	2.159090	-0.944417	-1.190120
O	0.673782	1.682550	-0.779694
O	-2.673600	-1.318050	-1.651660
H	-1.865850	1.116560	-1.139790
H	2.561670	-1.941650	-1.357400
O	3.062290	0.031762	-1.041920
C	4.449760	-0.364886	-1.095900
H	4.642550	-1.085810	-0.291097
C	5.296370	0.882206	-0.933458
H	4.642340	-0.854431	-2.059520
H	5.088390	1.367860	0.023956

H	5.089870	1.597020	-1.734850
H	6.357690	0.615520	-0.967310
C	0.958014	-3.439620	0.244745
C	-0.957391	-2.094050	1.186150
C	-1.325640	-3.900190	-0.596561
C	-1.159090	-3.970430	-2.136600
H	0.836777	-3.223930	-2.497800
C	-0.392856	-2.292280	-3.981910
H	-0.723620	-4.924880	-2.444260
O	-2.417650	-3.927100	-2.795300
H	-2.365530	-3.642610	-0.378848
H	-1.126930	-4.861010	-0.111491
H	-1.048160	-2.807200	2.011300
H	-0.321333	-1.269010	1.523920
H	-1.956560	-1.697660	0.987656
C	1.665660	-3.364500	1.376330
H	-2.850290	-3.099270	-2.520180
C	0.507962	-1.096610	-4.360960
C	-0.183961	-3.465550	-4.959800
H	-1.434840	-1.968760	-4.079010
H	-0.376594	-3.159080	-5.991020
H	0.849350	-3.836150	-4.911110
H	-0.863301	-4.290720	-4.738550
H	0.383267	-0.288309	-3.634000
H	1.563710	-1.397780	-4.295160
C	0.254947	-0.494621	-5.763310
C	-1.125490	0.089970	-5.917850
H	0.994249	0.308200	-5.904560
H	0.464933	-1.232510	-6.542250
C	-2.030150	-0.119180	-6.890230
C	-3.370070	0.579928	-6.864020
C	-1.829090	-1.028810	-8.078790
H	-0.863061	-1.537240	-8.077860
H	-2.615310	-1.794500	-8.115440
H	-1.905420	-0.459074	-9.014740
H	-4.192280	-0.148072	-6.844750
H	-3.473290	1.231320	-5.991380
H	-3.514150	1.190860	-7.765530
H	-1.407920	0.783696	-5.122790
H	2.589070	-3.925490	1.490420
H	1.360330	-2.760250	2.224560
H	1.346080	-4.085470	-0.543497

Conf 39

C	-0.489767	-2.158580	-1.400930
C	0.281006	-0.843206	-1.379570
C	-0.645348	0.270412	-1.109780
N	-1.932680	-0.312098	-1.081770
C	-1.949080	-1.664790	-1.302230
C	-0.178292	-3.107170	-0.132688
C	-0.316169	-3.139650	-2.612510
C	1.604790	-0.690157	-1.600920
O	-0.451056	1.462140	-0.953617
O	-2.972360	-2.335470	-1.388560
H	-2.775260	0.238344	-0.967576
H	2.228260	-1.549590	-1.840520

O	2.230380	0.491416	-1.562210
C	3.640930	0.480689	-1.872530
H	3.776260	0.097632	-2.892190
C	4.155380	1.901120	-1.746240
H	4.151940	-0.193077	-1.172680
H	5.225270	1.928490	-1.977030
H	3.631180	2.564600	-2.439540
H	4.007270	2.276910	-0.730020
C	1.314820	-3.368530	-0.026415
C	-0.743181	-2.549320	1.181440
C	-0.857064	-4.441290	-0.545936
C	-0.891829	-4.509930	-2.094550
H	0.768416	-3.277720	-2.724280
C	-0.852011	-2.742690	-4.015130
H	-0.267896	-5.325980	-2.468680
O	-2.196070	-4.814880	-2.569910
H	-1.887620	-4.462580	-0.181599
H	-0.344650	-5.300670	-0.102302
H	-0.528173	-3.235870	2.006110
H	-0.309298	-1.575840	1.433180
H	-1.829140	-2.436890	1.126670
C	2.123760	-3.075570	0.996588
H	-2.788820	-4.123160	-2.225620
C	-0.352954	-1.366570	-4.506800
C	-0.488767	-3.852460	-5.022400
H	-1.946460	-2.698060	-3.958820
H	-0.899681	-3.638400	-6.012630
H	0.601229	-3.941030	-5.128150
H	-0.890748	-4.817920	-4.710240
H	-0.591389	-0.596964	-3.766640
H	0.743923	-1.373120	-4.586760
C	-0.949283	-0.910751	-5.856630
C	-0.593788	0.517921	-6.176890
H	-0.631621	-1.579020	-6.660450
H	-2.045170	-1.000450	-5.796780
C	0.079852	1.000300	-7.236210
C	0.337062	2.483190	-7.378880
C	0.628912	0.164163	-8.368030
H	1.708990	0.329270	-8.479480
H	0.465078	-0.906975	-8.235840
H	0.170570	0.458361	-9.321900
H	1.413900	2.693100	-7.436800
H	-0.106180	2.872350	-8.305680
H	-0.075501	3.051230	-6.540160
H	-0.931243	1.243420	-5.434000
H	3.169870	-3.368240	0.976845
H	1.786900	-2.548960	1.883730
H	1.750230	-3.911430	-0.865868

Conf 11

C	-0.532513	-2.072290	-1.322630
C	0.200042	-0.734035	-1.269560
C	-0.773504	0.353500	-1.063870
N	-2.042300	-0.265016	-1.124370
C	-2.005790	-1.618810	-1.344380
C	-0.297960	-2.995060	-0.018060

C	-0.222736	-3.068600	-2.491800
C	1.526020	-0.543622	-1.446380
O	-0.622621	1.550600	-0.900634
O	-3.000780	-2.316440	-1.508610
H	-2.905600	0.262770	-1.077470
H	2.179080	-1.387280	-1.669300
O	2.123750	0.648975	-1.353890
C	3.509630	0.727019	-1.749340
H	3.931090	1.521340	-1.128790
C	3.647880	1.051030	-3.229100
H	4.011130	-0.215400	-1.492430
H	4.706980	1.162560	-3.486610
H	3.131880	1.985420	-3.466620
H	3.225500	0.256942	-3.853000
C	1.188570	-3.079160	0.294032
C	-0.984641	-2.442360	1.247980
C	-0.897572	-4.346000	-0.458848
C	-0.798762	-4.446820	-2.000420
H	0.870589	-3.177680	-2.489260
C	-0.646990	-2.719650	-3.944180
H	-0.120198	-5.248310	-2.304810
O	-2.048110	-4.802140	-2.579390
H	-1.956820	-4.376900	-0.190777
H	-0.423478	-5.187860	0.053027
H	-0.790784	-3.110460	2.093600
H	-0.600197	-1.451550	1.515000
H	-2.069140	-2.373100	1.122580
C	2.019790	-4.103250	0.076033
H	-2.689640	-4.124680	-2.301010
C	-0.186598	-1.325780	-4.422290
C	-0.136672	-3.824060	-4.891770
H	-1.742880	-2.735540	-3.986270
H	-0.467671	-3.650000	-5.919130
H	0.961461	-3.855830	-4.897430
H	-0.513641	-4.804790	-4.596000
H	-0.527515	-0.559308	-3.719710
H	0.911731	-1.270450	-4.415410
C	-0.698163	-0.928241	-5.824380
C	-0.406118	0.514357	-6.146260
H	-0.277707	-1.588460	-6.586590
H	-1.787910	-1.084770	-5.849250
C	0.301559	1.021930	-7.171160
C	0.475502	2.515740	-7.325990
C	0.968284	0.204922	-8.252670
H	2.040360	0.437641	-8.305140
H	0.865115	-0.872291	-8.109130
H	0.548948	0.453618	-9.236920
H	1.538830	2.791970	-7.323170
H	0.066801	2.862160	-8.285020
H	-0.022262	3.069660	-6.524880
H	-0.833116	1.228700	-5.439400
H	3.060440	-4.048630	0.383452
H	1.707940	-5.028470	-0.399968
H	1.592280	-2.196240	0.788239

Conf 17

C	-0.425318	-2.032940	-1.456950
C	0.342483	-0.714325	-1.511870
C	-0.607040	0.411998	-1.447830
N	-1.889680	-0.178370	-1.495600
C	-1.883320	-1.547580	-1.581860
C	-0.264847	-2.824040	-0.058666
C	-0.100588	-3.149390	-2.507380
C	1.676130	-0.574595	-1.675860
O	-0.428089	1.614560	-1.387430
O	-2.890720	-2.233700	-1.716670
H	-2.738820	0.372515	-1.533660
H	2.315100	-1.452580	-1.767860
O	2.290550	0.609309	-1.776770
C	3.729730	0.600921	-1.872510
H	3.974040	1.493230	-2.453420
C	4.379110	0.644690	-0.497228
H	4.049360	-0.280493	-2.443580
H	5.467920	0.705363	-0.602080
H	4.034930	1.519870	0.061169
H	4.143230	-0.252806	0.084090
C	1.206540	-2.911640	0.317381
C	-0.981247	-2.130060	1.118160
C	-0.885016	-4.197850	-0.384750
C	-0.731385	-4.456970	-1.903210
H	0.988550	-3.282710	-2.450960
C	-0.460626	-2.941200	-4.003720
H	-0.063922	-5.300750	-2.098100
O	-1.967480	-4.840450	-2.492470
H	-1.954040	-4.175560	-0.157836
H	-0.454518	-4.994570	0.228027
H	-0.836662	-2.713680	2.033320
H	-0.579827	-1.126610	1.299270
H	-2.058150	-2.048070	0.944409
C	2.015960	-3.972620	0.237936
H	-2.599940	-4.122880	-2.310730
C	0.042387	-1.607490	-4.597800
C	0.066948	-4.143320	-4.812670
H	-1.554080	-2.946840	-4.087910
H	-0.218313	-4.070940	-5.865480
H	1.163610	-4.191440	-4.768590
H	-0.339782	-5.083430	-4.435210
H	-0.306165	-0.768287	-3.989710
H	1.141410	-1.572230	-4.555120
C	-0.415312	-1.338280	-6.048990
C	0.049485	0.004992	-6.548690
H	-0.012413	-2.112860	-6.714030
H	-1.506120	-1.426320	-6.101130
C	-0.686325	1.075750	-6.894930
C	-0.024439	2.350480	-7.365940
C	-2.194920	1.137040	-6.859060
H	-2.658380	0.214746	-6.503850
H	-2.529310	1.955340	-6.207500
H	-2.596130	1.351750	-7.858680
H	-0.361279	2.619910	-8.376230
H	-0.286897	3.193690	-6.712890
H	1.065750	2.261280	-7.383660

H	1.134460	0.107202	-6.619920
H	3.046170	-3.912330	0.577775
H	1.695270	-4.934130	-0.152512
H	1.616250	-1.991700	0.732947

Conf 267

C	-0.506579	-2.228930	-1.254840
C	0.066140	-0.813839	-1.259930
C	-1.036990	0.164336	-1.270980
N	-2.214940	-0.603703	-1.408590
C	-2.006230	-1.957480	-1.486020
C	-0.333788	-2.993720	0.157411
C	0.047896	-3.283510	-2.272230
C	1.375380	-0.484000	-1.307600
O	-1.037160	1.380120	-1.209200
O	-2.892340	-2.780510	-1.689220
H	-3.129240	-0.180028	-1.511090
H	2.137610	-1.260670	-1.369090
O	1.825780	0.775028	-1.271570
C	3.234490	0.979408	-1.507610
H	3.797470	0.140121	-1.078260
C	3.531800	1.154500	-2.989220
H	3.481360	1.882760	-0.945018
H	4.596410	1.370840	-3.131090
H	3.289050	0.248661	-3.554050
H	2.950090	1.983890	-3.401050
C	1.104250	-2.871460	0.638587
C	-1.224530	-2.413360	1.275290
C	-0.726171	-4.440970	-0.202364
C	-0.428027	-4.670760	-1.703660
H	1.138440	-3.258160	-2.140930
C	-0.236656	-3.127270	-3.791090
H	0.366993	-5.408070	-1.844070
O	-1.550180	-5.228150	-2.376340
H	-1.800980	-4.572410	-0.052881
H	-0.231550	-5.169840	0.445407
H	-1.063240	-2.973000	2.202550
H	-0.984898	-1.363350	1.477340
H	-2.286980	-2.486300	1.025160
C	2.061300	-3.804690	0.619977
H	-2.291740	-4.611240	-2.244190
C	0.099028	-1.732410	-4.362050
C	0.518389	-4.235000	-4.553120
H	-1.308650	-3.296700	-3.948260
H	0.301038	-4.201800	-5.623970
H	1.604240	-4.121040	-4.431220
H	0.229174	-5.226240	-4.198870
H	-0.397647	-0.954086	-3.776500
H	1.177990	-1.540050	-4.262230
C	-0.317484	-1.527450	-5.836220
C	-0.011619	-0.135516	-6.325450
H	0.216005	-2.242480	-6.475210
H	-1.383130	-1.759880	-5.939680
C	-0.867502	0.838290	-6.682090
C	-0.360106	2.186200	-7.140760
C	-2.372500	0.713465	-6.670140

H	-2.814560	1.478310	-6.017810
H	-2.782010	0.886709	-7.674370
H	-2.724150	-0.262013	-6.329050
H	0.732967	2.231970	-7.141330
H	-0.711237	2.414970	-8.156150
H	-0.735150	2.988810	-6.491510
H	1.053620	0.099152	-6.378750
H	3.044990	-3.599390	1.033080
H	1.910960	-4.799250	0.209959
H	1.347320	-1.906020	1.080840

Conf 12

C	-0.617408	-2.087420	-1.398950
C	0.075073	-0.729128	-1.493580
C	-0.856084	0.333336	-1.071480
N	-2.083560	-0.320053	-0.828601
C	-2.062510	-1.673400	-1.049670
C	-0.051862	-3.037370	-0.222949
C	-0.589725	-3.044480	-2.642270
C	1.334170	-0.501672	-1.929380
O	-0.704426	1.535300	-0.949723
O	-3.048330	-2.397440	-0.961201
H	-2.925600	0.183203	-0.575976
H	1.956110	-1.328260	-2.269340
O	1.897800	0.710774	-1.970360
C	3.195560	0.797242	-2.602850
H	3.073220	0.608539	-3.676310
C	3.746610	2.186010	-2.346170
H	3.849240	0.023314	-2.179480
H	3.861850	2.366970	-1.273720
H	4.725470	2.288550	-2.825740
H	3.077300	2.947850	-2.754980
C	1.467640	-3.089010	-0.279099
C	-0.423733	-2.537520	1.188460
C	-0.709096	-4.395100	-0.548840
C	-1.008370	-4.447140	-2.067320
H	0.470890	-3.133690	-2.911860
C	-1.381610	-2.660380	-3.921380
H	-0.424086	-5.225830	-2.565530
O	-2.361830	-4.808970	-2.313570
H	-1.662390	-4.472530	-0.019934
H	-0.096781	-5.234260	-0.207945
H	-0.014182	-3.219090	1.941350
H	-0.009922	-1.541800	1.384210
H	-1.507470	-2.498990	1.331320
C	2.242720	-4.076130	-0.739680
H	-2.916310	-4.155810	-1.850820
C	-1.080640	-1.265630	-4.522360
C	-1.216760	-3.757030	-4.993820
H	-2.443010	-2.647880	-3.648150
H	-1.712180	-3.455090	-5.923880
H	-0.160999	-3.941170	-5.227710
H	-1.666090	-4.695740	-4.665030
H	-1.203430	-0.488641	-3.760230
H	-1.853770	-1.061950	-5.275190
C	0.293499	-1.085550	-5.201430

C	0.536190	0.345685	-5.606310
H	1.085900	-1.399140	-4.506350
H	0.370959	-1.755420	-6.061780
C	0.812645	0.840318	-6.826420
C	1.002160	2.325860	-7.033690
C	0.956998	0.016099	-8.083700
H	1.958360	0.144924	-8.516350
H	0.796826	-1.051760	-7.924010
H	0.244072	0.353690	-8.847650
H	0.273701	2.717100	-7.756720
H	0.887981	2.886050	-6.101160
H	1.996840	2.543990	-7.446100
H	0.450899	1.064700	-4.789010
H	3.325440	-4.002640	-0.687131
H	1.844210	-4.988790	-1.173370
H	1.960720	-2.216940	0.149013

Conf 30

C	-0.606888	-2.143280	-1.465180
C	0.087934	-0.788094	-1.559090
C	-0.840748	0.278300	-1.145670
N	-2.068560	-0.371786	-0.891096
C	-2.048680	-1.725900	-1.097970
C	-0.027035	-3.093080	-0.297550
C	-0.612731	-3.097140	-2.712490
C	1.360950	-0.566118	-1.955520
O	-0.689255	1.481330	-1.033900
O	-3.032960	-2.450080	-0.990937
H	-2.907570	0.133586	-0.632933
H	1.992780	-1.391640	-2.275990
O	1.927140	0.644869	-1.985720
C	3.258010	0.718447	-2.545510
H	3.890500	-0.033122	-2.055510
C	3.784610	2.120530	-2.310690
H	3.199620	0.488952	-3.616700
H	4.789690	2.212880	-2.734960
H	3.834620	2.342380	-1.240960
H	3.136200	2.860940	-2.787040
C	1.472010	-3.279410	-0.461777
C	-0.375964	-2.584820	1.108610
C	-0.699856	-4.457330	-0.615619
C	-1.028020	-4.499640	-2.130970
H	0.437665	-3.189270	-3.019200
C	-1.425930	-2.699180	-3.973800
H	-0.457803	-5.280980	-2.640800
O	-2.387170	-4.852440	-2.352700
H	-1.638400	-4.547050	-0.062330
H	-0.065720	-5.293070	-0.303750
H	0.013657	-3.271310	1.866630
H	0.049342	-1.594280	1.301920
H	-1.458490	-2.527060	1.248310
C	2.433240	-2.976330	0.416358
H	-2.928580	-4.196970	-1.877560
C	-1.105860	-1.308700	-4.575050
C	-1.301360	-3.795930	-5.051380
H	-2.481290	-2.666920	-3.679800

H	-1.809000	-3.482690	-5.970980
H	-0.253758	-3.997970	-5.306480
H	-1.760220	-4.727570	-4.715770
H	-1.876490	-1.093600	-5.327200
H	-1.216650	-0.530556	-3.812340
C	0.271206	-1.147790	-5.253240
C	0.532181	0.278857	-5.662630
H	1.058690	-1.465140	-4.554200
H	0.342750	-1.822320	-6.110520
C	0.800219	0.767658	-6.886840
C	1.013280	2.249470	-7.097860
C	0.912844	-0.059649	-8.145390
H	1.909760	0.052520	-8.592710
H	0.737500	-1.124690	-7.982600
H	0.194503	0.288953	-8.899260
H	2.006410	2.449520	-7.522990
H	0.282795	2.653200	-7.811940
H	0.921046	2.812070	-6.164380
H	0.471488	0.999053	-4.844300
H	3.471760	-3.215890	0.205417
H	2.233310	-2.492960	1.367230
H	1.777610	-3.775890	-1.383410

Conf 31

C	-0.607614	-2.149930	-1.473160
C	0.095662	-0.797428	-1.538670
C	-0.820687	0.263722	-1.086180
N	-2.049970	-0.384718	-0.834496
C	-2.042100	-1.732860	-1.078120
C	-0.021196	-3.135030	-0.338679
C	-0.634697	-3.069520	-2.745780
C	1.365740	-0.573550	-1.943380
O	-0.659535	1.462330	-0.944366
O	-3.030250	-2.452910	-0.979254
H	-2.882570	0.119180	-0.553694
H	1.988110	-1.394410	-2.293050
O	1.940180	0.633896	-1.947410
C	3.264780	0.713437	-2.520980
H	3.192250	0.512470	-3.597030
C	3.803610	2.105430	-2.255900
H	3.897890	-0.054816	-2.058390
H	3.867510	2.298860	-1.181390
H	4.804340	2.202280	-2.689340
H	3.154810	2.862260	-2.705130
C	1.474490	-3.327390	-0.525429
C	-0.350116	-2.662760	1.084760
C	-0.707524	-4.485480	-0.685626
C	-1.053440	-4.484320	-2.197600
H	0.411438	-3.160500	-3.067030
C	-1.459520	-2.631800	-3.986120
H	-0.494930	-5.255520	-2.735070
O	-2.417650	-4.821350	-2.412860
H	-1.640240	-4.583640	-0.123983
H	-0.075906	-5.333730	-0.403859
H	0.043228	-3.372270	1.819290
H	0.084603	-1.680810	1.299770

H	-1.430500	-2.601270	1.238730
C	2.447980	-3.055090	0.349276
H	-2.948640	-4.175330	-1.913630
C	-1.136170	-1.227780	-4.553220
C	-1.355610	-3.699670	-5.094490
H	-2.511150	-2.600050	-3.678930
H	-1.871380	-3.357750	-5.999220
H	-0.312565	-3.902260	-5.367190
H	-1.817600	-4.636750	-4.778920
H	-1.232610	-0.469842	-3.768540
H	-1.913610	-0.986999	-5.290390
C	0.234348	-1.058140	-5.242520
C	0.500942	0.377229	-5.616230
H	1.027240	-1.399580	-4.561190
H	0.291530	-1.709740	-6.118390
C	0.757772	0.897307	-6.829920
C	0.979192	2.382770	-7.003230
C	0.848980	0.103847	-8.111780
H	1.840790	0.222107	-8.568780
H	0.668899	-0.964138	-7.975670
H	0.123290	0.477146	-8.846550
H	0.243456	2.810870	-7.697430
H	0.901924	2.920430	-6.053830
H	1.968770	2.587340	-7.434440
H	0.455394	1.075300	-4.777980
H	3.482200	-3.296140	0.119743
H	2.262610	-2.596380	1.315180
H	1.765830	-3.800710	-1.463710

Conf 19

C	-0.574047	-2.044570	-1.424550
C	0.072034	-0.665081	-1.544110
C	-0.884517	0.370261	-1.112270
N	-2.084390	-0.320347	-0.836724
C	-2.024130	-1.674020	-1.047140
C	0.045052	-2.967850	-0.255242
C	-0.542806	-3.008780	-2.662390
C	1.311600	-0.398507	-2.012960
O	-0.768920	1.577300	-1.001050
O	-2.983660	-2.428770	-0.930675
H	-2.936720	0.157655	-0.569955
H	1.962780	-1.207380	-2.341310
O	1.806380	0.837733	-2.137670
C	3.177520	0.958050	-2.572950
H	3.395890	0.167074	-3.301500
C	4.139970	0.922568	-1.395140
H	3.219910	1.919430	-3.089400
H	5.164540	1.082910	-1.748280
H	4.105980	-0.043270	-0.880204
H	3.894270	1.708250	-0.675029
C	1.564020	-2.971700	-0.342452
C	-0.312926	-2.470560	1.160710
C	-0.574753	-4.348260	-0.558803
C	-0.905093	-4.419760	-2.070130
H	0.514287	-3.066750	-2.953650
C	-1.372550	-2.656710	-3.926540

H	-0.307561	-5.183130	-2.576240
O	-2.251520	-4.825610	-2.284190
H	-1.513300	-4.453030	-0.008685
H	0.071646	-5.165090	-0.226567
H	0.133860	-3.133510	1.909030
H	0.072700	-1.460730	1.341290
H	-1.394100	-2.465500	1.326070
C	2.361090	-3.936460	-0.812743
H	-2.816160	-4.186960	-1.813620
C	-1.119800	-1.260380	-4.546570
C	-1.204310	-3.758500	-4.993210
H	-2.427650	-2.668170	-3.629450
H	-1.727980	-3.477090	-5.914180
H	-0.149764	-3.917860	-5.249570
H	-1.622200	-4.705230	-4.646550
H	-1.914650	-1.083300	-5.283290
H	-1.244490	-0.478817	-3.789470
C	0.233470	-1.052960	-5.259800
C	0.430222	0.378538	-5.687330
H	1.050210	-1.335690	-4.579730
H	0.308165	-1.732010	-6.113160
C	0.619628	0.867981	-6.925770
C	0.778615	2.354150	-7.153310
C	0.690048	0.037689	-8.185460
H	0.558812	-1.031570	-8.009180
H	-0.079871	0.358292	-8.899890
H	1.656550	0.179780	-8.687690
H	1.742630	2.580060	-7.629530
H	0.001250	2.733370	-7.830420
H	0.718465	2.918700	-6.218370
H	0.392129	1.100790	-4.869730
H	3.441800	-3.828520	-0.782823
H	1.983350	-4.864110	-1.232900
H	2.036880	-2.081220	0.070461

Conf 33

C	-0.229314	-1.843290	-1.555540
C	0.703904	-0.657730	-1.331590
C	-0.088728	0.573623	-1.168330
N	-1.429960	0.187674	-1.387580
C	-1.598830	-1.141390	-1.678400
C	-0.284576	-2.867670	-0.310855
C	0.015125	-2.798700	-2.775990
C	2.054250	-0.694926	-1.318010
O	0.241724	1.718800	-0.918989
O	-2.675690	-1.650510	-1.969600
H	-2.193140	0.853568	-1.388710
H	2.585300	-1.633210	-1.470660
O	2.823260	0.388916	-1.167850
C	4.245000	0.180117	-1.045050
H	4.696370	1.079860	-1.469720
C	4.653590	-0.009459	0.408148
H	4.539010	-0.678248	-1.663560
H	5.742410	-0.109582	0.477927
H	4.345200	0.851907	1.007440
H	4.197600	-0.909037	0.833683

C	1.113080	-3.354750	0.033192
C	-0.988588	-2.275810	0.918456
C	-1.061300	-4.071630	-0.910509
C	-0.829708	-4.084340	-2.443610
H	1.072140	-3.092750	-2.708480
C	-0.202876	-2.282990	-4.224800
H	-0.269674	-4.971350	-2.751610
O	-2.058490	-4.178500	-3.151400
H	-2.132510	-3.949170	-0.729833
H	-0.763266	-5.011790	-0.435950
H	-1.025730	-3.014940	1.724700
H	-0.471164	-1.388880	1.299290
H	-2.019680	-1.997870	0.685274
C	1.752950	-3.239080	1.201170
H	-2.599020	-3.415990	-2.878200
C	0.562869	-0.980660	-4.544540
C	0.182589	-3.400400	-5.214430
H	-1.271580	-2.083490	-4.358980
H	-0.006226	-3.095350	-6.246760
H	1.250420	-3.645800	-5.130770
H	-0.400507	-4.305650	-5.036030
H	0.310667	-0.208339	-3.811610
H	1.643380	-1.154540	-4.435970
C	0.299695	-0.384565	-5.947550
C	-1.134200	0.029370	-6.156970
H	0.939893	0.505514	-6.041630
H	0.633322	-1.074640	-6.727150
C	-1.961660	-0.267177	-7.174350
C	-3.377630	0.261247	-7.199520
C	-1.596550	-1.117820	-8.367530
H	-2.278870	-1.973860	-8.453870
H	-1.701820	-0.540891	-9.296230
H	-0.575673	-1.502710	-8.330210
H	-3.555440	0.870903	-8.095870
H	-4.103500	-0.562426	-7.232370
H	-3.599830	0.874387	-6.321370
H	-1.535580	0.664864	-5.364380
H	2.731930	-3.688530	1.343120
H	1.335770	-2.711950	2.053180
H	1.614050	-3.916950	-0.755453

Conf 41

C	-0.394791	-2.106970	-1.523260
C	0.378657	-0.792853	-1.560890
C	-0.561829	0.338302	-1.478720
N	-1.849950	-0.242966	-1.510840
C	-1.854090	-1.610000	-1.605110
C	-0.205006	-2.926250	-0.146484
C	-0.118963	-3.200360	-2.613600
C	1.716790	-0.656260	-1.685970
O	-0.376024	1.539530	-1.411350
O	-2.868750	-2.289490	-1.721380
H	-2.696080	0.313554	-1.525360
H	2.358510	-1.532030	-1.770410
O	2.336570	0.526187	-1.759280
C	3.778580	0.518823	-1.775970

H	4.055020	1.397400	-2.363630
C	4.348880	0.594625	-0.367535
H	4.129460	-0.375739	-2.307330
H	5.442490	0.644700	-0.411641
H	3.981090	1.487360	0.146229
H	4.068370	-0.284487	0.221316
C	1.270600	-3.173850	0.118647
C	-0.882185	-2.245890	1.051590
C	-0.852143	-4.296100	-0.487337
C	-0.743875	-4.516840	-2.018020
H	0.970736	-3.343110	-2.615370
C	-0.527872	-2.947620	-4.090710
H	-0.090752	-5.362080	-2.250760
O	-1.999850	-4.875050	-2.578700
H	-1.912140	-4.282230	-0.220050
H	-0.389828	-5.106720	0.084526
H	-0.749990	-2.851030	1.953840
H	-0.464491	-1.252910	1.248710
H	-1.957580	-2.139270	0.887118
C	1.981020	-2.801910	1.188150
H	-2.619350	-4.156070	-2.360440
C	-0.007372	-1.611740	-4.664800
C	-0.058591	-4.140640	-4.947550
H	-1.623200	-2.923260	-4.136790
H	-0.378766	-4.033860	-5.987260
H	1.037580	-4.215160	-4.944720
H	-0.474655	-5.080200	-4.579310
H	-0.315925	-0.780324	-4.025480
H	1.093000	-1.606220	-4.651970
C	-0.497911	-1.292970	-6.095030
C	-0.012277	0.050778	-6.573110
H	-0.133547	-2.059610	-6.790780
H	-1.591690	-1.352230	-6.118590
C	-0.729345	1.147920	-6.872840
C	-0.047670	2.417580	-7.328920
C	-2.234400	1.245740	-6.795190
H	-2.712340	0.324530	-6.456700
H	-2.530590	2.051040	-6.109800
H	-2.655470	1.502070	-7.776650
H	-0.402351	2.720300	-8.323570
H	-0.273015	3.250200	-6.649000
H	1.039210	2.302460	-7.376100
H	1.072740	0.127856	-6.670100
H	3.021780	-3.096350	1.291280
H	1.564910	-2.208830	1.996190
H	1.779570	-3.780870	-0.630673

Conf 301

C	-0.459765	-2.337470	-1.371240
C	0.092889	-0.918226	-1.294680
C	-1.020360	0.044423	-1.231290
N	-2.193480	-0.729770	-1.383320
C	-1.971450	-2.073320	-1.536450
C	-0.228112	-3.187570	-0.018526
C	0.057000	-3.315770	-2.482900
C	1.397820	-0.568470	-1.297950

O	-1.034930	1.254960	-1.102650
O	-2.853720	-2.896970	-1.755670
H	-3.115320	-0.313448	-1.435310
H	2.174120	-1.325530	-1.398230
O	1.828320	0.691481	-1.176120
C	3.241210	0.924821	-1.349110
H	3.799840	0.073329	-0.938882
C	3.590610	1.175950	-2.808450
H	3.453980	1.802820	-0.734847
H	4.656600	1.411820	-2.899990
H	3.381600	0.296106	-3.425700
H	3.013070	2.017490	-3.201160
C	1.248510	-3.212980	0.339363
C	-1.079590	-2.683150	1.155140
C	-0.624756	-4.621830	-0.459961
C	-0.383160	-4.743890	-1.986400
H	1.153490	-3.283720	-2.414750
C	-0.296736	-3.057370	-3.973170
H	0.411977	-5.461510	-2.205450
O	-1.525720	-5.268100	-2.649740
H	-1.688440	-4.788190	-0.269871
H	-0.076979	-5.378460	0.110447
H	-0.906089	-3.302320	2.040680
H	-0.841846	-1.646970	1.417960
H	-2.145870	-2.741560	0.921377
C	1.823960	-2.769380	1.461300
H	-2.266450	-4.669370	-2.446740
C	0.027738	-1.627470	-4.457870
C	0.415265	-4.112530	-4.843490
H	-1.376000	-3.209650	-4.092840
H	0.148332	-4.004380	-5.898030
H	1.506390	-4.009490	-4.766010
H	0.137054	-5.124940	-4.545000
H	-0.439381	-0.889773	-3.800160
H	1.111340	-1.448840	-4.385810
C	-0.442035	-1.317550	-5.897170
C	-0.151779	0.106204	-6.295790
H	0.066850	-1.984490	-6.604720
H	-1.511150	-1.542830	-5.978470
C	-1.018500	1.098660	-6.563660
C	-0.525521	2.476970	-6.940390
C	-2.522470	0.967592	-6.523620
H	-2.956840	1.206600	-7.503630
H	-2.863720	-0.029967	-6.240740
H	-2.949930	1.685020	-5.810540
H	-0.886040	3.231320	-6.228120
H	0.567101	2.526860	-6.964560
H	-0.902245	2.773940	-7.928600
H	0.911305	0.348189	-6.358510
H	2.890250	-2.897770	1.625310
H	1.270560	-2.274330	2.252800
H	1.892220	-3.707140	-0.388988

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C	-0.271818	-1.875490	-1.514310
C	0.627585	-0.644240	-1.431860

C	-0.203706	0.573589	-1.408520
N	-1.529520	0.124661	-1.591370
C	-1.655930	-1.233620	-1.738940
C	-0.322243	-2.745480	-0.156280
C	0.034297	-2.967780	-2.596010
C	1.978150	-0.641003	-1.460240
O	0.092698	1.748410	-1.287330
O	-2.712690	-1.803160	-1.987630
H	-2.310110	0.763259	-1.685060
H	2.530310	-1.578070	-1.527750
O	2.717670	0.474313	-1.452360
C	4.149910	0.315746	-1.389890
H	4.548600	1.195130	-1.900880
C	4.640420	0.246190	0.048740
H	4.440530	-0.576059	-1.960440
H	5.734530	0.193500	0.066310
H	4.326760	1.134870	0.603765
H	4.249390	-0.639009	0.561134
C	1.091020	-3.005950	0.342962
C	-1.072010	-2.037550	0.991241
C	-1.044160	-4.029690	-0.614320
C	-0.781529	-4.227040	-2.127430
H	1.093780	-3.220210	-2.450300
C	-0.159355	-2.645790	-4.102740
H	-0.190423	-5.127550	-2.315120
O	-1.992260	-4.443260	-2.841510
H	-2.121650	-3.907910	-0.476994
H	-0.751120	-4.896450	-0.015643
H	-1.072390	-2.676320	1.880650
H	-0.590415	-1.091650	1.263810
H	-2.114330	-1.834750	0.728744
C	1.795220	-4.139990	0.271011
H	-2.560960	-3.671670	-2.670360
C	0.559142	-1.359090	-4.565350
C	0.296330	-3.860980	-4.935000
H	-1.232370	-2.512940	-4.277230
H	0.124368	-3.699170	-6.002760
H	1.370360	-4.047680	-4.798720
H	-0.253775	-4.761110	-4.654670
H	0.218800	-0.508314	-3.968330
H	1.637970	-1.456600	-4.373080
C	0.367300	-0.975866	-6.054300
C	-1.070000	-0.777968	-6.464090
H	0.948881	-0.066715	-6.237520
H	0.815286	-1.748490	-6.692600
C	-1.703980	0.374987	-6.745130
C	-3.161100	0.378468	-7.147340
C	-1.069250	1.744800	-6.701340
H	-1.135820	2.232000	-7.683500
H	-1.604980	2.394040	-5.996190
H	-0.019049	1.728140	-6.404260
H	-3.759800	0.986643	-6.455770
H	-3.292740	0.820159	-8.144560
H	-3.582400	-0.630784	-7.163630
H	-1.661650	-1.691280	-6.535690
H	2.789550	-4.205190	0.704061

H	1.419150	-5.041240	-0.204471
H	1.548830	-2.156710	0.849096