

# Waikikiamides A-C: Complex Diketopiperazine Dimer and Diketopiperazine-polyketide Hybrids from a Hawaiian Marine Fungal Strain *Aspergillus* sp. FM242

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**Abstract:** Waikikiamides A-C (**1-3**), structurally complex diketopiperazine derivatives, and three putative biogenic precursors, (+)-semivioxanthin (**4**), notoamide F (**5**) and notoamide A (**6**), were isolated from *Aspergillus* sp. FM242. Comprehensive spectroscopic analyses revealed the structures of Waikikiamides A-B (**1-2**) bearing a hendecacyclic ring system fused between (+)-avrainvillamide or aspergamide B and the polyketide **4**, which represents a novel skeleton. Waikikiamide C (**3**) featured the first heterodimer of two notoamide analogs with an N–O–C bridge. Compounds **1** and **3** exhibited potent antiproliferative activity against HT1080, PC3, Jurkat, and A2780 cancer cell lines with IC<sub>50</sub> values in the range of 0.52 to 1.86  $\mu$ M. Their biosynthetic pathways were supported by the gene clusters mined from the sequenced genome of *Aspergillus* sp. FM242.

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## Experimental section

### General experimental procedures

HRESIMS data were recorded on a Agilent 6530 accurate- Mass Q-TOF LC-MS spectrometer. NMR spectra were obtained on a Bruker AM-400 spectrometer. Optical rotations were carried out on a Rudolph research analytical autoPol automatic polarimeter. UV, CD and FT-IR spectra were recorded on Shimadzu UV-1800, JASCO J-815 CD and Thermo scientific nicolet iS10 IR spectrometer respectively. X-ray diffraction data were collected on Bruker APEX DUO CCD diffractometer. Preparative HPLC was carried out on an Ultimate 3000 chromatographic system with a Phenomenex preparative column (Phenyl-Hexyl,  $5\mu$ ,  $100 \times 21.20$  mm) and Semi-preparative HPLC on an Ultimate 3000 chromatographic system with an Dionex Ultimate 3000 DAD detector, Dionex Ultimate 3000 automated fraction collector and a Phenomenex semi-preparative column ( $C_{18}$ ,  $5\mu$ ,  $250 \times 10$  mm). Thermo SpeedVac 2010 system. Alfa Aesar Diaion HP 20, GeneAmp PCR System 9700, Eppendorf centrifuge 5810 R, BIO-RAD Molecular Imager ChemiDoc™ XRS+, Shimadzu Biotech BioSpec-nano. Galaxy 170 R CO<sub>2</sub> Incubator, Synergy H1 hybrid reader, Axiovert 40 CFL Inverted Microscope.

### Fungal material

The strain *Aspergillus* sp. FM 242 was isolated from a soil sample collected at Waikiki beach of Oahu, Honolulu, Hawaii. The rDNA ITS1-4 region sequence of fungus has been submitted to GenBank (Accession number MH879469). The strain was deposited at College of Pharmacy, University of Hawaii, HI, USA.

### Fermentation, extraction and isolation

The strain was grown on PDA plates at 28 °C, then it was cut into pieces ( $0.5 \times 0.5$  cm) and inoculated into 30 L autoclaving sterilized liquid medium (mannitol 20 g, glucose 10 g, monosodium glutamate 5 g, KH<sub>2</sub>PO<sub>4</sub> (0.5 g), MgSO<sub>4</sub>·7H<sub>2</sub>O 0.3 g, yeast extract 3 g, sea salt 30 g for 1 L distilled water; pH 6.5 prior sterilization.) for fermentation at 25°C for 21 days.

After filtering, the mycelia were extracted with MeOH under ultrasonic ( $1 \text{ L} \times 3$  times), then removed methanol under reduced pressure to afford an aqueous solution. Combined the mycelia extraction and supernatant solution then it was subjected to HP-20 column eluted with MeOH-H<sub>2</sub>O (10%, 50%, 70%, 100%) to afford four fractions (Fr.1-4). Fraction 4 (9.99 g) was separated by prep-HPLC (Phenyl-Hexyl,  $5\mu$ ,  $100 \times 21.20$  mm; 8 mL/min) eluted with 45%-100% MeOH-H<sub>2</sub>O in 35 minutes to get sub-fractions (SFr. 1-35). SFr 31 and 32 was purified by semi-preparative HPLC (50% - 96% CH<sub>3</sub>CN with 0.1% formic acid in 25 min; 3 mL/min) to afford compound **1** (10.1 mg,  $t_R$  18.5 min) and compound **2** (1.4 mg,  $t_R$  21.4 min). Similarly, compound **3** (3.5 mg,  $t_R$  15.3 min) was obtained from SFr 27 (45% CH<sub>3</sub>CN with 0.1% formic acid; 3 mL/min). Further separation of SFr 19 and 20 (45% - 85% CH<sub>3</sub>CN with 0.1% formic acid in 34 min; 3 mL/min) to afford compound **4** (15 mg,  $t_R$  16.5 min). Compound **5** (7.5 mg,  $t_R$  11.2 min) was got from SFr 29 (65% MeOH with 0.1% formic acid; 3 mL/min). Compound **6** (2.0 mg,  $t_R$  15.9 min) was obtained from SFr 28 by further separation (40% - 90% CH<sub>3</sub>CN with 0.1% formic acid in 30 min; 3 mL/min).

### Physical constants and spectral data of 1-6

**Compound 1** (Konamide A): Gray amorphous powder,  $[\alpha]_D^{20} + 39$  ( $c$  0.03 g/100ml, MeOH); UV (MeOH)  $\lambda_{max}$  (log  $\epsilon$ ): 234 (4.06), 265 (4.51), 362 (3.77) nm; CD ( $c$   $1.39 \times 10^{-5}$  M, MeOH)  $\lambda_{max}(\Delta\epsilon)$  225 (+22.4), 251 (+22.0), 265 (-0.3), 275 (+17.6), 324 (+15.1), 360 (-9.5) nm; IR (KBr)  $\nu_{max}$ : 1709, 1685, 1640, 1413, 1357, 1114 cm<sup>-1</sup>; <sup>1</sup>H and <sup>13</sup>C NMR data, see S29; HRESIMS (ESI)  $m/z$ : [M + H]<sup>+</sup> Calcd for C<sub>41</sub>H<sub>40</sub>N<sub>3</sub>O<sub>9</sub> 718.2759; Found 718.2743.

**Compound 2** (Konamide B): Gray amorphous powder,  $[\alpha]_D^{20} + 66$  ( $c$  0.03 g/100ml, MeOH); UV ( $c$  0.01 mg/ml, MeOH)  $\lambda_{max}$  (log  $\epsilon$ ): 234 (4.35), 265 (4.81), 362 (4.07) nm; CD ( $c$   $7.13 \times 10^{-5}$  M, MeOH)  $\lambda_{max}(\Delta\epsilon)$  235 (+7.5), 248 (+6.6), 265 (-12.1), 276 (+5.9), 324 (+5.4), 362 (-4.3) nm; IR (KBr)  $\nu_{max}$ : 3329, 2937, 1691, 1640, 1578, 1391, 1357, 1114 cm<sup>-1</sup>; <sup>1</sup>H and <sup>13</sup>C NMR, see S29 in main text; HRESIMS (ESI)  $m/z$ : [M + H]<sup>+</sup> Calcd for C<sub>41</sub>H<sub>40</sub>N<sub>3</sub>O<sub>8</sub> 702.2810; Found 702.2845.

**Compound 3** (Konamide C): Faint yellow needle crystal (CH<sub>3</sub>CN).  $[\alpha]_D^{20} - 75$  ( $c$  0.03 g/100ml, MeOH); UV ( $c$  0.01 mg/ml, MeOH)  $\lambda_{max}$  (log  $\epsilon$ ): 232 (4.55) nm; CD ( $c$   $3.43 \times 10^{-5}$  M, MeOH)  $\lambda_{max}(\Delta\epsilon)$  229 (+33.0), 245 (-70.5), 280 (+1.2), 301 (-5.4), 325 (-6.2) nm; IR (KBr)  $\nu_{max}$ : 2934, 1687, 1614, 1439, 1390, 1188, 1084 cm<sup>-1</sup>; <sup>1</sup>H and <sup>13</sup>C NMR data, see S30; HRESIMS (ESI)  $m/z$ : [M + H]<sup>+</sup> Calcd for C<sub>54</sub>H<sub>63</sub>N<sub>6</sub>O<sub>11</sub>, 971.4549; Found 971.4545.

**Compound 4** ((+)-semiovioxanthin): White amorphous powder; HRESIMS (ESI)  $m/z$ : [M + H]<sup>+</sup> Calcd for C<sub>15</sub>H<sub>15</sub>O<sub>5</sub> 275.0914; Found 275.0910. <sup>1</sup>H data matched the literature; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 13.76 (1H, s, 10-OH), 9.48 (1H, s, 9-OH), 6.88 (1H, s, H-5), 6.57 (1H, d,  $J$  = 2.4 Hz, H-6), 6.53 (1H, d,  $J$  = 2.3 Hz, H-8), 4.75 (1H, m, H-3), 3.88 (3H, s, H-7-OMe), 2.98 (2H, m, H-4), 1.55 (3H, d,  $J$  = 6.3 Hz, H-3-CH<sub>3</sub>).

**Compound 5** (Notoamide F): Colorless needle crystal (CH<sub>3</sub>OH); HRESIMS (ESI)  $m/z$ : [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>32</sub>N<sub>3</sub>O<sub>4</sub> 462.2387; Found 462.2396. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 10.73 (1H, s, 1-NH), 8.05 (1H, s, 19-NH), 7.35 (1H, d,  $J$  = 8.5 Hz, H-4), 6.96 (1H, d,  $J$  = 9.8 Hz, H-25), 6.53 (1H, d,  $J$  = 8.5 Hz, H-5), 5.75 (1H, d,  $J$  = 9.8 Hz, H-26), 4.76 (1H, s, H-10), 3.37 (3H, s, 10-OMe), 3.29 (1H, m, H-14a), 3.18 (1H, m, H-14b), 2.68 (1H, t,  $J$  = 7.3 Hz, H-21), 2.52 (1H, m, H-16a), 2.03 (2H, d,  $J$  = 7.4 Hz, H-20), 1.96 (1H, m, H-15a), 1.84 (2H, overlap, H-15b and 16b), 1.39 (6H, s, Me-28 and 29), 1.32 (3H, s, Me-23), 1.00 (3H, s, Me-24). Due to different NMR solvent, the NMR data are not quite consistent with literature; ultimately, the structure was confirmed by single crystal X-Ray and NOESY analysis.

**Compound 6** (Notoamide-A): White amorphous powder; HRESIMS (ESI)  $m/z$ : [M + H]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>30</sub>N<sub>3</sub>O<sub>5</sub> 464.2180; Found 464.2182. <sup>1</sup>H data matched the literature; <sup>1</sup>H NMR (400 MHz, Acetone-*d*<sub>6</sub>)  $\delta$ : 7.24 (1H, d,  $J$  = 10.4 Hz, H-25), 7.10 (1H, d,  $J$  = 8.0 Hz, H-4), 6.45 (1H, d,  $J$  = 8.0 Hz, H-5), 5.72 (1H, d,  $J$  = 10.4 Hz, H-26), 3.53 - 3.43 (2H, m, H-14), 3.32 (1H, d,  $J$  = 10.0 Hz, H-21), 3.05 (1H, s, H-10b), 2.65 (1H, m, H-16b), 2.21 (1H, d,  $J$  = 14.7 Hz, H-10a), 2.00 (1H, m, H-20b), 1.90 (1H, m, H-15b), 1.84 - 1.79 (3H, m, H-15a, 16a and 20a), 1.41 (3H, s, H-29), 1.38 (3H, s, H-28), 0.81 (3H, s, H-24), 0.74 (3H, s, H-23).

## X-ray Crystallography

Suitable crystals (0.16 × 0.10 × 0.08 mm) of compound **3** for an X-ray crystallographic study were obtained from acetonitrile at room temperature after repeated re-crystallization, while compound **5** crystallized with appropriate sizes (0.18 × 0.12 × 0.10 mm) in methanol at room temperature.

Crystals mounted on a diffractometer were collected data at 100 K. The intensities of the reflections were collected by means of a Bruker APEX DUO CCD diffractometer (Cu<sub>Kα</sub> radiation, λ=1.54178 Å), and equipped with an Oxford Cryosystems nitrogen flow apparatus. The collection method involved 1.0° scans in ω at -30°, -55°, -80°, 30°, 55°, 80° and 115° in 2θ. Data integration down to 0.84 Å resolution was carried out using SAINT V8.37 A<sup>[1]</sup> with reflection spot size optimization. Absorption corrections were made with the program SADABS<sup>[1]</sup>. The structure was solved by the Intrinsic Phasing methods and refined by least-squares methods against F<sup>2</sup> using SHELXT-2014<sup>[2]</sup> and SHELXL-2014<sup>[3]</sup> with OLEX 2 interface<sup>[4]</sup>. Crystallographic refinement details have been delineated within in each crystallographic information file (\*.cif). Deposition Number 1994346 (Compound5) and 1994347 (compound 3) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service [www.ccdc.cam.ac.uk/structures](http://www.ccdc.cam.ac.uk/structures). Crystal data as well as details of data collection and refinement are summarized in Table 1, geometric parameters are shown in Table 2, and hydrogen-bond parameters are listed in Table 3. The Ortep plots produced with SHELXL-2014 program,<sup>[3]</sup> and the drawings of three-dimensional supramolecular architectures were produced with Accelrys DS Visualizer 2.0<sup>[5]</sup>.

## Antiproliferative Assays

Antiproliferative assays was carried out as previously described.<sup>[6]</sup> Briefly, cells were cultured in 96-well plates at 1000 cells per well for 24 h and subsequently treated with compounds a series of concentrations for 72 h and analyzed. Relative viability of the treated cells was normalized to the DMSO-treated control cells. Taxol was used as a positive control. All experiments were performed in triplicate.

## Biosynthesis

### Fungal genomic DNA preparation

The genomic DNA of frozen lyophilized *Aspergillus* sp. FM242 mycelium was isolated with MasterPure Yeast DNA Purification kit (Epicentre Biotechnologies) following the manufacture's protocols. The quality of isolated genomic DNA was assessed by agarose gel and Nanodrop analysis. Further quality control and sequencing analysis were performed by Beijing Genome Institute (BGI) Genomics. One pair-end library (2 x 150 bp) was constructed for the sequencing using Illumina HiSeq4000 platform.

### Genome assembly

Quality control and filtering were conducted using the FAsTqC tool<sup>[7]</sup> with a cutoff Phred quality score of >= 25. This process yielded a total of 9,047,867 of paired-end reads with 150 bp length on average. Genome assembly was performed using Spades V3.11<sup>[8]</sup>, using kmer sizes of 21,33,55 and 77. Assembled contigs were corrected and polished by mapping again the Illumina reads and calling errors using Pilon correction tool<sup>[9]</sup>. The procedure was repeated twice. Polished assembled contigs shorter than 1 Kb and with biased read coverage were filtered and discarded. Final assembly produced a genome of 36,603,342 bp covered by 395 contigs (>= 1 kb). With the max sequence length was 767,409 bp and the N50 was 170,900 bp. The average read coverage for contig was 74X, with a GC content of 49.1 %. The assembled genome was then analyzed by AntiSMASH 4.2.0 fungal version<sup>[10]</sup> that led to the identification of one putative semiovioxanthin gene cluster (~34 kb) and the putative notoamide gene cluster (~47 kb) located at two different chromosomal regions. BLAST programs<sup>[11]</sup> were then used to predict function of each encoded pathway gene.

## Biosynthesis and Genome sequencing

### S1. Genome sequencing statistics for the assembly of *Aspergillus* sp. FM242.

Number of contigs	395
Total bases (bp)	36,603,342
Min sequence length (bp)	1,002
Max sequence length (bp)	767,409
Average sequence length (bp)	92,667
Median sequence length (bp)	60,454
N50 length (bp)	170,900
(A + T)s (%)	50.9
(G + C)s (%)	49.1

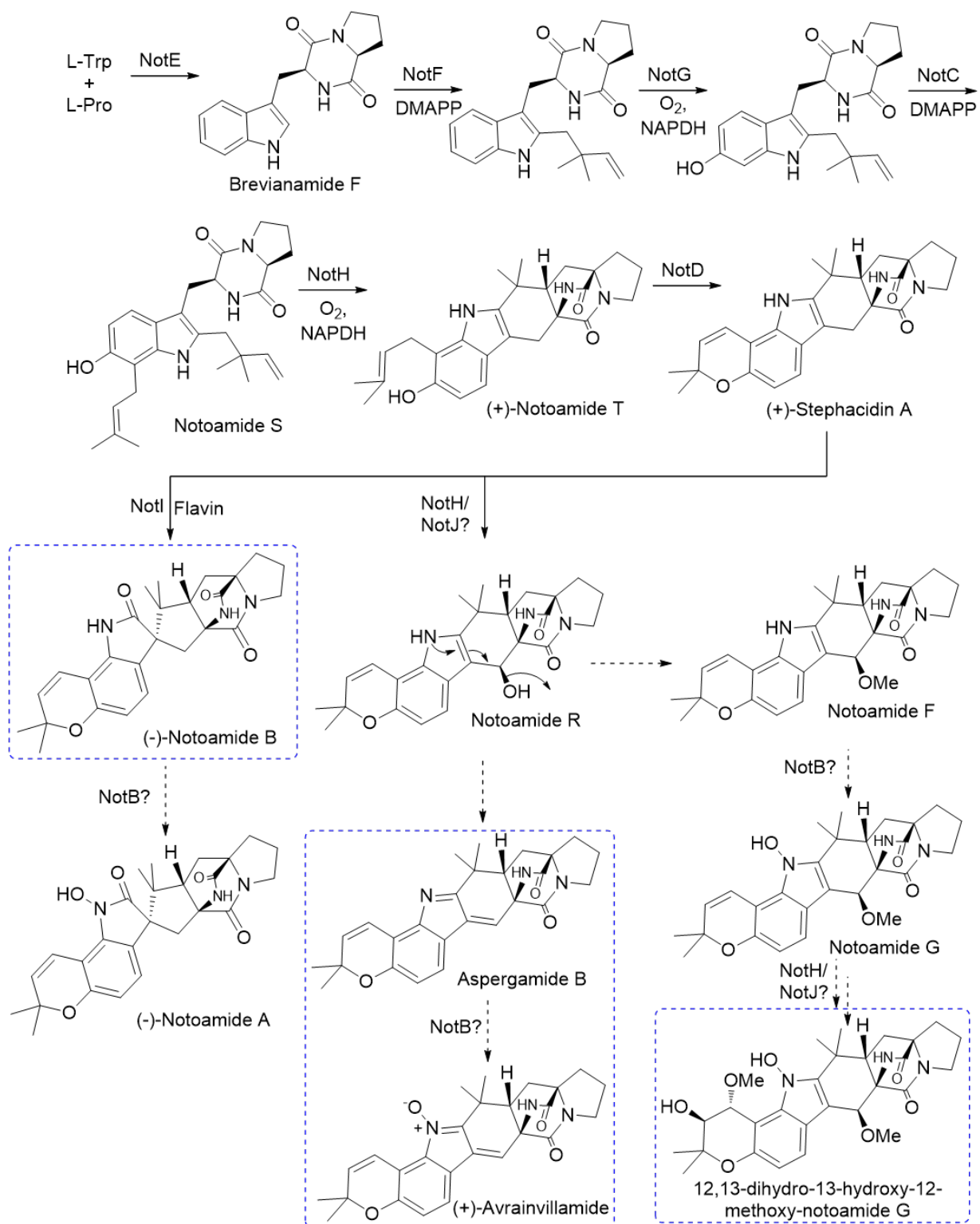
### S2. Predicted function of genes of the *not* cluster (~47 kb) in *Aspergillus* sp. FM242.

Gene	Length (AA, bp)	Putative function	BLAST-hit (identity/similarity [%])	Accession number
Orf1	1427, 4424	Hydrolase	Ubiquitin carbon terminal hydrolase from <i>A. steynii</i> IBT 23096 (90/93)	XP_024711203
Orf2	71, 215	Cold shock protein	Cold shock protein from <i>Pseudomonas fulva</i> (91/95)	AVF56731
NotD	617, 1987	FAD/FMN oxidoreductase	Oxidoreductase from <i>Aspergillus</i> sp. MF297-2 (67/78)	ADM34137
NotC	429, 1340	Normal prenyltransferase	Prenyltransferase from <i>Aspergillus versicolor</i> (75/83)	AGC83574
NotB	453, 1569	Flavin monooxygenase	FAD monooxygenase from <i>Aspergillus versicolor</i> (71/81)	AGC83573
NotA	344, 1217	Transcription regulator	NmrA family protein from <i>Aspergillus</i> sp. MF297-2 (66/78)	ADM34134
Orf1'	386, 1236	Capsule polysaccharide biosynthesis protein	Capsule polysaccharide biosynthesis protein from <i>Aspergillus</i> sp. MF297-2 (72/81)	ADM34133
NotE	2252, 6759	NRPS (A-T-C-A-T-C)	Non-ribosomal peptide synthetase from <i>Aspergillus</i> sp. MF297-2 (61/74)	ADM34138
NotF	451, 1460	Reverse prenyltransferase	Reverse prenyltransferase from <i>Aspergillus</i> sp. MF297-2 (69/82)	ADM34132
NotG	539, 1870	P450	P450 from <i>Aspergillus</i> sp. MF297-2 (73/83)	ADM34140
NotH	489, 1843	P450	P450 from <i>Aspergillus</i> sp. MF297-2 (67/81)	ADM34141
NotI	435, 1437	Flavin monooxygenase	FAD binding domain protein from <i>Aspergillus</i> sp. MF297-2 (70/80)	ADM34142
NotJ	369, 1110	P450	NotJ' from <i>Aspergillus</i> sp. MF297-2 (67/79)	ADM34143
WaiA1	777, 2913	Lysophospholipid acyltransferase	Uncharacterized protein from <i>A. steynii</i> IBT 23096 (83/90)	XP_024711194
WaiA2	384, 1378	Tafazzin	Hypothetical protein from <i>A. carbonarius</i> ITEM 5010 (88/94)	OOF99527
WaiB	108, 526	Ribosomal protein L31	Mitochondrial 54S ribosomal protein YmL31 from <i>A. steynii</i> IBT 23096 (98/100)	XP_024711193
WaiC	740, 2223	Hypothetical protein	Uncharacterized protein from <i>A. steynii</i> IBT 23096 (72/80)	XP_024711192
WaiD	483, 1682	P450	Benzoate 4-monooxygenase cytochrome P450 from <i>A. steynii</i> IBT 23096 (83/90)	XP_024711191

**S3: Predicted function of genes of the *svio* cluster (~34 kb) in *Aspergillus* sp. FM242.**

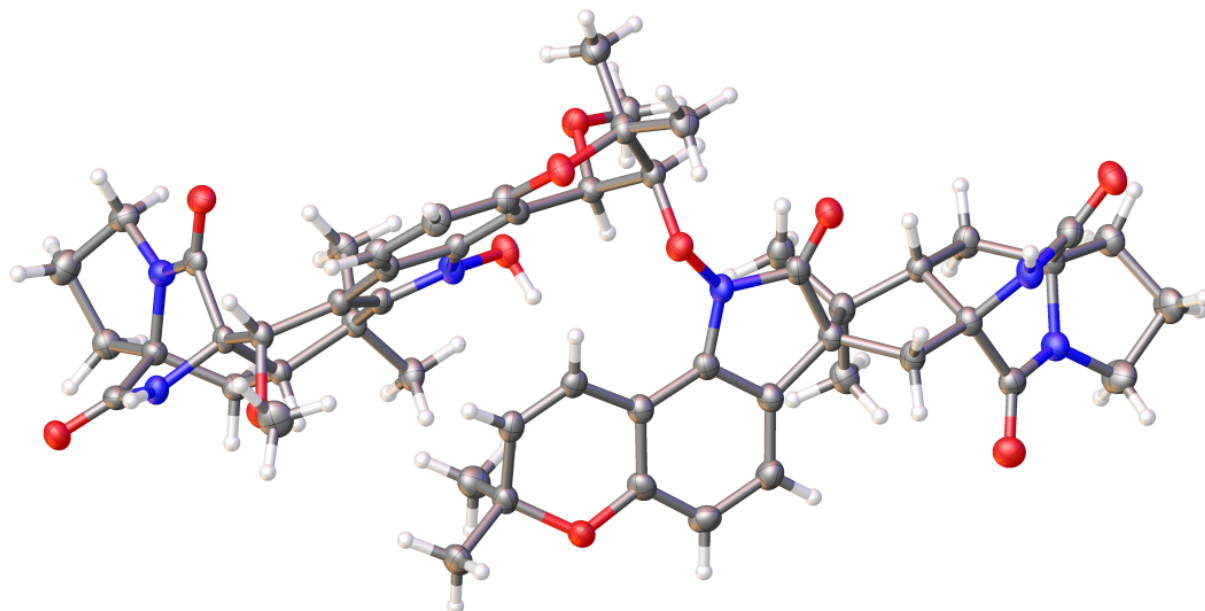
Gene	Length (AA, bp)	Putative function	BLAST-hit (identity/similarity [%])	Accession number
Orf1	217, 842	Cupin	Oxalate decarboxylase/oxidase from <i>Aspergillus steynii</i> IBT 23096 (90/95)	XP_024709122
Orf2	449, 1653	Peptide hydrolase	Zn-dependent exopeptidase from <i>A. steynii</i> IBT 23096 (94/95)	XP_024709123
SvioM	405, 1582	O-methyltransferase	SAM-dependent methyltransferase from <i>A. steynii</i> IBT 23096 (79/84)	XP_024703759
SvioL	606, 2190	Laccase	Conidial pigment biosynthesis oxidase methyltransferase from <i>A. steynii</i> IBT 23096 (91/95)	XP_024703758
SvioC	544, 2568	Enoyl reductase	Short chain dehydrogenase/reductase from <i>A. steynii</i> IBT 23096 (92/97)	XP_024703756
SvioX	247, 864	Unknown	hypothetical protein ATNIH1004_010670 from <i>A. tanneri</i> (90/94)	KAA8641731
SvioT	777, 3725	Transporter	MFS general substrate transporter from <i>A. tanneri</i> (86/89)	KAA8641732
SvioA	2076, 6539	Non-reducing polyketide synthase (SAT-KS-PT-T-T-TE)	Polyketide synthase from <i>Penicillium freii</i> (86/94)	KUM56377
SvioR1	446, 1358	Transcription regulator	Aurofusarin biosynthesis regulatory protein from <i>A. steynii</i> IBT 23096 (78/84)	XP_024703760
SvioR2	794, 2591	Transcription regulator	Fungal specific transcription factor domain from <i>Penicillium freii</i> (75/80)	KUM55655
Orf3	364, 1050	Glycosyl hydrolase	Class III chitinase from <i>A. steynii</i> IBT 23096 (86/91)	XP_024709124

**S4: The putative biosynthetic pathway of notoamides**

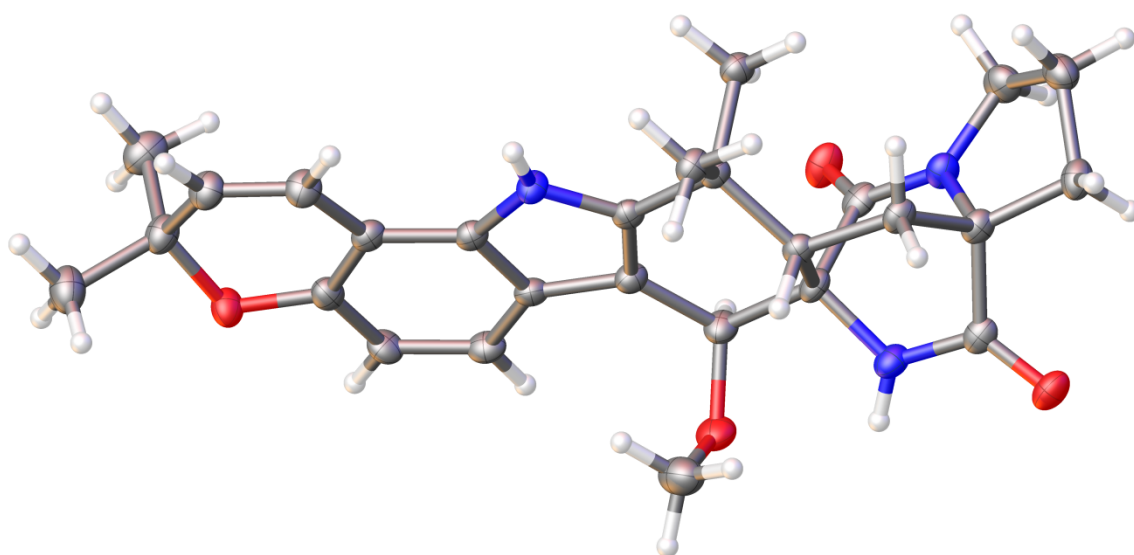


## X-ray crystallography

**S5:** X-ray crystal structure of **3**



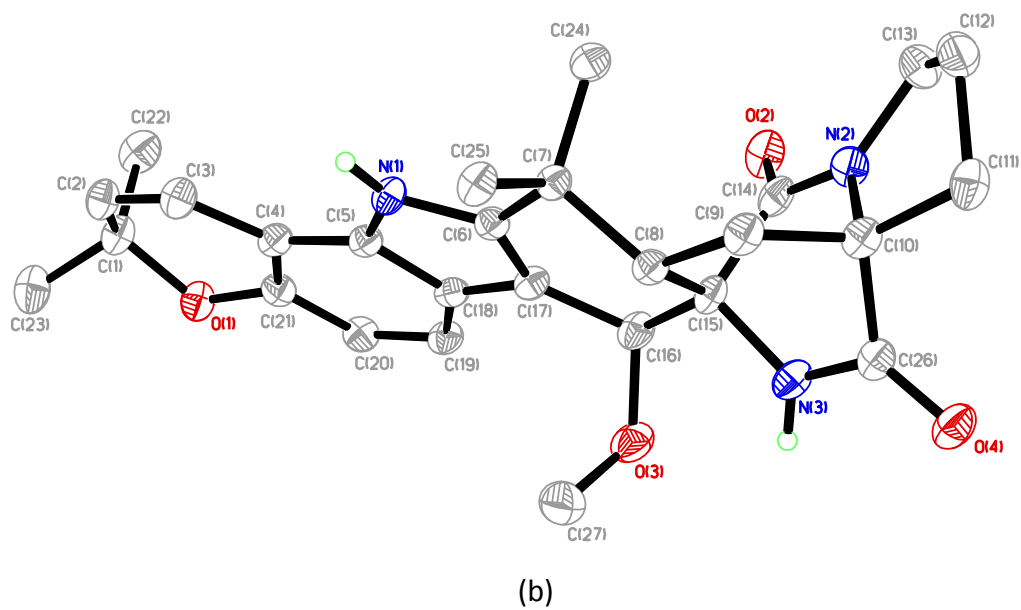
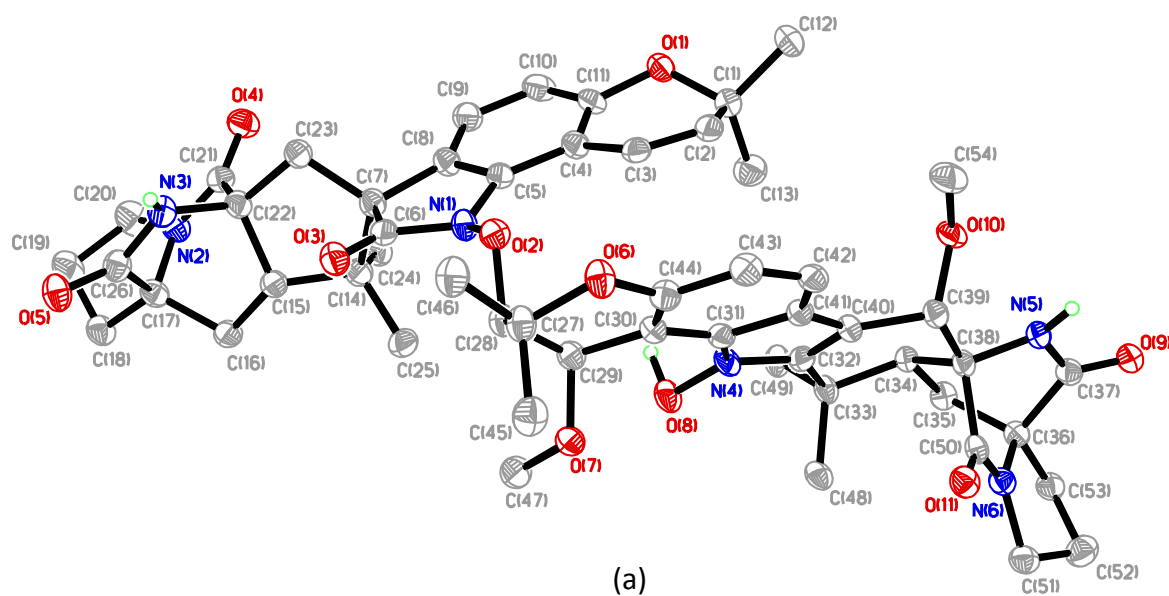
**S6:** X-ray crystal structure of **5**



### S7: X-ray crystallography details

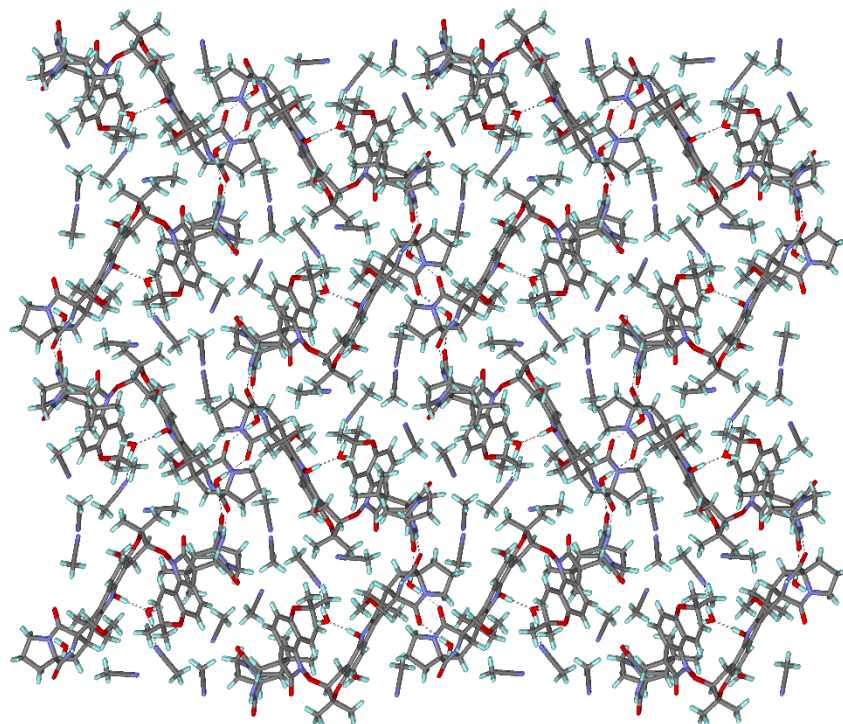
	Compound 3	Compound 5
CCDC Identifier	1994347	1994346
Crystal data		
Chemical formula	C <sub>64</sub> H <sub>81</sub> N <sub>11</sub> O <sub>13</sub>	C <sub>27</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub>
<i>M<sub>r</sub></i>	1212.39	461.55
Crystal system, space group	Orthorhombic, <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Orthorhombic, <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Temperature (K)	100	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.5082 (3), 23.6528 (8), 27.6237 (10)	8.1514 (3), 10.9209 (3), 25.9651 (8)
<i>V</i> (Å <sup>3</sup> )	6212.4 (4)	2311.43 (13)
<i>Z</i>	4	4
Radiation type	Cu <i>K</i> α	Cu <i>K</i> α
<i>m</i> (mm <sup>-1</sup> )	0.75	0.72
Crystal size (mm)	0.16 × 0.10 × 0.08	0.18 × 0.12 × 0.10
Data collection		
Diffractometer	Bruker D8 goniometer with CCD area detector	Bruker D8 goniometer with CCD area detector
Absorption correction	Multi-scan <i>SADABS</i>	Multi-scan <i>SADABS</i>
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.666, 0.806	0.793, 0.864
No. of measured, independent and observed [ <i>I</i> > 2 <i>s</i> ( <i>I</i> )] reflections	70587, 11009, 10444	22974, 3928, 3802
<i>R<sub>int</sub></i>	0.054	0.041
( <i>sin q</i> / <i>l</i> ) <sub>max</sub> (Å <sup>-1</sup> )	0.597	0.596
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 <i>s</i> ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.048, 0.131, 1.08	0.035, 0.090, 1.05
No. of reflections	11009	3928
No. of parameters	820	320
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
<i>Dρ<sub>max</sub></i> , <i>Dρ<sub>min</sub></i> (e Å <sup>-3</sup> )	0.45, -0.26	0.32, -0.21
Absolute structure	Flack <i>x</i> determined using 4363 quotients [( <i>I</i> <sup>+</sup> )-( <i>I</i> <sup>-</sup> )]/[( <i>I</i> <sup>+</sup> )+( <i>I</i> <sup>-</sup> )].	Flack <i>x</i> determined using 1531 quotients [( <i>I</i> <sup>+</sup> )-( <i>I</i> <sup>-</sup> )]/[( <i>I</i> <sup>+</sup> )+( <i>I</i> <sup>-</sup> )].
Absolute structure parameter	0.02 (6)	0.00 (12)

**S8:** Perspective views showing 50% probability displacement for 3 (a) and 5 (b) . The H atoms that ride on C atoms were omitted.

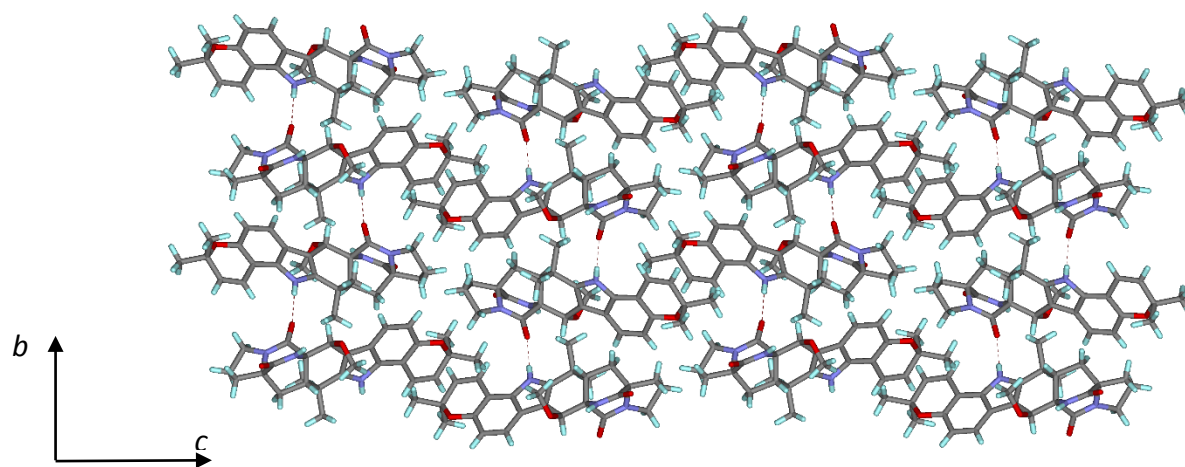




**S9: 3-D supramolecular architecture viewed along the a-axis direction for 3 (a) and 5 (b)**



(a)



(b)

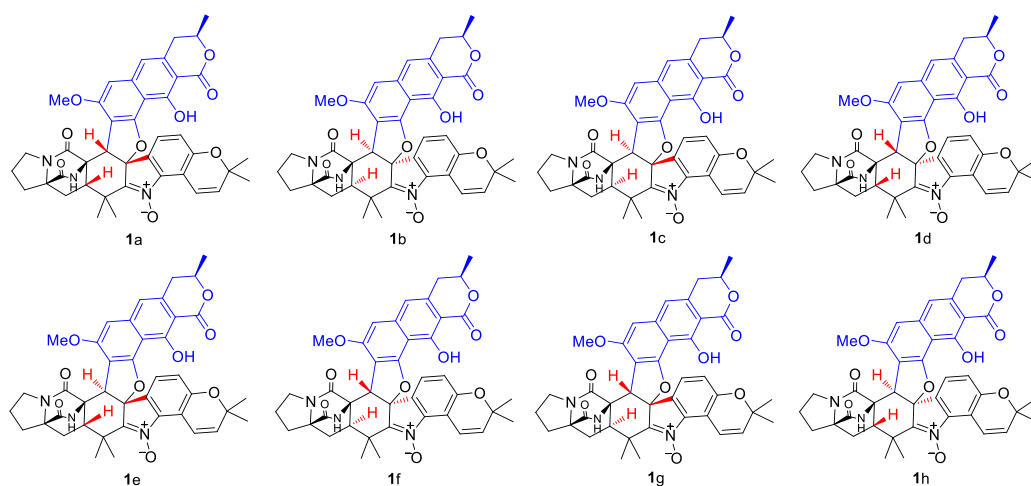
## Computational

### S10: Computational details

All the quantum mechanical calculations were performed using Gaussian 09.<sup>[12]</sup> Systematic conformational searches were done for each compound in the gas phase using the MMFF force field, implemented in Spartan 14,<sup>[13]</sup> and the results were validated using MacroModel<sup>[14]</sup> (MMFF force field, mixed torsional/low-mode sampling protocol) using an energy cutoff of 10 kcal/mol. The choice for the 10 kcal/mol of cutoff was set as a balance between reducing the overall CPU calculation time and minimizing the possibility of losing further contributing conformers. The number of unique conformations found within these boundaries ranged 8-17 depending on the relative configuration of the system under study. All conformers were kept for full geometry optimization at the B3LYP/6-31G\* level in gas phase. Frequency calculations were done at the same level to determine the nature of the stationary points found. All the B3LYP/6-31G\* optimized geometries (after removing duplicates) were next subjected to NMR calculations. The magnetic shielding constants ( $\sigma$ ) were computed using the *gauge including atomic orbitals* (GIAO) approach,<sup>[15]</sup> the method of choice to solve the gauge origin problem,<sup>[16]</sup> at the PCM/mPW1PW91/6-31+G\*\* level of theory (with methanol as solvent), the recommended for DP4+ calculations.<sup>[17]</sup> The unscaled chemical shifts ( $\delta_u$ ) were computed using TMS as reference standard according to  $\delta_u = \delta_0 - \delta_x$ , where  $\delta_x$  is the Boltzmann averaged isotropic shielding constant (over all significantly populated conformations) and  $\delta_0$  is the isotropic shielding constant of TMS computed at the same level of theory. The Boltzmann averaging was done according to eq 1:

$$\sigma^x = \frac{\sum_i \sigma_i^x e^{-E_i/RT}}{\sum_i e^{-E_i/RT}} \quad (\text{eq. 1})$$

where  $\sigma_i^x$  is the shielding constant for nucleus  $x$  in conformer  $i$ ,  $R$  is the molar gas constant ( $8.3145 \text{ J K}^{-1} \text{ mol}^{-1}$ ),  $T$  is the temperature (298 K), and  $E_i$  is the SCF energy of conformer  $i$  (relative to the lowest energy conformer), obtained at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level of theory. The scaled chemical shifts ( $\delta_s$ ) were computed as  $\delta_s = (\delta_u - b)/m$ , where  $m$  and  $b$  are the slope and intercept, respectively, resulting from a linear regression calculation on a plot of  $\delta_u$  against  $\delta_{exp}$ .<sup>[14]</sup> The DP4+ calculations were carried out using the Excel spreadsheet available for free at sarottinmr.weebly.com, or as part of the Supporting Information of the original paper.<sup>[17]</sup> The ECD calculations were carried out using the B3LYP/6-31G\* optimized geometries previously employed for DP4+ calculations. The excitation energies (nm) and rotatory strength ( $R$ ) in dipole velocity ( $R_{vel}$ ) of the first forty singlet excitations were calculated using TDDFT implemented in Gaussian 09 at the B3LYP/6-31G\* level of theory from all significantly populated conformers, which were averaged using Boltzmann weighting. The calculated rotatory strengths were simulated into the ECD curve as the sum of Gaussians with 0.5 eV width at half-heights ( $\sigma$ ). Geometry reoptimizations at CAM-B3LYP/6-31G\* and/or TDDFT calculations at other levels (including  $\omega$ B97XD, CAM-B3LYP and B3LYP) at gas phase or with the PCM model for the solvent were also carried out, and similar results were observed to those shown for B3LYP/6-31G\*.<sup>[18]</sup>



Structures (1a-h) used for NMR DP4+ calculation

**S11: NMR Boltzmann averaged isotropic magnetic shielding values ( $\sigma$ ) calculated at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level of theory for all significantly populated conformers of Isomers 1a-h.**

Atom	Isomer 1a	Isomer 1b	Isomer 1c	Isomer 1d	Isomer 1e	Isomer 1f	Isomer 1g	Isomer 1h
C-1	150.7682	149.9234	150.2642	151.2266	150.7385	151.3972	150.4025	149.5462
C-2	169.1348	169.8494	169.3850	168.8327	169.0354	168.9389	168.8210	169.1754
C-3	164.9362	166.3279	166.1252	163.3750	165.4470	166.8395	164.8481	164.9203
C-4	125.3265	126.1453	124.8992	125.3620	126.9843	125.1834	126.4028	126.6129
C-5	162.3031	161.4062	163.7568	159.9246	159.0914	162.8607	160.7466	164.5491
C-6	140.9378	142.4776	133.9091	126.2263	138.3490	141.6090	148.8011	149.5291
C-7	152.5430	151.5298	147.9288	148.0509	144.5183	144.5959	152.7288	153.0232
C-8	47.3481	48.1723	50.8395	50.9715	44.3127	44.2562	45.3630	45.0154
C-10	57.8554	57.8661	56.8945	58.5882	55.7926	55.0131	56.9312	57.3324
C-11	84.6760	84.4260	83.8860	85.4782	83.1753	85.5422	84.6451	84.9193
C-12	80.8279	80.7084	80.8393	80.2136	80.6086	80.0768	80.4574	80.8284
C-13	64.0347	64.6012	63.4636	64.7196	62.5215	62.4190	65.1811	64.0841
C-14	117.0291	117.4045	117.6712	118.8370	117.3062	117.2385	116.5337	116.7664
C-16	42.0628	42.1464	41.7574	43.5927	42.4127	43.0028	41.8985	41.5278
C-17	80.6185	82.3254	81.4173	82.2587	81.3852	79.6121	81.8493	83.1453
C-18	77.7254	76.8923	77.0941	76.5349	78.9313	75.7682	77.6847	76.4007
C-19	68.5626	68.2493	70.5110	69.2778	67.3948	67.8005	71.2288	70.5897
C-20	102.3990	102.0623	98.1357	96.8233	96.5562	96.1544	102.3343	100.9032
C-21	145.6276	150.8369	147.5043	144.3513	151.1094	149.0170	147.5089	152.4333
C-22	129.9819	130.7088	130.0603	132.5465	133.1179	133.2812	130.1834	130.3267
C-23	31.1630	30.5107	31.7430	33.4240	31.6217	31.3804	33.0035	29.5106
C-25	26.1529	26.8864	25.5494	26.2633	25.5790	24.2981	26.9865	24.5176
C-27	170.7004	170.4375	161.3159	162.4581	169.8736	167.8906	168.7756	168.6509
C-28	175.7435	173.1077	170.1346	171.5200	173.9586	173.2311	179.3392	178.5688
C-29	168.5947	168.3534	168.9808	169.1158	168.0918	168.5038	168.6710	168.3704
C-30	166.5689	166.9809	167.6640	167.4463	166.6740	166.3221	166.6565	166.6824
C-1'	27.2446	26.5019	27.1751	26.4753	29.0244	27.7895	27.5052	27.2897
C-10'	36.0429	34.7318	36.1527	37.2216	37.1871	38.5881	36.4807	35.2160
C-10'a	96.4730	96.7212	95.0192	94.0172	95.3575	95.6763	94.0683	94.8013
C-3'	119.1770	118.8363	118.7685	119.1999	119.8825	118.3123	119.1203	119.5653
C-3'-Me	175.1694	175.0200	174.7668	174.7465	174.4076	174.7559	175.2272	174.7307
C-4'	159.8432	158.9497	158.4594	159.0841	158.8946	159.4245	158.8602	158.7137
C-4'a	63.7410	59.0722	61.6875	61.3933	62.7060	63.3455	60.7294	58.5150
C-5'	81.0805	83.7278	82.7374	81.6954	82.9119	83.0507	82.9661	83.8175
C-5'a	53.8266	57.1846	58.0793	57.0707	53.4687	52.6282	58.6840	59.3077
C-6'	98.2349	98.2077	96.7360	97.6861	98.5521	99.6791	98.6538	98.1421
C-7'	41.9164	40.1891	42.4094	42.6415	42.2219	40.7531	36.7943	40.4645
C-7'-OMe	143.9173	141.3277	141.2934	140.9061	142.2925	140.6417	141.3065	140.6134
C-8'	84.5905	86.0854	82.9092	84.4161	85.4664	84.4619	81.8904	84.7533
C-9'	37.0871	39.1632	37.3415	38.5640	39.2812	39.8724	41.1961	39.3406
C-9'a	89.2064	90.2671	87.1627	85.1547	87.9359	87.1736	89.1427	88.7841
H-1	28.1295	27.9218	27.9909	28.2292	27.9860	28.3666	28.1356	28.0583
H-1	28.3399	28.1778	28.1203	28.3218	27.9896	28.4381	28.2372	28.0937
H-2	29.5247	29.4872	29.5025	29.5691	29.4483	29.5326	29.6042	29.5102
H-2	29.5216	29.4844	29.4826	29.5530	29.4378	29.4849	29.5217	29.4377
H-3	29.6470	29.6664	29.7022	29.7189	29.5761	29.5864	29.6603	29.6695
H-3	28.9105	28.9147	28.9458	28.9275	28.8817	28.8296	28.8951	28.8794
H-5	29.5023	29.3960	29.4370	29.1984	29.8043	29.6128	29.6010	29.6854
H-5	29.2260	29.1690	29.1218	29.0280	29.6498	29.5961	29.3965	29.4079
H-6	29.1801	29.2846	28.9677	28.8982	28.2128	29.4567	28.6764	28.8256
H-12	23.1579	23.1202	23.4302	23.4820	23.2038	23.2344	23.1177	23.2571
H-13	25.3268	25.3339	25.3920	25.4098	25.2345	25.2312	25.3469	25.3210
H-17	24.7532	24.7123	24.9426	24.8419	24.9308	24.9548	24.7253	24.6681
H-18	24.6157	24.4152	25.0732	24.7494	24.6273	24.5329	24.5603	24.3917
H-21	27.7676	26.0715	26.1842	26.1801	25.6993	26.3797	27.6590	26.7865
H-27	30.3339	30.2779	29.7903	29.8738	30.1622	29.9278	30.0159	30.0893
H-28	29.8431	29.8674	29.7665	29.8088	29.9966	29.8922	29.8072	30.0274
H-29	30.2001	30.2151	30.2313	30.2384	30.1925	30.2023	30.2118	30.1794
H-30	30.0874	30.0311	30.0802	30.0964	30.0954	30.1106	30.0770	30.0331
H-3'	26.7296	26.7808	26.7894	26.7685	26.8087	26.7579	26.7926	26.8047
H-4'	28.4828	28.5576	28.6871	28.5139	28.5492	28.6431	28.6467	28.6520
H-4'	28.4185	28.5472	28.2948	28.4526	28.4372	28.5292	28.5779	28.5894
H-5'	24.3773	24.2779	24.4266	24.3425	24.2705	24.3540	24.3552	24.3004
H-6'	24.4600	24.5437	24.4948	24.3093	24.5961	24.5050	24.5834	24.4470
H-3'-Me	30.0391	30.0550	30.1076	30.0819	30.1398	30.0517	30.1173	30.1287
H-7'-OMe	27.4491	27.6315	27.5935	27.3952	27.4849	27.5873	27.4810	27.4423

**S12: Unscaled chemical shifts computed for compounds 1a-h at the PCM/mPW1PW91/6-31+G\*\*/B3LYP/6-31G\* level of theory, using TMS as reference standard.**

Atom	Isomer 1a	Isomer 1b	Isomer 1c	Isomer 1d	Isomer 1e	Isomer 1f	Isomer 1g	Isomer 1h
C-1	46.0	46.9	46.5	45.6	46.0	45.4	46.4	47.2
C-2	27.6	26.9	27.4	27.9	27.7	27.8	28.0	27.6
C-3	31.8	30.5	30.7	33.4	31.3	29.9	31.9	31.9
C-4	71.5	70.6	71.9	71.4	69.8	71.6	70.4	70.2
C-5	34.5	35.4	33.0	36.9	37.7	33.9	36.0	32.2
C-6	55.8	54.3	62.9	70.6	58.4	55.2	48.0	47.3
C-7	44.2	45.2	48.9	48.7	52.3	52.2	44.1	43.8
C-8	149.4	148.6	145.9	145.8	152.5	152.5	151.4	151.8
C-10	138.9	138.9	139.9	138.2	141.0	141.8	139.8	139.4
C-11	112.1	112.4	112.9	111.3	113.6	111.2	112.1	111.9
C-12	116.0	116.1	115.9	116.6	116.2	116.7	116.3	116.0
C-13	132.7	132.2	133.3	132.1	134.3	134.4	131.6	132.7
C-14	79.8	79.4	79.1	77.9	79.5	79.5	80.2	80.0
C-16	154.7	154.6	155.0	153.2	154.4	153.8	154.9	155.3
C-17	116.2	114.5	115.4	114.5	115.4	117.2	114.9	113.6
C-18	119.1	119.9	119.9	120.2	117.8	121.0	119.1	120.4
C-19	128.2	128.5	126.3	127.5	129.4	129.0	125.6	126.2
C-20	94.4	94.7	98.6	100.0	100.2	100.6	94.4	95.9
C-21	51.2	45.9	49.3	52.4	45.7	47.8	49.3	44.3
C-22	66.8	66.1	66.7	64.2	63.7	63.5	66.6	66.5
C-23	165.6	166.3	165.0	163.4	165.2	165.4	163.8	167.3
C-25	170.6	169.9	171.2	170.5	171.2	172.5	169.8	172.3
C-27	26.1	26.3	35.5	34.3	26.9	28.9	28.0	28.1
C-28	21.0	23.7	26.6	25.3	22.8	23.5	17.4	18.2
C-29	28.2	28.4	27.8	27.7	28.7	28.3	28.1	28.4
C-30	30.2	29.8	29.1	29.3	30.1	30.5	30.1	30.1
C-1'	169.5	170.3	169.6	170.3	167.8	169.0	169.3	169.5
C-10'	160.7	162.0	160.6	159.6	159.6	158.2	160.3	161.6
C-10'a	100.3	100.1	101.8	102.8	101.4	101.1	102.7	102.0
C-3'	77.6	77.9	78.0	77.6	76.9	78.5	77.7	77.2
C-3'-Me	21.6	21.8	22.0	22.0	22.4	22.0	21.6	22.0
C-4'	36.9	37.8	38.3	37.7	37.9	37.4	37.9	38.1
C-4'a	133.0	137.7	135.1	135.4	134.1	133.4	136.0	138.3
C-5'	115.7	113.1	114.0	115.1	113.9	113.7	113.0	113.0
C-5'a	143.0	139.6	138.7	139.7	143.3	144.2	138.1	137.5
C-6'	98.5	98.6	100.0	99.1	98.2	97.1	98.1	98.6
C-7'	154.9	156.6	154.4	154.1	154.6	156.0	160.0	156.3
C-7'-OMe	52.9	55.5	55.5	55.9	54.5	56.1	55.5	56.2
C-8'	112.2	110.7	113.9	112.4	111.3	112.3	114.9	112.0
C-9'	159.7	157.6	159.4	158.2	157.5	156.9	155.6	157.4
C-9'a	107.6	106.5	109.6	111.6	108.8	109.6	107.6	108.0
H-1	3.42	3.63	3.56	3.32	3.56	3.18	3.41	3.49
H-1	3.21	3.37	3.43	3.23	3.56	3.11	3.31	3.46
H-2	2.03	2.06	2.05	1.98	2.10	2.02	1.95	2.04
H-2	2.03	2.07	2.07	2.00	2.11	2.07	2.03	2.11
H-3	1.90	1.88	1.85	1.83	1.97	1.96	1.89	1.88
H-3	2.64	2.64	2.60	2.62	2.67	2.72	2.66	2.67
H-5	2.05	2.15	2.11	2.35	1.75	1.94	1.95	1.87
H-5	2.32	2.38	2.43	2.52	1.90	1.95	2.15	2.14
H-6	2.37	2.27	2.58	2.65	2.34	2.09	2.87	2.72
H-12	8.39	8.43	8.12	8.07	8.35	8.32	8.43	8.29
H-13	6.22	6.22	6.16	6.14	6.32	6.32	6.20	6.23
H-17	6.80	6.84	6.61	6.71	6.62	6.60	6.83	6.88
H-18	6.93	7.14	6.48	6.80	6.92	7.02	6.99	7.16
H-21	3.78	5.48	5.37	5.37	5.85	5.17	3.89	4.76
H-27	1.22	1.27	1.76	1.68	1.39	1.62	1.53	1.46
H-28	1.71	1.68	1.78	1.74	1.55	1.66	1.74	1.52
H-29	1.35	1.34	1.32	1.31	1.36	1.35	1.34	1.37
H-30	1.46	1.52	1.47	1.45	1.46	1.44	1.47	1.52
H-3'	4.82	4.77	4.76	4.78	4.74	4.79	4.76	4.75
H-4'	3.07	2.99	2.86	3.04	3.00	2.91	2.90	2.90
H-4'	3.13	3.00	3.26	3.10	3.11	3.02	2.97	2.96
H-5'	7.17	7.27	7.12	7.21	7.28	7.20	7.20	7.25
H-6'	7.09	7.01	7.06	7.24	6.95	7.05	6.97	7.10
H-3'-Me	1.51	1.50	1.44	1.47	1.41	1.50	1.43	1.42
H-7'-OMe	4.10	3.92	3.96	4.16	4.07	3.96	4.07	4.11

**S13: Scaled chemical shifts computed for compounds 1a-h by correlating the unscaled shifts (S14) with the experimental NMR data of Waikikiamide A collected in CD<sub>3</sub>OD.**

Atom	Isomer 1a	Isomer 1b	Isomer 1c	Isomer 1d	Isomer 1e	Isomer 1f	Isomer 1g	Isomer 1h
C-1	43.8	44.8	42.7	41.0	43.0	42.4	44.5	45.8
C-2	24.6	24.0	22.4	22.1	23.8	24.1	25.3	25.5
C-3	29.0	27.7	25.8	27.9	27.6	26.3	29.4	29.9
C-4	70.3	69.6	69.6	68.7	68.0	69.8	69.5	69.5
C-5	31.8	32.8	28.3	31.6	34.3	30.4	33.7	30.3
C-6	54.0	52.6	60.1	67.8	56.1	52.7	46.1	45.8
C-7	41.9	43.1	45.2	44.4	49.6	49.5	42.0	42.2
C-8	151.7	151.0	148.3	148.6	154.9	154.5	154.0	153.8
C-10	140.7	140.9	141.9	140.4	142.8	143.3	141.9	141.1
C-11	112.8	113.2	113.2	111.6	114.0	111.3	113.0	112.6
C-12	116.8	117.0	116.4	117.2	116.7	117.0	117.4	116.8
C-13	134.3	133.9	134.9	133.9	135.7	135.5	133.3	134.1
C-14	79.0	78.7	77.3	75.7	78.2	78.2	79.8	79.7
C-16	157.2	157.3	157.9	156.5	156.9	155.8	157.6	157.4
C-17	117.0	115.4	115.8	115.0	115.9	117.5	115.9	114.4
C-18	120.0	121.0	120.4	121.2	118.5	121.5	120.3	121.4
C-19	129.6	130.0	127.4	129.0	130.6	129.9	127.0	127.4
C-20	94.3	94.7	98.1	99.4	100.0	100.2	94.6	96.1
C-21	49.2	43.8	45.6	48.3	42.6	44.9	47.5	42.8
C-22	65.5	64.8	64.1	61.0	61.5	61.4	65.5	65.7
C-23	168.6	169.4	168.6	167.5	168.2	168.0	166.9	169.8
C-25	173.8	173.2	175.2	175.1	174.6	175.4	173.1	175.0
C-27	23.0	23.4	30.9	28.9	22.9	25.2	25.3	26.1
C-28	17.7	20.6	21.6	19.2	18.6	19.6	14.3	15.8
C-29	25.2	25.5	22.8	21.8	24.8	24.5	25.4	26.4
C-30	27.3	27.0	24.2	23.6	26.3	26.8	27.5	28.1
C-1'	172.7	173.6	173.4	174.9	170.9	171.7	172.6	172.1
C-10'	163.5	165.0	163.9	163.4	162.4	160.4	163.2	163.9
C-10'a	100.4	100.3	101.4	102.4	101.2	100.7	103.2	102.4
C-3'	76.8	77.2	76.1	75.4	75.5	77.0	77.1	76.8
C-3'-Me	18.3	18.6	16.7	15.7	18.2	18.0	18.6	19.8
C-4'	34.3	35.4	34.0	32.5	34.5	34.0	35.6	36.4
C-4'a	134.6	139.6	136.8	137.4	135.5	134.5	137.9	139.9
C-5'	116.5	113.9	114.4	115.6	114.3	113.9	114.8	113.7
C-5'a	145.0	141.6	140.6	142.1	145.3	145.8	140.1	139.1
C-6'	98.6	98.8	99.5	98.5	97.9	96.5	98.4	98.9
C-7'	157.4	159.3	157.3	157.6	157.1	158.2	162.9	158.5
C-7'-OMe	50.9	53.8	52.2	52.0	51.9	53.7	53.9	55.1
C-8'	112.8	111.4	114.2	112.7	111.6	112.5	115.9	112.8
C-9'	162.4	160.4	162.6	161.9	160.2	159.1	158.3	159.7
C-9'a	108.0	107.1	109.7	111.9	109.0	109.6	108.3	108.6
H-1	3.44	3.56	3.51	3.26	3.52	3.21	3.43	3.46
H-1	3.24	3.32	3.38	3.17	3.52	3.14	3.33	3.43
H-2	2.10	2.09	2.01	1.96	2.14	2.10	2.01	2.09
H-2	2.10	2.09	2.03	1.97	2.15	2.15	2.09	2.16
H-3	1.98	1.92	1.82	1.81	2.02	2.05	1.96	1.94
H-3	2.69	2.63	2.57	2.58	2.68	2.77	2.69	2.69
H-5	2.12	2.18	2.08	2.32	1.81	2.02	2.02	1.93
H-5	2.39	2.39	2.39	2.49	1.95	2.04	2.21	2.19
H-6	2.43	2.28	2.54	2.61	2.37	2.17	2.90	2.74
H-12	8.21	8.07	8.03	7.87	8.01	8.08	8.25	7.99
H-13	6.13	5.99	6.09	6.00	6.10	6.19	6.11	6.04
H-17	6.68	6.58	6.53	6.55	6.39	6.45	6.70	6.66
H-18	6.81	6.86	6.40	6.64	6.67	6.85	6.86	6.92
H-21	3.79	5.30	5.30	5.25	5.67	5.10	3.88	4.66
H-27	1.32	1.35	1.73	1.66	1.47	1.72	1.62	1.55
H-28	1.79	1.73	1.75	1.73	1.63	1.76	1.82	1.60
H-29	1.45	1.41	1.29	1.31	1.44	1.46	1.43	1.46
H-30	1.56	1.58	1.44	1.45	1.54	1.55	1.56	1.60
H-3'	4.78	4.63	4.70	4.68	4.62	4.74	4.72	4.64
H-4'	3.10	2.96	2.82	2.98	2.99	2.95	2.93	2.90
H-4'	3.16	2.97	3.21	3.04	3.09	3.05	3.00	2.96
H-5'	7.04	6.99	7.04	7.04	7.01	7.02	7.06	7.00
H-6'	6.96	6.74	6.98	7.07	6.70	6.88	6.84	6.86
H-3'-Me	1.61	1.56	1.42	1.46	1.49	1.61	1.52	1.51
H-7'-OMe	4.09	3.83	3.91	4.07	3.99	3.95	4.05	4.04

**S14: Absolute unscaled and scaled errors computed for compounds 1a-h and DP4+ results.**

	Absolute unscaled error ( $abs[\delta_{exp} - \delta_{u}]$ )								Absolute scaled error ( $abs[\delta_{exp} - \delta_{s}]$ )							
	1a	1b	1c	1d	1e	1f	1g	1h	1a	1b	1c	1d	1e	1f	1g	1h
C-1	0.7	1.6	1.2	0.3	0.7	0.1	1.1	1.9	1.5	0.5	2.6	4.3	2.3	2.9	0.8	0.5
C-2	2.1	1.4	1.9	2.4	2.2	2.3	2.5	2.1	0.9	1.5	3.1	3.4	1.7	1.4	0.2	0.0
C-3	2.1	0.8	1.0	3.7	1.6	0.2	2.2	2.2	0.7	2.0	3.9	1.8	2.1	3.4	0.3	0.2
C-4	3.9	3.0	4.3	3.8	2.2	4.0	2.8	2.6	2.7	2.0	2.0	1.1	0.4	2.2	1.9	1.9
C-5	5.0	5.9	3.5	7.4	8.2	4.4	6.5	2.7	2.3	3.3	1.2	2.1	4.8	0.9	4.2	0.8
C-6	9.8	8.3	16.9	24.6	12.4	9.2	2.0	1.3	8.0	6.6	14.1	21.8	10.1	6.7	0.1	0.2
C-7	5.1	6.1	9.8	9.6	13.2	13.1	5.0	4.7	2.8	4.0	6.1	5.3	10.5	10.4	2.9	3.1
C-8	0.5	1.3	4.0	4.1	2.6	2.6	1.5	1.9	1.8	1.1	1.6	1.3	5.0	4.6	4.1	3.9
C-10	2.3	2.3	1.3	3.0	0.2	0.6	1.4	1.8	0.5	0.3	0.7	0.8	1.6	2.1	0.7	0.1
C-11	1.9	1.6	1.1	2.7	0.4	2.8	1.9	2.1	1.2	0.8	0.8	2.4	0.0	2.7	1.0	1.4
C-12	0.6	0.5	0.7	0.0	0.4	0.1	0.3	0.6	0.2	0.4	0.2	0.6	0.1	0.4	0.8	0.2
C-13	2.1	2.6	1.5	2.7	0.5	0.4	3.2	2.1	0.5	0.9	0.1	0.9	0.9	0.7	1.5	0.7
C-14	2.0	1.6	1.3	0.1	1.7	1.7	2.4	2.2	1.2	0.9	0.5	2.1	0.4	0.4	2.0	1.9
C-16	2.5	2.6	2.2	4.0	2.8	3.4	2.3	1.9	0.0	0.1	0.7	0.7	0.3	1.4	0.4	0.2
C-17	1.9	3.6	2.7	3.6	2.7	0.9	3.2	4.5	1.1	2.7	2.3	3.1	2.2	0.6	2.2	3.7
C-18	2.0	1.2	1.4	0.9	3.3	0.1	2.0	0.7	1.1	0.1	0.7	0.1	2.6	0.4	0.8	0.3
C-19	0.4	0.7	1.5	0.3	1.6	1.2	2.2	1.6	1.8	2.2	0.4	1.2	2.8	2.1	0.8	0.4
C-20	0.3	0.6	4.5	5.9	6.1	6.5	0.3	1.8	0.2	0.6	4.0	5.3	5.9	6.1	0.5	2.0
C-21	8.0	2.7	6.1	9.2	2.5	4.6	6.1	1.1	6.0	0.6	2.4	5.1	0.6	1.7	4.3	0.4
C-22	2.6	1.9	2.5	0.0	0.5	0.7	2.4	2.3	1.3	0.6	0.1	3.2	2.7	2.8	1.3	1.5
C-23	3.8	3.1	4.4	6.0	4.2	4.0	5.6	2.1	0.8	0.0	0.8	1.9	1.2	1.4	2.5	0.4
C-25	4.9	5.6	4.3	5.0	4.3	3.0	5.7	3.2	1.7	2.3	0.3	0.4	0.9	0.1	2.4	0.5
C-27	0.5	0.3	8.9	7.7	0.3	2.3	1.4	1.5	3.6	3.2	4.3	2.3	3.7	1.4	1.3	0.5
C-28	4.4	7.1	10.0	8.7	6.2	6.9	0.8	1.6	1.1	4.0	5.0	2.6	2.0	3.0	2.3	0.8
C-29	0.2	0.4	0.2	0.4	0.7	0.2	0.1	0.4	2.8	2.5	5.2	6.3	3.2	3.5	2.6	1.7
C-30	2.2	1.8	1.1	1.3	2.1	2.4	2.1	2.1	0.7	1.1	3.8	4.5	1.8	1.2	0.5	0.1
C-1'	2.8	2.0	2.7	2.0	4.5	3.3	3.0	2.8	0.4	1.3	1.1	2.6	1.4	0.6	0.3	0.2
C-10'	2.6	1.3	2.7	3.7	3.7	5.1	3.0	1.7	0.2	1.7	0.6	0.1	0.9	2.9	0.1	0.6
C-10'a	2.0	2.2	0.5	0.5	0.9	1.2	0.4	0.3	1.9	2.0	0.9	0.1	1.1	1.6	0.9	0.1
C-3'	0.0	0.3	0.4	0.0	0.7	0.9	0.1	0.4	0.8	0.4	1.5	2.2	2.1	0.6	0.5	0.8
C-3'-Me	0.7	0.9	1.1	1.1	1.5	1.1	0.7	1.1	2.6	2.3	4.2	5.2	2.7	2.9	2.3	1.1
C-4'	1.2	2.1	2.6	2.0	2.2	1.7	2.2	2.4	1.4	0.3	1.7	3.2	1.2	1.7	0.1	0.7
C-4'a	1.8	2.9	0.3	0.6	0.7	1.4	1.2	3.5	0.2	4.8	2.0	2.6	0.7	0.3	3.1	5.1
C-5'	1.1	3.7	2.8	1.7	2.9	3.1	3.0	3.8	0.3	2.9	2.4	1.2	2.5	2.9	2.0	3.1
C-5'a	0.1	3.5	4.4	3.4	0.2	1.1	5.0	5.6	1.9	1.5	2.5	1.0	2.2	2.7	3.0	4.0
C-6'	3.4	3.3	1.9	2.8	3.7	4.8	3.8	3.3	3.3	3.1	2.4	3.4	4.0	5.4	3.5	3.0
C-7'	3.6	1.9	4.1	4.4	3.9	2.5	1.5	2.2	1.1	0.8	1.2	0.9	1.4	0.3	4.4	0.0
C-7'-OMe	4.1	1.5	1.5	1.1	2.5	0.9	1.5	0.8	6.1	3.2	4.8	5.0	5.1	3.3	3.1	1.9
C-8'	0.4	1.1	2.1	0.6	0.5	0.5	3.1	0.2	1.0	0.4	2.4	0.9	0.2	0.7	4.1	1.0
C-9'	0.1	2.0	0.2	1.4	2.1	2.7	4.0	2.2	2.8	0.8	3.0	2.3	0.6	0.5	1.3	0.1
C-9'a	1.4	2.5	0.6	2.6	0.2	0.6	1.4	1.0	1.0	1.9	0.7	2.9	0.0	0.6	0.7	0.4
Average	2.4	2.4	3.1	3.5	2.8	2.6	2.5	2.1	1.7	1.8	2.4	2.9	2.3	2.2	1.8	1.2
H-1a	0.01	0.20	0.13	0.11	0.13	0.25	0.02	0.06	0.01	0.13	0.08	0.17	0.09	0.22	0.00	0.03
H-1b	0.22	0.06	0.00	0.20	0.13	0.32	0.12	0.03	0.19	0.11	0.05	0.26	0.09	0.29	0.10	0.00
H-2a	0.07	0.10	0.09	0.02	0.14	0.06	0.01	0.08	0.14	0.13	0.05	0.00	0.18	0.14	0.05	0.13
H-2b	0.05	0.01	0.01	0.08	0.03	0.01	0.05	0.03	0.02	0.01	0.05	0.11	0.07	0.07	0.01	0.08
H-3a	0.04	0.06	0.09	0.11	0.03	0.02	0.05	0.06	0.04	0.02	0.12	0.13	0.08	0.11	0.02	0.00
H-3b	0.01	0.01	0.03	0.01	0.04	0.09	0.03	0.04	0.06	0.00	0.06	0.05	0.05	0.14	0.06	0.06
H-5a	0.08	0.18	0.14	0.38	0.22	0.03	0.02	0.10	0.15	0.21	0.11	0.35	0.16	0.05	0.05	0.04
H-5b	0.04	0.10	0.15	0.24	0.38	0.33	0.13	0.14	0.11	0.11	0.11	0.21	0.33	0.24	0.07	0.09
H-6	0.53	0.63	0.32	0.25	0.56	0.81	0.03	0.18	0.47	0.62	0.36	0.29	0.53	0.73	0.00	0.16
H-12	0.65	0.69	0.38	0.33	0.61	0.58	0.69	0.55	0.47	0.33	0.29	0.13	0.27	0.34	0.51	0.25
H-13	0.30	0.30	0.24	0.22	0.40	0.40	0.28	0.31	0.21	0.07	0.17	0.08	0.18	0.27	0.19	0.12
H-17	0.17	0.21	0.02	0.08	0.01	0.03	0.20	0.25	0.05	0.05	0.10	0.08	0.24	0.18	0.07	0.03
H-18	0.17	0.38	0.28	0.04	0.16	0.26	0.23	0.40	0.05	0.10	0.36	0.12	0.09	0.09	0.10	0.16
H-21	0.98	0.72	0.61	0.61	1.09	0.41	0.87	0.00	0.97	0.54	0.54	0.49	0.91	0.34	0.88	0.10
H-27	0.32	0.27	0.22	0.14	0.15	0.08	0.01	0.08	0.22	0.19	0.19	0.12	0.07	0.18	0.08	0.01
H-28	0.10	0.07	0.17	0.13	0.06	0.05	0.13	0.09	0.18	0.12	0.14	0.12	0.02	0.15	0.21	0.01
H-29	0.07	0.08	0.10	0.11	0.06	0.07	0.08	0.05	0.03	0.01	0.13	0.11	0.02	0.04	0.01	0.04
H-30	0.04	0.10	0.05	0.03	0.04	0.02	0.05	0.10	0.14	0.16	0.02	0.03	0.12	0.13	0.14	0.18
H-3'	0.10	0.05	0.04	0.06	0.02	0.07	0.04	0.03	0.06	0.09	0.02	0.04	0.10	0.02	0.00	0.08
H-4'a	0.09	0.01	0.12	0.06	0.02	0.07	0.08	0.08	0.12	0.02	0.16	0.00	0.01	0.03	0.05	0.08
H-4'b	0.04	0.09	0.17	0.01	0.02	0.07	0.12	0.13	0.07	0.12	0.12	0.05	0.00	0.04	0.09	0.13
H-5'	0.04	0.14	0.01	0.08	0.15	0.07	0.07	0.12	0.09	0.14	0.09	0.09	0.12	0.11	0.07	0.13
H-6'	0.03	0.05	0.00	0.18	0.11	0.01	0.09	0.04	0.10	0.32	0.08	0.01	0.36	0.18	0.22	0.20
H-3'-Me	0.02	0.01	0.05	0.02	0.08	0.01	0.06	0.07	0.12	0.07	0.07	0.03	0.00	0.12	0.03	0.02
H-7'-OMe	0.01	0.19	0.15	0.05	0.04	0.15	0.04	0.00	0.02	0.28	0.20	0.04	0.12	0.16	0.06	0.07
Average	0.17	0.19	0.14	0.14	0.19	0.17	0.14	0.12	0.16	0.16	0.15	0.12	0.17	0.17	0.12	0.09

Functional	Solvent?	Basis Set	Type of Data													
mPW1PW91	PCM	6-31+G(d,p)	Shielding Tensors													
	1a	1b	1c	1d	1e	1f	1g	1h								
sDP4+ (H data)	0.00%	0.00%	0.00%	0.04%	0.00%	0.00%	0.66%	99.30%								
sDP4+ (C data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								
sDP4+ (all data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								
uDP4+ (H data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.19%	99.81%								
uDP4+ (C data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								
uDP4+ (all data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								
DP4+ (H data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								
DP4+ (C data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								
DP4+ (all data)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	100.00%								

**S15: NMR Boltzmann averaged isotropic magnetic shielding values ( $\sigma$ ), unscaled chemical shifts ( $\delta_u$ ) and scaled chemical shifts ( $\delta_s$ ) computed for 3'epi-16 at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level of theory.**

Atom	$\sigma$	$\delta_u$	$\delta_s$
C-1	151.1661	45.6	44.2
C-2	167.8199	29.0	27.0
C-3	164.4214	32.4	30.5
C-4	124.8652	71.9	71.4
C-5	165.6927	31.1	29.2
C-6	148.2413	48.5	47.2
C-7	151.9229	44.9	43.4
C-8	45.6130	151.2	153.1
C-10	57.5495	139.2	140.8
C-11	83.9041	112.9	113.6
C-12	80.6655	116.1	117.0
C-13	64.8216	132.0	133.3
C-14	116.0607	80.7	80.4
C-16	41.3148	155.5	157.6
C-17	82.5954	114.2	115.0
C-18	77.1756	119.6	120.6
C-19	70.6609	126.1	127.3
C-20	101.1089	95.7	95.9
C-21	153.3871	43.4	41.9
C-22	130.4943	66.3	65.5
C-23	30.3757	166.4	168.9
C-25	24.5078	172.3	174.9
C-27	170.0198	26.8	24.8
C-28	178.6386	18.1	15.9
C-29	169.0130	27.8	25.8
C-30	166.6804	30.1	28.2
C-1'	27.0995	169.7	172.2
C-10'	34.9646	161.8	164.1
C-10'a	95.5669	101.2	101.6
C-3'	118.6170	78.2	77.8
C-3'-Me	174.9517	21.8	19.7
C-4'	159.7393	37.0	35.4
C-4'a	61.5891	135.2	136.6
C-5'	82.8045	114.0	114.8
C-5'a	55.0653	141.7	143.4
C-6'	98.4332	98.3	98.6
C-7'	40.6214	156.2	158.3
C-7'-OMe	140.9844	55.8	54.7
C-8'	84.8890	111.9	112.6
C-9'	39.0349	157.7	159.9
C-9'a	89.1512	107.6	108.2
H-1	28.1092	3.44	3.41
H-1	28.1241	3.43	3.39
H-2	29.5316	2.02	2.06
H-2	29.4683	2.08	2.12
H-3	29.6421	1.91	1.96
H-3	28.8230	2.73	2.73
H-5	29.7143	1.84	1.89
H-5	29.4794	2.07	2.11
H-6	28.8710	2.68	2.69
H-12	23.1990	8.35	8.05
H-13	25.3407	6.21	6.02
H-17	24.6324	6.92	6.69
H-18	24.4400	7.11	6.88
H-21	26.7214	4.83	4.72
H-27	30.0234	1.53	1.60
H-28	30.0116	1.54	1.61
H-29	30.1419	1.41	1.48
H-30	30.0499	1.50	1.57
H-3'	26.7607	4.79	4.68
H-4'	28.6044	2.95	2.94
H-4'	28.4866	3.06	3.05
H-5'	24.3837	7.17	6.93
H-6'	24.4889	7.06	6.83
H-3'-Me	30.0959	1.45	1.53
H-7'-OMe	27.4199	4.13	4.06

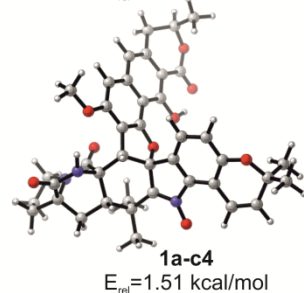
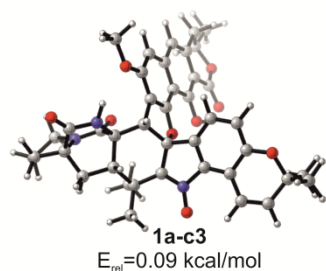
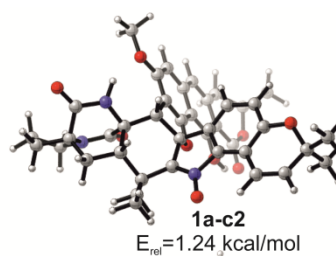
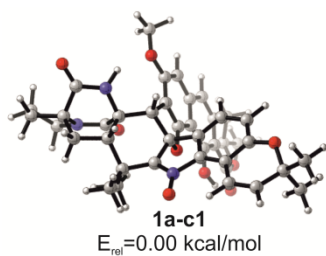
**S16:** Absolute unscaled and scaled errors computed for compounds 1h and 3'epi-1h, and DP4+ results.

	abs[ $\delta_{exp} - \delta_{u}$ ]		abs[ $\delta_{exp} - \delta_{s}$ ]	
	1h	3'epi-1h	1h	3'epi-1h
C-1	1.9	0.3	0.5	1.1
C-2	2.1	3.5	0.0	1.5
C-3	2.2	2.7	0.2	0.8
C-4	2.6	4.3	1.9	3.8
C-5	2.7	1.6	0.8	0.3
C-6	1.3	2.5	0.2	1.2
C-7	4.7	5.8	3.1	4.3
C-8	1.9	1.3	3.9	3.2
C-10	1.8	2.0	0.1	0.4
C-11	2.1	1.1	1.4	0.4
C-12	0.6	0.5	0.2	0.4
C-13	2.1	2.8	0.7	1.5
C-14	2.2	2.9	1.9	2.6
C-16	1.9	1.7	0.2	0.4
C-17	4.5	3.9	3.7	3.1
C-18	0.7	1.5	0.3	0.5
C-19	1.6	1.7	0.4	0.5
C-20	1.8	1.6	2.0	1.8
C-21	1.1	0.2	0.4	1.3
C-22	2.3	2.1	1.5	1.3
C-23	2.1	3.0	0.4	0.5
C-25	3.2	3.2	0.5	0.6
C-27	1.5	0.2	0.5	1.8
C-28	1.6	1.5	0.8	0.7
C-29	0.4	0.3	1.7	2.2
C-30	2.1	2.1	0.1	0.2
C-1'	2.8	2.6	0.2	0.1
C-10'	1.7	1.5	0.6	0.8
C-10'a	0.3	1.1	0.1	0.7
C-3'	0.4	0.6	0.8	0.2
C-3'-Me	1.1	0.9	1.1	1.2
C-4'	2.4	1.3	0.7	0.3
C-4'a	3.5	0.4	5.1	1.8
C-5'	3.8	2.8	3.1	2.0
C-5'a	5.6	1.4	4.0	0.3
C-6'	3.3	3.6	3.0	3.3
C-7'	2.2	2.3	0.0	0.2
C-7'-OMe	0.8	1.2	1.9	2.3
C-8'	0.2	0.1	1.0	0.8
C-9'	2.2	1.9	0.1	0.3
C-9'a	1.0	1.4	0.4	0.8
<b>Average</b>	<b>2.1</b>	<b>1.9</b>	<b>1.2</b>	<b>1.3</b>
H-1a	0.06	0.01	0.03	0.02
H-1b	0.03	0.00	0.00	0.04
H-2a	0.08	0.06	0.13	0.10
H-2b	0.03	0.00	0.08	0.04
H-3a	0.06	0.03	0.00	0.02
H-3b	0.04	0.10	0.06	0.10
H-5a	0.10	0.13	0.04	0.08
H-5b	0.14	0.21	0.09	0.17
H-6	0.18	0.22	0.16	0.21
H-12	0.55	0.61	0.25	0.31
H-13	0.31	0.29	0.12	0.10
H-17	0.25	0.29	0.03	0.06
H-18	0.40	0.35	0.16	0.12
H-21	0.00	0.07	0.10	0.04
H-27	0.08	0.01	0.01	0.06
H-28	0.09	0.07	0.01	0.00
H-29	0.05	0.01	0.04	0.06
H-30	0.10	0.08	0.18	0.15
H-3'	0.03	0.07	0.08	0.04
H-4'a	0.08	0.03	0.08	0.04
H-4'b	0.13	0.03	0.13	0.04
H-5'	0.12	0.04	0.13	0.20
H-6'	0.04	0.00	0.20	0.23
H-3'-Me	0.07	0.04	0.02	0.04
H-7'-OMe	0.00	0.02	0.07	0.05
<b>Average</b>	<b>0.12</b>	<b>0.11</b>	<b>0.09</b>	<b>0.09</b>

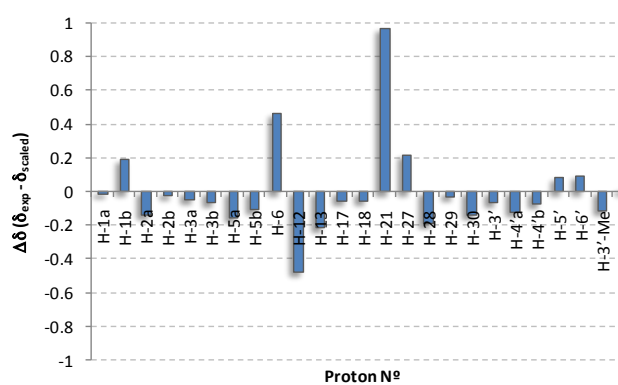
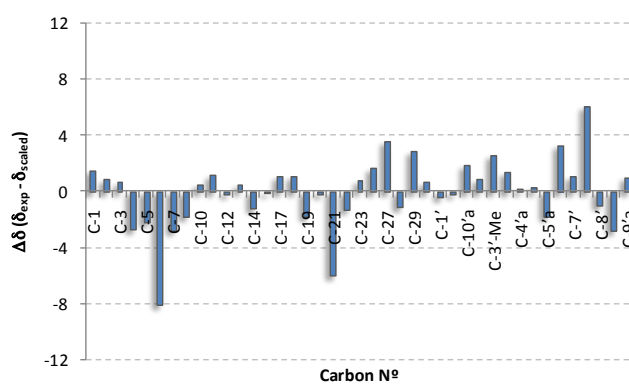
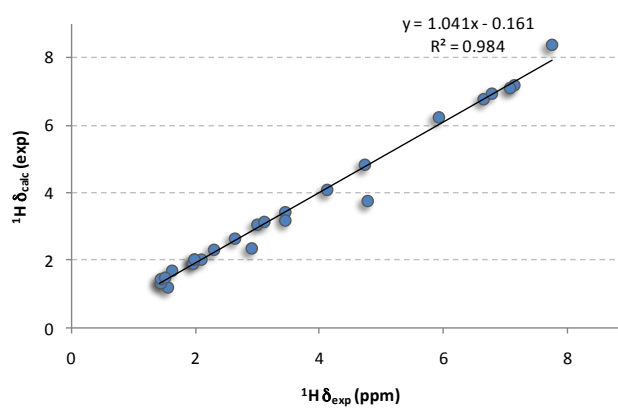
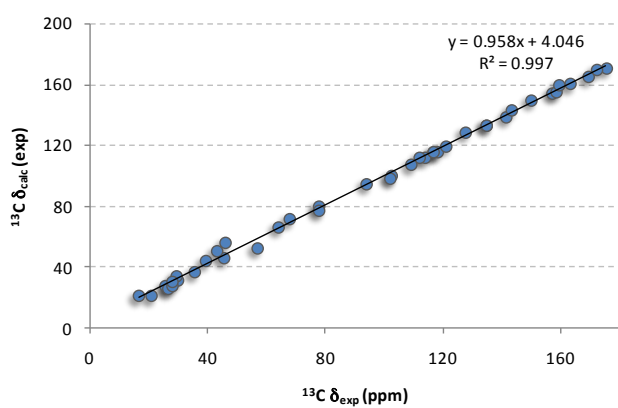
	1h	3'epi-1h
sDP4+ (H data)	77.25%	22.75%
sDP4+ (C data)	69.41%	30.59%
sDP4+ (all data)	88.51%	11.49%
uDP4+ (H data)	60.40%	39.60%
uDP4+ (C data)	26.28%	73.72%
uDP4+ (all data)	35.21%	64.79%
<b>DP4+ (H data)</b>	<b>83.81%</b>	<b>16.19%</b>
<b>DP4+ (C data)</b>	<b>44.71%</b>	<b>55.29%</b>
<b>DP4+ (all data)</b>	<b>80.72%</b>	<b>19.28%</b>



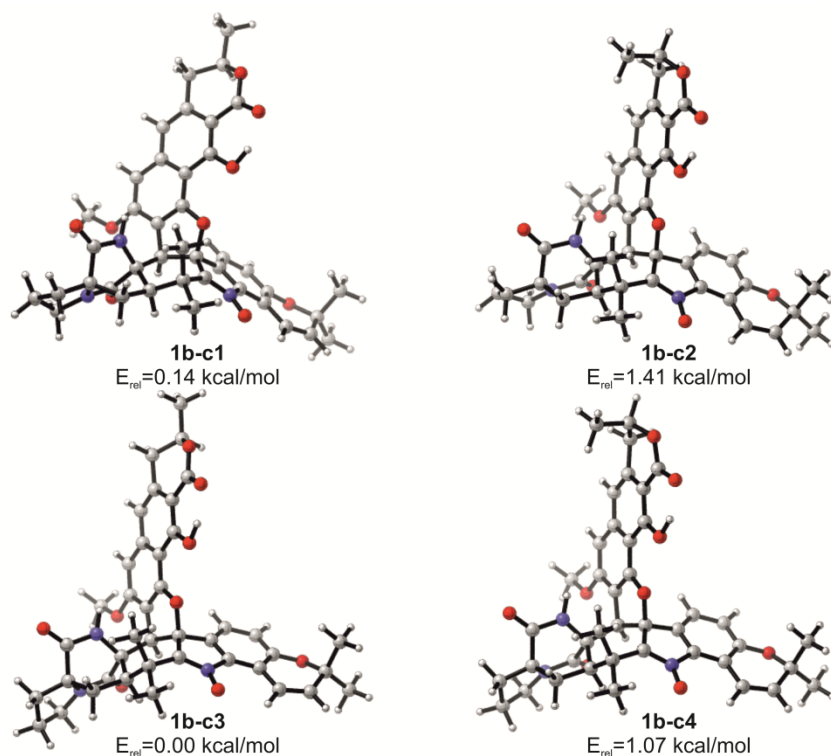
## S17: Computational NMR data of 1a



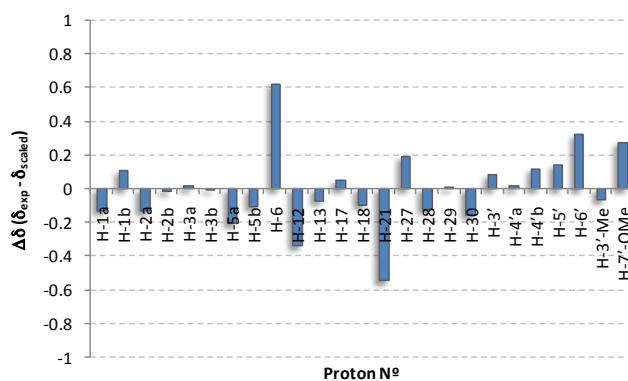
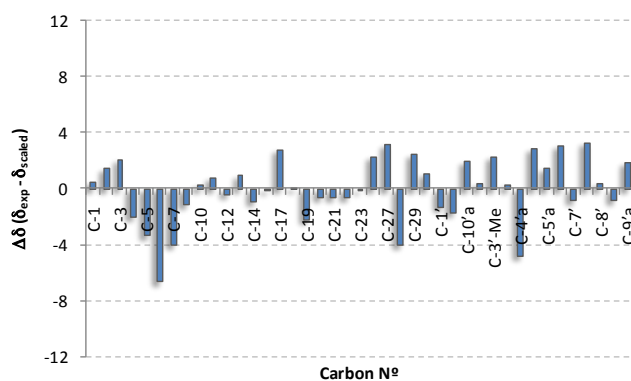
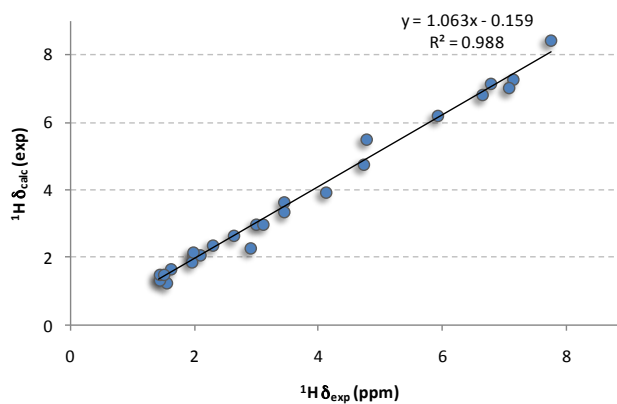
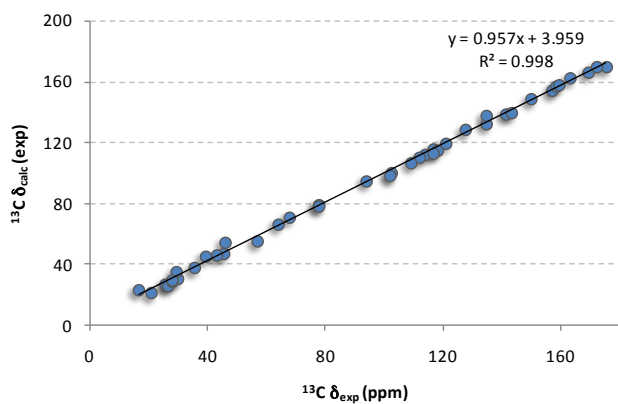
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1a** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



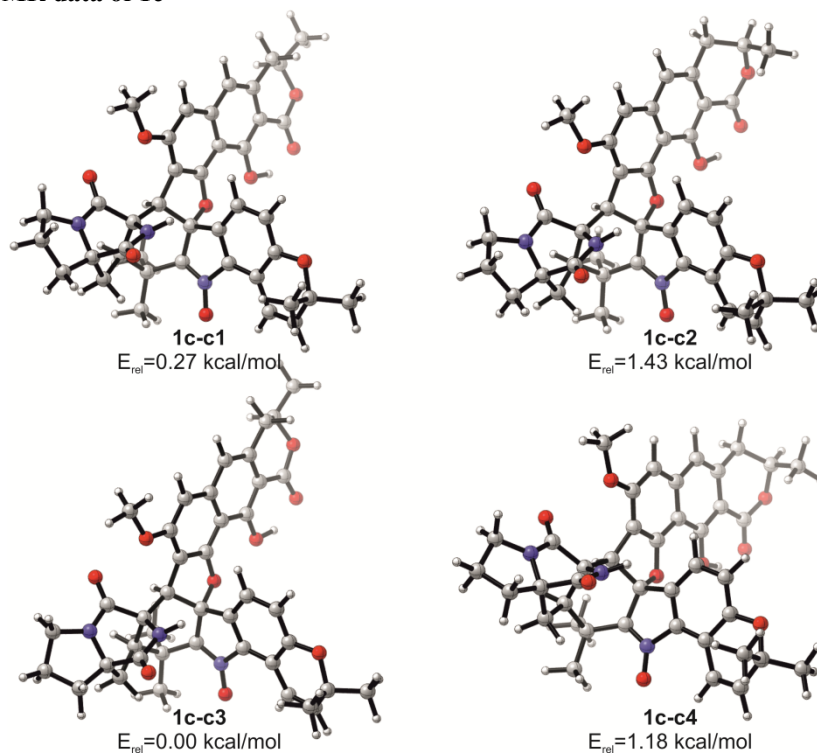
**S18: Computational NMR data of 1b**



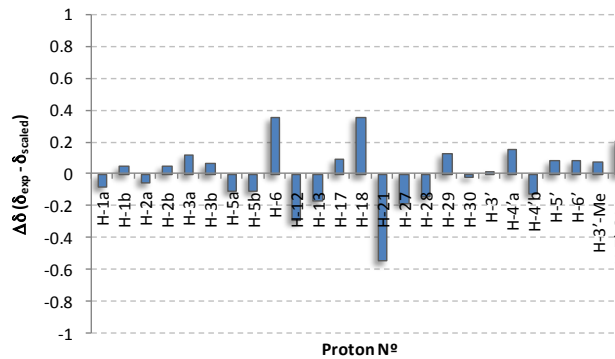
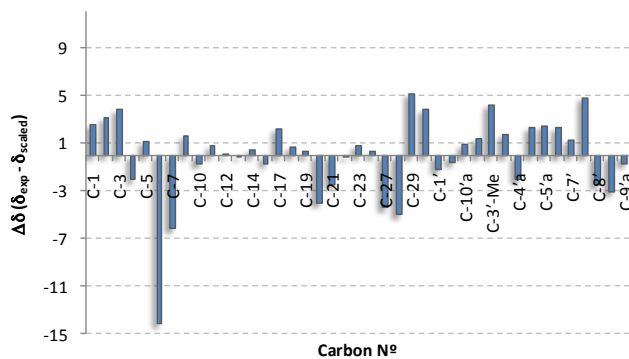
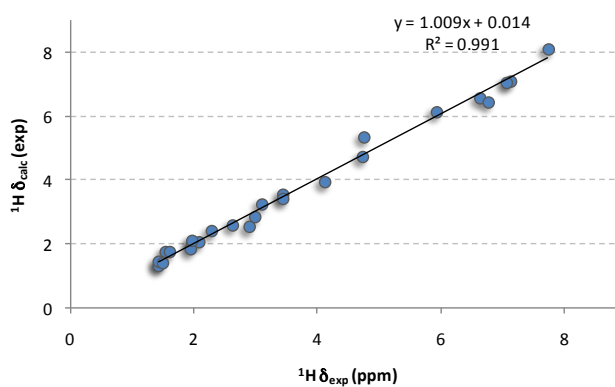
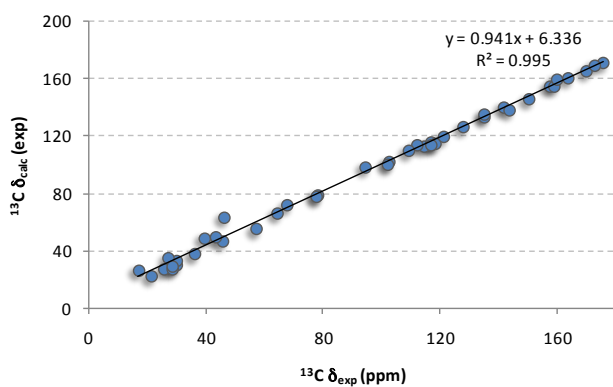
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1b** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



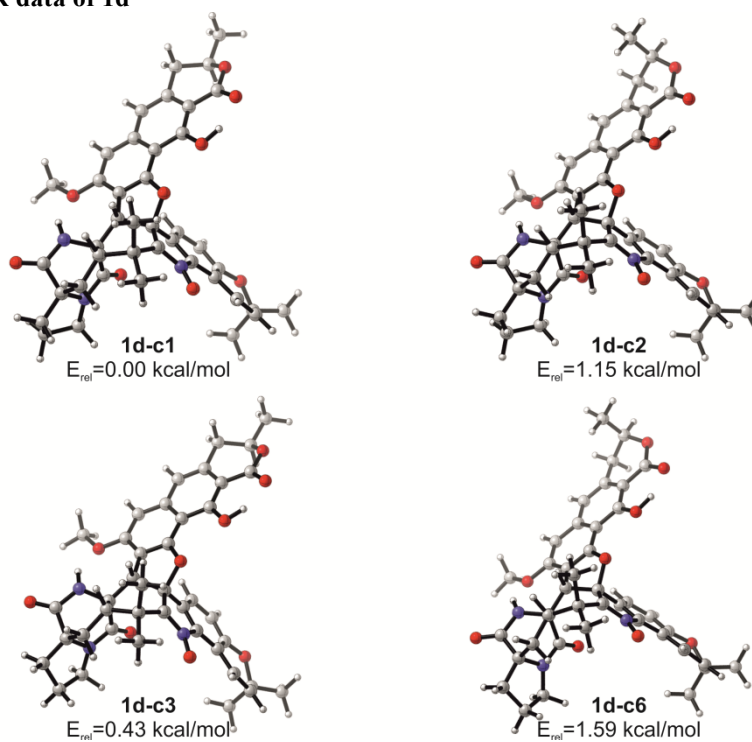
**S19: Computational NMR data of 1c**



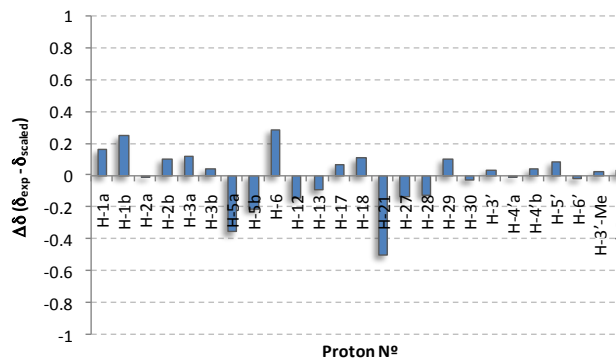
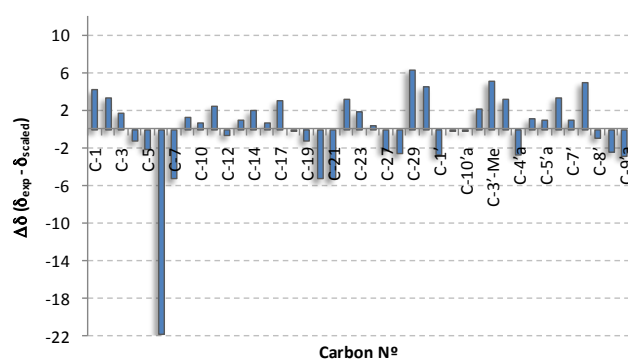
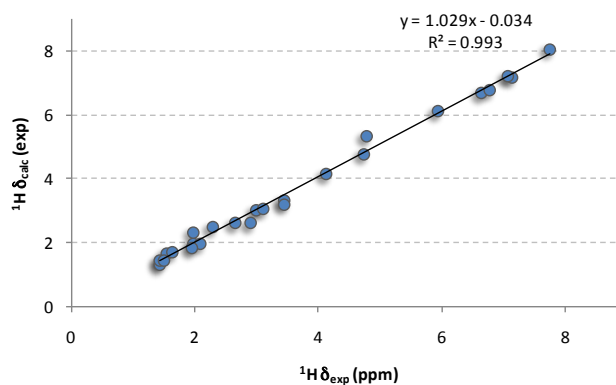
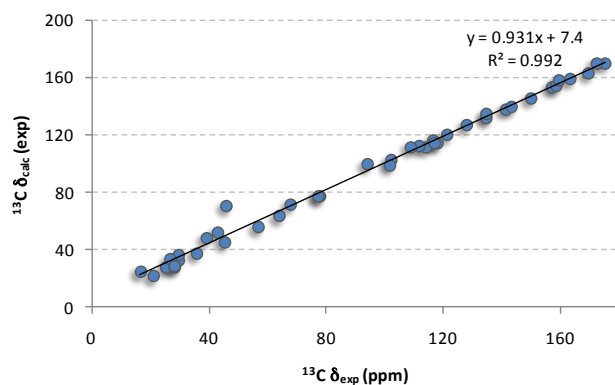
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for 1c with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



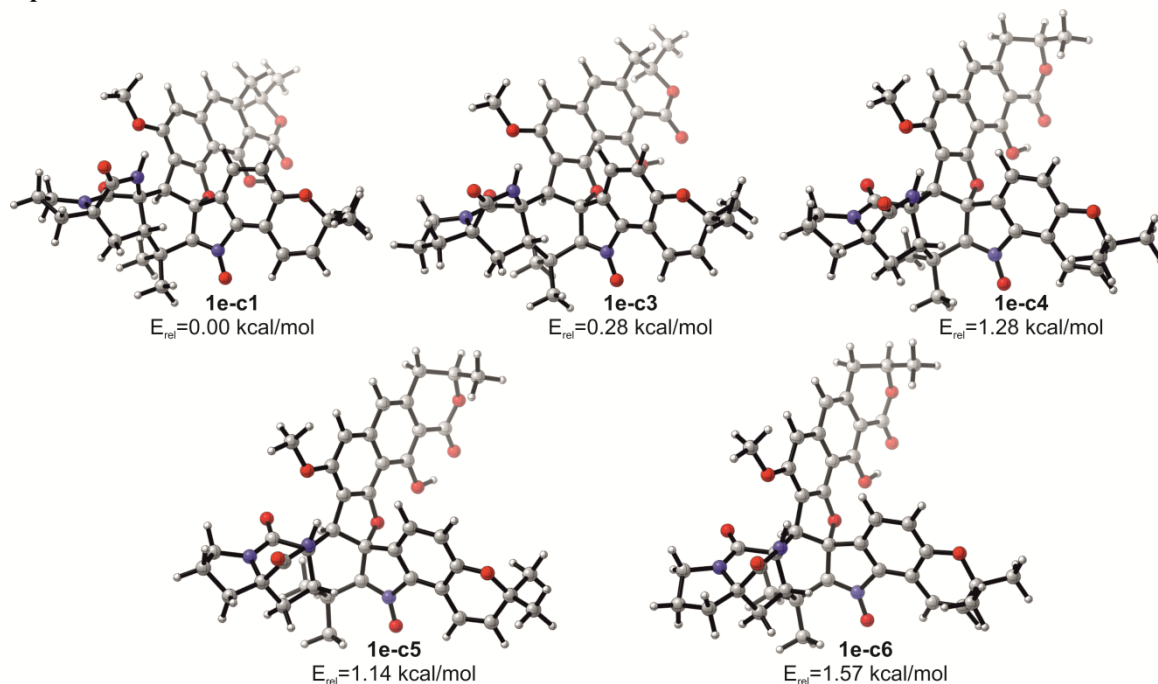
## S20: Computational NMR data of 1d



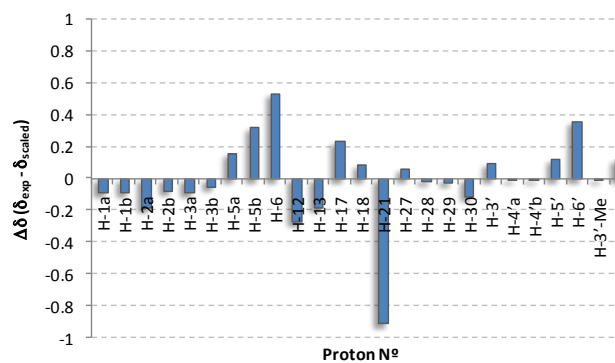
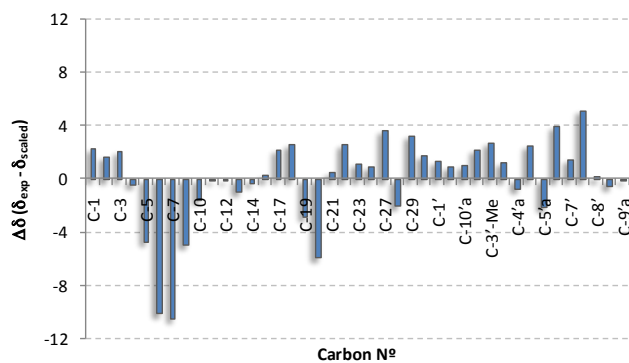
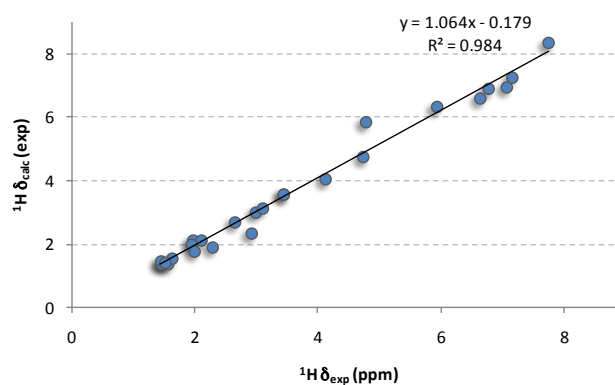
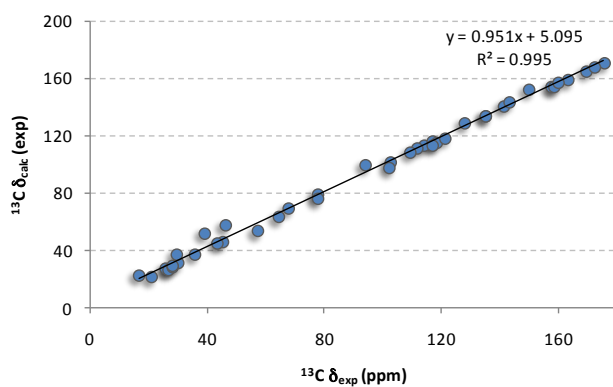
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1d** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



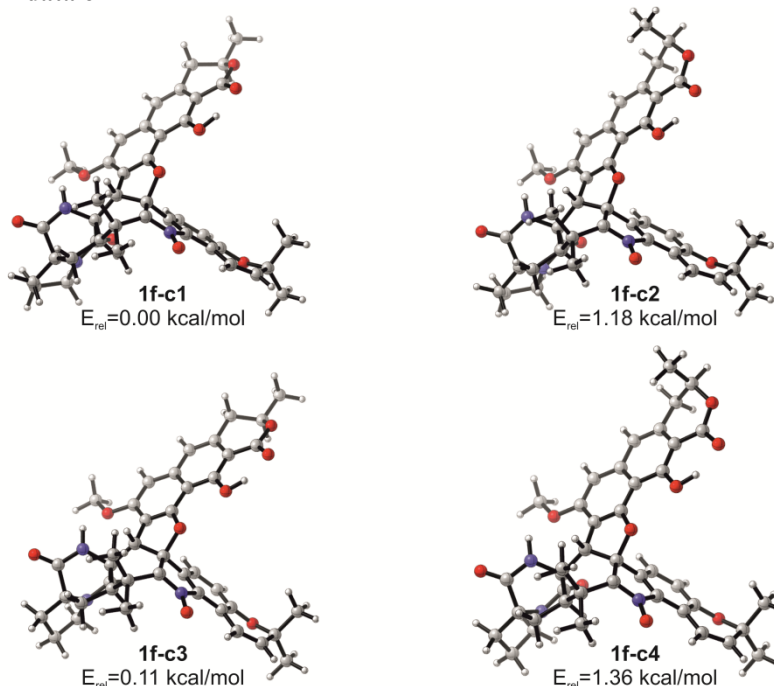
## S21: Computational NMR data of 1e



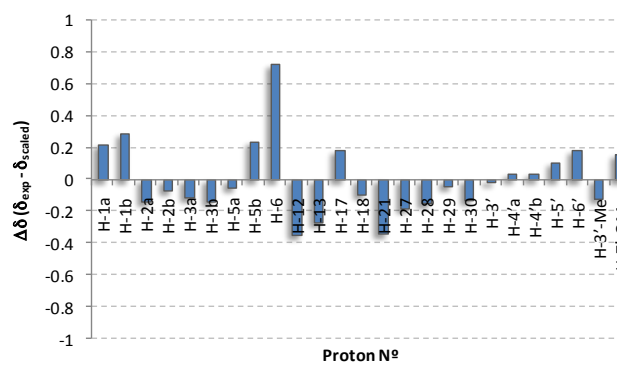
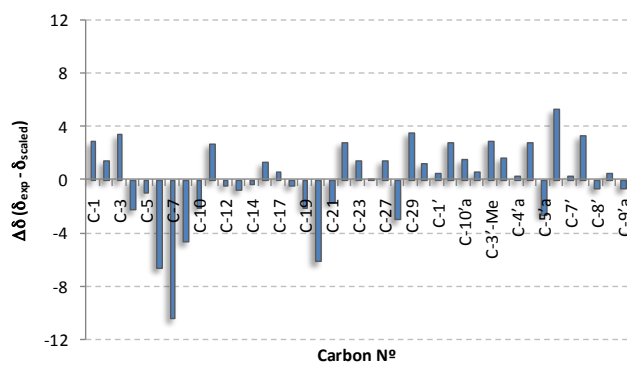
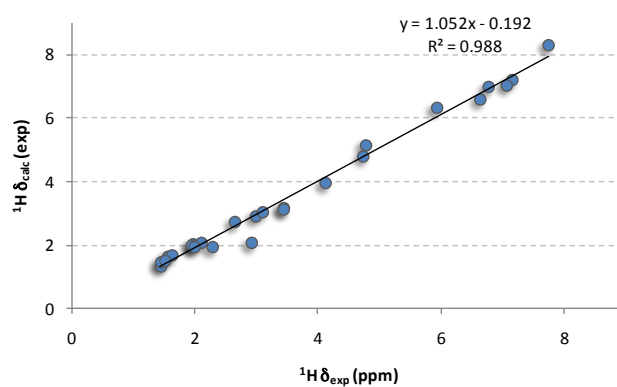
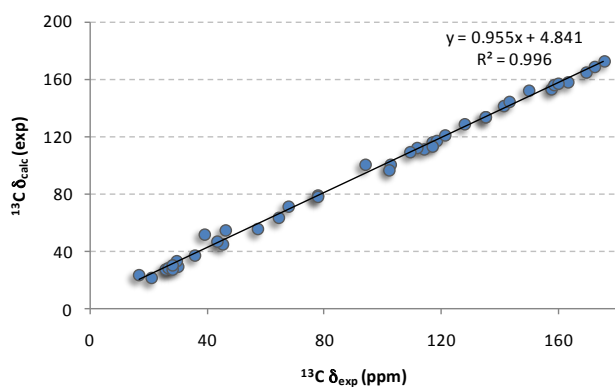
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1e** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



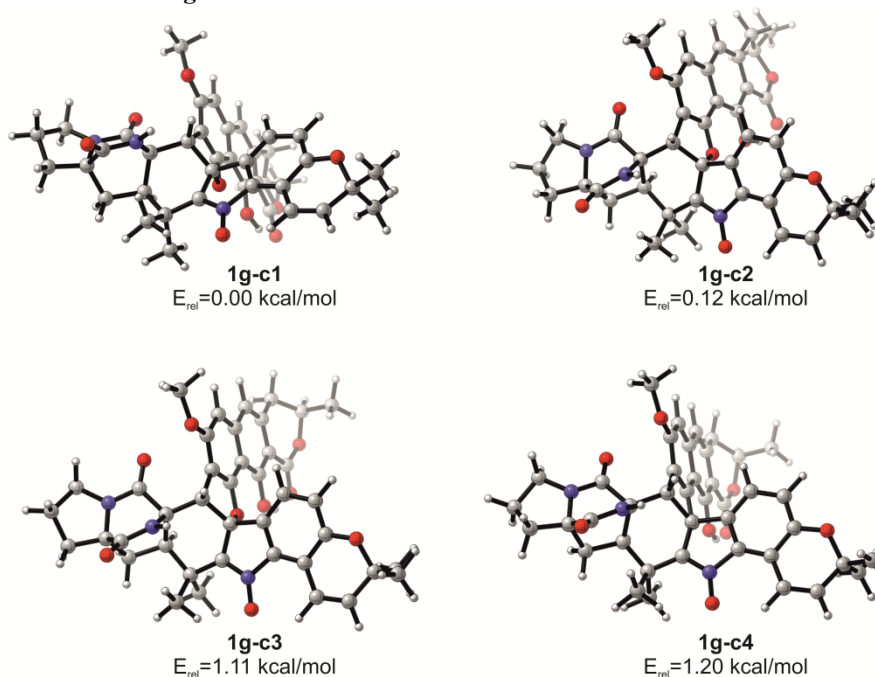
**S22: Computational NMR data of 1f**



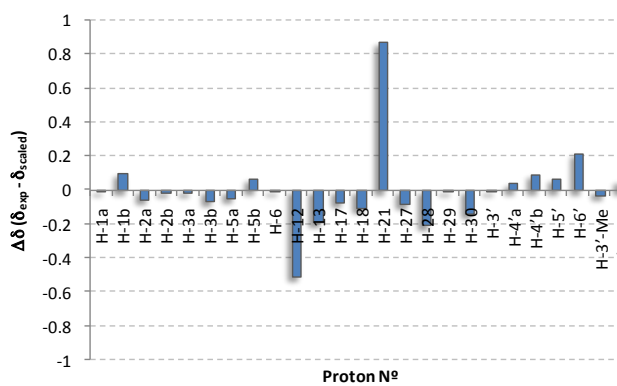
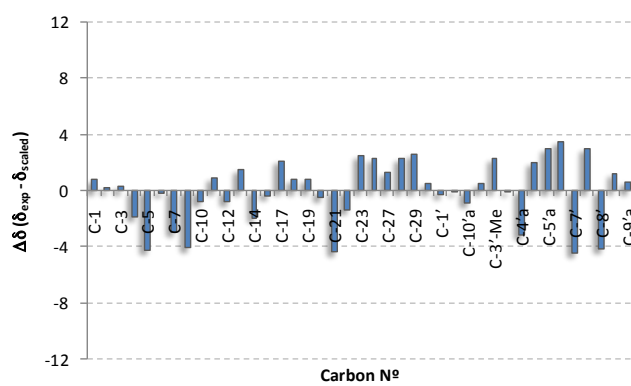
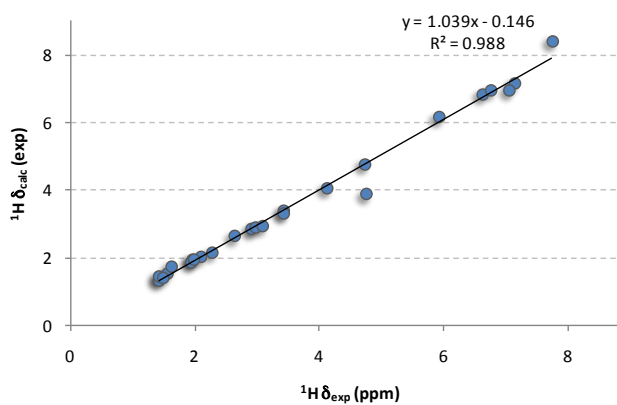
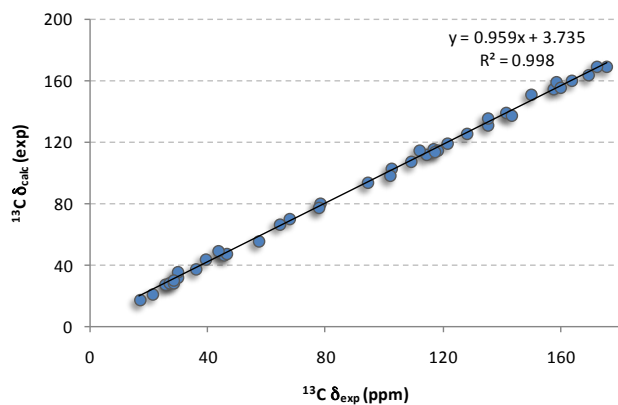
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1f** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



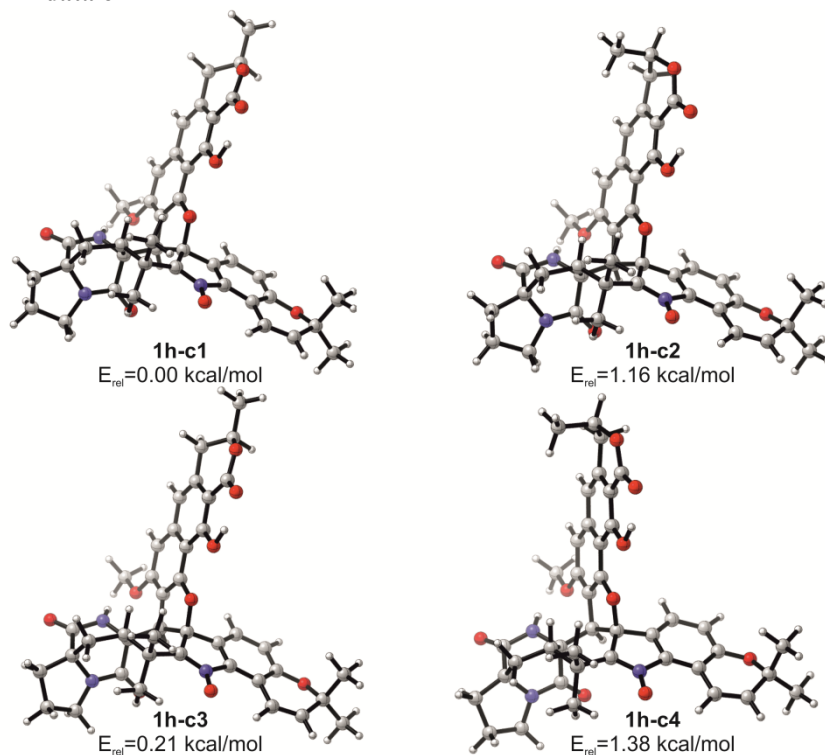
**S23: Computational NMR data of 1g**



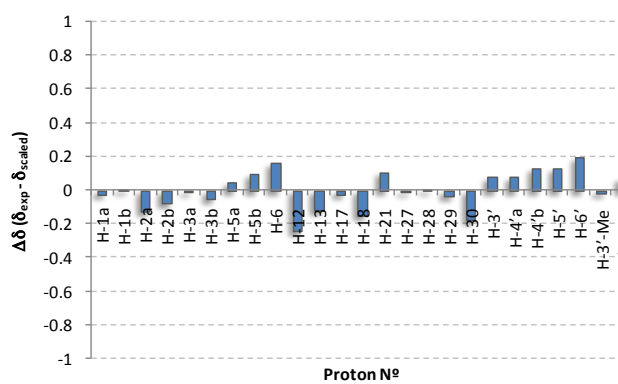
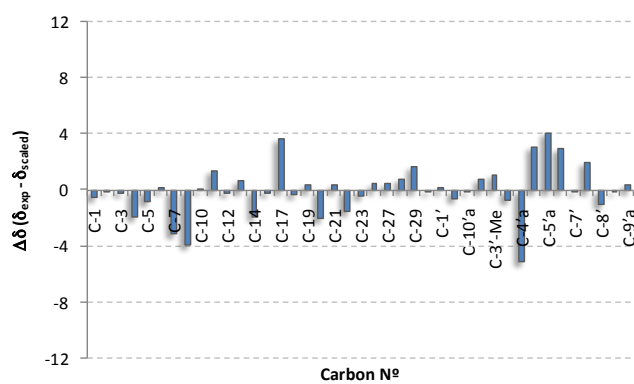
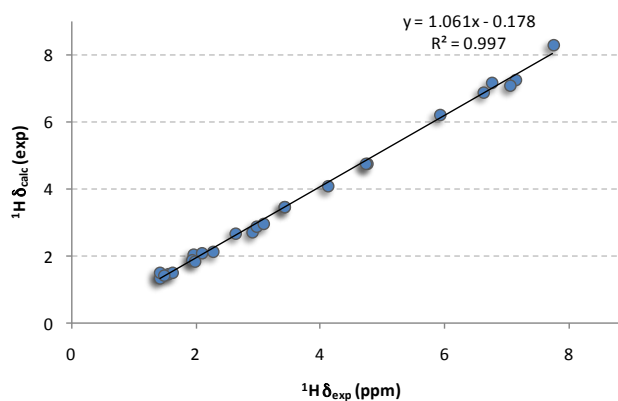
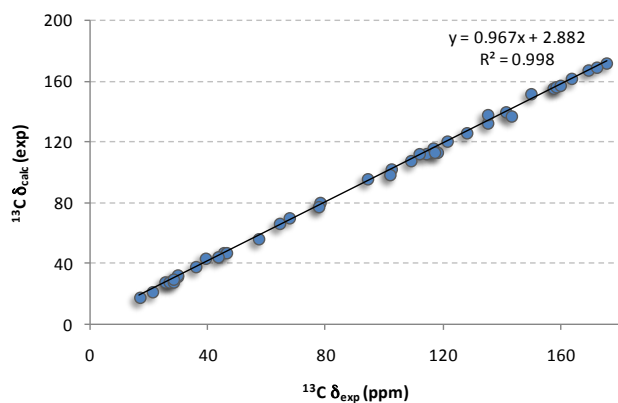
B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1g** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



**S24: Computational NMR data of 1h**

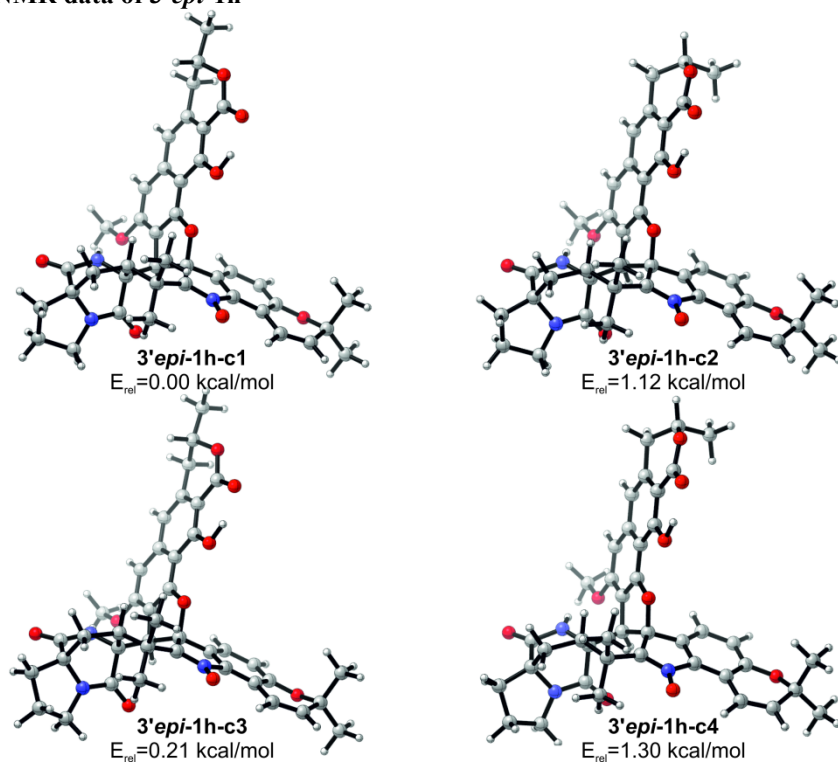


B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for **1h** with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.

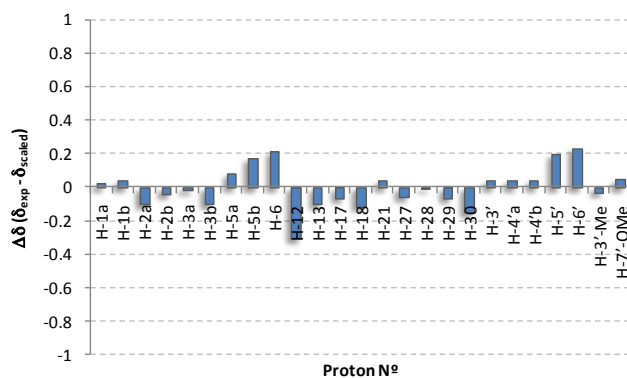
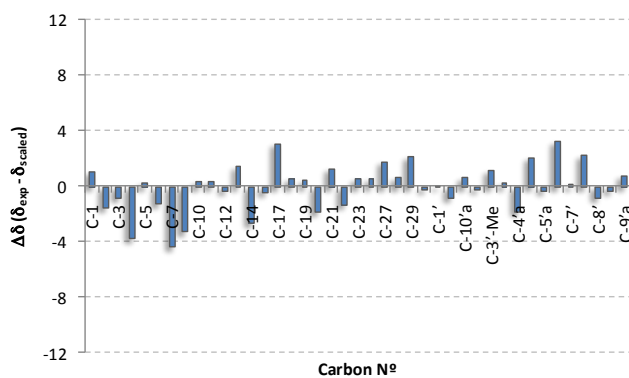
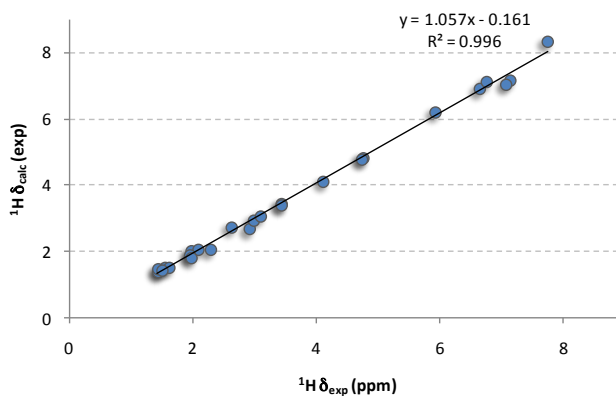
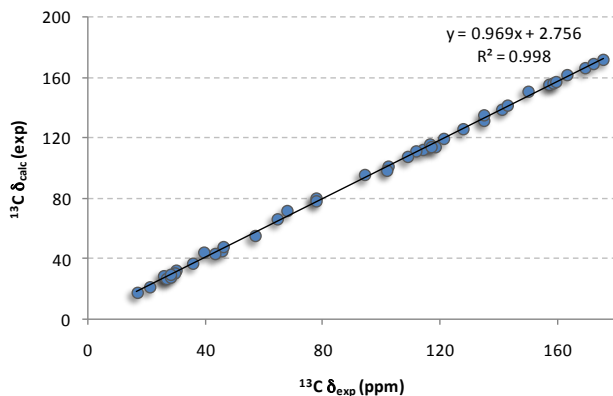




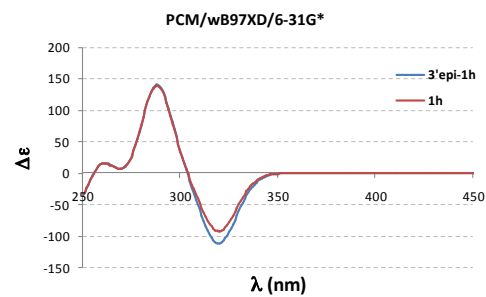
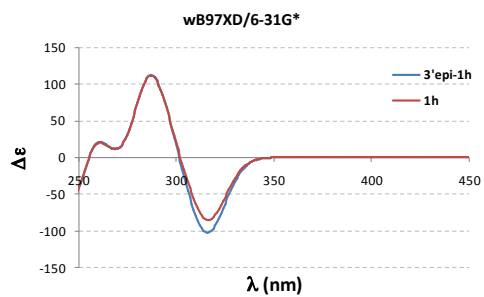
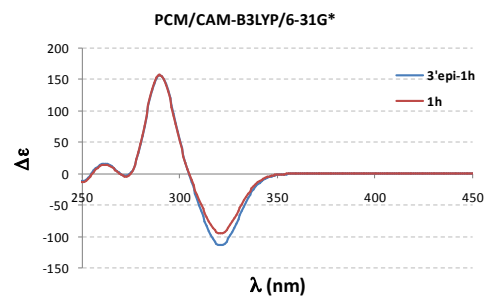
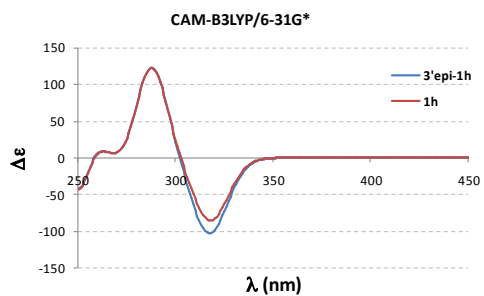
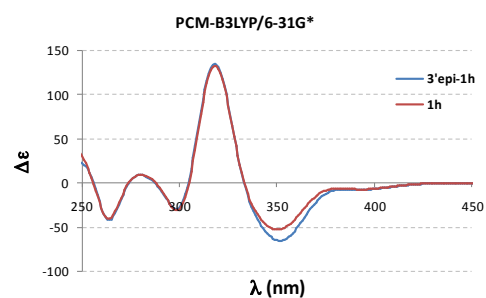
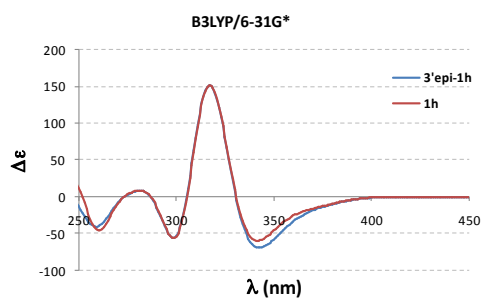
**S25: Computational NMR data of 3'epi-1h**



B3LYP/6-31G\* geometry optimized geometries of the most stable conformations found for 3'epi-1h with relative energies computed at the PCM/mPW1PW91/6-31+G\*\*//B3LYP/6-31G\* level.



**S26: Comparison of the ECD spectra of 1h and 3'epi-1h calculated at different levels of theory**



## NMR, HRESIMS, UV, and IR spectra

### S27: NMR data of compounds 1 and 2

no	1						2	
	Recorded in Pyr- <i>d</i> <sub>5</sub>		Recorded in DMSO- <i>d</i> <sub>6</sub>		Recorded in CD <sub>3</sub> OD		Recorded in Pyr- <i>d</i> <sub>5</sub>	
	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)
1	44.9	3.46 m 3.37 m	43.8	3.31 m	45.3	3.43 m	44.9	3.41 m 3.29 m
2	25.3	1.87 m (overlap)	24.0	1.85 m (overlap) 1.98 m	25.5	1.96 m (overlap) 2.08 m	25.4	1.80 m (overlap) 1.80 m (overlap)
3	29.8	1.87 m (overlap) 2.85 m	28.2	1.85 m (overlap) 2.44 m	29.7	1.94 m (overlap) 2.63 m	29.9	2.79 m
4	66.9		65.5		67.6		66.9	
5	29.4	2.09 dd (14.1, 10.4) 2.23 dd (14.1, 2.0)	27.6	1.93 m (overlap) 2.19 dd (14.4, 2.5)	29.5	1.97 m (overlap) 2.28 d (14.4)	30.5	2.05 dd (14.0, 9.68) 2.15 d (14.0)
6	45.8	3.20 dd (10.4, 2.0)	44.0	2.75 dd (10.3, 2.6)	46.0	2.90 dd (10.4, 2.4)	45.2	3.11 d (10.8)
7	38.5		37.0		39.1		41.0	
8	147.3		146.4		149.9		186.5	
10	141.3		139.3		141.2		151.3	
11	113.6		112.0		114.0		115.8	
12	116.7	8.15 d (10.3)	114.7	7.69 d (10.2)	116.6	7.74 d (10.3)	118.6	7.13 d (9.9)
13	133.8	5.76 d (10.3)	134.1	6.00 d (10.2)	134.8	5.92 d (10.1)	132.5	5.67 d (10.0)
14	77.4		76.6		77.8		77.4	
16	156.5		155.1		157.2		156.3	
17	117.3	6.66 d (8.1)	116.6	6.67 d (8.7)	118.1	6.63 d (7.5)	114.1	6.55 d (7.9)
18	120.7	7.02 d (8.1)	120.0	6.76 d (8.7)	121.1	6.76 d (8.3)	121.9	6.97 d (7.9)
19	127.8		126.2		127.8		131.4	
20	94.2		92.4		94.1		97.3	
21	43.0	5.34 s	41.2	4.61 s	43.2	4.76 s	45.7	5.11 s
22	63.8		62.0		64.2		64.2	
23	168.5		166.9		169.4		168.3	
25	174.1		172.5		175.5		174.2	
26 -NH		7.23 s		6.66 s				7.48 s
27	26.8	1.77 s	25.7	1.38 s	26.6	1.54 s	32.2	1.70 s
28	16.6	1.92 s	15.1	1.47 s	16.6	1.61 s	23.1	1.56 s
29	28.5	1.31 s (overlap)	27.4	1.39 s	28.03	1.42 (overlap)	28.5	1.33 s
30	28.3	1.31 s (overlap)	27.5	1.40 s	28.04	1.42 (overlap)	28.7	1.31 s
1'	171.7		170.4		172.3		171.9	
3'	76.7	4.71 m	75.9	4.77 m	77.6	4.72 m	76.9	4.69 m
4'	35.3	2.96 m	33.9	2.94 dd (16.2, 10.7) 3.10 dd (16.2, 2.6)	35.7	2.98 d (10.9) 3.09 d (15.0)	35.3	2.93 m
4'a	136.4		135.5		134.8		136.4	
5'	116.3	7.11 s	115.5	7.15 s (overlap)	116.8	7.13 s	116.5	7.11 s
5'a	142.4		141.0		143.1		142.5	
6'	101.6	7.10 s	101.0	7.15 s (overlap)	101.9	7.06 s	101.6	7.08 s
7'	158.2		156.9		158.5		158.5	
8'	112.1		110.6		111.8		111.7	
9'	159.6		157.5		159.6		160.5	
9'a	109.0		107.6		109.0		108.9	
10'	163.5		161.1		163.3		163.5	
10'-OH				12.50 s				
10'a	102.2		101.0		102.3		102.2	
3'-Me	21.1	1.39 d (6.2)	20.2	1.42 d (6.3)	20.9	1.49 d (6.3)	21.2	1.36 d (6.3)
7'-OMe	56.9	4.01 s	56.5	4.06 s	57.0	4.11 s	57.0	3.99 s

<sup>1</sup>H spectra recorded at 400 MHz. <sup>13</sup>C Spectra recorded at 100 MHz. Data based on <sup>1</sup>H, <sup>13</sup>C, HSQC, and HMBC experiments.

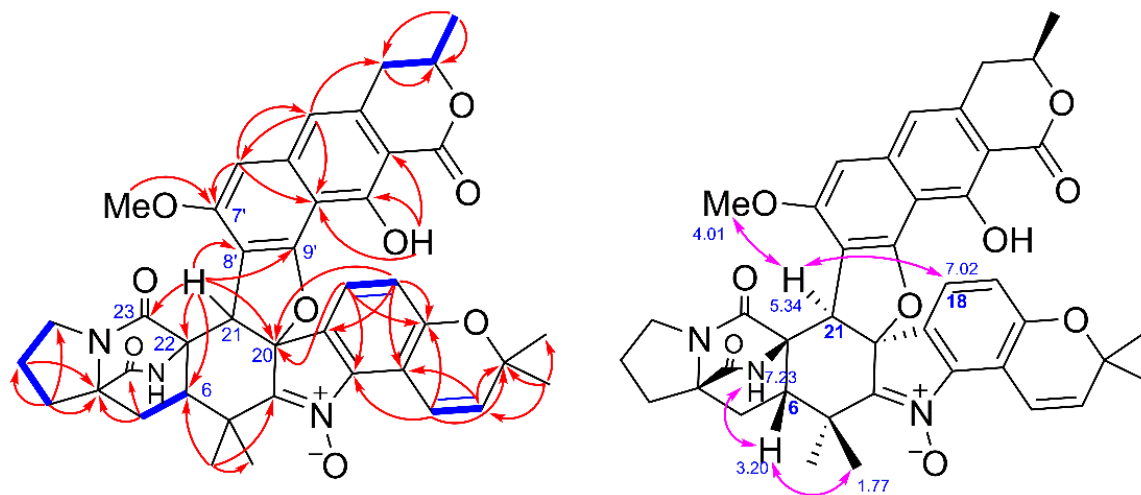
**S28: NMR data of compound 3**

no	$\delta_C$	$\delta_H$ ( <i>J</i> in Hz)
2	182.5	
3	61.5	
4	127.6	7.11 (1H, d, <i>J</i> = 8.2 Hz)
5	111.7	6.41 (1H, d, <i>J</i> = 8.2 Hz)
6	155.0	
7	107.4	
8	138.1	
9	119.9	
10 $\alpha$	35.9	2.31 (1H, d, <i>J</i> = 14.7 Hz)
10 $\beta$		3.02 (1H, d, <i>J</i> = 14.7 Hz)
11	67.3	
12	171.8	
14	44.9	3.52 (1H, m) 3.49 (1H, m)
15	25.7	2.09 (1H, overlap) 1.96 (1H, m)
16	30.4	1.93 (1H, m) 2.70 (1H, m)
17	70.3	
18	175.9	
20	31.1	1.86 (1H, m) 2.09 (1H, overlap)
21	58.2	3.35 (1H, m)
22	47.1	
23	20.3	1.07 (3H, s)
24	25.3	0.91 (3H, s)
25	117.3	6.07 (1H, d, <i>J</i> = 10.1 Hz)
26	129.8	4.41 (1H, d, <i>J</i> = 10.1 Hz)
27	76.3	
28	27.1	1.17 (3H, s)
29	28.4	0.92 (3H, s)
1'	45.0	3.32 (1H, m) 3.43 (1H, m)
2'	25.4	1.95 (1H, m) 2.04 (1H, m)
3'	30.0	1.94 (1H, m) 2.68 (1H, m)
4'	68.5	
5'	31.2	2.12 (2H, m)
6'	47.4	2.84 (dd, <i>J</i> = 9.1, 5.6 Hz, 1H).
7'	37.2	
8'	140.2	
10'	135.2	
11'	103.6	
12'	71.4	4.99 (1H, m)
13'	80.7	4.98 (1H, overlap)
14'	75.8	
16'	150.5	
17'	112.2	6.68 (1H, d, <i>J</i> = 8.4 Hz)
18'	121.9	7.63 (1H, d, <i>J</i> = 8.4 Hz)
19'	119.0	
20'	103.8	
21'	70.2	4.98 (1H, overlap)
22'	64.2	
23'	169.8	
26'	175.4	
27'	20.6	1.43 (3H, s)
28'	27.8	1.18 (3H, s)
29'	26.7	1.77 (3H, s)
30'	23.9	1.53 (3H, s)
31'	56.9	3.42 (3H, s)
32'	58.3	3.56 (3H, s)

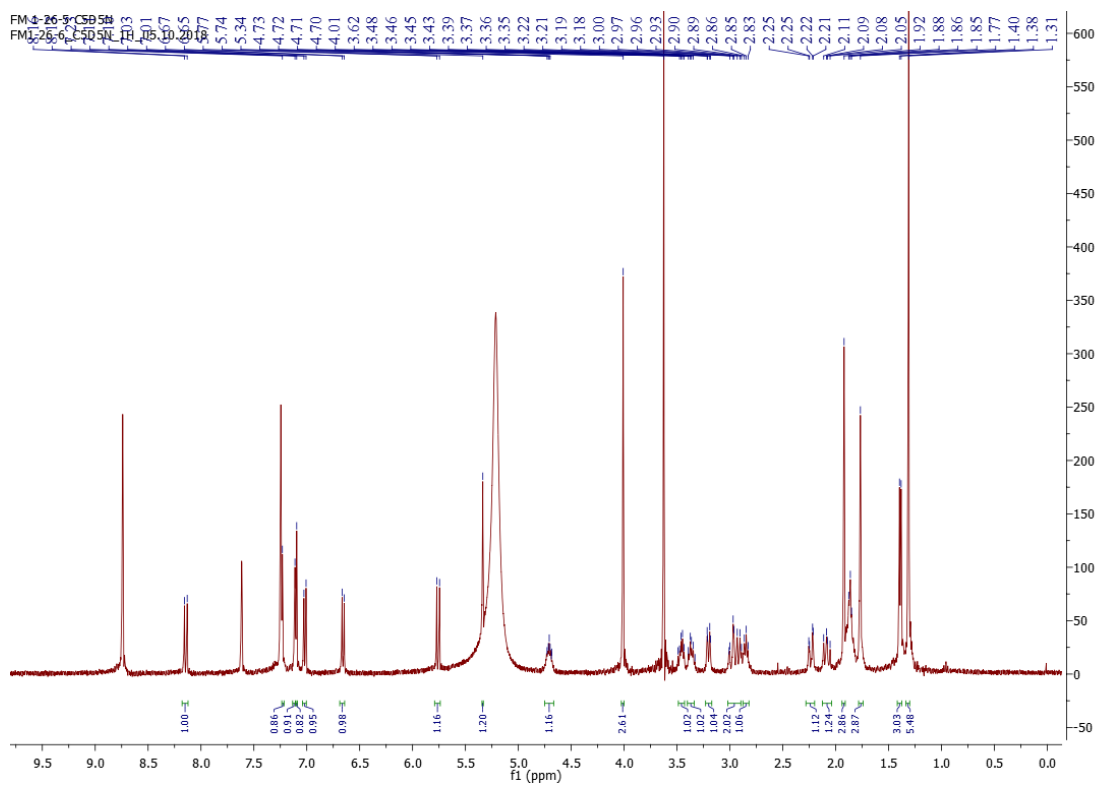
[a] <sup>1</sup>H spectra recorded at 400 MHz in Pyr-*d*<sub>5</sub>. <sup>13</sup>C Spectra recorded at 100MHz. Data based on <sup>1</sup>H, <sup>13</sup>C, HSQC, and HMBC experiments.

## For compound 1

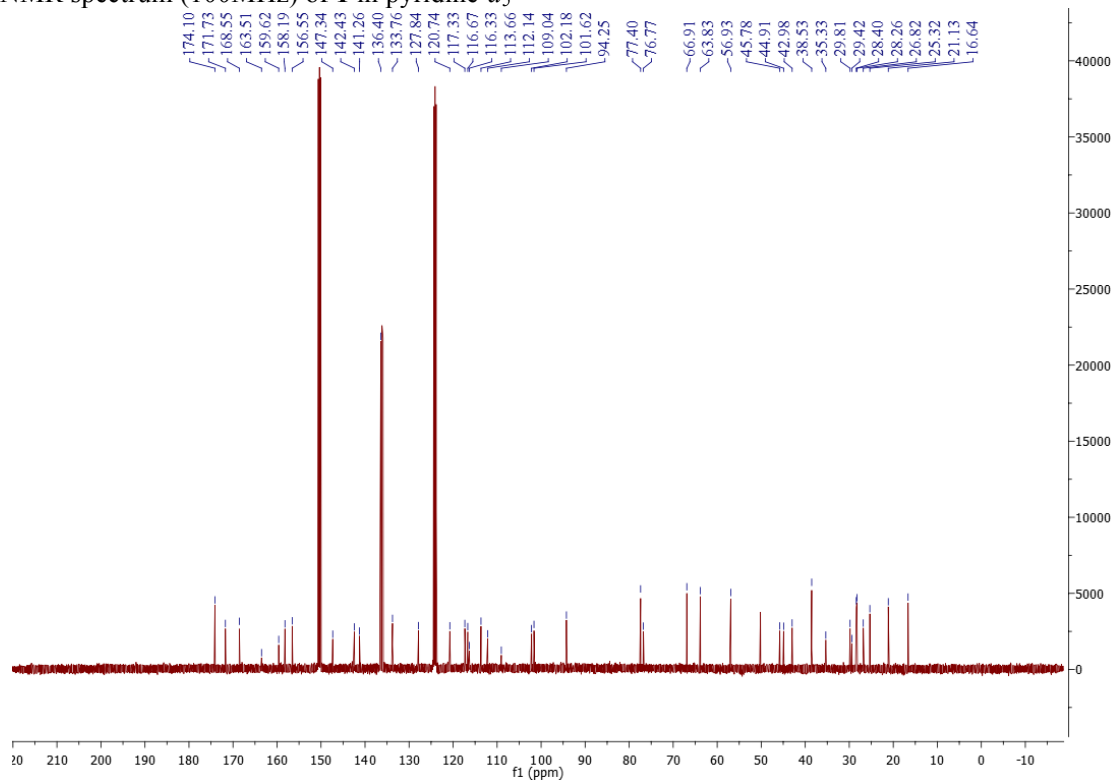
**S29:** Key 2D NMR correlations for compound 1



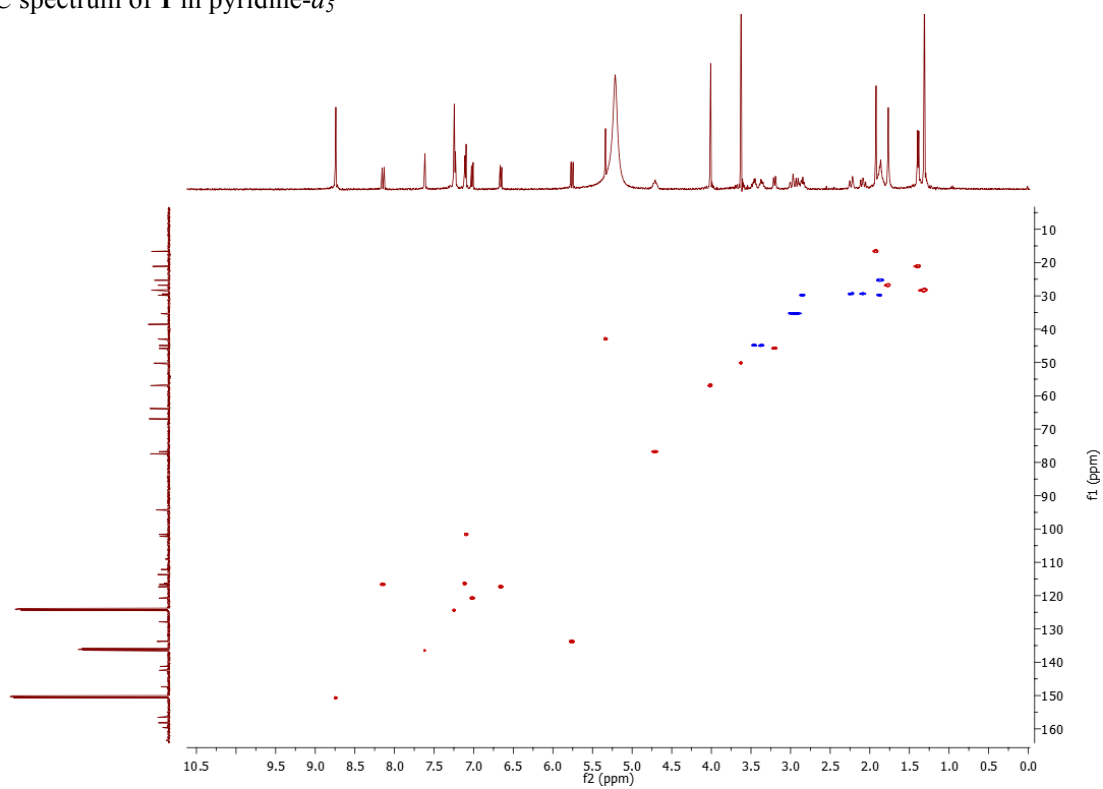
**S30:**  $^1\text{H}$  NMR spectrum (400MHz) of 1 in pyridine- $d_5$



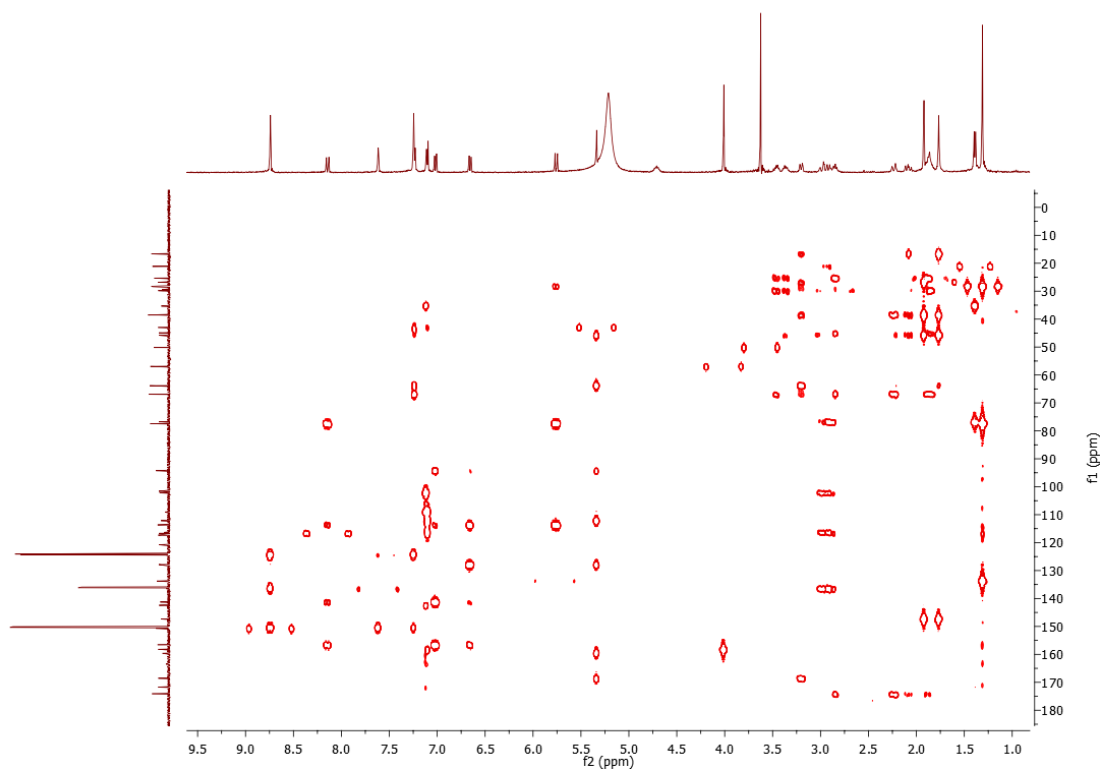
**S31:**  $^{13}\text{C}$  NMR spectrum (100MHz) of **1** in pyridine- $d_5$



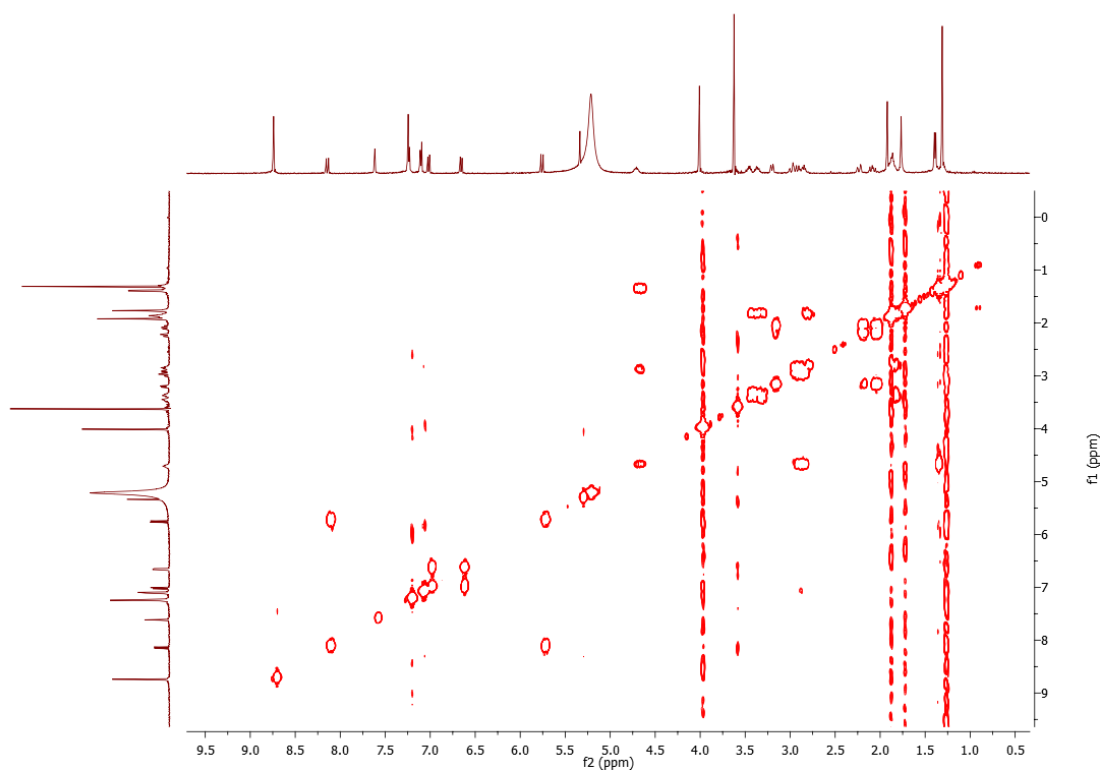
**S32:** HSQC spectrum of **1** in pyridine- $d_5$



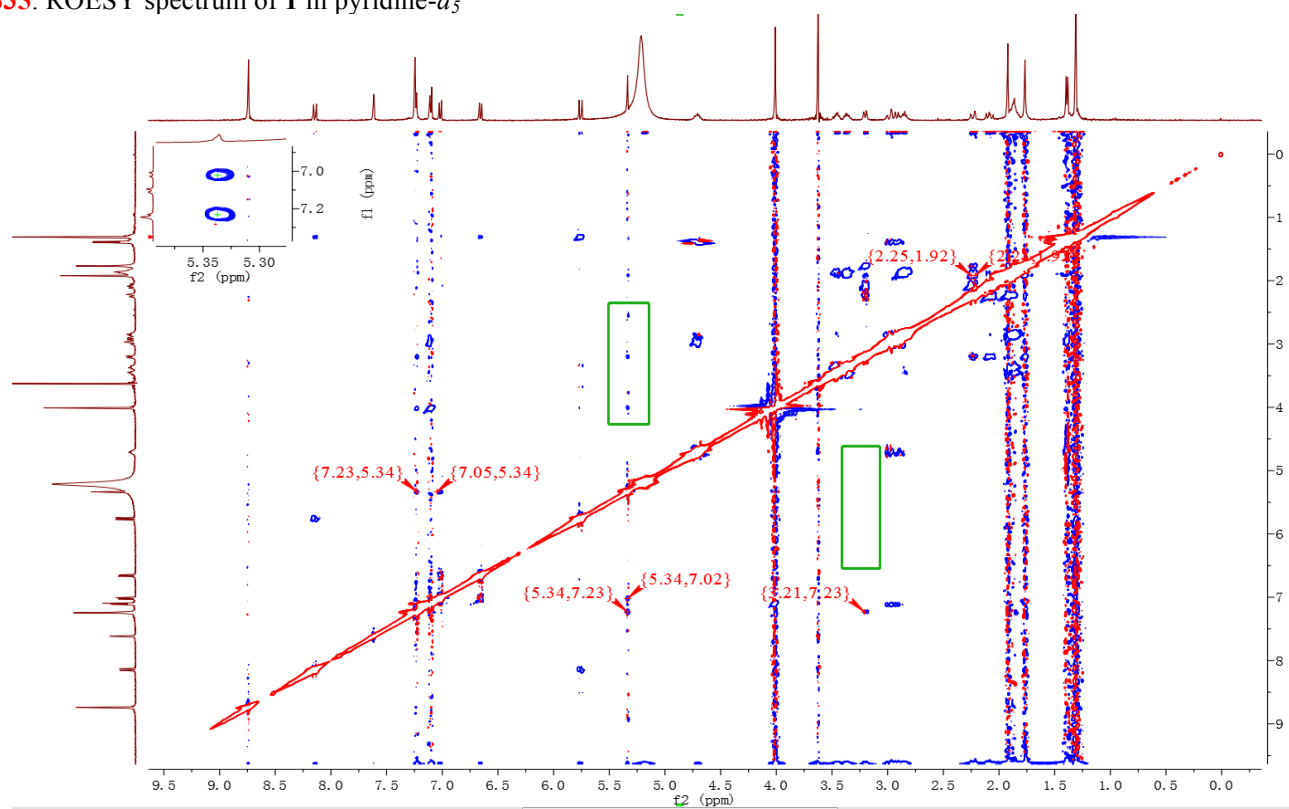
**S33:** HMBC spectrum of **1** in pyridine- $d_5$



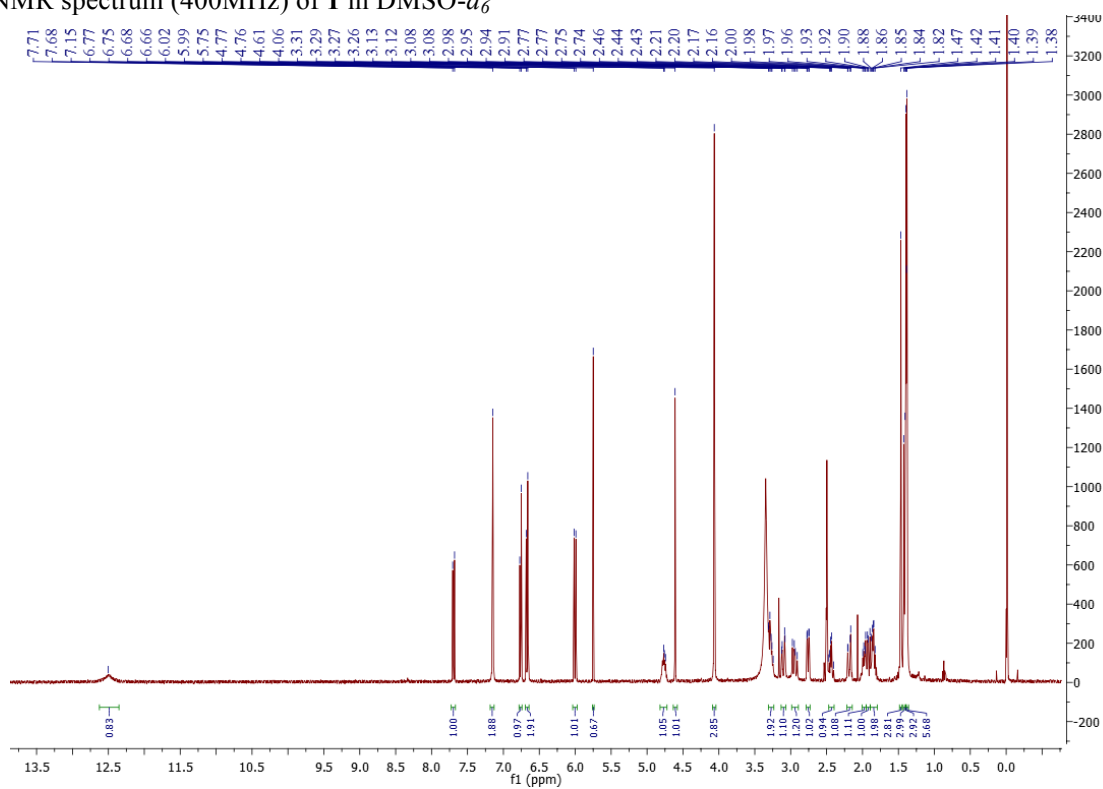
**S34:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in pyridine- $d_5$



S35: ROESY spectrum of **1** in pyridine-*d*<sub>5</sub>

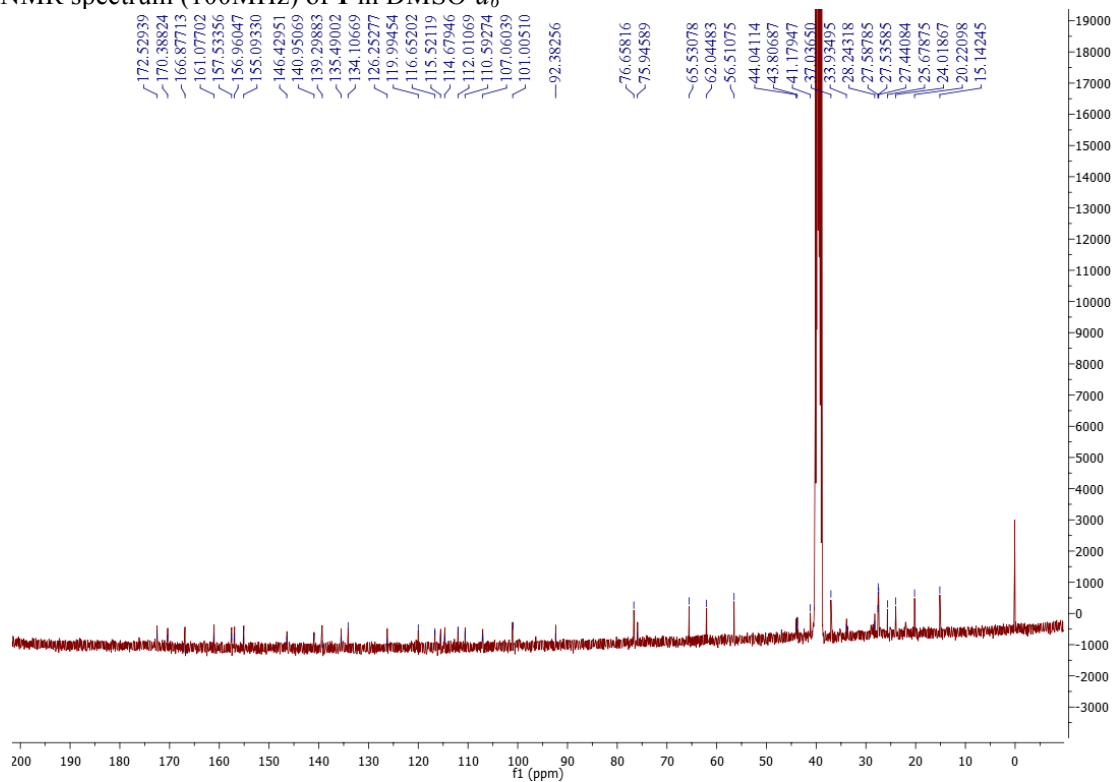


S36: <sup>1</sup>H NMR spectrum (400MHz) of **1** in DMSO-*d*<sub>6</sub>

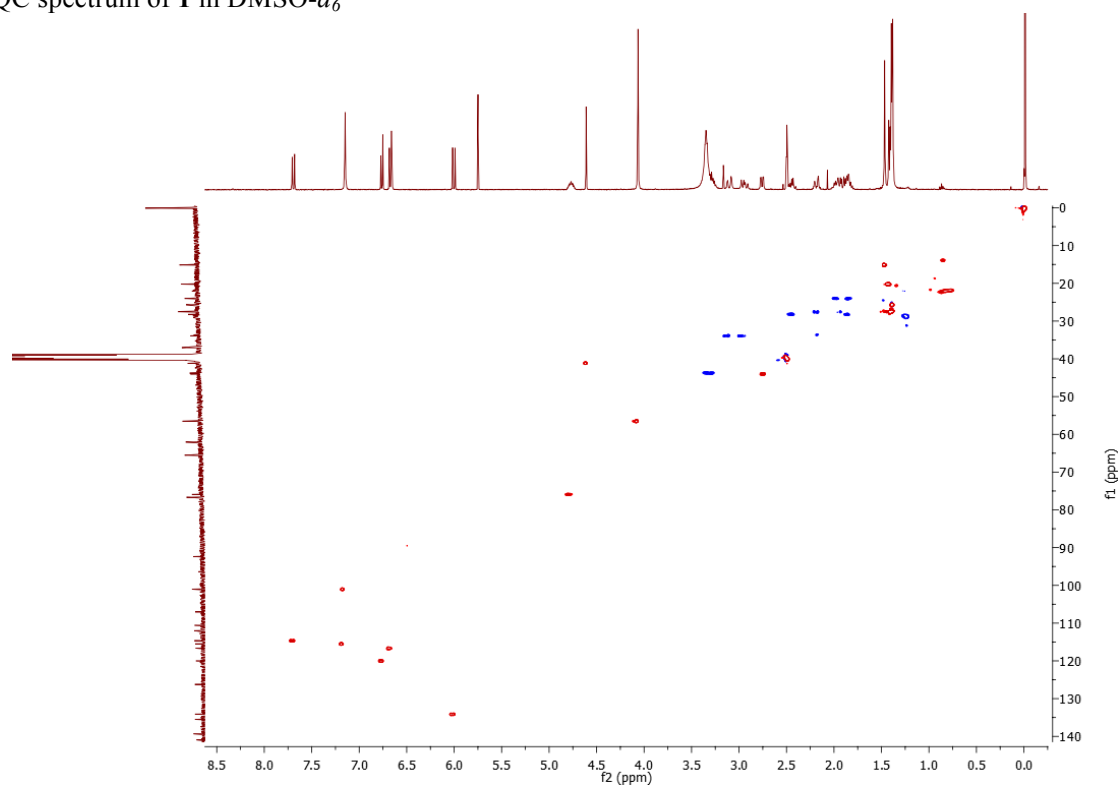




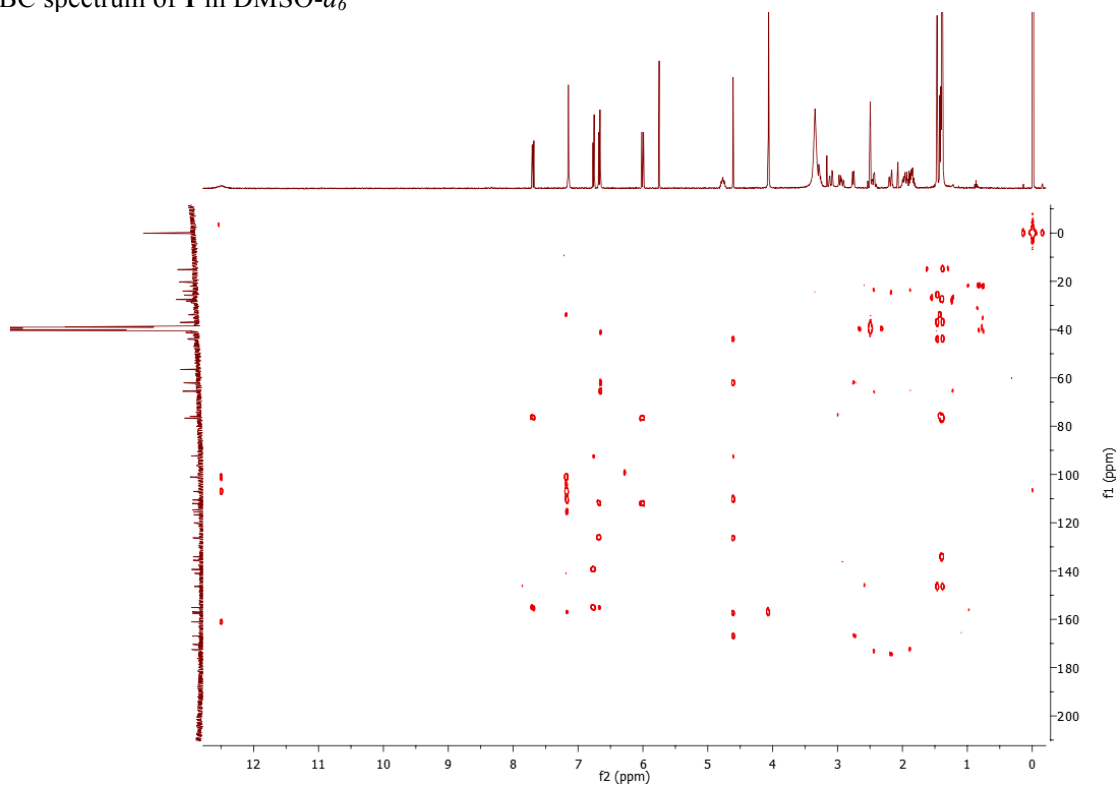
**S37:**  $^{13}\text{C}$  NMR spectrum (100MHz) of **1** in  $\text{DMSO-}d_6$



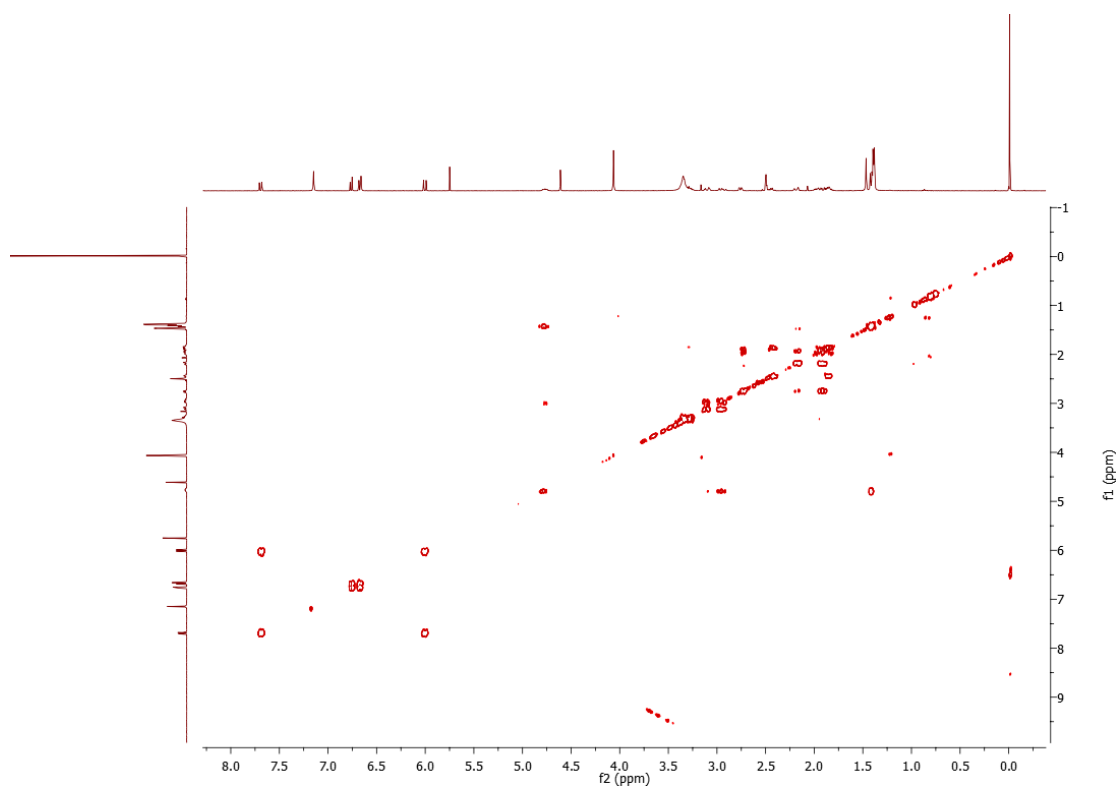
**S38:** HSQC spectrum of **1** in  $\text{DMSO-}d_6$



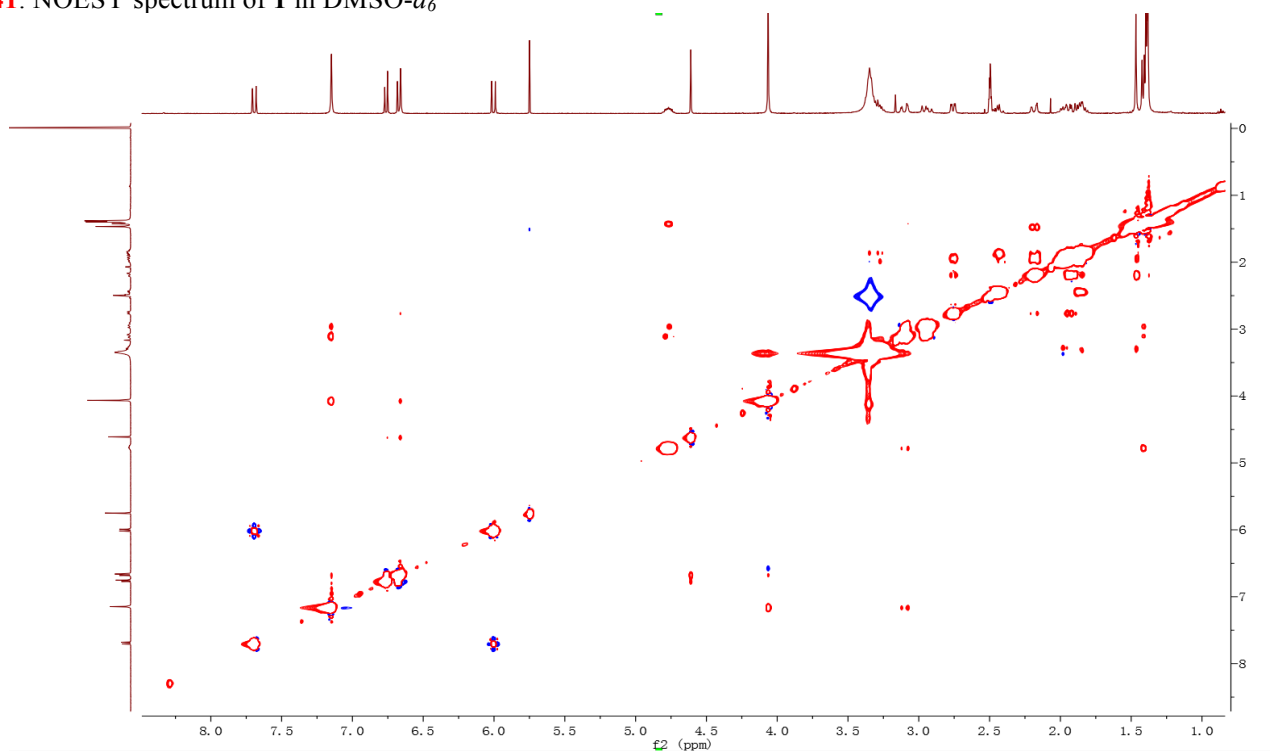
**S39:** HMBC spectrum of **1** in DMSO-*d*<sub>6</sub>



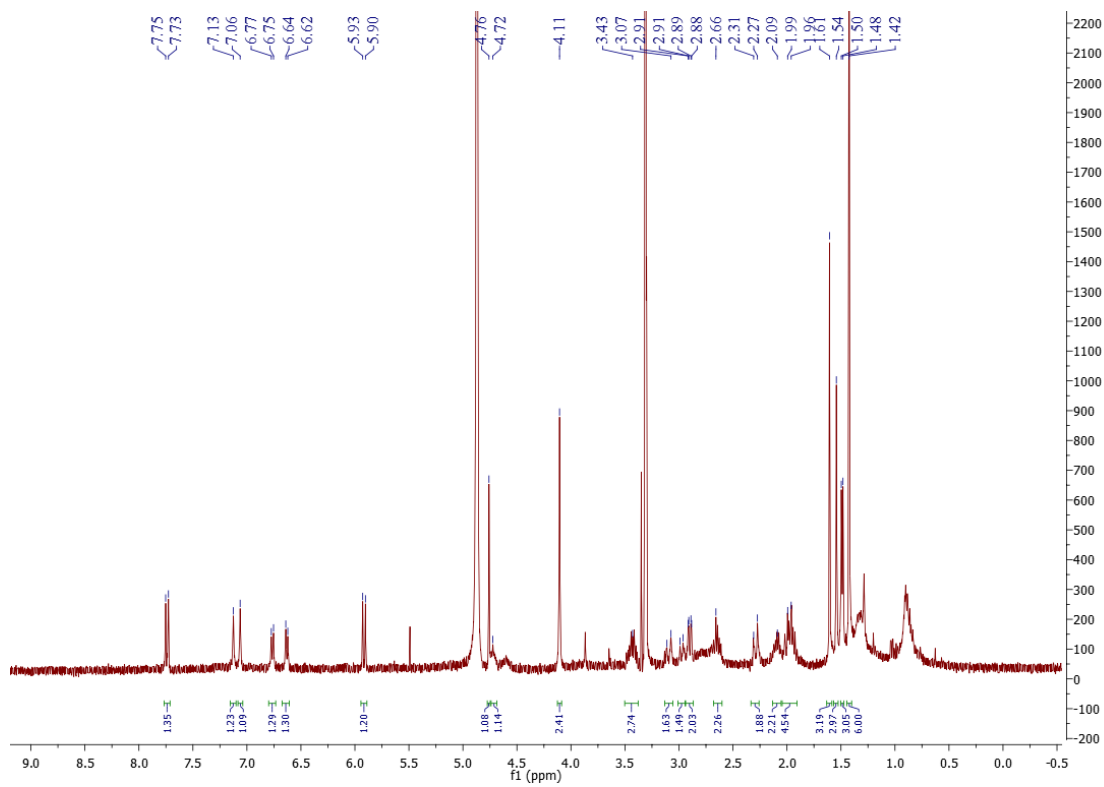
**S40:** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **1** in DMSO-*d*<sub>6</sub>



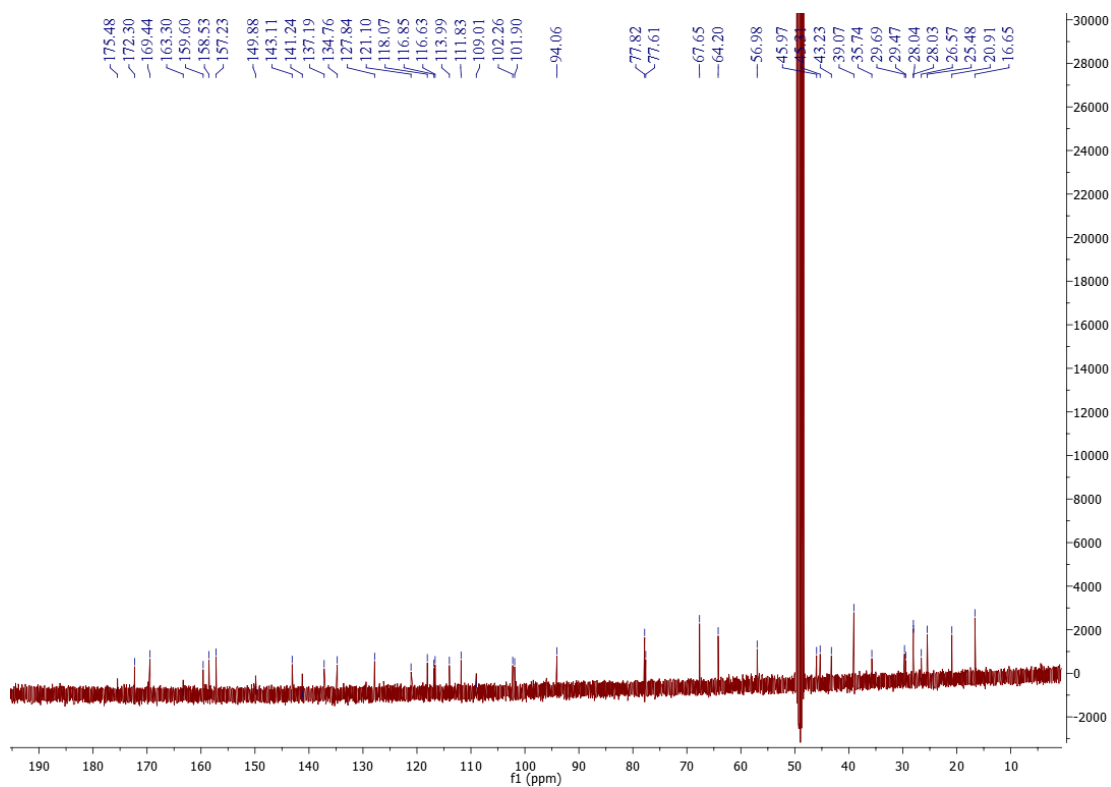
S41: NOESY spectrum of **1** in DMSO- $d_6$



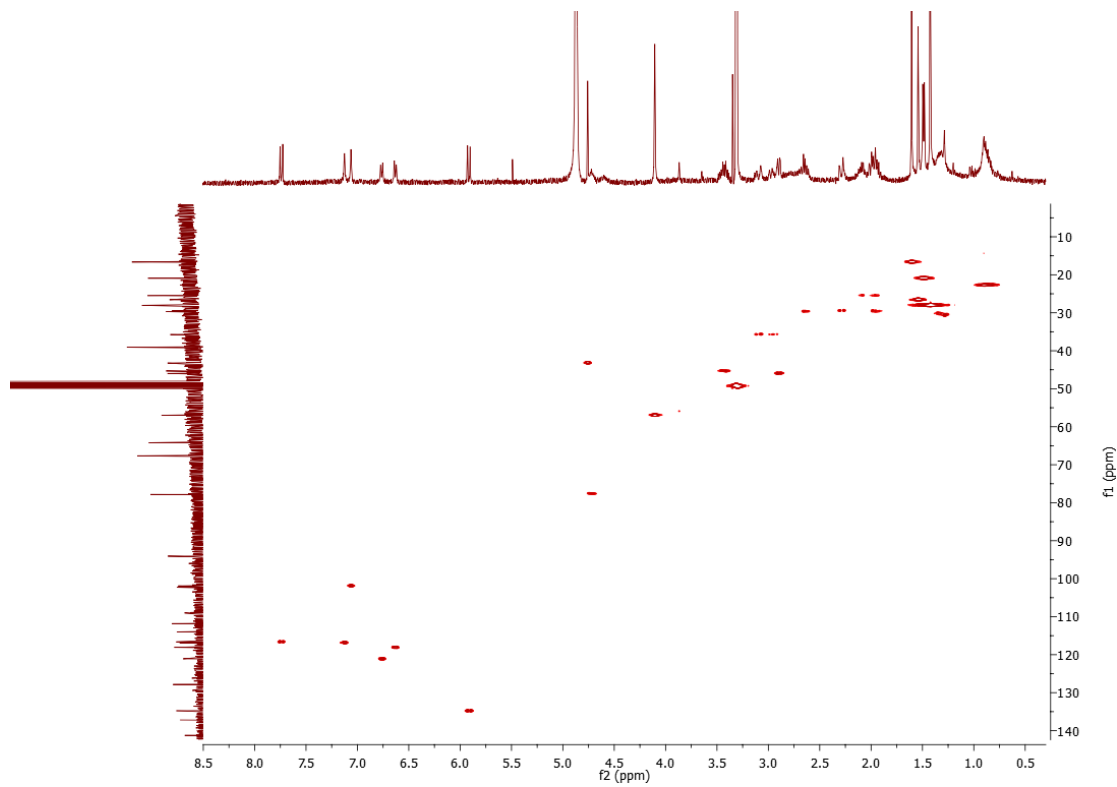
S42:  $^1\text{H}$  NMR spectrum (400MHz) of **1** in  $\text{CD}_3\text{OD}$



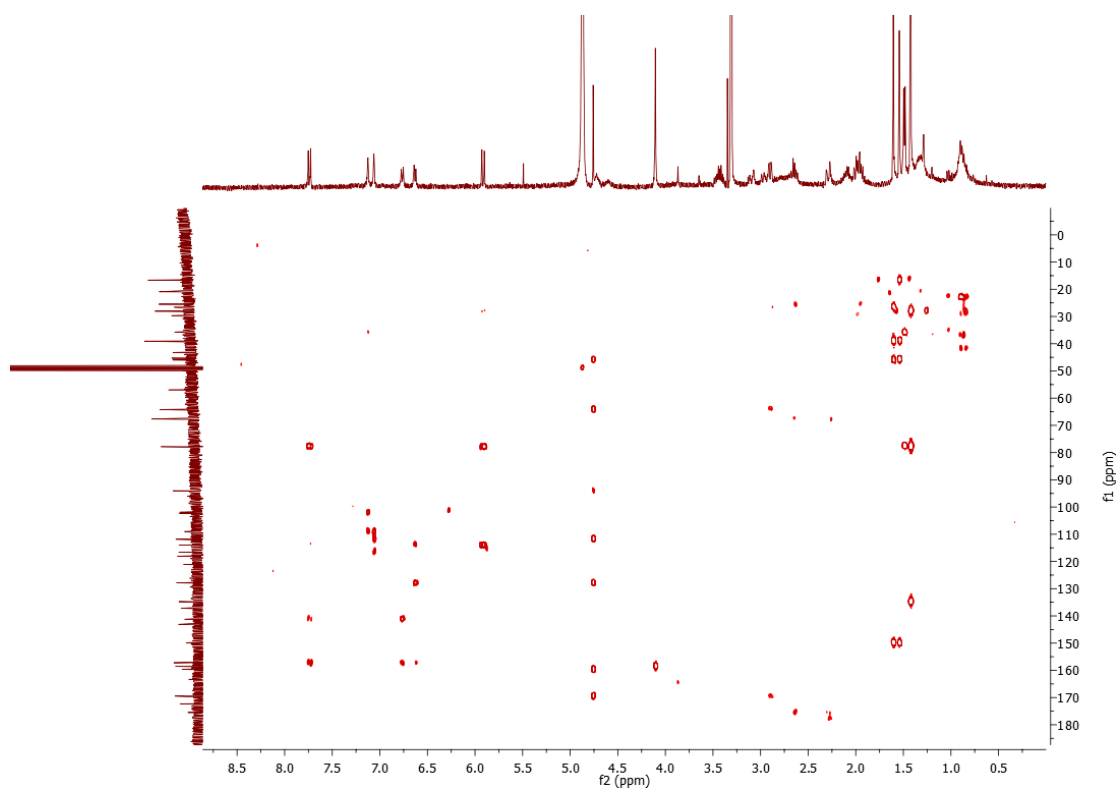
**S43:**  $^{13}\text{C}$  NMR spectrum (100MHz) of **1** in  $\text{CD}_3\text{OD}$



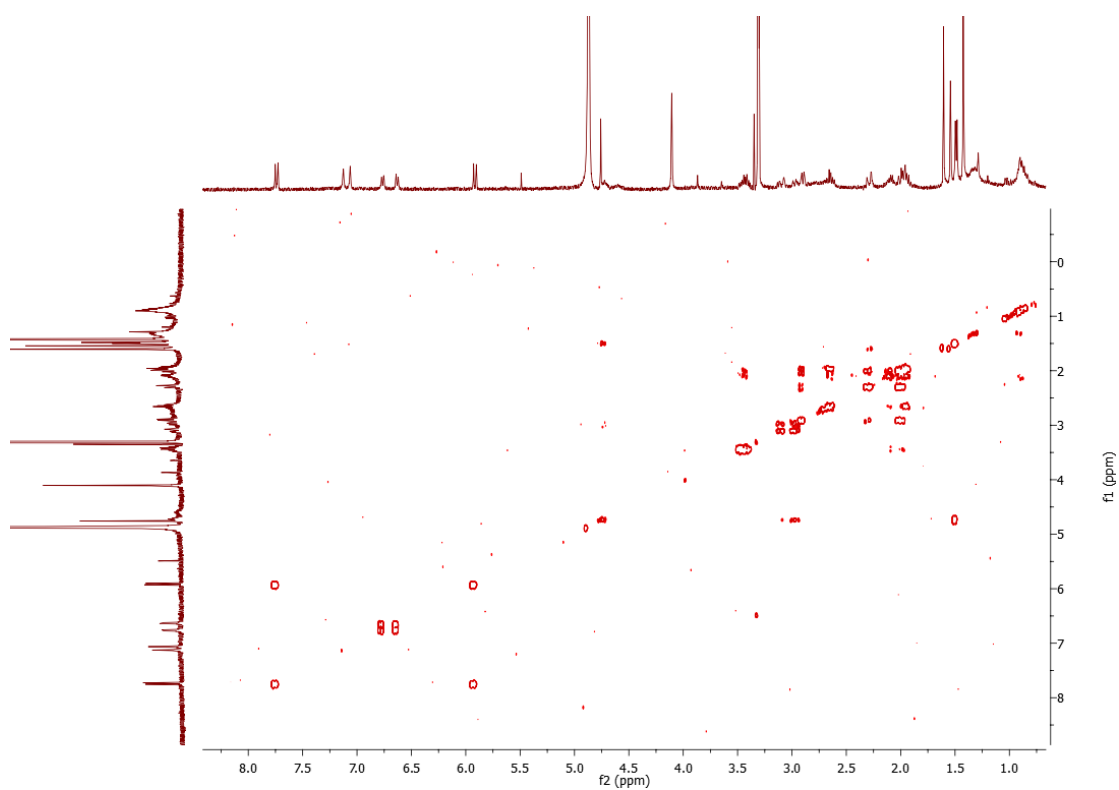
**S44:** HSQC spectrum of **1** in  $\text{CD}_3\text{OD}$



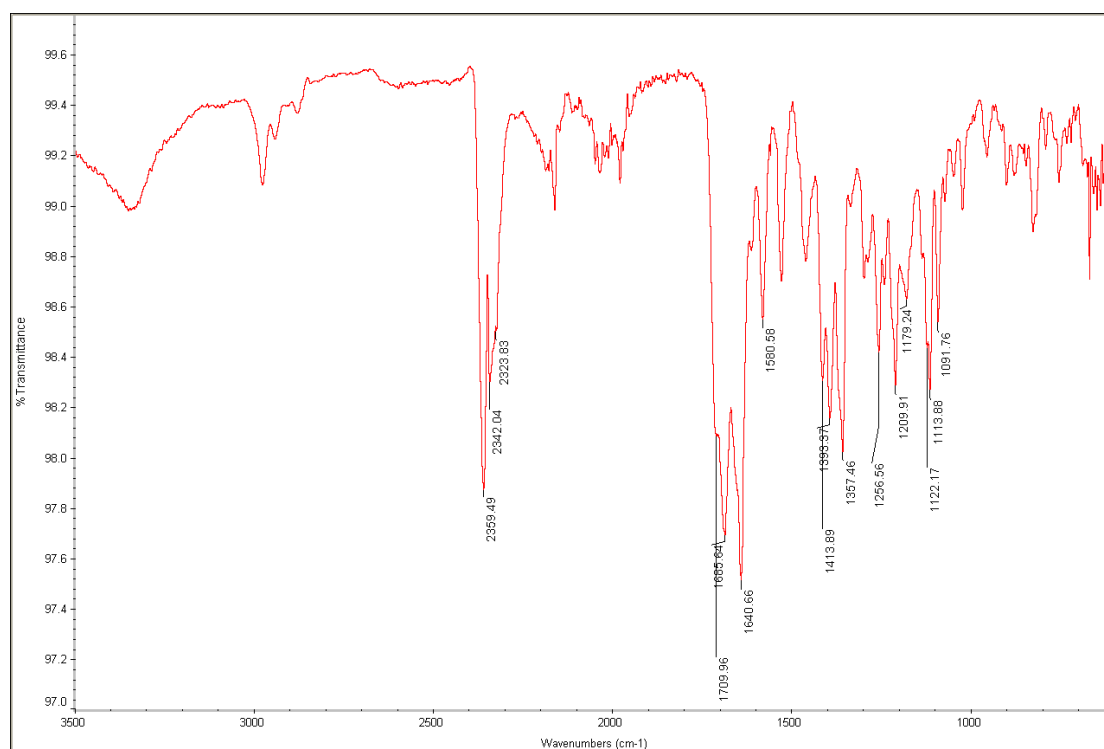
**S45:** HMBC spectrum of **1** in CD<sub>3</sub>OD



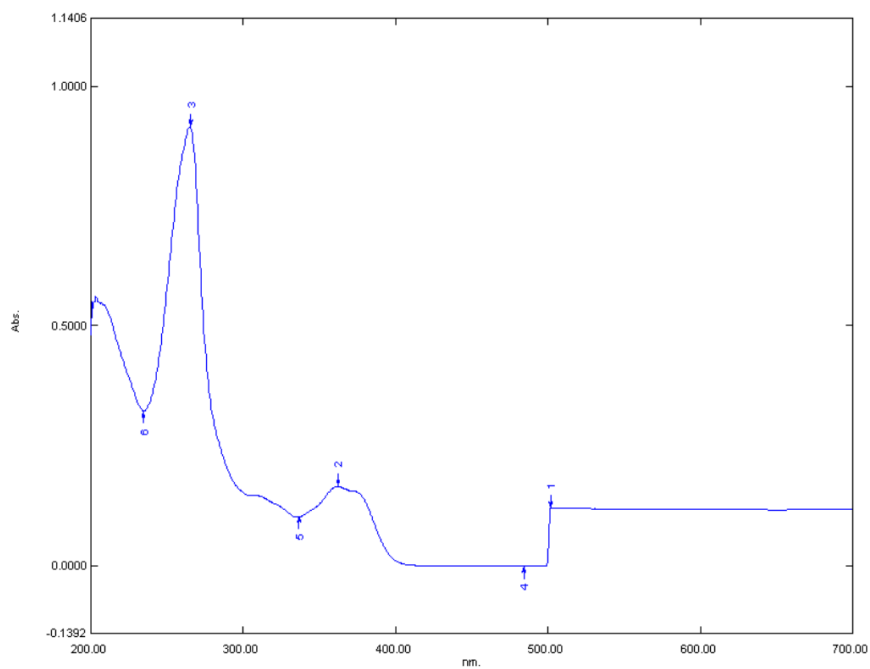
**S46:** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **1** in CD<sub>3</sub>OD



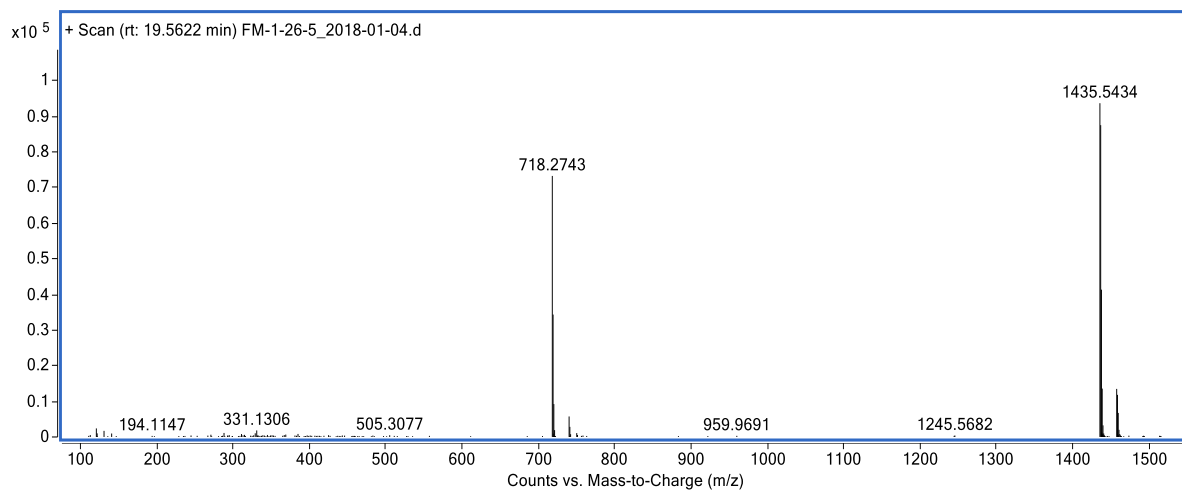
**S47:** IR spectrum of **1** (2359 and 2342 are CO<sub>2</sub> absorption bands)



**S48:** UV spectrum of **1**

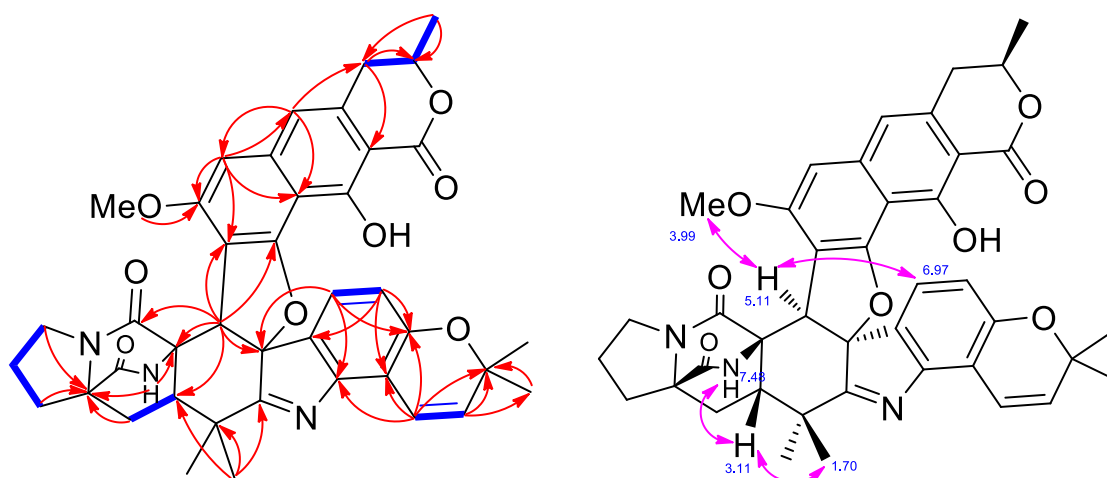


**S49:** (+)-HR-MS spectrum of **1**

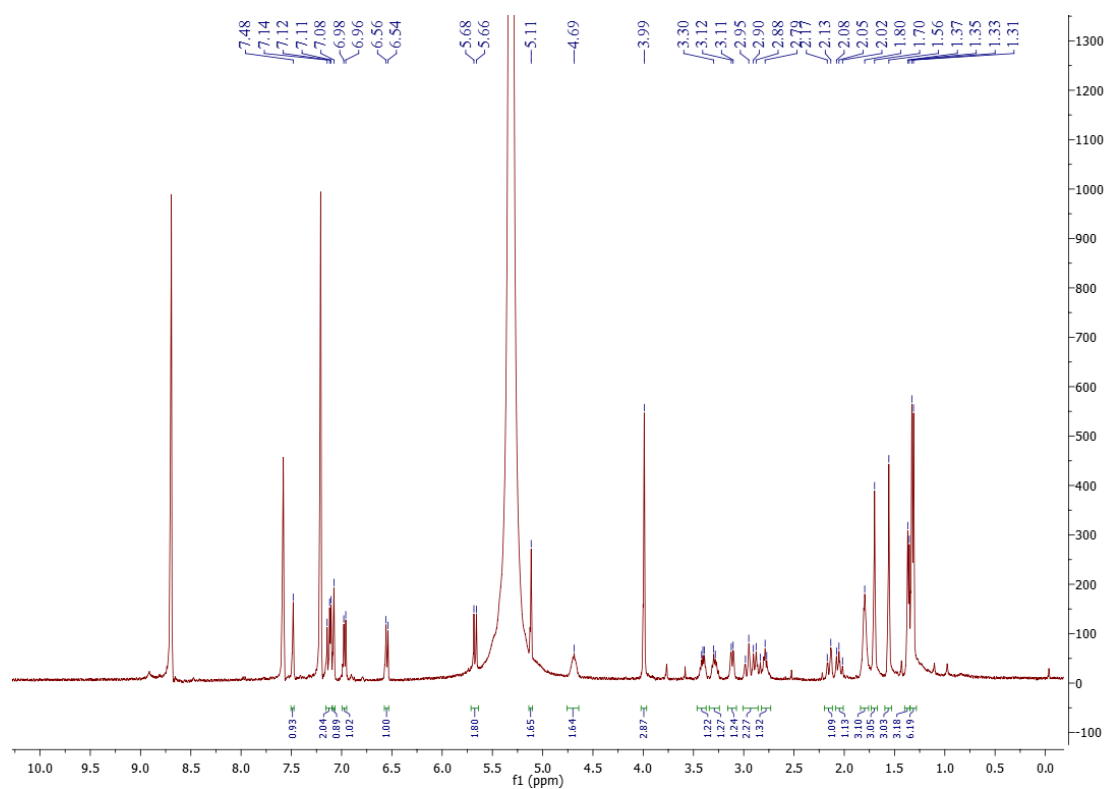


**For compound 2**

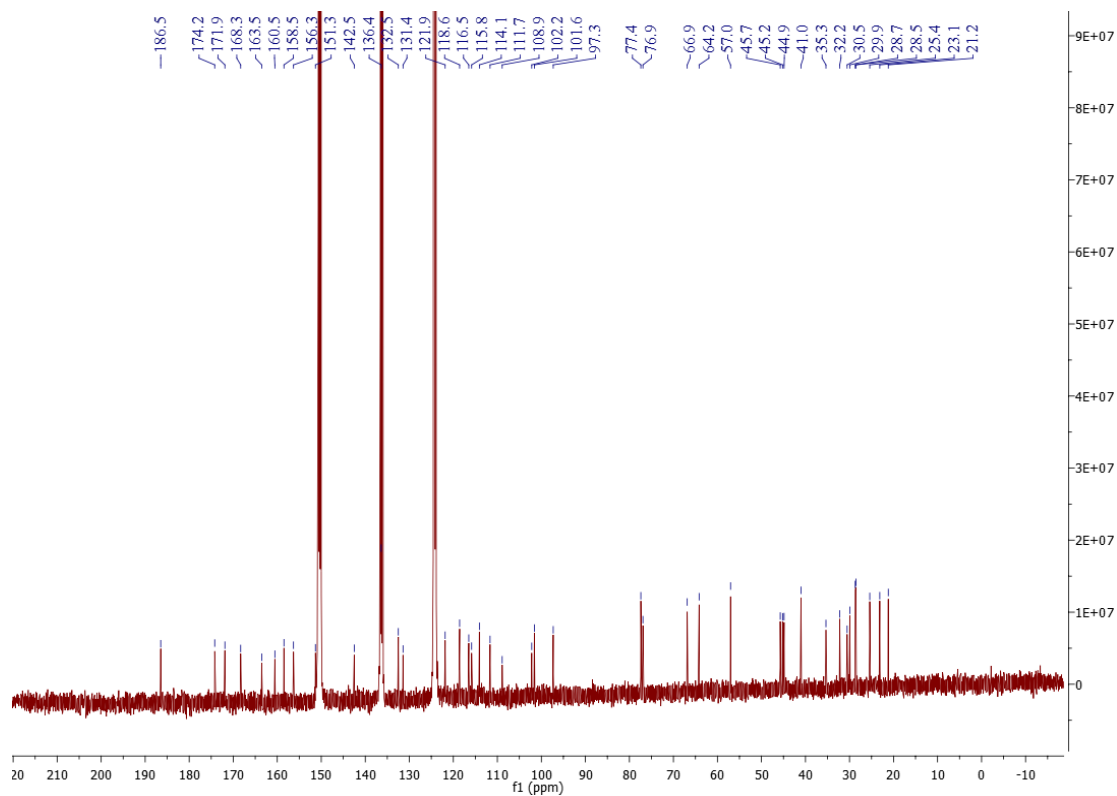
**S50:** Key 2D NMR correlations for compound **2**



**S51:**  $^1\text{H}$  NMR spectrum (400MHz) of **2** in pyridine- $d_5$

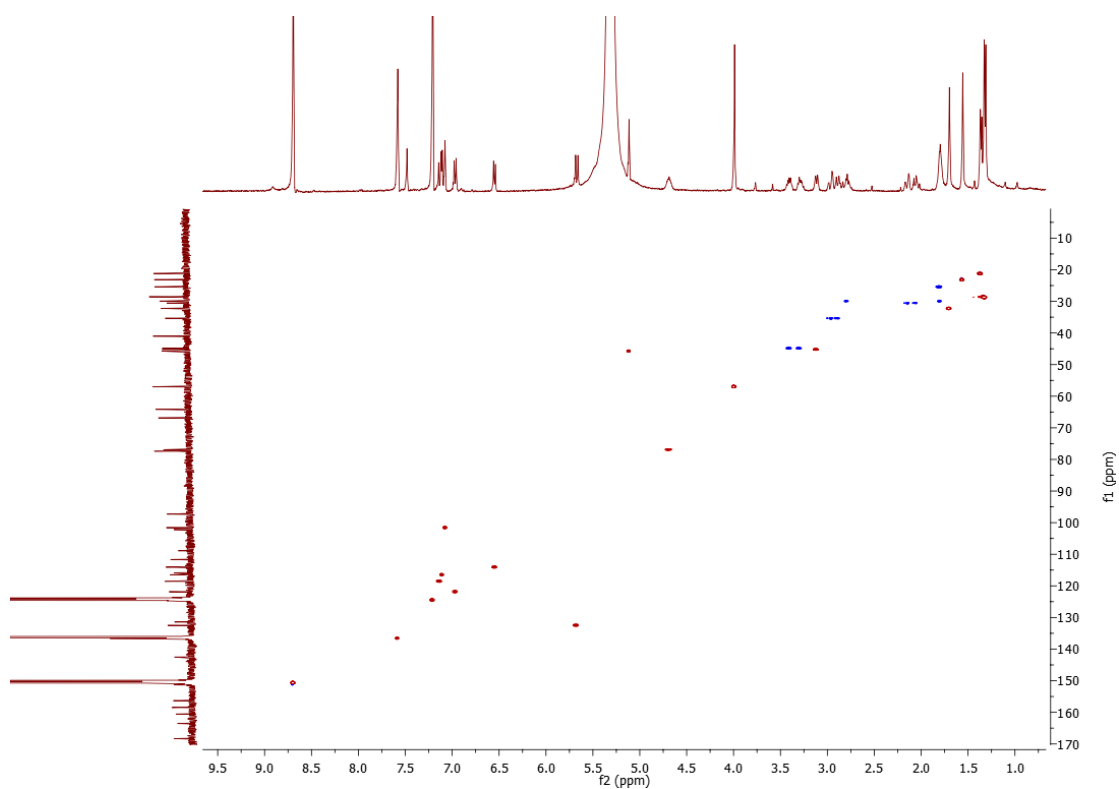


**S52:**  $^{13}\text{C}$  NMR spectrum (100MHz) of **2** in pyridine- $d_5$

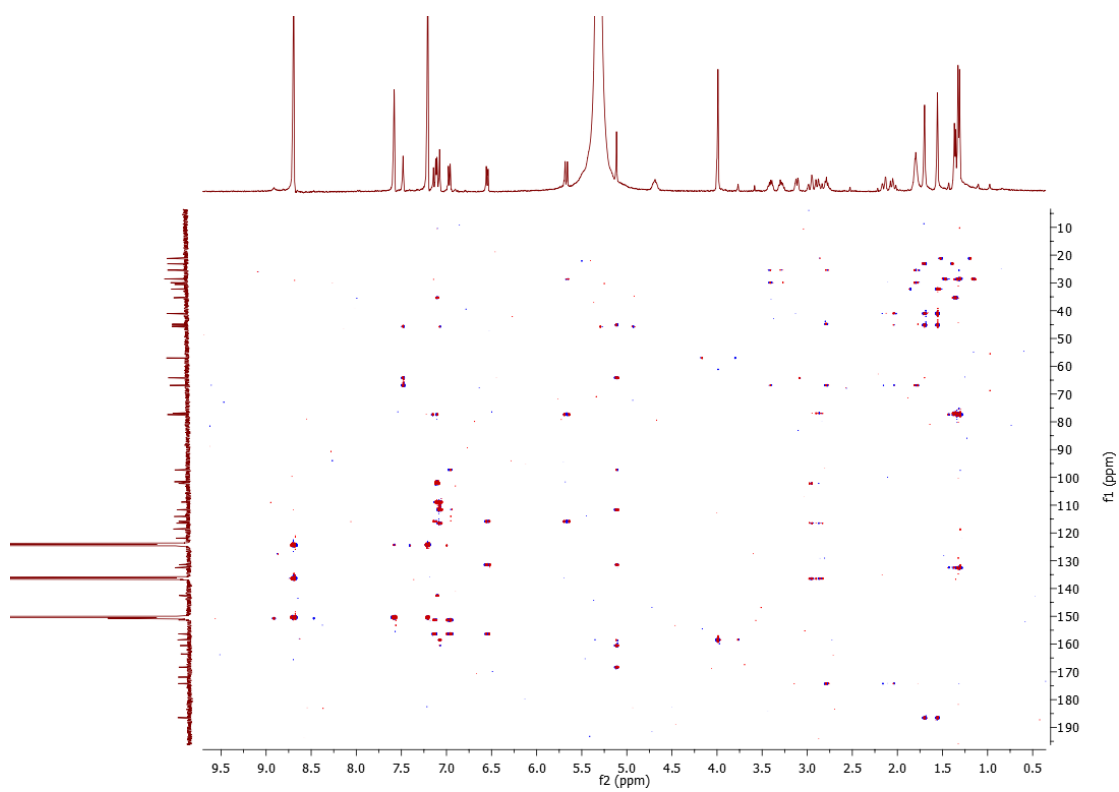




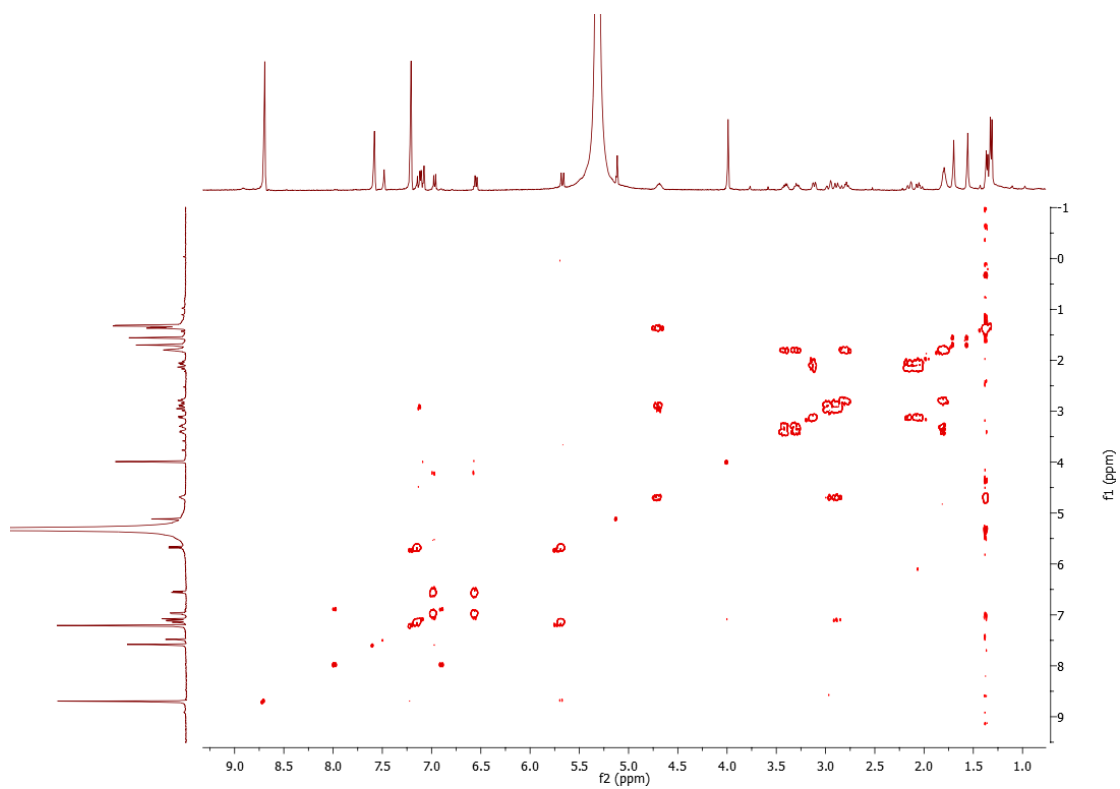
**S53:** HSQC spectrum of **2** in pyridine-*d*<sub>5</sub>



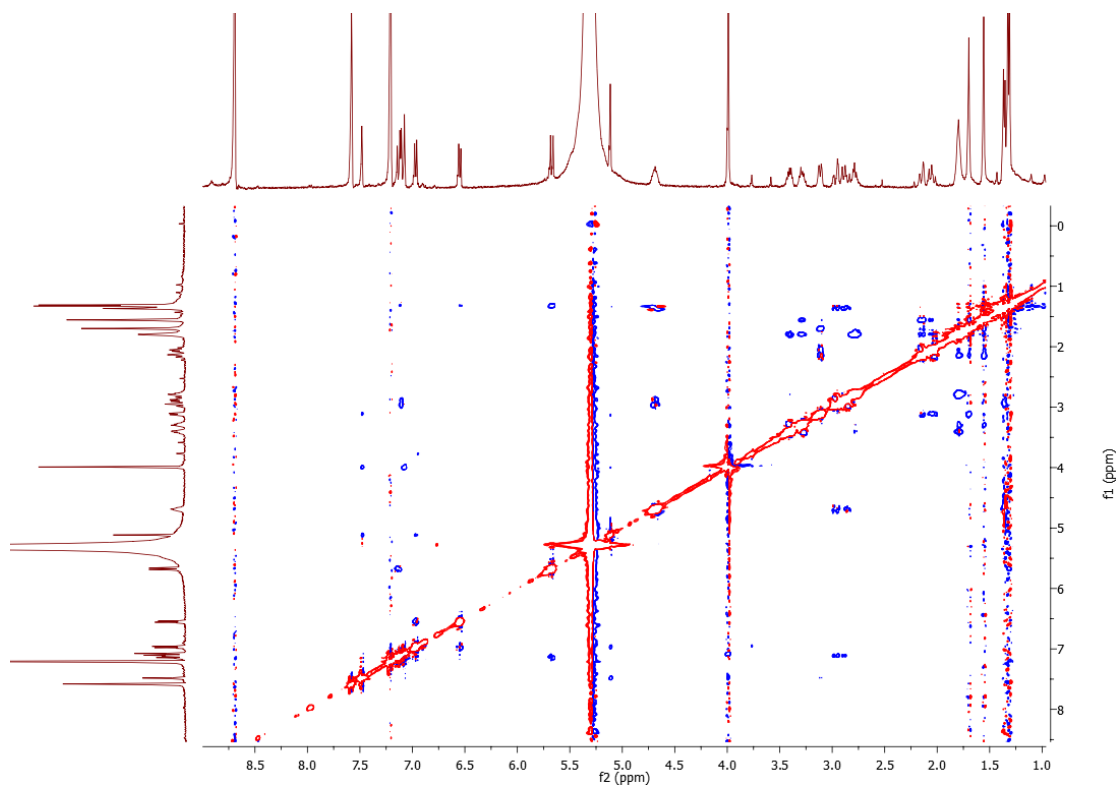
**S54:** HMBC spectrum of **2** in pyridine-*d*<sub>5</sub>



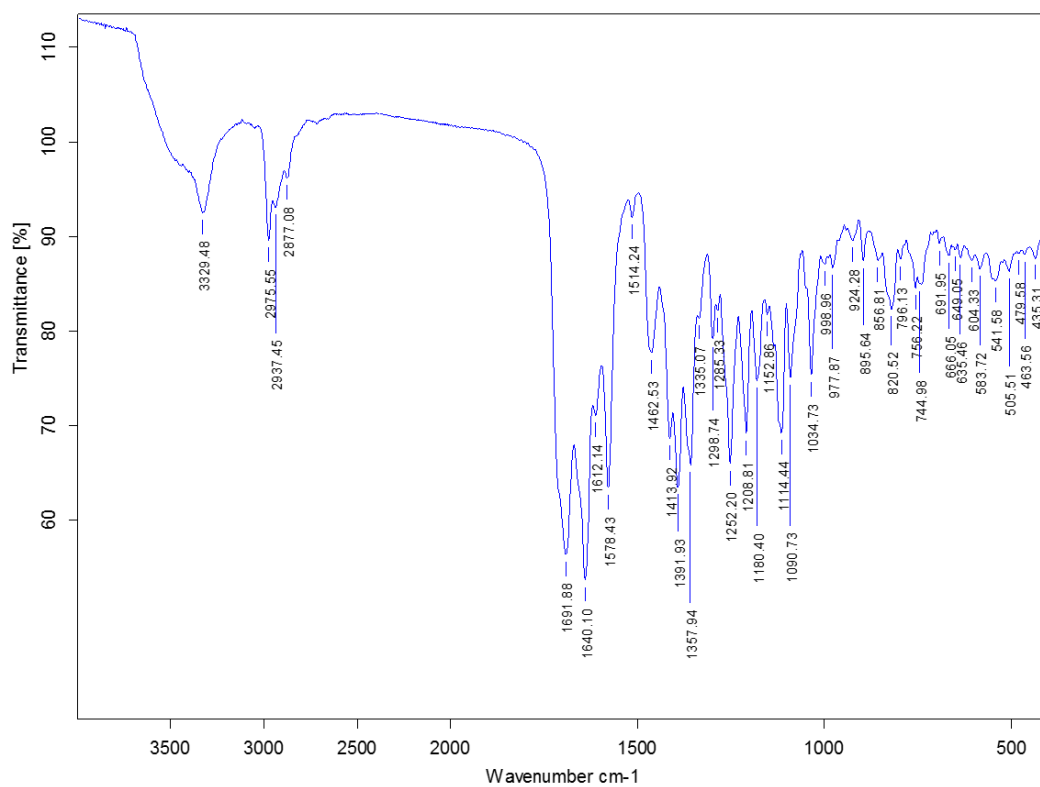
**S55:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in pyridine- $d_5$



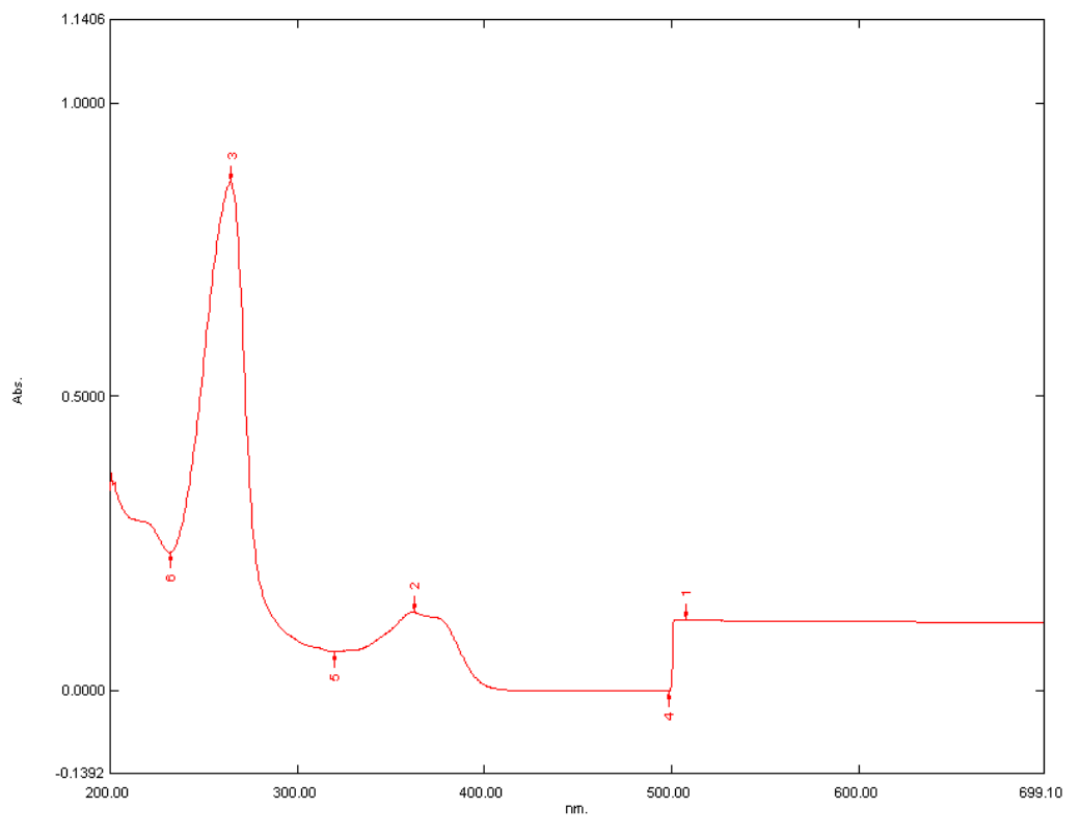
**S56:** NOESY spectrum of **2** in pyridine- $d_5$



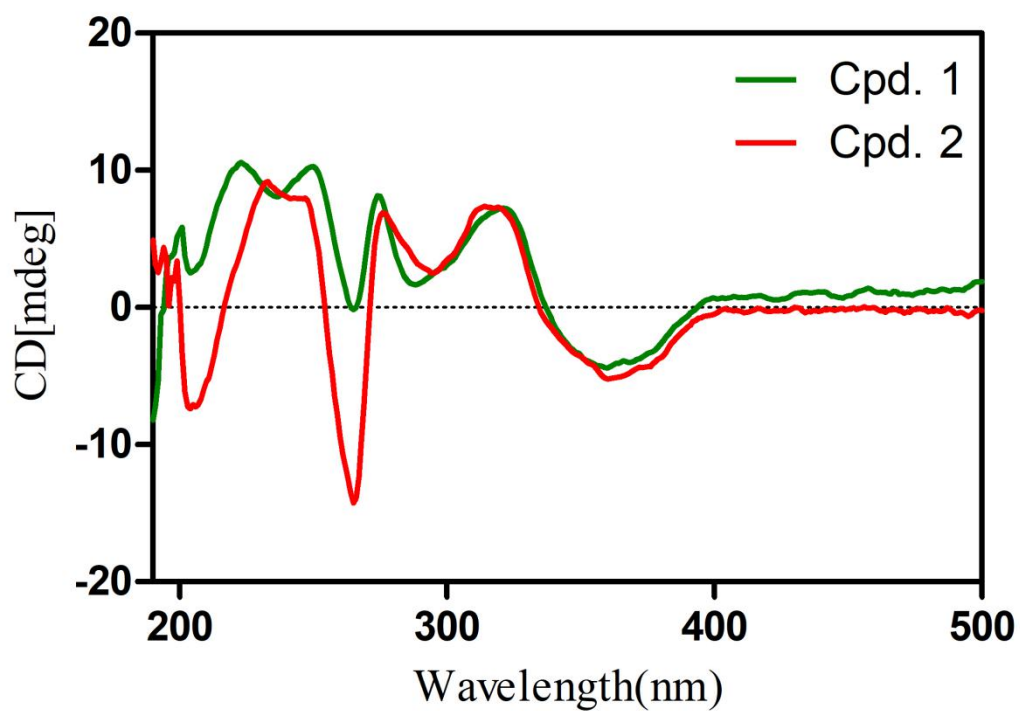
S57: IR spectrum of 2



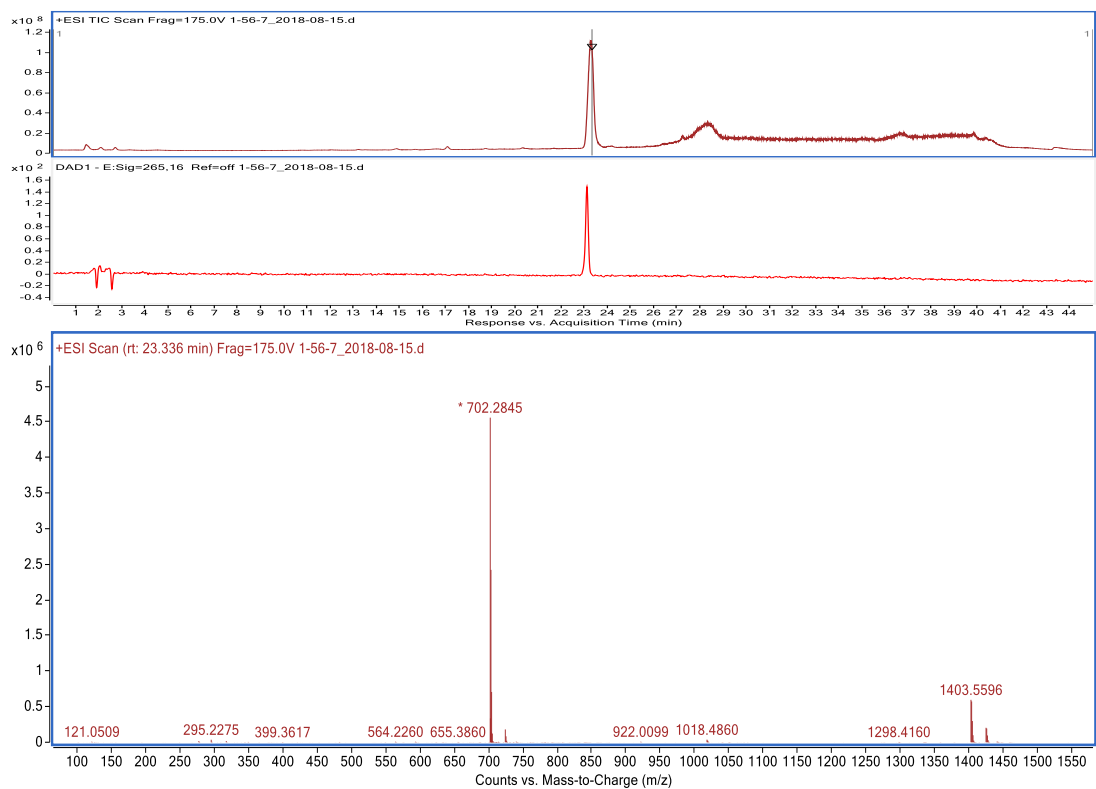
S58: UV spectrum of 2



S59: CD spectrum of 1 and 2

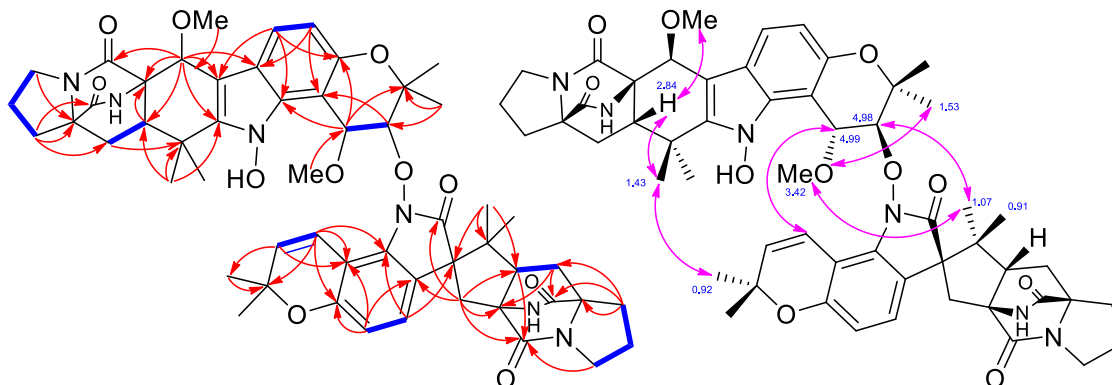


S60: (+)-HR-MS spectrum of 2

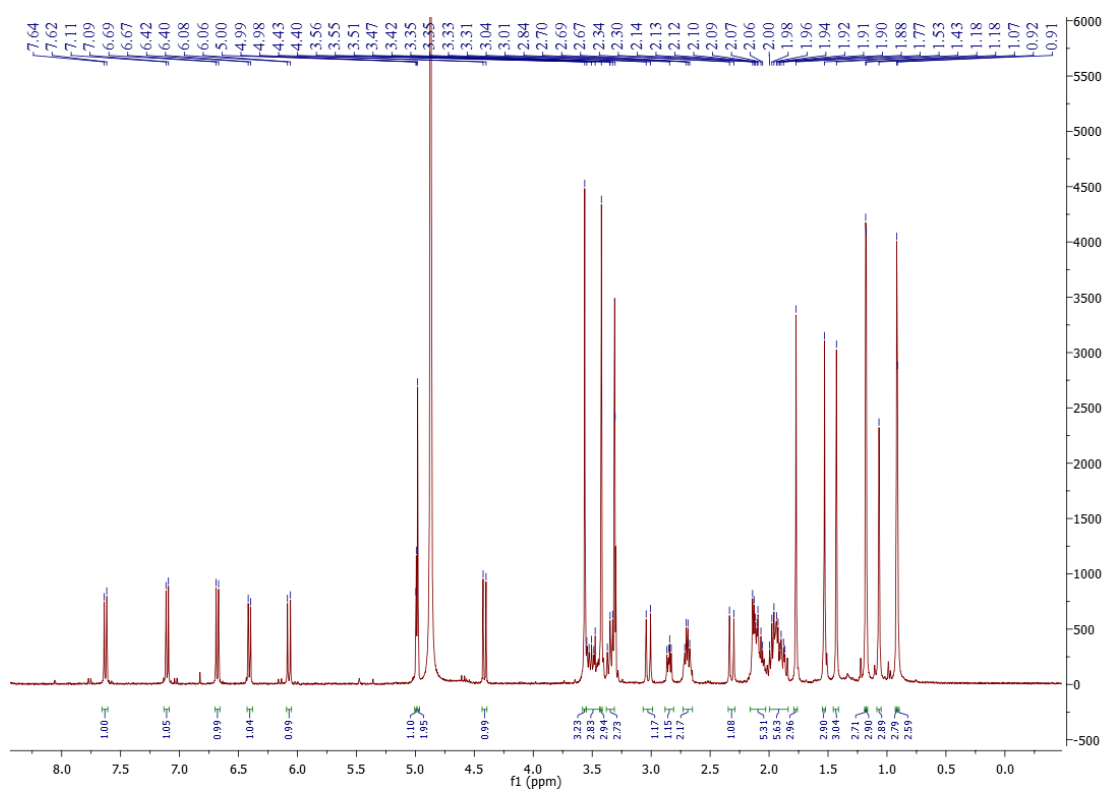


### For compound 3

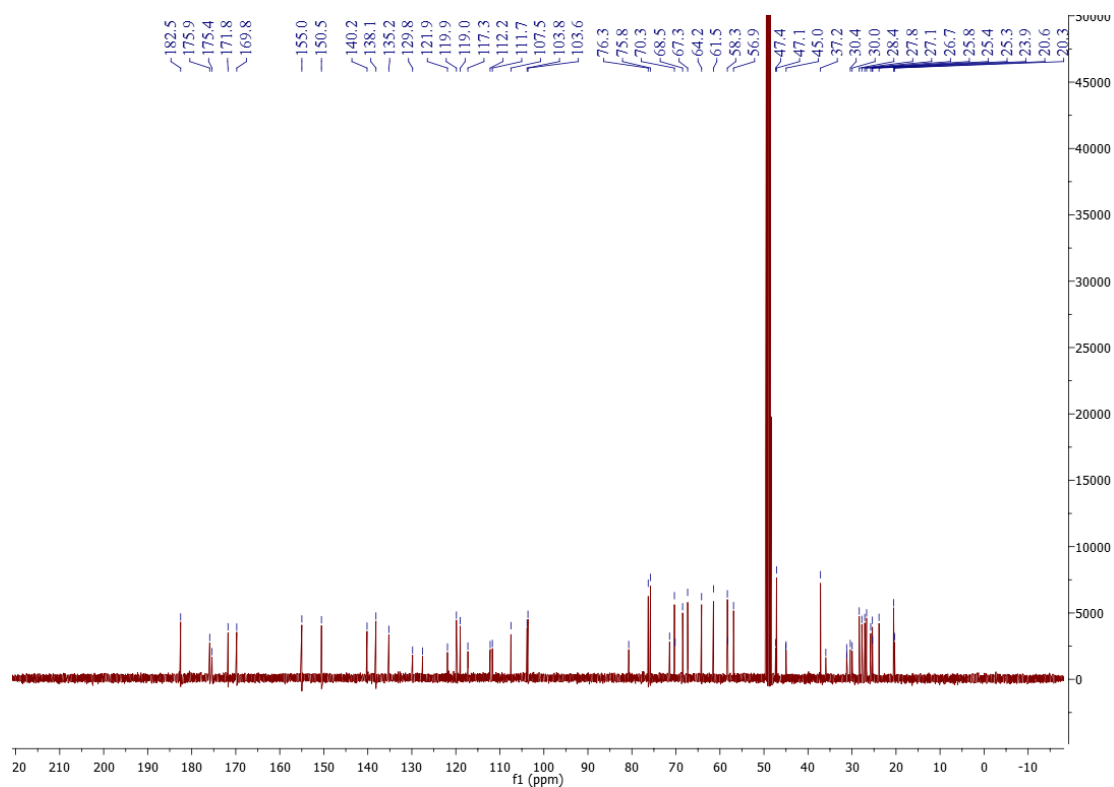
#### S61: Key 2D NMR correlations of 3



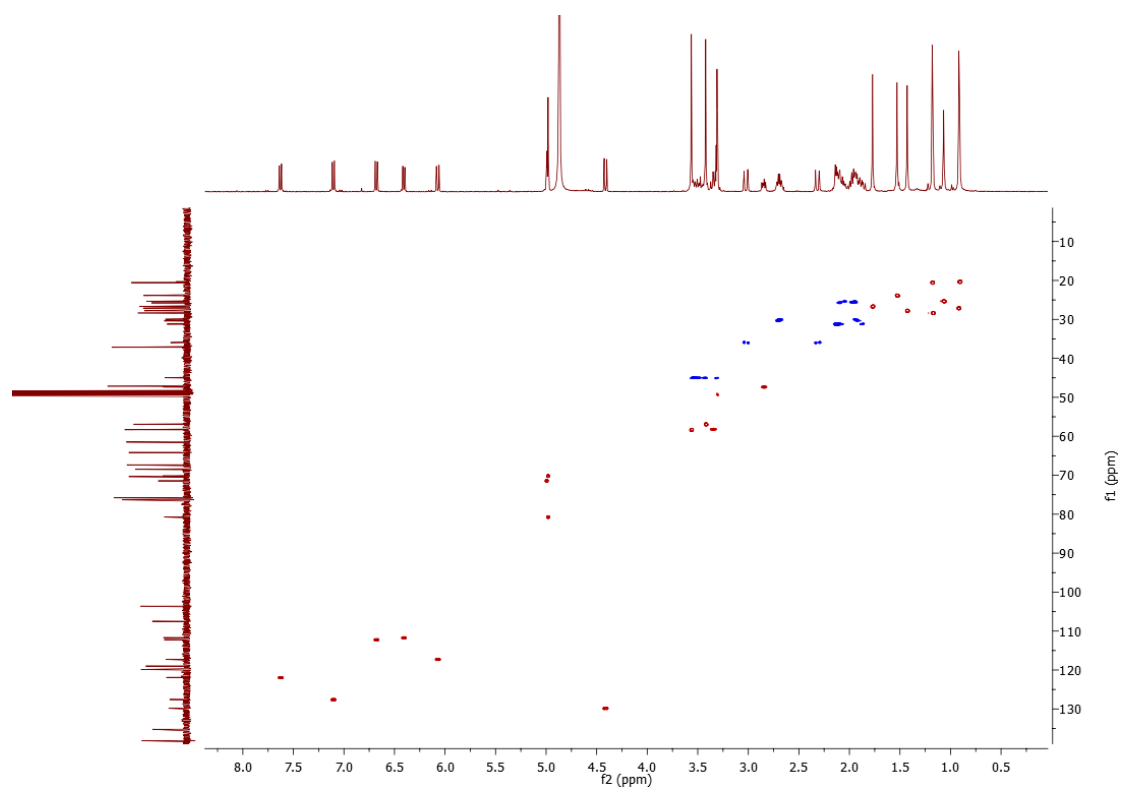
#### S62: $^1\text{H}$ NMR spectrum (400MHz) of 3 in $\text{CD}_3\text{OD}$



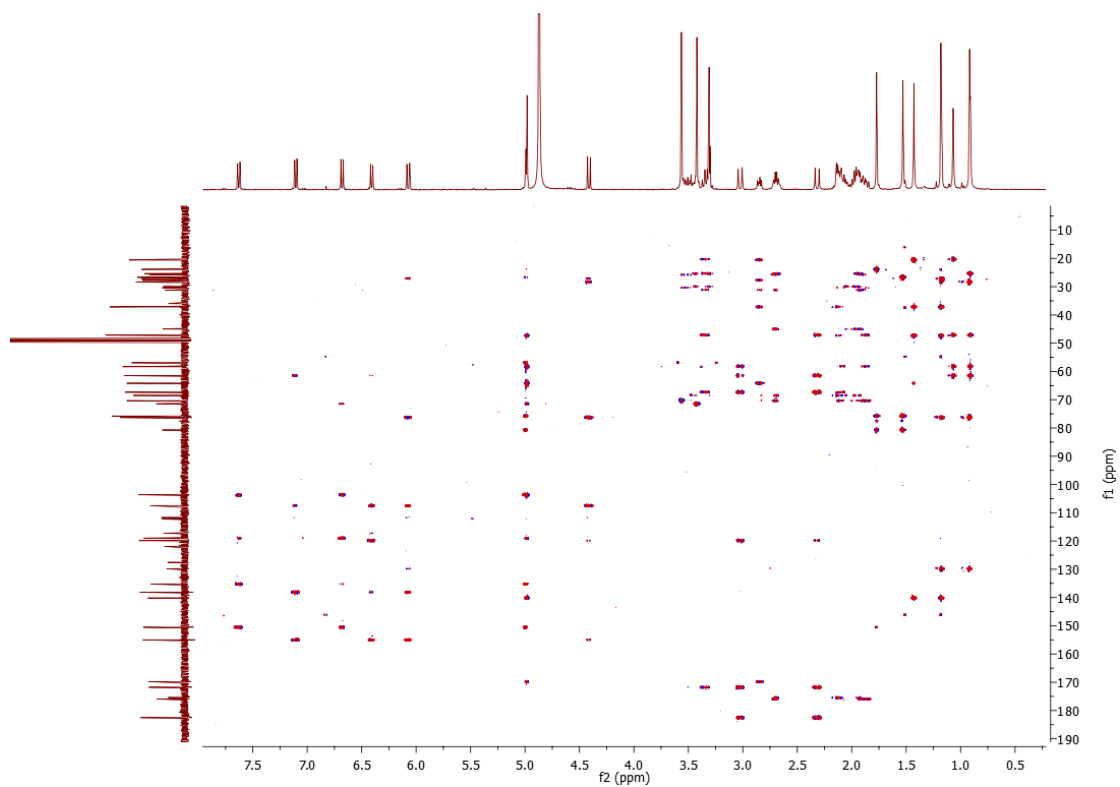
**S63:**  $^{13}\text{C}$  NMR spectrum (100MHz) of **3** in  $\text{CD}_3\text{OD}$



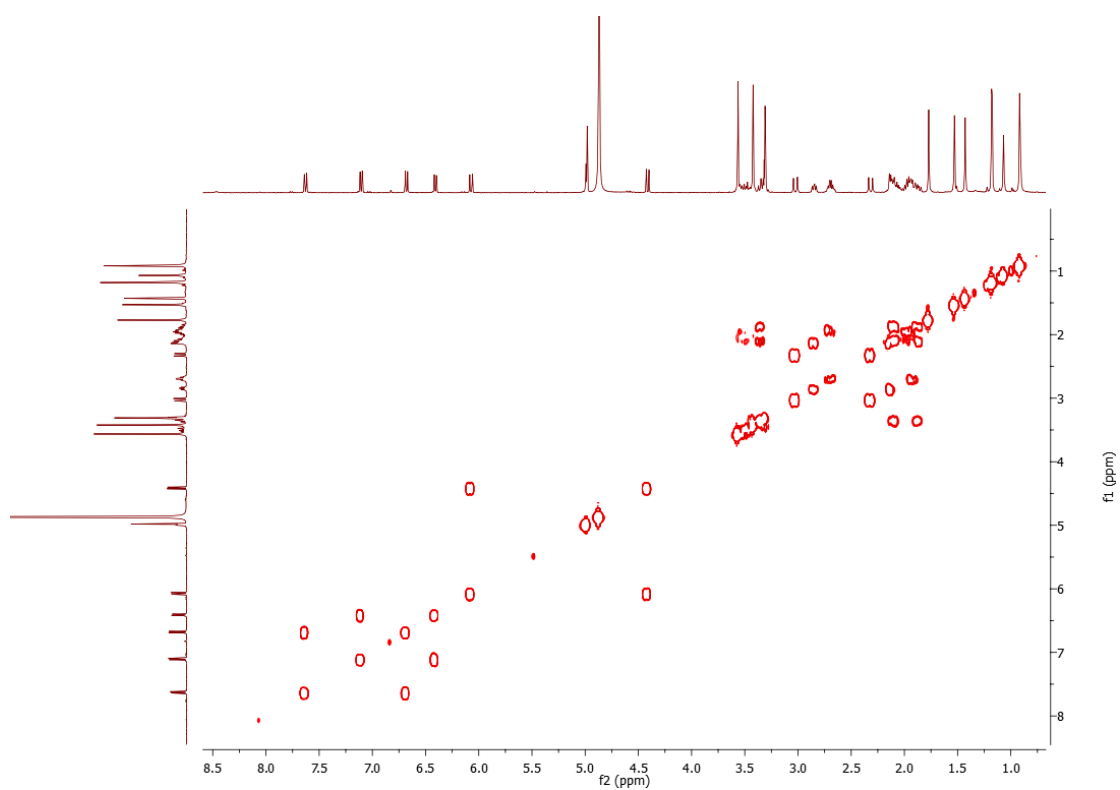
**S64:** HSQC spectrum of **3** in  $\text{CD}_3\text{OD}$



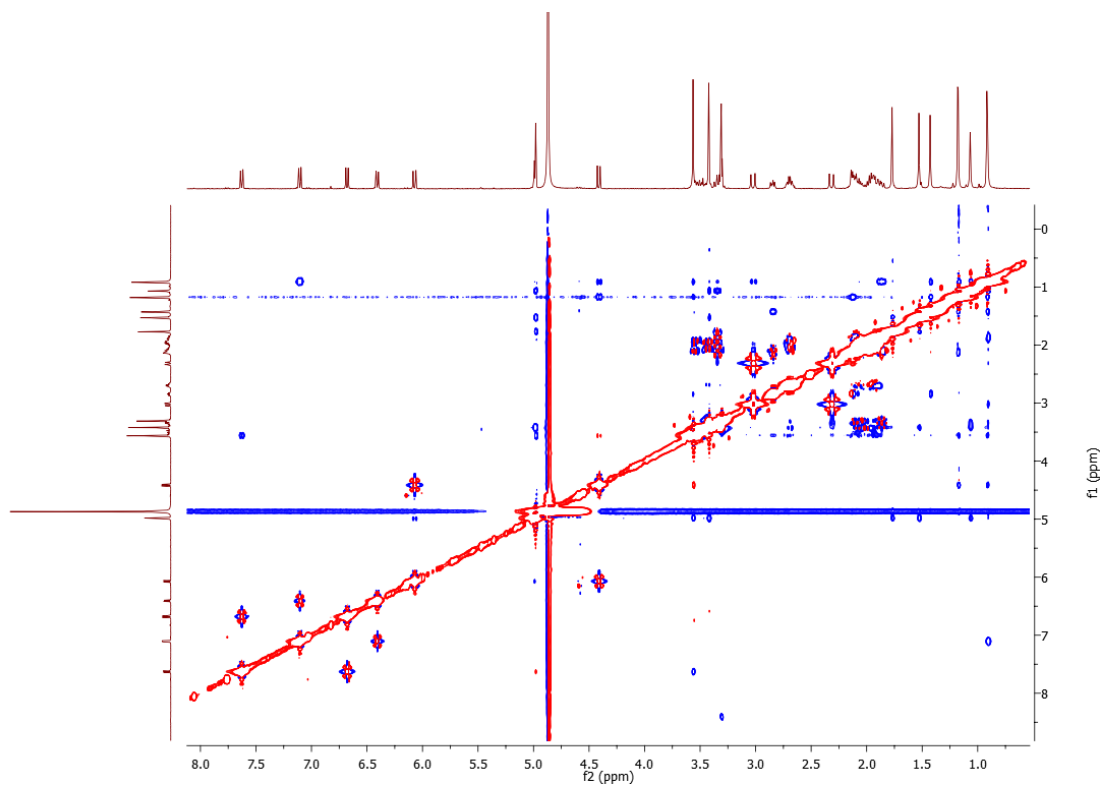
**S65:** HMBC spectrum of **3** in CD<sub>3</sub>OD



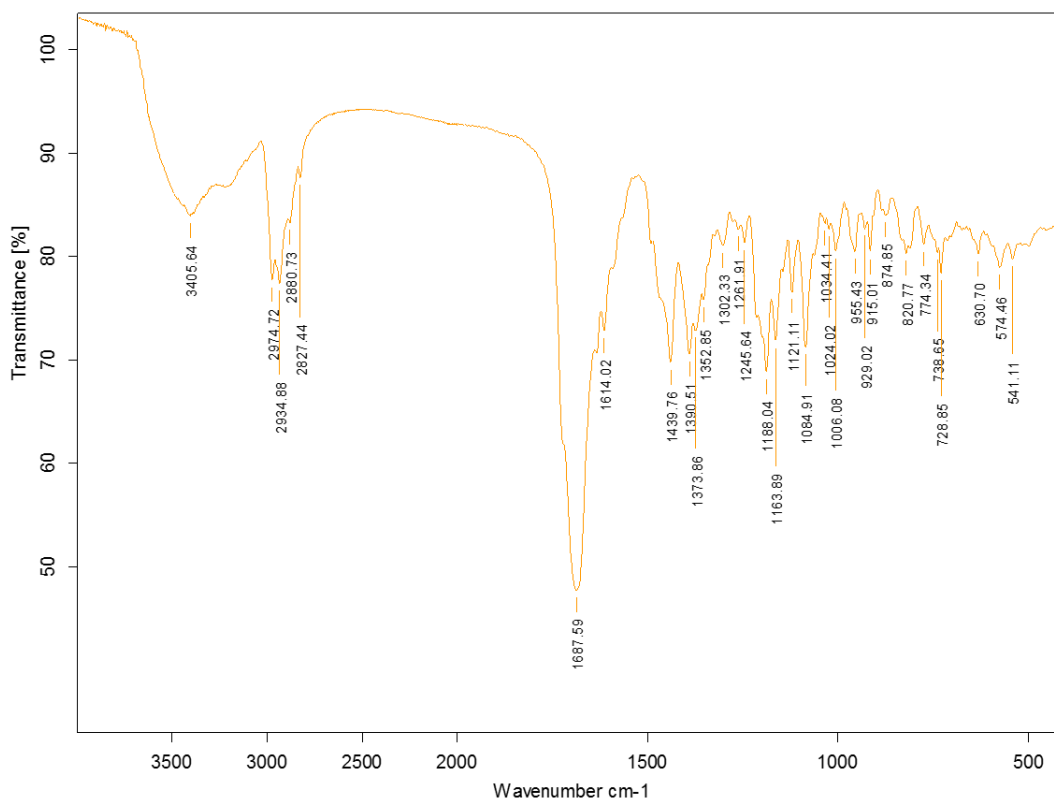
**S66:** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in CD<sub>3</sub>OD



**S67:** NOESY spectrum of **3** in CD<sub>3</sub>OD

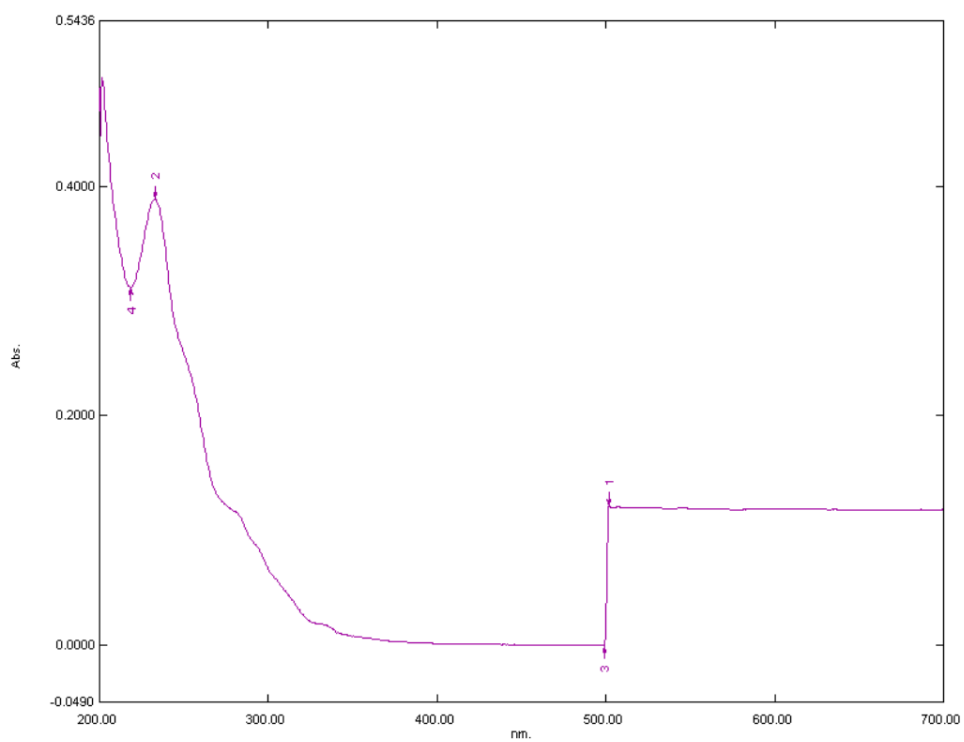


**S68:** IR spectrum of **3**

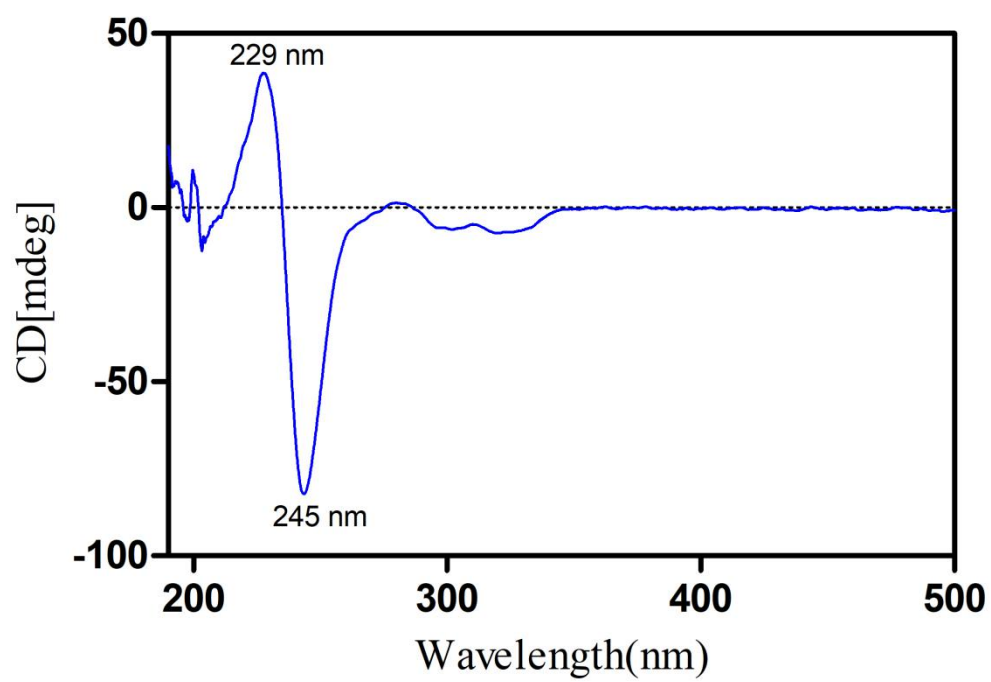




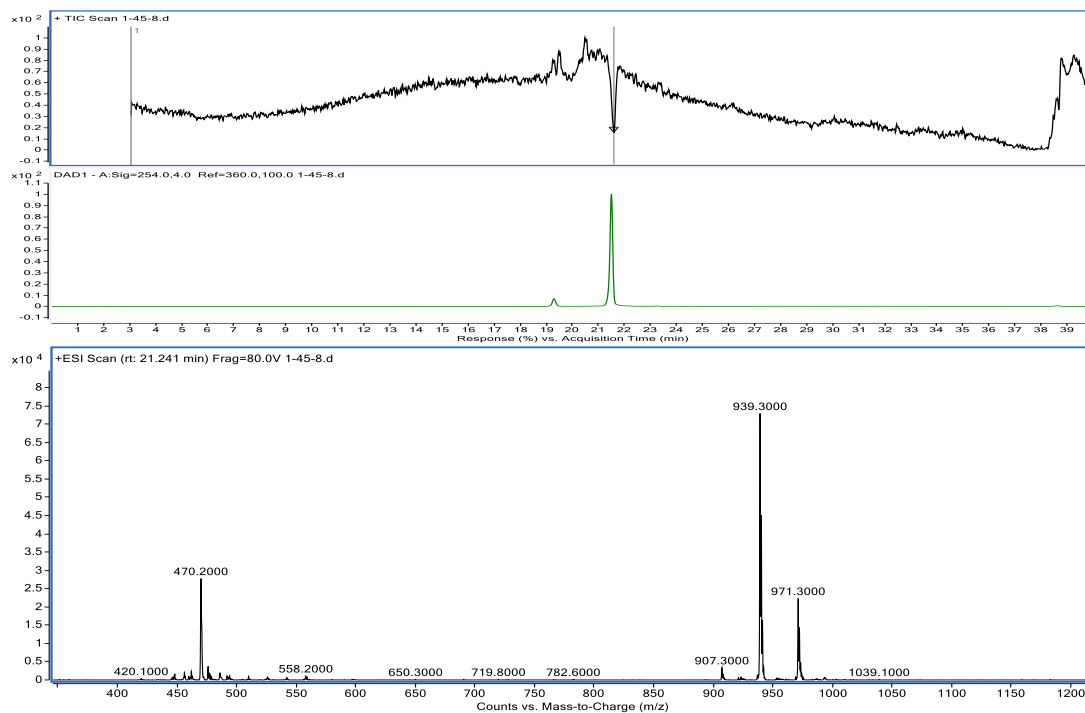
**S69:** UV spectrum of **3**



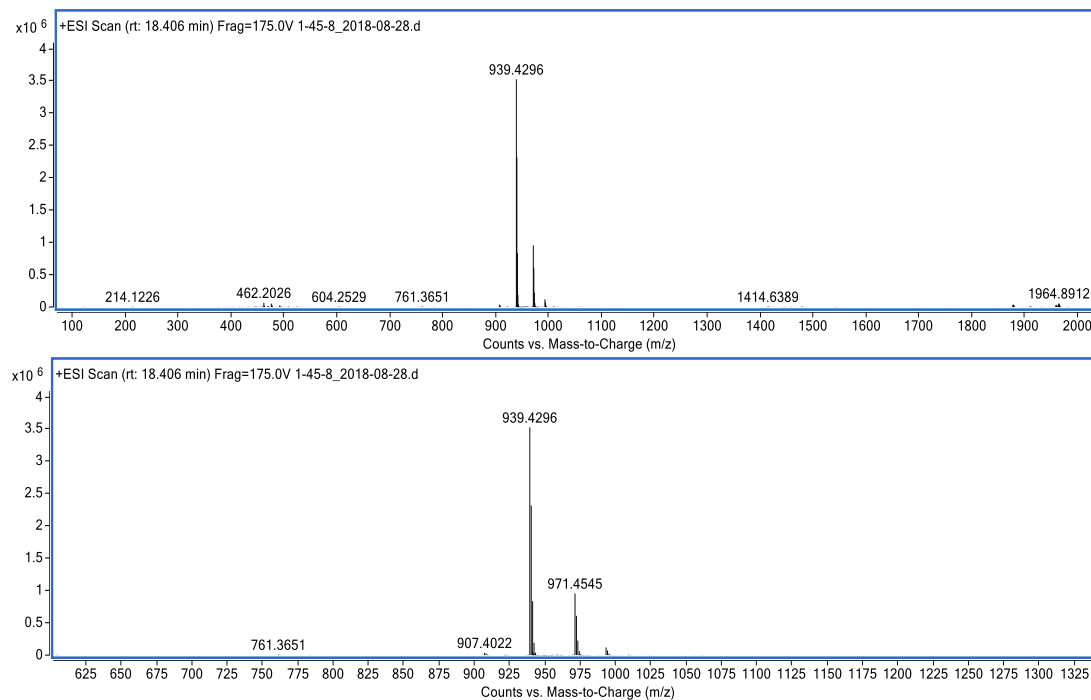
**S70:** CD spectrum of **3**



**S71:** (+)-LR-MS spectrum of **3**

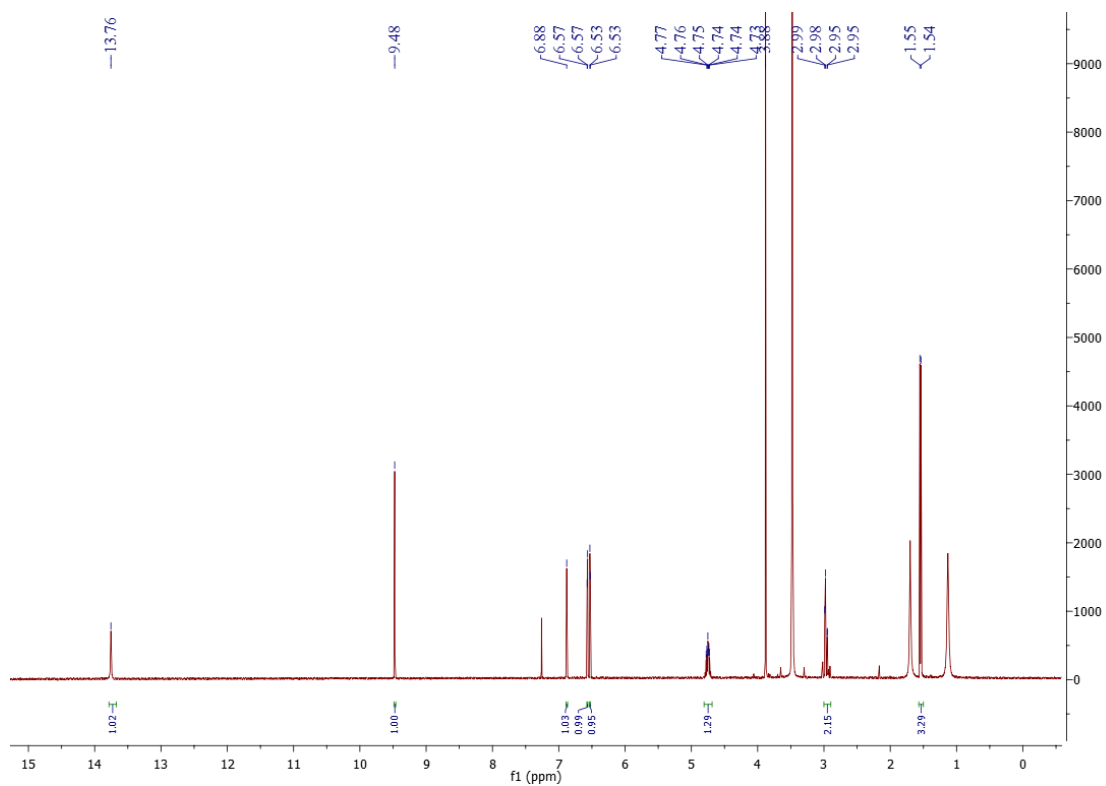


**S72:** (+)-HR-MS spectrum of **3**

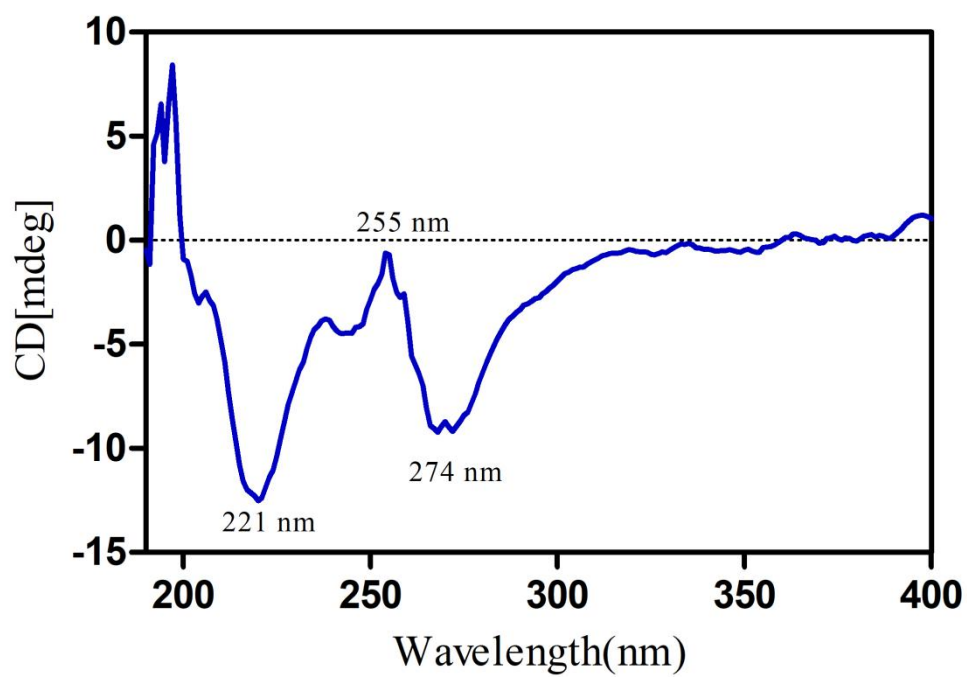


### For compound 4

**S73:**  $^1\text{H}$  NMR spectrum (400MHz) of 4 in  $\text{CCl}_3\text{D}$

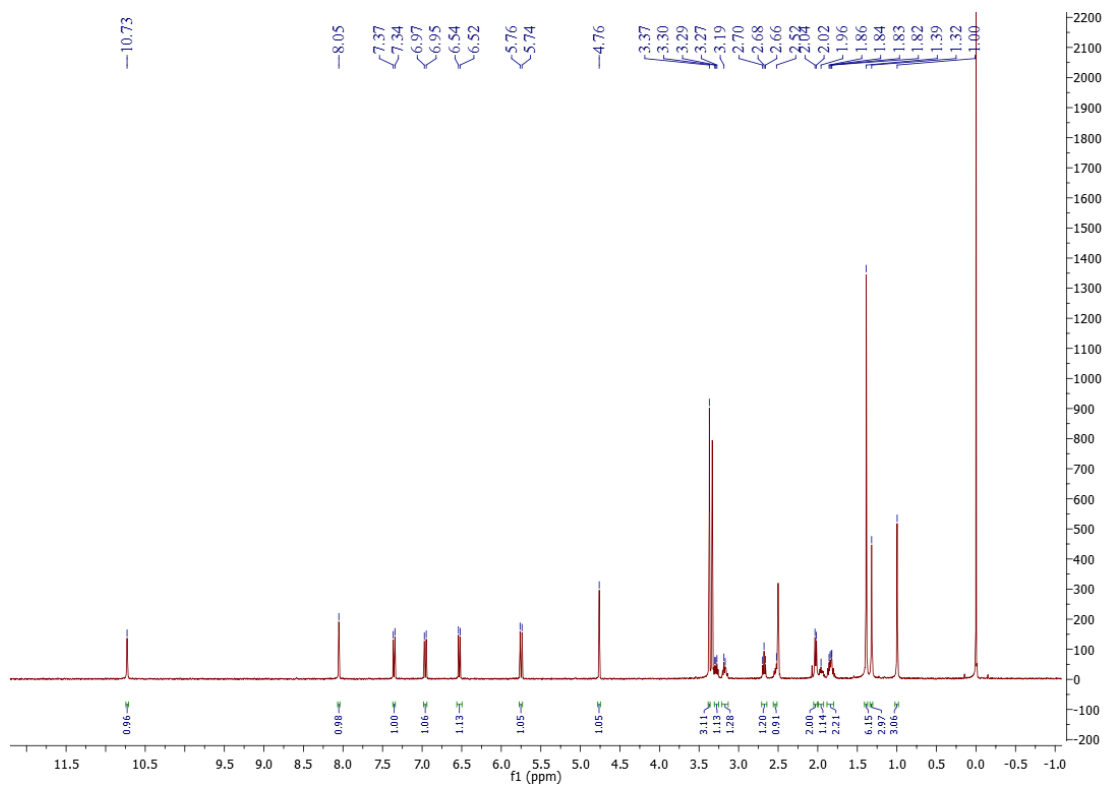


**S74:** CD spectrum of 4

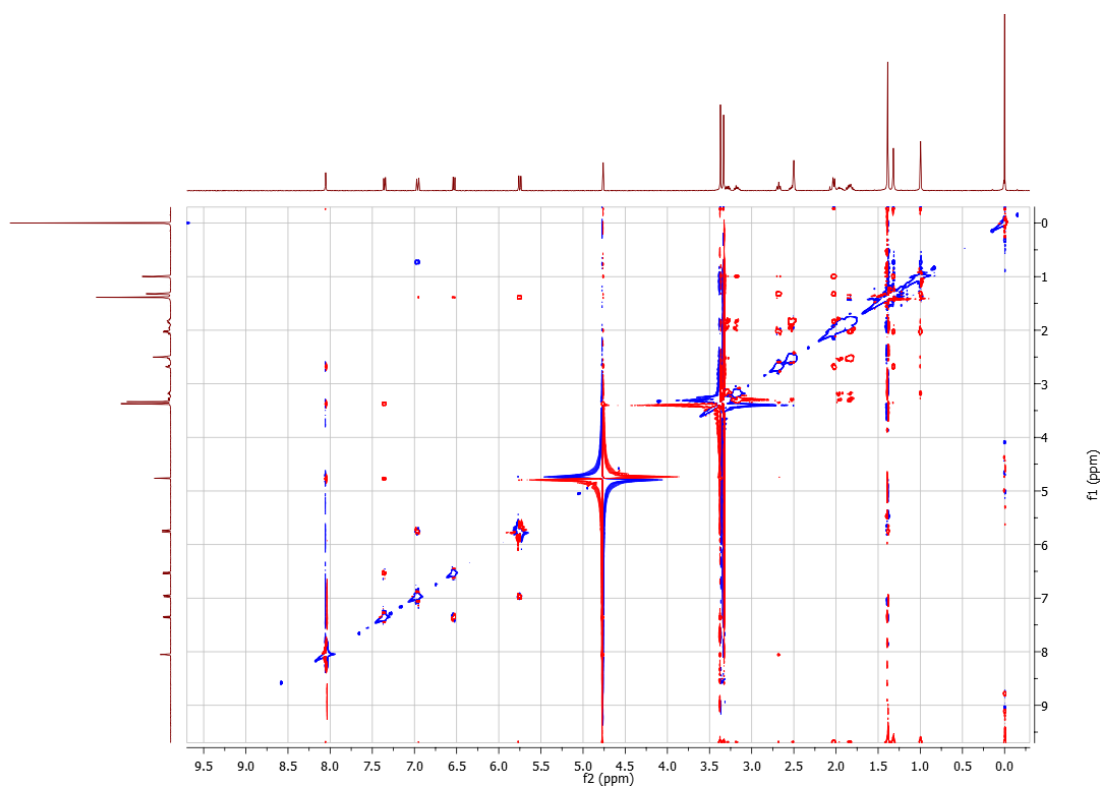


## For compound 5

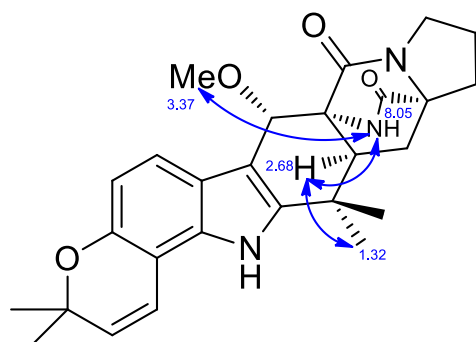
**S75:**  $^1\text{H}$  NMR spectrum (400MHz) of **5** in  $\text{DMSO-}d_6$



**S76:** ROESY spectrum of **5** in  $\text{DMSO-}d_6$

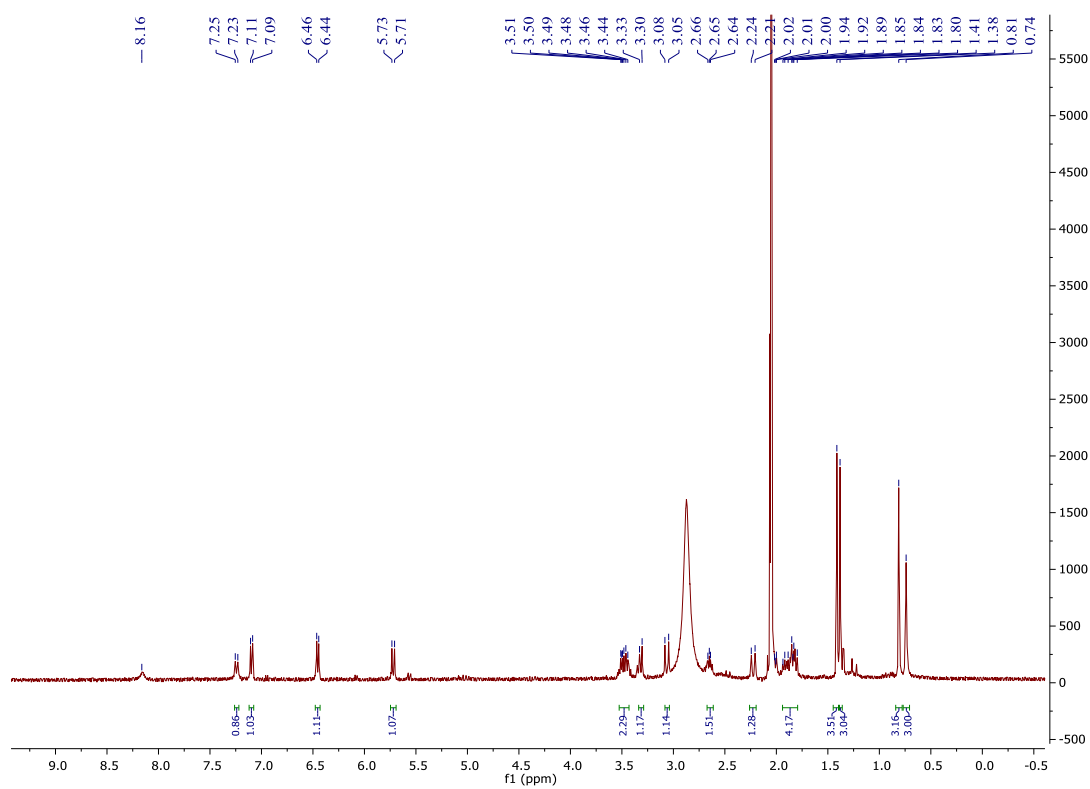


**S77:** Key ROESY correlations for compound **5**

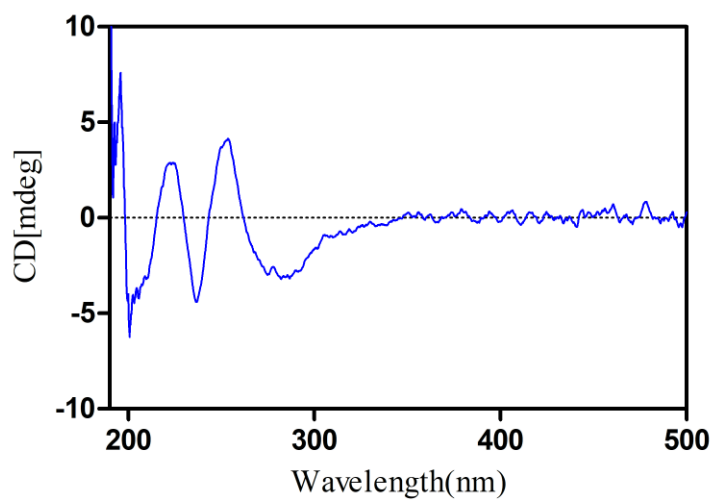


**For compound 6**

**S78:**  $^1\text{H}$  NMR spectrum (400MHz) of **6** in acetone- $d_6$



**S79:** CD spectrum of **6**



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## Cartesian Coordinates of the conformations found for each isomer at the B3LYP/6-31G\* level

1a\_c01  
B3LYP/6-31G\* Geometry  
C 5.093478 -4.466237 0.619595  
C 3.149559 -3.450382 -0.576239  
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C 3.315803 -4.468345 -1.613452  
C 5.557159 -4.849698 -0.782261  
C 4.032581 -3.396010 0.543944  
C 3.881634 -2.427741 1.500067  
C 2.841965 -1.454665 1.411776  
C 1.927561 -1.511628 0.304960  
C 2.086223 -2.531346 -0.684521  
C 0.908030 -0.527079 0.285763  
C 0.790590 0.435740 1.269197  
C 1.701706 0.489400 2.334558  
C 2.710168 -0.460059 2.413136  
C -0.322173 1.375777 0.878183  
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C -1.426118 2.434724 -1.847813  
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C 0.136016 2.741198 0.281238  
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N 1.790590 4.072355 -0.786866  
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C -0.508411 4.793237 -1.056412  
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Number of imaginary frequencies = 0

1a\_c02

B3LYP/6-31G\* Geometry

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C 0.027796 3.316312 1.194078  
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 H -3.150249 1.093201 4.835293  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72779074  
 Number of imaginary frequencies = 0

1a\_c03

B3LYP/6-31G\* Geometry  
 C 5.410869 -4.081875 0.592725  
 C 3.400729 -3.187901 -0.590142  
 O 4.795941 -4.875265 -1.632510  
 C 3.640310 -4.173689 -1.643942  
 C 5.902298 -4.408096 -0.814174  
 C 4.277073 -3.088341 0.532305  
 C 4.056921 -2.148611 1.503380  
 C 2.949737 -1.251584 1.429224  
 C 2.041685 -1.357398 0.321042  
 C 2.273999 -2.346319 -0.684892  
 C 0.952403 -0.450477 0.316947  
 C 0.764757 0.485875 1.315155  
 C 1.670638 0.589847 2.381395  
 C 2.746069 -0.284602 2.445334  
 C -0.416484 1.345593 0.938700  
 C -1.122301 0.389212 -0.057759  
 O -0.008951 -0.392204 -0.645989  
 C -1.969070 1.046230 -1.119138  
 C -1.593919 2.358102 -1.778191  
 C -1.195609 3.295265 -0.571083  
 C -0.060770 2.749925 0.363842  
 C 1.313023 2.900205 -0.380057  
 N 1.496442 4.214703 -0.667472  
 C 0.465209 5.189000 -0.254795  
 C -0.848047 4.765595 -0.950591  
 O 2.837885 -4.414685 -2.548731  
 H 6.239844 -3.693648 1.195049  
 H 5.073401 -5.014468 1.069339  
 H 6.284746 -3.491791 -1.284663  
 H 4.729424 -2.075315 2.354492  
 H 3.455510 -0.245581 3.263314

H -1.095799 1.529821 1.777834  
H -2.082704 3.324055 0.073558  
H -0.694057 4.874401 -2.028346  
H -1.661345 5.442264 -0.668720  
C -2.083221 -0.615708 0.558176  
C -4.150148 -2.393854 1.087991  
C -3.237379 -0.635687 -0.211894  
C -1.954865 -1.499031 1.621994  
C -3.004671 -2.385309 1.886427  
C -4.314261 -1.494280 0.001796  
H -1.061581 -1.516075 2.236733  
H -2.949621 -3.086608 2.712507  
N -3.129824 0.407439 -1.226186  
O -4.090888 0.626471 -2.024930  
O -5.142852 -3.254249 1.437297  
C -5.580731 -1.529327 -0.724526  
H -5.790288 -0.731210 -1.423381  
C -6.439467 -2.533490 -0.501835  
H -7.390972 -2.580103 -1.026061  
C -6.117373 -3.675663 0.433609  
C -5.521922 -4.864844 -0.338351  
H -4.603913 -4.565744 -0.853723  
H -6.231146 -5.227733 -1.090698  
H -5.290128 -5.685887 0.349100  
C -7.342455 -4.098135 1.247713  
H -7.743400 -3.247070 1.806287  
H -7.070122 -4.885298 1.957834  
H -8.125112 -4.482854 0.585144  
C -2.776622 3.030963 -2.511823  
H -2.442387 3.984735 -2.933639  
H -3.620763 3.224914 -1.843700  
H -3.142311 2.404910 -3.324553  
C -0.460573 2.115851 -2.807020  
H -0.085149 3.065859 -3.205340  
H -0.863804 1.541770 -3.647743  
H 0.378220 1.554718 -2.393723  
O 2.107700 2.017414 -0.675637  
C 2.657612 4.821165 -1.312217  
H 2.995287 4.194321 -2.141900  
H 3.489479 4.914147 -0.600437  
C 2.116322 6.196079 -1.740998  
H 1.649813 6.117574 -2.729894  
H 2.905749 6.950104 -1.807671  
C 1.055705 6.542734 -0.671456  
H 0.287496 7.225215 -1.046786  
H 1.509544 7.008241 0.208884  
C 0.327450 4.990231 1.268757  
N -0.015717 3.686526 1.512408  
H 0.204719 3.302377 2.426549  
O 0.537211 5.836054 2.123495  
C 6.957839 -5.499495 -0.868791  
H 7.858486 -5.181098 -0.332768  
H 7.228505 -5.716872 -1.906173  
H 6.584124 -6.420722 -0.409264  
O 1.408234 -2.440436 -1.691864  
H 1.711158 -3.207487 -2.253823  
O 1.402360 1.577359 3.290421  
C 2.303299 1.751561 4.380241  
H 3.314476 1.981274 4.024026  
H 2.332877 0.857533 5.014710  
H 1.917969 2.594698 4.955520  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72963029  
Number of imaginary frequencies = 0

1a\_c04  
B3LYP/6-31G\* Geometry  
C 2.227265 6.467417 0.096565  
C 2.063412 4.173862 -0.870772  
O 3.607099 5.797046 -1.811367  
C 2.979400 4.605745 -1.927038  
C 3.620499 6.493645 -0.534561  
C 1.704142 5.056352 0.191871  
C 0.884970 4.630190 1.202569  
C 0.349408 3.307389 1.213899  
C 0.680693 2.414032 0.138510  
C 1.534674 2.868448 -0.914771  
C 0.113018 1.117098 0.206369

C -0.709427 0.723307 1.244218  
C -1.037040 1.611821 2.279127  
C -0.495550 2.889401 2.272468  
C -1.215063 -0.665614 0.943481  
C -0.122900 -1.125543 -0.055824  
O 0.305060 0.132258 -0.714604  
C -0.539512 -2.170116 -1.060765  
C -1.918810 -2.210810 -1.686920  
C -2.903318 -2.025021 -0.465874  
C -2.674607 -0.739305 0.402155  
C -3.214781 0.500797 -0.393361  
N -4.534604 0.301380 -0.642237  
C -5.176301 -0.937434 -0.155756  
C -4.420509 -2.115299 -0.811063  
O 3.213645 3.938968 -2.937927  
H 1.551226 7.065215 -0.531200  
H 2.255589 6.946269 1.081685  
H 3.875258 7.519482 -0.815324  
H 0.615824 5.308070 2.008832  
H -0.716659 3.598390 3.061401  
H -1.186478 -1.329252 1.814437  
H -2.673063 -2.852382 0.216712  
H -4.588853 -2.049969 -1.890112  
H -4.839683 -3.068970 -0.473999  
C 1.123357 -1.738851 0.562949  
C 3.417897 -3.202342 1.115036  
C 1.452131 -2.872963 -0.166070  
C 1.953489 -1.323776 1.595684  
C 3.102953 -2.072210 1.872094  
C 2.582097 -3.656589 0.060979  
H 1.729473 -0.436614 2.177994  
H 3.774916 -1.789390 2.675663  
N 0.399906 -3.106469 -1.149579  
O 0.444499 -4.122901 -1.907536  
O 4.527759 -3.899812 1.475681  
C 2.958992 -4.891347 -0.621848  
H 2.240753 -5.343397 -1.292037  
C 4.166476 -5.426161 -0.395895  
H 4.469110 -6.347160 -0.888381  
C 5.187430 -4.762793 0.498866  
C 6.157195 -3.898395 -0.324022  
H 5.612016 -3.119097 -0.865606  
H 6.688897 -4.513595 -1.058535  
H 6.893653 -3.423085 0.333407  
C 5.941826 -5.789608 1.346796  
H 5.241603 -6.386448 1.938833  
H 6.631836 -5.281878 2.028104  
H 6.519529 -6.462126 0.703682  
C -2.250732 -3.572759 -2.337992  
H -3.272342 -3.543659 -2.731261  
H -2.178796 -4.399111 -1.624791  
H -1.570823 -3.792368 -3.159891  
C -2.027159 -1.111816 -2.773946  
H -3.051694 -1.041358 -3.157714  
H -1.377693 -1.379416 -3.613885  
H -1.720545 -0.128184 -2.416617  
O -2.592062 1.490783 -0.754082  
C -5.450480 1.213384 -1.321534  
H -4.956102 1.667612 -2.184469  
H -5.760184 2.023131 -0.646589  
C -6.627252 0.289960 -1.682423  
H -6.436499 -0.191306 -2.648834  
H -7.571973 0.834730 -1.765523  
C -6.648446 -0.763215 -0.551804  
H -7.102417 -1.708089 -0.864741  
H -7.201782 -0.404154 0.321502  
C -4.915541 -0.940864 1.364498  
N -3.562788 -0.899667 1.578728  
H -3.236027 -0.536604 2.469403  
O -5.768452 -0.930456 2.237633  
C 4.727708 5.924943 0.349766  
H 4.842345 6.540719 1.249110  
H 5.677800 5.924035 -0.192578  
H 4.504613 4.899981 0.662657  
O 1.810923 2.029809 -1.910981  
H 2.380115 2.536325 -2.555951  
O -1.890677 1.120906 3.229945

C -2.288277 1.986286 4.289460  
H -2.800248 2.875157 3.902310  
H -1.425543 2.294077 4.892573  
H -2.977048 1.407404 4.906543  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72735943  
Number of imaginary frequencies = 0

1a\_c05

B3LYP/6-31G\* Geometry  
C -1.746622 6.497606 0.518420  
C -0.588284 4.570638 -0.581716  
O -0.649429 6.776887 -1.616504  
C -0.035330 5.549630 -1.557945  
C -1.886187 7.008344 -0.911739  
C -1.411067 5.027034 0.492504  
C -1.882781 4.164113 1.453647  
C -1.576895 2.779587 1.409663  
C -0.771010 2.301854 0.324130  
C -0.272748 3.208267 -0.667310  
C -0.508282 0.913948 0.324294  
C -0.953841 0.051094 1.294571  
C -1.752653 0.532064 2.349436  
C -2.051116 1.883542 2.408087  
C -0.540004 -1.348824 0.909536  
C 0.632604 -1.033647 -0.054274  
O 0.224216 0.278192 -0.652288  
C 0.925581 -2.061858 -1.114668  
C -0.145500 -2.900293 -1.783497  
C -1.072966 -3.374922 -0.596469  
C -1.666095 -2.231385 0.294639  
C -2.802270 -1.503901 -0.506845  
N -3.739487 -2.426933 -0.846427  
C -3.559465 -3.823064 -0.392650  
C -2.237798 -4.326941 -1.006962  
O 0.923144 5.365814 -2.271207  
H -2.669941 6.672994 1.081984  
H -0.947714 7.069991 1.012938  
H -2.680490 6.442230 -1.420015  
H -2.506213 4.539583 2.261307  
H -2.655181 2.289851 3.210803  
H -0.140293 -1.921424 1.753611  
H -0.412548 -3.930666 0.080609  
H -2.372264 -4.346716 -2.092082  
H -2.033730 -5.353680 -0.686215  
C 1.992643 -0.806739 0.581515  
C 4.706619 -0.603941 1.133242  
C 2.941448 -1.459053 -0.194797  
C 2.402601 -0.037880 1.662819  
C 3.771589 0.050280 1.938161  
C 4.315596 -1.405065 0.026746  
H 1.688102 0.492541 2.282656  
H 4.136086 0.632061 2.778173  
N 2.242005 -2.224483 -1.222866  
O 2.888718 -2.953520 -2.031825  
O 6.010905 -0.502707 1.494935  
C 5.363855 -2.104494 -0.710923  
H 5.068661 -2.851090 -1.435269  
C 6.647970 -1.808171 -0.469226  
H 7.446417 -2.316169 -1.004669  
C 7.060834 -0.728539 0.503331  
C 7.317038 0.599209 -0.228494  
H 6.416401 0.928418 -0.756034  
H 8.118687 0.481728 -0.966143  
H 7.610584 1.375441 0.486608  
C 8.277886 -1.153786 1.328265  
H 8.074920 -2.090221 1.856457  
H 8.521929 -0.382335 2.065287  
H 9.146034 -1.299660 0.676708  
C 0.418773 -4.173066 -2.455729  
H -0.408851 -4.760045 -2.866808  
H 0.967922 -4.801960 -1.748357  
H 1.100256 -3.922012 -3.266964  
C -0.864569 -2.054251 -2.865844  
H -1.717207 -2.597863 -3.288275  
H -0.163055 -1.854752 -3.682631  
H -1.220864 -1.095003 -2.487375  
O -2.876845 -0.314463 -0.785604

C -5.066557 -2.159927 -1.401847  
H -5.018693 -2.112447 -2.498045  
H -5.434320 -1.195359 -1.041532  
C -5.883266 -3.370661 -0.915244  
H -6.721969 -3.601261 -1.578288  
H -6.284370 -3.171987 0.084188  
C -4.851672 -4.516976 -0.833585  
H -4.706787 -4.980444 -1.816585  
H -5.140774 -5.290477 -0.118933  
C -3.407288 -3.722103 1.140226  
N -2.338345 -2.914313 1.425869  
H -2.318065 -2.455302 2.332559  
O -4.142915 -4.239673 1.965946  
C -2.168673 8.498736 -1.016420  
H -3.133123 8.737748 -0.554519  
H -2.198908 8.806329 -2.065935  
H -1.385362 9.074972 -0.512373  
O 0.480657 2.762362 -1.684878  
H 0.606210 1.797068 -1.601104  
O -2.175346 -0.414459 3.244601  
C -3.004757 0.006394 4.324146  
H -3.933967 0.456482 3.955137  
H -2.480199 0.723789 4.966552  
H -3.235413 -0.894854 4.893970  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72050880  
Number of imaginary frequencies = 0

1b\_c01

B3LYP/6-31G\* Geometry  
C -2.140076 -1.687548 0.061797  
C -2.379726 -0.241444 -2.173139  
C -0.844229 0.600297 -0.204595  
C -1.786721 0.875219 -1.345731  
C -1.199357 -0.617341 0.701462  
C -3.065046 -1.172332 -1.103538  
C -3.808377 -2.411037 -1.693321  
C -3.602083 -3.631413 -0.765026  
N -3.882494 -3.209607 0.625685  
C -3.157548 -2.191034 1.146441  
C -4.814673 -4.090157 1.325667  
C -4.773465 -5.364551 0.463513  
C -4.516621 -4.843343 -0.967412  
O 0.512008 0.304649 -0.731779  
C -1.263354 -0.937547 -2.992493  
C -3.469805 0.230370 -3.161346  
O -3.301406 -1.713279 2.264222  
N -1.401117 -2.863614 -0.426434  
C -2.098824 -3.967556 -0.817278  
O -1.613075 -5.036475 -1.157422  
H -1.729118 -0.270819 1.593489  
H -3.816863 -0.533852 -0.622511  
H -3.441952 -2.663368 -2.693189  
H -4.878946 -2.202302 -1.783354  
H -5.819913 -3.647337 1.351146  
H -4.486995 -4.235881 2.358701  
H -5.692040 -5.953040 0.542860  
H -3.935698 -5.997216 0.776069  
H -5.454772 -4.527995 -1.438975  
H -4.035588 -5.587994 -1.605278  
H -1.666334 -1.788636 -3.551659  
H -0.436448 -1.293076 -2.378811  
H -0.854733 -0.226598 -3.718027  
H -3.852350 -0.635866 -3.712148  
H -3.064081 0.941805 -3.881955  
H -4.304410 0.720890 -2.655075  
H -0.401564 -2.934124 -0.282265  
N -2.113028 2.162308 -1.365243  
O -2.871258 2.783540 -2.171562  
C -1.492357 2.861680 -0.243117  
C -0.172725 3.696649 2.013184  
C -1.605213 4.213369 0.076410  
C -0.771429 1.939004 0.501307  
C -0.100247 2.349171 1.644576  
C -0.897153 4.608674 1.242118  
H 0.474825 1.650213 2.243299  
H 0.330793 4.062441 2.901886  
C -2.395508 5.227131 -0.616457

H -3.081707 4.900517 -1.385899  
 C -2.254131 6.515968 -0.278521  
 H -2.834262 7.289954 -0.775227  
 C -1.253552 6.971222 0.758443  
 O -0.958979 5.889118 1.694379  
 C -1.823346 8.088050 1.636273  
 H -1.103979 8.359652 2.415252  
 H -2.751307 7.762461 2.115711  
 H -2.033749 8.976729 1.031629  
 C 0.065483 7.400247 0.094545  
 H 0.786768 7.720509 0.854634  
 H -0.107078 8.232191 -0.597370  
 H 0.496356 6.569893 -0.473613  
 C 0.194371 -1.110834 1.031987  
 C 1.094407 -0.555505 0.140559  
 C 1.990676 -2.334922 2.088172  
 C 2.482942 -0.861993 0.155812  
 C 0.640303 -2.015508 2.021693  
 C 2.917948 -1.778403 1.172097  
 C 3.440002 -0.318463 -0.756446  
 H 4.619411 -2.830515 2.007641  
 H 2.362890 -3.020739 2.839830  
 C 4.801711 -0.657190 -0.622391  
 C 5.213885 -1.586528 0.378624  
 C 4.300005 -2.123370 1.246308  
 O 3.009210 0.499221 -1.714597  
 H 3.807544 0.732897 -2.267032  
 O -0.323152 -2.512155 2.832457  
 C 0.045668 -3.434009 3.850180  
 H 0.748388 -2.981796 4.561090  
 H 0.491549 -4.341121 3.423233  
 H -0.882014 -3.686999 4.364817  
 C 5.774089 -0.063121 -1.541199  
 O 7.090904 -0.269060 -1.321158  
 C 7.527145 -0.760699 -0.024588  
 H 7.380117 0.057663 0.693754  
 C 6.676652 -1.955584 0.394935  
 H 6.982847 -2.298721 1.389469  
 H 6.865624 -2.782958 -0.305157  
 O 5.459005 0.615132 -2.521355  
 C 9.008258 -1.067788 -0.165987  
 H 9.549644 -0.183243 -0.513919  
 H 9.167313 -1.876046 -0.887618  
 H 9.424378 -1.373700 0.799957  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73580092  
 Number of imaginary frequencies = 0

1b\_c02

B3LYP/6-31G\* Geometry  
 C 0.131580 2.623780 0.055225  
 C 1.292875 1.815573 -2.213007  
 C 1.029278 0.150857 -0.188157  
 C 1.795966 0.661455 -1.378508  
 C 0.377453 1.233534 0.724769  
 C 1.069692 2.966533 -1.162216  
 C 0.576001 4.316445 -1.769130  
 C -0.454283 4.968477 -0.816912  
 N 0.105185 4.952507 0.553197  
 C 0.445933 3.758519 1.094337  
 C 0.063281 6.253780 1.215881  
 C -0.974175 7.018003 0.374052  
 C -0.803499 6.441623 -1.048909  
 O -0.101777 -0.697696 -0.642133  
 C 0.008110 1.392770 -2.970273  
 C 2.313891 2.319521 -3.257883  
 O 0.955757 3.594857 2.195005  
 N -1.263961 2.800223 -0.379905  
 C -1.678035 4.032139 -0.791106  
 O -2.822535 4.336950 -1.093733  
 H 1.029956 1.439153 1.578099  
 H 2.062401 3.141177 -0.728280  
 H 0.108593 4.171544 -2.748040  
 H 1.419617 4.999200 -1.909751  
 H 1.049988 6.736120 1.183511  
 H -0.214210 6.129379 2.266253  
 H -0.829060 8.101418 0.413476  
 H -1.983187 6.796234 0.738038

H 0.019482 6.941514 -1.572955  
 H -1.710557 6.533202 -1.650284  
 H -0.412539 2.238579 -3.524492  
 H -0.765012 0.994499 -2.314540  
 H 0.261334 0.612337 -3.695204  
 H 1.875517 3.159387 -3.807850  
 H 2.563050 1.534421 -3.972912  
 H 3.248877 2.649623 -2.799167  
 H -1.954223 2.084916 -0.188310  
 N 2.984047 0.071619 -1.440880  
 O 3.909041 0.224634 -2.296314  
 C 3.165839 -0.827868 -0.304568  
 C 3.051657 -2.317977 1.996273  
 C 4.281633 -1.611965 -0.018133  
 C 2.032118 -0.758451 0.492438  
 C 1.962377 -1.508205 1.657980  
 C 4.179035 -2.377043 1.173550  
 H 1.085624 -1.478278 2.296721  
 H 3.045123 -2.916543 2.901147  
 C 5.530682 -1.687239 -0.770788  
 H 5.686522 -0.977875 -1.572128  
 C 6.439188 -2.617318 -0.447197  
 H 7.378822 -2.691504 -0.989381  
 C 6.194951 -3.641912 0.636092  
 O 5.214135 -3.148320 1.599148  
 C 7.455186 -3.887791 1.469408  
 H 7.239086 -4.587119 2.283300  
 H 7.817239 -2.950158 1.901638  
 H 8.246994 -4.314937 0.844701  
 C 5.656451 -4.952337 0.037697  
 H 5.478356 -5.687189 0.830611  
 H 6.375541 -5.372499 -0.674426  
 H 4.717003 -4.773291 -0.494627  
 C -0.880761 0.499214 1.139938  
 C -1.089124 -0.562669 0.278430  
 C -2.929450 -0.038455 2.303571  
 C -2.229725 -1.407807 0.358701  
 C -1.808064 0.770965 2.170950  
 C -3.159154 -1.117979 1.414435  
 C -2.487146 -2.503180 -0.523710  
 H -5.004645 -1.727906 2.375922  
 H -3.653665 0.140594 3.089244  
 C -3.658677 -3.268988 -0.360255  
 C -4.556669 -2.985964 0.711394  
 C -4.315388 -1.940488 1.562691  
 O -1.606815 -2.759978 -1.488852  
 H -1.939441 -3.572774 -1.964553  
 O -1.513013 1.836044 2.952187  
 C -2.399987 2.178468 4.009286  
 H -2.484817 1.362301 4.737573  
 H -3.396912 2.431256 3.626825  
 H -1.957684 3.052071 4.489531  
 C -3.937998 -4.350364 -1.307499  
 O -5.131747 -4.979078 -1.258234  
 C -6.229302 -4.402711 -0.495550  
 H -6.906172 -5.250485 -0.358382  
 C -5.728787 -3.921823 0.867773  
 H -5.419732 -4.799112 1.453662  
 H -6.546868 -3.442574 1.416729  
 O -3.130924 -4.730614 -2.158950  
 C -6.926490 -3.330059 -1.328456  
 H -7.198823 -3.733470 -2.308116  
 H -6.283171 -2.457175 -1.477732  
 H -7.841066 -2.999235 -0.823400  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73378059  
 Number of imaginary frequencies = 0

1b\_c03  
 B3LYP/6-31G\* Geometry  
 C -2.128820 -1.689139 0.094797  
 C -2.386672 -0.248577 -2.142297  
 C -0.824083 0.588983 -0.191707  
 C -1.773027 0.866128 -1.327195  
 C -1.184470 -0.618161 0.725196  
 C -3.065610 -1.171095 -1.060341  
 C -3.819128 -2.408660 -1.636061  
 C -3.595008 -3.635397 -0.714441



N -3.854622 -3.220147 0.681730  
C -3.147927 -2.180098 1.182896  
C -4.942108 -3.953586 1.324238  
C -5.658168 -4.606340 0.127922  
C -4.539207 -4.824781 -0.914913  
O 0.525696 0.274265 -0.725937  
C -1.286535 -0.953797 -2.975837  
C -3.487686 0.228545 -3.115828  
O -3.324038 -1.660273 2.277433  
N -1.395660 -2.862919 -0.405144  
C -2.095672 -3.968757 -0.790433  
O -1.611788 -5.035525 -1.136785  
H -1.713119 -0.261239 1.613858  
H -3.806296 -0.525176 -0.571957  
H -3.469174 -2.662459 -2.641464  
H -4.891437 -2.200655 -1.710787  
H -5.569930 -3.267965 1.900597  
H -4.540639 -4.705587 2.016940  
H -6.417592 -3.921334 -0.267126  
H -6.163380 -5.536473 0.403126  
H -4.920100 -4.878514 -1.938907  
H -3.983549 -5.747952 -0.721672  
H -1.701252 -1.804678 -3.526740  
H -0.452200 -1.310840 -2.373254  
H -0.885716 -0.246761 -3.709564  
H -3.887163 -0.637075 -3.655436  
H -3.087203 0.932379 -3.846594  
H -4.309554 0.729380 -2.598711  
H -0.394238 -2.932683 -0.274467  
N -2.082160 2.157291 -1.355596  
O -2.837812 2.781566 -2.161990  
C -1.444789 2.857893 -0.243824  
C -0.100224 3.694814 1.996719  
C -1.538303 4.213571 0.064782  
C -0.730713 1.932195 0.503521  
C -0.046991 2.343493 1.638965  
C -0.817873 4.609571 1.222600  
H 0.523277 1.642438 2.239774  
H 0.413608 4.061539 2.879115  
C -2.319491 5.231614 -0.632148  
H -3.014331 4.907522 -1.394881  
C -2.159291 6.521330 -0.306201  
H -2.732045 7.298568 -0.806394  
C -1.147281 6.972440 0.721413  
O -0.860481 5.894462 1.664409  
C -1.698582 8.103166 1.593265  
H -0.971692 8.372114 2.366153  
H -2.627853 7.792840 2.080220  
H -1.901349 8.989459 0.982540  
C 0.173051 7.380095 0.046674  
H 0.902532 7.697401 0.800133  
H 0.006784 8.208647 -0.650844  
H 0.590542 6.540106 -0.517307  
C 0.206241 -1.117591 1.056107  
C 1.106086 -0.580743 0.153489  
C 1.994320 -2.350384 2.114532  
C 2.491479 -0.901081 0.164883  
C 0.646939 -2.018051 2.051370  
C 2.922293 -1.811877 1.188192  
C 3.449080 -0.377052 -0.758084  
H 4.617440 -2.873236 2.024949  
H 2.363544 -3.032989 2.870591  
C 4.807802 -0.728895 -0.628210  
C 5.215721 -1.652237 0.380067  
C 4.301156 -2.170351 1.258382  
O 3.021358 0.435409 -1.722092  
H 3.818876 0.654873 -2.281461  
O -0.319065 -2.497225 2.869791  
C 0.042762 -3.420125 3.889371  
H 0.752553 -2.973290 4.596666  
H 0.477439 -4.333074 3.463462  
H -0.885962 -3.661747 4.407505  
C 5.781033 -0.155145 -1.558953  
O 7.096809 -0.373662 -1.344946  
C 7.535767 -0.856790 -0.046104  
H 7.402978 -0.029294 0.664502  
C 6.674389 -2.037330 0.391489

H 6.982891 -2.373302 1.387757  
H 6.849625 -2.874231 -0.300812  
O 5.467424 0.516603 -2.544058  
C 9.012235 -1.182682 -0.193822  
H 9.561551 -0.308426 -0.555079  
H 9.156951 -2.000661 -0.907482  
H 9.431240 -1.482838 0.772682  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73602588  
Number of imaginary frequencies = 0

1b\_c04

B3LYP/6-31G\* Geometry  
C 0.714609 2.529312 0.089954  
C 1.671957 1.499861 -2.184379  
C 1.001007 -0.082047 -0.184025  
C 1.876207 0.246991 -1.364230  
C 0.618812 1.113354 0.740063  
C 1.721587 2.655458 -1.115056  
C 1.568301 4.093035 -1.698280  
C 0.704432 4.958000 -0.744033  
N 1.223597 4.790885 0.631203  
C 1.296273 3.539260 1.141283  
C 1.705642 6.030110 1.236253  
C 1.837771 6.966357 0.021379  
C 0.752945 6.473435 -0.961794  
O -0.296438 -0.632456 -0.653175  
C 0.331416 1.408485 -2.956547  
C 2.795365 1.757939 -3.212999  
O 1.800546 3.235282 2.214849  
N -0.593307 3.036022 -0.354640  
C -0.702801 4.337649 -0.748427  
O -1.739798 4.906648 -1.053449  
H 1.297060 1.148391 1.597638  
H 2.722313 2.578579 -0.671254  
H 1.088980 4.080089 -2.682110  
H 2.550738 4.559633 -1.824022  
H 2.645948 5.849720 1.765134  
H 0.976728 6.409626 1.964987  
H 2.833249 6.855060 -0.424092  
H 1.712824 8.018619 0.292042  
H 0.974929 6.731626 -2.001252  
H -0.229132 6.892530 -0.720584  
H 0.133385 2.336730 -3.503153  
H -0.522293 1.201383 -2.312614  
H 0.396047 0.598241 -3.690152  
H 2.576393 2.683323 -3.757130  
H 2.859676 0.943162 -3.935106  
H 3.776213 1.851788 -2.741098  
H -1.434511 2.501094 -0.178303  
N 2.890681 -0.607682 -1.428529  
O 3.832434 -0.668836 -2.277294  
C 2.845237 -1.538139 -0.303806  
C 2.363156 -2.986275 1.976534  
C 3.741221 -2.567664 -0.022168  
C 1.754147 -1.211582 0.488889  
C 1.499962 -1.936846 1.644241  
C 3.450711 -3.301178 1.158373  
H 0.651189 -1.706994 2.280116  
H 2.208232 -3.576795 2.873396  
C 4.943662 -2.926710 -0.768430  
H 5.270460 -2.264179 -1.558340  
C 5.604019 -4.048964 -0.453217  
H 6.504709 -4.335418 -0.990825  
C 5.115778 -5.000333 0.614096  
O 4.270472 -4.300759 1.578605  
C 6.275247 -5.546675 1.450729  
H 5.893601 -6.190024 2.249870  
H 6.841192 -4.726497 1.902385  
H 6.952398 -6.135896 0.823052  
C 4.288130 -6.139654 -0.004182  
H 3.937666 -6.821707 0.778365  
H 4.892391 -6.708691 -0.719590  
H 3.420437 -5.738099 -0.536908  
C -0.779623 0.694937 1.141241  
C -1.228273 -0.279305 0.268008  
C -2.898008 0.638071 2.301678  
C -2.533804 -0.837455 0.342486

C -1.619811 1.167275 2.173749  
C -3.369811 -0.352816 1.404768  
C -3.037157 -1.836363 -0.548296  
H -5.301323 -0.536883 2.372222  
H -3.561719 0.972433 3.090166  
C -4.349439 -2.322255 -0.380965  
C -5.155229 -1.853341 0.698744  
C -4.681602 -0.893524 1.553429  
O -2.243295 -2.273685 -1.523311  
H -2.752818 -2.986729 -2.002710  
O -1.086773 2.129874 2.962481  
C -1.873318 2.660530 4.021699  
H -2.145666 1.880580 4.743518  
H -2.783897 3.139272 3.640230  
H -1.242786 3.405156 4.508889  
C -4.866978 -3.310577 -1.329484  
O -6.167660 -3.667263 -1.268001  
C -7.107789 -2.869140 -0.495037  
H -7.949818 -3.551576 -0.350173  
C -6.503570 -2.508199 0.863115  
H -6.390455 -3.431018 1.449687  
H -7.192862 -1.860774 1.416375  
O -4.170534 -3.851434 -2.191797  
C -7.567045 -1.671572 -1.323022  
H -7.928704 -2.007186 -2.299379  
H -6.754043 -0.955668 -1.480521  
H -8.385159 -1.153097 -0.810258  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73432092  
Number of imaginary frequencies = 0

1b\_c05

B3LYP/6-31G\* Geometry

C -1.842342 -1.987621 0.070345  
C -2.283790 -0.623533 -2.184723  
C -0.905177 0.465224 -0.218735  
C -1.866051 0.580138 -1.372462  
C -1.105564 -0.769498 0.710162  
C -2.826650 -1.634870 -1.106245  
C -3.363720 -2.980267 -1.685746  
C -2.962499 -4.145705 -0.751867  
N -3.314227 -3.770690 0.636585  
C -2.769172 -2.646723 1.151994  
C -4.088310 -4.792507 1.339166  
C -3.838122 -6.044282 0.479041  
C -3.665879 -5.490975 -0.952756  
O 0.485928 0.343843 -0.714685  
C -1.072287 -1.151205 -2.995212  
C -3.429994 -0.334572 -3.179693  
O -2.995505 -2.189785 2.267510  
N -0.915609 -3.025958 -0.409242  
C -1.424054 -4.232005 -0.795490  
O -0.770595 -5.209482 -1.126425  
H -1.726225 -0.479992 1.561545  
H -3.671397 -1.114129 -0.637373  
H -2.963205 -3.177846 -2.684825  
H -4.454034 -2.946574 -1.773310  
H -5.152208 -4.519609 1.364429  
H -3.739126 -4.880538 2.371503  
H -4.649384 -6.773726 0.557029  
H -2.910014 -6.531842 0.795822  
H -4.641389 -5.333571 -1.427509  
H -3.067683 -6.148417 -1.587300  
H -1.330752 -2.074403 -3.524450  
H -0.195791 -1.343548 -2.378173  
H -0.792340 -0.404492 -3.745482  
H -3.671167 -1.254683 -3.723129  
H -3.136473 0.424966 -3.905145  
H -4.332549 0.025026 -2.679885  
H 0.076476 -2.951469 -0.221762  
N -2.377110 1.805390 -1.417075  
O -3.213157 2.294202 -2.237208  
C -1.872465 2.608818 -0.306890  
C -0.697301 3.673716 1.932288  
C -2.180407 3.936641 -0.017068  
C -1.030341 1.815308 0.458760  
C -0.429392 2.343421 1.592784  
C -1.543217 4.454945 1.141294

H 0.240985 1.749045 2.205103  
 H -0.254396 4.127609 2.812612  
 C -3.104174 4.810441 -0.734844  
 H -3.726977 4.372308 -1.502696  
 C -3.157602 6.111764 -0.420740  
 H -3.840842 6.781950 -0.936890  
 C -2.246927 6.731016 0.613483  
 O -1.790204 5.721837 1.566315  
 C -2.990021 7.756182 1.473469  
 H -2.326163 8.149928 2.249600  
 H -3.856687 7.294840 1.956315  
 H -3.336463 8.591531 0.855567  
 C -1.007289 7.353355 -0.050578  
 H -0.354099 7.798831 0.707862  
 H -1.303883 8.134309 -0.759701  
 H -0.443413 6.592881 -0.599758  
 C 0.333386 -1.042018 1.103774  
 C 1.165477 -0.399165 0.196265  
 C 2.267857 -2.021331 2.166181  
 C 2.579493 -0.529858 0.220515  
 C 0.892539 -1.873572 2.098423  
 C 3.127062 -1.373780 1.246641  
 C 3.466032 0.110214 -0.704500  
 H 4.940419 -2.206941 2.091176  
 H 2.685214 -2.669945 2.929757  
 C 4.857098 -0.064804 -0.570149  
 C 5.381006 -0.924982 0.441956  
 C 4.540003 -1.552189 1.321647  
 O 2.939628 0.858612 -1.671084  
 H 3.703408 1.175315 -2.231259  
 O 0.096476 -2.599265 2.946199  
 C -0.437091 -1.880529 4.064548  
 H -1.042007 -2.597276 4.621134  
 H -1.080291 -1.055523 3.745118  
 H 0.375256 -1.502753 4.699222  
 C 5.751155 0.626948 -1.502182  
 O 7.082643 0.582012 -1.284855  
 C 7.580312 0.160688 0.014877  
 H 7.343099 0.965705 0.724008  
 C 6.876891 -1.119751 0.453938  
 H 7.225162 -1.412465 1.450676  
 H 7.157910 -1.928304 -0.237188  
 O 5.354669 1.247765 -2.490608  
 C 9.086122 0.025262 -0.133096  
 H 9.520492 0.962697 -0.492368  
 H 9.333342 -0.766530 -0.848049  
 H 9.539176 -0.221468 0.833159  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72806310  
 Number of imaginary frequencies = 0

1b\_c06  
 B3LYP/6-31G\* Geometry  
 C 0.113402 2.614667 0.059398  
 C 1.229968 1.807690 -2.230721  
 C 0.999917 0.139438 -0.203230  
 C 1.743286 0.648193 -1.409479  
 C 0.383605 1.228598 0.724876  
 C 1.029561 2.957828 -1.173487  
 C 0.527609 4.310094 -1.768377  
 C -0.487933 4.958333 -0.799234  
 N 0.093818 4.941418 0.562777  
 C 0.437700 3.747835 1.095606  
 C 0.042023 6.238353 1.235493  
 C -1.009123 6.997582 0.406247  
 C -0.845332 6.430709 -1.021217  
 O -0.149374 -0.695395 -0.623259  
 C -0.068811 1.390264 -2.966991  
 C 2.234803 2.311303 -3.291316  
 O 0.959313 3.579634 2.192825  
 N -1.288959 2.784538 -0.355425  
 C -1.710375 4.020631 -0.751979  
 O -2.859887 4.327839 -1.028456  
 H 1.080345 1.439112 1.539889  
 H 2.030546 3.129365 -0.757567  
 H 0.045138 4.168770 -2.740387  
 H 1.369278 4.993014 -1.919357  
 H 1.023783 6.729925 1.199122

H -0.227927 6.102447 2.286213  
H -0.872760 8.081887 0.450670  
H -2.012803 6.764577 0.777310  
H -0.028383 6.937174 -1.548517  
H -1.757343 6.521074 -1.615135  
H -0.494470 2.237407 -3.515354  
H -0.833103 0.997007 -2.298117  
H 0.169952 0.608420 -3.695334  
H 1.790803 3.155806 -3.829411  
H 2.467151 1.528489 -4.014410  
H 3.179568 2.634771 -2.848156  
H -1.982567 2.091075 -0.104583  
N 2.927840 0.053932 -1.496884  
O 3.836111 0.205565 -2.370044  
C 3.129524 -0.848820 -0.366689  
C 3.056089 -2.347553 1.930314  
C 4.247691 -1.638467 -0.105835  
C 2.012727 -0.777121 0.453709  
C 1.963226 -1.532572 1.616702  
C 4.166887 -2.407151 1.085248  
H 1.098080 -1.505106 2.271353  
H 3.064724 -2.950849 2.832032  
C 5.479942 -1.717156 -0.885323  
H 5.621368 -1.006929 -1.688535  
C 6.391225 -2.651825 -0.583559  
H 7.318275 -2.728828 -1.146583  
C 6.167432 -3.677462 0.503008  
O 5.207402 -3.183307 1.487110  
C 7.444235 -3.926734 1.309615  
H 7.243537 -4.625962 2.127520  
H 7.817668 -2.990230 1.734548  
H 8.221630 -4.355543 0.668210  
C 5.614009 -4.985911 -0.085778  
H 5.452797 -5.722184 0.709386  
H 6.316615 -5.405399 -0.814523  
H 4.663190 -4.804643 -0.596736  
C -0.863099 0.503080 1.194334  
C -1.108508 -0.553715 0.326838  
C -2.929227 0.019404 2.346982  
C -2.264890 -1.372892 0.416427  
C -1.791157 0.797933 2.216698  
C -3.192942 -1.057364 1.467204  
C -2.549529 -2.467787 -0.462647  
H -5.056834 -1.609842 2.425702  
H -3.637991 0.259845 3.132944  
C -3.741342 -3.199361 -0.298398  
C -4.637569 -2.888262 0.768298  
C -4.371629 -1.846691 1.616079  
O -1.671488 -2.755441 -1.420654  
H -2.023921 -3.562170 -1.892921  
O -1.626973 1.888206 3.031306  
C -0.703184 1.720777 4.113414  
H 0.306294 1.501818 3.753555  
H -1.044842 0.924455 4.787596  
H -0.684447 2.674258 4.642508  
C -4.046109 -4.279255 -1.241583  
O -5.256787 -4.872633 -1.196470  
C -6.342568 -4.262638 -0.441974  
H -7.043195 -5.090945 -0.305688  
C -5.835743 -3.790906 0.922001  
H -5.554453 -4.674232 1.512800  
H -6.642627 -3.286596 1.464880  
O -3.244234 -4.687003 -2.084994  
C -7.004602 -3.174580 -1.283400  
H -7.282902 -3.574677 -2.262741  
H -6.336654 -2.320421 -1.433132  
H -7.912216 -2.816000 -0.784869  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72598605  
Number of imaginary frequencies = 0

1b\_c07  
B3LYP/6-31G\* Geometry  
C -2.004689 -1.822285 0.100022  
C -2.337096 -0.428889 -2.155442  
C -0.838316 0.526643 -0.207500  
C -1.792685 0.731395 -1.354429  
C -1.150842 -0.678656 0.727901

C -2.965702 -1.377410 -1.064716  
C -3.638365 -2.665707 -1.629408  
C -3.333190 -3.867245 -0.699282  
N -3.626058 -3.458952 0.693063  
C -2.988290 -2.376992 1.189160  
C -4.645019 -4.277156 1.346879  
C -5.316852 -4.985419 0.156981  
C -4.191444 -5.121817 -0.892686  
O 0.530666 0.267933 -0.713016  
C -1.191636 -1.075823 -2.975387  
C -3.460512 -0.031937 -3.139236  
O -3.195330 -1.865413 2.285039  
N -1.188610 -2.943646 -0.390818  
C -1.813704 -4.098669 -0.766074  
O -1.259216 -5.133912 -1.098894  
H -1.737457 -0.326982 1.580142  
H -3.747282 -0.771965 -0.588138  
H -3.273821 -2.903800 -2.633359  
H -4.722060 -2.528784 -1.703066  
H -5.320229 -3.643395 1.928707  
H -4.175319 -4.992516 2.034937  
H -6.128899 -4.361288 -0.234079  
H -5.747688 -5.950496 0.438060  
H -4.574313 -5.202927 -1.914108  
H -3.568924 -6.001906 -0.703094  
H -1.543398 -1.971335 -3.498423  
H -0.331577 -1.350343 -2.366191  
H -0.847965 -0.362642 -3.731904  
H -3.799816 -0.926192 -3.673488  
H -3.101843 0.690187 -3.873624  
H -4.316578 0.418815 -2.631335  
H -0.191893 -2.965264 -0.214631  
N -2.176036 2.002063 -1.404489  
O -2.963263 2.568464 -2.222993  
C -1.585012 2.756517 -0.302538  
C -0.294521 3.709890 1.923279  
C -1.754418 4.110627 -0.019961  
C -0.823529 1.885789 0.463743  
C -0.165746 2.357067 1.591474  
C -1.060186 4.568547 1.131029  
H 0.444231 1.702126 2.205165  
H 0.197432 4.121442 2.798363  
C -2.589940 5.069780 -0.737065  
H -3.263253 4.692478 -1.494500  
C -2.504538 6.372217 -0.434464  
H -3.119998 7.105822 -0.949551  
C -1.521580 6.899659 0.584726  
O -1.174705 5.857000 1.547840  
C -2.137308 8.012732 1.435878  
H -1.428223 8.335846 2.204566  
H -3.048610 7.659448 1.927534  
H -2.388401 8.875549 0.809717  
C -0.225691 7.369429 -0.096869  
H 0.482503 7.743885 0.650610  
H -0.438728 8.172629 -0.811071  
H 0.240996 6.544004 -0.643494  
C 0.257089 -1.087561 1.113906  
C 1.141801 -0.530772 0.199587  
C 2.092410 -2.249201 2.167791  
C 2.537024 -0.795065 0.219234  
C 0.737464 -1.969704 2.105575  
C 3.005820 -1.686192 1.244523  
C 3.476981 -0.241237 -0.708670  
H 4.735672 -2.685157 2.084434  
H 2.449078 -2.934829 2.929806  
C 4.845980 -0.544698 -0.577270  
C 5.289875 -1.449907 0.433764  
C 4.396112 -1.996201 1.315493  
O 3.020140 0.552783 -1.674185  
H 3.808834 0.797837 -2.235776  
O -0.123901 -2.615846 2.954075  
C -0.583275 -1.851263 4.075018  
H -1.269313 -2.500275 4.620437  
H -1.126626 -0.956113 3.758669  
H 0.260679 -1.571527 4.719220  
C 5.798475 0.061633 -1.510912  
O 7.120492 -0.106797 -1.296411

C 7.579264 -0.572481 0.002564  
H 7.418433 0.251003 0.711944  
C 6.761320 -1.782407 0.442935  
H 7.083034 -2.106026 1.439030  
H 6.965182 -2.613442 -0.248561  
O 5.459240 0.717388 -2.498102  
C 9.066023 -0.845756 -0.147931  
H 9.583586 0.047403 -0.509794  
H 9.238419 -1.658064 -0.861866  
H 9.496738 -1.131103 0.817896  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72809016  
Number of imaginary frequencies = 0

1b\_c08

B3LYP/6-31G\* Geometry

C 0.655160 2.535730 0.094805  
C 1.588596 1.536635 -2.201067  
C 0.969198 -0.070498 -0.203040  
C 1.819519 0.277949 -1.396589  
C 0.603978 1.115927 0.737830  
C 1.642109 2.684756 -1.122831  
C 1.461862 4.124625 -1.692448  
C 0.594885 4.967621 -0.722776  
N 1.135254 4.799732 0.644981  
C 1.225383 3.549597 1.147520  
C 1.574560 6.048090 1.264422  
C 1.683394 6.997339 0.057870  
C 0.611119 6.485749 -0.929728  
O -0.334335 -0.622877 -0.639881  
C 0.237500 1.434641 -2.953442  
C 2.692750 1.817596 -3.244602  
O 1.736817 3.246064 2.220789  
N -0.667436 3.017715 -0.333217  
C -0.802191 4.323038 -0.712187  
O -1.851426 4.878685 -0.995678  
H 1.324243 1.154805 1.558789  
H 2.650585 2.616657 -0.695273  
H 0.972812 4.112588 -2.671327  
H 2.435816 4.607150 -1.823826  
H 2.517165 5.892336 1.796749  
H 0.828849 6.396202 1.991391  
H 2.681512 6.914718 -0.387949  
H 1.531522 8.043590 0.337652  
H 0.828912 6.755591 -1.967109  
H -0.380456 6.880978 -0.687464  
H 0.017213 2.365704 -3.486525  
H -0.602642 1.208373 -2.298344  
H 0.303281 0.633667 -3.697120  
H 2.453369 2.744380 -3.777606  
H 2.756323 1.009863 -3.974631  
H 3.679525 1.920549 -2.787212  
H -1.500164 2.489131 -0.104739  
N 2.845419 -0.561408 -1.482646  
O 3.776031 -0.601206 -2.344636  
C 2.829950 -1.502442 -0.366213  
C 2.399124 -2.982965 1.903434  
C 3.743837 -2.522741 -0.108881  
C 1.746651 -1.198432 0.445804  
C 1.517487 -1.941610 1.595244  
C 3.480051 -3.273122 1.067364  
H 0.672384 -1.733529 2.243398  
H 2.263551 -3.587102 2.794351  
C 4.940333 -2.857140 -0.875788  
H 5.246148 -2.182013 -1.663322  
C 5.620923 -3.972954 -0.581212  
H 6.517717 -4.240950 -1.134641  
C 5.161859 -4.942471 0.482569  
O 4.318700 -4.265607 1.465455  
C 6.340727 -5.479047 1.298167  
H 5.979858 -6.136385 2.095553  
H 6.899986 -4.654762 1.750670  
H 7.018464 -6.051292 0.655596  
C 4.343633 -6.087975 -0.136486  
H 4.012558 -6.782181 0.643795  
H 4.947942 -6.641498 -0.863891  
H 3.464080 -5.694440 -0.655514  
C -0.775568 0.681113 1.191579

C -1.242932 -0.286288 0.311605  
 C -2.895875 0.641836 2.345294  
 C -2.548209 -0.838525 0.396925  
 C -1.618148 1.160810 2.217145  
 C -3.383814 -0.346859 1.457639  
 C -3.061837 -1.837249 -0.492489  
 H -5.314809 -0.511219 2.427893  
 H -3.535660 1.020845 3.135850  
 C -4.376854 -2.310783 -0.321781  
 C -5.180485 -1.833994 0.757478  
 C -4.699650 -0.876265 1.609646  
 O -2.271250 -2.285200 -1.464874  
 H -2.786546 -2.995758 -1.942189  
 O -1.221846 2.185505 3.037168  
 C -0.361784 1.816405 4.122093  
 H -0.148232 2.739119 4.662987  
 H 0.582127 1.395112 3.764277  
 H -0.867298 1.102194 4.785147  
 C -4.903391 -3.297884 -1.268816  
 O -6.206720 -3.640988 -1.208629  
 C -7.140802 -2.833740 -0.436550  
 H -7.988734 -3.508867 -0.292457  
 C -6.533773 -2.478417 0.921705  
 H -6.428109 -3.402476 1.507723  
 H -7.217531 -1.825633 1.475352  
 O -4.210086 -3.847609 -2.127836  
 C -7.588106 -1.632482 -1.265426  
 H -7.951715 -1.964956 -2.242127  
 H -6.768749 -0.923646 -1.421911  
 H -8.402063 -1.106719 -0.753578  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72633785  
 Number of imaginary frequencies = 0

1b\_c09

B3LYP/6-31G\* Geometry

C -2.454811 -1.226537 0.068707  
 C -2.436872 0.272506 -2.146348  
 C -0.727245 0.750899 -0.195866  
 C -1.600055 1.225550 -1.323816  
 C -1.313251 -0.375571 0.708647  
 C -3.274720 -0.517107 -1.072880  
 C -4.261151 -1.572006 -1.662570  
 C -4.286368 -2.825620 -0.756235  
 N -4.455196 -2.382458 0.645787  
 C -3.539140 -1.531034 1.163825  
 C -5.543623 -3.061279 1.345622  
 C -5.775093 -4.303057 0.466218  
 C -5.428859 -3.825221 -0.961290  
 O 0.535629 0.156424 -0.744151  
 C -1.513876 -0.622682 -3.012690  
 C -3.431146 0.982301 -3.092563  
 O -3.572530 -1.040441 2.284784  
 N -1.970281 -2.515995 -0.450339  
 C -2.881633 -3.454209 -0.839114  
 O -2.624210 -4.593672 -1.196460  
 H -1.758775 0.071476 1.602262  
 H -3.873874 0.252217 -0.569390  
 H -3.971106 -1.875185 -2.673306  
 H -5.269915 -1.152749 -1.726366  
 H -6.434319 -2.419361 1.389106  
 H -5.243868 -3.287579 2.372552  
 H -6.795121 -4.689206 0.548053  
 H -5.084936 -5.100751 0.761312  
 H -6.287625 -3.320654 -1.419154  
 H -5.113709 -4.643303 -1.612561  
 H -2.099822 -1.362488 -3.568005  
 H -0.761549 -1.154534 -2.431095  
 H -0.992330 0.002135 -3.745364  
 H -4.006201 0.226387 -3.638330  
 H -2.906817 1.603958 -3.819098  
 H -4.126814 1.629290 -2.552843  
 H -1.006260 -2.793247 -0.311911  
 N -1.626830 2.554800 -1.342648  
 O -2.232814 3.329387 -2.141621  
 C -0.849756 3.097266 -0.229955  
 C 0.652411 3.610657 2.007917  
 C -0.649810 4.438993 0.086344



C -0.346574 2.034758 0.508174  
 C 0.413409 2.281583 1.642991  
 C 0.144611 4.663731 1.242874  
 H 0.821841 1.471051 2.237726  
 H 1.236131 3.852610 2.889751  
 C -1.198724 5.604906 -0.599975  
 H -1.945997 5.442528 -1.364559  
 C -0.770949 6.828793 -0.262292  
 H -1.168010 7.712820 -0.755293  
 C 0.312276 7.052024 0.766391  
 O 0.382344 5.922420 1.691924  
 C -0.001326 8.255281 1.658858  
 H 0.765971 8.361891 2.432118  
 H -0.972769 8.128172 2.145858  
 H -0.024938 9.174224 1.063482  
 C 1.686073 7.198612 0.091629  
 H 2.464416 7.357645 0.845984  
 H 1.685605 8.051606 -0.596060  
 H 1.929847 6.299761 -0.483308  
 C -0.053291 -1.150753 1.038284  
 C 0.937314 -0.802511 0.150665  
 C 1.464490 -2.727791 2.064465  
 C 2.238859 -1.362859 0.145789  
 C 0.209738 -2.138481 2.021400  
 C 2.485409 -2.361058 1.144551  
 C 3.272502 -0.974681 -0.767496  
 H 3.977600 -3.706264 1.949412  
 H 1.695839 -3.484649 2.804723  
 C 4.528807 -1.591775 -0.693640  
 C 4.757400 -2.585087 0.305593  
 C 3.772938 -2.952976 1.193012  
 O 3.057382 -0.011827 -1.678071  
 H 2.152490 0.341785 -1.573863  
 O -0.826526 -2.429932 2.842555  
 C -0.641716 -3.415601 3.850621  
 H 0.151987 -3.124527 4.549803  
 H -0.401579 -4.392509 3.412433  
 H -1.593083 -3.473470 4.380665  
 C 5.606052 -1.258362 -1.667270  
 O 6.881874 -1.637772 -1.331082  
 C 7.171871 -2.145007 -0.012395  
 H 7.102315 -1.308125 0.698063  
 C 6.133804 -3.199747 0.355922  
 H 6.337694 -3.609413 1.351541  
 H 6.213778 -4.029560 -0.361759  
 O 5.442298 -0.715529 -2.734519  
 C 8.599769 -2.665683 -0.056199  
 H 9.282368 -1.874649 -0.380550  
 H 8.682753 -3.500689 -0.760114  
 H 8.910864 -3.010523 0.936193  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72609020  
 Number of imaginary frequencies = 0

1b\_c10  
 B3LYP/6-31G\* Geometry  
 C -2.309905 -1.455796 0.094180  
 C -2.433659 0.017559 -2.132503  
 C -0.759495 0.660372 -0.197411  
 C -1.674523 1.047606 -1.325928  
 C -1.241737 -0.505107 0.717673  
 C -3.198062 -0.823795 -1.042793  
 C -4.100217 -1.961778 -1.610581  
 C -4.003967 -3.212813 -0.698817  
 N -4.191203 -2.780088 0.703717  
 C -3.363583 -1.829844 1.196095  
 C -5.347714 -3.384905 1.360153  
 C -6.153317 -3.941658 0.172304  
 C -5.084241 -4.282567 -0.889367  
 O 0.550438 0.176507 -0.744254  
 C -1.443805 -0.809338 -2.992183  
 C -3.488008 0.629905 -3.081776  
 O -3.462760 -1.293321 2.292265  
 N -1.723735 -2.701195 -0.424980  
 C -2.554953 -3.717675 -0.800208  
 O -2.203589 -4.831862 -1.154435  
 H -1.719511 -0.089914 1.610162  
 H -3.848970 -0.097974 -0.539126

H -3.798571 -2.247236 -2.623084  
H -5.142196 -1.630411 -1.665036  
H -5.881289 -2.633622 1.949350  
H -5.026361 -4.182958 2.042903  
H -6.834086 -3.170325 -0.206417  
H -6.759253 -4.808231 0.451463  
H -5.484375 -4.284490 -1.907345  
H -4.637133 -5.265437 -0.709596  
H -1.968381 -1.600465 -3.538582  
H -0.649651 -1.272018 -2.407129  
H -0.976475 -0.151644 -3.732699  
H -4.003375 -0.178876 -3.611125  
H -3.019915 1.279208 -3.822638  
H -4.229728 1.227675 -2.546925  
H -0.738225 -2.895163 -0.296973  
N -1.821034 2.368883 -1.352500  
O -2.497985 3.080434 -2.153183  
C -1.093031 2.986254 -0.245775  
C 0.358011 3.646303 1.987271  
C -1.018107 4.342110 0.064521  
C -0.493119 1.978239 0.496414  
C 0.243342 2.299296 1.628096  
C -0.248317 4.644295 1.219935  
H 0.725841 1.532076 2.224840  
H 0.917751 3.945495 2.867071  
C -1.672594 5.448747 -0.627161  
H -2.396497 5.213930 -1.395408  
C -1.366399 6.708726 -0.290378  
H -1.843241 7.549334 -0.788631  
C -0.317031 7.039597 0.744325  
O -0.130328 5.920615 1.666374  
C -0.760207 8.199759 1.639206  
H -0.011802 8.383769 2.416381  
H -1.715000 7.968922 2.120923  
H -0.878101 9.113078 1.046392  
C 1.036327 7.333966 0.076542  
H 1.790157 7.570881 0.835352  
H 0.948825 8.185431 -0.607526  
H 1.376678 6.468674 -0.500832  
C 0.080334 -1.167936 1.045440  
C 1.035224 -0.740142 0.153919  
C 1.726337 -2.608364 2.073168  
C 2.379708 -1.187789 0.149069  
C 0.426503 -2.126873 2.030538  
C 2.711150 -2.158680 1.150361  
C 3.375593 -0.715462 -0.766502  
H 4.313135 -3.370546 1.955858  
H 2.022143 -3.340291 2.815497  
C 4.680423 -1.221604 -0.691445  
C 4.993218 -2.190106 0.309228  
C 4.044419 -2.638808 1.198321  
O 3.077240 0.221763 -1.680408  
H 2.144555 0.494422 -1.578048  
O -0.582287 -2.500973 2.852861  
C -0.317724 -3.469890 3.859764  
H 0.448573 -3.115378 4.560263  
H 0.002427 -4.422733 3.419908  
H -1.261507 -3.607165 4.388677  
C 5.725773 -0.796572 -1.664359  
O 7.029415 -1.065493 -1.327645  
C 7.361623 -1.547466 -0.009310  
H 7.221605 -0.719933 0.701731  
C 6.416528 -2.686295 0.358333  
H 6.654950 -3.078348 1.353367  
H 6.565232 -3.505628 -0.360469  
O 5.516836 -0.268420 -2.731058  
C 8.828572 -1.944958 -0.053787  
H 9.441238 -1.098402 -0.377658  
H 8.982026 -2.769243 -0.758421  
H 9.168228 -2.262741 0.938271  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72637720  
Number of imaginary frequencies = 0

1b\_c11  
B3LYP/6-31G\* Geometry  
C -0.057381 2.650286 0.051205  
C 1.168973 1.921143 -2.209465

C 0.999302 0.242121 -0.185968  
C 1.733120 0.794178 -1.375620  
C 0.263572 1.276090 0.720168  
C 0.870189 3.052308 -1.155837  
C 0.303562 4.374141 -1.760351  
C -0.771611 4.959951 -0.814823  
N -0.224699 4.970228 0.560579  
C 0.181670 3.796239 1.098576  
C -0.342392 6.266077 1.225480  
C -1.415308 6.973298 0.378435  
C -1.203643 6.411463 -1.044879  
O -0.091037 -0.676657 -0.648927  
C -0.082645 1.430983 -2.981029  
C 2.169625 2.487344 -3.241775  
O 0.693334 3.654337 2.201394  
N -1.456209 2.743842 -0.397698  
C -1.939021 3.954164 -0.802437  
O -3.097507 4.193920 -1.107641  
H 0.896196 1.519719 1.578932  
H 1.847503 3.282597 -0.713003  
H -0.145382 4.208960 -2.744762  
H 1.107126 5.105799 -1.889254  
H 0.616537 6.801723 1.199389  
H -0.618833 6.124551 2.273874  
H -1.330969 8.062924 0.421264  
H -2.412660 6.694804 0.735467  
H -0.408215 6.959381 -1.563405  
H -2.111221 6.452672 -1.651002  
H -0.548052 2.255895 -3.530351  
H -0.838906 0.985788 -2.335213  
H 0.220420 0.675108 -3.713335  
H 1.689760 3.303068 -3.792919  
H 2.470908 1.721605 -3.957539  
H 3.078807 2.869266 -2.771372  
H -2.108329 1.995302 -0.198757  
N 2.951274 0.265433 -1.438374  
O 3.863261 0.463422 -2.295395  
C 3.181324 -0.622769 -0.300511  
C 3.144871 -2.110657 2.004228  
C 4.336515 -1.345922 -0.013053  
C 2.045009 -0.611421 0.496907  
C 2.014375 -1.359967 1.665052  
C 4.274191 -2.112738 1.181517  
H 1.138082 -1.373962 2.304961  
H 3.169807 -2.706304 2.910556  
C 5.587316 -1.358023 -0.766090  
H 5.705510 -0.647100 -1.572399  
C 6.544652 -2.235973 -0.437936  
H 7.485504 -2.262687 -0.982313  
C 6.361778 -3.264638 0.652905  
O 5.346411 -2.826473 1.609023  
C 7.631673 -3.421506 1.492951  
H 7.457341 -4.126378 2.311983  
H 7.931018 -2.458900 1.918138  
H 8.451824 -3.802237 0.874997  
C 5.909250 -4.611605 0.065326  
H 5.777633 -5.348980 0.864703  
H 6.655166 -4.991313 -0.641801  
H 4.961262 -4.498571 -0.469871  
C -0.952011 0.469036 1.133387  
C -1.088601 -0.607818 0.289000  
C -2.970450 -0.213447 2.274961  
C -2.140386 -1.554279 0.363320  
C -1.912585 0.675825 2.156011  
C -3.105745 -1.324144 1.397169  
C -2.258521 -2.687556 -0.506649  
H -4.937917 -2.062967 2.281767  
H -3.720771 -0.081144 3.045422  
C -3.342698 -3.563022 -0.358017  
C -4.305699 -3.308619 0.664282  
C -4.190567 -2.230560 1.510452  
O -1.354498 -2.905029 -1.474951  
H -0.656975 -2.222286 -1.432089  
O -1.706303 1.763869 2.935266  
C -2.627442 2.036358 3.983921  
H -2.659884 1.212664 4.707815  
H -3.636025 2.216592 3.591030

H -2.255960 2.938088 4.472076  
C -3.487333 -4.762679 -1.230567  
O -4.718700 -5.368303 -1.263574  
C -5.862723 -4.784319 -0.602824  
H -6.552046 -5.627372 -0.491555  
C -5.447266 -4.285960 0.781478  
H -5.134601 -5.153880 1.379226  
H -6.299831 -3.829934 1.296799  
O -2.602491 -5.256229 -1.889838  
C -6.514448 -3.726411 -1.492223  
H -6.725320 -4.149906 -2.478735  
H -5.866044 -2.854430 -1.622280  
H -7.459728 -3.389361 -1.050903  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72399269  
Number of imaginary frequencies = 0

1b\_c12

B3LYP/6-31G\* Geometry  
C 0.689505 2.549581 0.084739  
C 1.660392 1.518856 -2.183118  
C 0.995382 -0.059776 -0.177205  
C 1.862391 0.265523 -1.361641  
C 0.594663 1.136323 0.739169  
C 1.702084 2.675648 -1.115150  
C 1.547755 4.112164 -1.700949  
C 0.678983 4.976782 -0.750966  
N 1.193219 4.812023 0.626639  
C 1.265627 3.561463 1.137885  
C 1.669110 6.053614 1.232744  
C 1.805199 6.988354 0.017225  
C 0.726083 6.492054 -0.970577  
O -0.316405 -0.615000 -0.645580  
C 0.324669 1.427066 -2.963715  
C 2.790124 1.776387 -3.204997  
O 1.766598 3.256355 2.212635  
N -0.617512 3.050691 -0.368209  
C -0.727654 4.355043 -0.757454  
O -1.765341 4.923576 -1.058366  
H 1.272157 1.176537 1.597528  
H 2.700838 2.601668 -0.666504  
H 1.071961 4.097201 -2.686421  
H 2.529696 4.580434 -1.823697  
H 2.607012 5.876093 1.766726  
H 0.935134 6.431699 1.956914  
H 2.803095 6.878821 -0.423174  
H 1.676436 8.040593 0.285872  
H 0.952751 6.749114 -2.009278  
H -0.257913 6.909622 -0.734816  
H 0.137973 2.348803 -3.524701  
H -0.536213 1.242138 -2.321998  
H 0.387406 0.607715 -3.687676  
H 2.577721 2.704998 -3.745784  
H 2.855496 0.965122 -3.930932  
H 3.768672 1.865172 -2.727249  
H -1.460409 2.524048 -0.174944  
N 2.872664 -0.596192 -1.429174  
O 3.805865 -0.665369 -2.283540  
C 2.829385 -1.523977 -0.300876  
C 2.351144 -2.959988 1.987717  
C 3.721658 -2.556245 -0.020712  
C 1.743728 -1.188704 0.496704  
C 1.491682 -1.907128 1.657015  
C 3.432677 -3.284437 1.164715  
H 0.648368 -1.669903 2.297373  
H 2.197780 -3.546372 2.887405  
C 4.918487 -2.924090 -0.771424  
H 5.244715 -2.268236 -1.567036  
C 5.575752 -4.047329 -0.453375  
H 6.471817 -4.340059 -0.995190  
C 5.092343 -4.991736 0.621685  
O 4.246606 -4.286548 1.583598  
C 6.255053 -5.528692 1.459876  
H 5.876449 -6.166367 2.264859  
H 6.820797 -4.704039 1.903532  
H 6.931415 -6.121774 0.835116  
C 4.265347 -6.136806 0.014109  
H 3.917807 -6.813080 0.802760

H 4.869539 -6.710510 -0.697502  
H 3.395805 -5.741808 -0.520436  
C -0.803679 0.719374 1.146759  
C -1.250449 -0.262813 0.294707  
C -2.936581 0.662535 2.281908  
C -2.534889 -0.856771 0.364790  
C -1.662262 1.198237 2.167984  
C -3.391687 -0.355339 1.398686  
C -2.979981 -1.902957 -0.508384  
H -5.363796 -0.519640 2.274958  
H -3.616248 1.008580 3.051731  
C -4.274249 -2.420666 -0.363528  
C -5.123044 -1.893629 0.655738  
C -4.696723 -0.899854 1.505570  
O -2.178021 -2.375156 -1.475861  
H -1.311292 -1.926296 -1.432226  
O -1.143414 2.174842 2.949986  
C -1.945559 2.708300 3.996323  
H -2.222743 1.930964 4.719062  
H -2.853943 3.179525 3.600477  
H -1.325219 3.459394 4.486611  
C -4.762008 -3.526584 -1.235507  
O -6.116947 -3.742883 -1.273392  
C -7.039904 -2.842473 -0.622182  
H -7.950035 -3.441355 -0.516098  
C -6.504635 -2.486883 0.765126  
H -6.469171 -3.406796 1.365879  
H -7.186147 -1.795837 1.273505  
O -4.058727 -4.261145 -1.888984  
C -7.338890 -1.640343 -1.516845  
H -7.660734 -1.983548 -2.504577  
H -6.457421 -1.004032 -1.642424  
H -8.142039 -1.034120 -1.081820  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72430248  
Number of imaginary frequencies = 0

1b\_c13

B3LYP/6-31G\* Geometry

C -2.277496 -1.513341 0.067815  
C -2.401526 -0.068419 -2.176000  
C -0.776654 0.640447 -0.222953  
C -1.683411 0.990969 -1.369944  
C -1.250315 -0.523327 0.697927  
C -3.161927 -0.918557 -1.089771  
C -4.027941 -2.084138 -1.660812  
C -3.916676 -3.316757 -0.733461  
N -4.139931 -2.871135 0.661272  
C -3.320186 -1.923753 1.166779  
C -5.127080 -3.675714 1.380074  
C -5.211033 -4.945014 0.513589  
C -4.937972 -4.442375 -0.920950  
O 0.550572 0.180487 -0.736009  
C -1.375853 -0.877828 -3.010294  
C -3.455909 0.505150 -3.149314  
O -3.401631 -1.430202 2.286696  
N -1.646807 -2.746890 -0.429371  
C -2.450418 -3.787140 -0.801632  
O -2.069199 -4.897539 -1.136268  
H -1.766110 -0.096858 1.562260  
H -3.841583 -0.206017 -0.605308  
H -3.705368 -2.370802 -2.666294  
H -5.076276 -1.777996 -1.730992  
H -6.089804 -3.149028 1.429092  
H -4.788066 -3.853577 2.404145  
H -6.175068 -5.452621 0.609019  
H -4.424957 -5.647948 0.809014  
H -5.853471 -4.043175 -1.373012  
H -4.537023 -5.224003 -1.569755  
H -1.871993 -1.683389 -3.562001  
H -0.583628 -1.320557 -2.407358  
H -0.909276 -0.213972 -3.745763  
H -3.940879 -0.322639 -3.677567  
H -2.992879 1.158099 -3.890228  
H -4.222056 1.089010 -2.633931  
H -0.669680 -2.932527 -0.239322  
N -1.867988 2.307233 -1.411078  
O -2.553561 2.991537 -2.227724

C -1.173870 2.956007 -0.300692  
 C 0.231159 3.680425 1.941972  
 C -1.140634 4.316732 -0.004534  
 C -0.555968 1.972965 0.460088  
 C 0.158374 2.326999 1.596272  
 C -0.393809 4.652718 1.156681  
 H 0.657636 1.580521 2.205558  
 H 0.773057 4.004982 2.823962  
 C -1.816530 5.397478 -0.716370  
 H -2.524729 5.134870 -1.490247  
 C -1.548090 6.668941 -0.390590  
 H -2.041234 7.490757 -0.904048  
 C -0.520157 7.039413 0.652252  
 O -0.316585 5.936287 1.590032  
 C -1.003316 8.198430 1.527627  
 H -0.268590 8.411039 2.310477  
 H -1.957309 7.949069 2.001578  
 H -1.137757 9.101024 0.922082  
 C 0.833192 7.360151 -0.003140  
 H 1.572142 7.623073 0.761713  
 H 0.732726 8.202425 -0.696702  
 H 1.201368 6.497900 -0.567859  
 C 0.080242 -1.149345 1.073489  
 C 1.040247 -0.712993 0.183874  
 C 1.738404 -2.580789 2.090948  
 C 2.388777 -1.143827 0.189013  
 C 0.436892 -2.116342 2.045983  
 C 2.729308 -2.119768 1.183486  
 C 3.386118 -0.657208 -0.721001  
 H 4.336788 -3.321694 1.991038  
 H 1.998030 -3.329929 2.832357  
 C 4.694609 -1.150073 -0.639621  
 C 5.014988 -2.121950 0.356620  
 C 4.066758 -2.587288 1.236866  
 O 3.084122 0.281684 -1.631499  
 H 2.145040 0.536159 -1.541443  
 O -0.507456 -2.652185 2.883128  
 C -0.816480 -1.873136 4.044969  
 H -1.574192 -2.435803 4.591629  
 H -1.232146 -0.897074 3.776875  
 H 0.077452 -1.744354 4.669037  
 C 5.741627 -0.707275 -1.604921  
 O 7.045732 -0.958380 -1.260291  
 C 7.376654 -1.446658 0.056624  
 H 7.221888 -0.626384 0.772909  
 C 6.444113 -2.600405 0.409297  
 H 6.681839 -2.997938 1.402232  
 H 6.606963 -3.411688 -0.315489  
 O 5.531037 -0.179176 -2.671142  
 C 8.848790 -1.824781 0.017325  
 H 9.452327 -0.967722 -0.295848  
 H 9.016938 -2.641133 -0.693118  
 H 9.186684 -2.146395 1.008709  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71832675  
 Number of imaginary frequencies = 0

1b\_c14

B3LYP/6-31G\* Geometry  
 C 0.018084 2.642196 0.053940  
 C 1.176931 1.872496 -2.227485  
 C 0.977384 0.194374 -0.204836  
 C 1.709480 0.719566 -1.407984  
 C 0.312282 1.261001 0.717278  
 C 0.940064 3.011907 -1.166439  
 C 0.414550 4.356086 -1.759032  
 C -0.625073 4.976294 -0.797238  
 N -0.057904 4.964328 0.571288  
 C 0.306408 3.775900 1.100658  
 C -0.143368 6.257140 1.249353  
 C -1.201743 6.998052 0.412904  
 C -1.011849 6.441842 -1.015546  
 O -0.162093 -0.672286 -0.634991  
 C -0.104998 1.432196 -2.979691  
 C 2.181753 2.403226 -3.274696  
 O 0.820456 3.609998 2.201823  
 N -1.382739 2.780638 -0.376862  
 C -1.827501 4.012453 -0.766088

O -2.981226 4.297274 -1.046036  
H 0.995027 1.485883 1.540799  
H 1.932622 3.203028 -0.739067  
H -0.054247 4.210519 -2.737121  
H 1.242598 5.058080 -1.897050  
H 0.828466 6.768574 1.224683  
H -0.420824 6.110801 2.296649  
H -1.088362 8.084653 0.463630  
H -2.204001 6.742571 0.772763  
H -0.201014 6.968227 -1.532598  
H -1.919861 6.515863 -1.617763  
H -0.543557 2.273436 -3.526378  
H -0.869761 1.022579 -2.320604  
H 0.157056 0.661916 -3.712780  
H 1.726872 3.243128 -3.810413  
H 2.435961 1.631091 -4.001828  
H 3.115545 2.742042 -2.819731  
H -2.065904 2.078746 -0.119913  
N 2.905745 0.145459 -1.493271  
O 3.809624 0.312338 -2.365119  
C 3.122343 -0.754457 -0.362156  
C 3.069470 -2.251675 1.936189  
C 4.254020 -1.522507 -0.098312  
C 2.001845 -0.702522 0.455780  
C 1.962608 -1.457068 1.619953  
C 4.183881 -2.291870 1.094185  
H 1.096328 -1.444231 2.273488  
H 3.086786 -2.853850 2.838384  
C 5.489416 -1.579439 -0.874382  
H 5.619392 -0.871176 -1.681171  
C 6.418922 -2.493722 -0.565946  
H 7.347790 -2.554168 -1.127874  
C 6.218477 -3.518206 0.525583  
O 5.234988 -3.047806 1.499918  
C 7.496158 -3.721739 1.343560  
H 7.310915 -4.421792 2.164326  
H 7.836884 -2.771356 1.765100  
H 8.291464 -4.130098 0.710965  
C 5.709327 -4.846732 -0.057418  
H 5.565231 -5.581457 0.742238  
H 6.429768 -5.250067 -0.777720  
H 4.757130 -4.699161 -0.576528  
C -0.920922 0.506680 1.180661  
C -1.130093 -0.560798 0.331446  
C -2.979817 -0.052464 2.313412  
C -2.232510 -1.444855 0.414270  
C -1.876152 0.771880 2.193583  
C -3.186595 -1.157988 1.446055  
C -2.420101 -2.572418 -0.454546  
H -5.058969 -1.781076 2.333376  
H -3.711499 0.167674 3.084397  
C -3.551590 -3.382880 -0.298636  
C -4.500128 -3.070312 0.722177  
C -4.323162 -1.997668 1.563521  
O -1.533355 -2.845385 -1.424434  
H -0.804184 -2.195755 -1.395482  
O -1.763487 1.877513 2.996573  
C -0.871480 1.744345 4.109883  
H -0.896045 2.702094 4.631086  
H 0.154702 1.550713 3.783450  
H -1.212251 0.944199 4.779734  
C -3.764054 -4.579111 -1.164215  
O -5.027879 -5.110688 -1.198420  
C -6.137865 -4.457153 -0.543378  
H -6.875375 -5.258122 -0.430629  
C -5.697073 -3.978748 0.840001  
H -5.437788 -4.861222 1.441983  
H -6.522398 -3.471076 1.351231  
O -2.905877 -5.128342 -1.814438  
C -6.723756 -3.367302 -1.439757  
H -6.959223 -3.783561 -2.423782  
H -6.024408 -2.536359 -1.575131  
H -7.647224 -2.971193 -1.001462  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71610484  
Number of imaginary frequencies = 0

1b\_c15

B3LYP/6-31G\* Geometry  
C -2.243666 -1.552348 0.096786  
C -2.400066 -0.118793 -2.152126  
C -0.759973 0.609469 -0.218278  
C -1.678134 0.948626 -1.359892  
C -1.220558 -0.551164 0.712867  
C -3.145397 -0.966124 -1.052493  
C -4.009035 -2.139716 -1.607395  
C -3.874725 -3.373543 -0.678807  
N -4.083058 -2.926525 0.717120  
C -3.281708 -1.954695 1.202515  
C -5.201872 -3.585155 1.387707  
C -5.991100 -4.181191 0.208469  
C -4.914950 -4.484837 -0.857444  
O 0.566486 0.153359 -0.737288  
C -1.378901 -0.927385 -2.992640  
C -3.467627 0.443898 -3.117409  
O -3.389309 -1.419375 2.301342  
N -1.609800 -2.780766 -0.406540  
C -2.408298 -3.830928 -0.766131  
O -2.020410 -4.938398 -1.099618  
H -1.735516 -0.121621 1.576310  
H -3.821159 -0.252996 -0.563471  
H -3.695322 -2.429204 -2.614951  
H -5.060929 -1.842617 -1.669100  
H -5.764602 -2.859074 1.981110  
H -4.833437 -4.365203 2.067032  
H -6.704726 -3.440323 -0.170720  
H -6.559032 -5.070194 0.496555  
H -5.320453 -4.507114 -1.873063  
H -4.428826 -5.448546 -0.675708  
H -1.875543 -1.740404 -3.532883  
H -0.576583 -1.360021 -2.395808  
H -0.925708 -0.265347 -3.738090  
H -3.953853 -0.389553 -3.635556  
H -3.016006 1.094827 -3.867073  
H -4.231267 1.026832 -2.597247  
H -0.629091 -2.958581 -0.227845  
N -1.870226 2.263629 -1.406862  
O -2.566680 2.939370 -2.221482  
C -1.170958 2.922502 -0.305809  
C 0.245753 3.667296 1.922665  
C -1.143980 4.284992 -0.017005  
C -0.541622 1.947185 0.455530  
C 0.178954 2.311670 1.584496  
C -0.391132 4.631596 1.137107  
H 0.687173 1.571563 2.194135  
H 0.791844 3.999742 2.799113  
C -1.831500 5.357899 -0.729637  
H -2.543180 5.087035 -1.497441  
C -1.568877 6.632669 -0.412089  
H -2.070461 7.448801 -0.926446  
C -0.536633 7.014949 0.622186  
O -0.319424 5.917736 1.563745  
C -1.022004 8.174797 1.495280  
H -0.283869 8.395828 2.272575  
H -1.971362 7.921305 1.976302  
H -1.166176 9.073684 0.886474  
C 0.810195 7.341780 -0.043557  
H 1.552407 7.612682 0.715321  
H 0.699660 8.180482 -0.739911  
H 1.180262 6.479559 -0.607088  
C 0.115529 -1.165610 1.084895  
C 1.067776 -0.729157 0.187381  
C 1.786697 -2.578289 2.105873  
C 2.419436 -1.149793 0.190878  
C 0.481687 -2.123693 2.061987  
C 2.770924 -2.115425 1.191832  
C 3.409799 -0.661766 -0.725880  
H 4.391278 -3.297040 2.003664  
H 2.054666 -3.320623 2.851141  
C 4.722831 -1.142117 -0.644158  
C 5.054476 -2.103408 0.358700  
C 4.112662 -2.570761 1.244758  
O 3.096721 0.267105 -1.642946  
H 2.155789 0.514284 -1.551788  
O -0.458002 -2.660727 2.903836



C -0.773495 -1.876461 4.060545  
H -1.522758 -2.444427 4.613406  
H -1.201685 -0.907464 3.786318  
H 0.120214 -1.732050 4.681441  
C 5.763429 -0.696828 -1.615197  
O 7.070609 -0.932717 -1.271450  
C 7.408786 -1.407695 0.048493  
H 7.247211 -0.583585 0.758857  
C 6.488252 -2.567852 0.411631  
H 6.731974 -2.955848 1.406872  
H 6.657439 -3.382688 -0.307686  
O 5.545499 -0.179098 -2.685019  
C 8.884567 -1.771356 0.009197  
H 9.478759 -0.910745 -0.312022  
H 9.059591 -2.591578 -0.695099  
H 9.227683 -2.081593 1.002405  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71845407  
Number of imaginary frequencies = 0

1b\_c16

B3LYP/6-31G\* Geometry

C 0.680991 2.545655 0.088775  
C 1.612715 1.526307 -2.198750  
C 0.963602 -0.064960 -0.196702  
C 1.814364 0.262691 -1.392694  
C 0.600771 1.129757 0.735867  
C 1.679018 2.674493 -1.121787  
C 1.527914 4.116487 -1.694858  
C 0.671439 4.976682 -0.731136  
N 1.200554 4.800415 0.640263  
C 1.262944 3.549908 1.144915  
C 1.658826 6.041871 1.260971  
C 1.792261 6.987237 0.053812  
C 0.717125 6.493936 -0.939853  
O -0.363711 -0.596874 -0.635217  
C 0.266032 1.451057 -2.962296  
C 2.730811 1.784104 -3.233424  
O 1.760459 3.235816 2.221654  
N -0.629999 3.048677 -0.350302  
C -0.737790 4.359137 -0.725502  
O -1.775440 4.935207 -1.007981  
H 1.317511 1.159140 1.560864  
H 2.683071 2.589254 -0.687048  
H 1.043831 4.111886 -2.676270  
H 2.511207 4.580732 -1.821806  
H 2.595191 5.869637 1.799101  
H 0.914916 6.403937 1.982775  
H 2.791605 6.886581 -0.385483  
H 1.657111 8.036277 0.331426  
H 0.946251 6.758237 -1.976192  
H -0.268485 6.907481 -0.704158  
H 0.076554 2.380269 -3.509768  
H -0.586773 1.263384 -2.310800  
H 0.315493 0.640022 -3.696604  
H 2.518418 2.719047 -3.763093  
H 2.779792 0.978998 -3.967402  
H 3.716461 1.861174 -2.768387  
H -1.474592 2.545547 -0.107486  
N 2.818181 -0.604996 -1.481280  
O 3.739864 -0.672092 -2.348005  
C 2.784212 -1.542919 -0.361373  
C 2.324596 -3.001865 1.916524  
C 3.672106 -2.585209 -0.104826  
C 1.712505 -1.207499 0.454763  
C 1.469197 -1.938736 1.609096  
C 3.393454 -3.324435 1.076235  
H 0.633976 -1.705139 2.261323  
H 2.177428 -3.598654 2.810395  
C 4.855673 -2.954021 -0.875789  
H 5.175472 -2.292584 -1.669332  
C 5.509233 -4.084960 -0.577995  
H 6.395473 -4.378361 -1.135375  
C 5.034777 -5.037180 0.494015  
O 4.204701 -4.337038 1.473495  
C 6.205318 -5.587957 1.312054  
H 5.833788 -6.231364 2.115757  
H 6.781122 -4.770500 1.756080

H 6.870493 -6.178578 0.673101  
 C 4.194039 -6.171960 -0.113827  
 H 3.852766 -6.853742 0.672790  
 H 4.786178 -6.742177 -0.838235  
 H 3.320053 -5.767403 -0.633795  
 C -0.788026 0.724208 1.191598  
 C -1.269493 -0.243076 0.333721  
 C -2.921866 0.721366 2.322214  
 C -2.565572 -0.806667 0.412986  
 C -1.640134 1.226835 2.205713  
 C -3.410917 -0.286126 1.448332  
 C -3.041906 -1.840582 -0.461820  
 H -5.381756 -0.400766 2.333521  
 H -3.570709 1.122452 3.094504  
 C -4.346060 -2.327547 -0.308541  
 C -5.180119 -1.782507 0.714569  
 C -4.728157 -0.798747 1.561855  
 O -2.257450 -2.330400 -1.434567  
 H -1.383633 -1.894431 -1.403132  
 O -1.239632 2.261300 3.011644  
 C -0.415774 1.895545 4.125544  
 H -0.199071 2.823390 4.656412  
 H 0.529077 1.450663 3.799218  
 H -0.951296 1.202189 4.786919  
 C -4.863685 -3.422571 -1.179295  
 O -6.222802 -3.603169 -1.216562  
 C -7.122552 -2.682784 -0.559555  
 H -8.045801 -3.260878 -0.452221  
 C -6.574338 -2.344452 0.827028  
 H -6.557957 -3.267012 1.424536  
 H -7.237731 -1.639597 1.340212  
 O -4.178712 -4.175592 -1.830976  
 C -7.396111 -1.471689 -1.449929  
 H -7.728872 -1.804466 -2.437597  
 H -6.500826 -0.855171 -1.576524  
 H -8.183636 -0.848355 -1.010677  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71641532  
 Number of imaginary frequencies = 0

1c\_c01

B3LYP/6-31G\* Geometry  
 C -2.091800 -1.766765 0.262719  
 C -2.208778 -0.653497 2.783580  
 C -0.451320 0.028425 0.955391  
 C -1.444292 0.408747 2.021521  
 C -0.635265 -1.424782 0.480777  
 C -2.814189 -1.678180 1.696999  
 C -4.333596 -1.593416 1.392243  
 C -4.590829 -2.156201 -0.035962  
 N -3.749410 -3.356851 -0.260415  
 C -2.400577 -3.241805 -0.121192  
 C -4.502893 -4.513594 -0.734655  
 C -5.790583 -3.866542 -1.275422  
 C -6.007324 -2.640419 -0.361802  
 O 0.987116 -0.040366 1.347297  
 C -3.337820 -0.110546 3.688659  
 C -1.237774 -1.405474 3.737907  
 O -1.591786 -4.155774 -0.194747  
 N -2.741796 -0.873055 -0.703970  
 C -4.057342 -1.083690 -1.003899  
 O -4.695223 -0.511883 -1.873808  
 H -0.388614 -2.037956 1.354452  
 H -2.638817 -2.663858 2.141999  
 H -4.703164 -0.564652 1.425330  
 H -4.904111 -2.167704 2.128821  
 H -4.712185 -5.207613 0.091768  
 H -3.923175 -5.055021 -1.487337  
 H -6.640222 -4.555449 -1.269420  
 H -5.631421 -3.530569 -2.305716  
 H -6.522859 -2.931770 0.560660  
 H -6.582608 -1.850439 -0.849771  
 H -3.840228 -0.960198 4.167038  
 H -4.075123 0.486559 3.156569  
 H -2.922091 0.524751 4.474019  
 H -1.762468 -2.232011 4.231719  
 H -0.884940 -0.717346 4.512902  
 H -0.352390 -1.811205 3.244396

H -2.183107 -0.291426 -1.316377  
 N -1.845840 1.664693 1.841336  
 O -2.686471 2.333217 2.514195  
 C -1.266702 2.218398 0.627309  
 C -0.112425 2.773229 -1.791843  
 C -1.455259 3.506357 0.130924  
 C -0.539278 1.217842 -0.009034  
 C 0.068750 1.504870 -1.228410  
 C -0.855254 3.752527 -1.131034  
 H 0.661341 0.766949 -1.754895  
 H 0.325148 3.021797 -2.753020  
 O -0.931690 4.974651 -1.717164  
 C -2.146767 4.614330 0.783549  
 H -2.445773 4.496091 1.815913  
 C -2.381717 5.739577 0.095405  
 H -2.885319 6.582854 0.561749  
 C -2.019501 5.884718 -1.364050  
 C -1.462960 7.278009 -1.667021  
 H -0.595250 7.489552 -1.035157  
 H -2.226763 8.040691 -1.481145  
 H -1.155873 7.341674 -2.715661  
 C -3.223428 5.555227 -2.261879  
 H -2.949598 5.659663 -3.317567  
 H -4.057588 6.232770 -2.047966  
 H -3.564823 4.530482 -2.085138  
 C 0.625512 -1.549969 -0.358242  
 C 1.557446 -0.790580 0.343296  
 C 2.364582 -2.307357 -1.841393  
 C 2.940100 -0.797312 0.036897  
 C 1.017294 -2.288060 -1.489233  
 C 3.331554 -1.597075 -1.091997  
 C 3.935837 -0.063336 0.756285  
 H 4.993483 -2.222525 -2.337385  
 H 2.698333 -2.858091 -2.713150  
 C 5.286881 -0.155876 0.368599  
 C 5.655085 -0.932536 -0.772577  
 C 4.707912 -1.631193 -1.470906  
 O 0.026344 -2.891561 -2.186461  
 C 0.374237 -3.832037 -3.192858  
 H -0.566465 -4.280300 -3.515213  
 H 1.032359 -4.612466 -2.793246  
 H 0.859816 -3.345115 -4.048696  
 O 3.548789 0.681999 1.789615  
 H 4.367038 1.145193 2.125155  
 C 6.296525 0.569301 1.140005  
 C 7.111903 -0.904753 -1.163631  
 H 7.314950 -0.036485 -1.808177  
 H 7.381625 -1.800439 -1.734338  
 C 7.989953 -0.798348 0.079509  
 H 7.829227 -1.681939 0.712503  
 O 7.603395 0.361916 0.864404  
 O 6.024511 1.375514 2.032587  
 C 9.471074 -0.633385 -0.216230  
 H 10.035290 -0.514562 0.713367  
 H 9.643025 0.250303 -0.839955  
 H 9.850938 -1.514389 -0.744830  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.69107263  
 Number of imaginary frequencies = 0

1c\_c02

B3LYP/6-31G\* Geometry  
 C -2.194958 -1.651875 0.230144  
 C -2.296383 -0.542688 2.754567  
 C -0.433899 -0.001113 0.983985  
 C -1.422136 0.454799 2.024476  
 C -0.722725 -1.431195 0.494240  
 C -2.950038 -1.510603 1.643123  
 C -4.448044 -1.302602 1.294884  
 C -4.707607 -1.838822 -0.143285  
 N -3.958614 -3.102498 -0.349278  
 C -2.609471 -3.095799 -0.171508  
 C -4.786080 -4.191042 -0.861034  
 C -6.000034 -3.438510 -1.434070  
 C -6.147494 -2.207144 -0.513782  
 O 0.980787 -0.189311 1.419810  
 C -3.405421 0.090550 3.625211  
 C -1.423904 -1.377039 3.735129

O -1.874228 -4.070963 -0.228617  
N -2.742481 -0.705763 -0.749659  
C -4.061336 -0.809295 -1.089019  
O -4.625462 -0.184875 -1.973638  
H -0.555537 -2.065490 1.371714  
H -2.868059 -2.508777 2.087073  
H -4.734396 -0.247437 1.322097  
H -5.084370 -1.830725 2.011857  
H -5.075570 -4.874271 -0.050044  
H -4.227100 -4.769481 -1.601798  
H -6.901638 -4.057236 -1.462650  
H -5.781671 -3.106835 -2.454877  
H -6.709832 -2.465760 0.390880  
H -6.645121 -1.370338 -1.008933  
H -3.993235 -0.715013 4.082132  
H -4.072333 0.748699 3.072084  
H -2.964545 0.686869 4.427169  
H -2.033140 -2.157102 4.206726  
H -1.039121 -0.724038 4.525193  
H -0.560740 -1.855967 3.268236  
H -2.121573 -0.166209 -1.340293  
N -1.706821 1.742554 1.847151  
O -2.502489 2.477258 2.505519  
C -1.051751 2.251475 0.651999  
C 0.195172 2.717263 -1.739495  
C -1.121886 3.552420 0.159088  
C -0.396242 1.196100 0.026046  
C 0.259949 1.436471 -1.178449  
C -0.478068 3.752462 -1.089551  
H 0.800825 0.654405 -1.697062  
H 0.671232 2.931676 -2.690590  
O -0.442969 4.978412 -1.671493  
C -1.731471 4.711901 0.803902  
H -2.057160 4.616406 1.830494  
C -1.860372 5.854357 0.116101  
H -2.300020 6.735670 0.576715  
C -1.462916 5.970584 -1.336924  
C -0.794489 7.315842 -1.629818  
H 0.076770 7.458923 -0.983791  
H -1.498906 8.136243 -1.455697  
H -0.466436 7.354632 -2.673294  
C -2.673268 5.734774 -2.255461  
H -2.374455 5.817676 -3.306300  
H -3.456076 6.474751 -2.054736  
H -3.095825 4.739488 -2.085888  
C 0.550312 -1.659806 -0.303879  
C 1.519069 -0.986368 0.434734  
C 2.270427 -2.573397 -1.719491  
C 2.906217 -1.117008 0.181418  
C 0.917490 -2.430550 -1.421413  
C 3.267498 -1.955912 -0.928653  
C 3.935663 -0.480334 0.945430  
H 4.917152 -2.792499 -2.062056  
H 2.587612 -3.158512 -2.574798  
C 5.285236 -0.667839 0.589297  
C 5.628204 -1.528384 -0.497856  
C 4.650362 -2.139784 -1.234590  
O -0.095663 -2.942746 -2.158659  
C 0.205298 -3.913280 -3.151527  
H 0.770729 -3.475354 -3.984517  
H -0.758577 -4.271725 -3.515187  
H 0.769343 -4.751502 -2.725946  
O 3.578055 0.273432 1.983113  
H 4.425633 0.592620 2.404036  
C 6.323494 0.027671 1.351101  
C 7.100184 -1.757548 -0.731150  
H 7.292713 -2.077006 -1.761386  
H 7.452270 -2.565428 -0.073976  
C 7.906841 -0.496047 -0.419060  
H 8.969612 -0.746802 -0.359163  
O 7.604224 -0.025668 0.924385  
O 6.096627 0.665841 2.382080  
C 7.713815 0.642581 -1.417739  
H 8.269295 1.526512 -1.090842  
H 6.657861 0.912683 -1.519033  
H 8.087290 0.343562 -2.403783  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68922716

Number of imaginary frequencies = 0

1c\_c03

B3LYP/6-31G\* Geometry

C -2.101925 -1.741768 0.160523  
C -2.251577 -0.683056 2.702852  
C -0.462341 0.028266 0.913934  
C -1.468435 0.390178 1.974461  
C -0.647626 -1.412797 0.407612  
C -2.839336 -1.691348 1.588985  
C -4.354825 -1.613957 1.267710  
C -4.593958 -2.124366 -0.187225  
N -3.748186 -3.314599 -0.445790  
C -2.406665 -3.209967 -0.248150  
C -4.509806 -4.527595 -0.732167  
C -5.933076 -4.145277 -0.286352  
C -6.006461 -2.618671 -0.509875  
O 0.971369 -0.055523 1.321920  
C -3.395774 -0.150427 3.594524  
C -1.300387 -1.454632 3.661355  
O -1.604885 -4.133467 -0.268090  
N -2.740927 -0.819806 -0.785029  
C -4.054166 -1.018398 -1.107373  
O -4.680836 -0.416657 -1.963927  
H -0.418591 -2.044892 1.272677  
H -2.656411 -2.684077 2.014791  
H -4.737974 -0.591614 1.330893  
H -4.929975 -2.219375 1.976199  
H -4.084983 -5.376535 -0.188112  
H -4.469961 -4.761347 -1.804534  
H -6.063684 -4.380236 0.776685  
H -6.702910 -4.688938 -0.841320  
H -6.763329 -2.134033 0.113564  
H -6.233250 -2.376107 -1.553110  
H -3.913666 -1.006042 4.044956  
H -4.117813 0.461953 3.058573  
H -2.993095 0.466738 4.400771  
H -1.836411 -2.287420 4.131990  
H -0.958001 -0.781289 4.453839  
H -0.408665 -1.855530 3.175023  
H -2.177340 -0.210892 -1.365569  
N -1.856865 1.653714 1.819194  
O -2.699743 2.313790 2.497396  
C -1.258521 2.230448 0.625280  
C -0.072717 2.829399 -1.768231  
C -1.431562 3.530525 0.155557  
C -0.531088 1.238871 -0.024971  
C 0.092898 1.547699 -1.230860  
C -0.815758 3.799511 -1.094158  
H 0.685593 0.816570 -1.766699  
H 0.377080 3.095662 -2.718959  
O -0.877188 5.034530 -1.654347  
C -2.121355 4.629586 0.824881  
H -2.431442 4.491763 1.851542  
C -2.340822 5.771091 0.158698  
H -2.842364 6.608292 0.638018  
C -1.963275 5.943805 -1.293856  
C -1.395583 7.339473 -1.563078  
H -0.532741 7.532644 -0.918792  
H -2.156514 8.102951 -1.368890  
H -1.078084 7.422544 -2.607237  
C -3.160119 5.639565 -2.209862  
H -2.875335 5.763449 -3.260543  
H -3.992362 6.317710 -1.990506  
H -3.509213 4.613569 -2.057002  
C 0.623359 -1.532315 -0.414707  
C 1.550388 -0.791575 0.312231  
C 2.377441 -2.288629 -1.879892  
C 2.937310 -0.805594 0.025343  
C 1.025735 -2.263620 -1.546093  
C 3.338499 -1.594106 -1.108226  
C 3.928724 -0.090398 0.769132  
H 5.013293 -2.217899 -2.337064  
H 2.720045 -2.833563 -2.751875  
C 5.284629 -0.190644 0.400739  
C 5.662869 -0.955287 -0.745217  
C 4.719988 -1.635402 -1.467193

O 0.039763 -2.857483 -2.258668  
C 0.394882 -3.786950 -3.272911  
H 0.892459 -3.291331 -4.116762  
H -0.544102 -4.226624 -3.611602  
H 1.045034 -4.575232 -2.875610  
O 3.532790 0.645202 1.806109  
H 4.350037 1.096113 2.160257  
C 6.289285 0.513748 1.197436  
C 7.125752 -0.936550 -1.113544  
H 7.347234 -0.061308 -1.742412  
H 7.395462 -1.826764 -1.692750  
C 7.985171 -0.856729 0.144498  
H 7.805092 -1.747275 0.762342  
O 7.598193 0.296545 0.939462  
O 6.011465 1.310673 2.096550  
C 9.472448 -0.703630 -0.125564  
H 10.022984 -0.603378 0.814364  
H 9.663650 0.186378 -0.734501  
H 9.851339 -1.581533 -0.659994  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.69150631  
Number of imaginary frequencies = 0

1c\_c04

B3LYP/6-31G\* Geometry  
C -2.203931 -1.621728 0.131468  
C -2.339218 -0.567017 2.677352  
C -0.441162 -0.005871 0.948597  
C -1.443112 0.436971 1.982077  
C -0.734839 -1.422960 0.426698  
C -2.978516 -1.512538 1.537030  
C -4.470181 -1.298161 1.170402  
C -4.708371 -1.779809 -0.294473  
N -3.964780 -3.039856 -0.533356  
C -2.625173 -3.055232 -0.297826  
C -4.821741 -4.176224 -0.862163  
C -6.220429 -3.671560 -0.461299  
C -6.148132 -2.142332 -0.666780  
O 0.965547 -0.213511 1.400831  
C -3.460258 0.059568 3.537088  
C -1.491362 -1.425180 3.658647  
O -1.907539 -4.045610 -0.303740  
N -2.729005 -0.642807 -0.826661  
C -4.043813 -0.723101 -1.190500  
O -4.587576 -0.065142 -2.062340  
H -0.590585 -2.076159 1.294362  
H -2.898717 -2.519786 1.960511  
H -4.762748 -0.245943 1.228484  
H -5.118382 -1.852276 1.857368  
H -4.494967 -5.065573 -0.315031  
H -4.764641 -4.401490 -1.935589  
H -6.410166 -3.904774 0.593133  
H -7.015217 -4.137734 -1.050495  
H -6.878073 -1.597807 -0.060901  
H -6.318244 -1.868809 -1.713069  
H -4.067233 -0.749376 3.961684  
H -4.107005 0.737837 2.984191  
H -3.031338 0.632539 4.362246  
H -2.115656 -2.206656 4.107780  
H -1.113102 -0.788704 4.465165  
H -0.625681 -1.905265 3.197467  
H -2.096292 -0.083555 -1.385554  
N -1.713753 1.730718 1.826550  
O -2.512749 2.459102 2.487808  
C -1.036456 2.257808 0.651892  
C 0.249189 2.758933 -1.712157  
C -1.090291 3.568153 0.182280  
C -0.379449 1.209678 0.015432  
C 0.296480 1.467432 -1.174408  
C -0.426646 3.786568 -1.052940  
H 0.838650 0.690655 -1.699614  
H 0.740564 2.987601 -2.652066  
O -0.375159 5.022769 -1.611500  
C -1.702132 4.719830 0.838828  
H -2.043008 4.608327 1.858853  
C -1.814746 5.874883 0.169418  
H -2.255886 6.750627 0.639126  
C -1.395918 6.013668 -1.275597

C -0.717744 7.360616 -1.536349  
 H 0.144445 7.489385 -0.875292  
 H -1.421361 8.181035 -1.359159  
 H -0.374071 7.415159 -2.574077  
 C -2.593661 5.798466 -2.215544  
 H -2.279156 5.898296 -3.260311  
 H -3.376522 6.538046 -2.013560  
 H -3.022697 4.802219 -2.069532  
 C 0.548237 -1.651098 -0.353429  
 C 1.511479 -0.998365 0.409999  
 C 2.279851 -2.566248 -1.753391  
 C 2.900951 -1.137834 0.174199  
 C 0.924297 -2.416205 -1.471582  
 C 3.270570 -1.965100 -0.941990  
 C 3.924942 -0.520545 0.961035  
 H 4.928961 -2.799447 -2.064261  
 H 2.604376 -3.145968 -2.609618  
 C 5.277748 -0.714296 0.620786  
 C 5.628563 -1.562441 -0.473542  
 C 4.656021 -2.155825 -1.231699  
 O -0.084127 -2.918184 -2.222316  
 C 0.222878 -3.876970 -3.224873  
 H 0.798726 -3.430341 -4.046000  
 H -0.738758 -4.226334 -3.602899  
 H 0.779266 -4.722998 -2.804615  
 O 3.559178 0.221888 2.004031  
 H 4.403436 0.527934 2.441060  
 C 6.311016 -0.038016 1.406271  
 C 7.101749 -1.800295 -0.690298  
 H 7.305576 -2.106644 -1.722345  
 H 7.438403 -2.620372 -0.040177  
 C 7.914291 -0.550085 -0.349267  
 H 8.974052 -0.810553 -0.278435  
 O 7.597055 -0.096266 0.996475  
 O 6.075211 0.587693 2.442871  
 C 7.744506 0.604094 -1.334215  
 H 8.303227 1.478405 -0.987569  
 H 6.692404 0.884943 -1.445715  
 H 8.128520 0.315483 -2.319309  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68962418  
 Number of imaginary frequencies = 0

1c\_c05

B3LYP/6-31G\* Geometry  
 C -2.134332 -1.739361 0.270389  
 C -2.239363 -0.606523 2.782572  
 C -0.459602 0.019559 0.957918  
 C -1.438475 0.429806 2.021510  
 C -0.669198 -1.435533 0.492197  
 C -2.862598 -1.622947 1.698720  
 C -4.377896 -1.504708 1.383830  
 C -4.639579 -2.070927 -0.042169  
 N -3.825692 -3.293025 -0.253217  
 C -2.475890 -3.209690 -0.104061  
 C -4.604227 -4.434884 -0.724353  
 C -5.872279 -3.760461 -1.277727  
 C -6.065302 -2.523493 -0.373443  
 O 0.988581 -0.100655 1.358489  
 C -3.360781 -0.023668 3.672254  
 C -1.299948 -1.379514 3.751540  
 O -1.687238 -4.141826 -0.161615  
 N -2.755451 -0.834673 -0.704801  
 C -4.073774 -1.019837 -1.014848  
 O -4.689320 -0.442872 -1.896668  
 H -0.442396 -2.048114 1.371330  
 H -2.713668 -2.609195 2.151770  
 H -4.724306 -0.467678 1.408457  
 H -4.965629 -2.061136 2.120478  
 H -4.835032 -5.117583 0.105634  
 H -4.033103 -4.995184 -1.469655  
 H -6.738279 -4.428576 -1.272680  
 H -5.698524 -3.435368 -2.309111  
 H -6.592540 -2.796642 0.547907  
 H -6.619202 -1.723543 -0.869787  
 H -3.894768 -0.854511 4.149090  
 H -4.073864 0.592049 3.128154  
 H -2.935130 0.602914 4.459234

H -1.855908 -2.180819 4.252229  
H -0.927107 -0.695680 4.521099  
H -0.428229 -1.825095 3.267412  
H -2.177919 -0.285360 -1.329530  
N -1.795120 1.700632 1.839670  
O -2.609017 2.397407 2.512537  
C -1.195830 2.233075 0.624715  
C -0.023119 2.739570 -1.795988  
C -1.342186 3.524301 0.124202  
C -0.500690 1.206481 -0.007762  
C 0.116590 1.467929 -1.228472  
C -0.734052 3.745543 -1.139674  
H 0.683865 0.709335 -1.753304  
H 0.423265 2.970108 -2.757465  
O -0.771858 4.964024 -1.732065  
C -1.996618 4.656927 0.772291  
H -2.302317 4.553102 1.804178  
C -2.190028 5.788170 0.081071  
H -2.664801 6.649146 0.545149  
C -1.819892 5.920500 -1.377129  
C -1.203186 7.288824 -1.676976  
H -0.327178 7.461170 -1.044793  
H -1.933132 8.083568 -1.489737  
H -0.893613 7.340774 -2.725436  
C -3.035508 5.643563 -2.276717  
H -2.755755 5.737457 -3.331743  
H -3.839890 6.356266 -2.063288  
H -3.420853 4.634183 -2.101721  
C 0.586879 -1.603885 -0.349415  
C 1.537508 -0.864606 0.331356  
C 2.322698 -2.411686 -1.812445  
C 2.915261 -0.859824 0.023828  
C 0.975026 -2.364985 -1.473279  
C 3.302229 -1.693240 -1.077761  
C 3.891953 -0.075949 0.723357  
H 4.990281 -2.391776 -2.239955  
H 2.653893 -2.988435 -2.668274  
C 5.239982 -0.159768 0.353514  
C 5.613569 -1.019444 -0.725697  
C 4.679280 -1.751890 -1.417948  
O -0.023284 -2.960628 -2.167232  
C 0.316060 -3.906878 -3.171275  
H 0.818878 -3.428224 -4.021746  
H -0.629796 -4.337303 -3.502648  
H 0.956080 -4.699512 -2.766110  
O 3.526361 0.716568 1.743586  
H 2.554882 0.684906 1.848451  
C 6.274324 0.672543 1.028296  
C 7.081387 -1.087910 -1.066717  
H 7.361254 -0.266596 -1.743143  
H 7.315098 -2.027030 -1.580747  
C 7.903676 -0.956534 0.210744  
H 7.632652 -1.770884 0.898670  
O 7.583102 0.295842 0.850031  
O 6.059295 1.662384 1.687811  
C 9.407532 -0.952269 -0.014034  
H 9.932480 -0.798209 0.933415  
H 9.691457 -0.145986 -0.698820  
H 9.732108 -1.907307 -0.442004  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68191644  
Number of imaginary frequencies = 0

1c\_c06  
B3LYP/6-31G\* Geometry  
C -2.250026 -1.602058 0.231272  
C -2.338875 -0.475475 2.748349  
C -0.445584 -0.007953 0.990893  
C -1.418112 0.485359 2.024871  
C -0.772426 -1.434319 0.506585  
C -3.014136 -1.424878 1.634517  
C -4.499551 -1.165676 1.268112  
C -4.762952 -1.705800 -0.168118  
N -4.055398 -2.996111 -0.356487  
C -2.709174 -3.034323 -0.163680  
C -4.914779 -4.060476 -0.867673  
C -6.096582 -3.271861 -1.458728  
C -6.210855 -2.028013 -0.550480



O 0.969549 -0.262624 1.441426  
C -3.433545 0.205878 3.600497  
C -1.511936 -1.337472 3.744253  
O -2.005320 -4.032854 -0.203180  
N -2.753107 -0.642866 -0.759782  
C -4.071267 -0.709375 -1.116686  
O -4.600924 -0.079388 -2.017790  
H -0.635165 -2.068612 1.388889  
H -2.973114 -2.422623 2.084822  
H -4.746715 -0.100390 1.282107  
H -5.162464 -1.662953 1.982920  
H -5.234389 -4.726323 -0.053745  
H -4.368659 -4.663470 -1.598263  
H -7.018564 -3.859480 -1.490580  
H -5.857647 -2.957031 -2.480229  
H -6.790950 -2.258965 0.350423  
H -6.674672 -1.179231 -1.057909  
H -4.059074 -0.573061 4.052817  
H -4.067498 0.885966 3.034848  
H -2.981174 0.788675 4.405904  
H -2.158648 -2.085460 4.217530  
H -1.105513 -0.695477 4.532595  
H -0.668398 -1.860900 3.288830  
H -2.107341 -0.147624 -1.362625  
N -1.646220 1.785504 1.844681  
O -2.411107 2.552144 2.498994  
C -0.961752 2.266109 0.653159  
C 0.325804 2.674617 -1.727098  
C -0.973950 3.567627 0.158375  
C -0.345549 1.182585 0.033907  
C 0.330917 1.392599 -1.165255  
C -0.309614 3.738584 -1.085000  
H 0.842235 0.588147 -1.679520  
H 0.820127 2.867421 -2.673364  
O -0.217451 4.958696 -1.668406  
C -1.542196 4.752329 0.794763  
H -1.886346 4.672793 1.816610  
C -1.612149 5.898921 0.105329  
H -2.020555 6.797753 0.560685  
C -1.189509 6.001460 -1.341070  
C -0.448663 7.311809 -1.617496  
H 0.417846 7.409213 -0.956796  
H -1.113625 8.166238 -1.452533  
H -0.101646 7.336591 -2.655184  
C -2.397235 5.831788 -2.277242  
H -2.079467 5.905111 -3.323098  
H -3.144116 6.609657 -2.083179  
H -2.872576 4.858528 -2.119812  
C 0.492732 -1.716316 -0.289731  
C 1.482662 -1.075566 0.433731  
C 2.198982 -2.686792 -1.686691  
C 2.865919 -1.212313 0.187656  
C 0.849585 -2.508933 -1.401992  
C 3.213162 -2.075886 -0.903659  
C 3.886842 -0.545553 0.944176  
H 4.870199 -2.911268 -2.020058  
H 2.507186 -3.290204 -2.532601  
C 5.234153 -0.770197 0.635721  
C 5.563453 -1.643079 -0.447029  
C 4.590563 -2.262211 -1.194064  
O -0.173004 -3.001101 -2.140342  
C 0.112379 -3.976808 -3.133005  
H 0.695506 -3.550772 -3.959897  
H -0.856786 -4.311002 -3.505512  
H 0.652767 -4.828991 -2.704386  
O 3.558149 0.302684 1.931765  
H 2.585109 0.382413 1.981768  
C 6.320045 -0.128347 1.427962  
C 7.029236 -1.856202 -0.725194  
H 7.185118 -2.206994 -1.751455  
H 7.426680 -2.631190 -0.054494  
C 7.809766 -0.565433 -0.477023  
H 8.882661 -0.782583 -0.494826  
O 7.577968 -0.117723 0.876112  
O 6.187634 0.360083 2.525880  
C 7.516191 0.557838 -1.470708  
H 8.068549 1.458389 -1.186070

H 6.449543 0.801566 -1.498569  
H 7.828863 0.263996 -2.479654  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67966405  
Number of imaginary frequencies = 0

1c\_c07

B3LYP/6-31G\* Geometry  
C -2.146079 -1.712084 0.169780  
C -2.284144 -0.632665 2.703465  
C -0.469747 0.018303 0.918885  
C -1.462147 0.412592 1.976316  
C -0.683078 -1.424583 0.421528  
C -2.891067 -1.631522 1.591952  
C -4.402029 -1.516625 1.259676  
C -4.644542 -2.030377 -0.193409  
N -3.829223 -3.244827 -0.437561  
C -2.487096 -3.174832 -0.230483  
C -4.621499 -4.438310 -0.724788  
C -6.037312 -4.015343 -0.292133  
C -6.067592 -2.488329 -0.523396  
O 0.972576 -0.119426 1.335914  
C -3.419889 -0.057593 3.579552  
C -1.367343 -1.426894 3.676730  
O -1.708589 -4.117841 -0.235528  
N -2.752413 -0.777440 -0.784572  
C -4.068089 -0.947300 -1.118338  
O -4.669155 -0.339319 -1.988042  
H -0.476037 -2.056255 1.292091  
H -2.737749 -2.625602 2.025985  
H -4.759619 -0.484580 1.314372  
H -4.996928 -2.102824 1.967881  
H -4.224084 -5.295709 -0.173486  
H -4.579128 -4.677474 -1.795735  
H -6.183074 -4.241873 0.770733  
H -6.817037 -4.540343 -0.851105  
H -6.815320 -1.980301 0.092383  
H -6.280594 -2.244891 -1.569293  
H -3.971265 -0.893158 4.027414  
H -4.115483 0.574899 3.031789  
H -3.007053 0.549796 4.388067  
H -1.937145 -2.232394 4.154627  
H -1.003438 -0.758068 4.463569  
H -0.490541 -1.870630 3.199811  
H -2.167089 -0.203252 -1.378887  
N -1.804235 1.690746 1.818075  
O -2.620543 2.380320 2.495284  
C -1.183825 2.244139 0.623218  
C 0.023763 2.790683 -1.771807  
C -1.313041 3.546730 0.147992  
C -0.488940 1.225330 -0.021964  
C 0.145989 1.506483 -1.229139  
C -0.687210 3.788745 -1.103498  
H 0.713060 0.753636 -1.762468  
H 0.483798 3.037316 -2.722787  
O -0.707944 5.019407 -1.670936  
C -1.965705 4.671548 0.811275  
H -2.283836 4.549758 1.837434  
C -2.142001 5.817977 0.140752  
H -2.614608 6.673645 0.616690  
C -1.754572 5.975435 -1.310467  
C -1.126437 7.345217 -1.577802  
H -0.256721 7.500406 -0.932609  
H -1.853749 8.140819 -1.384067  
H -0.804562 7.414763 -2.621519  
C -2.961347 5.722480 -2.228834  
H -2.669031 5.834714 -3.278654  
H -3.764103 6.435704 -2.011076  
H -3.354469 4.712287 -2.077440  
C 0.583265 -1.589486 -0.403203  
C 1.529879 -0.869890 0.303163  
C 2.332368 -2.396931 -1.849732  
C 2.912027 -0.873909 0.015527  
C 0.980774 -2.343577 -1.528167  
C 3.307022 -1.695290 -1.092411  
C 3.885878 -0.110020 0.740568  
H 5.004994 -2.391671 -2.241327  
H 2.671218 -2.967476 -2.706740

C 5.238186 -0.200646 0.388304  
C 5.619059 -1.047242 -0.698645  
C 4.688118 -1.761093 -1.414386  
O -0.013362 -2.928125 -2.237536  
C 0.331871 -3.863983 -3.249470  
H 0.846265 -3.377421 -4.088437  
H -0.612592 -4.285282 -3.596093  
H 0.963634 -4.664654 -2.847114  
O 3.513207 0.670303 1.767708  
H 2.540240 0.645286 1.859716  
C 6.270412 0.611656 1.090061  
C 7.090635 -1.123204 -1.021162  
H 7.386176 -0.293958 -1.681063  
H 7.323292 -2.056247 -1.546612  
C 7.897024 -1.018591 0.268837  
H 7.610410 -1.841349 0.940278  
O 7.578226 0.226257 0.923549  
O 6.054995 1.592791 1.762355  
C 9.403685 -1.023557 0.063800  
H 9.917359 -0.888867 1.020339  
H 9.703376 -0.209142 -0.604415  
H 9.725899 -1.974552 -0.374855  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68231209  
Number of imaginary frequencies = 0

1c\_c08

B3LYP/6-31G\* Geometry

C -2.270086 -1.563384 0.131061  
C -2.390488 -0.484708 2.667565  
C -0.458031 -0.011715 0.952722  
C -1.443329 0.476124 1.977593  
C -0.796063 -1.424336 0.438113  
C -3.054705 -1.410593 1.526562  
C -4.531183 -1.136899 1.140538  
C -4.773563 -1.625940 -0.321455  
N -4.078278 -2.917172 -0.539394  
C -2.743194 -2.983498 -0.289125  
C -4.977045 -4.022572 -0.864106  
C -6.357736 -3.457929 -0.481998  
C -6.223032 -1.935405 -0.704468  
O 0.945953 -0.292747 1.421870  
C -3.493588 0.196970 3.508342  
C -1.592904 -1.371586 3.665364  
O -2.063599 -3.999919 -0.276308  
N -2.744169 -0.571339 -0.840322  
C -4.057263 -0.608191 -1.222428  
O -4.561710 0.056661 -2.111757  
H -0.686373 -2.075997 1.311591  
H -3.022267 -2.416977 1.958078  
H -4.777970 -0.072236 1.182274  
H -5.210099 -1.653492 1.826813  
H -4.690785 -4.917865 -0.304203  
H -4.918833 -4.261699 -1.934318  
H -6.565953 -3.670748 0.573226  
H -7.165240 -3.898959 -1.073109  
H -6.936696 -1.355205 -0.112522  
H -6.371598 -1.667957 -1.755577  
H -4.141525 -0.580977 3.929610  
H -4.103529 0.898627 2.942576  
H -3.051160 0.755969 4.335866  
H -2.257632 -2.116831 4.117698  
H -1.190663 -0.746127 4.468987  
H -0.749501 -1.900546 3.216079  
H -2.083234 -0.058831 -1.411330  
N -1.650322 1.782436 1.816888  
O -2.416368 2.547775 2.471342  
C -0.937180 2.275067 0.647219  
C 0.403106 2.707872 -1.699719  
C -0.920731 3.585472 0.176494  
C -0.324843 1.194146 0.019490  
C 0.377572 1.415643 -1.162454  
C -0.228275 3.769436 -1.049620  
H 0.886131 0.612731 -1.681861  
H 0.918883 2.910770 -2.632313  
O -0.104272 4.998493 -1.607517  
C -1.486432 4.766294 0.822249  
H -1.857556 4.671847 1.833329

C -1.522420 5.927220 0.154565  
H -1.929599 6.822536 0.617907  
C -1.061091 6.054414 -1.277779  
C -0.284816 7.354332 -1.502797  
H 0.565451 7.417314 -0.817249  
H -0.935440 8.219263 -1.335337  
H 0.090714 7.395573 -2.530015  
C -2.247750 5.935410 -2.248014  
H -1.901262 6.027289 -3.283191  
H -2.982036 6.725085 -2.053519  
H -2.748457 4.969682 -2.127349  
C 0.478423 -1.713716 -0.338515  
C 1.464666 -1.097102 0.409954  
C 2.192572 -2.695491 -1.717197  
C 2.849667 -1.249218 0.183204  
C 0.841491 -2.504007 -1.450065  
C 3.202252 -2.104030 -0.913390  
C 3.867309 -0.604617 0.962892  
H 4.865419 -2.945637 -2.015956  
H 2.506079 -3.296067 -2.563183  
C 5.216223 -0.841047 0.670552  
C 5.550732 -1.704385 -0.418185  
C 4.581468 -2.303125 -1.186322  
O -0.177727 -2.982251 -2.202178  
C 0.110269 -3.949723 -3.202333  
H 0.706267 -3.519574 -4.017810  
H -0.857567 -4.271331 -3.588974  
H 0.638784 -4.811019 -2.777070  
O 3.534386 0.234517 1.956858  
H 2.561691 0.324466 1.994864  
C 6.297974 -0.221678 1.485919  
C 7.017772 -1.931644 -0.678083  
H 7.184294 -2.271720 -1.706284  
H 7.396237 -2.719575 -0.011501  
C 7.809999 -0.653608 -0.402708  
H 8.880360 -0.883580 -0.407645  
O 7.563819 -0.219596 0.952376  
O 6.155479 0.255355 2.587595  
C 7.544669 0.485178 -1.386687  
H 8.102819 1.375671 -1.082395  
H 6.481453 0.741684 -1.428052  
H 7.869600 0.200087 -2.394277  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68004741  
Number of imaginary frequencies = 0

1d\_c01

B3LYP/6-31G\* Geometry  
C 2.213890 -1.797718 0.241140  
C 2.358282 -0.617256 2.715962  
C 0.503140 -0.025466 0.915352  
C 1.525111 0.392012 1.940252  
C 0.745410 -1.478099 0.474808  
C 2.863552 -1.769136 1.698575  
C 4.392420 -1.982947 1.528870  
C 4.678532 -2.414398 0.073518  
N 4.284401 -1.272055 -0.783377  
C 2.972628 -0.918227 -0.790382  
C 5.286526 -0.926005 -1.792595  
C 6.237652 -2.137131 -1.758951  
C 6.140768 -2.657140 -0.308259  
O -0.924342 -0.182313 1.370885  
C 1.460442 -1.276472 3.801950  
C 3.549951 0.012310 3.469558  
O 2.464892 -0.100536 -1.545884  
N 2.433849 -3.188052 -0.201525  
C 3.739395 -3.576139 -0.353909  
O 4.107895 -4.647790 -0.810524  
H 0.554398 -2.034541 1.403277  
H 2.474913 -2.700165 2.120996  
H 4.761742 -2.733198 2.236978  
H 4.960724 -1.065381 1.694281  
H 5.799694 0.003829 -1.514200  
H 4.800953 -0.763803 -2.759185  
H 7.258972 -1.872390 -2.047462  
H 5.880325 -2.912385 -2.444622  
H 6.796272 -2.081911 0.356434  
H 6.395284 -3.715839 -0.224995

H 2.020911 -2.054111 4.335308  
 H 0.553177 -1.729534 3.392430  
 H 1.146687 -0.522423 4.531099  
 H 4.113346 -0.786941 3.965363  
 H 3.195907 0.707165 4.232477  
 H 4.224932 0.572759 2.822454  
 H 1.711625 -3.635854 -0.760056  
 N 1.823017 1.679200 1.770426  
 O 2.641045 2.395311 2.419176  
 C 1.130028 2.218432 0.609107  
 C -0.243350 2.753101 -1.693446  
 C 1.181035 3.534345 0.148477  
 C 0.442600 1.186305 -0.011702  
 C -0.277558 1.459151 -1.168811  
 C 0.471314 3.768472 -1.054562  
 H -0.827263 0.684659 -1.688794  
 H -0.767796 2.995172 -2.612019  
 C 1.824003 4.676464 0.791600  
 H 2.194855 4.557508 1.800462  
 C 1.924899 5.835201 0.126151  
 H 2.386078 6.705834 0.586198  
 C 1.459361 5.980000 -1.304756  
 O 0.405735 5.014249 -1.599002  
 C 2.619017 5.735447 -2.285313  
 H 2.271178 5.841193 -3.319023  
 H 3.026473 4.728453 -2.151649  
 H 3.426378 6.455869 -2.111714  
 C 0.805100 7.342271 -1.546657  
 H 0.426521 7.402555 -2.571945  
 H 1.533288 8.146638 -1.396488  
 H -0.030531 7.492656 -0.856605  
 C -0.540548 -1.743905 -0.280232  
 C -1.485800 -0.998520 0.422830  
 C -2.300675 -2.751686 -1.581905  
 C -2.876672 -1.096209 0.169735  
 C -0.949793 -2.648092 -1.271855  
 C -3.270421 -2.000765 -0.875212  
 C -3.882877 -0.360898 0.875362  
 H -4.945500 -2.832393 -1.973327  
 H -2.643452 -3.421905 -2.360981  
 C -5.235370 -0.500966 0.507881  
 C -5.609840 -1.417148 -0.521751  
 C -4.656022 -2.135758 -1.190482  
 O -3.501084 0.437864 1.868646  
 H -4.335401 0.823750 2.258166  
 O 0.038884 -3.383337 -1.867607  
 C -0.315324 -4.285120 -2.913354  
 H -0.770845 -3.749460 -3.754113  
 H -1.002743 -5.060036 -2.553826  
 H 0.619280 -4.745962 -3.236138  
 C -6.247155 0.284477 1.216957  
 O -7.521948 0.263475 0.769757  
 C -7.798479 -0.232553 -0.568422  
 H -7.402322 0.510871 -1.273877  
 C -7.087309 -1.563744 -0.789517  
 H -7.266998 -1.915685 -1.811527  
 H -7.523554 -2.309920 -0.108731  
 O -6.005060 0.964334 2.216377  
 C -9.311355 -0.305997 -0.686880  
 H -9.758583 0.668340 -0.469640  
 H -9.718318 -1.037801 0.018998  
 H -9.596651 -0.602269 -1.702056  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68898951  
 Number of imaginary frequencies = 0

1d\_c02  
 B3LYP/6-31G\* Geometry  
 C 2.003238 -1.920660 0.255680  
 C 2.142239 -0.778220 2.749257  
 C 0.437026 0.000898 0.874545  
 C 1.446806 0.312152 1.947809  
 C 0.562698 -1.463591 0.424369  
 C 2.581158 -1.966392 1.742489  
 C 4.088086 -2.327750 1.644010  
 C 4.400915 -2.773889 0.198963  
 N 4.161913 -1.592413 -0.662769  
 C 2.892475 -1.111612 -0.728223

C 5.241282 -1.341316 -1.619762  
C 6.067354 -2.639600 -1.553024  
C 5.849251 -3.156224 -0.114358  
O -1.019214 -0.027818 1.263015  
C 1.135323 -1.355996 3.784676  
C 3.352095 -0.272308 3.564379  
O 2.503653 -0.242948 -1.497269  
N 2.107996 -3.322651 -0.192669  
C 3.375713 -3.835161 -0.287179  
O 3.660139 -4.933868 -0.739484  
H 0.275190 -2.009946 1.333799  
H 2.083381 -2.857893 2.134732  
H 4.347024 -3.116185 2.359496  
H 4.734953 -1.471963 1.847506  
H 5.828597 -0.467544 -1.308278  
H 4.821686 -1.127472 -2.607016  
H 7.122496 -2.473967 -1.788931  
H 5.670645 -3.372240 -2.263507  
H 6.524346 -2.651911 0.587316  
H 5.994874 -4.235265 -0.030458  
H 1.591608 -2.192137 4.328570  
H 0.206580 -1.710127 3.328513  
H 0.866306 -0.582930 4.511779  
H 3.808856 -1.125220 4.080217  
H 3.031332 0.451650 4.314842  
H 4.109498 0.221035 2.955156  
H 1.376035 -3.691215 -0.794742  
N 1.877303 1.564512 1.802139  
O 2.734390 2.192749 2.490261  
C 1.288522 2.176666 0.619738  
C 0.058965 2.859877 -1.724957  
C 1.481909 3.485588 0.176992  
C 0.530443 1.220382 -0.039001  
C -0.115951 1.570079 -1.218644  
C 0.842209 3.796680 -1.047617  
H -0.717090 0.855485 -1.766570  
H -0.406130 3.159311 -2.658429  
C 2.207535 4.555389 0.855708  
H 2.529393 4.392666 1.875263  
C 2.442696 5.704594 0.207717  
H 2.968886 6.522711 0.693688  
C 2.043582 5.906484 -1.236202  
O 0.914281 5.048150 -1.578155  
C 3.208431 5.561774 -2.179522  
H 2.908877 5.709636 -3.223124  
H 3.513176 4.519291 -2.044386  
H 4.074053 6.200152 -1.969408  
C 1.530490 7.327322 -1.482345  
H 1.193192 7.432764 -2.518334  
H 2.327278 8.056456 -1.299700  
H 0.691043 7.551228 -0.817337  
C -0.703892 -1.596725 -0.395576  
C -1.608381 -0.774245 0.274683  
C -2.482155 -2.409702 -1.803795  
C -2.988393 -0.738568 -0.044953  
C -1.145191 -2.441239 -1.424953  
C -3.410753 -1.580773 -1.130233  
C -3.956077 0.077567 0.625915  
H -5.086250 -2.181674 -2.370041  
H -2.845777 -3.026990 -2.616494  
C -5.303718 0.036915 0.219533  
C -5.697256 -0.774872 -0.887370  
C -4.781023 -1.561896 -1.530644  
O -3.545641 0.846369 1.631321  
H -4.344802 1.361654 1.936599  
O -0.201030 -3.256464 -1.987332  
C -0.583299 -4.099106 -3.071685  
H -0.944050 -3.505895 -3.919786  
H -1.356763 -4.813788 -2.766090  
H 0.319943 -4.638459 -3.360296  
C -6.290511 0.832496 0.953103  
O -7.603121 0.676473 0.675459  
C -8.054011 -0.463864 -0.107710  
H -9.045708 -0.153199 -0.448056  
C -7.138793 -0.667863 -1.316448  
H -7.256301 0.193488 -1.989316  
H -7.452339 -1.556127 -1.876001

O -5.988702 1.654214 1.821534  
C -8.190871 -1.686742 0.795720  
H -8.809290 -1.444679 1.665016  
H -7.214927 -2.034942 1.148483  
H -8.669325 -2.506048 0.247117  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68715772  
Number of imaginary frequencies = 0

1d\_c03

B3LYP/6-31G\* Geometry

C 2.184162 -1.848881 0.174906  
C 2.366944 -0.693359 2.659230  
C 0.503604 -0.056519 0.881520  
C 1.541510 0.335367 1.900282  
C 0.722463 -1.506300 0.420988  
C 2.838763 -1.849954 1.630832  
C 4.359767 -2.109347 1.456449  
C 4.636585 -2.523800 -0.009512  
N 4.261317 -1.359705 -0.842448  
C 2.964517 -0.960123 -0.832088  
C 5.325956 -0.908423 -1.733074  
C 6.582198 -1.464002 -1.041761  
C 6.106115 -2.777112 -0.379377  
O -0.921555 -0.202328 1.350454  
C 1.469629 -1.342937 3.751434  
C 3.578240 -0.088702 3.401342  
O 2.489758 -0.082260 -1.540423  
N 2.374236 -3.237588 -0.283550  
C 3.669470 -3.655463 -0.450478  
O 4.005707 -4.727307 -0.928786  
H 0.529203 -2.070521 1.344499  
H 2.425374 -2.773342 2.046251  
H 4.700993 -2.888835 2.146760  
H 4.959880 -1.216829 1.646251  
H 5.308010 0.181282 -1.818444  
H 5.194383 -1.328542 -2.740223  
H 6.926053 -0.755378 -0.279499  
H 7.406440 -1.623394 -1.742786  
H 6.705589 -3.046257 0.495205  
H 6.145894 -3.617711 -1.078788  
H 2.020554 -2.135869 4.272113  
H 0.549014 -1.774328 3.348170  
H 1.179311 -0.588680 4.490047  
H 4.131767 -0.899793 3.888877  
H 3.246154 0.611115 4.169415  
H 4.256528 0.460193 2.747500  
H 1.640724 -3.663713 -0.844239  
N 1.854016 1.620541 1.742446  
O 2.689315 2.318085 2.389745  
C 1.153676 2.183314 0.597048  
C -0.240752 2.764530 -1.681506  
C 1.214473 3.504525 0.153260  
C 0.446487 1.167762 -0.028861  
C -0.284071 1.464122 -1.173440  
C 0.492977 3.762941 -1.037729  
H -0.849871 0.703296 -1.696381  
H -0.773600 3.025024 -2.590160  
C 1.877941 4.630595 0.803781  
H 2.260035 4.493461 1.806152  
C 1.983214 5.797418 0.153311  
H 2.459650 6.656441 0.619607  
C 1.501151 5.967588 -1.269310  
O 0.434250 5.016956 -1.564138  
C 2.645914 5.726103 -2.267996  
H 2.286106 5.850388 -3.295517  
H 3.044954 4.713321 -2.154222  
H 3.462478 6.436059 -2.094246  
C 0.857877 7.339833 -1.483004  
H 0.466909 7.419004 -2.502344  
H 1.596141 8.134536 -1.330528  
H 0.032638 7.488546 -0.780194  
C -0.573610 -1.745170 -0.326077  
C -1.502587 -0.998566 0.397235  
C -2.358740 -2.712514 -1.624446  
C -2.897096 -1.077049 0.157826  
C -1.003625 -2.629342 -1.326948  
C -3.312227 -1.961558 -0.895970

C -3.887332 -0.341891 0.885763  
H -5.008360 -2.758552 -1.987395  
H -2.717439 -3.366884 -2.409826  
C -5.245372 -0.462474 0.532048  
C -5.641212 -1.358921 -0.506910  
C -4.702648 -2.076957 -1.197519  
O -3.485778 0.437661 1.886506  
H -4.311467 0.826050 2.291583  
O -0.029596 -3.366340 -1.943916  
C -0.404075 -4.248095 -2.999671  
H -0.861358 -3.694578 -3.827832  
H -1.096923 -5.020505 -2.645213  
H 0.522122 -4.714451 -3.338309  
C -6.240580 0.322073 1.265029  
O -7.520906 0.319940 0.833481  
C -7.818682 -0.152415 -0.508659  
H -7.424330 0.598283 -1.207389  
C -7.123169 -1.486640 -0.759456  
H -7.318380 -1.820464 -1.784698  
H -7.558695 -2.239415 -0.085509  
O -5.979617 0.984381 2.271474  
C -9.333568 -0.209821 -0.609076  
H -9.768667 0.765068 -0.370716  
H -9.738549 -0.948954 0.090282  
H -9.634587 -0.487144 -1.625069  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68830516  
Number of imaginary frequencies = 0

1d\_c04

B3LYP/6-31G\* Geometry  
C 2.175660 -1.835217 0.238897  
C 2.315364 -0.692050 2.734080  
C 0.475289 -0.055014 0.935396  
C 1.494558 0.337950 1.972734  
C 0.713440 -1.500418 0.470551  
C 2.823505 -1.825471 1.697098  
C 4.351794 -2.035518 1.526229  
C 4.633973 -2.462118 0.069498  
N 4.247522 -1.312418 -0.784062  
C 2.935938 -0.968766 -0.799956  
C 5.245184 -0.984485 -1.805354  
C 6.188169 -2.201931 -1.768673  
C 6.093495 -2.713763 -0.315151  
O -0.958673 -0.213897 1.375508  
C 1.404380 -1.368057 3.798499  
C 3.505131 -0.087143 3.510811  
O 2.418510 -0.180605 -1.584986  
N 2.382400 -3.224342 -0.218510  
C 3.687381 -3.620467 -0.362263  
O 4.056479 -4.693998 -0.811686  
H 0.507609 -2.072883 1.386066  
H 2.434898 -2.763349 2.104040  
H 4.723446 -2.788182 2.230293  
H 4.918997 -1.117580 1.694271  
H 5.766088 -0.055955 -1.538523  
H 4.752484 -0.827036 -2.769168  
H 7.209852 -1.944959 -2.062531  
H 5.823674 -2.978693 -2.448744  
H 6.753664 -2.138432 0.344813  
H 6.342510 -3.773333 -0.227623  
H 1.954982 -2.161196 4.318933  
H 0.496552 -1.804981 3.373132  
H 1.091092 -0.627524 4.541514  
H 4.057689 -0.900920 3.995051  
H 3.149382 0.594304 4.285084  
H 4.190125 0.481371 2.881790  
H 1.648861 -3.676715 -0.762999  
N 1.810006 1.623318 1.820689  
O 2.635090 2.320334 2.480965  
C 1.129230 2.186434 0.663424  
C -0.231984 2.769745 -1.634635  
C 1.196502 3.508130 0.222097  
C 0.431764 1.170833 0.026262  
C -0.282613 1.469079 -1.128299  
C 0.492926 3.767561 -0.979577  
H -0.843577 0.709601 -1.658305  
H -0.752517 3.031491 -2.550013



C 1.849541 4.633694 0.883990  
H 2.217160 4.495340 1.891565  
C 1.962986 5.801659 0.237058  
H 2.431744 6.660188 0.711901  
C 1.501610 5.974988 -1.191850  
O 0.442828 5.020800 -1.506619  
C 2.662001 5.741070 -2.174018  
H 2.317076 5.867100 -3.206390  
H 3.063735 4.729675 -2.057244  
H 3.472926 6.453804 -1.986040  
C 0.856197 7.345406 -1.410460  
H 0.480824 7.426821 -2.435438  
H 1.588899 8.142333 -1.243630  
H 0.019676 7.488315 -0.719936  
C -0.559673 -1.744692 -0.303902  
C -1.514735 -1.013365 0.408012  
C -2.298399 -2.732107 -1.641713  
C -2.899310 -1.118840 0.137156  
C -0.953791 -2.615507 -1.322835  
C -3.282343 -2.011513 -0.926561  
C -3.919269 -0.403696 0.848520  
H -4.944152 -2.848176 -2.039636  
H -2.598290 -3.409252 -2.435497  
C -5.266721 -0.553691 0.472975  
C -5.629304 -1.461303 -0.570334  
C -4.666213 -2.158834 -1.246459  
O -3.548205 0.385360 1.853440  
H -4.387609 0.757449 2.245837  
O -0.007389 -3.383008 -1.979654  
C 0.486391 -2.790778 -3.195346  
H 1.197478 -3.506382 -3.613404  
H 0.987510 -1.838427 -2.988330  
H -0.334694 -2.632876 -3.904438  
C -6.289918 0.213636 1.187595  
O -7.561745 0.186574 0.734717  
C -7.830442 -0.299477 -0.609354  
H -7.441033 0.455519 -1.306157  
C -7.104560 -1.620690 -0.841947  
H -7.278811 -1.964842 -1.867483  
H -7.533886 -2.377940 -0.169066  
O -6.057491 0.883050 2.196224  
C -9.342157 -0.388076 -0.731323  
H -9.800502 0.579010 -0.505063  
H -9.742314 -1.131633 -0.033926  
H -9.622181 -0.677044 -1.750047  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68222553  
Number of imaginary frequencies = 0

1d\_c05

B3LYP/6-31G\* Geometry  
C 1.952726 -1.954696 0.246574  
C 2.080128 -0.858497 2.763249  
C 0.400756 -0.022505 0.890516  
C 1.405077 0.256427 1.978147  
C 0.521259 -1.477851 0.411610  
C 2.520975 -2.028567 1.735699  
C 4.025752 -2.395401 1.640750  
C 4.338740 -2.830322 0.193227  
N 4.117919 -1.636307 -0.659121  
C 2.851054 -1.157966 -0.736106  
C 5.197492 -1.402835 -1.622188  
C 6.007045 -2.711578 -1.557084  
C 5.782768 -3.227475 -0.119321  
O -1.061718 -0.049621 1.260558  
C 1.054791 -1.448968 3.773172  
C 3.285005 -0.384518 3.604749  
O 2.459475 -0.310216 -1.531816  
N 2.039429 -3.351958 -0.224001  
C 3.302975 -3.878844 -0.307769  
O 3.583288 -4.978323 -0.758489  
H 0.214498 -2.040035 1.304871  
H 2.015880 -2.924598 2.107661  
H 4.278626 -3.191942 2.349154  
H 4.675874 -1.544421 1.854366  
H 5.796396 -0.536286 -1.313750  
H 4.776038 -1.184520 -2.607695  
H 7.063962 -2.558169 -1.792913

H 5.601769 -3.438579 -2.268435  
 H 6.462627 -2.731411 0.583620  
 H 5.916216 -4.308133 -0.037159  
 H 1.496580 -2.300620 4.304677  
 H 0.128504 -1.784885 3.298742  
 H 0.783878 -0.688959 4.513146  
 H 3.723888 -1.253754 4.108690  
 H 2.962752 0.327248 4.366256  
 H 4.056749 0.111940 3.016701  
 H 1.297124 -3.713906 -0.821891  
 N 1.860100 1.502643 1.853522  
 O 2.725323 2.104133 2.555013  
 C 1.290094 2.143591 0.677193  
 C 0.078978 2.888413 -1.658385  
 C 1.508076 3.456104 0.257353  
 C 0.517926 1.211522 0.000115  
 C -0.120196 1.593655 -1.174179  
 C 0.877904 3.799283 -0.963893  
 H -0.737726 0.901607 -1.732876  
 H -0.380161 3.212597 -2.586512  
 C 2.249951 4.501482 0.956400  
 H 2.566334 4.315711 1.973678  
 C 2.505904 5.657732 0.329181  
 H 3.044442 6.458101 0.830885  
 C 2.114341 5.892834 -1.111571  
 O 0.974040 5.057008 -1.473672  
 C 3.277088 5.549397 -2.057848  
 H 2.982760 5.720652 -3.099326  
 H 3.567159 4.500503 -1.941097  
 H 4.150752 6.171754 -1.833595  
 C 1.622252 7.325268 -1.332056  
 H 1.289206 7.455017 -2.366641  
 H 2.428995 8.039218 -1.133967  
 H 0.784445 7.548816 -0.664894  
 C -0.728582 -1.585352 -0.428894  
 C -1.643550 -0.776187 0.251251  
 C -2.483093 -2.374085 -1.873112  
 C -3.017133 -0.746406 -0.085649  
 C -1.151564 -2.395212 -1.485436  
 C -3.428092 -1.574602 -1.190513  
 C -4.000034 0.048432 0.593670  
 H -5.091611 -2.175709 -2.445125  
 H -2.805370 -3.000544 -2.699103  
 C -5.343580 -0.002774 0.180997  
 C -5.725111 -0.801438 -0.941397  
 C -4.797985 -1.565818 -1.594630  
 O -3.600795 0.805663 1.612152  
 H -4.406881 1.306300 1.924060  
 O -0.250595 -3.238388 -2.112400  
 C 0.354487 -2.677708 -3.292390  
 H 1.014171 -3.451453 -3.690658  
 H 0.932609 -1.780424 -3.044219  
 H -0.413037 -2.432152 -4.035661  
 C -6.343474 0.767405 0.925951  
 O -7.652509 0.596499 0.644611  
 C -8.086499 -0.536501 -0.159687  
 H -9.082199 -0.233635 -0.495145  
 C -7.167193 -0.704527 -1.370893  
 H -7.295453 0.168524 -2.026504  
 H -7.468047 -1.585559 -1.948429  
 O -6.053382 1.579368 1.807368  
 C -8.206157 -1.777101 0.721402  
 H -8.828642 -1.559794 1.594319  
 H -7.225676 -2.118009 1.068629  
 H -8.672405 -2.592988 0.157519  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68047731  
 Number of imaginary frequencies = 0

1d\_c06

B3LYP/6-31G\* Geometry  
 C 1.968215 -1.968536 0.187898  
 C 2.149593 -0.860796 2.693625  
 C 0.432912 -0.032920 0.849064  
 C 1.460268 0.249448 1.913608  
 C 0.535909 -1.492027 0.376010  
 C 2.555568 -2.046770 1.670300  
 C 4.051828 -2.446785 1.557842

C 4.352117 -2.870214 0.099064  
N 4.124419 -1.667062 -0.732001  
C 2.871489 -1.147260 -0.772012  
C 5.263848 -1.308281 -1.570431  
C 6.431653 -1.989620 -0.837689  
C 5.805525 -3.258053 -0.213426  
O -1.019424 -0.051514 1.254073  
C 1.146668 -1.432944 3.736052  
C 3.377709 -0.382098 3.497484  
O 2.512831 -0.222037 -1.488394  
N 2.046802 -3.364256 -0.281782  
C 3.303206 -3.901037 -0.398599  
O 3.557898 -4.994993 -0.877205  
H 0.249182 -2.047285 1.280395  
H 2.039338 -2.931108 2.054481  
H 4.287396 -3.261798 2.251157  
H 4.723788 -1.616596 1.785257  
H 5.352896 -0.220816 -1.638175  
H 5.135487 -1.700838 -2.589010  
H 6.810998 -1.325267 -0.052696  
H 7.264528 -2.220315 -1.508004  
H 6.339739 -3.591466 0.681059  
H 5.795238 -4.091622 -0.922252  
H 1.595125 -2.283262 4.264280  
H 0.206044 -1.765309 3.287790  
H 0.900626 -0.663888 4.475479  
H 3.825699 -1.246378 4.002004  
H 3.079015 0.342341 4.256402  
H 4.136155 0.101993 2.881949  
H 1.303297 -3.712429 -0.881755  
N 1.906650 1.497528 1.778962  
O 2.782994 2.103507 2.463045  
C 1.309989 2.134964 0.614420  
C 0.057588 2.869465 -1.702458  
C 1.517987 3.446458 0.186237  
C 0.528484 1.199446 -0.046569  
C -0.130387 1.575668 -1.210955  
C 0.866097 3.784167 -1.024805  
H -0.751558 0.878719 -1.759347  
H -0.416699 3.188925 -2.624613  
C 2.270928 4.495355 0.867922  
H 2.603162 4.314975 1.881154  
C 2.517784 5.647844 0.230116  
H 3.064451 6.451051 0.718361  
C 2.103242 5.872771 -1.206104  
O 0.951799 5.041421 -1.539990  
C 3.247646 5.513839 -2.169009  
H 2.936932 5.678595 -3.206802  
H 3.532456 4.463928 -2.048705  
H 4.129143 6.132039 -1.964543  
C 1.616467 7.306277 -1.431072  
H 1.267066 7.429139 -2.461114  
H 2.430741 8.016894 -1.252573  
H 0.791179 7.540813 -0.752152  
C -0.740475 -1.596969 -0.432963  
C -1.627880 -0.774497 0.259930  
C -2.542254 -2.363910 -1.836978  
C -3.010289 -0.715952 -0.045743  
C -1.202310 -2.418902 -1.471592  
C -3.453534 -1.534234 -1.141009  
C -3.960865 0.101823 0.647240  
H -5.148115 -2.092049 -2.375113  
H -2.921597 -2.963170 -2.656007  
C -5.312501 0.085814 0.252587  
C -5.726704 -0.702125 -0.863892  
C -4.826949 -1.490530 -1.528421  
O -3.531144 0.848487 1.661261  
H -4.320431 1.369556 1.981914  
O -0.273865 -3.236415 -2.056119  
C -0.676375 -4.056400 -3.150513  
H -1.036618 -3.444881 -3.985727  
H -1.456442 -4.765843 -2.849550  
H 0.217301 -4.602538 -3.455600  
C -6.281974 0.882344 1.007900  
O -7.598998 0.748057 0.739947  
C -8.071962 -0.373303 -0.057533  
H -9.062542 -0.044205 -0.383518

C -7.170517 -0.569173 -1.277901  
H -7.282792 0.304643 -1.935414  
H -7.500676 -1.443919 -1.849096  
O -5.961367 1.685869 1.886550  
C -8.216659 -1.608951 0.827045  
H -8.824358 -1.373312 1.705611  
H -7.242239 -1.975213 1.165419  
H -8.710325 -2.413017 0.269447  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68645867  
Number of imaginary frequencies = 0

1d\_c07

B3LYP/6-31G\* Geometry  
C 2.143478 -1.886186 0.173118  
C 2.319105 -0.773012 2.679384  
C 0.473859 -0.087211 0.903238  
C 1.508433 0.277841 1.935381  
C 0.688209 -1.528770 0.416417  
C 2.794522 -1.909512 1.629832  
C 4.315371 -2.165714 1.455455  
C 4.590579 -2.567601 -0.013212  
N 4.223096 -1.391771 -0.835942  
C 2.923637 -1.009696 -0.841579  
C 5.277993 -0.971548 -1.754049  
C 6.537397 -1.529225 -1.071242  
C 6.058220 -2.830033 -0.386719  
O -0.958607 -0.234774 1.354666  
C 1.405933 -1.440233 3.747491  
C 3.527404 -0.195167 3.447454  
O 2.434709 -0.168181 -1.588608  
N 2.321797 -3.271673 -0.304112  
C 3.617081 -3.695014 -0.463872  
O 3.955332 -4.766595 -0.939284  
H 0.478194 -2.110474 1.325315  
H 2.380027 -2.840069 2.027721  
H 4.656928 -2.951377 2.138304  
H 4.914800 -1.274389 1.653131  
H 5.271951 0.116158 -1.861338  
H 5.123981 -1.411079 -2.749788  
H 6.895680 -0.813609 -0.322335  
H 7.351485 -1.704313 -1.780207  
H 6.660752 -3.086971 0.489361  
H 6.092183 -3.681989 -1.072416  
H 1.944793 -2.250470 4.253741  
H 0.484593 -1.852761 3.326697  
H 1.116523 -0.701003 4.501438  
H 4.068260 -1.021597 3.923442  
H 3.192672 0.490494 4.227175  
H 4.217724 0.361852 2.813651  
H 1.577864 -3.701744 -0.852410  
N 1.840515 1.560519 1.796502  
O 2.683424 2.236863 2.456032  
C 1.154029 2.149011 0.655537  
C -0.226547 2.783042 -1.617475  
C 1.232979 3.476048 0.232453  
C 0.435886 1.151934 0.012278  
C -0.287882 1.475859 -1.129344  
C 0.518331 3.762022 -0.956488  
H -0.865173 0.731408 -1.663147  
H -0.754725 3.064775 -2.522487  
C 1.907833 4.583575 0.902880  
H 2.286391 4.425418 1.903470  
C 2.027036 5.759998 0.272480  
H 2.512063 6.605491 0.754343  
C 1.549421 5.961325 -1.147323  
O 0.476626 5.023730 -1.463952  
C 2.694645 5.731566 -2.148142  
H 2.337747 5.877841 -3.173743  
H 3.087236 4.714332 -2.052947  
H 3.515278 6.432874 -1.959295  
C 0.916131 7.341983 -1.335303  
H 0.528240 7.444044 -2.353767  
H 1.659608 8.128221 -1.165417  
H 0.090250 7.482713 -0.631626  
C -0.593760 -1.743257 -0.352533  
C -1.533241 -1.011961 0.379861  
C -2.355980 -2.687380 -1.690748

C -2.921502 -1.098124 0.121307  
 C -1.007266 -2.591371 -1.382820  
 C -3.324876 -1.968896 -0.953096  
 C -3.926473 -0.384870 0.855454  
 H -5.006891 -2.769723 -2.062092  
 H -2.670717 -3.346899 -2.493550  
 C -5.279396 -0.515809 0.492765  
 C -5.662290 -1.401877 -0.561705  
 C -4.713503 -2.096811 -1.260420  
 O -3.536614 0.383782 1.869025  
 H -4.368052 0.757077 2.276908  
 O -0.076074 -3.357538 -2.062407  
 C 0.433088 -2.736701 -3.257379  
 H 1.134768 -3.450482 -3.693862  
 H 0.948461 -1.798793 -3.020858  
 H -0.382230 -2.543994 -3.964573  
 C -6.287084 0.248214 1.232498  
 O -7.564329 0.239925 0.794669  
 C -7.853396 -0.219868 -0.554389  
 H -7.465909 0.544066 -1.242463  
 C -7.142066 -1.542978 -0.819160  
 H -7.331130 -1.867022 -1.848607  
 H -7.570521 -2.308427 -0.155066  
 O -6.036696 0.898109 2.249563  
 C -9.367220 -0.293270 -0.659244  
 H -9.814143 0.673340 -0.409336  
 H -9.765310 -1.046234 0.029195  
 H -9.662384 -0.560693 -1.679573  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68146685  
 Number of imaginary frequencies = 0

1d\_c08

B3LYP/6-31G\* Geometry  
 C 1.920616 -1.999562 0.181449  
 C 2.088755 -0.938409 2.709951  
 C 0.396452 -0.057845 0.868382  
 C 1.417243 0.194357 1.947194  
 C 0.496658 -1.507410 0.367162  
 C 2.500750 -2.103387 1.664613  
 C 3.996555 -2.501866 1.553185  
 C 4.297275 -2.911020 0.091559  
 N 4.080823 -1.695230 -0.727175  
 C 2.825239 -1.190169 -0.783721  
 C 5.210998 -1.365620 -1.590895  
 C 6.379703 -2.052268 -0.865588  
 C 5.747828 -3.309297 -0.223924  
 O -1.062456 -0.076908 1.254364  
 C 1.068654 -1.527020 3.726267  
 C 3.310217 -0.488809 3.540633  
 O 2.452976 -0.297436 -1.538587  
 N 1.986619 -3.389904 -0.310252  
 C 3.241731 -3.933854 -0.419732  
 O 3.497175 -5.026589 -0.898603  
 H 0.191505 -2.078660 1.255310  
 H 1.981675 -2.994362 2.029074  
 H 4.230617 -3.323978 2.238325  
 H 4.668128 -1.673861 1.789909  
 H 5.314161 -0.280930 -1.677537  
 H 5.059722 -1.773133 -2.600538  
 H 6.773517 -1.384618 -0.090639  
 H 7.202615 -2.296639 -1.543200  
 H 6.284260 -3.634797 0.672069  
 H 5.729509 -4.151366 -0.922324  
 H 1.505216 -2.391176 4.241700  
 H 0.131822 -1.844230 3.259596  
 H 0.817726 -0.772501 4.478834  
 H 3.743058 -1.368268 4.031960  
 H 3.007643 0.221130 4.311731  
 H 4.081562 0.001619 2.946819  
 H 1.233979 -3.734973 -0.905064  
 N 1.884888 1.437045 1.834068  
 O 2.766969 2.018266 2.531844  
 C 1.306645 2.101521 0.675221  
 C 0.074520 2.894069 -1.633352  
 C 1.536117 3.416804 0.270385  
 C 0.514422 1.188568 -0.004474  
 C -0.134971 1.595356 -1.164207

C 0.894760 3.784798 -0.937701  
 H -0.768943 0.919357 -1.724197  
 H -0.392902 3.236821 -2.550619  
 C 2.300857 4.442920 0.973394  
 H 2.626756 4.240065 1.984376  
 C 2.565524 5.603234 0.357328  
 H 3.121107 6.389863 0.862167  
 C 2.160016 5.860907 -1.075775  
 O 1.001569 5.048040 -1.431914  
 C 3.304990 5.508935 -2.040458  
 H 3.000545 5.696530 -3.076202  
 H 3.579010 4.454153 -1.938929  
 H 4.191600 6.114314 -1.820502  
 C 1.689157 7.303583 -1.274486  
 H 1.345530 7.450268 -2.303336  
 H 2.510049 8.001908 -1.078813  
 H 0.863494 7.533563 -0.594501  
 C -0.761958 -1.588283 -0.462962  
 C -1.661708 -0.780603 0.238856  
 C -2.536728 -2.332039 -1.905893  
 C -3.037611 -0.729679 -0.085858  
 C -1.202325 -2.374478 -1.530204  
 C -3.466945 -1.534072 -1.201352  
 C -4.005499 0.065602 0.614160  
 H -5.147455 -2.094341 -2.452276  
 H -2.872771 -2.939891 -2.740248  
 C -5.352628 0.037668 0.211114  
 C -5.752449 -0.737697 -0.921135  
 C -4.839762 -1.502330 -1.594161  
 O -3.589244 0.801091 1.641752  
 H -4.386560 1.306751 1.967680  
 O -0.315602 -3.215214 -2.180240  
 C 0.297263 -2.633292 -3.345825  
 H 0.950478 -3.403763 -3.760612  
 H 0.883732 -1.747390 -3.076923  
 H -0.466523 -2.363007 -4.084386  
 C -6.337148 0.808283 0.975810  
 O -7.650275 0.658393 0.701645  
 C -8.104423 -0.456393 -0.116868  
 H -9.098804 -0.136048 -0.439777  
 C -7.196539 -0.616590 -1.337710  
 H -7.319228 0.268053 -1.978686  
 H -7.512465 -1.484825 -1.926479  
 O -6.030211 1.602449 1.867658  
 C -8.232823 -1.709032 0.745736  
 H -8.846300 -1.497774 1.626477  
 H -7.254102 -2.067101 1.080433  
 H -8.713054 -2.510355 0.172787  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67966643  
 Number of imaginary frequencies = 0

1d\_c09

B3LYP/6-31G\* Geometry  
 C 2.284864 -1.745113 0.240767  
 C 2.422119 -0.534501 2.699770  
 C 0.527742 -0.025947 0.915464  
 C 1.537066 0.434737 1.928748  
 C 0.807705 -1.477914 0.489294  
 C 2.953530 -1.678879 1.687623  
 C 4.486390 -1.840255 1.496257  
 C 4.766039 -2.274545 0.040171  
 N 4.318328 -1.154190 -0.819825  
 C 2.996317 -0.844886 -0.806418  
 C 5.294838 -0.778095 -1.843926  
 C 6.287587 -1.955270 -1.816791  
 C 6.230242 -2.468610 -0.361764  
 O -0.904099 -0.248202 1.392047  
 C 1.571673 -1.216484 3.809668  
 C 3.600937 0.151458 3.424172  
 O 2.447545 -0.045273 -1.553041  
 N 2.545982 -3.129893 -0.193624  
 C 3.862689 -3.472504 -0.363356  
 O 4.261907 -4.533840 -0.816892  
 H 0.648276 -2.028895 1.426558  
 H 2.604154 -2.618340 2.125291  
 H 4.892424 -2.570459 2.205098  
 H 5.024125 -0.901701 1.645019

H 5.778688 0.170333 -1.576117  
H 4.791393 -0.637900 -2.804725  
H 7.294705 -1.657141 -2.121900  
H 5.947539 -2.746678 -2.492640  
H 6.875045 -1.866694 0.289554  
H 6.522350 -3.517289 -0.275695  
H 2.175860 -1.959112 4.344723  
H 0.681647 -1.719732 3.420900  
H 1.234497 -0.467537 4.533678  
H 4.204752 -0.618597 3.918039  
H 3.233739 0.840205 4.186273  
H 4.241956 0.729997 2.758328  
H 1.832296 -3.607376 -0.739106  
N 1.770320 1.736537 1.756012  
O 2.556380 2.489851 2.397810  
C 1.039758 2.241996 0.601266  
C -0.386125 2.705625 -1.684771  
C 1.019814 3.558302 0.141038  
C 0.396843 1.175997 -0.012017  
C -0.347419 1.410734 -1.162328  
C 0.282060 3.756623 -1.052841  
H -0.860264 0.609137 -1.678766  
H -0.933404 2.920841 -2.596525  
C 1.615211 4.730754 0.775056  
H 2.014726 4.629555 1.774793  
C 1.640214 5.895346 0.112771  
H 2.066321 6.786322 0.567534  
C 1.135536 6.026768 -1.305402  
O 0.143295 4.995340 -1.594450  
C 2.287127 5.873722 -2.313226  
H 1.909761 5.970160 -3.337276  
H 2.764048 4.894708 -2.203697  
H 3.048300 6.644237 -2.146378  
C 0.385732 7.344938 -1.513115  
H -0.019970 7.391924 -2.528617  
H 1.061822 8.194496 -1.368728  
H -0.441727 7.430781 -0.802534  
C -0.470551 -1.805365 -0.257007  
C -1.438674 -1.090330 0.427754  
C -2.214675 -2.887312 -1.523356  
C -2.825586 -1.202042 0.185266  
C -0.865887 -2.741007 -1.232813  
C -3.204920 -2.140828 -0.830098  
C -3.822096 -0.434622 0.876258  
H -4.886271 -2.984416 -1.902302  
H -2.546036 -3.585184 -2.283089  
C -5.175232 -0.624050 0.569793  
C -5.535731 -1.559809 -0.447961  
C -4.585386 -2.285995 -1.125486  
O -3.465265 0.475192 1.795128  
H -2.489154 0.516914 1.849476  
O 0.139763 -3.455766 -1.825660  
C -0.199322 -4.390873 -2.847313  
H 0.744979 -4.829102 -3.173137  
H -0.683084 -3.887575 -3.692249  
H -0.857306 -5.178395 -2.461227  
C -6.239488 0.101737 1.318495  
O -7.486373 0.133703 0.744549  
C -7.682926 -0.340384 -0.603452  
H -7.210964 0.377571 -1.290209  
C -7.005351 -1.697832 -0.758061  
H -7.151296 -2.087663 -1.771719  
H -7.484028 -2.404408 -0.063912  
O -6.101609 0.628210 2.397461  
C -9.185416 -0.363591 -0.836066  
H -9.612552 0.627099 -0.654543  
H -9.668323 -1.075077 -0.157702  
H -9.407268 -0.656084 -1.868413  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68008373  
Number of imaginary frequencies = 0

1d\_c10  
B3LYP/6-31G\* Geometry  
C 2.252659 -1.801081 0.175877  
C 2.431102 -0.614687 2.644376  
C 0.527356 -0.058877 0.882976  
C 1.554026 0.375467 1.890388

C 0.781947 -1.509334 0.437174  
C 2.928394 -1.764488 1.620906  
C 4.454884 -1.970955 1.423689  
C 4.722928 -2.390272 -0.042856  
N 4.293365 -1.248059 -0.880282  
C 2.985518 -0.891033 -0.847583  
C 5.329658 -0.762580 -1.786885  
C 6.614218 -1.269444 -1.110323  
C 6.194558 -2.594451 -0.433676  
O -0.902909 -0.267980 1.372506  
C 1.580697 -1.287100 3.760105  
C 3.631063 0.045462 3.357401  
O 2.468335 -0.029471 -1.546724  
N 2.482698 -3.185661 -0.273664  
C 3.789683 -3.559331 -0.457843  
O 4.155662 -4.622753 -0.931820  
H 0.620302 -2.067835 1.369793  
H 2.554937 -2.697603 2.051947  
H 4.835062 -2.730556 2.115695  
H 5.025179 -1.055467 1.594945  
H 5.271252 0.325355 -1.876543  
H 5.199343 -1.191967 -2.790109  
H 6.943864 -0.544480 -0.357229  
H 7.433434 -1.403996 -1.822255  
H 6.816359 -2.837069 0.432965  
H 6.253279 -3.437418 -1.128863  
H 2.176192 -2.044771 4.283755  
H 0.677071 -1.770491 3.377367  
H 1.265932 -0.536533 4.492513  
H 4.225716 -0.738262 3.840622  
H 3.286776 0.738279 4.126335  
H 4.275021 0.613890 2.685412  
H 1.756310 -3.641811 -0.820527  
N 1.803875 1.675678 1.729919  
O 2.608864 2.409974 2.370602  
C 1.066512 2.205490 0.590835  
C -0.379041 2.716955 -1.672593  
C 1.059412 3.527486 0.146964  
C 0.401454 1.156259 -0.027685  
C -0.352867 1.415325 -1.166046  
C 0.311006 3.750658 -1.035855  
H -0.883761 0.627624 -1.685656  
H -0.933949 2.950994 -2.575061  
C 1.677711 4.683879 0.788483  
H 2.086643 4.564908 1.782464  
C 1.711453 5.856145 0.140250  
H 2.154558 6.735603 0.601151  
C 1.192927 6.011766 -1.270475  
O 0.183230 4.997960 -1.560634  
C 2.331016 5.855249 -2.292999  
H 1.943650 5.969216 -3.311498  
H 2.795418 4.868486 -2.200578  
H 3.104574 6.613196 -2.125566  
C 0.459481 7.342745 -1.453741  
H 0.043577 7.408063 -2.464092  
H 1.148901 8.180980 -1.306232  
H -0.359037 7.431152 -0.733186  
C -0.507849 -1.809065 -0.301135  
C -1.459011 -1.089939 0.402991  
C -2.279426 -2.850047 -1.563771  
C -2.849760 -1.180249 0.173983  
C -0.925858 -2.725833 -1.285420  
C -3.252207 -2.100165 -0.849759  
C -3.828671 -0.409876 0.886568  
H -4.955988 -2.907184 -1.914708  
H -2.628120 -3.532801 -2.329449  
C -5.187419 -0.577795 0.592558  
C -5.570984 -1.494679 -0.433904  
C -4.637555 -2.223454 -1.131852  
O -3.450022 0.482088 1.814142  
H -2.472907 0.510153 1.858420  
O 0.064109 -3.445256 -1.898360  
C -0.297022 -4.362909 -2.928311  
H -0.782023 -3.842706 -3.762243  
H -0.961667 -5.146530 -2.545734  
H 0.638346 -4.809206 -3.268576  
C -6.234017 0.150753 1.363137



O -7.486856 0.205967 0.804077  
C -7.704480 -0.246709 -0.548053  
H -7.231553 0.475053 -1.230137  
C -7.045583 -1.610011 -0.729403  
H -7.207650 -1.983395 -1.746776  
H -7.525266 -2.320534 -0.039996  
O -6.077362 0.660724 2.447462  
C -9.209705 -0.248306 -0.763540  
H -9.622362 0.744931 -0.563425  
H -9.693577 -0.963127 -0.089383  
H -9.447060 -0.523685 -1.797120  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67940367  
Number of imaginary frequencies = 0

1d\_c11

B3LYP/6-31G\* Geometry  
C 2.061728 -1.886413 0.259980  
C 2.184984 -0.721700 2.742738  
C 0.448320 -0.009588 0.871379  
C 1.442699 0.339173 1.942111  
C 0.606833 -1.477157 0.435072  
C 2.653106 -1.902528 1.741028  
C 4.170329 -2.215574 1.630379  
C 4.485353 -2.657875 0.184323  
N 4.198392 -1.489558 -0.680654  
C 2.914377 -1.050402 -0.733707  
C 5.262042 -1.202167 -1.645079  
C 6.132638 -2.471252 -1.581779  
C 5.943263 -2.991751 -0.140268  
O -1.022701 -0.096445 1.268470  
C 1.212167 -1.326243 3.795222  
C 3.386021 -0.165481 3.537962  
O 2.488526 -0.193784 -1.497024  
N 2.207991 -3.286021 -0.181768  
C 3.492212 -3.755450 -0.287129  
O 3.809026 -4.845680 -0.737078  
H 0.343868 -2.022689 1.352043  
H 2.188162 -2.806598 2.144684  
H 4.460531 -2.992232 2.346661  
H 4.791213 -1.338784 1.825172  
H 5.820537 -0.308199 -1.338121  
H 4.828695 -1.004495 -2.629676  
H 7.179643 -2.269942 -1.825717  
H 5.756269 -3.218571 -2.287996  
H 6.606710 -2.463706 0.554967  
H 6.125893 -4.065054 -0.055490  
H 1.706661 -2.136107 4.345161  
H 0.295575 -1.726385 3.352036  
H 0.918438 -0.556241 4.516108  
H 3.883500 -0.997613 4.049521  
H 3.049544 0.548506 4.290973  
H 4.115143 0.353143 2.914934  
H 1.483503 -3.681768 -0.776231  
N 1.815059 1.611999 1.798428  
O 2.639263 2.276180 2.488740  
C 1.199221 2.198658 0.615726  
C -0.054977 2.822637 -1.732362  
C 1.334893 3.514069 0.172702  
C 0.484405 1.208536 -0.043344  
C -0.173678 1.526535 -1.225663  
C 0.684045 3.794752 -1.054644  
H -0.738479 0.784765 -1.775936  
H -0.531303 3.100023 -2.666798  
C 2.009095 4.616066 0.852413  
H 2.339613 4.468534 1.871464  
C 2.187457 5.776588 0.206655  
H 2.673855 6.617590 0.694839  
C 1.778605 5.965551 -1.235764  
O 0.701550 5.044619 -1.587676  
C 2.962528 5.695428 -2.179472  
H 2.655485 5.832424 -3.222268  
H 3.328178 4.671832 -2.050812  
H 3.788722 6.382444 -1.964387  
C 1.183493 7.355637 -1.472223  
H 0.844469 7.449381 -2.508667  
H 1.935119 8.128928 -1.280299  
H 0.329828 7.523994 -0.809075

C -0.654555 -1.665823 -0.384466  
C -1.583811 -0.866414 0.259946  
C -2.424709 -2.555452 -1.759512  
C -2.958860 -0.833873 -0.061147  
C -1.085237 -2.544140 -1.397534  
C -3.372454 -1.721330 -1.108566  
C -3.909525 0.030234 0.580368  
H -5.075696 -2.413868 -2.252509  
H -2.781538 -3.209027 -2.546602  
C -5.256198 -0.020385 0.198615  
C -5.653590 -0.923595 -0.834909  
C -4.745871 -1.739935 -1.465899  
O -3.518136 0.866426 1.553132  
H -2.549226 0.797281 1.671496  
O -0.122935 -3.344754 -1.950846  
C -0.493450 -4.223715 -3.010647  
H -0.883245 -3.660838 -3.866480  
H -1.241129 -4.953401 -2.677752  
H 0.421800 -4.742480 -3.298949  
C -6.267871 0.871285 0.832890  
O -7.590105 0.543672 0.658007  
C -7.981431 -0.693119 0.023783  
H -9.013266 -0.504860 -0.289841  
C -7.112968 -0.925057 -1.212520  
H -7.313360 -0.115494 -1.928686  
H -7.388025 -1.865152 -1.703507  
O -6.018362 1.868959 1.467829  
C -7.973701 -1.840092 1.033615  
H -8.571289 -1.567643 1.908686  
H -6.958687 -2.075351 1.368719  
H -8.406377 -2.742668 0.586220  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67787786  
Number of imaginary frequencies = 0

1d\_c12

B3LYP/6-31G\* Geometry

C 2.245378 -1.785394 0.244072  
C 2.381343 -0.607269 2.722273  
C 0.499859 -0.055914 0.938777  
C 1.506839 0.381696 1.964874  
C 0.774384 -1.502083 0.490925  
C 2.915219 -1.733240 1.690753  
C 4.447278 -1.887879 1.495799  
C 4.720694 -2.323610 0.039810  
N 4.278120 -1.199660 -0.821287  
C 2.955561 -0.903664 -0.817150  
C 5.246759 -0.849055 -1.863460  
C 6.232892 -2.031714 -1.827987  
C 6.181768 -2.527356 -0.366823  
O -0.939171 -0.278448 1.399060  
C 1.519613 -1.306734 3.812358  
C 3.559761 0.055731 3.468646  
O 2.394312 -0.142397 -1.598901  
N 2.493417 -3.171315 -0.199867  
C 3.810095 -3.521230 -0.361444  
O 4.210396 -4.585804 -0.804125  
H 0.600662 -2.067968 1.416764  
H 2.568852 -2.679781 2.115240  
H 4.858982 -2.616079 2.203189  
H 4.981822 -0.946828 1.641535  
H 5.738351 0.100580 -1.616220  
H 4.732838 -0.721403 -2.820523  
H 7.239473 -1.742480 -2.142961  
H 5.884807 -2.829601 -2.491905  
H 6.831712 -1.920022 0.274278  
H 6.470253 -3.576033 -0.270209  
H 2.115944 -2.063196 4.336558  
H 0.629079 -1.797049 3.408653  
H 1.182089 -0.570273 4.548853  
H 4.155650 -0.728951 3.948829  
H 3.191931 0.729324 4.244019  
H 4.208506 0.645019 2.820206  
H 1.768441 -3.656805 -0.727683  
N 1.756852 1.682592 1.809315  
O 2.548895 2.418481 2.463654  
C 1.039756 2.210600 0.656162  
C -0.367790 2.719751 -1.631505

C 1.038129 3.532633 0.212622  
 C 0.387689 1.159496 0.026412  
 C -0.347978 1.418319 -1.124493  
 C 0.310162 3.754644 -0.983381  
 H -0.871221 0.630622 -1.651727  
 H -0.908325 2.953140 -2.542798  
 C 1.642779 4.689995 0.865340  
 H 2.034588 4.571428 1.866210  
 C 1.684991 5.862642 0.218409  
 H 2.117876 6.742755 0.687628  
 C 1.190804 6.018796 -1.200823  
 O 0.190772 5.000551 -1.511293  
 C 2.347312 5.868882 -2.203342  
 H 1.977543 5.983246 -3.228283  
 H 2.814538 4.884058 -2.104463  
 H 3.114477 6.629797 -2.020858  
 C 0.454735 7.346767 -1.394646  
 H 0.056200 7.411947 -2.411953  
 H 1.137911 8.187644 -1.233895  
 H -0.376472 7.430553 -0.688234  
 C -0.491844 -1.808001 -0.275030  
 C -1.468345 -1.105304 0.416460  
 C -2.214989 -2.870016 -1.578099  
 C -2.849463 -1.224004 0.156329  
 C -0.872712 -2.711634 -1.278179  
 C -3.218423 -2.151969 -0.877276  
 C -3.858812 -0.475929 0.853684  
 H -4.887104 -2.998674 -1.965744  
 H -2.503751 -3.573243 -2.353329  
 C -5.206918 -0.673602 0.536887  
 C -5.556119 -1.600313 -0.494949  
 C -4.597170 -2.307649 -1.178472  
 O -3.513721 0.423197 1.787745  
 H -2.538517 0.470002 1.851594  
 O 0.091327 -3.461891 -1.929162  
 C 0.551613 -2.880812 -3.163387  
 H 1.285563 -3.578834 -3.571402  
 H 1.018117 -1.905448 -2.983628  
 H -0.281131 -2.770450 -3.867622  
 C -6.281863 0.035514 1.288345  
 O -7.524393 0.067246 0.706950  
 C -7.712026 -0.395999 -0.646609  
 H -7.242877 0.332197 -1.324405  
 C -7.023524 -1.746779 -0.810874  
 H -7.163287 -2.128946 -1.828232  
 H -7.498800 -2.462978 -0.124344  
 O -6.153066 0.548779 2.374670  
 C -9.213325 -0.428413 -0.885311  
 H -9.648829 0.557240 -0.696436  
 H -9.693393 -1.149904 -0.215601  
 H -9.428684 -0.713033 -1.921203  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67320228  
 Number of imaginary frequencies = 0

1d\_c13  
 B3LYP/6-31G\* Geometry  
 C 2.028202 -1.936806 0.193669  
 C 2.196586 -0.801038 2.687058  
 C 0.446735 -0.042750 0.845140  
 C 1.459636 0.279146 1.906689  
 C 0.581504 -1.506027 0.387308  
 C 2.630098 -1.982660 1.670523  
 C 4.137310 -2.336137 1.546600  
 C 4.437941 -2.761229 0.088102  
 N 4.163619 -1.572862 -0.750332  
 C 2.896109 -1.091183 -0.777786  
 C 5.285754 -1.179995 -1.597600  
 C 6.480196 -1.818462 -0.869217  
 C 5.900578 -3.103383 -0.234093  
 O -1.021015 -0.118736 1.259764  
 C 1.228107 -1.398066 3.747796  
 C 3.417541 -0.270795 3.469189  
 O 2.500661 -0.176608 -1.488923  
 N 2.145697 -3.332405 -0.265881  
 C 3.418459 -3.828979 -0.391831  
 O 3.703538 -4.917136 -0.865212  
 H 0.319032 -2.059652 1.299717

H 2.145782 -2.879181 2.067865  
 H 4.404726 -3.137988 2.243602  
 H 4.785047 -1.483723 1.761794  
 H 5.337690 -0.090517 -1.671056  
 H 5.163813 -1.581865 -2.613156  
 H 6.843121 -1.137824 -0.090451  
 H 7.315503 -2.025439 -1.544105  
 H 6.452121 -3.415178 0.657629  
 H 5.911779 -3.940251 -0.938963  
 H 1.714906 -2.222684 4.282490  
 H 0.298157 -1.776251 3.313083  
 H 0.958904 -0.630214 4.480489  
 H 3.906550 -1.114281 3.970193  
 H 3.104086 0.445648 4.229616  
 H 4.147652 0.237508 2.838617  
 H 1.408977 -3.707987 -0.858249  
 N 1.847797 1.548347 1.773043  
 O 2.692039 2.191957 2.458886  
 C 1.222619 2.158890 0.607829  
 C -0.058326 2.831210 -1.712300  
 C 1.371144 3.477615 0.179036  
 C 0.483900 1.187651 -0.052861  
 C -0.188176 1.530442 -1.220170  
 C 0.705741 3.783439 -1.034382  
 H -0.773104 0.804573 -1.770647  
 H -0.545374 3.127520 -2.635340  
 C 2.072709 4.560882 0.861225  
 H 2.415752 4.396275 1.873507  
 C 2.260177 5.725810 0.226011  
 H 2.767143 6.553353 0.716290  
 C 1.832694 5.937533 -1.207912  
 O 0.733941 5.039890 -1.551906  
 C 2.996889 5.656462 -2.172773  
 H 2.676213 5.809851 -3.209160  
 H 3.346106 4.625236 -2.060412  
 H 3.838417 6.326490 -1.963586  
 C 1.259380 7.340564 -1.420596  
 H 0.905359 7.451196 -2.450341  
 H 2.028163 8.097982 -1.233346  
 H 0.419794 7.517623 -0.741920  
 C -0.690763 -1.666124 -0.421691  
 C -1.602883 -0.865576 0.245524  
 C -2.485252 -2.507259 -1.795587  
 C -2.980424 -0.809624 -0.061434  
 C -1.142540 -2.520686 -1.445810  
 C -3.415412 -1.672162 -1.120982  
 C -3.913477 0.054992 0.604769  
 H -5.138013 -2.319084 -2.262877  
 H -2.858287 -3.141642 -2.590861  
 C -5.264133 0.029297 0.234835  
 C -5.682720 -0.848290 -0.812324  
 C -4.791973 -1.665028 -1.466527  
 O -3.501954 0.867461 1.589255  
 H -2.532729 0.784687 1.695858  
 O -0.196050 -3.323828 -2.021772  
 C -0.586867 -4.178672 -3.093965  
 H -0.975620 -3.595426 -3.936542  
 H -1.341840 -4.903952 -2.767974  
 H 0.318949 -4.704486 -3.398746  
 C -6.258447 0.920766 0.896237  
 O -7.586311 0.612718 0.728316  
 C -7.999470 -0.605078 0.071527  
 H -9.031487 -0.396857 -0.228616  
 C -7.145026 -0.821647 -1.177253  
 H -7.340117 0.006381 -1.873480  
 H -7.437249 -1.746697 -1.686571  
 O -5.990477 1.902492 1.548291  
 C -7.997750 -1.773470 1.056479  
 H -8.584663 -1.512699 1.942261  
 H -6.983007 -2.028279 1.377768  
 H -8.445244 -2.660841 0.593498  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67719716  
 Number of imaginary frequencies = 0

1d\_c14  
 B3LYP/6-31G\* Geometry  
 C 2.210469 -1.841566 0.179323

C 2.384137 -0.694188 2.669560  
C 0.497061 -0.090774 0.908044  
C 1.520475 0.317745 1.929747  
C 0.745951 -1.534195 0.437575  
C 2.884971 -1.823490 1.624785  
C 4.411254 -2.023735 1.426252  
C 4.675948 -2.436226 -0.041706  
N 4.252084 -1.285417 -0.873185  
C 2.941066 -0.948368 -0.857476  
C 5.277001 -0.836956 -1.812176  
C 6.566277 -1.340885 -1.143654  
C 6.145823 -2.650020 -0.436752  
O -0.941167 -0.300269 1.378958  
C 1.518990 -1.385612 3.762024  
C 3.582357 -0.059718 3.408609  
O 2.407742 -0.129994 -1.600119  
N 2.428944 -3.225195 -0.284373  
C 3.736490 -3.603708 -0.461410  
O 4.104806 -4.667908 -0.929737  
H 0.567719 -2.109838 1.356703  
H 2.512829 -2.764350 2.039718  
H 4.794973 -2.785429 2.113729  
H 4.978905 -1.107002 1.600186  
H 5.229371 0.248544 -1.930752  
H 5.123398 -1.292867 -2.800455  
H 6.910501 -0.604074 -0.408874  
H 7.374689 -1.494893 -1.863829  
H 6.771663 -2.874349 0.431830  
H 6.199635 -3.508361 -1.113130  
H 2.104165 -2.159388 4.273426  
H 0.614779 -1.853213 3.361612  
H 1.203853 -0.649330 4.508582  
H 4.166606 -0.859233 3.878458  
H 3.235899 0.616949 4.190988  
H 4.236796 0.519742 2.756756  
H 1.692303 -3.688431 -0.815839  
N 1.789705 1.616350 1.787790  
O 2.601376 2.330846 2.442031  
C 1.067821 2.171056 0.650503  
C -0.357911 2.733139 -1.613443  
C 1.081350 3.498968 0.224990  
C 0.392223 1.138973 0.014296  
C -0.352623 1.424752 -1.124201  
C 0.343306 3.748478 -0.959297  
H -0.894447 0.652605 -1.655639  
H -0.905401 2.987353 -2.514968  
C 1.710715 4.638072 0.886400  
H 2.111809 4.499829 1.881065  
C 1.763418 5.818830 0.255142  
H 2.214786 6.685784 0.731395  
C 1.255417 6.002048 -1.155949  
O 0.236717 5.003389 -1.468664  
C 2.397974 5.849120 -2.173912  
H 2.018109 5.982814 -3.192805  
H 2.851685 4.856302 -2.093859  
H 3.178261 6.596272 -1.990214  
C 0.537330 7.343503 -1.322791  
H 0.128746 7.429220 -2.334582  
H 1.234782 8.171721 -1.157686  
H -0.284814 7.429511 -0.606110  
C -0.530518 -1.808751 -0.323436  
C -1.490813 -1.103871 0.388303  
C -2.279686 -2.824710 -1.628491  
C -2.875817 -1.200723 0.140180  
C -0.932728 -2.689266 -1.338746  
C -3.266867 -2.106452 -0.905000  
C -3.868515 -0.452634 0.861043  
H -4.957154 -2.913860 -1.989968  
H -2.584755 -3.510010 -2.413436  
C -5.222190 -0.628621 0.555400  
C -5.593464 -1.533097 -0.488378  
C -4.650469 -2.239998 -1.194218  
O -3.502565 0.425543 1.807011  
H -2.526254 0.458856 1.861593  
O 0.014654 -3.440334 -2.012590  
C 0.491108 -2.829832 -3.226244  
H 1.213942 -3.528149 -3.653023

H 0.974969 -1.869038 -3.015752  
H -0.336608 -2.681918 -3.929575  
C -6.280434 0.079948 1.330722  
O -7.528772 0.136180 0.763817  
C -7.736638 -0.301270 -0.595361  
H -7.266582 0.433218 -1.265694  
C -7.065854 -1.656798 -0.790744  
H -7.221118 -2.019267 -1.813025  
H -7.542082 -2.379434 -0.111657  
O -6.133721 0.572929 2.424151  
C -9.240788 -0.312253 -0.817573  
H -9.662487 0.674949 -0.606762  
H -9.721763 -1.039604 -0.154885  
H -9.471101 -0.576346 -1.855654  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67245424  
Number of imaginary frequencies = 0

1d\_c15

B3LYP/6-31G\* Geometry  
C 2.304459 -1.720259 0.274388  
C 2.341555 -0.436335 2.703890  
C 0.529770 0.029450 0.827203  
C 1.488275 0.513838 1.876148  
C 0.824077 -1.432863 0.451087  
C 2.917410 -1.602446 1.742071  
C 4.456388 -1.759256 1.613102  
C 4.786999 -2.253568 0.187971  
N 4.374126 -1.169557 -0.736705  
C 3.050830 -0.882655 -0.797095  
C 5.380867 -0.857734 -1.754846  
C 6.371947 -2.030402 -1.629713  
C 6.263579 -2.465937 -0.152243  
O -0.927858 -0.181097 1.239500  
C 1.446534 -1.094883 3.792617  
C 3.489363 0.267959 3.460229  
O 2.515346 -0.162560 -1.633655  
N 2.573675 -3.123154 -0.098786  
C 3.897173 -3.471886 -0.196596  
O 4.317860 -4.551763 -0.579169  
H 0.615485 -1.960738 1.392159  
H 2.557393 -2.531380 2.193333  
H 4.841619 -2.456838 2.364850  
H 4.983292 -0.811352 1.740994  
H 5.856615 0.105554 -1.530813  
H 4.904278 -0.775673 -2.735916  
H 7.388961 -1.746314 -1.914382  
H 6.057157 -2.857611 -2.274146  
H 6.885283 -1.829282 0.488387  
H 6.552371 -3.508122 -0.001218  
H 2.027849 -1.824858 4.368807  
H 0.573422 -1.607846 3.378679  
H 1.079613 -0.330319 4.485120  
H 4.076241 -0.489232 3.992956  
H 3.090892 0.970744 4.193007  
H 4.154346 0.834867 2.807853  
H 1.872249 -3.632527 -0.635940  
N 1.722554 1.814004 1.691520  
O 2.467537 2.582717 2.362650  
C 1.048318 2.293040 0.490376  
C -0.268677 2.697327 -1.872606  
C 1.036687 3.600442 0.004250  
C 0.447950 1.207805 -0.134711  
C -0.228657 1.410096 -1.331722  
C 0.332862 3.772219 -1.215043  
H -0.704828 0.592800 -1.858434  
H -0.769153 2.888766 -2.815973  
C 1.691546 4.771668 0.579979  
H 2.382758 4.623322 1.397889  
C 1.429169 5.985844 0.077144  
H 1.908216 6.872601 0.485209  
C 0.426850 6.200302 -1.032711  
O 0.278163 4.983788 -1.827335  
C 0.913674 7.251217 -2.033178  
H 0.199723 7.345994 -2.857344  
H 1.886730 6.966882 -2.444747  
H 1.010827 8.226132 -1.543552  
C -0.952291 6.568994 -0.461125

H -1.671588 6.719976 -1.273469  
 H -0.889222 7.491441 0.126870  
 H -1.322165 5.773701 0.193454  
 C -0.410011 -1.774734 -0.351888  
 C -1.414834 -1.045785 0.268589  
 C -2.077808 -2.897404 -1.675789  
 C -2.783267 -1.174144 -0.047324  
 C -0.748405 -2.721032 -1.330394  
 C -3.109022 -2.149387 -1.051076  
 C -3.818746 -0.385361 0.562558  
 H -4.736662 -3.077084 -2.136663  
 H -2.334588 -3.635792 -2.429277  
 C -5.152489 -0.594935 0.195874  
 C -5.460515 -1.587368 -0.786923  
 C -4.476248 -2.332995 -1.388371  
 O -3.512050 0.533112 1.491112  
 H -2.541132 0.567671 1.608076  
 O 0.242478 -3.495216 -1.908753  
 C 0.748305 -2.968914 -3.149960  
 H 1.500148 -3.681022 -3.496377  
 H 1.204042 -1.983985 -2.997265  
 H -0.056743 -2.895694 -3.890265  
 C -6.248602 0.221506 0.792137  
 O -7.528859 -0.252540 0.654609  
 C -7.791511 -1.557710 0.093580  
 H -8.840498 -1.497505 -0.213449  
 C -6.915086 -1.762079 -1.142231  
 H -7.207227 -1.017140 -1.895996  
 H -7.093522 -2.750472 -1.579973  
 O -6.099421 1.276424 1.363048  
 C -7.650659 -2.640190 1.162849  
 H -8.267145 -2.386984 2.030556  
 H -6.613431 -2.746194 1.495689  
 H -7.986189 -3.607143 0.770067  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67085375  
 Number of imaginary frequencies = 0

1d\_c16

B3LYP/6-31G\* Geometry  
 C 2.258865 -1.791182 0.212698  
 C 2.345208 -0.533574 2.654258  
 C 0.527068 -0.006572 0.798778  
 C 1.507195 0.444243 1.842833  
 C 0.786803 -1.469774 0.401791  
 C 2.880390 -1.708184 1.679275  
 C 4.412521 -1.919091 1.545513  
 C 4.728737 -2.397384 0.107683  
 N 4.338071 -1.285042 -0.789708  
 C 3.027785 -0.947962 -0.837455  
 C 5.396790 -0.879723 -1.710812  
 C 6.660190 -1.355440 -0.975370  
 C 6.211089 -2.630306 -0.224695  
 O -0.931001 -0.193363 1.223201  
 C 1.444164 -1.176709 3.747239  
 C 3.518612 0.135417 3.402795  
 O 2.521686 -0.167119 -1.637042  
 N 2.489759 -3.195108 -0.179001  
 C 3.802062 -3.582023 -0.291928  
 O 4.184165 -4.666775 -0.697909  
 H 0.572266 -2.003837 1.338167  
 H 2.491231 -2.629226 2.122253  
 H 4.768368 -2.649622 2.280188  
 H 4.976210 -0.996282 1.698907  
 H 5.356349 0.199561 -1.878486  
 H 5.276542 -1.378283 -2.682958  
 H 6.981413 -0.586551 -0.263390  
 H 7.492554 -1.543737 -1.659160  
 H 6.805168 -2.815416 0.674929  
 H 6.286848 -3.518948 -0.858568  
 H 2.011634 -1.925935 4.312467  
 H 0.554311 -1.663686 3.337450  
 H 1.103706 -0.408175 4.448864  
 H 4.090791 -0.640712 3.923983  
 H 3.147058 0.843753 4.144291  
 H 4.191422 0.688704 2.746540  
 H 1.772320 -3.679964 -0.717465  
 N 1.769957 1.740441 1.668847

O 2.541297 2.483951 2.338796  
C 1.092370 2.248777 0.482063  
C -0.244897 2.710968 -1.858903  
C 1.105405 3.561595 0.010523  
C 0.458715 1.185295 -0.147287  
C -0.228655 1.417129 -1.332739  
C 0.390473 3.763754 -1.197539  
H -0.731683 0.617647 -1.861847  
H -0.753287 2.925023 -2.793136  
C 1.794511 4.710677 0.590904  
H 2.492318 4.536992 1.398165  
C 1.553957 5.936333 0.105292  
H 2.058397 6.807041 0.517344  
C 0.542954 6.186675 -0.989081  
O 0.356712 4.983318 -1.795669  
C 1.041097 7.237922 -1.983613  
H 0.319024 7.358591 -2.797248  
H 2.001989 6.936198 -2.411066  
H 1.166893 8.204529 -1.484172  
C -0.819974 6.580165 -0.395551  
H -1.545513 6.758842 -1.196672  
H -0.727730 7.493058 0.203418  
H -1.200622 5.785357 0.253420  
C -0.460734 -1.774620 -0.395172  
C -1.444733 -1.034431 0.245188  
C -2.163012 -2.845330 -1.718193  
C -2.818615 -1.132550 -0.057931  
C -0.827152 -2.699240 -1.384293  
C -3.173293 -2.087575 -1.071363  
C -3.832731 -0.333609 0.574302  
H -4.829221 -2.970386 -2.151195  
H -2.441025 -3.567163 -2.480125  
C -5.174082 -0.514174 0.220044  
C -5.511061 -1.487068 -0.772729  
C -4.547202 -2.241563 -1.395748  
O -3.498913 0.566152 1.511813  
H -2.526307 0.580870 1.618540  
O 0.142129 -3.483172 -1.985560  
C 0.664649 -2.932771 -3.209271  
H 1.400247 -3.652133 -3.574856  
H 1.143736 -1.963815 -3.027647  
H -0.136361 -2.817886 -3.948701  
C -6.248754 0.312730 0.840429  
O -7.538615 -0.137216 0.711875  
C -7.830616 -1.429567 0.135749  
H -8.881933 -1.346864 -0.157750  
C -6.972457 -1.631444 -1.113200  
H -7.260444 -0.871195 -1.853149  
H -7.173170 -2.610410 -1.562326  
O -6.074462 1.356871 1.423889  
C -7.696033 -2.529493 1.187886  
H -8.297533 -2.278035 2.066543  
H -6.656919 -2.658332 1.506499  
H -8.053192 -3.484734 0.785635  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67012011  
Number of imaginary frequencies = 0

1e\_c01

B3LYP/6-31G\* Geometry  
C -2.720206 -1.012229 0.070156  
C -2.823874 0.617201 2.214381  
C -0.654023 0.444019 0.714401  
C -1.467743 1.182915 1.749781  
C -1.236243 -0.924690 0.365087  
C -3.456805 0.161159 0.826942  
C -4.980145 -0.132617 0.778832  
C -5.235647 -1.273081 -0.234954  
N -4.580127 -2.475839 0.325118  
C -3.250745 -2.404542 0.562257  
C -5.461986 -3.635881 0.424433  
C -6.614766 -3.253601 -0.522217  
C -6.691070 -1.713450 -0.426666  
O 0.703696 -0.015806 1.187099  
C -3.750751 1.703095 2.807495  
C -2.708814 -0.498486 3.277671  
O -2.562003 -3.285063 1.063629  
N -3.144159 -0.861934 -1.332450



C -4.486334 -1.029311 -1.575299  
 O -5.003746 -1.064386 -2.680172  
 H -1.196646 -1.436391 1.333714  
 H -3.295859 1.017312 0.162583  
 H -5.540571 0.767553 0.506466  
 H -5.361531 -0.479640 1.745308  
 H -5.809313 -3.769572 1.458153  
 H -4.923731 -4.542108 0.132883  
 H -7.555345 -3.741995 -0.251950  
 H -6.363984 -3.541585 -1.548514  
 H -7.287046 -1.407463 0.441225  
 H -7.118525 -1.260020 -1.323449  
 H -4.702942 1.239958 3.088036  
 H -3.952390 2.513760 2.104224  
 H -3.311027 2.149923 3.700038  
 H -3.702111 -0.901900 3.507787  
 H -2.303068 -0.073571 4.201652  
 H -2.074807 -1.339110 2.992671  
 H -2.497149 -1.135227 -2.064394  
 N -1.232175 2.490980 1.612514  
 O -1.677334 3.449547 2.308790  
 C -0.474176 2.752017 0.390929  
 C 0.692110 2.766862 -2.090310  
 C -0.074115 3.993561 -0.099111  
 C -0.302537 1.544140 -0.281767  
 C 0.295772 1.544392 -1.534715  
 C 0.535283 3.958617 -1.381969  
 H 0.455685 0.624487 -2.085274  
 H 1.134932 2.812845 -3.079847  
 O 0.919149 5.105043 -2.003289  
 C -0.256930 5.298556 0.530047  
 H -0.879729 5.357968 1.411982  
 C 0.339547 6.374710 -0.000880  
 H 0.217981 7.357300 0.448742  
 C 1.248745 6.281911 -1.203964  
 C 2.719647 6.167925 -0.769953  
 H 2.867724 5.281628 -0.145163  
 H 3.017016 7.047503 -0.188119  
 H 3.369932 6.093071 -1.648543  
 C 1.039247 7.460362 -2.157890  
 H 1.663904 7.340170 -3.048599  
 H 1.311306 8.400534 -1.666384  
 H -0.007534 7.518567 -2.470869  
 C -0.054517 -1.548929 -0.342388  
 C 1.047506 -1.012663 0.312132  
 C 1.378510 -3.053390 -1.555596  
 C 2.365613 -1.484451 0.093554  
 C 0.102169 -2.570633 -1.290014  
 C 2.507780 -2.540717 -0.871673  
 C 3.528978 -0.976629 0.754037  
 H 3.913585 -3.836045 -1.896204  
 H 1.538535 -3.831763 -2.292219  
 C 4.791061 -1.535755 0.473364  
 C 4.918046 -2.566066 -0.507718  
 C 3.811654 -3.050150 -1.151913  
 O -1.039540 -2.989877 -1.909511  
 C -0.959167 -4.100384 -2.796756  
 H -1.980997 -4.289881 -3.128719  
 H -0.568257 -4.986124 -2.282726  
 H -0.329756 -3.872425 -3.666030  
 O 3.375699 0.014564 1.629621  
 H 4.291197 0.258295 1.943320  
 C 5.964643 -1.029443 1.185810  
 C 6.317353 -3.048478 -0.800125  
 H 6.789677 -2.405756 -1.558096  
 H 6.304400 -4.067141 -1.203660  
 C 7.165276 -3.005059 0.467435  
 H 6.726948 -3.676495 1.218649  
 O 7.146916 -1.666415 1.032932  
 O 5.942786 -0.038822 1.919614  
 C 8.628622 -3.352200 0.252069  
 H 9.185377 -3.254610 1.188618  
 H 9.078931 -2.682844 -0.488599  
 H 8.723626 -4.383587 -0.104262  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.69015629  
 Number of imaginary frequencies = 0

1e\_c03

B3LYP/6-31G\* Geometry

C -2.700729 -1.048284 -0.012232  
C -2.851956 0.547865 2.157710  
C -0.659599 0.417377 0.685354  
C -1.496038 1.134378 1.718137  
C -1.223444 -0.951627 0.309265  
C -3.461165 0.103541 0.755914  
C -4.979746 -0.205679 0.677208  
C -5.209764 -1.328335 -0.368315  
N -4.547854 -2.536462 0.173041  
C -3.230216 -2.446752 0.460916  
C -5.455776 -3.652442 0.423005  
C -6.836760 -2.972488 0.400441  
C -6.663394 -1.777070 -0.564449  
O 0.695855 -0.035130 1.171532  
C -3.799230 1.616392 2.750044  
C -2.738121 -0.577995 3.210291  
O -2.555827 -3.309509 1.011267  
N -3.104777 -0.871031 -1.416341  
C -4.441521 -1.042983 -1.688503  
O -4.935257 -1.054520 -2.803652  
H -1.196263 -1.476463 1.271373  
H -3.301848 0.972100 0.107598  
H -5.542801 0.694002 0.409172  
H -5.374711 -0.568978 1.632408  
H -5.208917 -4.131419 1.374712  
H -5.360881 -4.407445 -0.369022  
H -7.091415 -2.617416 1.405708  
H -7.629231 -3.655604 0.081950  
H -7.371534 -0.968197 -0.363203  
H -6.795294 -2.079953 -1.607708  
H -4.750732 1.139545 3.009277  
H -3.998365 2.433983 2.054148  
H -3.378331 2.056061 3.655127  
H -3.730310 -0.992692 3.425093  
H -2.347166 -0.158746 4.143199  
H -2.094020 -1.409948 2.923262  
H -2.444316 -1.116363 -2.145896  
N -1.273625 2.446622 1.600136  
O -1.739534 3.391305 2.301861  
C -0.501238 2.731394 0.393057  
C 0.701695 2.789917 -2.070058  
C -0.109309 3.983473 -0.076559  
C -0.305304 1.533888 -0.291350  
C 0.311684 1.556321 -1.535048  
C 0.519731 3.971234 -1.350280  
H 0.491038 0.645106 -2.094027  
H 1.158820 2.852959 -3.052122  
O 0.899101 5.129342 -1.952396  
C -0.318954 5.278610 0.564393  
H -0.955663 5.319631 1.437378  
C 0.270323 6.368734 0.054412  
H 0.128203 7.344420 0.512969  
C 1.198978 6.302227 -1.135328  
C 2.664542 6.204659 -0.679902  
H 2.816064 5.313285 -0.063222  
H 2.939759 7.081539 -0.083274  
H 3.329335 6.149825 -1.549058  
C 0.987078 7.487795 -2.079873  
H 1.626943 7.386055 -2.962053  
H 1.238049 8.426432 -1.574402  
H -0.055518 7.534471 -2.408367  
C -0.025496 -1.556507 -0.387101  
C 1.061726 -1.017911 0.289621  
C 1.437778 -3.034653 -1.596289  
C 2.387193 -1.474604 0.083630  
C 0.153320 -2.567362 -1.342255  
C 2.552687 -2.517934 -0.892030  
C 3.536462 -0.963287 0.765700  
H 3.985362 -3.785748 -1.913856  
H 1.615162 -3.803551 -2.338922  
C 4.807943 -1.505470 0.494427  
C 4.958346 -2.522057 -0.497588  
C 3.865439 -3.010155 -1.161481  
O -0.976966 -2.991831 -1.978494  
C -0.875892 -4.092872 -2.875394

H -0.239954 -3.849926 -3.735841  
H -1.892265 -4.289694 -3.219508  
H -0.480962 -4.979458 -2.365878  
O 3.361291 0.015053 1.651600  
H 4.270010 0.264485 1.980183  
C 5.966927 -0.995497 1.227794  
C 6.366382 -2.985261 -0.778749  
H 6.840463 -2.327782 -1.522835  
H 6.369776 -3.998834 -1.195090  
C 7.198679 -2.948286 0.499380  
H 6.759348 -3.634186 1.236814  
O 7.158087 -1.617241 1.081433  
O 5.925000 -0.014675 1.973818  
C 8.668381 -3.275763 0.297054  
H 9.213040 -3.183233 1.241207  
H 9.119356 -2.592168 -0.430080  
H 8.779703 -4.301525 -0.070630  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68971582  
Number of imaginary frequencies = 0

1e\_c04

B3LYP/6-31G\* Geometry

C -2.609642 -1.078691 0.067050  
C -2.773197 0.492732 2.251392  
C -0.552986 0.336498 0.824091  
C -1.398704 1.059440 1.845817  
C -1.136571 -1.015550 0.417344  
C -3.362442 0.079404 0.831607  
C -4.885616 -0.198454 0.722961  
C -5.114796 -1.303048 -0.335613  
N -4.491486 -2.529936 0.209103  
C -3.170725 -2.479808 0.495942  
C -5.385444 -3.685359 0.230241  
C -6.495905 -3.258352 -0.747038  
C -6.565609 -1.722584 -0.595507  
O 0.780087 -0.150566 1.334882  
C -3.711523 1.569745 2.842334  
C -2.700431 -0.651064 3.288228  
O -2.508484 -3.382829 0.992678  
N -2.980343 -0.881261 -1.344884  
C -4.314805 -1.024590 -1.640006  
O -4.792618 -1.017892 -2.763205  
H -1.136621 -1.554449 1.371900  
H -3.171989 0.952225 0.197451  
H -5.428964 0.715243 0.461156  
H -5.302617 -0.572785 1.664303  
H -5.775113 -3.853546 1.243581  
H -4.842468 -4.585023 -0.072659  
H -7.449876 -3.749339 -0.534620  
H -6.204576 -3.508075 -1.772580  
H -7.190128 -1.445044 0.261842  
H -6.957177 -1.231826 -1.488986  
H -4.674596 1.105625 3.080862  
H -3.886099 2.399212 2.154052  
H -3.297446 1.990969 3.759335  
H -3.704248 -1.047554 3.481630  
H -2.314514 -0.255082 4.233306  
H -2.069325 -1.492298 2.998649  
H -2.310774 -1.142932 -2.060755  
N -1.154336 2.369077 1.741561  
O -1.620379 3.319332 2.435807  
C -0.357115 2.650179 0.551797  
C 0.889530 2.718499 -1.886529  
C 0.047428 3.903296 0.097544  
C -0.155849 1.455824 -0.134362  
C 0.497213 1.481920 -1.360119  
C 0.676556 3.900172 -1.174810  
H 0.686346 0.573237 -1.919922  
H 1.369670 2.784324 -2.857353  
O 1.147029 5.050182 -1.725490  
C -0.069420 5.179035 0.797369  
H -0.376971 5.170663 1.834113  
C 0.212908 6.315236 0.145786  
H 0.145326 7.277438 0.647607  
C 0.582306 6.334488 -1.319315  
C 1.695272 7.346159 -1.603498  
H 2.574256 7.131045 -0.988665

H 1.351941 8.362229 -1.381339  
 H 1.986485 7.300271 -2.657612  
 C -0.655108 6.605960 -2.191224  
 H -0.378186 6.615125 -3.251263  
 H -1.098323 7.575164 -1.936522  
 H -1.413313 5.832992 -2.030919  
 C 0.064239 -1.631868 -0.264863  
 C 1.146163 -1.128547 0.447258  
 C 1.529089 -3.103572 -1.479764  
 C 2.467130 -1.605494 0.261265  
 C 0.247459 -2.619672 -1.242766  
 C 2.635914 -2.628513 -0.734703  
 C 3.607700 -1.140372 0.990661  
 H 4.060430 -3.939502 -1.713251  
 H 1.709455 -3.858789 -2.235577  
 C 4.881475 -1.667967 0.704030  
 C 5.028202 -2.699415 -0.272703  
 C 3.942474 -3.153339 -0.971628  
 O -0.874195 -3.006187 -1.918243  
 C -0.770763 -4.086926 -2.839075  
 H -0.109044 -3.835812 -3.677480  
 H -1.781508 -4.256072 -3.213339  
 H -0.405366 -4.992871 -2.341798  
 O 3.421602 -0.213276 1.927438  
 H 4.314090 -0.050408 2.344204  
 C 6.044504 -1.145156 1.423186  
 C 6.411373 -3.278726 -0.431791  
 H 6.534801 -3.744584 -1.415785  
 H 6.564803 -4.067719 0.318178  
 C 7.481355 -2.205008 -0.227616  
 H 8.458518 -2.680974 -0.106768  
 O 7.282885 -1.533952 1.047879  
 O 5.960221 -0.362255 2.372279  
 C 7.561114 -1.168756 -1.346214  
 H 8.303611 -0.404800 -1.097563  
 H 6.596327 -0.677197 -1.507047  
 H 7.860670 -1.651226 -2.283592  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68811728  
 Number of imaginary frequencies = 0

1e\_c05

B3LYP/6-31G\* Geometry  
 C -2.806180 -0.755593 0.044554  
 C -2.801875 0.923424 2.154642  
 C -0.608384 0.454937 0.755722  
 C -1.371019 1.313097 1.736880  
 C -1.337549 -0.841821 0.407386  
 C -3.427811 0.513074 0.750235  
 C -4.971649 0.401969 0.641511  
 C -5.318780 -0.714012 -0.372339  
 N -4.840431 -1.978172 0.230946  
 C -3.523867 -2.065073 0.527833  
 C -5.860283 -3.021980 0.297692  
 C -6.912003 -2.517564 -0.707255  
 C -6.806871 -0.978582 -0.626785  
 O 0.660881 -0.151850 1.300504  
 C -3.616259 2.124452 2.688061  
 C -2.863927 -0.171257 3.244290  
 O -2.970440 -3.014246 1.069583  
 N -3.145732 -0.580697 -1.378074  
 C -4.486478 -0.586051 -1.679504  
 O -4.955274 -0.576268 -2.806390  
 H -1.404760 -1.328823 1.387057  
 H -3.138998 1.329286 0.078869  
 H -5.408969 1.358885 0.339027  
 H -5.430350 0.114688 1.594032  
 H -6.269755 -3.096802 1.314450  
 H -5.422623 -3.990811 0.041268  
 H -7.916312 -2.886208 -0.479773  
 H -6.648809 -2.846968 -1.717848  
 H -7.398892 -0.592732 0.211509  
 H -7.136765 -0.488121 -1.544965  
 H -4.625072 1.780946 2.941064  
 H -3.697168 2.935257 1.961043  
 H -3.160411 2.539854 3.587689  
 H -3.907521 -0.441686 3.444873  
 H -2.440971 0.223107 4.174074

H -2.330955 -1.091897 3.002408  
 H -2.506496 -0.944177 -2.076847  
 N -0.977557 2.580432 1.579991  
 O -1.335729 3.603738 2.232933  
 C -0.143270 2.716608 0.388150  
 C 1.120687 2.523648 -2.037562  
 C 0.417046 3.889320 -0.114712  
 C -0.085342 1.478033 -0.246722  
 C 0.561753 1.372020 -1.470617  
 C 1.071424 3.746448 -1.367372  
 H 0.635627 0.423968 -1.990744  
 H 1.607241 2.489355 -3.006819  
 O 1.609141 4.822273 -2.000912  
 C 0.358975 5.225051 0.472349  
 H -0.287197 5.380526 1.325296  
 C 1.094051 6.211016 -0.059699  
 H 1.067264 7.214005 0.359402  
 C 2.031555 5.983077 -1.222154  
 C 3.465404 5.729560 -0.727438  
 H 3.497093 4.850948 -0.075613  
 H 3.831647 6.589997 -0.156322  
 H 4.135652 5.563270 -1.578037  
 C 1.983789 7.146094 -2.216188  
 H 2.628373 6.934974 -3.075277  
 H 2.331333 8.068636 -1.738934  
 H 0.962071 7.300891 -2.575603  
 C -0.210763 -1.623068 -0.229819  
 C 0.918425 -1.207016 0.465011  
 C 1.083047 -3.315203 -1.348444  
 C 2.179259 -1.835192 0.313347  
 C -0.137037 -2.678779 -1.149638  
 C 2.234916 -2.924467 -0.623319  
 C 3.364773 -1.455703 1.020081  
 H 3.506146 -4.437906 -1.517177  
 H 1.178395 -4.128246 -2.058351  
 C 4.573113 -2.134526 0.770654  
 C 4.605020 -3.231206 -0.143705  
 C 3.475752 -3.602666 -0.821866  
 O -1.293328 -2.976241 -1.810868  
 C -1.308423 -4.112022 -2.669176  
 H -2.331136 -4.189868 -3.040982  
 H -1.045689 -5.023066 -2.119218  
 H -0.621898 -3.982616 -3.515195  
 O 3.283273 -0.459656 1.899549  
 H 4.189330 -0.371049 2.309417  
 C 5.788112 -1.697517 1.460359  
 C 5.916778 -3.965248 -0.262113  
 H 5.986301 -4.500944 -1.215341  
 H 5.986636 -4.718898 0.535120  
 C 7.097148 -3.002892 -0.119651  
 H 8.017608 -3.573372 0.032779  
 O 6.976397 -2.238272 1.112288  
 O 5.792078 -0.853953 2.360138  
 C 7.284787 -2.050428 -1.298140  
 H 8.107128 -1.358525 -1.093730  
 H 6.378601 -1.467182 -1.490139  
 H 7.526083 -2.617616 -2.204332  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68833465  
 Number of imaginary frequencies = 0

1e\_c06  
 B3LYP/6-31G\* Geometry  
 C -2.602529 -1.092082 -0.023621  
 C -2.804246 0.450317 2.181616  
 C -0.562629 0.319708 0.784054  
 C -1.426277 1.026657 1.801839  
 C -1.136049 -1.027888 0.350676  
 C -3.372361 0.050276 0.749459  
 C -4.891574 -0.234633 0.612375  
 C -5.101779 -1.324441 -0.471397  
 N -4.475762 -2.556768 0.058186  
 C -3.167789 -2.494347 0.393334  
 C -5.407553 -3.664883 0.247659  
 C -6.776689 -2.962883 0.199539  
 C -6.554297 -1.746132 -0.727860  
 O 0.763815 -0.170984 1.309699  
 C -3.755134 1.518269 2.768961

C -2.740778 -0.702450 3.208997  
O -2.525223 -3.381326 0.943127  
N -2.955656 -0.871168 -1.435488  
C -4.285010 -1.015204 -1.756636  
O -4.740849 -0.989087 -2.887599  
H -1.151056 -1.578899 1.298358  
H -3.179453 0.933106 0.130136  
H -5.433066 0.680314 0.351545  
H -5.323515 -0.618743 1.543276  
H -5.198770 -4.173470 1.193088  
H -5.298114 -4.399418 -0.561581  
H -7.057483 -2.629419 1.205248  
H -7.568937 -3.624929 -0.161221  
H -7.257500 -0.932211 -0.529690  
H -6.654939 -2.020682 -1.782386  
H -4.720818 1.048937 2.985905  
H -3.920495 2.355035 2.087244  
H -3.357606 1.930133 3.697455  
H -3.746393 -1.100934 3.389089  
H -2.365021 -0.314134 4.161326  
H -2.107200 -1.541026 2.917806  
H -2.274794 -1.111657 -2.147905  
N -1.182474 2.337913 1.720421  
O -1.661313 3.277520 2.420502  
C -0.365618 2.637025 0.548243  
C 0.922367 2.741352 -1.867254  
C 0.047424 3.896478 0.120157  
C -0.152303 1.452932 -0.151999  
C 0.520746 1.497171 -1.366305  
C 0.698815 3.912118 -1.140917  
H 0.719344 0.596849 -1.936241  
H 1.419329 2.821555 -2.828475  
O 1.181668 5.069151 -1.665437  
C -0.079741 5.161106 0.837859  
H -0.408921 5.136964 1.867706  
C 0.220667 6.306751 0.211588  
H 0.145926 7.260678 0.727997  
C 0.621640 6.350652 -1.244491  
C 1.750772 7.356296 -1.483949  
H 2.614268 7.119069 -0.855469  
H 1.413207 8.371123 -1.247639  
H 2.063720 7.329262 -2.532477  
C -0.593628 6.653318 -2.137081  
H -0.293596 6.681280 -3.190494  
H -1.032135 7.621869 -1.871954  
H -1.363211 5.885531 -2.009580  
C 0.076587 -1.634209 -0.318717  
C 1.145899 -1.137800 0.416712  
C 1.561650 -3.092755 -1.524686  
C 2.470138 -1.611844 0.246896  
C 0.275934 -2.612653 -1.302669  
C 2.655885 -2.624058 -0.757200  
C 3.598182 -1.154382 1.000168  
H 4.097326 -3.923419 -1.726422  
H 1.754570 -3.840587 -2.284782  
C 4.876838 -1.678402 0.729033  
C 5.040275 -2.698964 -0.256417  
C 3.966577 -3.145481 -0.978307  
O -0.835858 -2.994981 -1.996380  
C -0.718431 -4.067021 -2.925803  
H -1.724135 -4.235075 -3.313781  
H -0.356785 -4.976608 -2.432419  
H -0.047012 -3.806437 -3.753545  
O 3.396059 -0.237602 1.943788  
H 4.281338 -0.079073 2.377245  
C 6.027434 -1.163189 1.473114  
C 6.426268 -3.275871 -0.399064  
H 6.566126 -3.730765 -1.385990  
H 6.567908 -4.073061 0.344533  
C 7.492079 -2.203923 -0.165311  
H 8.467410 -2.680794 -0.033702  
O 7.272127 -1.547299 1.114080  
O 5.927018 -0.390865 2.429283  
C 7.589640 -1.155362 -1.270946  
H 8.328092 -0.394372 -1.002007  
H 6.627577 -0.661863 -1.441783  
H 7.904098 -1.627602 -2.208649

SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68764923

Number of imaginary frequencies = 0

1e\_c08

B3LYP/6-31G\* Geometry

C -2.768391 -0.926314 0.073807  
C -2.824213 0.726413 2.201122  
C -0.654271 0.451595 0.721893  
C -1.440288 1.229355 1.745582  
C -1.284057 -0.901183 0.381190  
C -3.462610 0.283562 0.812302  
C -4.995923 0.051163 0.752631  
C -5.288194 -1.086734 -0.254148  
N -4.688068 -2.310772 0.322945  
C -3.359895 -2.291249 0.573986  
C -5.618328 -3.433303 0.421460  
C -6.744200 -3.011218 -0.540235  
C -6.758602 -1.468792 -0.456453  
O 0.687178 -0.084278 1.216706  
C -3.708881 1.857428 2.774142  
C -2.766276 -0.381448 3.277123  
O -2.711037 -3.192338 1.091590  
N -3.169658 -0.771332 -1.334621  
C -4.516442 -0.887263 -1.588769  
O -5.023210 -0.913366 -2.698240  
H -1.274667 -1.404654 1.354540  
H -3.260963 1.126016 0.141505  
H -5.516330 0.971257 0.467927  
H -5.399706 -0.271873 1.718226  
H -5.981144 -3.544044 1.452463  
H -5.114820 -4.362997 0.142244  
H -7.706731 -3.458461 -0.276337  
H -6.495146 -3.317291 -1.561658  
H -7.349069 -1.132276 0.403822  
H -7.159214 -1.004849 -1.360195  
H -4.681540 1.437187 3.051230  
H -3.872296 2.667703 2.060324  
H -3.259158 2.295451 3.666094  
H -3.778072 -0.736526 3.505638  
H -2.347194 0.034345 4.199319  
H -2.170704 -1.254100 3.005134  
H -2.530335 -1.089291 -2.055614  
N -1.143999 2.525967 1.600986  
O -1.550408 3.506374 2.286736  
C -0.358280 2.743723 0.387463  
C 0.846504 2.681657 -2.074573  
C 0.108125 3.960738 -0.104194  
C -0.233924 1.523109 -0.274087  
C 0.382672 1.483975 -1.517831  
C 0.736579 3.885595 -1.377267  
H 0.505377 0.553615 -2.059986  
H 1.308167 2.698338 -3.056222  
O 1.187325 5.004259 -1.998998  
C -0.021329 5.278105 0.511985  
H -0.653213 5.376409 1.383878  
C 0.635019 6.319412 -0.017940  
H 0.554687 7.309969 0.423199  
C 1.556335 6.175537 -1.206261  
C 3.014509 6.002717 -0.750844  
H 3.118380 5.117163 -0.116270  
H 3.341203 6.874635 -0.173372  
H 3.672140 5.892456 -1.619963  
C 1.410089 7.351308 -2.175124  
H 2.043528 7.195816 -3.053949  
H 1.713386 8.284361 -1.688535  
H 0.371712 7.449535 -2.505581  
C -0.130389 -1.585464 -0.319784  
C 0.990643 -1.096199 0.320079  
C 1.260029 -3.144550 -1.516746  
C 2.299671 -1.577023 0.098420  
C -0.000651 -2.621891 -1.263263  
C 2.412027 -2.650948 -0.846032  
C 3.466305 -1.042047 0.737865  
H 3.803209 -4.013379 -1.793422  
H 1.396927 -3.939725 -2.240128  
C 4.722621 -1.594001 0.458238  
C 4.814609 -2.682839 -0.462694

C 3.702535 -3.187392 -1.093753  
O -1.154282 -3.007890 -1.882680  
C -1.103460 -4.120626 -2.769793  
H -0.459823 -3.912858 -3.633622  
H -2.128270 -4.277030 -3.109519  
H -0.745036 -5.018229 -2.252643  
O 3.358309 -0.031422 1.614813  
H 2.421539 0.241247 1.684303  
C 5.961408 -1.027367 1.060053  
C 6.188234 -3.257360 -0.705135  
H 6.718575 -2.683084 -1.479348  
H 6.117104 -4.291963 -1.059143  
C 7.000702 -3.187557 0.583691  
H 6.481833 -3.758449 1.367699  
O 7.086702 -1.813084 1.012562  
O 6.063280 0.072052 1.552117  
C 8.430902 -3.685263 0.446291  
H 8.970390 -3.553859 1.388971  
H 8.959608 -3.125433 -0.332625  
H 8.441387 -4.748804 0.183206  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68119481  
Number of imaginary frequencies = 0

1e\_c09

B3LYP/6-31G\* Geometry

C 2.750333 -0.962797 0.009810  
C 2.854501 0.660875 -2.140955  
C 0.661174 0.429002 -0.687478  
C 1.470506 1.185111 -1.709329  
C 1.271944 -0.925315 -0.321006  
C 3.469748 0.226703 -0.739074  
C 4.998591 -0.024009 -0.651638  
C 5.264627 -1.149681 0.382161  
N 4.654299 -2.376180 -0.178923  
C 3.336842 -2.334228 -0.475984  
C 5.606583 -3.454357 -0.431573  
C 6.959937 -2.721900 -0.391055  
C 6.733406 -1.543837 0.584223  
O -0.679130 -0.099257 -1.194555  
C 3.760293 1.775686 -2.712729  
C 2.796890 -0.456311 -3.207164  
O 2.698842 -3.214167 -1.042190  
N 3.134406 -0.785961 1.419244  
C 4.475923 -0.911505 1.699430  
O 4.960357 -0.919959 2.818110  
H 1.273368 -1.440648 -1.288354  
H 3.271248 1.081147 -0.082787  
H 5.523326 0.893939 -0.368460  
H 5.414648 -0.359718 -1.607833  
H 5.385853 -3.933171 -1.389695  
H 5.533895 -4.219662 0.352698  
H 7.208762 -2.347328 -1.390704  
H 7.775512 -3.377253 -0.072739  
H 7.411058 -0.706252 0.396050  
H 6.869740 -1.851881 1.625372  
H 4.732339 1.341563 -2.970082  
H 3.921854 2.591864 -2.005254  
H 3.329195 2.208777 -3.616197  
H 3.807535 -0.824110 -3.420531  
H 2.393577 -0.044220 -4.138011  
H 2.189570 -1.320082 -2.933618  
H 2.481109 -1.076500 2.138992  
N 1.186607 2.486584 -1.585426  
O 1.613734 3.453608 -2.277601  
C 0.385692 2.728398 -0.386514  
C -0.855987 2.710933 2.057825  
C -0.074165 3.956634 0.082945  
C 0.237803 1.517696 0.288283  
C -0.397635 1.501206 1.523012  
C -0.722167 3.904708 1.347342  
H -0.539380 0.579204 2.074789  
H -1.331939 2.745079 3.032175  
O -1.169401 5.036091 1.948244  
C 0.079497 5.264531 -0.547642  
H 0.725072 5.344618 -1.411320  
C -0.572182 6.319934 -0.040360  
H -0.473648 7.303829 -0.492610



C -1.512599 6.201752 1.135675  
 C -2.965889 6.040366 0.660775  
 H -3.071088 5.148070 0.035939  
 H -3.273502 6.908635 0.067544  
 H -3.637502 5.949038 1.521351  
 C -1.366890 7.387621 2.092227  
 H -2.014515 7.249774 2.963626  
 H -1.652837 8.317933 1.590138  
 H -0.332320 7.478456 2.436442  
 C 0.101880 -1.590955 0.369806  
 C -1.004974 -1.098449 -0.291534  
 C -1.318165 -3.128260 1.559765  
 C -2.321146 -1.566078 -0.084134  
 C -0.049545 -2.618922 1.319152  
 C -2.456146 -2.630144 0.868605  
 C -3.473774 -1.027385 -0.745387  
 H -3.872720 -3.971216 1.808852  
 H -1.472260 -3.916055 2.287790  
 C -4.738767 -1.565763 -0.478614  
 C -4.853275 -2.644829 0.451261  
 C -3.754757 -3.152881 1.102916  
 O 1.093136 -3.010510 1.954793  
 C 1.022396 -4.116213 2.849360  
 H 0.371436 -3.895980 3.704593  
 H 2.042043 -4.279552 3.201044  
 H 0.661098 -5.014276 2.334989  
 O -3.344230 -0.026296 -1.630355  
 H -2.404060 0.236969 -1.689428  
 C -5.963871 -0.994520 -1.103579  
 C -6.235115 -3.204996 0.679907  
 H -6.771030 -2.618635 1.441106  
 H -6.178043 -4.236683 1.044820  
 C -7.029119 -3.140733 -0.620685  
 H -6.504783 -3.724064 -1.391797  
 O -7.096661 -1.769909 -1.064206  
 O -6.049191 0.100733 -1.607940  
 C -8.465590 -3.624052 -0.498202  
 H -8.990987 -3.496736 -1.449377  
 H -8.999625 -3.051959 0.268065  
 H -8.489643 -4.684909 -0.225305  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68073038  
 Number of imaginary frequencies = 0

1e\_c10  
 B3LYP/6-31G\* Geometry  
 C -2.834838 -0.686225 0.044261  
 C -2.793781 1.014887 2.134806  
 C -0.608193 0.461503 0.759430  
 C -1.345231 1.349718 1.728372  
 C -1.372136 -0.819851 0.418615  
 C -3.420194 0.609901 0.729409  
 C -4.966187 0.545681 0.610276  
 C -5.341117 -0.571622 -0.392146  
 N -4.907032 -1.842625 0.229888  
 C -3.596983 -1.965865 0.539871  
 C -5.960826 -2.851965 0.304850  
 C -6.989104 -2.328056 -0.714249  
 C -6.835173 -0.792125 -0.654196  
 O 0.640249 -0.207085 1.327984  
 C -3.568435 2.251283 2.645518  
 C -2.903939 -0.064397 3.235916  
 O -3.075967 -2.922387 1.100401  
 N -3.155730 -0.518663 -1.383240  
 C -4.495521 -0.486969 -1.694195  
 O -4.954609 -0.478930 -2.824441  
 H -1.463015 -1.295180 1.401849  
 H -3.100895 1.409381 0.051528  
 H -5.371270 1.511794 0.292720  
 H -5.440141 0.284659 1.562870  
 H -6.378425 -2.898472 1.319889  
 H -5.553195 -3.837947 0.065179  
 H -8.006138 -2.661101 -0.488794  
 H -6.729945 -2.679767 -1.718319  
 H -7.420658 -0.375550 0.173898  
 H -7.142622 -0.304410 -1.581564  
 H -4.592554 1.949336 2.889119  
 H -3.609882 3.056060 1.908481

H -3.108824 2.658993 3.546769  
 H -3.957997 -0.296067 3.428980  
 H -2.476838 0.325207 4.165805  
 H -2.401844 -1.006106 3.009111  
 H -2.528584 -0.926395 -2.068988  
 N -0.901256 2.601319 1.567196  
 O -1.224328 3.639307 2.211365  
 C -0.047162 2.697635 0.384342  
 C 1.239662 2.435057 -2.022538  
 C 0.563762 3.843735 -0.119401  
 C -0.028346 1.451695 -0.240206  
 C 0.629887 1.309953 -1.454707  
 C 1.228836 3.665009 -1.363064  
 H 0.673116 0.355864 -1.966863  
 H 1.737833 2.373828 -2.984388  
 O 1.815603 4.711621 -1.997227  
 C 0.550376 5.184934 0.457158  
 H -0.096008 5.372103 1.303434  
 C 1.326859 6.138287 -0.075359  
 H 1.334435 7.143950 0.337897  
 C 2.264216 5.871351 -1.228833  
 C 3.687597 5.584887 -0.722890  
 H 3.693204 4.713884 -0.060229  
 H 4.073772 6.442099 -0.160276  
 H 4.357498 5.390691 -1.567606  
 C 2.252551 7.023269 -2.236810  
 H 2.895389 6.784385 -3.089832  
 H 2.623136 7.941342 -1.768501  
 H 1.237269 7.201907 -2.603280  
 C -0.273869 -1.647457 -0.213030  
 C 0.865822 -1.272129 0.470033  
 C 0.985435 -3.374917 -1.320107  
 C 2.119512 -1.904568 0.322362  
 C -0.219696 -2.712200 -1.131630  
 C 2.153136 -3.001512 -0.601105  
 C 3.305909 -1.500049 1.020146  
 H 3.432851 -4.505455 -1.490196  
 H 1.064178 -4.194991 -2.024141  
 C 4.501501 -2.199987 0.815020  
 C 4.516565 -3.295413 -0.102880  
 C 3.388834 -3.674158 -0.791031  
 O -1.381181 -2.982553 -1.796078  
 C -1.417072 -4.116886 -2.656338  
 H -2.438793 -4.170747 -3.034890  
 H -1.178613 -5.033952 -2.105387  
 H -0.721670 -4.001997 -3.497119  
 O 3.278731 -0.444275 1.848693  
 H 2.382051 -0.053475 1.848613  
 C 5.742443 -1.830417 1.551236  
 C 5.826277 -4.021692 -0.272720  
 H 5.852683 -4.561804 -1.225724  
 H 5.942928 -4.768837 0.525178  
 C 6.995321 -3.041257 -0.181578  
 H 7.932542 -3.602510 -0.109388  
 O 6.929254 -2.330520 1.073402  
 O 5.785464 -1.147813 2.548057  
 C 7.096766 -2.059007 -1.348173  
 H 7.922893 -1.362645 -1.175709  
 H 6.176054 -1.479317 -1.467403  
 H 7.287686 -2.598257 -2.283490  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67914223  
 Number of imaginary frequencies = 0

1e\_c11  
 B3LYP/6-31G\* Geometry  
 C -2.812375 -0.739091 -0.035506  
 C -2.831223 0.933992 2.081029  
 C -0.616349 0.429974 0.733365  
 C -1.381757 1.295628 1.700963  
 C -1.356137 -0.858003 0.365777  
 C -3.429106 0.537586 0.660861  
 C -4.970717 0.453080 0.509006  
 C -5.311722 -0.651716 -0.525505  
 N -4.869677 -1.928555 0.079286  
 C -3.571092 -2.027567 0.440188  
 C -5.949256 -2.886304 0.305674  
 C -7.207766 -2.006739 0.188211

C -6.804207 -0.883263 -0.793505  
O 0.633817 -0.225846 1.312364  
C -3.633272 2.152500 2.592781  
C -2.942085 -0.158286 3.169106  
O -3.062969 -2.961198 1.049903  
N -3.108002 -0.547630 -1.464172  
C -4.441025 -0.526401 -1.806043  
O -4.871387 -0.501096 -2.946343  
H -1.459738 -1.345788 1.341673  
H -3.111136 1.351251 -0.000354  
H -5.380305 1.418715 0.196138  
H -5.461212 0.175129 1.448514  
H -5.827584 -3.365371 1.281229  
H -5.929538 -3.672317 -0.461017  
H -7.459622 -1.585564 1.168406  
H -8.076452 -2.572831 -0.159445  
H -7.390951 0.028944 -0.652947  
H -6.924963 -1.196689 -1.834942  
H -4.656360 1.831445 2.815692  
H -3.675596 2.965297 1.864670  
H -3.195271 2.556633 3.506350  
H -3.995629 -0.407961 3.342260  
H -2.537035 0.228929 4.109793  
H -2.422601 -1.089958 2.941040  
H -2.461078 -0.927504 -2.147190  
N -0.955869 2.556050 1.559382  
O -1.305281 3.581606 2.209702  
C -0.087227 2.679169 0.389767  
C 1.235780 2.463495 -2.002146  
C 0.510007 3.840952 -0.094490  
C -0.038243 1.440281 -0.246887  
C 0.638978 1.322200 -1.453456  
C 1.193692 3.686585 -1.331160  
H 0.706189 0.374146 -1.974230  
H 1.747436 2.420800 -2.957899  
O 1.768792 4.749661 -1.948236  
C 0.465919 5.175893 0.495087  
H -0.193142 5.343174 1.335763  
C 1.231116 6.148427 -0.018895  
H 1.215863 7.149762 0.404566  
C 2.186001 5.910665 -1.164371  
C 3.609241 5.647271 -0.645752  
H 3.624852 4.770728 0.009408  
H 3.973064 6.506824 -0.071920  
H 4.291348 5.473290 -1.485094  
C 2.162436 7.071516 -2.161874  
H 2.818883 6.853116 -3.010002  
H 2.509937 7.992271 -1.681316  
H 1.147804 7.233603 -2.537715  
C -0.236622 -1.663759 -0.255834  
C 0.887277 -1.278740 0.447328  
C 1.061330 -3.365532 -1.357773  
C 2.151891 -1.891820 0.311447  
C -0.155589 -2.721488 -1.180475  
C 2.213856 -2.980342 -0.620604  
C 3.322849 -1.475475 1.028067  
H 3.527660 -4.457601 -1.504803  
H 1.161279 -4.179253 -2.066494  
C 4.531616 -2.155152 0.832345  
C 4.574967 -3.242601 -0.094176  
C 3.461986 -3.632782 -0.799704  
O -1.305351 -3.003643 -1.859797  
C -1.315121 -4.131290 -2.729554  
H -2.331737 -4.196771 -3.119739  
H -1.069357 -5.049392 -2.183501  
H -0.612047 -3.999217 -3.561400  
O 3.268584 -0.427518 1.865163  
H 2.365971 -0.050698 1.856733  
C 5.757795 -1.771936 1.586109  
C 5.897834 -3.947148 -0.253142  
H 5.944223 -4.480213 -1.209323  
H 6.016860 -4.697662 0.541220  
C 7.049913 -2.948970 -0.141309  
H 7.995110 -3.495749 -0.062272  
O 6.958033 -2.248777 1.118016  
O 5.778325 -1.096830 2.588731  
C 7.149190 -1.956377 -1.299308

H 7.961894 -1.248216 -1.111745  
H 6.220751 -1.390568 -1.425160  
H 7.359855 -2.485240 -2.236310  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67869938  
Number of imaginary frequencies = 0

1f\_c01

B3LYP/6-31G\* Geometry

C 2.662430 -1.205255 0.252124  
C 2.787158 0.390486 2.450098  
C 0.654190 0.281695 0.898241  
C 1.478729 1.015684 1.930697  
C 1.193090 -1.121897 0.619934  
C 3.450175 -0.115638 1.091378  
C 4.935739 -0.552145 1.129171  
C 5.172803 -1.523017 -0.056664  
N 4.451519 -1.035999 -1.267499  
C 3.088346 -0.952142 -1.213974  
C 5.265553 -1.100835 -2.482833  
C 6.444736 -1.996147 -2.061448  
C 6.606802 -1.719667 -0.551816  
O -0.731101 -0.080384 1.353463  
C 2.587157 -0.685732 3.543033  
C 3.756131 1.436380 3.050550  
O 2.348063 -0.710643 -2.156960  
N 3.153882 -2.557114 0.615272  
C 4.464507 -2.838817 0.319042  
O 4.970868 -3.949315 0.335349  
H 1.199224 -1.560139 1.625096  
H 3.421515 0.780523 0.460666  
H 5.193543 -1.064354 2.062869  
H 5.592047 0.318588 1.040624  
H 5.600919 -0.095154 -2.769483  
H 4.669629 -1.502770 -3.306961  
H 7.353975 -1.785175 -2.631779  
H 6.185582 -3.049706 -2.208991  
H 7.185087 -0.803362 -0.383927  
H 7.092979 -2.544046 -0.025413  
H 3.530897 -1.206092 3.741037  
H 1.836492 -1.442712 3.312091  
H 2.275271 -0.195848 4.471514  
H 4.666178 0.923983 3.381864  
H 3.309244 1.935268 3.911532  
H 4.033209 2.212473 2.334097  
H 2.496570 -3.322541 0.496868  
N 1.319308 2.327771 1.735010  
O 1.802148 3.287989 2.402776  
C 0.604903 2.577487 0.482970  
C -0.459090 2.543304 -2.043611  
C 0.283323 3.815362 -0.070166  
C 0.397340 1.354869 -0.150388  
C -0.141395 1.326729 -1.428628  
C -0.278651 3.754138 -1.373407  
H -0.278884 0.392049 -1.957586  
H -0.849768 2.571273 -3.055518  
C 0.505448 5.135067 0.513266  
H 1.096507 5.201786 1.416475  
C -0.017780 6.215225 -0.082825  
H 0.132924 7.208936 0.332239  
C -0.881609 6.114997 -1.318581  
O -0.581263 4.891587 -2.055292  
C -0.574635 7.240812 -2.309315  
H -1.168476 7.113966 -3.220022  
H 0.485415 7.234111 -2.580172  
H -0.817862 8.213182 -1.867715  
C -2.372992 6.093185 -0.943026  
H -2.990022 6.012946 -1.844885  
H -2.648224 7.010721 -0.410919  
H -2.591557 5.242910 -0.289460  
C -0.012285 -1.774152 -0.016581  
C -1.100419 -1.128969 0.554812  
C -1.488656 -3.355655 -1.073821  
C -2.437357 -1.545244 0.330522  
C -0.196535 -2.925846 -0.796509  
C -2.610102 -2.687662 -0.524566  
C -3.589824 -0.907334 0.889370  
H -4.053364 -4.024922 -1.436961

H -1.665615 -4.224262 -1.697017  
C -4.876535 -1.377925 0.560761  
C -5.029293 -2.525492 -0.275354  
C -3.931539 -3.151043 -0.801737  
O -3.405342 0.124286 1.710472  
H -4.311443 0.400402 2.024989  
O 0.943144 -3.559995 -1.196655  
C 0.826685 -4.682023 -2.065809  
H 0.332442 -4.401510 -3.003153  
H 0.273432 -5.500553 -1.589025  
H 1.848209 -5.004299 -2.272340  
C -6.044957 -0.689668 1.110432  
O -7.275966 -1.046088 0.680702  
C -7.406106 -1.832164 -0.534936  
H -7.142441 -1.172336 -1.373054  
C -6.439320 -3.011743 -0.501287  
H -6.513192 -3.579214 -1.435763  
H -6.741931 -3.687496 0.312596  
O -5.975059 0.201311 1.959940  
C -8.869947 -2.228468 -0.626366  
H -9.508482 -1.340684 -0.598614  
H -9.145982 -2.878499 0.210708  
H -9.058258 -2.764478 -1.562871  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.69072327  
Number of imaginary frequencies = 0

1f\_c02

B3LYP/6-31G\* Geometry

C 2.536637 -1.317960 0.272622  
C 2.638736 0.206103 2.521529  
C 0.590639 0.273975 0.856406  
C 1.401710 0.926298 1.952513  
C 1.057217 -1.152818 0.564489  
C 3.342672 -0.303653 1.185253  
C 4.794571 -0.833523 1.286803  
C 5.035904 -1.781590 0.083261  
N 4.411153 -1.215759 -1.146884  
C 3.054348 -1.050386 -1.160845  
C 5.283816 -1.296380 -2.319989  
C 6.382562 -2.274697 -1.867111  
C 6.479712 -2.053150 -0.342827  
O -0.836779 -0.014006 1.227354  
C 2.310876 -0.882928 3.569911  
C 3.635434 1.170836 3.206369  
O 2.380571 -0.738498 -2.132501  
N 2.925333 -2.707181 0.618311  
C 4.230087 -3.061153 0.379553  
O 4.666441 -4.201097 0.385954  
H 0.980996 -1.617455 1.554943  
H 3.403386 0.609374 0.581674  
H 4.968280 -1.389690 2.214710  
H 5.506939 -0.003619 1.263466  
H 5.694151 -0.305677 -2.556917  
H 4.709628 -1.636731 -3.186231  
H 7.332142 -2.103757 -2.382442  
H 6.068890 -3.305478 -2.061950  
H 7.103586 -1.180772 -0.114960  
H 6.885024 -2.921807 0.180815  
H 3.209958 -1.459981 3.813397  
H 1.536591 -1.591634 3.272780  
H 1.967706 -0.397709 4.489777  
H 4.488898 0.591216 3.575501  
H 3.170869 1.676632 4.053792  
H 4.005772 1.944833 2.530712  
H 2.230477 -3.427242 0.443562  
N 1.334536 2.250681 1.788762  
O 1.840189 3.159798 2.509008  
C 0.702855 2.579228 0.511067  
C -0.237292 2.682565 -2.062342  
C 0.482283 3.849796 -0.017161  
C 0.455247 1.390094 -0.169906  
C -0.021387 1.431889 -1.472274  
C -0.018967 3.860426 -1.346173  
H -0.189890 0.523419 -2.036790  
H -0.577543 2.763072 -3.089509  
C 0.753073 5.136367 0.617618  
H 1.304897 5.141764 1.547730

C 0.320847 6.262527 0.033835  
 H 0.509492 7.233134 0.486376  
 C -0.489611 6.248916 -1.241449  
 O -0.222249 5.033499 -2.004084  
 C -0.076715 7.385286 -2.180235  
 H -0.635833 7.320491 -3.119013  
 H 0.992314 7.326501 -2.405706  
 H -0.285017 8.355963 -1.717535  
 C -1.995822 6.299220 -0.933901  
 H -2.572954 6.283664 -1.865075  
 H -2.244562 7.213193 -0.382960  
 H -2.291783 5.442033 -0.321121  
 C -0.148869 -1.710883 -0.154744  
 C -1.225399 -1.013570 0.376617  
 C -1.659526 -3.168701 -1.334356  
 C -2.570997 -1.340702 0.071693  
 C -0.360439 -2.827758 -0.977046  
 C -2.766052 -2.445274 -0.827149  
 C -3.711278 -0.642912 0.583144  
 H -4.233682 -3.625348 -1.903503  
 H -1.854783 -4.004452 -1.995844  
 C -5.005926 -1.052178 0.207969  
 C -5.179944 -2.128399 -0.714294  
 C -4.095458 -2.804064 -1.204681  
 O -3.507715 0.378300 1.412589  
 H -4.408565 0.754519 1.621936  
 O 0.758292 -3.520500 -1.337045  
 C 0.620622 -4.608860 -2.244936  
 H 0.195146 -4.272689 -3.197595  
 H -0.005956 -5.404171 -1.822654  
 H 1.630302 -4.988236 -2.408154  
 C -6.162485 -0.360198 0.779119  
 O -7.402434 -0.844692 0.548836  
 C -7.573422 -2.187193 0.014715  
 H -8.596779 -2.171195 -0.370547  
 C -6.596485 -2.424592 -1.138342  
 H -6.875037 -1.761922 -1.970096  
 H -6.693545 -3.453248 -1.502891  
 O -6.072239 0.660860 1.465154  
 C -7.477474 -3.207022 1.146805  
 H -8.160880 -2.934663 1.956457  
 H -6.462025 -3.261899 1.551735  
 H -7.754181 -4.201840 0.779516  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68883860  
 Number of imaginary frequencies = 0

1f\_c03

B3LYP/6-31G\* Geometry  
 C 2.632148 -1.298660 0.228658  
 C 2.803879 0.284155 2.431978  
 C 0.660211 0.233173 0.890676  
 C 1.506392 0.941109 1.923784  
 C 1.166298 -1.180139 0.600075  
 C 3.448530 -0.228816 1.066890  
 C 4.922728 -0.700598 1.094936  
 C 5.134005 -1.683442 -0.090508  
 N 4.418345 -1.177553 -1.293395  
 C 3.061866 -1.040446 -1.235978  
 C 5.267153 -1.094640 -2.478518  
 C 6.676257 -1.033497 -1.865801  
 C 6.571211 -1.890761 -0.584735  
 O -0.730773 -0.103668 1.350796  
 C 2.585145 -0.794140 3.519345  
 C 3.798403 1.304734 3.033790  
 O 2.332622 -0.732884 -2.168457  
 N 3.092537 -2.660438 0.592834  
 C 4.393730 -2.979250 0.289763  
 O 4.865540 -4.103967 0.300829  
 H 1.163344 -1.624638 1.602580  
 H 3.434122 0.670960 0.440673  
 H 5.175119 -1.217796 2.027424  
 H 5.600300 0.153611 1.000934  
 H 5.000844 -0.215599 -3.071962  
 H 5.137701 -1.982372 -3.113358  
 H 6.922031 0.004258 -1.611766  
 H 7.445198 -1.398329 -2.552712  
 H 7.308347 -1.607962 0.172510

H 6.711724 -2.954071 -0.803174  
H 3.519571 -1.332037 3.714624  
H 1.821605 -1.536711 3.284125  
H 2.281886 -0.303609 4.450355  
H 4.698804 0.770547 3.356898  
H 3.366914 1.807468 3.900345  
H 4.088444 2.079493 2.320999  
H 2.416777 -3.410493 0.481845  
N 1.373409 2.257800 1.739898  
O 1.880933 3.202258 2.411902  
C 0.655079 2.532917 0.495618  
C -0.431968 2.543082 -2.021261  
C 0.352663 3.781970 -0.043292  
C 0.418271 1.320481 -0.146914  
C -0.132198 1.314999 -1.420483  
C -0.222509 3.743905 -1.341527  
H -0.293259 0.388303 -1.956754  
H -0.831398 2.587908 -3.029145  
C 0.605871 5.091666 0.550003  
H 1.207489 5.138712 1.447469  
C 0.097185 6.187129 -0.030576  
H 0.271344 7.173883 0.391859  
C -0.781622 6.114412 -1.257674  
O -0.510006 4.893473 -2.009663  
C -0.466291 7.244640 -2.240671  
H -1.071681 7.136548 -3.146181  
H 0.590599 7.223104 -2.522887  
H -0.688681 8.216547 -1.787232  
C -2.269002 6.114139 -0.865940  
H -2.897164 6.054289 -1.761681  
H -2.522487 7.030438 -0.321046  
H -2.495060 5.260730 -0.219040  
C -0.055035 -1.799207 -0.038462  
C -1.126567 -1.135963 0.543240  
C -1.568442 -3.333994 -1.111291  
C -2.472964 -1.520018 0.318068  
C -0.266347 -2.936155 -0.832804  
C -2.673143 -2.648127 -0.550202  
C -3.609595 -0.863255 0.887278  
H -4.148147 -3.941454 -1.475052  
H -1.766456 -4.190190 -1.745231  
C -4.907235 -1.300694 0.555963  
C -5.087625 -2.434392 -0.293532  
C -4.005331 -3.078314 -0.829615  
O -3.400056 0.153874 1.720398  
H -4.298981 0.446514 2.040518  
O 0.858512 -3.588021 -1.245352  
C 0.716429 -4.696613 -2.127842  
H 0.225594 -4.394506 -3.060294  
H 0.147531 -5.509199 -1.659372  
H 1.730515 -5.037285 -2.341251  
C -6.058624 -0.592427 1.115948  
O -7.298127 -0.914976 0.683873  
C -7.447822 -1.683308 -0.540876  
H -7.169566 -1.019850 -1.371403  
C -6.508856 -2.885381 -0.522586  
H -6.597320 -3.439933 -1.463518  
H -6.825813 -3.563494 0.283848  
O -5.966973 0.286331 1.976058  
C -8.920778 -2.043638 -0.635326  
H -9.537825 -1.141264 -0.595018  
H -9.211403 -2.697776 0.193559  
H -9.122985 -2.562595 -1.578511  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.69054004  
Number of imaginary frequencies = 0

1f\_c04  
B3LYP/6-31G\* Geometry  
C 2.491710 -1.422616 0.248942  
C 2.652207 0.087401 2.503140  
C 0.594162 0.221109 0.852751  
C 1.428936 0.842825 1.948910  
C 1.019504 -1.216416 0.549640  
C 3.331846 -0.432297 1.157980  
C 4.768818 -1.001356 1.244192  
C 4.976957 -1.959357 0.037926  
N 4.355510 -1.373338 -1.181103

C 3.008575 -1.154021 -1.184948  
C 5.263768 -1.318940 -2.322759  
C 6.642160 -1.363039 -1.643613  
C 6.421562 -2.244434 -0.393518  
O -0.839253 -0.030846 1.228843  
C 2.305942 -0.999305 3.547575  
C 3.678107 1.023066 3.184987  
O 2.346075 -0.779933 -2.142570  
N 2.845715 -2.821224 0.592235  
C 4.137485 -3.214952 0.339546  
O 4.535359 -4.367951 0.334981  
H 0.933543 -1.683913 1.538035  
H 3.409290 0.482067 0.558300  
H 4.937553 -1.563447 2.169525  
H 5.504120 -0.191480 1.214552  
H 5.082480 -0.411343 -2.905068  
H 5.109360 -2.182056 -2.985425  
H 6.939673 -0.349937 -1.348779  
H 7.419190 -1.758661 -2.303857  
H 7.136497 -2.028038 0.405717  
H 6.506294 -3.308600 -0.635325  
H 3.194822 -1.593383 3.787358  
H 1.519084 -1.693278 3.248619  
H 1.972968 -0.511567 4.469863  
H 4.520516 0.420967 3.543349  
H 3.233214 1.534762 4.039336  
H 4.061375 1.792181 2.510923  
H 2.130294 -3.522289 0.424009  
N 1.394444 2.169894 1.796972  
O 1.926627 3.059509 2.522476  
C 0.764593 2.525618 0.525905  
C -0.187386 2.676372 -2.040610  
C 0.575685 3.806241 0.009522  
C 0.482054 1.349280 -0.163644  
C -0.001241 1.415348 -1.462654  
C 0.066818 3.841888 -1.316084  
H -0.196912 0.516930 -2.034389  
H -0.531445 2.774681 -3.064966  
C 0.887339 5.079505 0.652352  
H 1.445827 5.061698 1.578279  
C 0.484216 6.222237 0.080124  
H 0.704526 7.183399 0.538477  
C -0.335641 6.242027 -1.188912  
O -0.108744 5.025535 -1.963084  
C 0.102527 7.373541 -2.122131  
H -0.465286 7.332071 -3.057001  
H 1.167715 7.286068 -2.356346  
H -0.074399 8.346149 -1.650500  
C -1.837452 6.332923 -0.869466  
H -2.421800 6.342960 -1.796205  
H -2.055352 7.248398 -0.308059  
H -2.153602 5.478919 -0.262376  
C -0.203971 -1.735067 -0.168887  
C -1.258769 -1.011943 0.371037  
C -1.757007 -3.138876 -1.358344  
C -2.613622 -1.297712 0.065550  
C -0.448054 -2.837629 -1.001273  
C -2.841480 -2.388468 -0.842591  
C -3.732496 -0.570751 0.583471  
H -4.344108 -3.515505 -1.927655  
H -1.977190 -3.962455 -2.027235  
C -5.038830 -0.938372 0.205776  
C -5.244969 -2.001255 -0.725345  
C -4.181202 -2.704896 -1.221737  
O -3.498292 0.437295 1.420947  
H -4.387422 0.838683 1.633572  
O 0.650809 -3.556467 -1.370796  
C 0.482016 -4.633031 -2.287551  
H 0.064811 -4.277323 -3.236797  
H -0.165797 -5.414147 -1.870846  
H 1.480686 -5.038602 -2.455304  
C -6.174052 -0.216434 0.782532  
O -7.428052 -0.661296 0.548345  
C -7.639505 -1.993414 0.002812  
H -8.661727 -1.943075 -0.382509  
C -6.669705 -2.250546 -1.152044  
H -6.927413 -1.572221 -1.977874



H -6.797989 -3.272448 -1.525836  
O -6.053125 0.795855 1.476822  
C -7.575040 -3.025209 1.126221  
H -8.250707 -2.739424 1.937732  
H -6.562017 -3.113787 1.531296  
H -7.880992 -4.008155 0.750291  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68856043  
Number of imaginary frequencies = 0

1f\_c05

B3LYP/6-31G\* Geometry  
C 2.704216 -1.138594 0.250898  
C 2.802422 0.481090 2.431589  
C 0.662143 0.292776 0.901004  
C 1.466904 1.057558 1.922447  
C 1.236392 -1.101325 0.633178  
C 3.466073 -0.016742 1.070783  
C 4.965010 -0.406090 1.094514  
C 5.218200 -1.379082 -0.086685  
N 4.466594 -0.925520 -1.292557  
C 3.102979 -0.882673 -1.222016  
C 5.268044 -0.971883 -2.517267  
C 6.480502 -1.825722 -2.104060  
C 6.651619 -1.533541 -0.598310  
O -0.716342 -0.129741 1.378465  
C 2.652780 -0.589254 3.537661  
C 3.741166 1.567109 3.008441  
O 2.341464 -0.669066 -2.154956  
N 3.240583 -2.471130 0.619372  
C 4.556615 -2.713406 0.307671  
O 5.097228 -3.806995 0.325414  
H 1.267068 -1.527239 1.642875  
H 3.402813 0.871685 0.431704  
H 5.250110 -0.902031 2.029097  
H 5.592220 0.484128 0.990790  
H 5.566917 0.042306 -2.813865  
H 4.676017 -1.398686 -3.331563  
H 7.375581 -1.589324 -2.686536  
H 6.253907 -2.888058 -2.241770  
H 7.202516 -0.598256 -0.443699  
H 7.170086 -2.338344 -0.072464  
H 3.617489 -1.070773 3.731722  
H 1.930648 -1.378063 3.322023  
H 2.331284 -0.101818 4.464111  
H 4.673737 1.091090 3.330674  
H 3.289867 2.057813 3.871841  
H 3.980855 2.345347 2.280747  
H 2.607019 -3.257748 0.507912  
N 1.256967 2.363231 1.720990  
O 1.707886 3.342360 2.379877  
C 0.518166 2.580030 0.475976  
C -0.579248 2.488894 -2.034870  
C 0.141387 3.801230 -0.078051  
C 0.348689 1.345899 -0.148265  
C -0.205057 1.288744 -1.419410  
C -0.437909 3.710102 -1.373241  
H -0.311415 0.346592 -1.942153  
H -0.985685 2.495970 -3.040784  
C 0.321588 5.131983 0.494333  
H 0.923449 5.228494 1.387594  
C -0.252614 6.186925 -0.100040  
H -0.134033 7.188075 0.307279  
C -1.131773 6.046999 -1.320654  
O -0.798139 4.828496 -2.054123  
C -0.881219 7.175396 -2.323998  
H -1.484310 7.019990 -3.223992  
H 0.173976 7.205618 -2.611656  
H -1.153284 8.141306 -1.885277  
C -2.614643 5.972531 -0.920854  
H -3.242478 5.862923 -1.811905  
H -2.915008 6.883292 -0.390945  
H -2.792198 5.120068 -0.257862  
C 0.053551 -1.805200 0.006909  
C -1.052125 -1.197264 0.563199  
C -1.390828 -3.437616 -1.020024  
C -2.381850 -1.624020 0.347734  
C -0.108834 -2.974866 -0.760556

C -2.532788 -2.783306 -0.482741  
C -3.531066 -0.961238 0.891435  
H -3.979971 -4.118921 -1.382989  
H -1.550240 -4.321361 -1.626721  
C -4.811007 -1.461118 0.620180  
C -4.944990 -2.614822 -0.212006  
C -3.847818 -3.247312 -0.746829  
O -3.388957 0.146581 1.636160  
H -2.440405 0.377146 1.698678  
O 1.045783 -3.582943 -1.159753  
C 0.951488 -4.724798 -2.006011  
H 0.441146 -4.475459 -2.943530  
H 0.423912 -5.547412 -1.507746  
H 1.979209 -5.024302 -2.215832  
C -6.021584 -0.835519 1.220879  
O -7.230870 -1.160820 0.656659  
C -7.286412 -1.900772 -0.580099  
H -6.946784 -1.238326 -1.389986  
C -6.346754 -3.098178 -0.488145  
H -6.378374 -3.683939 -1.413726  
H -6.698001 -3.751653 0.324257  
O -6.028129 -0.097667 2.178233  
C -8.745952 -2.269126 -0.795206  
H -9.368296 -1.369296 -0.796463  
H -9.097819 -2.928456 0.005441  
H -8.872704 -2.782877 -1.754683  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68188230  
Number of imaginary frequencies = 0

1f\_c06

B3LYP/6-31G\* Geometry

C 2.603181 -1.219672 0.272246  
C 2.655949 0.323942 2.508500  
C 0.594222 0.281207 0.864009  
C 1.374571 0.975255 1.952581  
C 1.119882 -1.129066 0.579354  
C 3.367575 -0.158257 1.166687  
C 4.845854 -0.612427 1.251560  
C 5.118673 -1.557829 0.052450  
N 4.449893 -1.035329 -1.173650  
C 3.087461 -0.934710 -1.169463  
C 5.311446 -1.077872 -2.357284  
C 6.463911 -1.995962 -1.912162  
C 6.568993 -1.758425 -0.390754  
O -0.826147 -0.093907 1.252915  
C 2.400986 -0.774416 3.567628  
C 3.608541 1.346147 3.172207  
O 2.384419 -0.657974 -2.131151  
N 3.063831 -2.584781 0.623010  
C 4.382858 -2.873978 0.369041  
O 4.875767 -3.990005 0.377336  
H 1.077330 -1.588481 1.573825  
H 3.373758 0.752201 0.556061  
H 5.061481 -1.149936 2.181635  
H 5.513942 0.252816 1.210297  
H 5.667372 -0.068784 -2.604065  
H 4.745271 -1.452508 -3.214507  
H 7.397007 -1.780832 -2.440709  
H 6.200388 -3.042605 -2.096230  
H 7.150132 -0.853519 -0.177296  
H 7.025295 -2.601054 0.133454  
H 3.334214 -1.297456 3.804143  
H 1.666285 -1.528702 3.282559  
H 2.040882 -0.303757 4.488583  
H 4.499925 0.816756 3.526019  
H 3.133083 1.828290 4.027450  
H 3.922057 2.136348 2.486609  
H 2.404868 -3.339674 0.454412  
N 1.231266 2.295016 1.786372  
O 1.688981 3.230709 2.501101  
C 0.567774 2.584974 0.514306  
C -0.406130 2.624548 -2.048351  
C 0.264130 3.838488 -0.011810  
C 0.382545 1.380841 -0.162188  
C -0.109533 1.389926 -1.459554  
C -0.252024 3.815444 -1.336258  
H -0.228090 0.471287 -2.020113

H -0.763144 2.682386 -3.071187  
 C 0.458174 5.139865 0.620323  
 H 1.013398 5.182409 1.547404  
 C -0.049731 6.235406 0.039191  
 H 0.077990 7.215624 0.492152  
 C -0.864384 6.173279 -1.231477  
 O -0.534955 4.970202 -1.992110  
 C -0.516935 7.326727 -2.175867  
 H -1.075258 7.227850 -3.112022  
 H 0.552881 7.325892 -2.405224  
 H -0.776723 8.286030 -1.715684  
 C -2.369243 6.141943 -0.916993  
 H -2.948552 6.091470 -1.845349  
 H -2.665085 7.043247 -0.368616  
 H -2.616744 5.272608 -0.299969  
 C -0.056934 -1.757581 -0.132920  
 C -1.163708 -1.115093 0.381208  
 C -1.514376 -3.289493 -1.288425  
 C -2.497025 -1.466144 0.071927  
 C -0.229050 -2.894482 -0.945918  
 C -2.653465 -2.594085 -0.799420  
 C -3.643125 -0.751970 0.555391  
 H -4.108513 -3.854854 -1.791079  
 H -1.679482 -4.147453 -1.929661  
 C -4.926931 -1.175142 0.188468  
 C -5.066356 -2.312770 -0.664689  
 C -3.971884 -2.994473 -1.140700  
 O -3.491386 0.306171 1.367141  
 H -2.538048 0.474488 1.507657  
 O 0.917164 -3.543550 -1.302410  
 C 0.819243 -4.649330 -2.194827  
 H 0.370133 -4.344503 -3.147140  
 H 0.231619 -5.464962 -1.755706  
 H 1.842912 -4.986678 -2.362868  
 C -6.138190 -0.439748 0.647485  
 O -7.344267 -1.087214 0.536492  
 C -7.418826 -2.474370 0.142195  
 H -8.452992 -2.588506 -0.198456  
 C -6.471051 -2.718746 -1.032096  
 H -6.821461 -2.120550 -1.885249  
 H -6.505359 -3.769719 -1.340214  
 O -6.147123 0.687073 1.085526  
 C -7.192219 -3.387719 1.346358  
 H -7.871222 -3.107340 2.157202  
 H -6.164849 -3.318554 1.717273  
 H -7.390324 -4.431066 1.073982  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67963648  
 Number of imaginary frequencies = 0

1f\_c07

B3LYP/6-31G\* Geometry  
 C 2.676882 -1.232836 0.227782  
 C 2.822067 0.375288 2.413784  
 C 0.669636 0.244213 0.893172  
 C 1.496255 0.983556 1.915774  
 C 1.211293 -1.160494 0.613136  
 C 3.467725 -0.129686 1.046844  
 C 4.956209 -0.554852 1.061869  
 C 5.184570 -1.540590 -0.118377  
 N 4.438790 -1.067542 -1.316906  
 C 3.080118 -0.971662 -1.243596  
 C 5.270801 -0.968453 -2.513097  
 C 6.684152 -0.857168 -1.917862  
 C 6.621705 -1.706141 -0.628422  
 O -0.715859 -0.153269 1.374975  
 C 2.654589 -0.697950 3.514525  
 C 3.786809 1.437703 2.991545  
 O 2.328312 -0.691580 -2.166938  
 N 3.182409 -2.576222 0.597745  
 C 4.490287 -2.855889 0.280543  
 O 4.996748 -3.964819 0.294027  
 H 1.233335 -1.593247 1.620246  
 H 3.418570 0.762968 0.412243  
 H 5.235353 -1.056032 1.995499  
 H 5.605438 0.319324 0.952936  
 H 4.969723 -0.103699 -3.110828  
 H 5.161674 -1.865692 -3.138087

H 6.899896 0.190044 -1.675655  
 H 7.456140 -1.203629 -2.610723  
 H 7.358558 -1.393629 0.117280  
 H 6.793354 -2.766285 -0.839807  
 H 3.611503 -1.195289 3.707292  
 H 1.920898 -1.474457 3.293655  
 H 2.339577 -0.210033 4.442961  
 H 4.711473 0.940500 3.304431  
 H 3.351299 1.931804 3.861083  
 H 4.037432 2.215751 2.267328  
 H 2.530046 -3.348029 0.493263  
 N 1.311477 2.294864 1.727033  
 O 1.786544 3.259060 2.391006  
 C 0.568282 2.537322 0.489426  
 C -0.550487 2.490853 -2.013082  
 C 0.209518 3.770598 -0.049800  
 C 0.370785 1.312537 -0.144925  
 C -0.193920 1.278148 -1.412048  
 C -0.381687 3.702775 -1.340946  
 H -0.322746 0.343285 -1.942698  
 H -0.964866 2.515010 -3.015494  
 C 0.417519 5.092187 0.534325  
 H 1.028052 5.169343 1.423581  
 C -0.143338 6.162842 -0.044564  
 H -0.004273 7.157563 0.371950  
 C -1.034784 6.050284 -1.259111  
 O -0.727051 4.834283 -2.007877  
 C -0.774178 7.184824 -2.252895  
 H -1.386605 7.048028 -3.149607  
 H 0.279088 7.201478 -2.548627  
 H -1.027630 8.150357 -1.802377  
 C -2.515369 5.995796 -0.847671  
 H -3.152186 5.905471 -1.734504  
 H -2.796550 6.905832 -0.306117  
 H -2.701355 5.139591 -0.191850  
 C 0.011270 -1.831918 -0.015464  
 C -1.078640 -1.205107 0.550637  
 C -1.471544 -3.419140 -1.057658  
 C -2.418094 -1.599777 0.334289  
 C -0.178824 -2.987956 -0.796851  
 C -2.596981 -2.745957 -0.508958  
 C -3.550810 -0.917567 0.888379  
 H -4.076017 -4.038160 -1.420668  
 H -1.652407 -4.291511 -1.674700  
 C -4.842304 -1.385131 0.614380  
 C -5.004206 -2.526014 -0.230509  
 C -3.922796 -3.177144 -0.774896  
 O -3.381753 0.178045 1.645480  
 H -2.428081 0.386714 1.707202  
 O 0.961306 -3.614637 -1.207802  
 C 0.840842 -4.743675 -2.067871  
 H 0.332910 -4.472285 -3.000596  
 H 0.297829 -5.561265 -1.577989  
 H 1.861530 -5.061543 -2.284758  
 C -6.037179 -0.738688 1.224308  
 O -7.254455 -1.029296 0.658309  
 C -7.328662 -1.753895 -0.586625  
 H -6.974446 -1.090491 -1.389455  
 C -6.417215 -2.973813 -0.509433  
 H -6.463850 -3.548272 -1.441424  
 H -6.782417 -3.627969 0.296226  
 O -6.025306 -0.011913 2.190060  
 C -8.796811 -2.085091 -0.803887  
 H -9.397530 -1.170764 -0.792868  
 H -9.163176 -2.745823 -0.010929  
 H -8.937069 -2.583615 -1.769478  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.68166375  
 Number of imaginary frequencies = 0

1f\_c08  
 B3LYP/6-31G\* Geometry  
 C 2.558587 -1.333368 0.246930  
 C 2.669130 0.194327 2.491066  
 C 0.599333 0.228574 0.855608  
 C 1.405594 0.888977 1.946317  
 C 1.079865 -1.195284 0.557978  
 C 3.359458 -0.299104 1.142116

C 4.822266 -0.799957 1.216520  
C 5.062286 -1.757023 0.015111  
N 4.403365 -1.209427 -1.201956  
C 3.049192 -1.046603 -1.192690  
C 5.300492 -1.111033 -2.350133  
C 6.684420 -1.089659 -1.680594  
C 6.514202 -1.977969 -0.427774  
O -0.830622 -0.106984 1.247702  
C 2.384921 -0.903573 3.543028  
C 3.655205 1.181629 3.158592  
O 2.360365 -0.699207 -2.141880  
N 2.977359 -2.711615 0.596270  
C 4.284444 -3.047385 0.333930  
O 4.734248 -4.180558 0.333981  
H 1.023785 -1.660078 1.549359  
H 3.387441 0.614858 0.537229  
H 5.027110 -1.345674 2.144307  
H 5.518478 0.043146 1.172459  
H 5.072053 -0.212897 -2.930522  
H 5.182280 -1.980279 -3.011929  
H 6.936714 -0.063273 -1.389563  
H 7.474132 -1.449935 -2.345870  
H 7.225408 -1.728726 0.365150  
H 6.644754 -3.037630 -0.668907  
H 3.302804 -1.455615 3.773405  
H 1.627709 -1.634083 3.254849  
H 2.041114 -0.428951 4.468183  
H 4.530498 0.622265 3.506511  
H 3.197171 1.672490 4.018316  
H 3.991865 1.966586 2.477850  
H 2.294181 -3.445825 0.434023  
N 1.302052 2.213877 1.792350  
O 1.791863 3.128795 2.512763  
C 0.640823 2.535406 0.526923  
C -0.349217 2.628637 -2.028046  
C 0.372155 3.802528 0.014227  
C 0.415166 1.343751 -0.159276  
C -0.085650 1.380245 -1.452882  
C -0.154071 3.807662 -1.306332  
H -0.236503 0.471314 -2.021420  
H -0.711782 2.706635 -3.047592  
C 0.611711 5.091593 0.655998  
H 1.176275 5.108646 1.578242  
C 0.133279 6.207543 0.088831  
H 0.295844 7.179308 0.548807  
C -0.694321 6.181493 -1.174688  
O -0.406579 4.976641 -1.949445  
C -0.322227 7.333289 -2.111643  
H -0.891224 7.258985 -3.043635  
H 0.745110 7.304230 -2.350553  
H -0.550611 8.295310 -1.640611  
C -2.196580 6.190637 -0.846645  
H -2.785414 6.166421 -1.770060  
H -2.461108 7.094544 -0.286676  
H -2.463793 5.322652 -0.235967  
C -0.117581 -1.779959 -0.156600  
C -1.202459 -1.108954 0.367407  
C -1.623811 -3.253776 -1.324613  
C -2.546692 -1.416098 0.058668  
C -0.326027 -2.901200 -0.982547  
C -2.739725 -2.529796 -0.823765  
C -3.669128 -0.672199 0.552655  
H -4.235400 -3.735978 -1.822834  
H -1.816838 -4.098760 -1.975217  
C -4.966247 -1.052473 0.185701  
C -5.142642 -2.177133 -0.677883  
C -4.070784 -2.886780 -1.164318  
O -3.482781 0.372515 1.374520  
H -2.524323 0.509945 1.513751  
O 0.799568 -3.578315 -1.351425  
C 0.666746 -4.671088 -2.255312  
H 0.223412 -4.343230 -3.202700  
H 0.057270 -5.474052 -1.822678  
H 1.679717 -5.035804 -2.430683  
C -6.153291 -0.285157 0.655577  
O -7.378617 -0.895230 0.543440  
C -7.496002 -2.275646 0.136153

H -8.534305 -2.355501 -0.201688  
C -6.560154 -2.536953 -1.044017  
H -6.895413 -1.920151 -1.889988  
H -6.627264 -3.583336 -1.362161  
O -6.126882 0.837514 1.103500  
C -7.292643 -3.206784 1.330803  
H -7.960777 -2.914492 2.146453  
H -6.262603 -3.171040 1.699010  
H -7.521859 -4.241264 1.049181  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.67944323  
Number of imaginary frequencies = 0

1g\_c01

B3LYP/6-31G\* Geometry

C 1.519716 -2.247416 0.179021  
C 2.267818 -0.940650 -2.044295  
C 1.029649 0.282684 -0.052430  
C 2.035633 0.247863 -1.155913  
C 0.987226 -0.949134 0.890314  
C 1.520067 -2.183176 -1.406814  
C 2.083223 -3.540275 -1.934645  
C 2.603069 -4.394735 -0.753886  
N 1.439999 -4.635141 0.114844  
C 0.749653 -3.568978 0.581351  
C 1.180699 -6.047632 0.373761  
C 2.538642 -6.690822 0.039252  
C 3.110722 -5.802215 -1.087741  
O -0.320569 0.296729 -0.675991  
C 3.796972 -1.133463 -2.252056  
C 1.626557 -0.654103 -3.430473  
O -0.292855 -3.662467 1.213568  
N 2.921204 -2.476079 0.590294  
C 3.589779 -3.553284 0.083200  
O 4.770566 -3.806801 0.269092  
H 1.611475 -0.774261 1.771908  
H 0.469599 -2.098106 -1.702573  
H 2.876289 -3.394908 -2.668939  
H 1.292275 -4.118357 -2.423547  
H 0.378722 -6.422354 -0.277891  
H 0.861239 -6.186906 1.410192  
H 2.443191 -7.739884 -0.255040  
H 3.195917 -6.643002 0.914388  
H 2.720721 -6.115635 -2.063207  
H 4.202140 -5.819056 -1.126640  
H 3.996918 -1.813156 -3.085545  
H 4.302659 -1.517938 -1.364558  
H 4.238897 -0.169525 -2.508185  
H 1.744067 -1.521496 -4.091644  
H 2.121754 0.203005 -3.895957  
H 0.560246 -0.429492 -3.329963  
H 3.424229 -1.808662 1.160797  
N 2.614729 1.433754 -1.281840  
O 3.432748 1.821695 -2.177120  
C 2.200501 2.315243 -0.196766  
C 1.154088 3.555597 2.015439  
C 2.644732 3.610101 0.055393  
C 1.280949 1.632036 0.592144  
C 0.746882 2.250628 1.713710  
C 2.071837 4.223046 1.201740  
H 0.022090 1.746492 2.344116  
H 0.765548 4.076028 2.884503  
O 2.455632 5.466691 1.591894  
C 3.650583 4.361147 -0.689891  
H 4.216683 3.840342 -1.450550  
C 3.844342 5.657061 -0.410882  
H 4.589288 6.238147 -0.949044  
C 3.012953 6.396125 0.611784  
C 1.843307 7.132112 -0.062861  
H 1.199451 6.423913 -0.593742  
H 2.216830 7.861895 -0.789937  
H 1.244255 7.660414 0.687049  
C 3.869399 7.355647 1.441732  
H 3.258242 7.837776 2.211211  
H 4.298678 8.132896 0.800448  
H 4.685192 6.815251 1.931125  
C -0.483835 -0.902179 1.254591  
C -1.161530 -0.223710 0.266303

C -2.540969 -1.203686 2.469788  
C -2.572783 -0.069039 0.265843  
C -1.162595 -1.351010 2.405547  
C -3.260747 -0.593911 1.412319  
C -3.317254 0.568657 -0.771720  
H -5.193253 -0.837310 2.365108  
H -3.097122 -1.549836 3.333078  
C -4.720815 0.654918 -0.672419  
C -5.388122 0.153524 0.485712  
C -4.678823 -0.454419 1.487199  
O -0.382904 -1.863617 3.386475  
C -1.013722 -2.567122 4.448280  
H -1.633287 -1.900744 5.062330  
H -0.205064 -2.969813 5.060666  
H -1.625941 -3.388286 4.058830  
O -2.654000 1.054224 -1.821712  
H -3.333789 1.497029 -2.403077  
C -5.471766 1.278616 -1.761050  
C -6.881424 0.360738 0.545504  
H -7.110645 1.350792 0.967281  
H -7.354125 -0.383876 1.195826  
C -7.482446 0.280425 -0.854415  
H -7.302209 -0.721515 -1.268014  
O -6.822547 1.228251 -1.736593  
O -4.941917 1.863968 -2.708662  
C -8.964642 0.608561 -0.916109  
H -9.319531 0.578659 -1.950423  
H -9.154358 1.609832 -0.514875  
H -9.537176 -0.118096 -0.329588  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72441273  
Number of imaginary frequencies = 0

1g\_c02

B3LYP/6-31G\* Geometry

C -1.179589 2.440564 0.255531  
C -2.086986 1.303808 -2.002332  
C -1.072808 -0.128234 -0.021681  
C -2.055066 0.082522 -1.127753  
C -0.840496 1.066983 0.940612  
C -1.174908 2.413253 -1.331438  
C -1.538980 3.850083 -1.821937  
C -1.954104 4.738653 -0.618530  
N -0.780086 4.797685 0.270281  
C -0.222295 3.627688 0.664375  
C -0.175661 6.125714 0.365950  
C -0.865305 6.902527 -0.772417  
C -2.236407 6.209911 -0.937978  
O 0.260124 -0.347854 -0.643987  
C -3.564388 1.727887 -2.240260  
C -1.465466 0.939685 -3.379484  
O 0.867415 3.548833 1.214079  
N -2.538720 2.848386 0.664695  
C -3.052947 4.018474 0.181946  
O -4.190505 4.422962 0.365564  
H -1.479843 0.972940 1.823706  
H -0.144556 2.187074 -1.623683  
H -2.339578 3.835324 -2.561888  
H -0.672533 4.324045 -2.294991  
H 0.910636 6.051563 0.261595  
H -0.388754 6.568048 1.347991  
H -0.279883 6.810469 -1.694371  
H -0.958915 7.968812 -0.548049  
H -2.659230 6.339100 -1.938218  
H -2.969505 6.591629 -0.220389  
H -3.639592 2.433876 -3.072639  
H -4.026109 2.181272 -1.361347  
H -4.142205 0.844018 -2.513488  
H -1.430135 1.824547 -4.026866  
H -2.078028 0.178087 -3.870729  
H -0.450295 0.548771 -3.260938  
H -3.136397 2.235867 1.204569  
N -2.807679 -0.998614 -1.278691  
O -3.665014 -1.244189 -2.187414  
C -2.545306 -1.949810 -0.204763  
C -1.728389 -3.367644 1.997402  
C -3.189266 -3.162181 0.025206  
C -1.537740 -1.429770 0.600350

C -1.119188 -2.138620 1.717659  
 C -2.730304 -3.873013 1.166346  
 H -0.331639 -1.761921 2.361804  
 H -1.435013 -3.953155 2.862407  
 O -3.308065 -5.046395 1.534444  
 C -4.295748 -3.733770 -0.736552  
 H -4.766709 -3.117927 -1.490815  
 C -4.694047 -4.986459 -0.477888  
 H -5.519014 -5.434258 -1.026733  
 C -3.993001 -5.862519 0.534339  
 C -2.944824 -6.755781 -0.149756  
 H -2.195566 -6.144227 -0.662035  
 H -3.421644 -7.403343 -0.893953  
 H -2.440623 -7.385793 0.591449  
 C -4.991000 -6.695420 1.342555  
 H -4.465506 -7.277028 2.106548  
 H -5.527347 -7.388389 0.685636  
 H -5.719873 -6.046365 1.837058  
 C 0.607575 0.796081 1.295738  
 C 1.171765 0.030920 0.299981  
 C 2.693356 0.786472 2.498984  
 C 2.544649 -0.330610 0.290563  
 C 1.352429 1.138444 2.442038  
 C 3.308874 0.081284 1.434806  
 C 3.182050 -1.062282 -0.756166  
 H 5.262116 0.035612 2.374888  
 H 3.300181 1.044291 3.358911  
 C 4.559307 -1.349865 -0.668773  
 C 5.299888 -0.958756 0.487449  
 C 4.692136 -0.263096 1.498585  
 O 0.663199 1.767280 3.423504  
 C 1.396927 2.351278 4.491882  
 H 1.904579 1.588679 5.096409  
 H 0.661573 2.868708 5.110389  
 H 2.130361 3.070893 4.110832  
 O 2.448348 -1.439998 -1.803723  
 H 3.053542 -1.970761 -2.393797  
 C 5.205792 -2.063469 -1.769265  
 C 6.748474 -1.378177 0.532554  
 H 6.836403 -2.395423 0.942800  
 H 7.327774 -0.716083 1.185852  
 C 7.344394 -1.368783 -0.871671  
 H 7.304846 -0.346921 -1.273803  
 O 6.550422 -2.203672 -1.757411  
 O 4.591056 -2.559279 -2.716670  
 C 8.764928 -1.902272 -0.950310  
 H 9.113377 -1.908552 -1.987247  
 H 8.814321 -2.925644 -0.563550  
 H 9.438387 -1.271735 -0.359776  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72422147  
 Number of imaginary frequencies = 0

1g\_c03  
 B3LYP/6-31G\* Geometry  
 C 2.682254 -0.620030 0.203003  
 C 2.370732 0.911739 -1.980986  
 C 0.561200 0.841173 -0.054178  
 C 1.337297 1.561900 -1.106924  
 C 1.366299 -0.093367 0.886904  
 C 2.691422 -0.518810 -1.381226  
 C 4.063835 -1.068195 -1.882548  
 C 4.991818 -1.357230 -0.679474  
 N 4.302560 -2.375582 0.128945  
 C 3.049644 -2.114552 0.568410  
 C 5.100999 -3.572750 0.372383  
 C 6.530011 -3.066850 0.105567  
 C 6.351946 -1.992386 -0.990450  
 O -0.382428 -0.079381 -0.742671  
 C 3.598595 1.857470 -2.110739  
 C 1.764551 0.712593 -3.397925  
 O 2.356128 -2.931238 1.157742  
 N 3.825208 0.186945 0.679479  
 C 5.075594 -0.098838 0.211225  
 O 6.089222 0.535045 0.463778  
 H 1.655453 0.442045 1.796434  
 H 1.895551 -1.185361 -1.728256  
 H 4.550887 -0.378437 -2.572741



H 3.926247 -2.014868 -2.415117  
H 4.816033 -4.377882 -0.319518  
H 4.935148 -3.933916 1.391039  
H 7.208839 -3.870134 -0.194694  
H 6.933559 -2.603389 1.012450  
H 6.326188 -2.454414 -1.984260  
H 7.141846 -1.238239 -0.975937  
H 4.249783 1.545292 -2.932545  
H 4.195108 1.908280 -1.198054  
H 3.243142 2.862038 -2.344296  
H 2.483143 0.202751 -4.051259  
H 1.529065 1.685781 -3.838193  
H 0.846879 0.118213 -3.351560  
H 3.698452 0.981792 1.292589  
N 0.915680 2.814649 -1.206751  
O 1.254256 3.695778 -2.061419  
C -0.039764 3.111298 -0.146037  
C -1.739685 3.179460 2.006279  
C -0.651109 4.332786 0.121884  
C -0.236222 1.953437 0.599226  
C -1.092716 1.978597 1.690911  
C -1.533300 4.325260 1.235287  
H -1.271413 1.090549 2.287879  
H -2.414496 3.245595 2.853258  
O -2.157478 5.463466 1.637101  
C -0.441270 5.598177 -0.575340  
H 0.357045 5.652950 -1.303241  
C -1.230372 6.643257 -0.292845  
H -1.092173 7.598258 -0.793955  
C -2.382163 6.544796 0.680183  
C -3.698816 6.257601 -0.060568  
H -3.627176 5.319085 -0.619089  
H -3.920716 7.060447 -0.772501  
H -4.527259 6.182735 0.652482  
C -2.492983 7.801932 1.546206  
H -3.297648 7.686593 2.279262  
H -2.712986 8.674941 0.922449  
H -1.555852 7.981511 2.081584  
C 0.277621 -1.106828 1.181064  
C -0.644166 -1.072323 0.158622  
C -1.014006 -2.802614 2.300438  
C -1.755491 -1.953010 0.092665  
C 0.070046 -1.936140 2.301588  
C -1.913895 -2.845605 1.206526  
C -2.692182 -1.995541 -0.984084  
H -3.113901 -4.448525 2.039819  
H -1.194469 -3.468611 3.135940  
C -3.776448 -2.894150 -0.930451  
C -3.906585 -3.792905 0.170681  
C -3.008887 -3.760843 1.204357  
O 0.948535 -1.779829 3.319851  
C 0.948352 -2.746048 4.362307  
H 0.011269 -2.722985 4.933475  
H 1.775998 -2.474954 5.020042  
H 1.111944 -3.751659 3.958727  
O -2.503587 -1.178430 -2.020790  
H -3.228862 -1.384094 -2.675417  
C -4.755305 -2.892627 -2.017780  
C -5.034168 -4.791052 0.090084  
H -5.314719 -5.152558 1.085635  
H -4.706615 -5.666745 -0.488187  
C -6.254292 -4.184008 -0.604433  
H -6.958124 -4.978630 -0.867535  
O -5.876105 -3.638166 -1.899173  
O -4.614083 -2.245026 -3.058381  
C -6.982367 -3.117057 0.209710  
H -7.803895 -2.694142 -0.375978  
H -6.308321 -2.305216 0.500672  
H -7.398931 -3.560233 1.121444  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72263732  
Number of imaginary frequencies = 0

1g\_c04  
B3LYP/6-31G\* Geometry  
C 2.697034 -0.571703 0.279744  
C 2.396811 0.922737 -1.931064  
C 0.559881 0.854169 -0.027167

C 1.345162 1.571536 -1.076359  
C 1.359613 -0.065016 0.933535  
C 2.733975 -0.493565 -1.305478  
C 4.128891 -1.021948 -1.765778  
C 5.042973 -1.266154 -0.535097  
N 4.363541 -2.285747 0.283171  
C 3.077546 -2.060327 0.643715  
C 5.078832 -3.558337 0.360028  
C 6.155664 -3.415279 -0.732733  
C 6.409310 -1.894372 -0.829228  
O -0.368648 -0.078119 -0.719879  
C 3.612097 1.883925 -2.065772  
C 1.805692 0.692271 -3.349609  
O 2.354697 -2.913568 1.138983  
N 3.811155 0.266398 0.767253  
C 5.077800 0.009411 0.324045  
O 6.067383 0.678563 0.577601  
H 1.623572 0.478659 1.845927  
H 1.958162 -1.181116 -1.657108  
H 4.616165 -0.330699 -2.453973  
H 4.023184 -1.977441 -2.290150  
H 4.385516 -4.388428 0.197065  
H 5.523405 -3.683136 1.356220  
H 5.771929 -3.797740 -1.685463  
H 7.063340 -3.977198 -0.495108  
H 6.799549 -1.590569 -1.804638  
H 7.122699 -1.556424 -0.070975  
H 4.269778 1.572197 -2.882680  
H 4.205711 1.952033 -1.152321  
H 3.244163 2.881157 -2.310807  
H 2.536442 0.180853 -3.988137  
H 1.561736 1.654902 -3.808277  
H 0.895213 0.087155 -3.301040  
H 3.648750 1.084044 1.340805  
N 0.911013 2.818546 -1.196000  
O 1.249526 3.693604 -2.056759  
C -0.060465 3.117351 -0.150346  
C -1.787436 3.191127 1.980313  
C -0.686674 4.335628 0.097341  
C -0.255115 1.965711 0.604647  
C -1.125267 1.993405 1.685311  
C -1.582225 4.330895 1.200087  
H -1.302857 1.109556 2.288888  
H -2.473147 3.259593 2.818302  
O -2.221651 5.467167 1.582954  
C -0.480551 5.595873 -0.610247  
H 0.325697 5.651036 -1.329315  
C -1.282767 6.636187 -0.347739  
H -1.147821 7.587238 -0.857183  
C -2.444885 6.536856 0.612774  
C -3.750232 6.230649 -0.140222  
H -3.663766 5.287708 -0.689113  
H -3.971212 7.024825 -0.862091  
H -4.586096 6.154795 0.564013  
C -2.577075 7.801389 1.464991  
H -3.389382 7.685948 2.189553  
H -2.797443 8.666264 0.830125  
H -1.648043 7.994632 2.009645  
C 0.281716 -1.092803 1.213765  
C -0.629684 -1.070472 0.182175  
C -0.993463 -2.810890 2.317716  
C -1.729901 -1.964384 0.106749  
C 0.080560 -1.932390 2.327325  
C -1.886161 -2.860493 1.218140  
C -2.657864 -2.016644 -0.977134  
H -3.073494 -4.478525 2.040276  
H -1.169580 -3.483543 3.148793  
C -3.732076 -2.927761 -0.932688  
C -3.859980 -3.829497 0.166236  
C -2.970424 -3.788384 1.206600  
O 0.959164 -1.776224 3.345913  
C 0.961844 -2.745142 4.386036  
H 0.023720 -2.727492 4.955631  
H 1.787459 -2.472136 5.045471  
H 1.130186 -3.749120 3.980247  
O -2.471477 -1.195840 -2.011286  
H -3.189889 -1.408939 -2.671096

C -4.703410 -2.935220 -2.026664  
C -4.975548 -4.840242 0.075942  
H -5.258566 -5.207226 1.068793  
H -4.634484 -5.710830 -0.502215  
C -6.197740 -4.245054 -0.625309  
H -6.891284 -5.046692 -0.894419  
O -5.816959 -3.692876 -1.916654  
O -4.562181 -2.284512 -3.065355  
C -6.942278 -3.187532 0.186100  
H -7.764095 -2.771748 -0.404274  
H -6.278553 -2.369543 0.483522  
H -7.360531 -3.637065 1.093940  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72250237  
Number of imaginary frequencies = 0

1g\_c09

B3LYP/6-31G\* Geometry

C -1.014516 2.450370 0.198911  
C -1.739532 1.310929 -2.111486  
C -1.004939 -0.110606 -0.019415  
C -1.901134 0.134923 -1.190295  
C -0.790129 1.082926 0.945616  
C -0.828312 2.384618 -1.374525  
C -1.042269 3.822691 -1.940887  
C -1.559451 4.753884 -0.821339  
N -0.496470 4.786537 0.195897  
C -0.140882 3.622442 0.782407  
C -0.133704 6.136766 0.626603  
C -1.306324 6.981478 0.094301  
C -1.772082 6.228904 -1.171612  
O 0.343265 -0.368630 -0.557424  
C -3.136620 1.825674 -2.558642  
C -0.983972 0.833706 -3.384344  
O 0.683292 3.536944 1.682832  
N -2.399973 2.920793 0.439500  
C -2.789513 4.090757 -0.157682  
O -3.929906 4.527727 -0.172486  
H -1.522137 1.030917 1.752746  
H 0.209825 2.088347 -1.550953  
H -1.731715 3.830822 -2.785361  
H -0.093860 4.242470 -2.291119  
H 0.822776 6.436436 0.178242  
H -0.016639 6.163322 1.713546  
H -1.015685 8.015846 -0.109645  
H -2.118087 6.997485 0.829719  
H -1.150491 6.497454 -2.033978  
H -2.817957 6.422525 -1.419165  
H -3.048405 2.491004 -3.422421  
H -3.678861 2.354880 -1.772959  
H -3.738189 0.970245 -2.868096  
H -0.803345 1.681662 -4.056577  
H -1.591475 0.097026 -3.918710  
H -0.024863 0.375814 -3.126022  
H -3.116757 2.295683 0.787173  
N -2.714467 -0.897410 -1.365648  
O -3.525933 -1.114930 -2.321912  
C -2.573144 -1.842797 -0.263340  
C -1.943360 -3.292636 1.979785  
C -3.305078 -3.008252 -0.053177  
C -1.570135 -1.381343 0.582829  
C -1.245261 -2.107496 1.720456  
C -2.941817 -3.737686 1.110479  
H -0.458219 -1.781542 2.392480  
H -1.722214 -3.891690 2.856891  
O -3.607560 -4.868851 1.459572  
C -4.414232 -3.513145 -0.857398  
H -4.813299 -2.875740 -1.634990  
C -4.904482 -4.734683 -0.607850  
H -5.734151 -5.131732 -1.187655  
C -4.304426 -5.646779 0.436760  
C -3.290463 -6.611740 -0.199346  
H -2.482624 -6.053868 -0.683013  
H -3.778135 -7.231842 -0.959734  
H -2.859363 -7.268125 0.564614  
C -5.386912 -6.405415 1.208365  
H -4.932529 -7.011781 1.998156  
H -5.939090 -7.068851 0.534336

H -6.092432 -5.706262 1.667265  
C 0.631178 0.756871 1.421266  
C 1.222359 -0.007384 0.420134  
C 2.722149 0.632045 2.632303  
C 2.582479 -0.395851 0.404979  
C 1.385807 1.023335 2.594435  
C 3.346897 -0.036753 1.566315  
C 3.214489 -1.107888 -0.661698  
H 5.288127 -0.157698 2.527532  
H 3.282802 0.850887 3.535072  
C 4.583679 -1.427892 -0.569017  
C 5.322065 -1.092645 0.609595  
C 4.723245 -0.414842 1.635218  
O 0.956520 1.602999 3.740947  
C -0.421581 1.800969 4.009991  
H -0.856272 2.553933 3.347991  
H -0.466714 2.162530 5.039592  
H -0.981622 0.858901 3.941967  
O 2.488665 -1.433642 -1.731867  
H 3.093858 -1.956148 -2.331584  
C 5.226518 -2.115708 -1.686543  
C 6.758084 -1.552715 0.655087  
H 6.812770 -2.586623 1.027708  
H 7.346630 -0.931667 1.339556  
C 7.371548 -1.508798 -0.740837  
H 7.364463 -0.472553 -1.106341  
O 6.566958 -2.289705 -1.665476  
O 4.612059 -2.561500 -2.659844  
C 8.778148 -2.077794 -0.821860  
H 9.139474 -2.057430 -1.854205  
H 8.794855 -3.115002 -0.470796  
H 9.460789 -1.487039 -0.201508  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71671586  
Number of imaginary frequencies = 0

1g\_c10

B3LYP/6-31G\* Geometry  
C -0.931808 2.502999 0.268107  
C -1.719803 1.436805 -2.058141  
C -1.026656 -0.052761 0.002711  
C -1.919828 0.250638 -1.157117  
C -0.753942 1.113951 0.985834  
C -0.764142 2.462264 -1.308930  
C -0.936406 3.919132 -1.840062  
C -1.415255 4.846587 -0.693376  
N -0.345488 4.818564 0.316071  
C 0.013090 3.625550 0.837249  
C 0.245206 6.124708 0.596292  
C -0.204126 6.958379 -0.617400  
C -1.556396 6.336475 -1.033413  
O 0.305116 -0.362229 -0.547752  
C -3.099597 2.011545 -2.485586  
C -0.991086 0.954793 -3.344798  
O 0.914829 3.480709 1.651962  
N -2.295985 3.016776 0.533149  
C -2.656723 4.210743 -0.035746  
O -3.781954 4.683673 -0.026514  
H -1.481399 1.075378 1.797907  
H 0.261062 2.132725 -1.501463  
H -1.637001 3.967855 -2.673787  
H 0.020242 4.313524 -2.198034  
H 1.329607 6.032199 0.699400  
H -0.149035 6.528871 1.538639  
H 0.527259 6.856410 -1.427342  
H -0.287952 8.022734 -0.380689  
H -1.786034 6.494432 -2.090899  
H -2.386247 6.752862 -0.453851  
H -2.993417 2.682773 -3.342814  
H -3.613278 2.552461 -1.688807  
H -3.737667 1.184577 -2.799154  
H -0.780959 1.807746 -4.002001  
H -1.630125 0.252826 -3.888999  
H -0.049200 0.454623 -3.101768  
H -3.029444 2.406893 0.873064  
N -2.775369 -0.744963 -1.344828  
O -3.600825 -0.912903 -2.299062  
C -2.666338 -1.714566 -0.260186

C -2.082694 -3.227852 1.953399  
 C -3.441985 -2.854448 -0.066953  
 C -1.641716 -1.308294 0.588277  
 C -1.339795 -2.066538 1.711044  
 C -3.101557 -3.618232 1.081495  
 H -0.537020 -1.783652 2.383939  
 H -1.880954 -3.850814 2.818432  
 O -3.808415 -4.729606 1.413392  
 C -4.572706 -3.302624 -0.874648  
 H -4.951355 -2.636526 -1.638310  
 C -5.106553 -4.509824 -0.645690  
 H -5.952591 -4.865029 -1.228937  
 C -4.536763 -5.462594 0.379202  
 C -3.560583 -6.451760 -0.278465  
 H -2.735449 -5.914679 -0.756461  
 H -4.072893 -7.041305 -1.046983  
 H -3.149702 -7.136013 0.472064  
 C -5.643733 -6.195443 1.140813  
 H -5.209428 -6.834909 1.915654  
 H -6.223875 -6.823273 0.456157  
 H -6.320045 -5.479563 1.617537  
 C 0.654853 0.719262 1.445342  
 C 1.203806 -0.060130 0.432485  
 C 2.742257 0.480436 2.644860  
 C 2.542027 -0.518339 0.408740  
 C 1.429257 0.943466 2.613801  
 C 3.327120 -0.212320 1.571378  
 C 3.133347 -1.250848 -0.667417  
 H 5.261481 -0.445867 2.525712  
 H 3.318236 0.666087 3.545419  
 C 4.483948 -1.643825 -0.581904  
 C 5.241602 -1.360708 0.598017  
 C 4.681590 -0.663433 1.632496  
 O 1.039211 1.551120 3.760346  
 C -0.323009 1.832188 4.035023  
 H -0.720838 2.599995 3.366556  
 H -0.339818 2.210527 5.059397  
 H -0.937672 0.923731 3.984504  
 O 2.389162 -1.526387 -1.739026  
 H 2.964858 -2.073534 -2.345741  
 C 5.087089 -2.352806 -1.708234  
 C 6.651814 -1.895690 0.634673  
 H 6.653617 -2.934813 0.996706  
 H 7.273764 -1.313194 1.323489  
 C 7.263038 -1.869339 -0.762653  
 H 7.308477 -0.830380 -1.117514  
 O 6.416463 -2.597912 -1.692487  
 O 4.447894 -2.755113 -2.684571  
 C 8.638083 -2.509415 -0.854066  
 H 8.997328 -2.496877 -1.887268  
 H 8.602047 -3.549748 -0.513856  
 H 9.351920 -1.961316 -0.229692  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71649697  
 Number of imaginary frequencies = 0

1g\_c11  
 B3LYP/6-31G\* Geometry  
 C 2.364110 -1.290100 0.218705  
 C 2.256885 0.094522 -2.068656  
 C 0.694130 0.649279 -0.023017  
 C 1.578636 1.072156 -1.151332  
 C 1.273238 -0.415132 0.942892  
 C 2.238907 -1.328814 -1.361977  
 C 3.359319 -2.268151 -1.906481  
 C 4.317216 -2.658875 -0.758578  
 N 3.495928 -3.398524 0.213127  
 C 2.447449 -2.759591 0.776975  
 C 4.088510 -4.665314 0.643111  
 C 5.545978 -4.531276 0.163469  
 C 5.453240 -3.630666 -1.087881  
 O -0.472880 -0.024216 -0.621453  
 C 3.667585 0.623457 -2.452811  
 C 1.419987 -0.007857 -3.375553  
 O 1.737937 -3.249495 1.645262  
 N 3.710478 -0.747544 0.520203  
 C 4.791156 -1.369325 -0.047327  
 O 5.941091 -0.959849 -0.004964

H 1.762429 0.085241 1.779677  
 H 1.265944 -1.776817 -1.583653  
 H 3.917201 -1.808851 -2.722820  
 H 2.927616 -3.197953 -2.290268  
 H 3.575326 -5.509016 0.163092  
 H 3.980013 -4.780248 1.725229  
 H 6.006153 -5.501127 -0.045312  
 H 6.146714 -4.031101 0.930972  
 H 5.188707 -4.222044 -1.972417  
 H 6.380135 -3.090205 -1.291063  
 H 4.065858 0.079375 -3.314185  
 H 4.393889 0.557957 -1.640825  
 H 3.578484 1.670910 -2.743110  
 H 1.858936 -0.755425 -4.047827  
 H 1.421581 0.957779 -3.890042  
 H 0.385053 -0.288713 -3.160523  
 H 3.834271 0.181602 0.903177  
 N 1.526444 2.388207 -1.302737  
 O 2.036313 3.101819 -2.225313  
 C 0.757656 2.989472 -0.218326  
 C -0.754909 3.630990 1.979880  
 C 0.539481 4.345393 0.009446  
 C 0.267959 1.968336 0.589414  
 C -0.497396 2.282959 1.703800  
 C -0.257294 4.637281 1.148873  
 H -0.905894 1.507822 2.343696  
 H -1.348295 3.922541 2.840097  
 O -0.506568 5.921624 1.513886  
 C 1.076159 5.467561 -0.754796  
 H 1.822452 5.260228 -1.509849  
 C 0.637132 6.707051 -0.498836  
 H 1.024174 7.560527 -1.050206  
 C -0.449880 6.985736 0.512782  
 C -1.824468 7.067966 -0.171193  
 H -2.055469 6.128116 -0.682244  
 H -1.833343 7.870936 -0.916670  
 H -2.605972 7.269367 0.569761  
 C -0.153290 8.251425 1.320587  
 H -0.923471 8.401405 2.083747  
 H -0.139795 9.127266 0.663129  
 H 0.818780 8.170660 1.816200  
 C -0.032934 -1.106677 1.353639  
 C -0.939012 -0.894235 0.318952  
 C -1.741702 -2.408370 2.466739  
 C -2.220739 -1.487179 0.239984  
 C -0.475929 -1.827243 2.494216  
 C -2.607211 -2.289128 1.366553  
 C -3.121066 -1.338557 -0.861447  
 H -4.162666 -3.547274 2.206940  
 H -2.055948 -2.965873 3.342910  
 C -4.385047 -1.958943 -0.814149  
 C -4.743879 -2.775122 0.304338  
 C -3.886846 -2.925575 1.359126  
 O 0.179700 -2.009040 3.665409  
 C 1.341684 -1.267297 3.997496  
 H 2.188714 -1.542503 3.364347  
 H 1.568735 -1.532980 5.032270  
 H 1.155687 -0.186392 3.943939  
 O -2.731066 -0.619698 -1.914569  
 H -3.476571 -0.672009 -2.578955  
 C -5.314050 -1.760393 -1.925104  
 C -6.069777 -3.487707 0.212047  
 H -6.447084 -3.751101 1.206357  
 H -5.941086 -4.428851 -0.341385  
 C -7.100874 -2.632032 -0.525552  
 H -7.964668 -3.247933 -0.791338  
 O -6.579551 -2.221696 -1.820506  
 O -5.005819 -1.191106 -2.976553  
 C -7.577088 -1.405787 0.249418  
 H -8.263079 -0.815820 -0.365593  
 H -6.738385 -0.767824 0.545881  
 H -8.106476 -1.718808 1.156557  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71484748  
 Number of imaginary frequencies = 0

1g\_c12  
 B3LYP/6-31G\* Geometry

C 2.393102 -1.256550 0.287832  
C 2.299184 0.095585 -2.021582  
C 0.702786 0.658632 -0.002622  
C 1.598952 1.076807 -1.123908  
C 1.277056 -0.390692 0.982471  
C 2.296489 -1.318741 -1.294680  
C 3.447475 -2.241401 -1.803094  
C 4.396935 -2.596002 -0.629847  
N 3.573209 -3.332932 0.340652  
C 2.475667 -2.727179 0.841798  
C 4.052096 -4.682543 0.627149  
C 4.993591 -4.957386 -0.559271  
C 5.544002 -3.565727 -0.945522  
O -0.451965 -0.027938 -0.608732  
C 3.705431 0.639437 -2.401203  
C 1.475246 -0.037014 -3.333867  
O 1.707665 -3.255617 1.634866  
N 3.722569 -0.684536 0.605343  
C 4.828171 -1.287132 0.063044  
O 5.966112 -0.848668 0.116619  
H 1.745221 0.124384 1.822460  
H 1.336268 -1.789113 -1.526087  
H 4.013296 -1.777826 -2.611219  
H 3.042954 -3.182653 -2.189187  
H 3.207851 -5.373378 0.698628  
H 4.586334 -4.703902 1.586873  
H 4.423890 -5.385904 -1.391780  
H 5.786888 -5.665197 -0.303229  
H 5.850084 -3.509425 -1.993884  
H 6.412155 -3.292968 -0.337384  
H 4.115769 0.093297 -3.255657  
H 4.428015 0.590464 -1.584565  
H 3.605010 1.683031 -2.701373  
H 1.929841 -0.788505 -3.991266  
H 1.468868 0.920976 -3.862526  
H 0.442141 -0.327921 -3.123712  
H 3.817858 0.257419 0.964769  
N 1.535241 2.390687 -1.291185  
O 2.047546 3.099290 -2.216174  
C 0.749271 2.996994 -0.221920  
C -0.791646 3.648495 1.953581  
C 0.517815 4.353412 -0.010472  
C 0.259278 1.980461 0.591122  
C -0.520537 2.299889 1.694048  
C -0.293038 4.650252 1.117669  
H -0.929226 1.527890 2.337654  
H -1.396254 3.944104 2.804550  
O -0.555719 5.936190 1.467485  
C 1.053489 5.472207 -0.780353  
H 1.809093 5.263437 -1.525684  
C 0.602066 6.710635 -0.541320  
H 0.987827 7.561668 -1.097336  
C -0.497269 6.990658 0.456552  
C -1.865495 7.055565 -0.241887  
H -2.084022 6.109172 -0.746326  
H -1.873193 7.851465 -0.994913  
H -2.655942 7.257663 0.489335  
C -0.218659 8.266616 1.254641  
H -0.997723 8.418132 2.008430  
H -0.205257 9.135978 0.588636  
H 0.748879 8.198400 1.760895  
C -0.027962 -1.091824 1.379766  
C -0.924319 -0.891446 0.334812  
C -1.739339 -2.397738 2.483708  
C -2.203335 -1.489486 0.248415  
C -0.475259 -1.814000 2.517223  
C -2.597017 -2.285519 1.376556  
C -3.094394 -1.351126 -0.861805  
H -4.155885 -3.542829 2.211789  
H -2.057098 -2.955425 3.358494  
C -4.357020 -1.974917 -0.821361  
C -4.723128 -2.784713 0.299348  
C -3.874706 -2.925665 1.362411  
O 0.178071 -1.999312 3.689498  
C 1.341879 -1.262392 4.025187  
H 2.187725 -1.530249 3.387079  
H 1.572783 -1.539718 5.055994

H 1.157194 -0.180759 3.984280  
O -2.697413 -0.638052 -1.916267  
H -3.437097 -0.696742 -2.586527  
C -5.276802 -1.786830 -1.941775  
C -6.046161 -3.501764 0.200472  
H -6.431270 -3.759607 1.193254  
H -5.910056 -4.446207 -0.345521  
C -7.073232 -2.654105 -0.551840  
H -7.933002 -3.274261 -0.820773  
O -6.541808 -2.251413 -1.845110  
O -4.961270 -1.223612 -2.994319  
C -7.559604 -1.423864 0.210391  
H -8.241882 -0.840236 -0.414712  
H -6.725334 -0.781401 0.509615  
H -8.095957 -1.732052 1.115088  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.71446236  
Number of imaginary frequencies = 0

1h\_c01

B3LYP/6-31G\* Geometry  
C -1.858302 -1.931177 0.184682  
C -2.163189 -0.579993 -2.076463  
C -0.816175 0.408846 -0.010264  
C -1.767927 0.550013 -1.158949  
C -1.018527 -0.834576 0.900688  
C -1.704772 -1.924661 -1.381306  
C -2.410999 -3.203563 -1.925732  
C -3.226999 -3.864463 -0.788071  
N -4.030478 -2.824864 -0.095024  
C -3.372430 -1.801184 0.508217  
C -5.424205 -3.216664 0.115809  
C -5.390373 -4.735342 -0.132775  
C -4.262755 -4.923543 -1.170222  
O 0.547464 0.235529 -0.591437  
C -1.391925 -0.435277 -3.416120  
C -3.682661 -0.486324 -2.379764  
O -3.882348 -0.923926 1.196004  
N -1.456521 -3.273289 0.656545  
C -2.208031 -4.343801 0.262133  
O -2.095652 -5.484629 0.687506  
H -1.562542 -0.544600 1.803378  
H -0.629697 -2.020945 -1.563130  
H -1.675567 -3.923967 -2.298740  
H -3.079884 -2.971739 -2.756341  
H -6.076803 -2.700250 -0.601420  
H -5.742410 -2.934006 1.123084  
H -6.353426 -5.123733 -0.476450  
H -5.121936 -5.257364 0.791681  
H -4.631914 -4.732821 -2.184815  
H -3.826074 -5.924070 -1.136391  
H -1.638305 -1.264926 -4.090421  
H -0.310607 -0.428398 -3.247832  
H -1.673742 0.501218 -3.906148  
H -3.986816 -1.250775 -3.100483  
H -3.892067 0.490908 -2.815233  
H -4.295423 -0.586381 -1.482022  
H -0.946854 -3.352504 1.531236  
N -2.138536 1.815605 -1.284677  
O -2.835067 2.347188 -2.207525  
C -1.632733 2.603677 -0.165575  
C -0.481229 3.625974 2.106852  
C -1.869372 3.949416 0.097342  
C -0.870849 1.770178 0.644366  
C -0.284415 2.275608 1.794478  
C -1.247145 4.444958 1.274458  
H 0.320901 1.648907 2.442112  
H -0.047579 4.063814 2.999791  
C -2.717527 4.861673 -0.663491  
H -3.333125 4.446856 -1.450354  
C -2.716359 6.166929 -0.362274  
H -3.345245 6.866051 -0.908264  
C -1.812695 6.749567 0.699412  
O -1.437495 5.729408 1.675719  
C -2.534076 7.817619 1.525350  
H -1.880313 8.182225 2.324036  
H -3.440637 7.404436 1.977534  
H -2.813754 8.665354 0.890703



C -0.522318 7.305298 0.073975  
 H 0.125588 7.726109 0.850907  
 H -0.757057 8.092705 -0.650983  
 H 0.022027 6.513085 -0.449388  
 C 0.428793 -1.207585 1.170342  
 C 1.237950 -0.575299 0.244994  
 C 2.387456 -2.194786 2.194186  
 C 2.648247 -0.747300 0.203336  
 C 1.012622 -2.019205 2.164415  
 C 3.216935 -1.582076 1.222243  
 C 3.504980 -0.149277 -0.772662  
 H 5.048723 -2.434805 2.008627  
 H 2.854993 -2.815036 2.949364  
 C 4.897636 -0.351906 -0.695486  
 C 5.444497 -1.198849 0.314262  
 C 4.627773 -1.788804 1.242319  
 O 2.952135 0.582197 -1.738330  
 H 3.697392 0.868341 -2.338205  
 O 0.135402 -2.602924 3.037322  
 C 0.655427 -3.420503 4.084686  
 H 1.317583 -2.841273 4.738313  
 H 1.196633 -4.284224 3.681420  
 H -0.212277 -3.762879 4.649657  
 C 5.763855 0.292100 -1.684676  
 O 7.102992 0.220504 -1.524844  
 C 7.646062 -0.174447 -0.235403  
 H 7.455805 0.655185 0.459412  
 C 6.935336 -1.426131 0.270050  
 H 7.319321 -1.697134 1.259870  
 H 7.170805 -2.260216 -0.407656  
 O 5.338489 0.894848 -2.672353  
 C 9.141253 -0.346985 -0.441685  
 H 9.579172 0.570126 -0.846228  
 H 9.341821 -1.164040 -1.142756  
 H 9.629674 -0.575757 0.511675  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.74074331  
 Number of imaginary frequencies = 0

1h\_c02  
 B3LYP/6-31G\* Geometry  
 C -1.136066 -2.338852 0.197434  
 C -1.761887 -1.153287 -2.091047  
 C -0.888597 0.210573 0.015958  
 C -1.787402 0.041648 -1.171247  
 C -0.715687 -1.033535 0.931428  
 C -0.930920 -2.284387 -1.361794  
 C -1.174437 -3.720920 -1.915747  
 C -1.787600 -4.604651 -0.801497  
 N -2.903948 -3.870881 -0.153355  
 C -2.625581 -2.693322 0.463419  
 C -4.114410 -4.677252 0.000570  
 C -3.598674 -6.109711 -0.226814  
 C -2.421344 -5.936027 -1.210764  
 O 0.480092 0.486348 -0.512138  
 C -1.019337 -0.765594 -3.398206  
 C -3.217263 -1.548438 -2.459792  
 O -3.411907 -2.022293 1.122108  
 N -0.350621 -3.486146 0.700127  
 C -0.711714 -4.739000 0.291786  
 O -0.261939 -5.786496 0.733890  
 H -1.356413 -0.933783 1.811406  
 H 0.126179 -2.036988 -1.501442  
 H -0.234706 -4.173266 -2.249257  
 H -1.846931 -3.713749 -2.775115  
 H -4.861139 -4.388625 -0.751883  
 H -4.551191 -4.508760 0.988735  
 H -4.376185 -6.777443 -0.608993  
 H -3.225374 -6.524974 0.715270  
 H -2.784418 -5.873168 -2.243414  
 H -1.695302 -6.749073 -1.141772  
 H -0.960775 -1.627588 -4.074269  
 H -0.004392 -0.416844 -3.184193  
 H -1.561890 0.035550 -3.908571  
 H -3.228536 -2.353899 -3.199766  
 H -3.714292 -0.682255 -2.897149  
 H -3.798877 -1.861513 -1.590848  
 H 0.125806 -3.400374 1.592839

N -2.532555 1.125195 -1.330218  
O -3.319521 1.409240 -2.289168  
C -2.351738 2.032678 -0.201906  
C -1.685090 3.365850 2.103124  
C -3.011483 3.235337 0.030883  
C -1.402483 1.482522 0.651177  
C -1.058172 2.146983 1.818350  
C -2.630664 3.901859 1.226474  
H -0.315493 1.744155 2.500091  
H -1.452000 3.918366 3.007260  
C -4.066509 3.835581 -0.780025  
H -4.487660 3.247066 -1.584026  
C -4.482348 5.078411 -0.502165  
H -5.271668 5.546794 -1.085241  
C -3.848035 5.915335 0.584677  
O -3.232818 5.062153 1.598244  
C -4.895391 6.724174 1.353970  
H -4.420463 7.275144 2.171887  
H -5.657492 6.061857 1.775426  
H -5.384622 7.443042 0.688094  
C -2.754465 6.827290 0.003598  
H -2.299782 7.429149 0.798303  
H -3.178164 7.502336 -0.748339  
H -1.973863 6.230024 -0.477886  
C 0.764090 -0.925513 1.256122  
C 1.361889 -0.062331 0.356602  
C 2.897389 -1.241944 2.354990  
C 2.754056 0.223559 0.365429  
C 1.540113 -1.513327 2.275678  
C 3.521802 -0.389848 1.410516  
C 3.408053 1.075993 -0.578837  
H 5.490463 -0.570634 2.302192  
H 3.510058 -1.680518 3.133384  
C 4.796717 1.292257 -0.476597  
C 5.538193 0.702206 0.589727  
C 4.919708 -0.119298 1.494587  
O 2.677339 1.631524 -1.543369  
H 3.297507 2.213426 -2.067273  
O 0.863361 -2.348330 3.122359  
C 1.576543 -2.956676 4.198092  
H 0.842603 -3.558330 4.735371  
H 1.993203 -2.196002 4.868146  
H 2.380595 -3.602304 3.826211  
C 5.461782 2.124081 -1.482123  
O 6.809022 2.209808 -1.482330  
C 7.601848 1.263202 -0.712015  
H 8.569139 1.765646 -0.624468  
C 6.996294 1.075923 0.680102  
H 7.096240 2.021245 1.232128  
H 7.564464 0.320682 1.234222  
O 4.852080 2.767248 -2.339571  
C 7.776551 -0.027916 -1.507765  
H 8.158424 0.197157 -2.507861  
H 6.830763 -0.569502 -1.610617  
H 8.493988 -0.684644 -1.002773  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73889287  
Number of imaginary frequencies = 0

1h\_c03  
B3LYP/6-31G\* Geometry  
C -1.809631 -1.980951 0.260774  
C -2.172310 -0.664278 -2.015314  
C -0.816217 0.376938 0.019363  
C -1.785830 0.484812 -1.118020  
C -0.981266 -0.858375 0.949126  
C -1.681853 -1.991797 -1.308788  
C -2.371933 -3.291205 -1.822402  
C -3.156135 -3.956305 -0.660605  
N -3.964929 -2.920292 0.027250  
C -3.322508 -1.867459 0.593267  
C -5.384012 -3.251587 0.118675  
C -5.547634 -4.303861 -0.991362  
C -4.184793 -5.030734 -1.034799  
O 0.542596 0.223408 -0.578152  
C -1.420371 -0.525063 -3.366624  
C -3.696493 -0.600034 -2.301212  
O -3.846775 -0.965783 1.237827

N -1.372574 -3.308256 0.740302  
 C -2.111001 -4.399886 0.377545  
 O -1.970334 -5.528775 0.823434  
 H -1.517157 -0.566096 1.855914  
 H -0.608317 -2.072932 -1.506256  
 H -1.629174 -4.003509 -2.196601  
 H -3.058653 -3.085756 -2.645621  
 H -5.991498 -2.353829 -0.026938  
 H -5.621869 -3.662273 1.109532  
 H -5.743394 -3.802961 -1.946497  
 H -6.380786 -4.985258 -0.797098  
 H -3.975667 -5.472968 -2.013380  
 H -4.133218 -5.832862 -0.291833  
 H -1.661110 -1.367968 -4.026417  
 H -0.337296 -0.497880 -3.212374  
 H -1.723961 0.399792 -3.865684  
 H -3.999458 -1.387914 -2.996757  
 H -3.925175 0.362087 -2.759916  
 H -4.294880 -0.680310 -1.391812  
 H -0.847404 -3.366413 1.607371  
 N -2.184130 1.740802 -1.253711  
 O -2.904301 2.246671 -2.173048  
 C -1.679606 2.552708 -0.151364  
 C -0.519385 3.625947 2.093001  
 C -1.940636 3.896373 0.098819  
 C -0.889783 1.745040 0.657962  
 C -0.298522 2.276326 1.793820  
 C -1.313449 4.418733 1.261620  
 H 0.328467 1.670090 2.440274  
 H -0.083090 4.083469 2.974708  
 C -2.817287 4.781746 -0.661503  
 H -3.433802 4.345005 -1.435705  
 C -2.839631 6.090196 -0.375389  
 H -3.489588 6.769706 -0.921462  
 C -1.935565 6.704164 0.668009  
 O -1.525222 5.703645 1.650497  
 C -2.669854 7.765213 1.491612  
 H -2.013189 8.155448 2.275661  
 H -3.559301 7.336196 1.962649  
 H -2.979553 8.597866 0.850940  
 C -0.665810 7.281076 0.019947  
 H -0.017571 7.724408 0.783959  
 H -0.926774 8.055203 -0.710351  
 H -0.110853 6.495179 -0.501804  
 C 0.476821 -1.199365 1.202807  
 C 1.260514 -0.562809 0.258788  
 C 2.468477 -2.135020 2.211304  
 C 2.673343 -0.706667 0.200119  
 C 1.090148 -1.986841 2.198626  
 C 3.272296 -1.517728 1.220885  
 C 3.504803 -0.102387 -0.793702  
 H 5.131374 -2.324326 1.991949  
 H 2.958602 -2.736316 2.967457  
 C 4.902234 -0.275349 -0.732475  
 C 5.479455 -1.099660 0.279111  
 C 4.687203 -1.695731 1.224298  
 O 2.924603 0.606700 -1.760058  
 H 3.656137 0.901779 -2.372356  
 O 0.236630 -2.576290 3.090788  
 C 0.786503 -3.371623 4.140070  
 H 1.447092 -2.772587 4.777255  
 H 1.337753 -4.230058 3.739110  
 H -0.066633 -3.723060 4.721404  
 C 5.742222 0.376227 -1.739229  
 O 7.084485 0.334885 -1.595512  
 C 7.651815 -0.035584 -0.309129  
 H 7.452661 0.796880 0.379770  
 C 6.973950 -1.296644 0.217516  
 H 7.376380 -1.549824 1.204713  
 H 7.217885 -2.132230 -0.455312  
 O 5.291923 0.959317 -2.727661  
 C 9.147625 -0.178544 -0.532842  
 H 9.560403 0.743087 -0.953248  
 H 9.356755 -0.999019 -1.227390  
 H 9.653070 -0.385893 0.416511  
 SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.74040355  
 Number of imaginary frequencies = 0

1h\_c04

B3LYP/6-31G\* Geometry

C -1.181545 -2.326626 0.271386  
C -1.825689 -1.161825 -2.025862  
C -0.875628 0.214956 0.040631  
C -1.795765 0.051376 -1.130813  
C -0.721292 -1.017635 0.975198  
C -1.010461 -2.301520 -1.293640  
C -1.297795 -3.740874 -1.816697  
C -1.899232 -4.598589 -0.671473  
N -2.983165 -3.829025 -0.013285  
C -2.674194 -2.640793 0.564629  
C -4.255056 -4.543401 0.045404  
C -4.089780 -5.598620 -1.061482  
C -2.577593 -5.916446 -1.065642  
O 0.492310 0.446871 -0.510300  
C -1.104507 -0.824503 -3.358628  
C -3.301326 -1.518883 -2.350448  
O -3.445004 -1.923952 1.193293  
N -0.405031 -3.480191 0.771588  
C -0.799931 -4.734078 0.396338  
O -0.361573 -5.779577 0.852191  
H -1.348358 -0.886036 1.860831  
H 0.049328 -2.082610 -1.457878  
H -0.376370 -4.218963 -2.165285  
H -1.990861 -3.734674 -2.660044  
H -5.084985 -3.850949 -0.121395  
H -4.394067 -5.004912 1.032656  
H -4.392253 -5.171241 -2.024441  
H -4.704657 -6.485584 -0.884232  
H -2.228093 -6.281786 -2.035866  
H -2.324183 -6.673564 -0.316861  
H -1.090570 -1.700761 -4.018626  
H -0.073501 -0.505518 -3.177071  
H -1.633202 -0.015922 -3.871682  
H -3.358425 -2.353270 -3.055378  
H -3.775721 -0.653321 -2.813526  
H -3.875709 -1.770300 -1.456905  
H 0.090215 -3.391107 1.653509  
N -2.513186 1.152177 -1.297886  
O -3.307343 1.440174 -2.249841  
C -2.291478 2.073077 -0.188075  
C -1.559427 3.423506 2.086731  
C -2.914615 3.297267 0.033111  
C -1.346794 1.510381 0.661880  
C -0.969603 2.183537 1.813831  
C -2.500899 3.971616 1.213215  
H -0.229688 1.771277 2.492924  
H -1.300066 3.983310 2.979156  
C -3.961824 3.914282 -0.775270  
H -4.407919 3.325462 -1.565447  
C -4.339636 5.172436 -0.512524  
H -5.121862 5.653792 -1.094603  
C -3.671095 6.007753 0.554742  
O -3.066771 5.153493 1.573914  
C -4.687979 6.855056 1.323546  
H -4.189211 7.405461 2.127547  
H -5.462121 6.219236 1.763413  
H -5.165967 7.576654 0.652446  
C -2.560867 6.882480 -0.051578  
H -2.081493 7.483224 0.729406  
H -2.975430 7.558017 -0.808164  
H -1.801519 6.258664 -0.533417  
C 0.764276 -0.937677 1.281166  
C 1.371236 -0.104218 0.360074  
C 2.901244 -1.280807 2.364755  
C 2.768999 0.153078 0.351422  
C 1.537842 -1.524495 2.303097  
C 3.533842 -0.457756 1.400206  
C 3.431296 0.976747 -0.612422  
H 5.506413 -0.663155 2.277686  
H 3.512171 -1.719151 3.144657  
C 4.824719 1.167700 -0.525276  
C 5.563949 0.580546 0.544231  
C 4.937552 -0.213859 1.467605  
O 2.703215 1.530604 -1.579853

H 3.330024 2.091731 -2.118357  
O 0.851915 -2.331033 3.169536  
C 1.562088 -2.936326 4.248960  
H 2.002087 -2.173687 4.901635  
H 2.347941 -3.606111 3.880884  
H 0.820364 -3.512093 4.803627  
C 5.496925 1.970510 -1.549454  
O 6.845499 2.030747 -1.561803  
C 7.626419 1.080420 -0.783872  
H 8.604323 1.564564 -0.712888  
C 7.029904 0.926822 0.616136  
H 7.153234 1.878382 1.152508  
H 7.588072 0.169140 1.177048  
O 4.892288 2.611291 -2.412297  
C 7.767725 -0.226255 -1.560733  
H 8.144128 -0.024502 -2.567854  
H 6.810340 -0.750295 -1.645839  
H 8.476915 -0.889223 -1.052239  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73854612  
Number of imaginary frequencies = 0

1h\_c05

B3LYP/6-31G\* Geometry

C -2.137343 -1.681034 0.177886  
C -2.296832 -0.263517 -2.057529  
C -0.767109 0.485435 -0.013784  
C -1.697064 0.780516 -1.148387  
C -1.126678 -0.732728 0.884718  
C -2.026390 -1.670339 -1.391052  
C -2.928692 -2.819839 -1.931167  
C -3.807396 -3.367840 -0.779857  
N -4.426421 -2.231587 -0.050301  
C -3.605365 -1.331019 0.547799  
C -5.858238 -2.410697 0.192577  
C -6.063307 -3.911790 -0.080014  
C -5.001244 -4.251779 -1.147883  
O 0.560719 0.107549 -0.619923  
C -1.572365 -0.225441 -3.429956  
C -3.794496 0.071324 -2.295824  
O -3.955737 -0.397808 1.261664  
N -1.927288 -3.076129 0.619048  
C -2.845719 -4.013499 0.234421  
O -2.897342 -5.164092 0.643080  
H -1.605183 -0.373172 1.799833  
H -0.982527 -1.923070 -1.603838  
H -2.319480 -3.637188 -2.330534  
H -3.574269 -2.479858 -2.742926  
H -6.441021 -1.787083 -0.498950  
H -6.104134 -2.101552 1.212156  
H -7.081759 -4.140440 -0.406768  
H -5.860096 -4.486995 0.829434  
H -5.361362 -3.992316 -2.150454  
H -4.721107 -5.307388 -1.137283  
H -1.988510 -0.985440 -4.102125  
H -0.499931 -0.414400 -3.317894  
H -1.707235 0.755011 -3.895673  
H -4.245718 -0.630505 -3.002789  
H -3.865190 1.071629 -2.723677  
H -4.376222 0.062672 -1.372727  
H -1.414930 -3.246225 1.479511  
N -1.862823 2.091352 -1.261972  
O -2.480753 2.730068 -2.169857  
C -1.220858 2.782347 -0.147339  
C 0.105912 3.587147 2.116743  
C -1.230341 4.146832 0.122117  
C -0.596197 1.830173 0.650571  
C 0.075996 2.224631 1.797347  
C -0.522087 4.526072 1.295070  
H 0.575618 1.503055 2.436125  
H 0.614341 3.943115 3.006467  
C -1.920829 5.191637 -0.627550  
H -2.603869 4.891498 -1.410855  
C -1.697070 6.476689 -0.322276  
H -2.202705 7.273944 -0.861574  
C -0.701569 6.896123 0.733834  
O -0.490313 5.820495 1.701179  
C -1.231553 8.062152 1.572047

H -0.518448 8.311562 2.364019  
H -2.188299 7.799204 2.032904  
H -1.376512 8.946926 0.943001  
C 0.657341 7.235942 0.099640  
H 1.373681 7.532660 0.873659  
H 0.551578 8.060619 -0.614007  
H 1.057436 6.371020 -0.438686  
C 0.252695 -1.321516 1.134799  
C 1.141354 -0.797506 0.227309  
C 2.068351 -2.591965 2.111464  
C 2.518646 -1.124734 0.170879  
C 0.731963 -2.233180 2.105529  
C 2.975659 -2.060381 1.153884  
C 3.432506 -0.566173 -0.781596  
H 4.709252 -3.120142 1.899453  
H 2.453534 -3.290784 2.844359  
C 4.777068 -0.960780 -0.763515  
C 5.216216 -1.892287 0.224551  
C 4.347164 -2.419100 1.151757  
O 3.018617 0.342858 -1.678523  
H 2.076278 0.549749 -1.522731  
O -0.211003 -2.713025 2.973665  
C 0.198657 -3.632564 3.985267  
H 0.612197 -4.546828 3.544216  
H -0.703669 -3.872348 4.548765  
H 0.939760 -3.174559 4.650285  
C 5.737327 -0.458857 -1.786572  
O 7.072512 -0.607327 -1.505582  
C 7.500984 -1.040524 -0.198125  
H 7.314257 -0.220804 0.511162  
C 6.679875 -2.256673 0.217712  
H 6.993802 -2.613584 1.205010  
H 6.873926 -3.067630 -0.499769  
O 5.435079 0.031237 -2.849024  
C 8.995304 -1.302254 -0.300124  
H 9.513483 -0.406921 -0.656161  
H 9.195877 -2.117335 -1.003625  
H 9.402959 -1.575183 0.679586  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73109560  
Number of imaginary frequencies = 0

1h\_c06

B3LYP/6-31G\* Geometry  
C -1.497344 -2.169367 0.177036  
C -2.002770 -0.879379 -2.082459  
C -0.844667 0.313476 -0.002406  
C -1.769355 0.306005 -1.178693  
C -0.858171 -0.951134 0.904253  
C -1.337771 -2.131687 -1.386867  
C -1.822834 -3.505439 -1.940253  
C -2.529323 -4.294116 -0.811101  
N -3.495325 -3.402028 -0.120142  
C -3.013772 -2.290997 0.493565  
C -4.807309 -4.016598 0.084512  
C -4.526332 -5.508400 -0.171002  
C -3.377326 -5.506748 -1.202346  
O 0.562292 0.353646 -0.543904  
C -1.290836 -0.638676 -3.440781  
C -3.525848 -1.012754 -2.355808  
O -3.660119 -1.512536 1.186068  
N -0.881855 -3.429312 0.644912  
C -1.452346 -4.605996 0.244554  
O -1.161608 -5.714355 0.669515  
H -1.466969 -0.748299 1.789685  
H -0.259772 -2.051189 -1.561067  
H -0.977751 -4.095805 -2.308965  
H -2.513059 -3.382762 -2.776840  
H -5.532907 -3.609014 -0.632466  
H -5.168948 -3.793613 1.091988  
H -5.411964 -6.044926 -0.523267  
H -4.183201 -5.986393 0.752560  
H -3.767031 -5.376119 -2.218822  
H -2.784115 -6.423137 -1.168111  
H -1.446714 -1.492162 -4.111647  
H -0.213494 -0.499369 -3.304500  
H -1.699929 0.254546 -3.921205  
H -3.730860 -1.841839 -3.038861

H -3.878026 -0.093894 -2.825318  
H -4.103309 -1.159227 -1.441239  
H -0.380746 -3.430143 1.528517  
N -2.319566 1.504047 -1.323544  
O -3.065560 1.916608 -2.265393  
C -1.964471 2.364948 -0.199194  
C -1.041304 3.549210 2.098443  
C -2.395860 3.664973 0.042083  
C -1.118041 1.651257 0.641996  
C -0.645630 2.238890 1.805522  
C -1.886424 4.249036 1.234022  
H 0.021144 1.706933 2.476792  
H -0.702243 4.048432 2.999880  
C -3.335269 4.447112 -0.755302  
H -3.861536 3.948970 -1.558517  
C -3.522679 5.741929 -0.467507  
H -4.220846 6.345222 -1.042531  
C -2.747548 6.450379 0.618450  
O -2.263353 5.495769 1.614631  
C -3.641849 7.406368 1.411796  
H -3.072858 7.867597 2.225119  
H -4.492043 6.868070 1.841116  
H -4.022282 8.199908 0.759726  
C -1.528265 7.181032 0.032370  
H -0.970168 7.686181 0.828305  
H -1.846217 7.929764 -0.701758  
H -0.862075 6.473742 -0.471468  
C 0.621362 -1.088130 1.226058  
C 1.350410 -0.322817 0.347994  
C 2.689242 -1.749522 2.298155  
C 2.762787 -0.211713 0.360792  
C 1.308298 -1.807884 2.232314  
C 3.435480 -0.968235 1.373504  
C 3.506984 0.610424 -0.548491  
H 5.375845 -1.493746 2.176177  
H 3.234350 -2.299664 3.055863  
C 4.905546 0.644643 -0.463349  
C 5.560749 -0.137343 0.534775  
C 4.851317 -0.912632 1.422027  
O 2.879286 1.327775 -1.493465  
H 1.912541 1.223306 -1.395744  
O 0.515072 -2.545498 3.068917  
C 1.133970 -3.280304 4.124090  
H 1.673108 -2.608134 4.801311  
H 1.821404 -4.037401 3.729335  
H 0.319606 -3.768643 4.660338  
C 5.709983 1.506229 -1.375841  
O 7.053430 1.239976 -1.465991  
C 7.634791 0.080946 -0.829903  
H 8.698810 0.330342 -0.767008  
C 7.065620 -0.059742 0.581983  
H 7.375079 0.818775 1.165791  
H 7.486088 -0.941089 1.078843  
O 5.278044 2.433228 -2.020077  
C 7.468262 -1.155786 -1.711799  
H 7.849129 -0.948605 -2.716311  
H 6.418278 -1.453005 -1.795254  
H 8.032297 -1.998206 -1.294589  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*) = -2426.72873164  
Number of imaginary frequencies = 0

1h\_c07  
B3LYP/6-31G\* Geometry  
C -2.066957 -1.768306 0.252671  
C -2.309362 -0.378756 -1.996888  
C -0.781253 0.446427 0.018010  
C -1.735951 0.695807 -1.106723  
C -1.084845 -0.773129 0.935381  
C -1.980680 -1.768079 -1.319275  
C -2.845407 -2.956883 -1.832555  
C -3.682321 -3.534164 -0.659886  
N -4.331859 -2.415124 0.066390  
C -3.543233 -1.465727 0.629210  
C -5.779556 -2.561665 0.191318  
C -6.105906 -3.559193 -0.932801  
C -4.851499 -4.457179 -1.024645  
O 0.550936 0.109271 -0.601915

C -1.603406 -0.331104 -3.378677  
C -3.820442 -0.099191 -2.220498  
O -3.926307 -0.513951 1.300965  
N -1.792179 -3.149298 0.699688  
C -2.678040 -4.128806 0.342363  
O -2.675424 -5.273166 0.768927  
H -1.565520 -0.419151 1.851495  
H -0.931527 -1.985864 -1.544305  
H -2.211202 -3.753869 -2.234532  
H -3.518178 -2.652811 -2.636945  
H -6.268439 -1.589782 0.079504  
H -6.043194 -2.959881 1.180627  
H -6.256227 -3.016462 -1.873140  
H -7.016357 -4.130069 -0.729797  
H -4.725720 -4.903106 -2.015645  
H -4.888621 -5.273923 -0.296934  
H -2.001798 -1.111936 -4.037648  
H -0.524002 -0.482895 -3.277932  
H -1.776743 0.639143 -3.852919  
H -4.256922 -0.829315 -2.907812  
H -3.931068 0.889758 -2.665949  
H -4.387586 -0.106655 -1.288232  
H -1.261531 -3.290909 1.554090  
N -1.950882 1.998403 -1.231153  
O -2.603936 2.604758 -2.136770  
C -1.319469 2.723936 -0.132530  
C 0.007570 3.599854 2.104921  
C -1.374655 4.089986 0.123409  
C -0.650038 1.803439 0.666132  
C 0.022611 2.233870 1.799662  
C -0.664599 4.506849 1.282416  
H 0.556407 1.537650 2.438990  
H 0.514617 3.983121 2.984039  
C -2.112212 5.101679 -0.626960  
H -2.796097 4.769125 -1.396313  
C -1.928266 6.397176 -0.339478  
H -2.469269 7.170333 -0.879556  
C -0.931864 6.861850 0.696819  
O -0.674324 5.805967 1.674617  
C -1.486367 8.021657 1.527647  
H -0.771465 8.302000 2.307576  
H -2.429041 7.735874 2.003650  
H -1.665376 8.893924 0.889987  
C 0.406950 7.234942 0.039075  
H 1.124767 7.562450 0.799179  
H 0.266116 8.047302 -0.682569  
H 0.825252 6.375861 -0.494751  
C 0.318674 -1.306375 1.175135  
C 1.175354 -0.763180 0.248390  
C 2.191832 -2.498326 2.142187  
C 2.562284 -1.043089 0.175778  
C 0.843530 -2.187288 2.150637  
C 3.065908 -1.948743 1.164155  
C 3.441830 -0.467914 -0.798733  
H 4.845796 -2.938506 1.896672  
H 2.611528 -3.174081 2.877815  
C 4.798917 -0.817549 -0.797451  
C 5.284681 -1.719251 0.196474  
C 4.448647 -2.260784 1.145289  
O 2.983641 0.414165 -1.701104  
H 2.037502 0.591902 -1.532939  
O -0.069993 -2.689471 3.037200  
C 0.386583 -3.578496 4.055992  
H 1.120478 -3.084294 4.702796  
H 0.826010 -4.484157 3.622284  
H -0.498475 -3.841494 4.636246  
C 5.724990 -0.300724 -1.844203  
O 7.068759 -0.401658 -1.584218  
C 7.533305 -0.800476 -0.278218  
H 7.332584 0.023791 0.421925  
C 6.759222 -2.035768 0.170305  
H 7.100789 -2.366634 1.157518  
H 6.967768 -2.851465 -0.537705  
O 5.389175 0.162633 -2.908601  
C 9.033257 -1.016295 -0.402520  
H 9.516880 -0.110289 -0.779545  
H 9.247537 -1.834577 -1.098207



H 9.465647 -1.262566 0.573665  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.73076637  
Number of imaginary frequencies = 0

1h\_c08

B3LYP/6-31G\* Geometry

C -1.462960 -2.198175 0.256275  
C -2.011004 -0.943737 -2.017271  
C -0.843896 0.290396 0.032920  
C -1.782158 0.256401 -1.132228  
C -0.830490 -0.961154 0.957462  
C -1.326518 -2.179688 -1.311719  
C -1.802618 -3.566425 -1.837126  
C -2.478910 -4.353777 -0.684234  
N -3.443730 -3.463225 0.006750  
C -2.975825 -2.328728 0.584365  
C -4.792306 -4.017422 0.093358  
C -4.785360 -5.072911 -1.025224  
C -3.324139 -5.573494 -1.072568  
O 0.555361 0.339176 -0.527719  
C -1.313534 -0.714145 -3.385068  
C -3.534661 -1.096650 -2.275890  
O -3.634970 -1.526578 1.237010  
N -0.821468 -3.442493 0.728477  
C -1.380927 -4.634549 0.356332  
O -1.067579 -5.729384 0.797526  
H -1.430000 -0.752170 1.847784  
H -0.251596 -2.092596 -1.500968  
H -0.956375 -4.151964 -2.211134  
H -2.508023 -3.466132 -2.664393  
H -5.534720 -3.226483 -0.045688  
H -4.961081 -4.468786 1.080528  
H -5.059207 -4.602455 -1.976639  
H -5.498675 -5.880436 -0.837712  
H -3.046366 -5.965991 -2.055206  
H -3.146817 -6.365615 -0.338321  
H -1.465988 -1.578628 -4.042557  
H -0.236660 -0.561673 -3.259908  
H -1.736208 0.167950 -3.874254  
H -3.900826 -0.186988 -2.752584  
H -4.101683 -1.236881 -1.353896  
H -3.736414 -1.935258 -2.948288  
H -0.306959 -3.425289 1.604031  
N -2.345582 1.446595 -1.288590  
O -3.105834 1.838015 -2.228344  
C -1.986549 2.327489 -0.181183  
C -1.049679 3.554734 2.088192  
C -2.426856 3.627245 0.044909  
C -1.124245 1.634424 0.661208  
C -0.644884 2.243856 1.810612  
C -1.910278 4.233707 1.222469  
H 0.034257 1.728460 2.482417  
H -0.705598 4.070659 2.978247  
C -3.380244 4.389669 -0.754968  
H -3.909898 3.875191 -1.545540  
C -3.574926 5.687355 -0.485427  
H -4.282941 6.276403 -1.063184  
C -2.795535 6.418286 0.582448  
O -2.294532 5.482672 1.588215  
C -3.690165 7.378986 1.369723  
H -3.117373 7.857097 2.170532  
H -4.531826 6.840410 1.815192  
H -4.083224 8.159458 0.709403  
C -1.587599 7.149762 -0.025819  
H -1.025745 7.670212 0.757490  
H -1.918195 7.885800 -0.767192  
H -0.920857 6.440562 -0.526227  
C 0.654739 -1.075105 1.262330  
C 1.363108 -0.314729 0.363374  
C 2.744107 -1.695934 2.316865  
C 2.774135 -0.187487 0.355379  
C 1.363190 -1.771559 2.270048  
C 3.468871 -0.920459 1.370514  
C 3.496548 0.628274 -0.576898  
H 5.425824 -1.410195 2.155614  
H 3.305613 -2.228068 3.075470  
C 4.895652 0.679479 -0.511498

C 5.572966 -0.078622 0.490332  
C 4.884495 -0.847683 1.399240  
O 2.847810 1.323216 -1.524406  
H 1.883770 1.209910 -1.411139  
O 0.589601 -2.506128 3.127217  
C 1.230517 -3.218676 4.184534  
H 1.769822 -2.530753 4.845638  
H 1.922186 -3.972843 3.791603  
H 0.428924 -3.709304 4.737647  
C 5.677911 1.534755 -1.448831  
O 7.023219 1.282989 -1.551975  
C 7.627118 0.142246 -0.903981  
H 8.688560 0.406013 -0.858464  
C 7.077163 0.018120 0.517038  
H 7.382688 0.910180 1.082074  
H 7.514872 -0.849412 1.023222  
O 5.226563 2.445143 -2.103388  
C 7.465664 -1.111014 -1.763238  
H 7.832129 -0.916061 -2.775526  
H 6.418543 -1.422397 -1.829260  
H 8.044920 -1.939444 -1.338900  
SCF Energy (PCM/mPW1PW91/6-31+G\*\*)= -2426.72837248  
Number of imaginary frequencies = 0