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

Fuqian Wang,[a,b] Ariel M. Sarotti,[c] Guangde Jiang,[d] José C. Huguet-Tapia,[e] Shao-Liang Zheng,[f] Xiaohua Wu,[a] Chunshun Li,[a] Yousong Ding, *[d] and Shugeng Cao* [a, g]

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_{50} values in the range of 0.52 to 1.86 μM. Their biosynthetic pathways were supported by the gene clusters mined from the sequenced genome of *Aspergillus* sp. FM242.

[a] *Daniel K. Inouye College of Pharmacy, University of Hawaii at Hilo, 200 West Kawili Street, Hilo, Hawai'i 96720, USA.*
[b] *Department of Pharmacy, Wuhan No. 1 Hospital, Wuhan 430022, China.*
[c] *Instituto de Química Rosario (CONICET), Facultad de CienciasBioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Suipacha 531, Rosario 2000, Argentina.*
[d] *Department of Medicinal Chemistry, Center for Natural Products, Drug Discovery and Development, College of Pharmacy, University of Florida, Gainesville, Florida, 32610, USA*
[e] *Department of Plant Pathology, University of Florida, Gainesville, Florida, 32611, USA.*
[f] *Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, Massachusetts 02138, USA.*
[g] *Cancer Biology Program, University of Hawaii Cancer Center, 701 Ilalo Street, Honolulu, Hawai'i 96813, USA*

CONTENTS

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, 5μ, 100 × 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}, 5μ, 250 × 10 mm). Thermo SpeedVac 2010 system. Alfa Aesar Diaion HP 20, GeneAmp PCR System 9700, Eppendrof centifuage 5810 R, BIO-RAD Molecular Imager ChemiDoc^{TM} XRS+, Shimadzu Biotech BioSpec-nano . Galaxy 170 R CO_2 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 × 0.5 cm) and inoculated into 30 L autoclaving sterilized liquid medium (mannitol 20 g, glucose 10 g, monosodium glutamate 5 g, KH_2PO_4 (0.5 g), $MgSO_4 \cdot 7H_2O$ 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 L × 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_2O (10%, 50%, 70%, 100%) to afford four fractions (Fr.1-4). Fraction 4 (9.99 g) was separated by prep-HPLC (Phenyl-Hexyl, 5μ, 100 × 21.20 mm; 8 mL/min) eluted with 45%-100% MeOH–H_2O in 35 minutes to get sub-fractions (SFr. 1–35). SFr 31 and 32 was purified by semi-preparative HPLC (50 % – 96% CH_3CN 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_3CN with 0.1% formic acid; 3 mL/min). Further separation of SFr 19 and 20 (45% - 85% CH_3CN 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_3CN 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) λ_{max} (log ε): 234 (4.06), 265 (4.51), 362 (3.77) nm; CD (*c* 1.39 × 10^{-5} M, MeOH) $\lambda_{max}(\Delta\varepsilon)$ 225 (+22.4), 251 (+22.0), 265 (–0.3), 275 (+17.6), 324 (+15.1), 360 (–9.5) nm; IR (KBr) ν_{max}: 1709, 1685, 1640, 1413, 1357, 1114 cm^{-1}; ^1H and ^{13}C NMR data, see S29; HRESIMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{41}H_{40}N_3O_9$ 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) λ_{max} (log ε): 234 (4.35), 265 (4.81), 362 (4.07) nm; CD (*c* 7.13 × 10^{-5} M, MeOH) $\lambda_{max}(\Delta\varepsilon)$ 235 (+7.5), 248 (+6.6), 265 (–12.1), 276 (+5.9), 324 (+5.4), 362 (–4.3) nm; IR (KBr) ν_{max}: 3329, 2937, 1691, 1640, 1578, 1391, 1357, 1114 cm^{-1}; ^1H and ^{13}C NMR, see S29 in main text; HRESIMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{41}H_{40}N_3O_8$ 702.2810; Found 702.2845.

Compound 3 (Konamide C)**:** Faint yellow needle crystal (CH_3CN). $[\alpha]_D^{20}$ – 75 (*c* 0.03 g/100ml, MeOH,); UV (*c* 0.01 mg/ml, MeOH) λ_{max} (log ε): 232 (4.55) nm; CD (*c* 3.43 × 10^{-5} M, MeOH) $\lambda_{max}(\Delta\varepsilon)$ 229 (+33.0), 245 (–70.5), 280 (+1.2), 301 (–5.4), 325 (–6.2) nm; IR (KBr) ν_{max}: 2934, 1687, 1614, 1439, 1390, 1188, 1084 cm^{-1}; ^1H and ^{13}C NMR data, see S30; HRESIMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{54}H_{63}N_6O_{11}$, 971.4549; Found 971.4545.

Compound 4 ((+)-semivioxanthin): White amorphous powder; HRESIMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{15}O_5$ 275.0914; Found 275.0910. ^1H data matched the literature; ^1H NMR (400 MHz, $CDCl_3$) δ: 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_3).

Compound 5 (Notoamide F): Colorless needle crystal (CH_3OH); HRESIMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{32}N_3O_4$ 462.2387; Found 462.2396. ^1H NMR (400 MHz, DMSO-d_6) δ: 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*: $[M + H]^+$ Calcd for $C_{26}H_{30}N_3O_5$ 464.2180; Found 464.2182. ^1H data matched the literature; ^1H NMR (400 MHz, Acetone-d_6) δ: 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** crystalized 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 ($Cu_{K\alpha}$ 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[1] with reflection spot size optimization. Absorption corrections were made with the program SADABS[1]. The structure was solved by the Intrinsic Phasing methods and refined by least-squares methods again F^2 using SHELXT-2014[2] and SHELXL-2014[3] with OLEX 2 interface[4]. 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. 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,[3] and the drawings of three-dimensional supramolecular architectures were produced with Accelrys DS Visualizer 2.0 [5].

Antiproliferative Assays

Antiproliferative assays was carried out as previously described.[6] 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 [7] 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[8] , 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 [9]. 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[10] that led to the identification of one putative semivioxanthin gene cluster (~34 kb) and the putative notoammide gene cluster (~47 kb) located at two different chromosomal regions. BLAST programs[11] 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

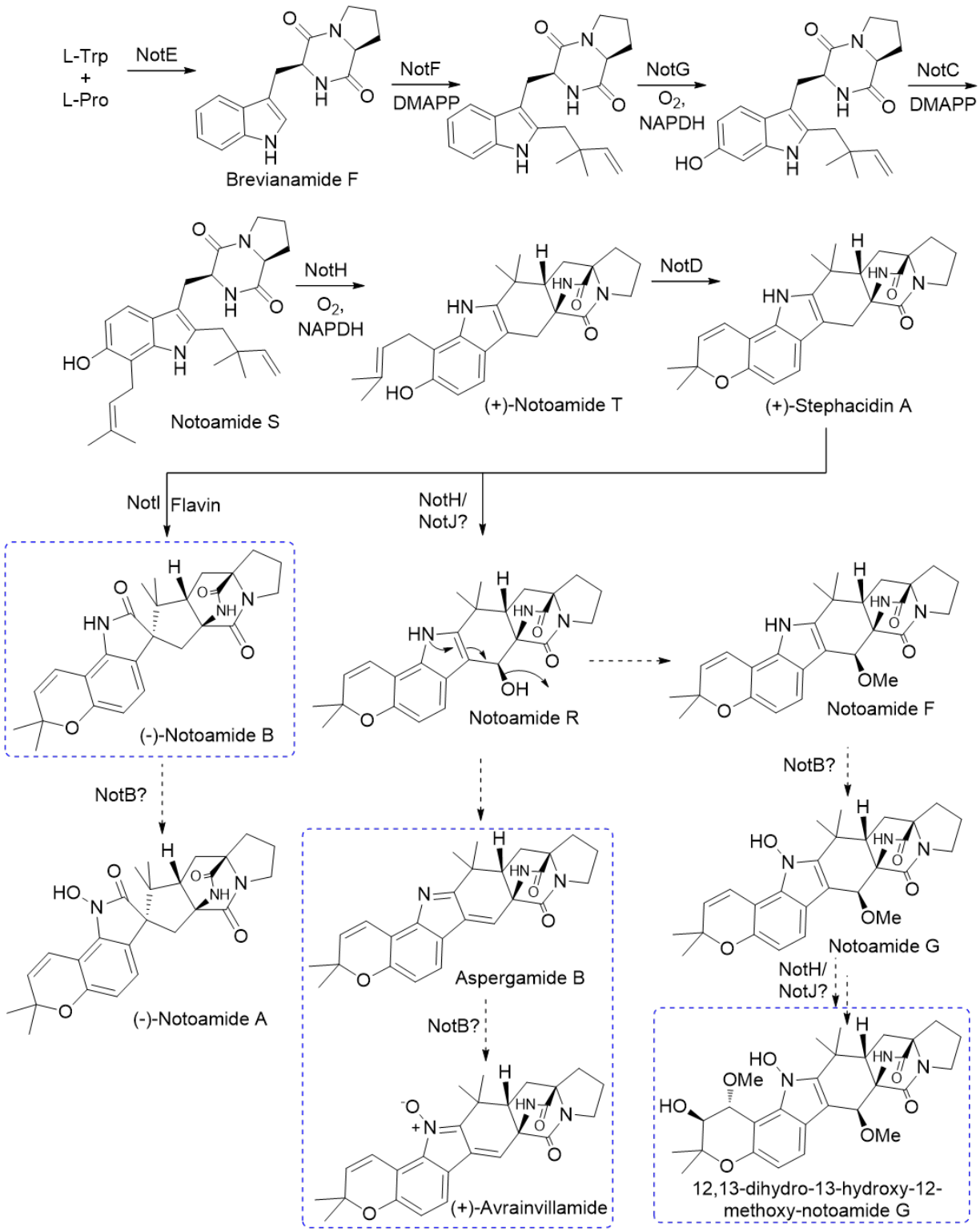
S2. Predicted function of genes of the *not* cluster (~47 kb) in *Aspergillus* sp. FM242.

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

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

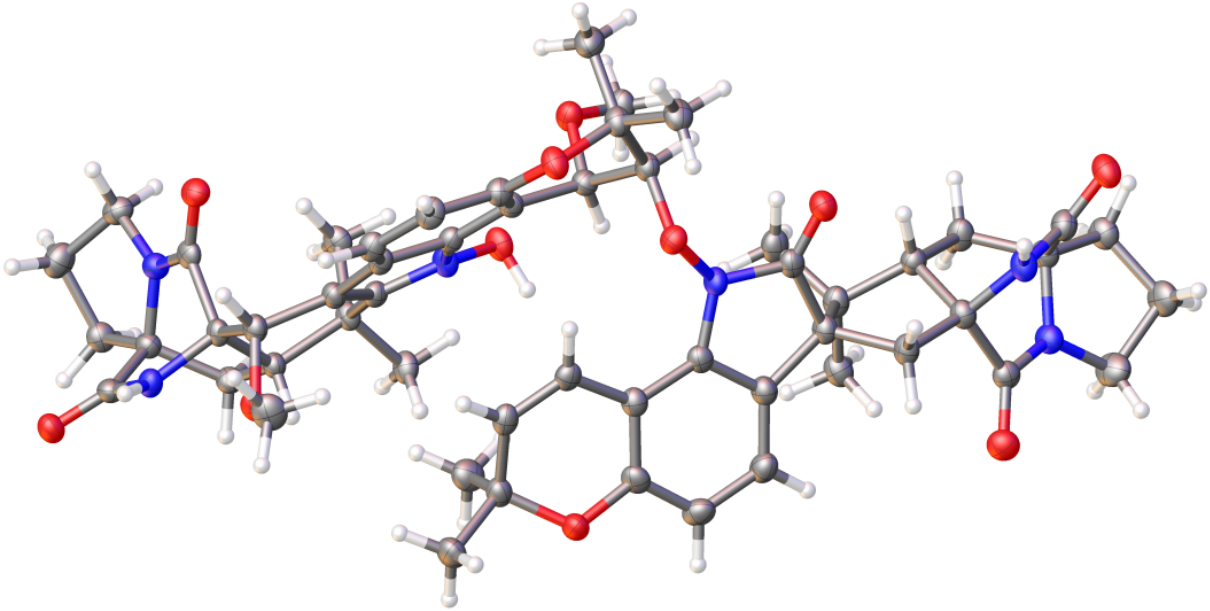
Gene	Length (AA, bp)	Putative function	BLAST-hit (identity/similarity [%])	Accession number
Orf1	217, 842	Cupin	Oxalate decarboxylase/oxidase from *Aspergillus steynii* IBT 23096 (90/95)	XP_024709122
Orf2	449, 1653	Peptide hydrolase	Zn-dependent exopeptidase from *A. steynii* IBT 23096 (94/95)	XP_024709123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

S4: The putative biosynthetic pathway of notoamides

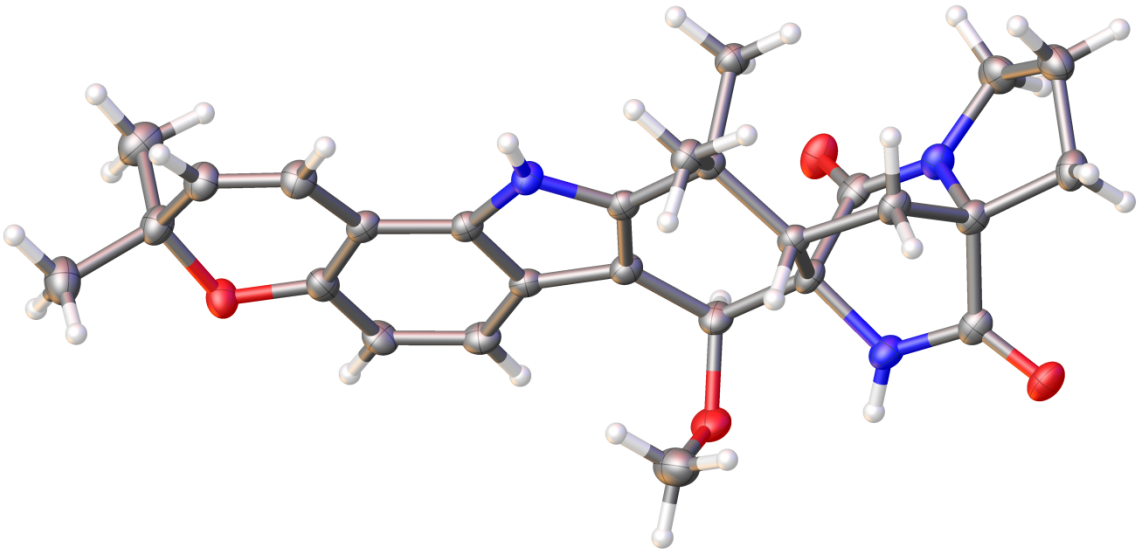


X-ray crystallography

S5: X-ray crystal structure of 3



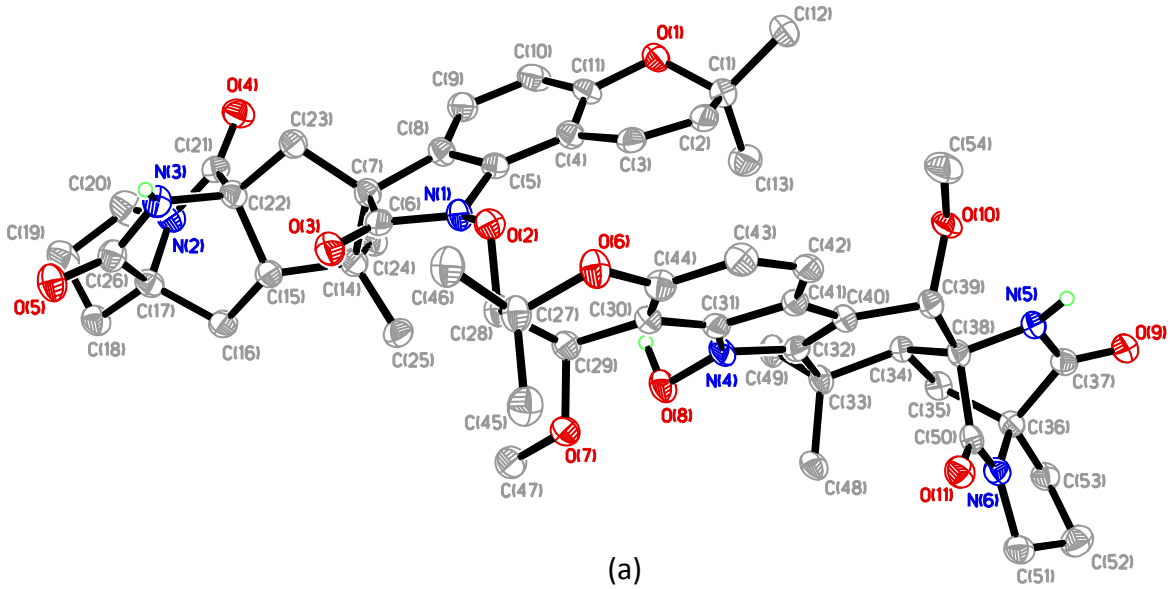
S6: X-ray crystal structure of 5



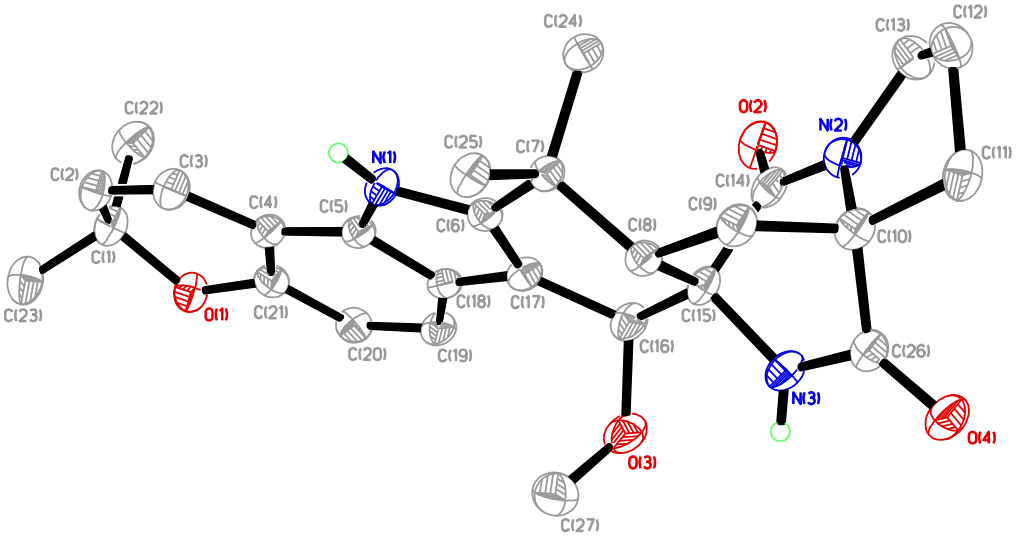
S7: X-ray crystallography details

	Compound 3	**Compound 5**
CCDC Identifier	1994347	1994346
Crystal data		
Chemical formula	$C_{64}H_{81}N_{11}O_{13}$	$C_{27}H_{31}N_3O_4$
M_r	1212.39	461.55
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	100	100
a, *b*, *c* (Å)	9.5082 (3), 23.6528 (8), 27.6237 (10)	8.1514 (3), 10.9209 (3), 25.9651 (8)
V (Å^3)	6212.4 (4)	2311.43 (13)
Z	4	4
Radiation type	Cu *K*a	Cu *K*a
m (mm^{-1})	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 *SADABS*	Multi-scan *SADABS*
T_{min}, T_{max}	0.666, 0.806	0.793, 0.864
No. of measured, independent and observed [$I > 2s(I)$] reflections	70587, 11009, 10444	22974, 3928, 3802
R_{int}	0.054	0.041
(sin q/l)$_{max}$ (Å^{-1})	0.597	0.596
Refinement		
$R[F^2 > 2s(F^2)]$, $wR(F^2)$, *S*	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
Dρ$_{max}$, Dρ$_{min}$ (e Å^{-3})	0.45, -0.26	0.32, -0.21
Absolute structure	Flack x determined using 4363 quotients [(I+)-(I-)]/[(I+)+(I-)].	Flack x determined using 1531 quotients [(I+)-(I-)]/[(I+)+(I-)].
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.

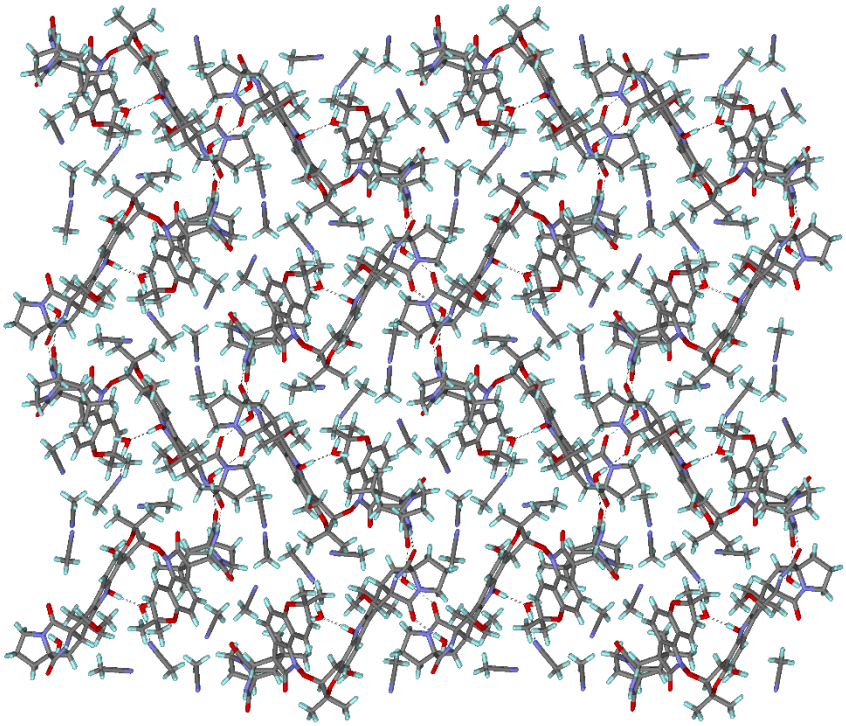


(a)

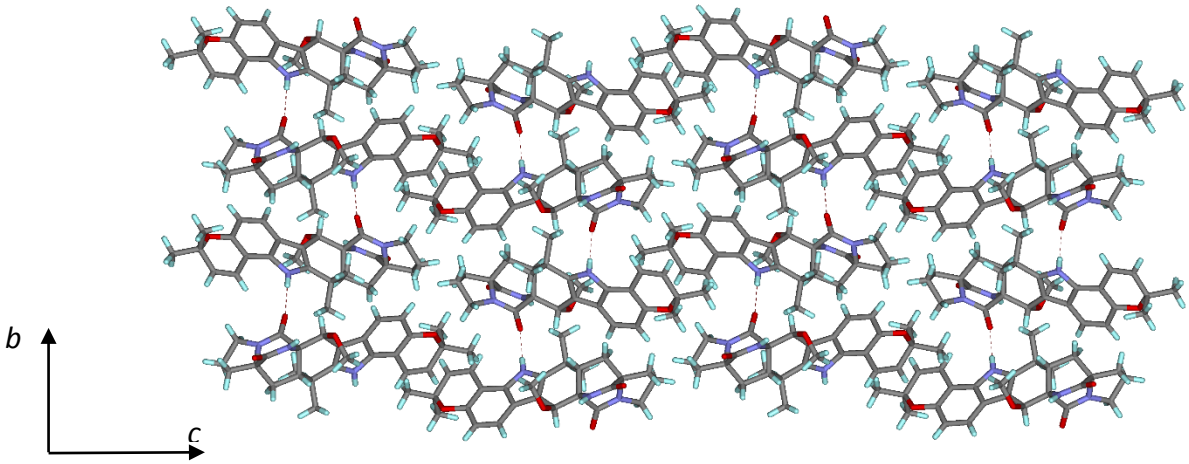


(b)

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



(a)



(b)

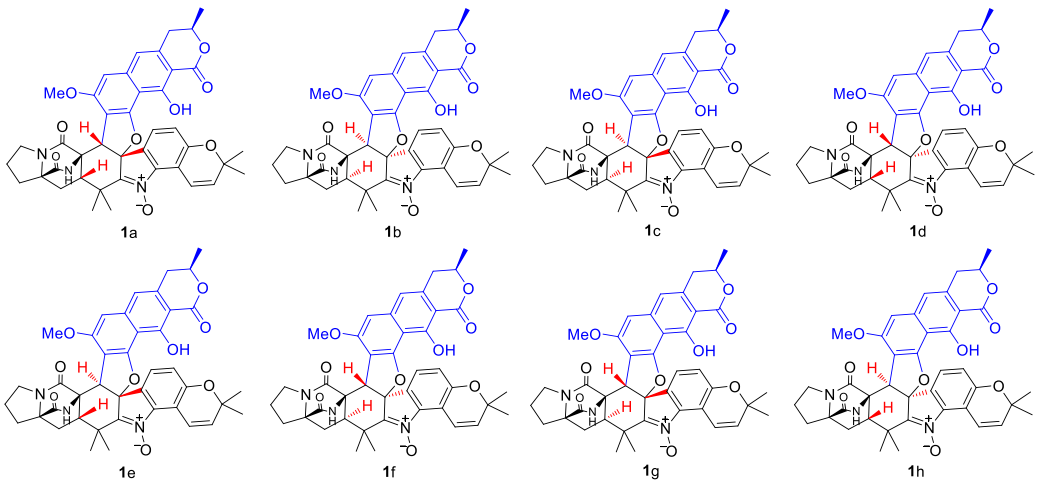
Computational

S10: Computational details

All the quantum mechanical calculations were performed using Gaussian 09.[12] Systematic conformational searches were done for each compound in the gas phase using the MMFF force field, implemented in Spartan 14,[13] and the results were validated using Macromodel[14] (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 (σ) were computed using the *gauge including atomic orbitals* (GIAO) approach,[15] the method of choice to solve the gauge origin problem,[16] at the PCM/mPW1PW91/6-31+G** level of theory (with methanol as solvent), the recommended for DP4+ calculations.[17] The unscaled chemical shifts (δu) were computed using TMS as reference standard according to $\delta u = \delta_0 - \delta_x$, where δ_x is the Boltzmann averaged isotropic shielding constant (over all significantly populated conformations) and δ_0 is the isotropic shielding constant of TMS computed at the same level of theory. The Boltzmann averaging was done according to eq 1:

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

where $\sigma_i{}^x$ is the shielding constant for nucleus x in conformer i, R is the molar gas constant (8.3145 J K^{-1} 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 (δ_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 δ_u against δ_{exp}.[14] 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.[17] The ECD calculations were carried out using the B3LYP/6-31G* optimized geometries previously employed for DP4+ calculations. The excitation energies (nm) and rotatory strenght (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 significanlty pouplated conformers, which were averaged using Boltzmann weighting. The calculated rotatory strenghts were simulated into the ECD curve as the sum of Gaussians with 0.5 eV width at half-heights (σ). Geometry reoptimizations at CAM-B3LYP/6-31G* and/or TDDFT calculations at other levels (including ωB97XD, CAM-B3LYP and B3LYP) at gas phase of with the PCM model for the solvent were also carried out, and similar results were observed to those shown for B3LYP/6-31G*.[18]



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

S11: NMR Boltzmann averaged isotropic magnetic shielding values (σ) 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	29.2128	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	119.7	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	113.8	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_3OD.

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[δ_{exp}-δ_u])							
	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
C-2	2.1	1.4	1.9	2.4	2.2	2.3	2.5	2.1
C-3	2.1	0.8	1.0	3.7	1.6	0.2	2.2	2.2
C-4	3.9	3.0	4.3	3.8	2.2	4.0	2.8	2.6
C-5	5.0	5.9	3.5	7.4	8.2	4.4	6.5	2.7
C-6	9.8	8.3	16.9	24.6	12.4	9.2	2.0	1.3
C-7	5.1	6.1	9.8	9.6	13.2	13.1	5.0	4.7
C-8	0.5	1.3	4.0	4.1	2.6	2.6	1.5	1.9
C-10	2.3	2.3	1.3	3.0	0.2	0.6	1.4	1.8
C-11	1.9	1.6	1.1	2.7	0.4	2.8	1.9	2.1
C-12	0.6	0.5	0.7	0.0	0.4	0.1	0.3	0.6
C-13	2.1	2.6	1.5	2.7	0.5	0.4	3.2	2.1
C-14	2.0	1.6	1.3	0.1	1.7	1.7	2.4	2.2
C-16	2.5	2.6	2.2	4.0	2.8	3.4	2.3	1.9
C-17	1.9	3.6	2.7	3.6	2.7	0.9	3.2	4.5
C-18	2.0	1.2	1.4	0.9	3.3	0.1	2.0	0.7
C-19	0.4	0.7	1.5	0.3	1.6	1.2	2.2	1.6
C-20	0.3	0.6	4.5	5.9	6.1	6.5	0.3	1.8
C-21	8.0	2.7	6.1	9.2	2.5	4.6	6.1	1.1
C-22	2.6	1.9	2.5	0.0	0.5	0.7	2.4	2.3
C-23	3.8	3.1	4.4	6.0	4.2	4.0	5.6	2.1
C-25	4.9	5.6	4.3	5.0	4.3	3.0	5.7	3.2
C-27	0.5	0.3	8.9	7.7	0.3	2.3	1.4	1.5
C-28	4.4	7.1	10.0	8.7	6.2	6.9	0.8	1.6
C-29	0.2	0.4	0.2	0.4	0.7	0.2	0.1	0.4
C-30	2.2	1.8	1.1	1.3	2.1	2.4	2.1	2.1
C-1'	2.8	2.0	2.7	2.0	4.5	3.3	3.0	2.8
C-10'	2.6	1.3	2.7	3.7	3.7	5.1	3.0	1.7
C-10'a	2.0	2.2	0.5	0.5	0.9	1.2	0.4	0.3
C-3'	0.0	0.3	0.4	0.0	0.7	0.9	0.1	0.4
C-3'-Me	0.7	0.9	1.1	1.1	1.5	1.1	0.7	1.1
C-4'	1.2	2.1	2.6	2.0	2.2	1.7	2.2	2.4
C-4'a	1.8	2.9	0.3	0.6	0.7	1.4	1.2	3.5
C-5'	1.1	3.7	2.8	1.7	2.9	3.1	3.0	3.8
C-5'a	0.1	3.5	4.4	3.4	0.2	1.1	5.0	5.6
C-6'	3.4	3.3	1.9	2.8	3.7	4.8	3.8	3.3
C-7'	3.6	1.9	4.1	4.4	3.9	2.5	1.5	2.2
C-7'-OMe	4.1	1.5	1.5	1.1	2.5	0.9	1.5	0.8
C-8'	0.4	1.1	2.1	0.6	0.5	0.5	3.1	0.2
C-9'	0.1	2.0	0.2	1.4	2.1	2.7	4.0	2.2
C-9'a	1.4	2.5	0.6	2.6	0.2	0.6	1.4	1.0
Average	2.4	2.4	3.1	3.5	2.8	2.6	2.5	2.1

	Absolute scaled error (abs[δ_{exp}-δ_s])							
	1a	1b	1c	1d	1e	1f	1g	1h
C-1	1.5	0.5	2.6	4.3	2.3	2.9	0.8	0.5
C-2	0.9	1.5	3.1	3.4	1.7	1.4	0.2	0.0
C-3	0.7	2.0	3.9	1.8	2.1	3.4	0.3	0.2
C-4	2.7	2.0	2.0	1.1	0.4	2.2	1.9	1.9
C-5	2.3	3.3	1.2	2.1	4.8	0.9	4.2	0.8
C-6	8.0	6.6	14.1	21.8	10.1	6.7	0.1	0.2
C-7	2.8	4.0	6.1	5.3	10.5	10.4	2.9	3.1
C-8	1.8	1.1	1.6	1.3	5.0	4.6	4.1	3.9
C-10	0.5	0.3	0.7	0.8	1.6	2.1	0.7	0.1
C-11	1.2	0.8	0.8	2.4	0.0	2.7	1.0	1.4
C-12	0.2	0.4	0.2	0.6	0.1	0.4	0.8	0.2
C-13	0.5	0.9	0.1	0.9	0.9	0.7	1.5	0.7
C-14	1.2	0.9	0.5	2.1	0.4	0.4	2.0	1.9
C-16	0.0	0.1	0.7	0.7	0.3	1.4	0.4	0.2
C-17	1.1	2.7	2.3	3.1	2.2	0.6	2.2	3.7
C-18	1.1	0.1	0.7	0.1	2.6	0.4	0.8	0.3
C-19	1.8	2.2	0.4	1.2	2.8	2.1	0.8	0.4
C-20	0.2	0.6	4.0	5.3	5.9	6.1	0.5	2.0
C-21	6.0	0.6	2.4	5.1	0.6	1.7	4.3	0.4
C-22	1.3	0.6	0.1	3.2	2.7	2.8	1.3	1.5
C-23	0.8	0.0	0.8	1.9	1.2	1.4	2.5	0.4
C-25	1.7	2.3	0.3	0.4	0.9	0.1	2.4	0.5
C-27	3.6	3.2	4.3	2.3	3.7	1.4	1.3	0.5
C-28	1.1	4.0	5.0	2.6	2.0	3.0	2.3	0.8
C-29	2.8	2.5	5.2	6.3	3.2	3.5	2.6	1.7
C-30	0.7	1.1	3.8	4.5	1.8	1.2	0.5	0.1
C-1'	0.4	1.3	1.1	2.6	1.4	0.6	0.3	0.2
C-10'	0.2	1.7	0.6	0.1	0.9	2.9	0.1	0.6
C-10'a	1.9	2.0	0.9	0.1	1.1	1.6	0.9	0.1
C-3'	0.8	0.4	1.5	2.2	2.1	0.6	0.5	0.8
C-3'-Me	2.6	2.3	4.2	5.2	2.7	2.9	2.3	1.1
C-4'	1.4	0.3	1.7	3.2	1.2	1.7	0.1	0.7
C-4'a	0.2	4.8	2.0	2.6	0.7	0.3	3.1	5.1
C-5'	0.3	2.9	2.4	1.2	2.5	2.9	2.0	3.1
C-5'a	1.9	1.5	2.5	1.0	2.2	2.7	3.0	4.0
C-6'	3.3	3.1	2.4	3.4	4.0	5.4	3.5	3.0
C-7'	1.1	0.8	1.2	0.9	1.4	0.3	4.4	0.0
C-7'-OMe	6.1	3.2	4.8	5.0	5.1	3.3	3.1	1.9
C-8'	1.0	0.4	2.4	0.9	0.2	0.7	4.1	1.0
C-9'	2.8	0.8	3.0	2.3	0.6	0.5	1.3	0.1
C-9'a	1.0	1.9	0.7	2.9	0.0	0.6	0.7	0.4
Average	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
H-1b	0.22	0.06	0.00	0.20	0.13	0.32	0.12	0.03
H-2a	0.07	0.10	0.09	0.02	0.14	0.06	0.01	0.08
H-2b	0.05	0.01	0.01	0.08	0.03	0.01	0.05	0.03
H-3a	0.04	0.06	0.09	0.11	0.03	0.02	0.05	0.06
H-3b	0.01	0.01	0.03	0.01	0.04	0.09	0.03	0.04
H-5a	0.08	0.18	0.14	0.38	0.22	0.03	0.02	0.10
H-5b	0.04	0.10	0.15	0.24	0.38	0.33	0.13	0.14
H-6	0.53	0.63	0.32	0.25	0.56	0.81	0.03	0.18
H-12	0.65	0.69	0.38	0.33	0.61	0.58	0.69	0.55
H-13	0.30	0.30	0.24	0.22	0.40	0.40	0.28	0.31
H-17	0.17	0.21	0.02	0.08	0.01	0.03	0.20	0.25
H-18	0.17	0.38	0.28	0.04	0.16	0.26	0.23	0.40
H-21	0.98	0.72	0.61	0.61	1.09	0.41	0.87	0.00
H-27	0.32	0.27	0.22	0.14	0.15	0.08	0.01	0.08
H-28	0.10	0.07	0.17	0.13	0.06	0.05	0.13	0.09
H-29	0.07	0.08	0.10	0.11	0.06	0.07	0.08	0.05
H-30	0.04	0.10	0.05	0.03	0.04	0.02	0.05	0.10
H-3'	0.10	0.05	0.04	0.06	0.02	0.07	0.04	0.03
H-4'a	0.09	0.01	0.12	0.06	0.02	0.07	0.08	0.08
H-4'b	0.04	0.09	0.17	0.01	0.02	0.07	0.12	0.13
H-5'	0.04	0.14	0.01	0.08	0.15	0.07	0.07	0.12
H-6'	0.03	0.05	0.00	0.18	0.11	0.01	0.09	0.04
H-3'-Me	0.02	0.01	0.05	0.02	0.08	0.01	0.06	0.07
H-7'-OMe	0.01	0.19	0.15	0.05	0.04	0.15	0.04	0.00
Average	0.17	0.19	0.14	0.14	0.19	0.17	0.14	0.12

H-1a	0.01	0.13	0.08	0.17	0.09	0.22	0.00	0.03
H-1b	0.19	0.11	0.05	0.26	0.09	0.29	0.10	0.00
H-2a	0.14	0.13	0.05	0.00	0.18	0.14	0.05	0.13
H-2b	0.02	0.01	0.05	0.11	0.07	0.07	0.01	0.08
H-3a	0.04	0.02	0.12	0.13	0.08	0.11	0.02	0.00
H-3b	0.06	0.00	0.06	0.05	0.05	0.14	0.06	0.06
H-5a	0.15	0.21	0.11	0.35	0.16	0.05	0.05	0.04
H-5b	0.11	0.11	0.11	0.21	0.33	0.24	0.07	0.09
H-6	0.47	0.62	0.36	0.29	0.53	0.73	0.00	0.16
H-12	0.47	0.33	0.29	0.13	0.27	0.34	0.51	0.25
H-13	0.21	0.07	0.17	0.08	0.18	0.27	0.19	0.12
H-17	0.05	0.05	0.10	0.08	0.24	0.18	0.07	0.03
H-18	0.05	0.10	0.36	0.12	0.09	0.09	0.10	0.16
H-21	0.97	0.54	0.54	0.49	0.91	0.34	0.88	0.10
H-27	0.22	0.19	0.19	0.12	0.07	0.18	0.08	0.01
H-28	0.18	0.12	0.14	0.12	0.02	0.15	0.21	0.01
H-29	0.03	0.01	0.13	0.11	0.02	0.04	0.01	0.04
H-30	0.14	0.16	0.02	0.03	0.12	0.13	0.14	0.18
H-3'	0.06	0.09	0.02	0.04	0.10	0.02	0.00	0.08
H-4'a	0.12	0.02	0.16	0.00	0.01	0.03	0.05	0.08
H-4'b	0.07	0.12	0.12	0.05	0.00	0.04	0.09	0.13
H-5'	0.09	0.14	0.09	0.09	0.12	0.11	0.07	0.13
H-6'	0.10	0.32	0.08	0.01	0.36	0.18	0.22	0.20
H-3'-Me	0.12	0.07	0.07	0.03	0.00	0.12	0.03	0.02
H-7'-OMe	0.02	0.28	0.20	0.04	0.12	0.16	0.06	0.07
Average	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 (σ), unscaled chemical shifts (δ_u) and scaled chemical shifts (δ_s) computed for 3'*epi*-16 at the PCM/mPW1PW91/6-31+G//B3LYP/6-31G* level of theory.**

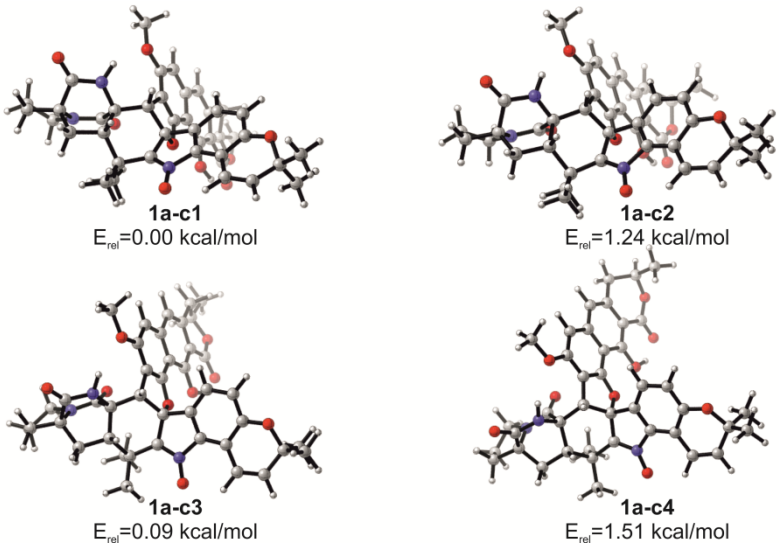
Atom	σ	δ_u	δ_s
C-1	151.1661	45.6	44.2
C-2	167.8199	29.0	27.0
C-3	164.4214	32.4	30.5
C-4	124.8652	71.9	71.4
C-5	165.6927	31.1	29.2
C-6	148.2413	48.5	47.2
C-7	151.9229	44.9	43.4
C-8	45.6130	151.2	153.1
C-10	57.5495	139.2	140.8
C-11	83.9041	112.9	113.6
C-12	80.6655	116.1	117.0
C-13	64.8216	132.0	133.3
C-14	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.

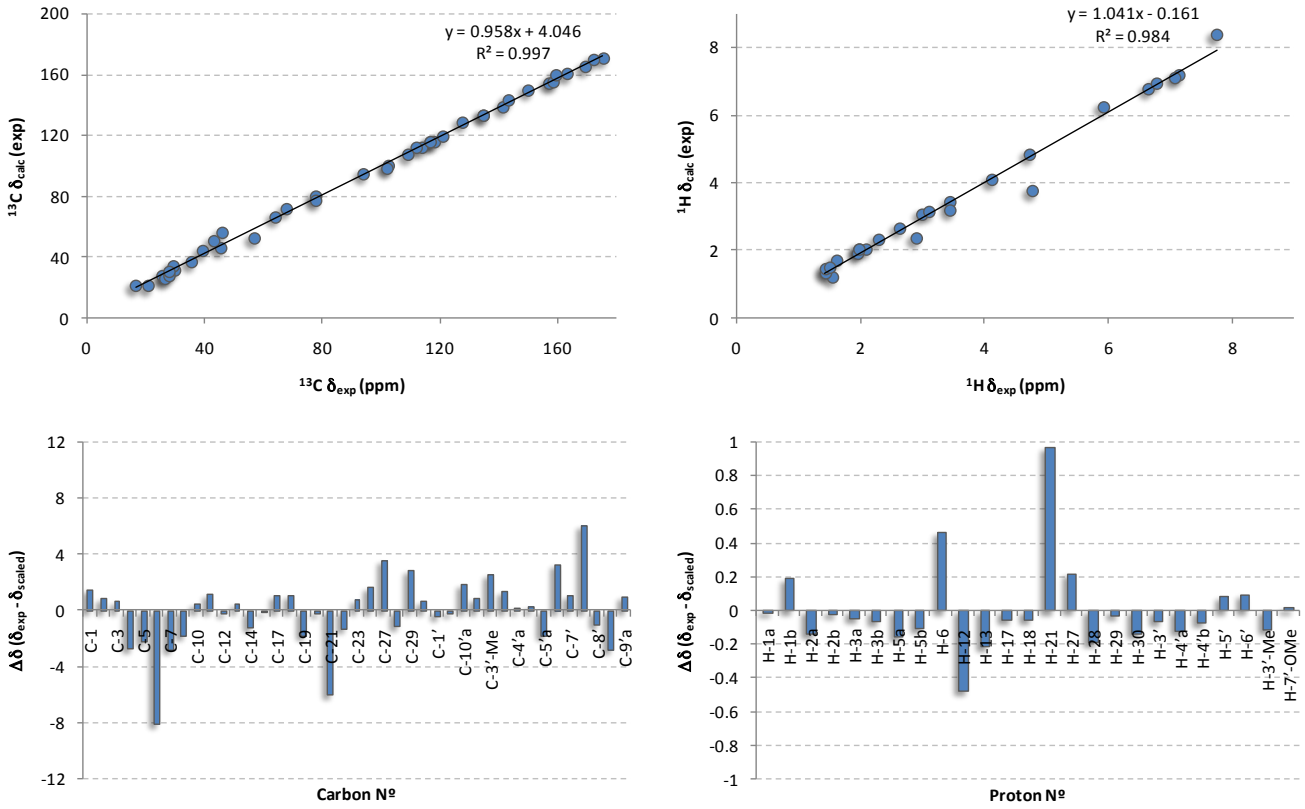
	abs[δ_{exp}-δ_u]		abs[δ_{exp}-δ_s]	
	1h	3'*epi* -1h	1h	3'*epi* -1h
C-1	1.9	0.3	0.5	1.1
C-2	2.1	3.5	0.0	1.5
C-3	2.2	2.7	0.2	0.8
C-4	2.6	4.3	1.9	3.8
C-5	2.7	1.6	0.8	0.3
C-6	1.3	2.5	0.2	1.2
C-7	4.7	5.8	3.1	4.3
C-8	1.9	1.3	3.9	3.2
C-10	1.8	2.0	0.1	0.4
C-11	2.1	1.1	1.4	0.4
C-12	0.6	0.5	0.2	0.4
C-13	2.1	2.8	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
Average	**2.1**	**1.9**	**1.2**	**1.3**
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
Average	**0.12**	**0.11**	**0.09**	**0.09**

	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%
DP4+ (H data)	83.81%	16.19%
DP4+ (C data)	44.71%	55.29%
DP4+ (all data)	80.72%	19.28%

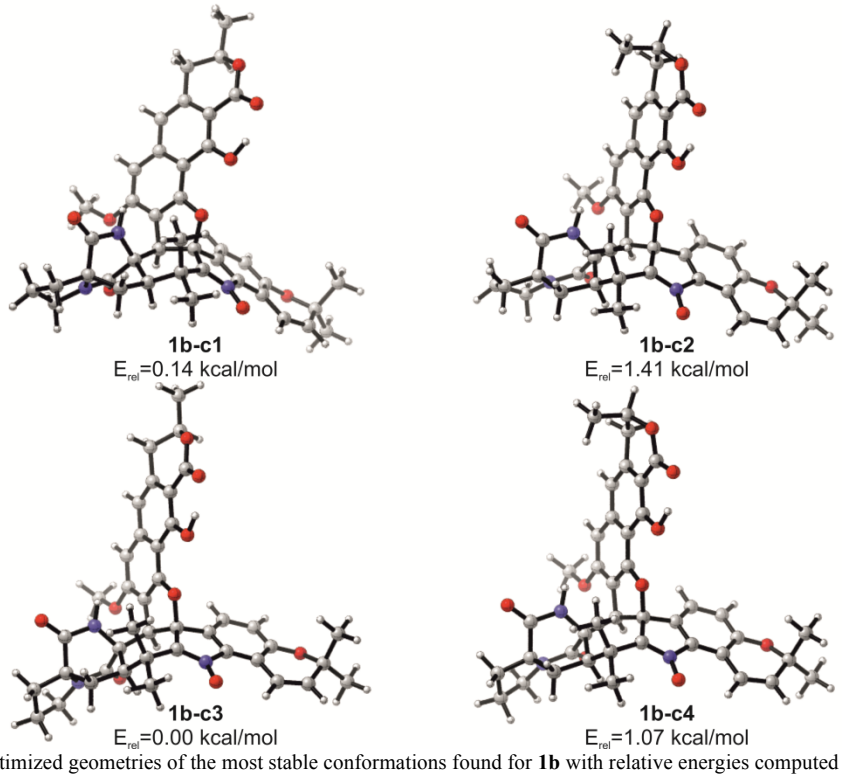
S17: Computational NMR data of 1a



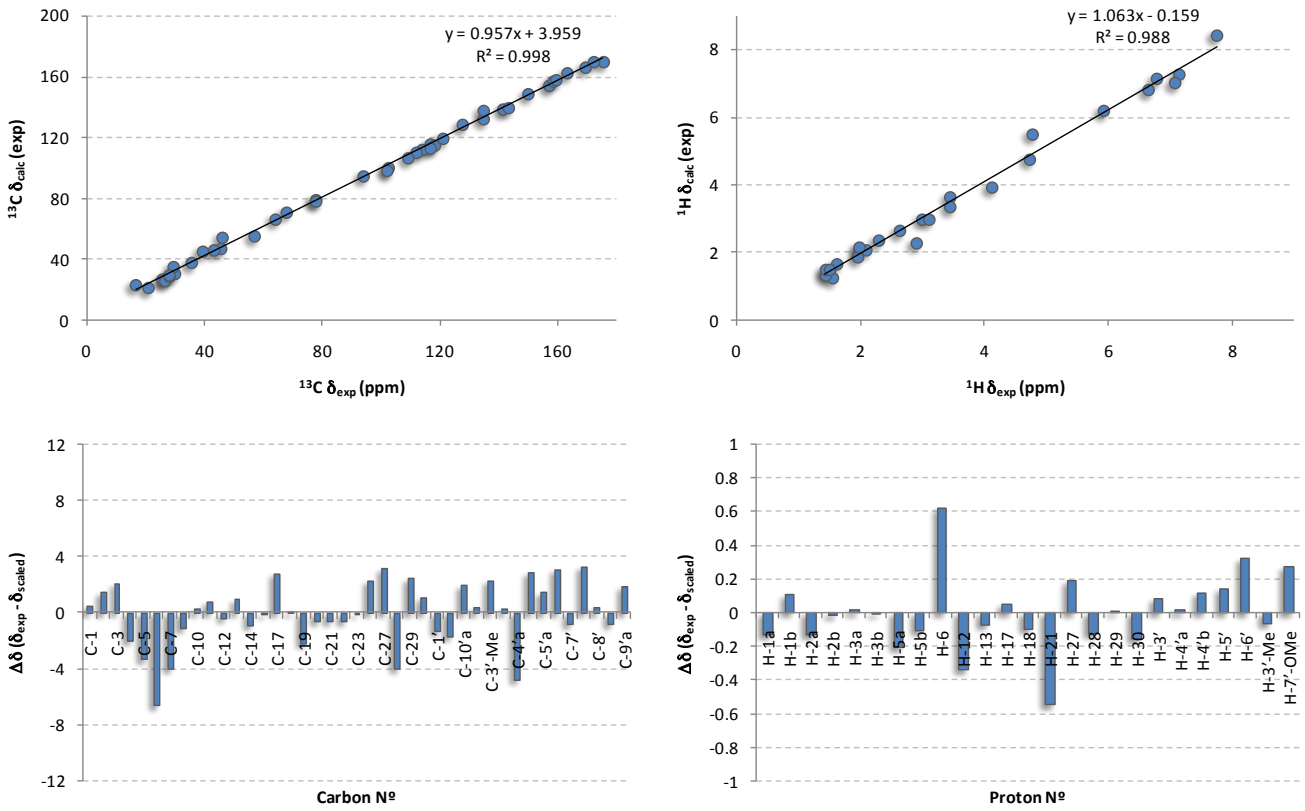
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1a** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



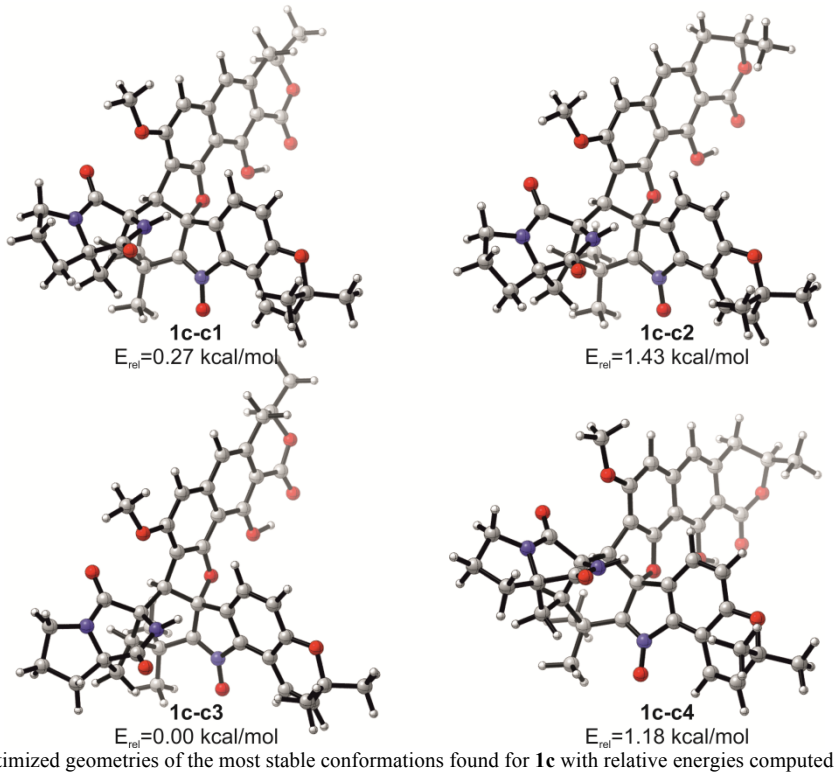
S18: Computational NMR data of 1b



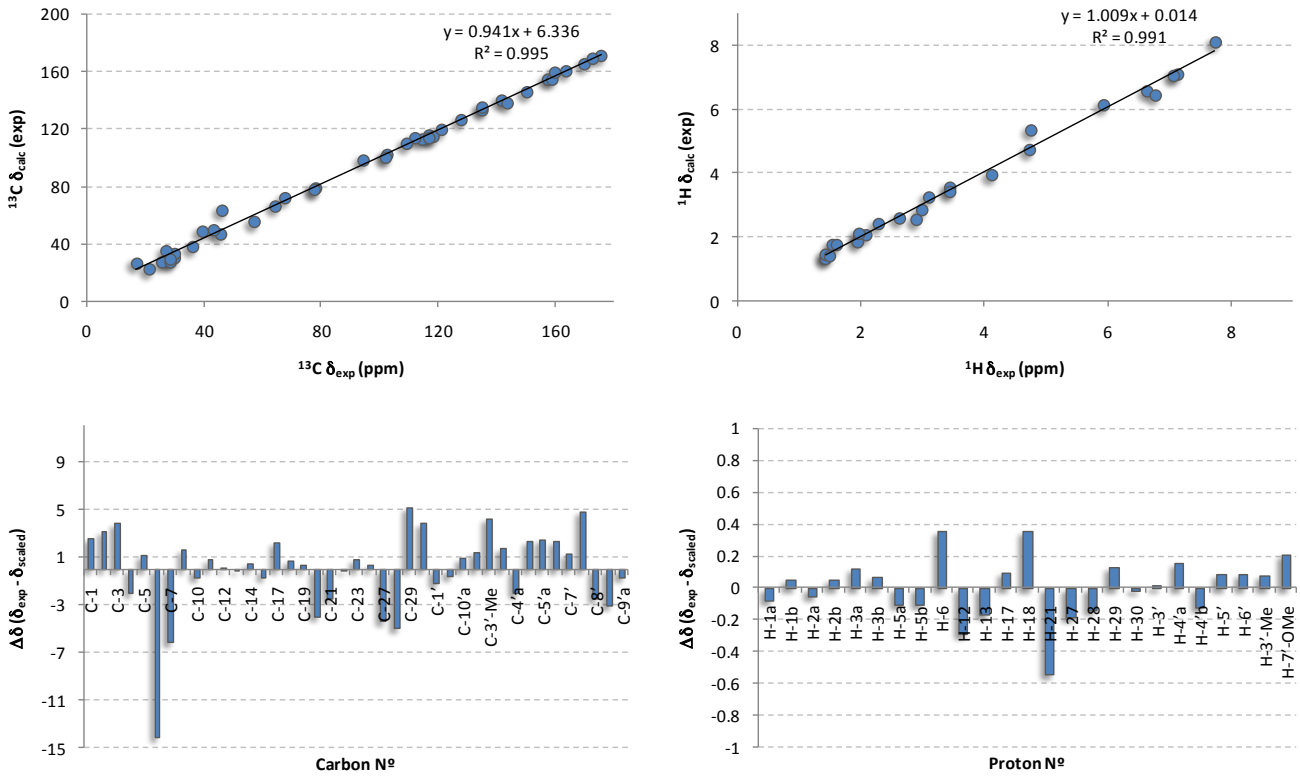
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1b** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



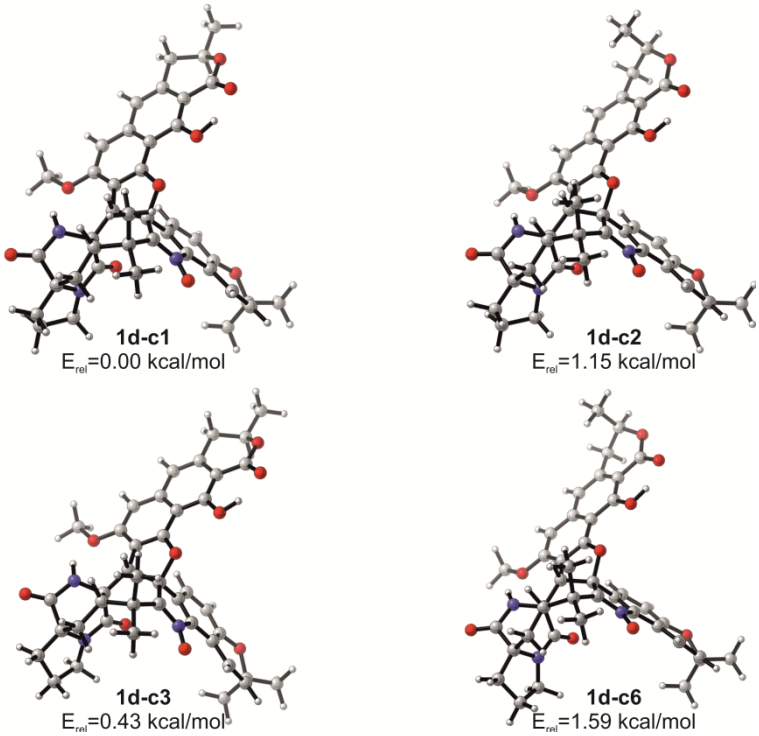
S19: Computational NMR data of 1c



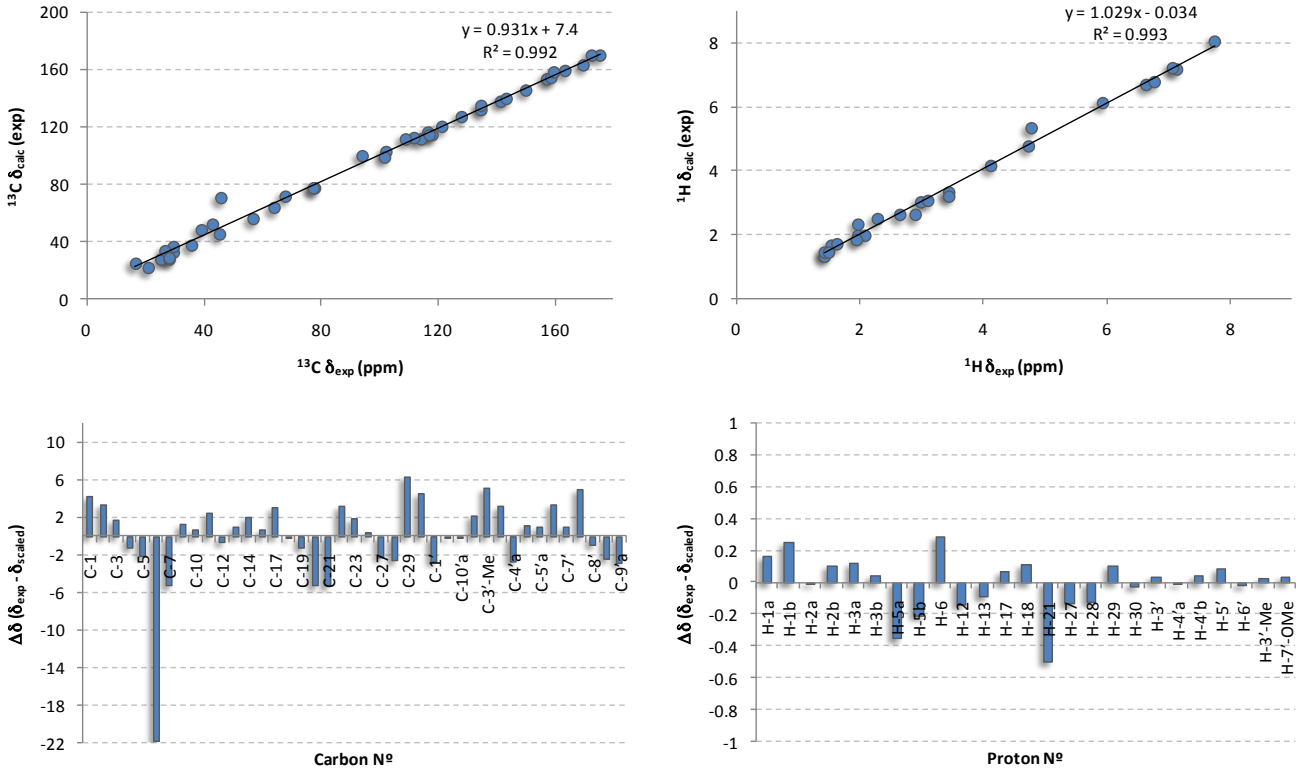
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1c** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



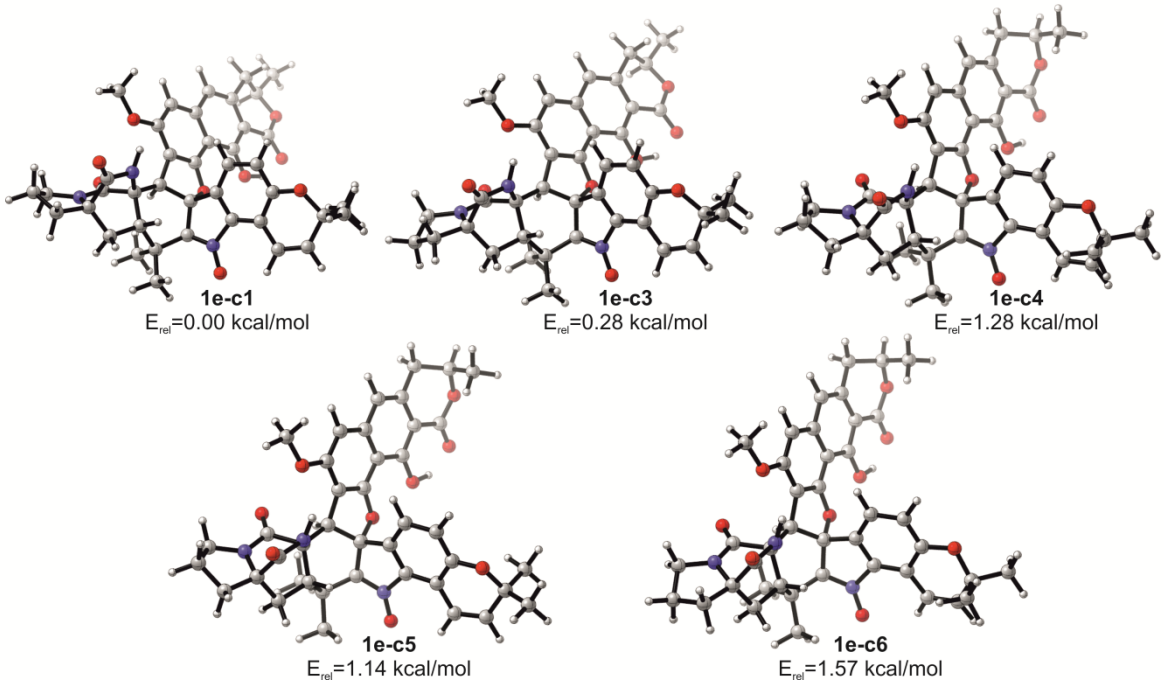
S20: Computational NMR data of 1d



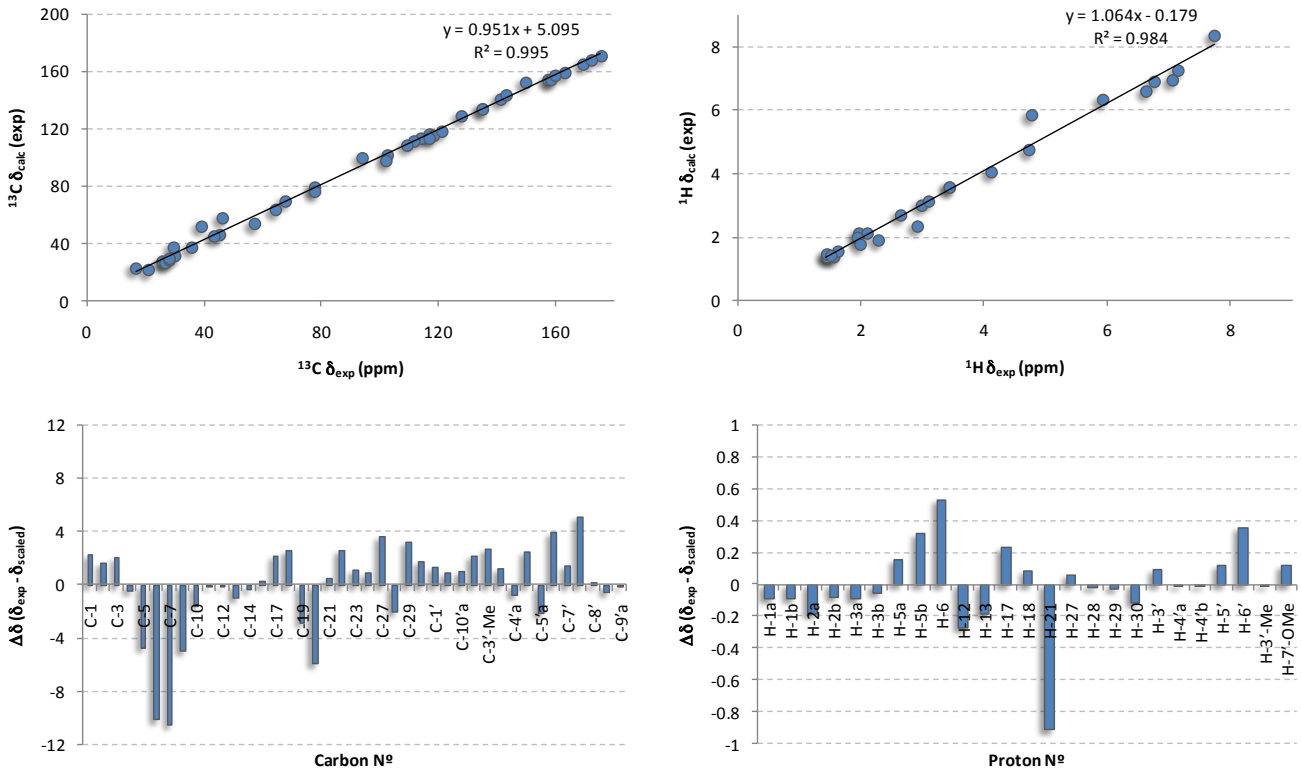
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1d** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



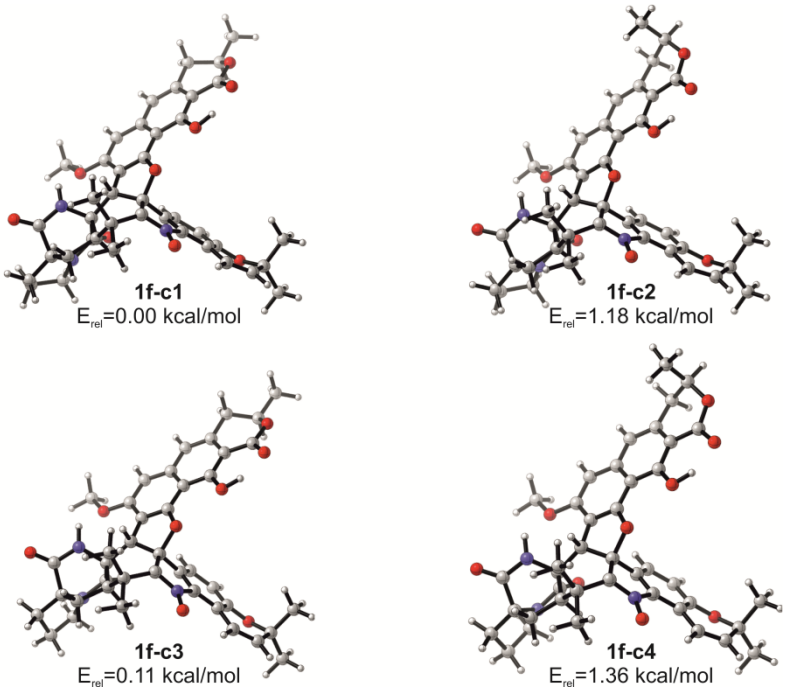
S21: Computational NMR data of 1e



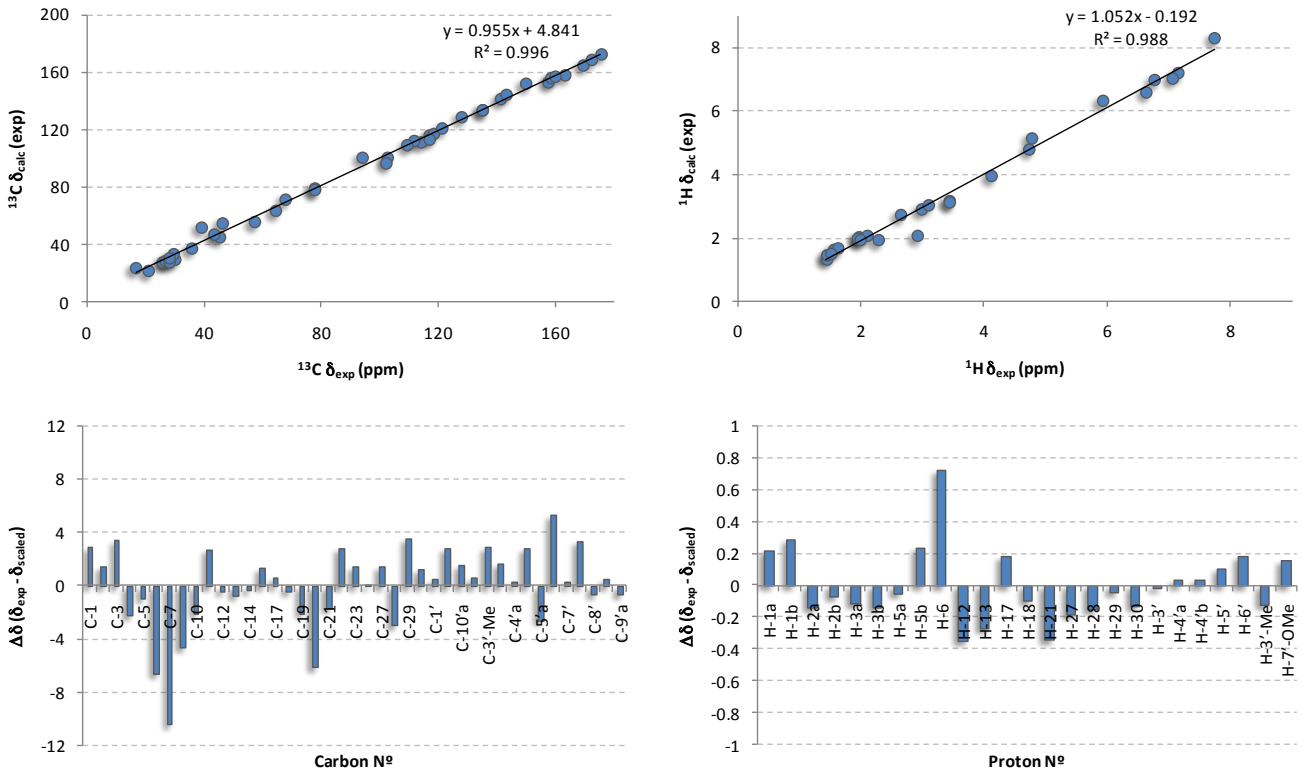
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1e** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



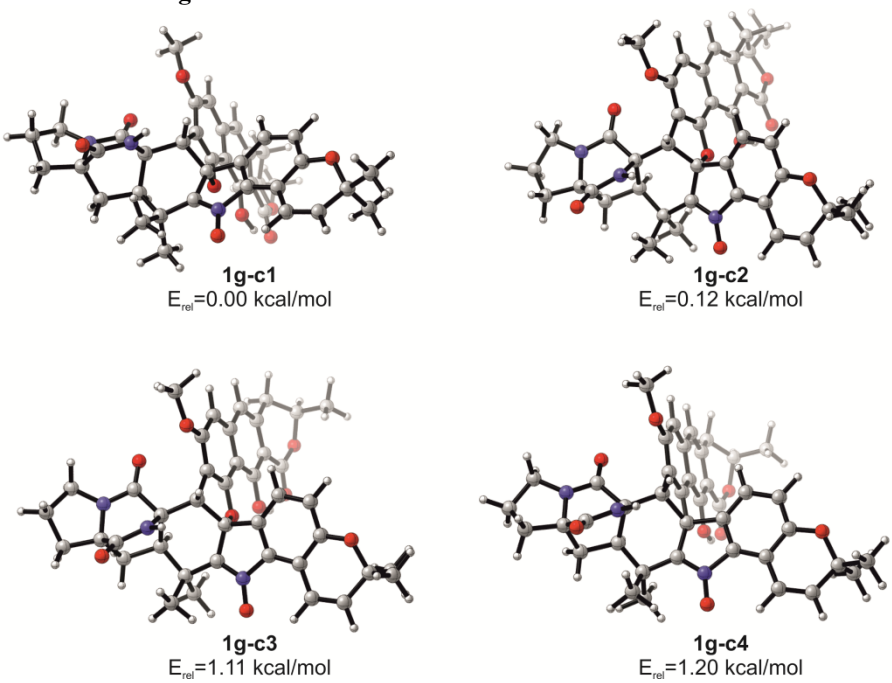
S22: Computational NMR data of 1f



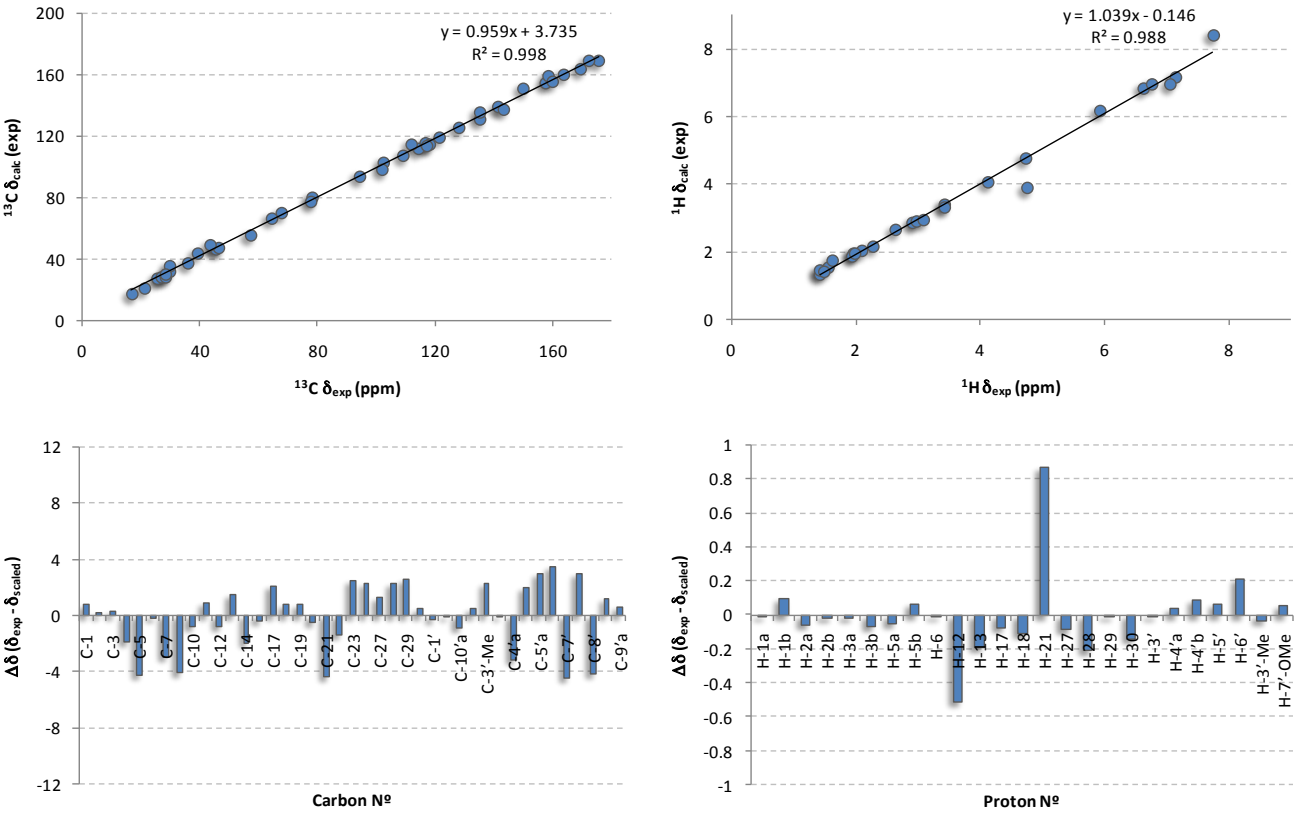
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1f** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



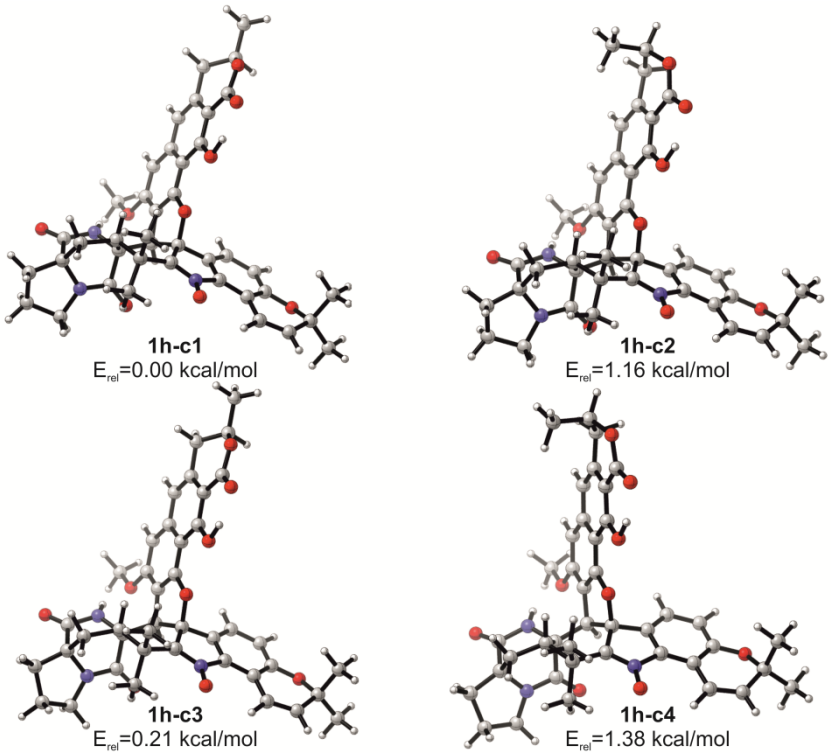
S23: Computational NMR data of 1g



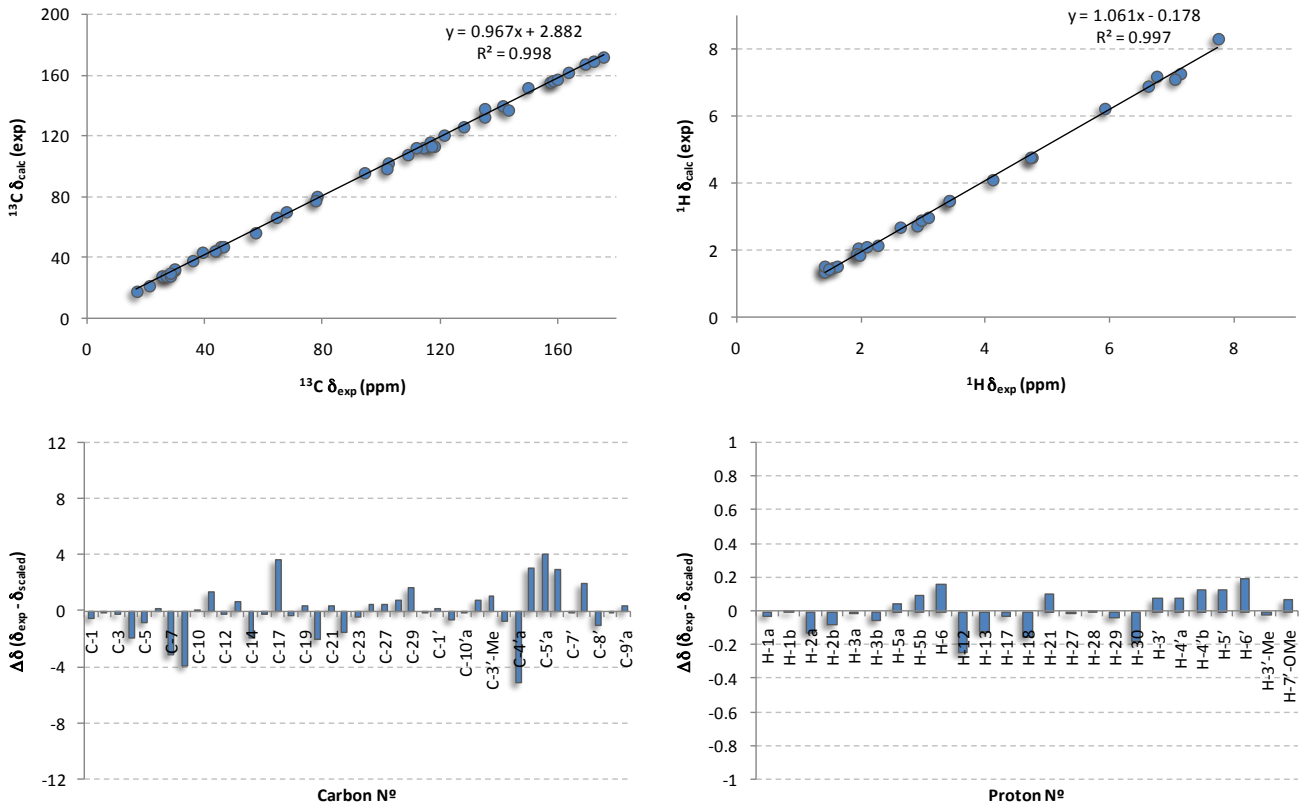
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1g** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.



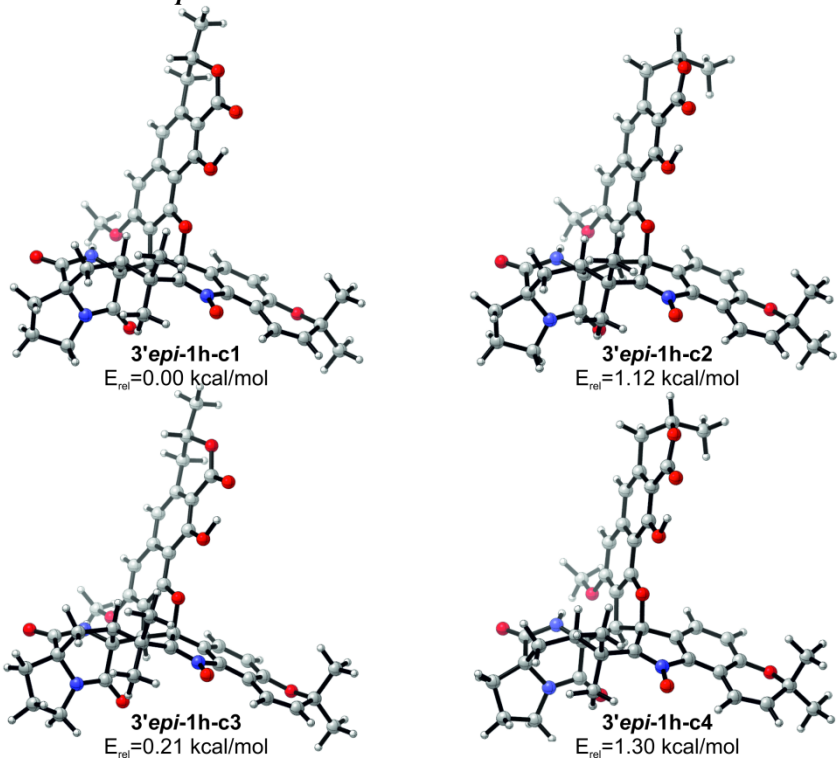
S24: Computational NMR data of 1h



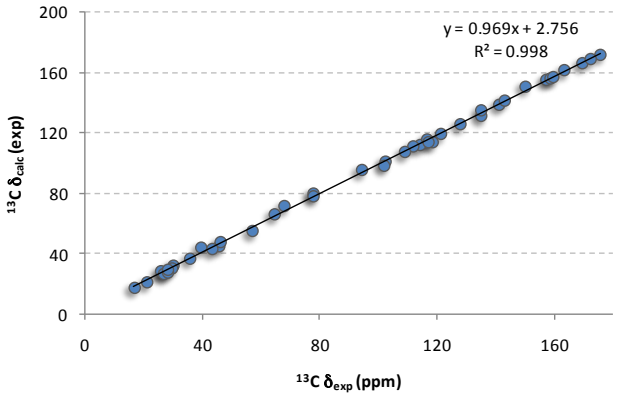
B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for **1h** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.

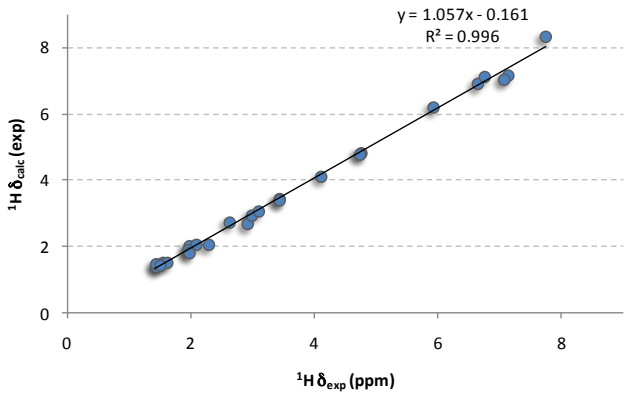


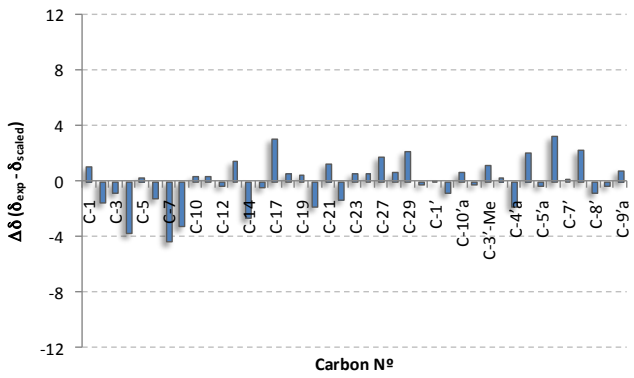
S25: Computational NMR data of 3'*epi*-1h

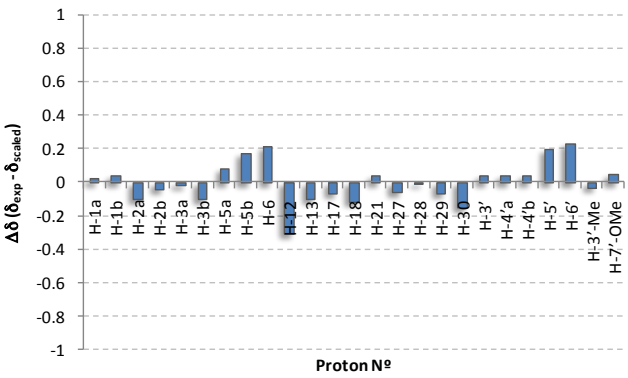


B3LYP/6-31G* geometry optimized geometries of the most stable conformations found for 3'*epi*-**1h** with relative energies computed at the PCM/mPW1PW91/6-31+G**//B3LYP/6-31G* level.

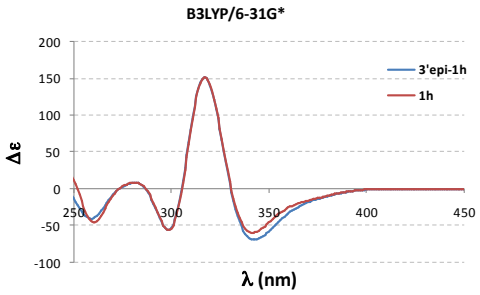


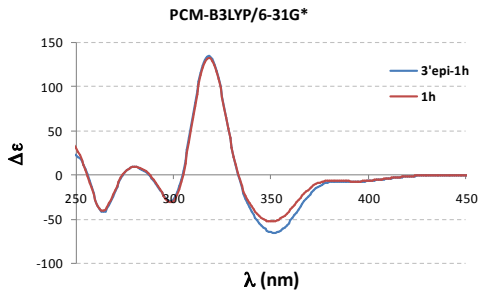


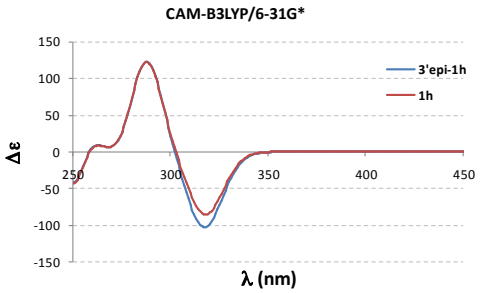


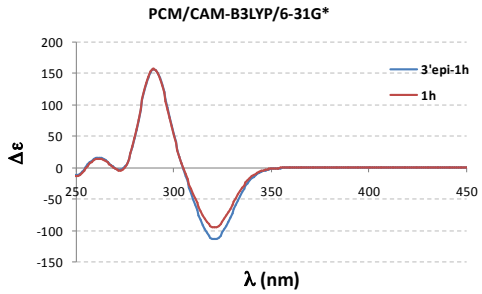


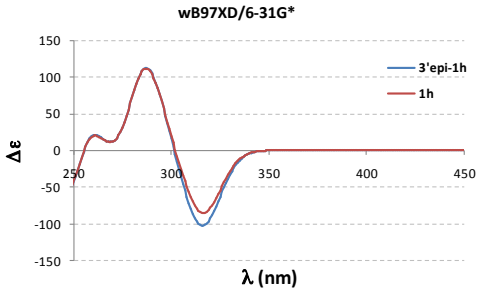
S26: Comparison of the ECD spectra of 1h and 3'*epi*-1h calculated at different levels of theory

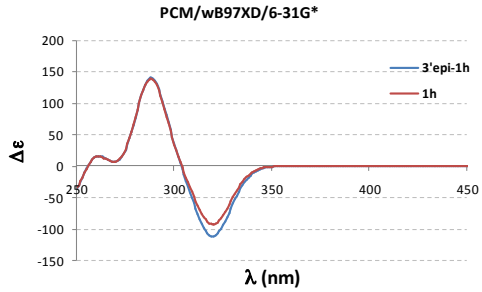












NMR, HRESIMS, UV, and IR spectra

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

	1						2	
no	**Recorded in Pyr-d_5**		**Recorded in DMSO-d_6**		**Recorded in CD_3OD**		**Recorded in Pyr-d_5**	
	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_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

[a] ^1H spectra recorded at 400 MHz. ^{13}C Spectra recorded at 100 MHz. Data based on ^1H, ^{13}C, HSQC, and HMBC experiments.

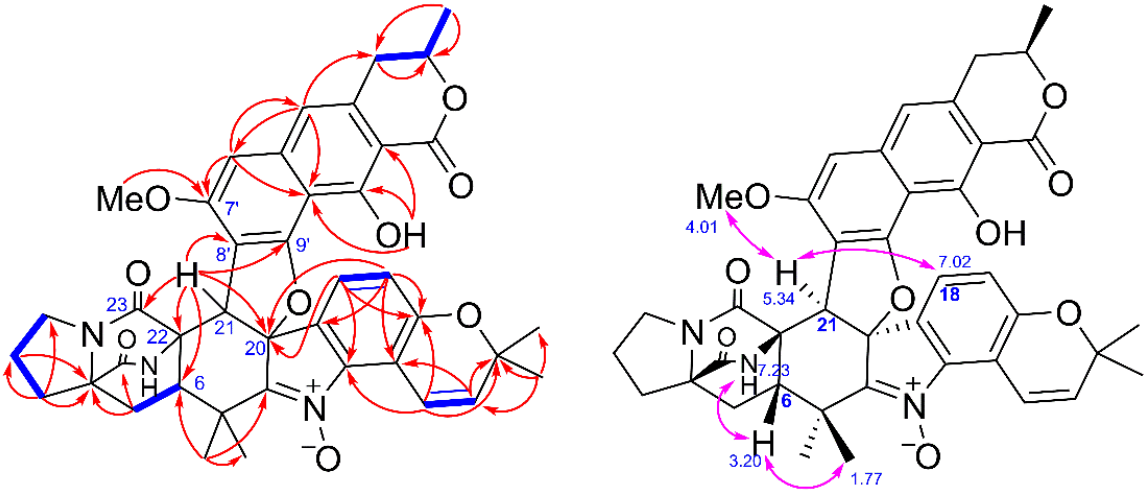
S28: NMR data of compound **3**

no	δ_C	δ_H (*J* in Hz)
2	182.5	
3	61.5	
4	127.6	7.11 (1H, d, *J* = 8.2 Hz)
5	111.7	6.41 (1H, d, *J* = 8.2 Hz)
6	155.0	
7	107.4	
8	138.1	
9	119.9	
10*α*	35.9	2.31 (1H, d, *J* = 14.7 Hz)
10*β*		3.02 (1H, d, *J* = 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, *J* = 10.1 Hz)
26	129.8	4.41 (1H, d, *J* = 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, *J* = 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, *J* = 8.4 Hz)
18’	121.9	7.63 (1H, d, *J* = 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)

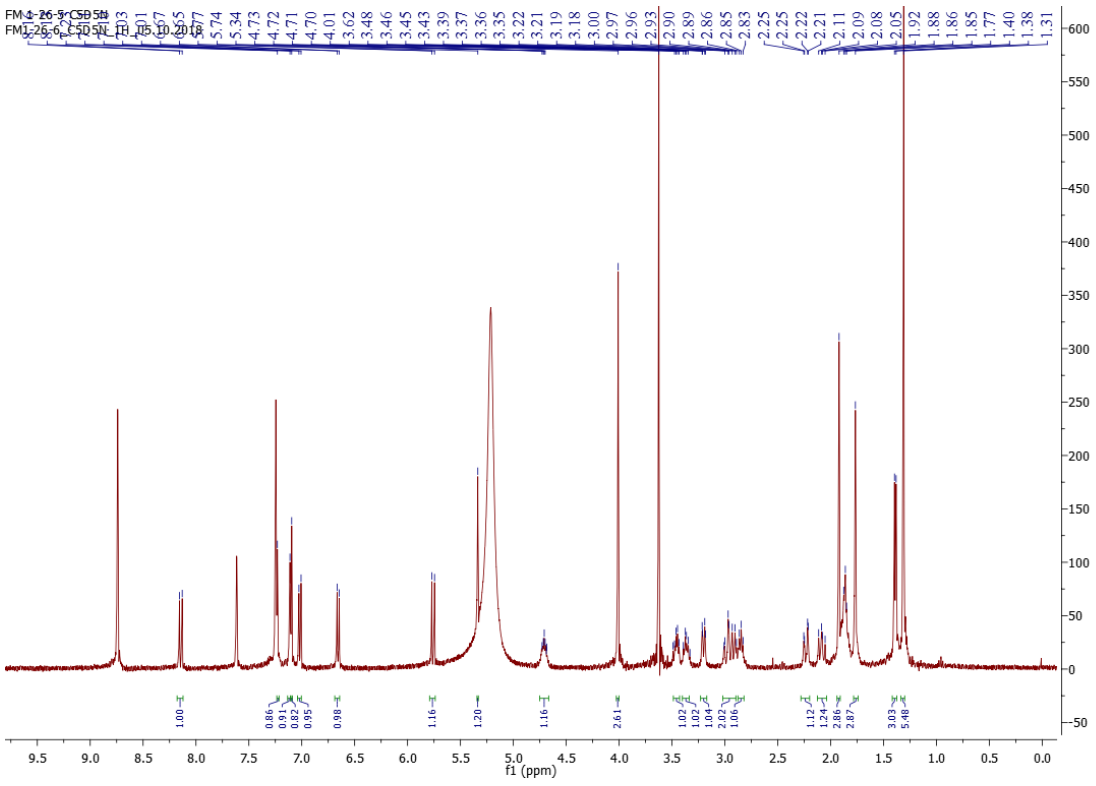
[a] ^{1}H spectra recorded at 400 MHz in Pyr-d_5. ^{13}C Spectra recorded at 100MHz. Data based on ^{1}H, ^{13}C, HSQC, and HMBC experiments.

For compound 1

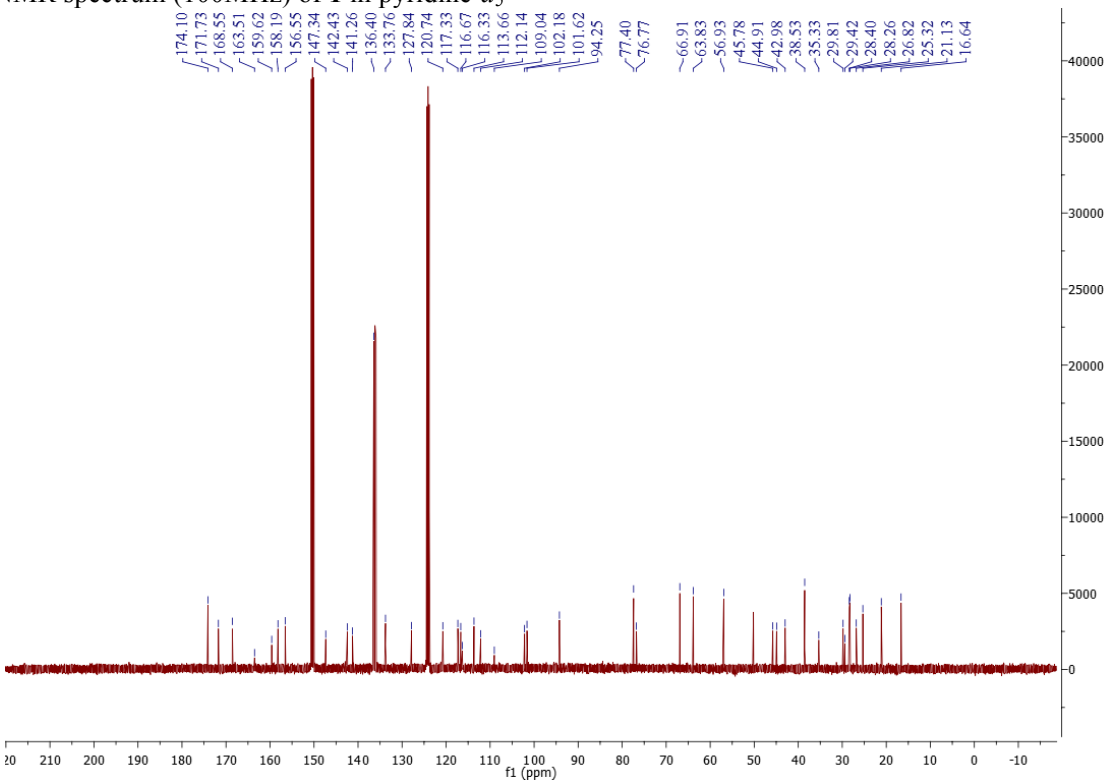
S29: Key 2D NMR correlations for compound **1**



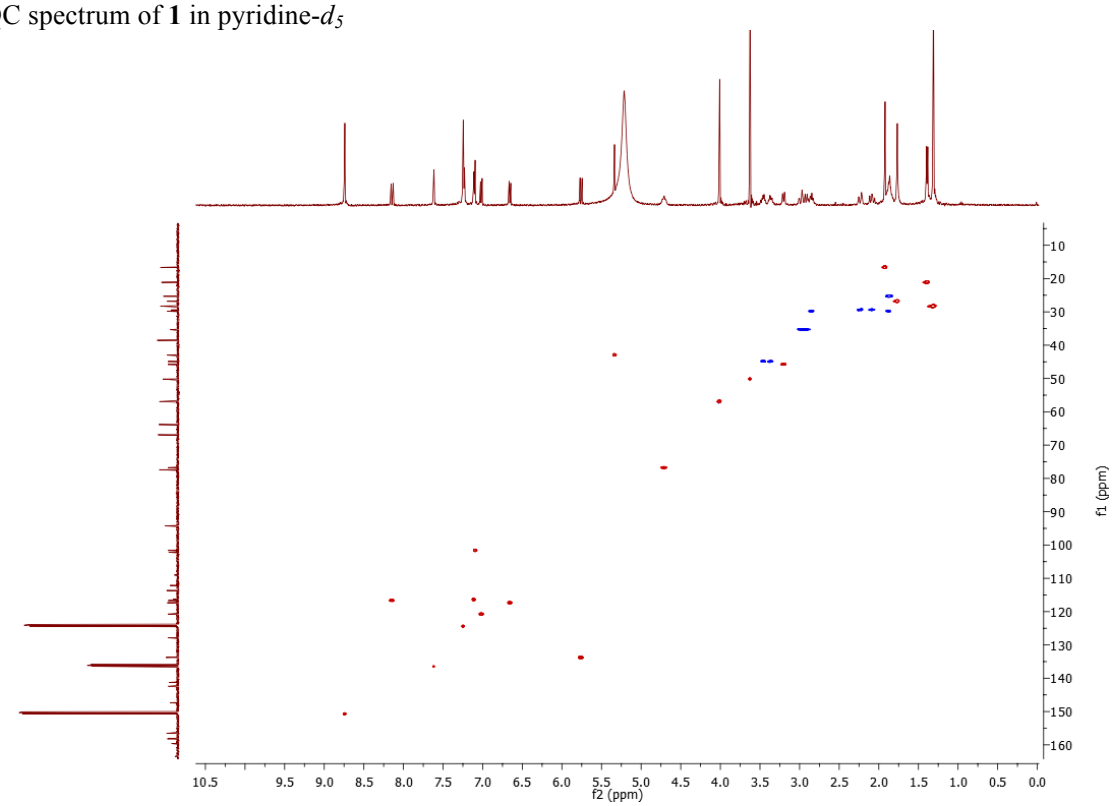
S30: ^{1}H NMR spectrum (400MHz) of **1** in pyridine-d_5



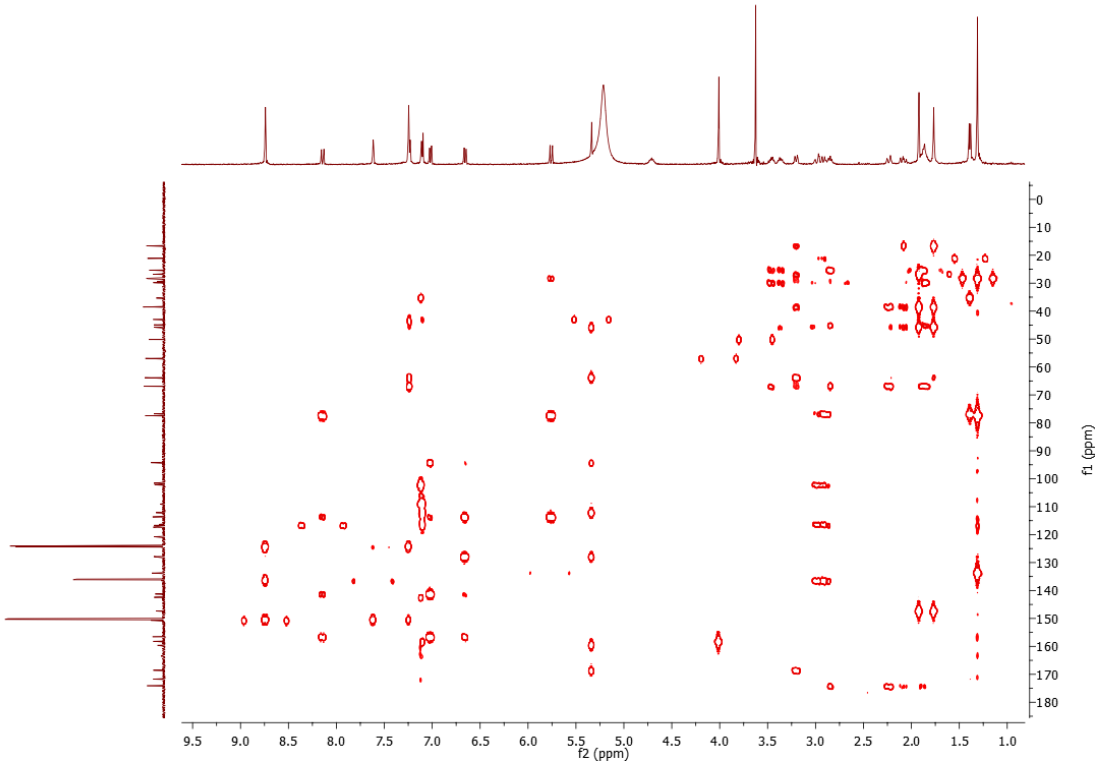
S31: ^{13}C NMR spectrum (100MHz) of **1** in pyridine-d_5



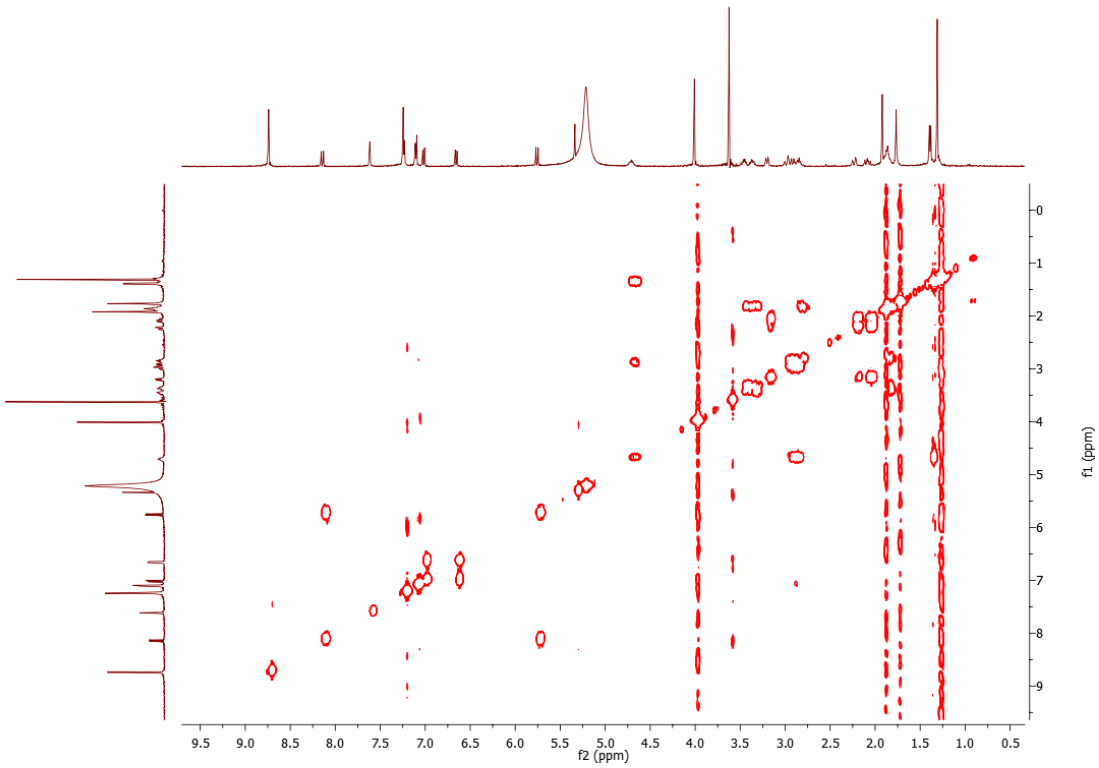
S32: HSQC spectrum of **1** in pyridine-d_5



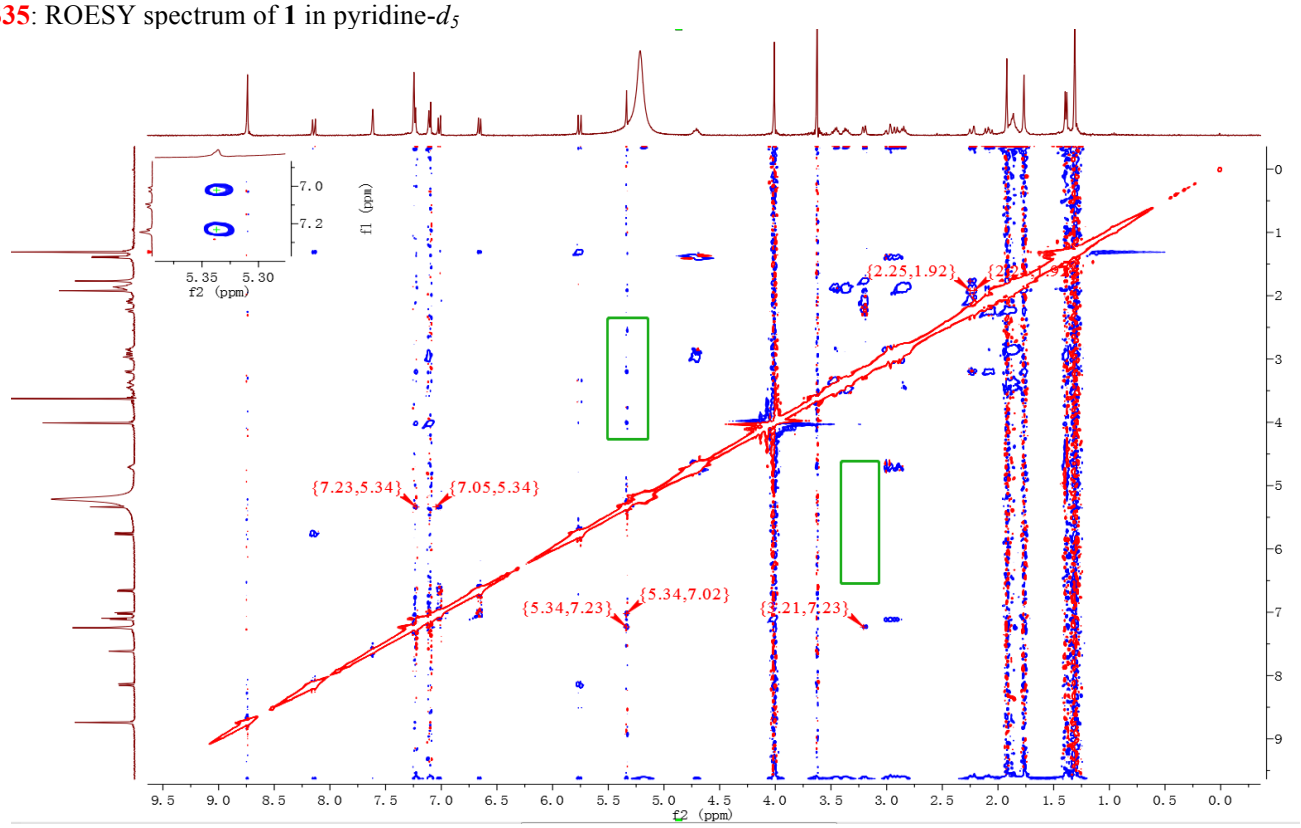
S33: HMBC spectrum of **1** in pyridine-d_5



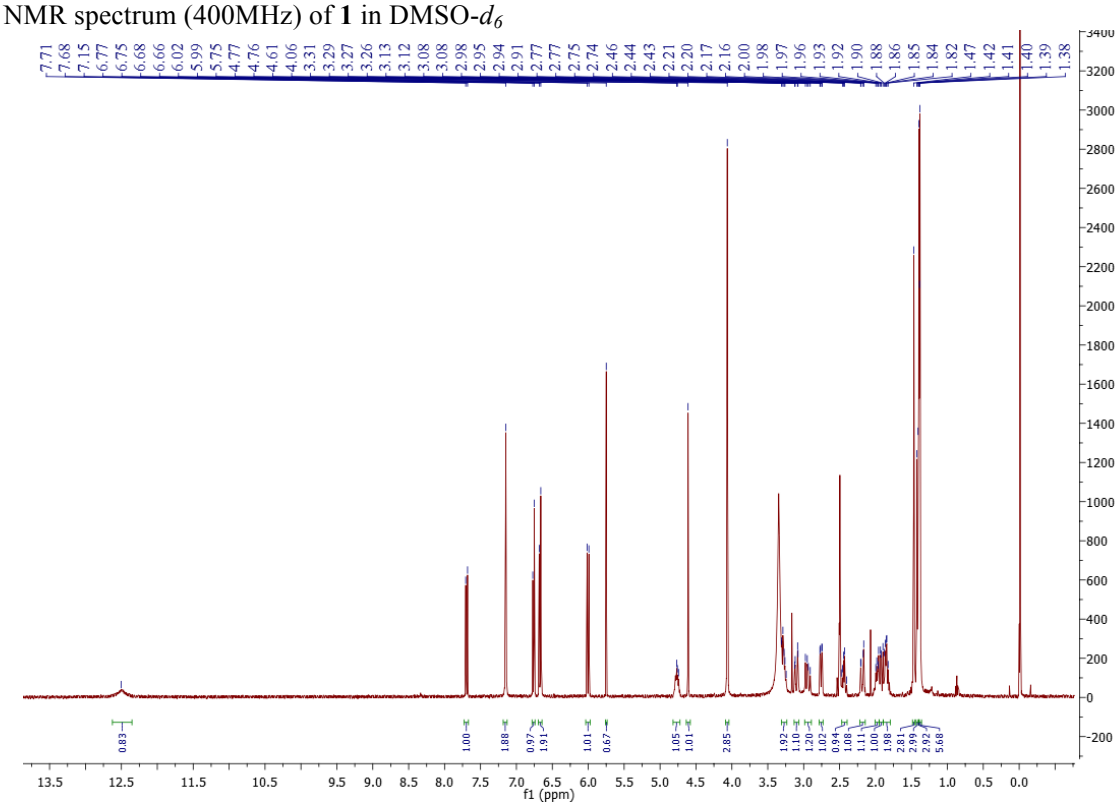
S34: ^{1}H-^{1}H COSY spectrum of **1** in pyridine-d_5



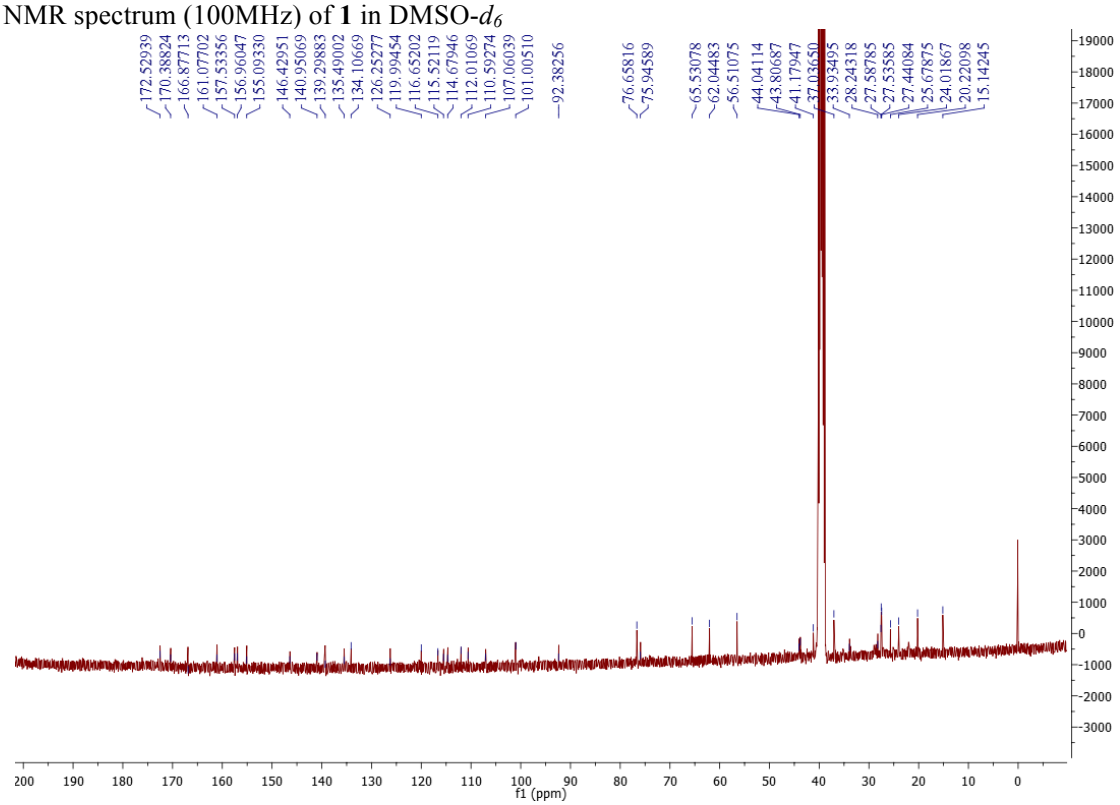
S35: ROESY spectrum of **1** in pyridine-d_5



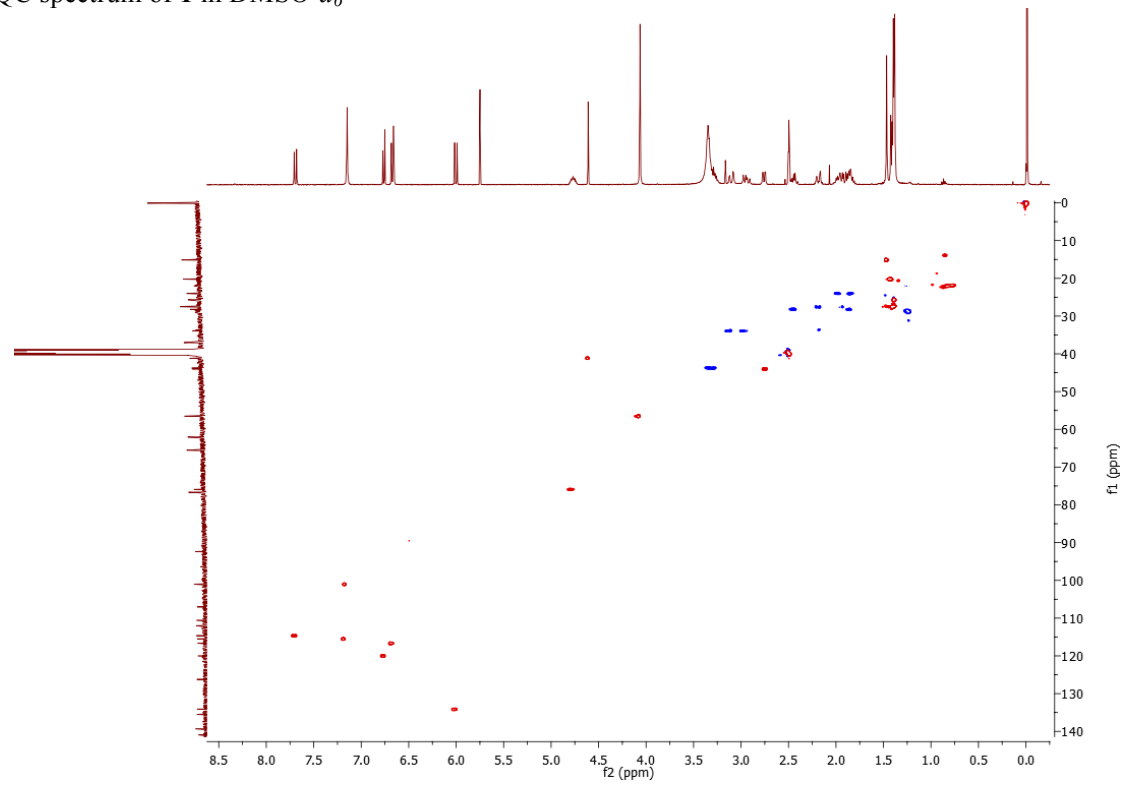
S36: ^{1}H NMR spectrum (400MHz) of **1** in DMSO-d_6



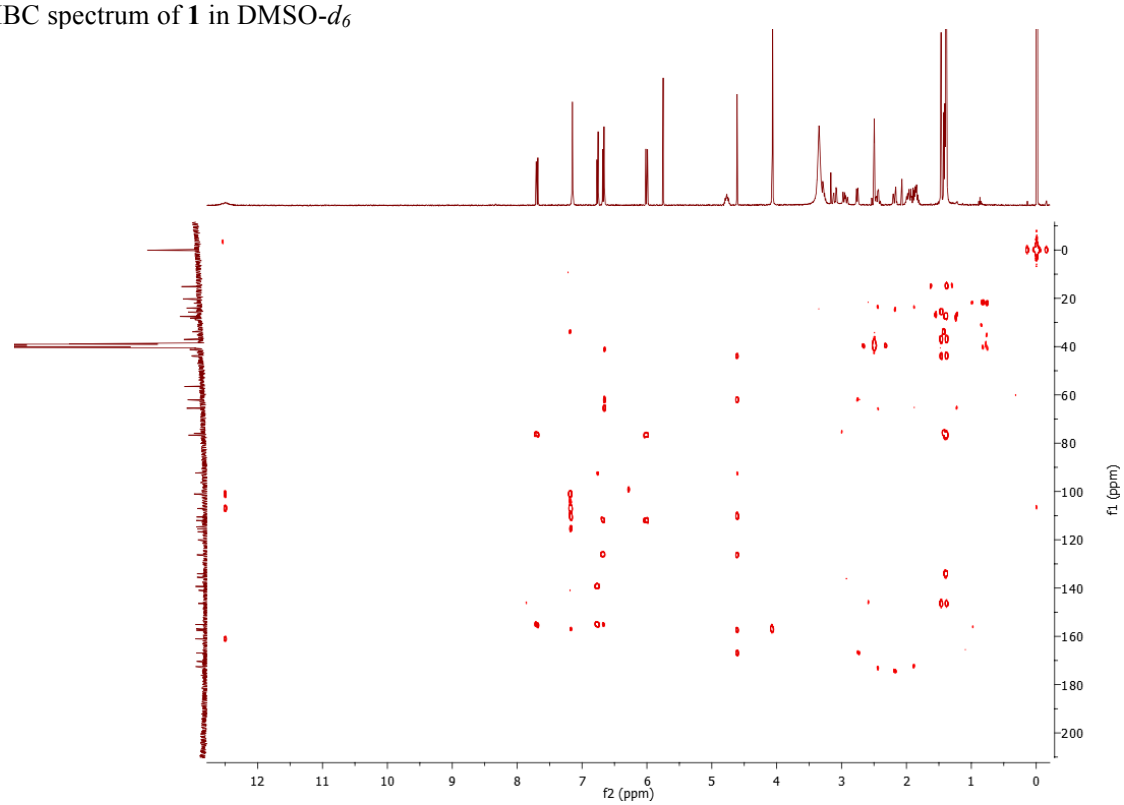
S37: ^{13}C NMR spectrum (100MHz) of **1** in DMSO-d_6



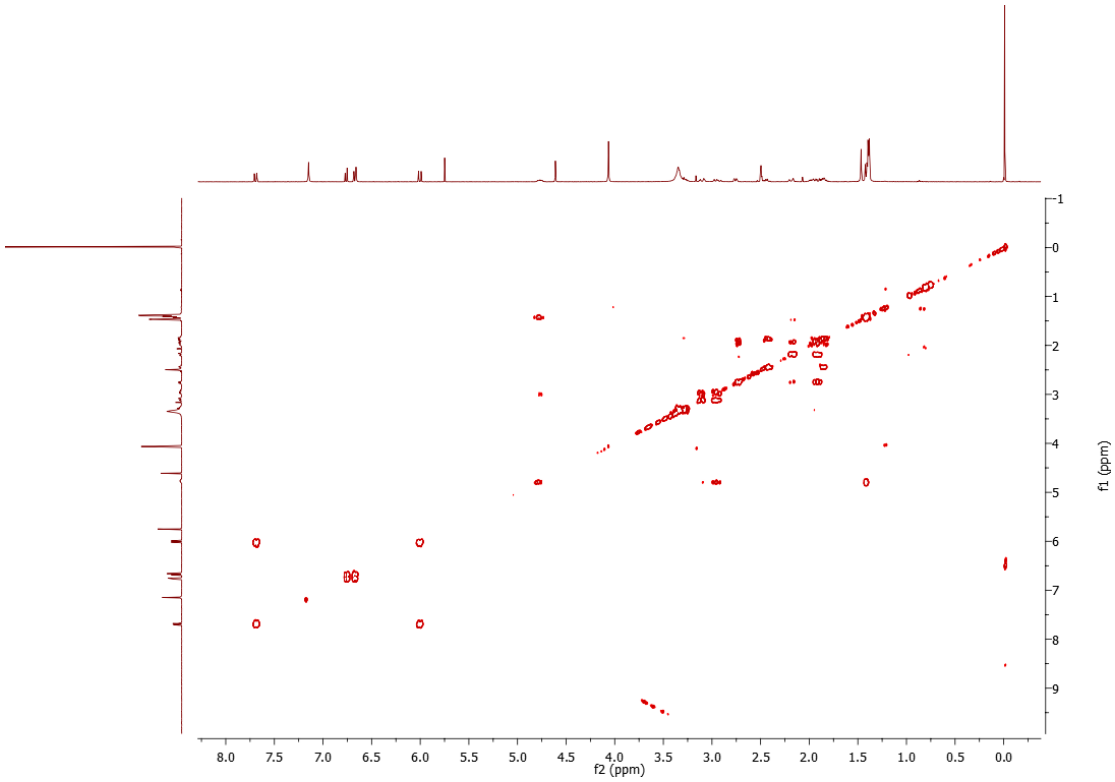
S38: HSQC spectrum of **1** in DMSO-d_6



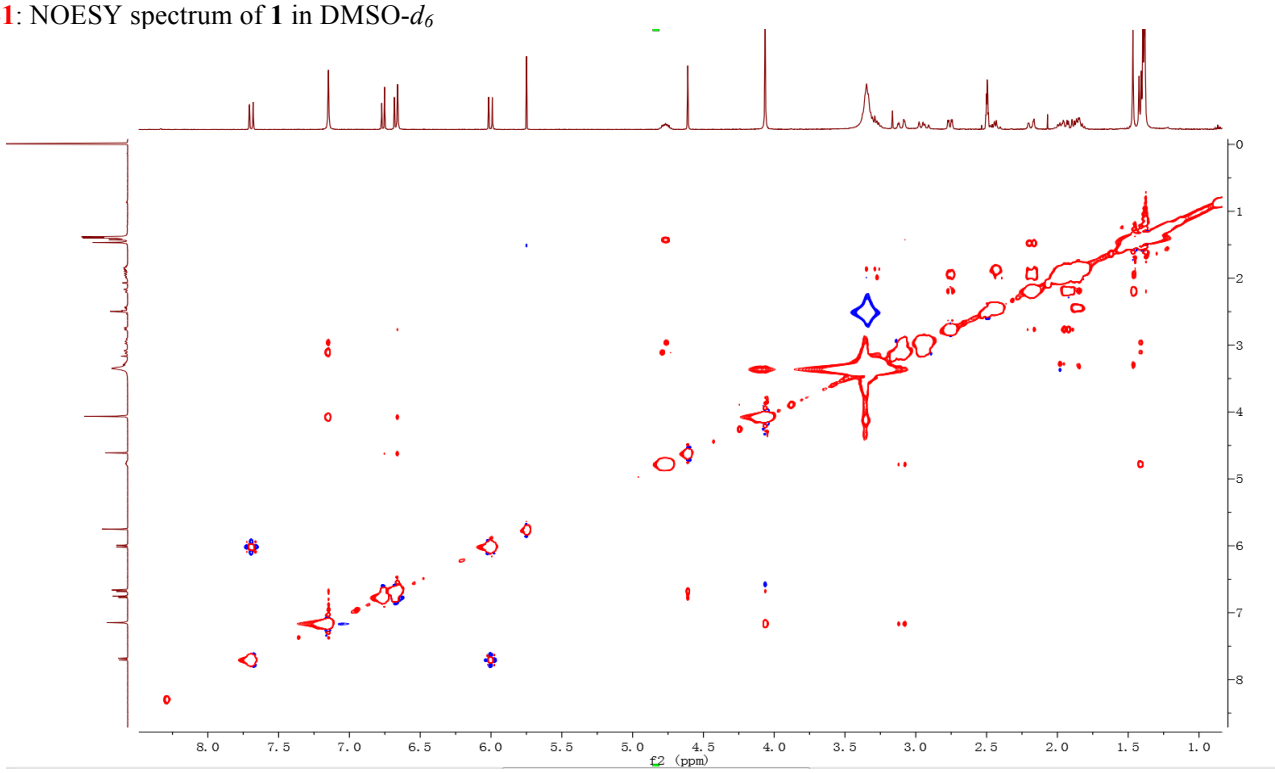
S39: HMBC spectrum of **1** in DMSO-d_6



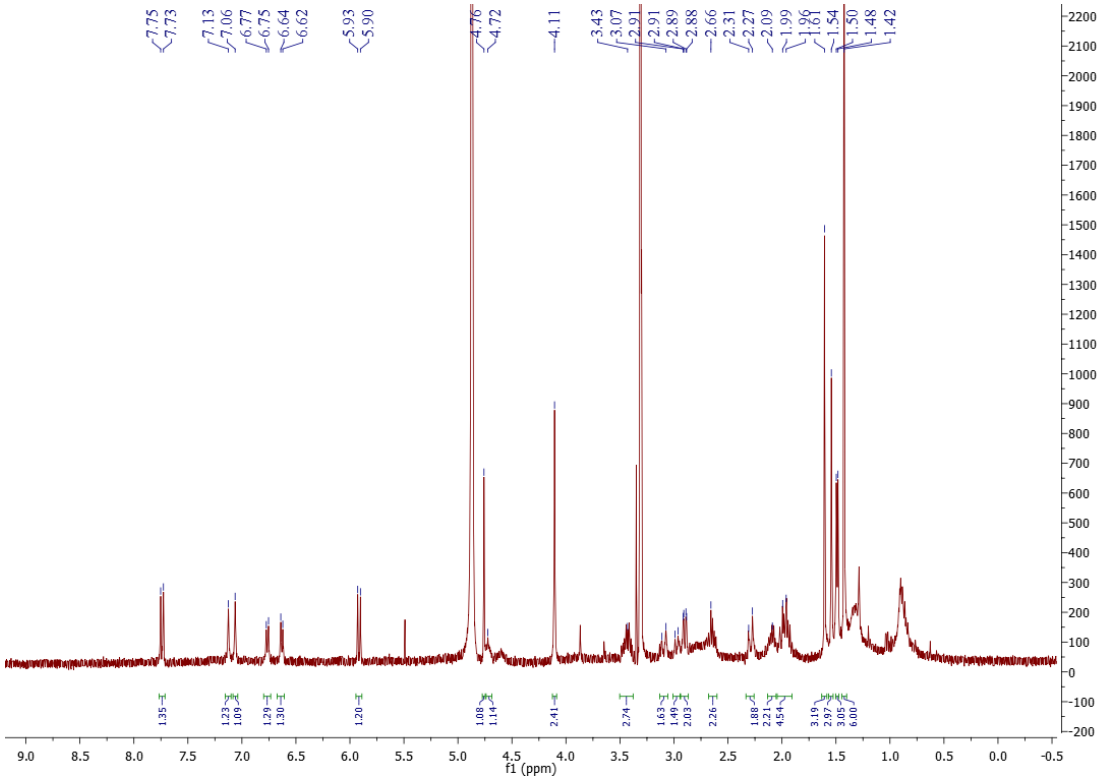
S40: ^{1}H-^{1}H COSY spectrum of **1** in DMSO-d_6



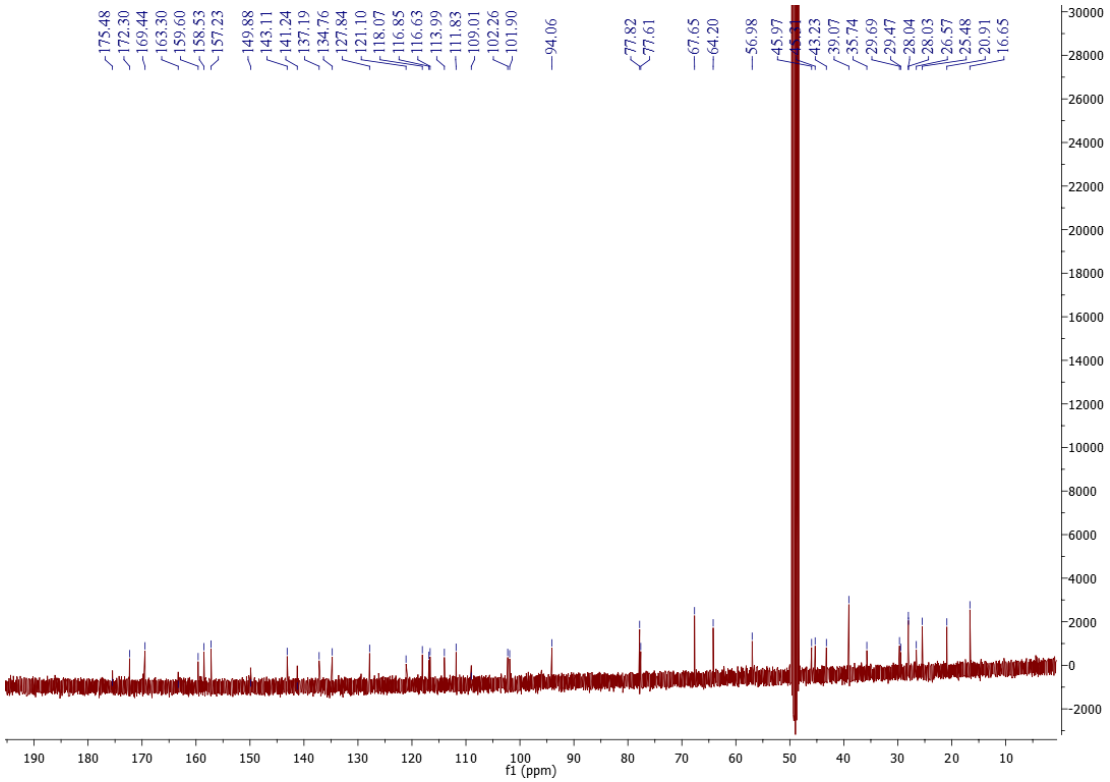
S41: NOESY spectrum of **1** in DMSO-d_6



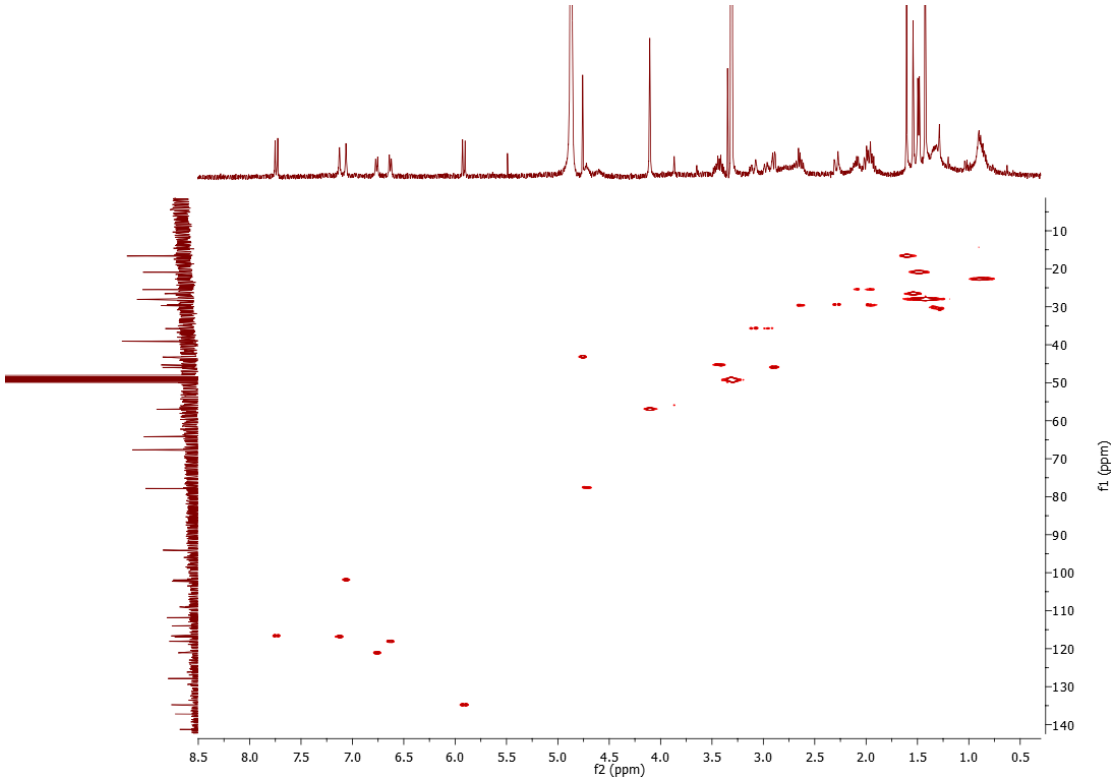
S42: ^{1}H NMR spectrum (400MHz) of **1** in CD_3OD



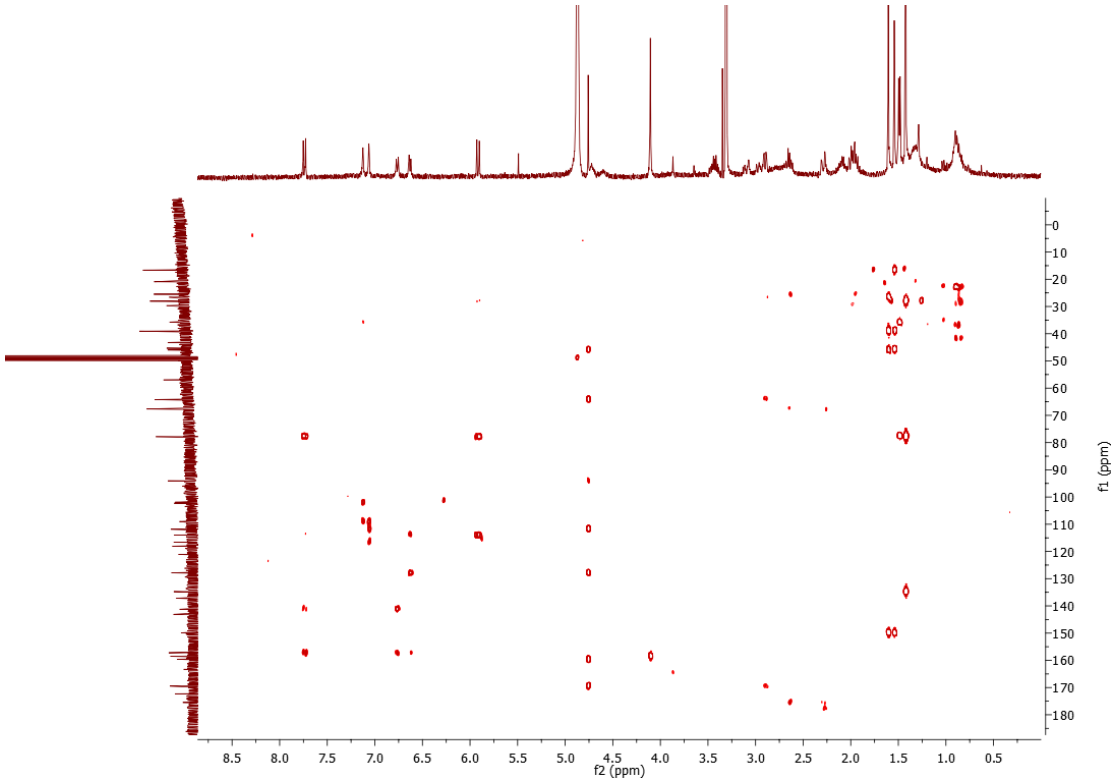
S43: ^{13}C NMR spectrum (100MHz) of **1** in CD_3OD



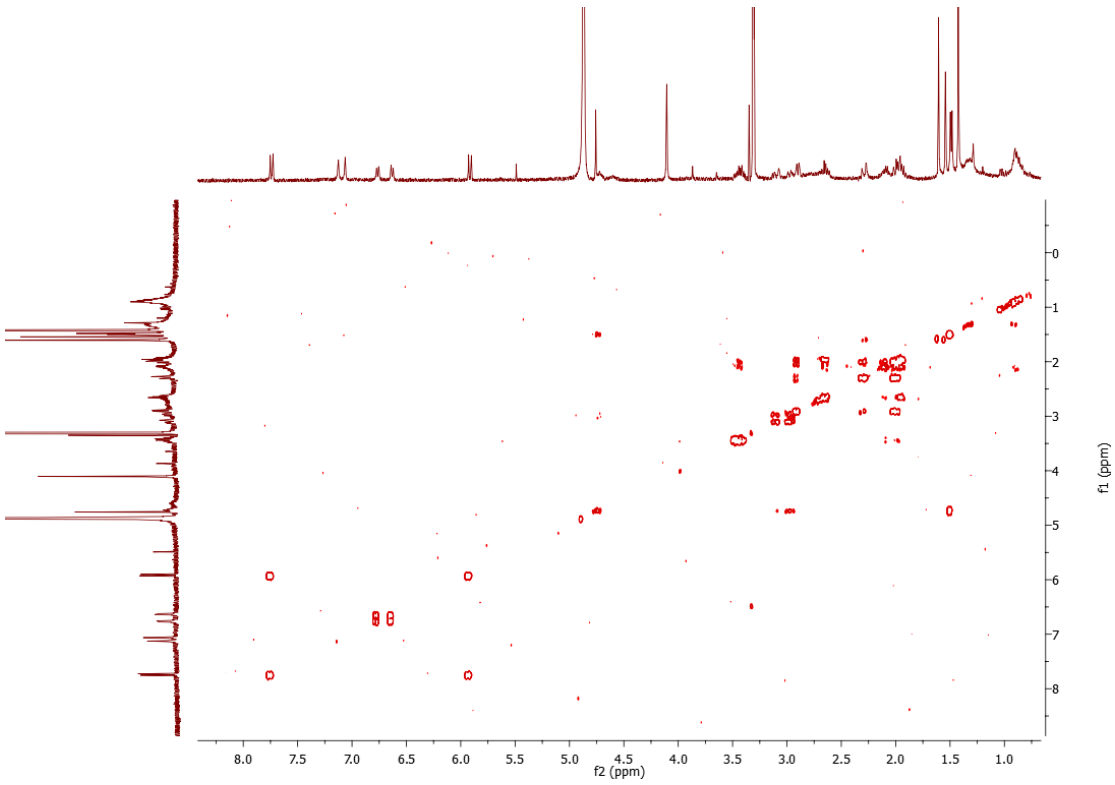
S44: HSQC spectrum of **1** in CD_3OD



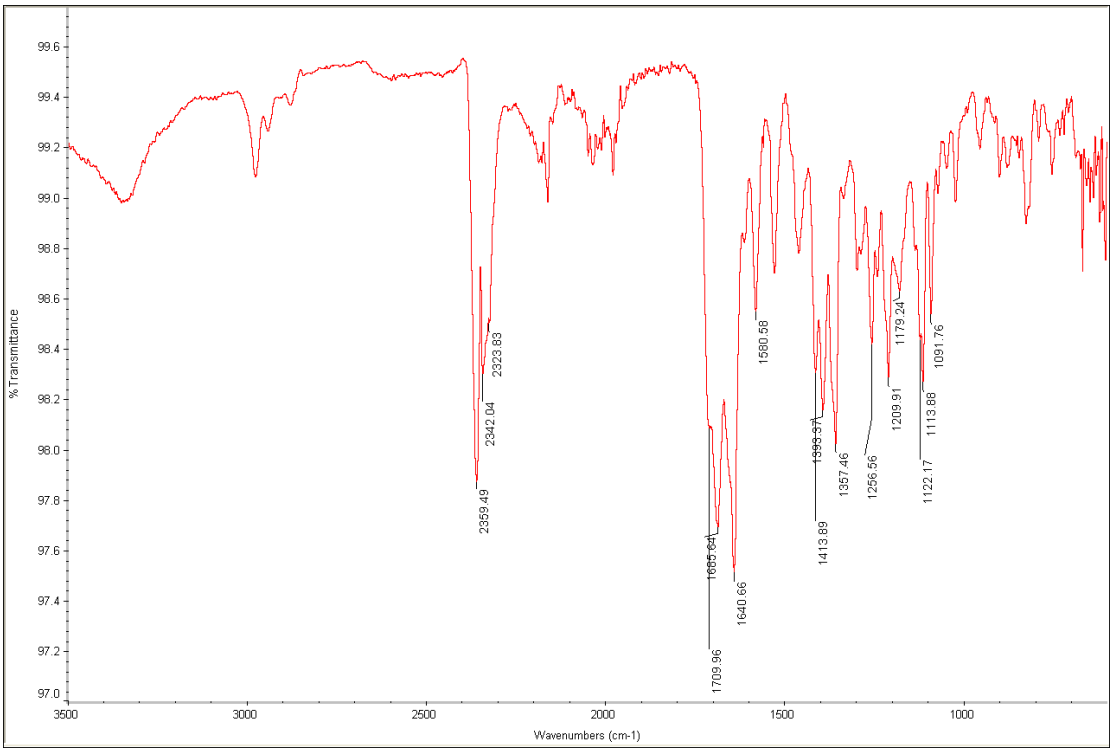
S45: HMBC spectrum of **1** in CD_3OD



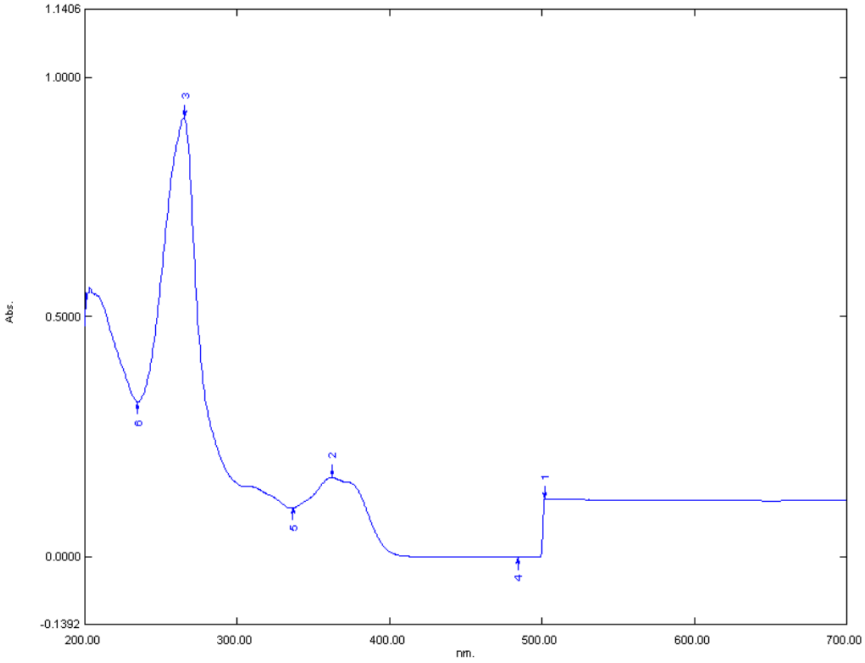
S46: ^{1}H-^{1}H COSY spectrum of **1** in CD_3OD



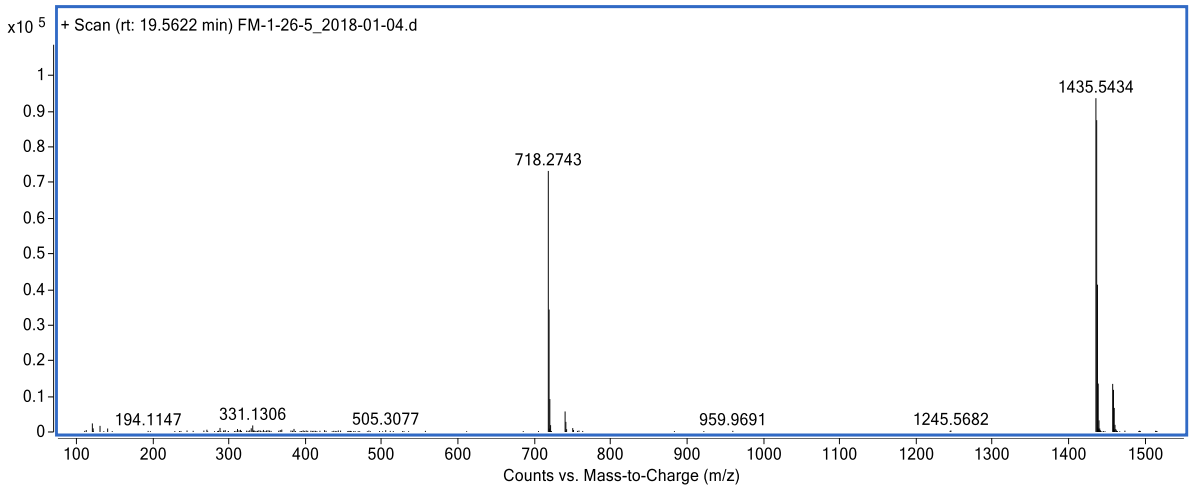
S47: IR spectrum of **1** (2359 and 2342 are CO_2 absorption bands)



S48: UV spectrum of **1**

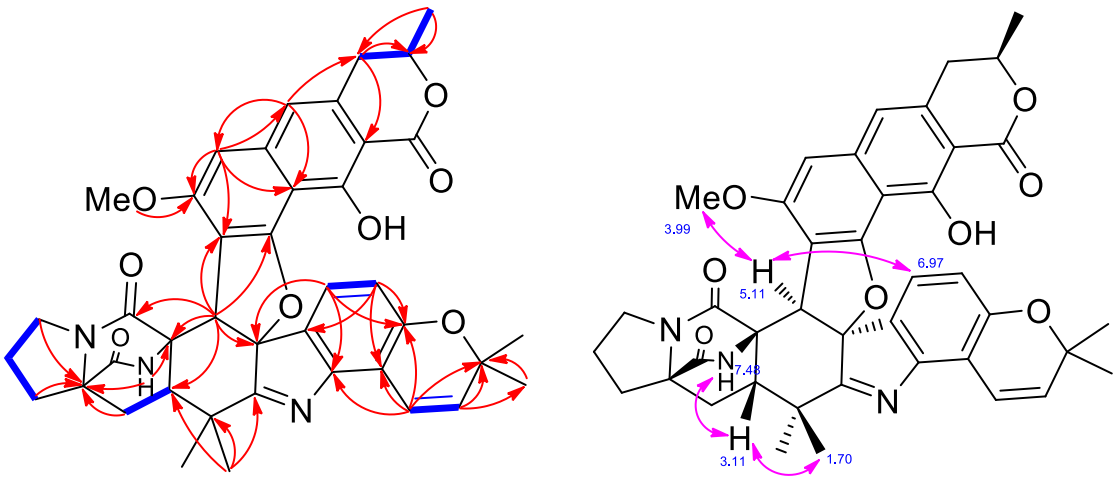


S49: (+)-HR-MS spectrum of **1**

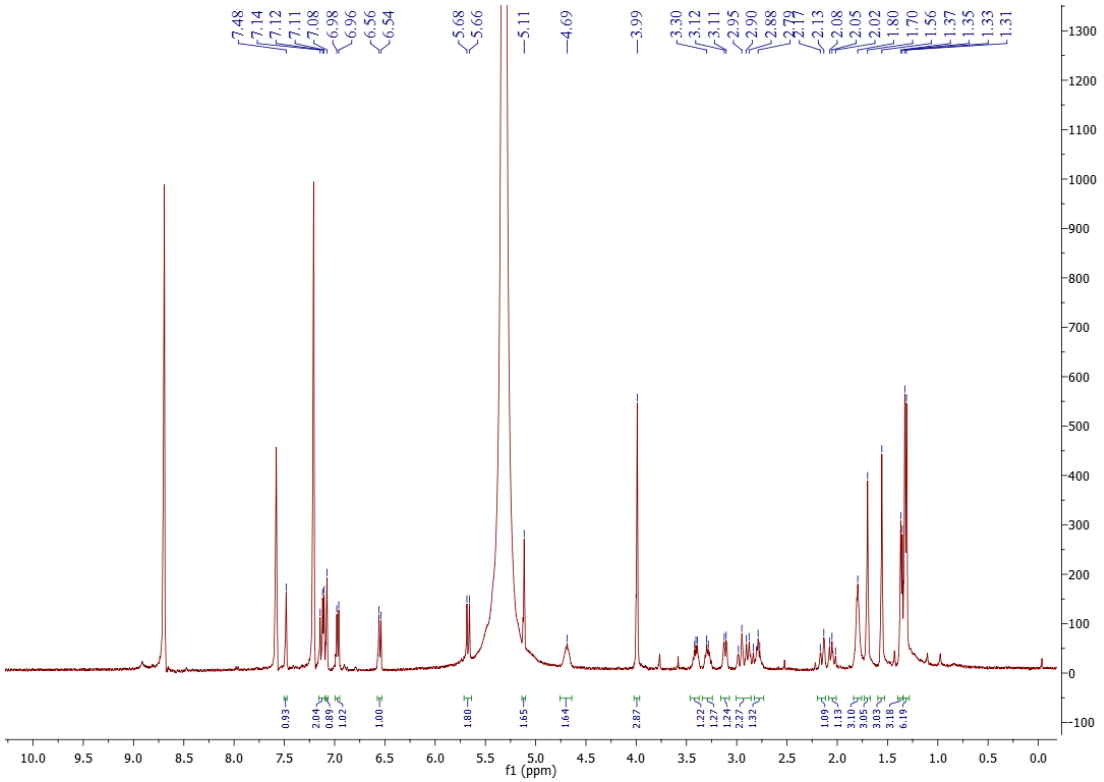


For compound 2

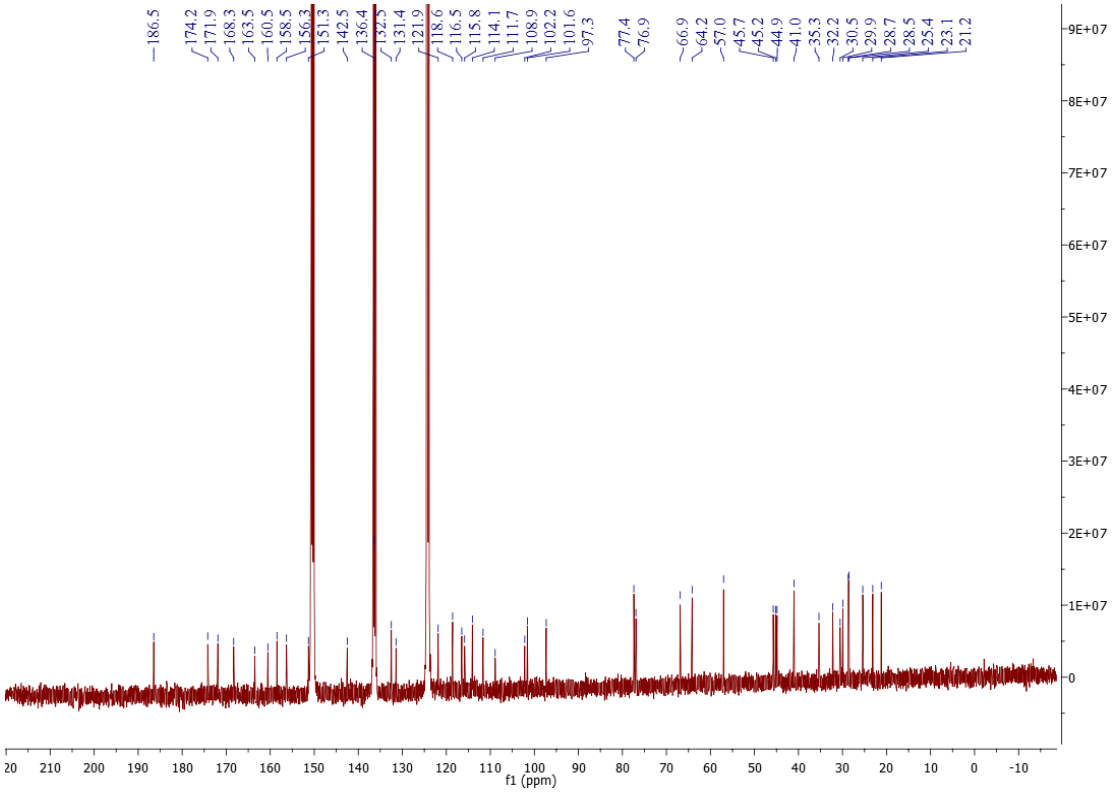
S50: Key 2D NMR correlations for compound **2**



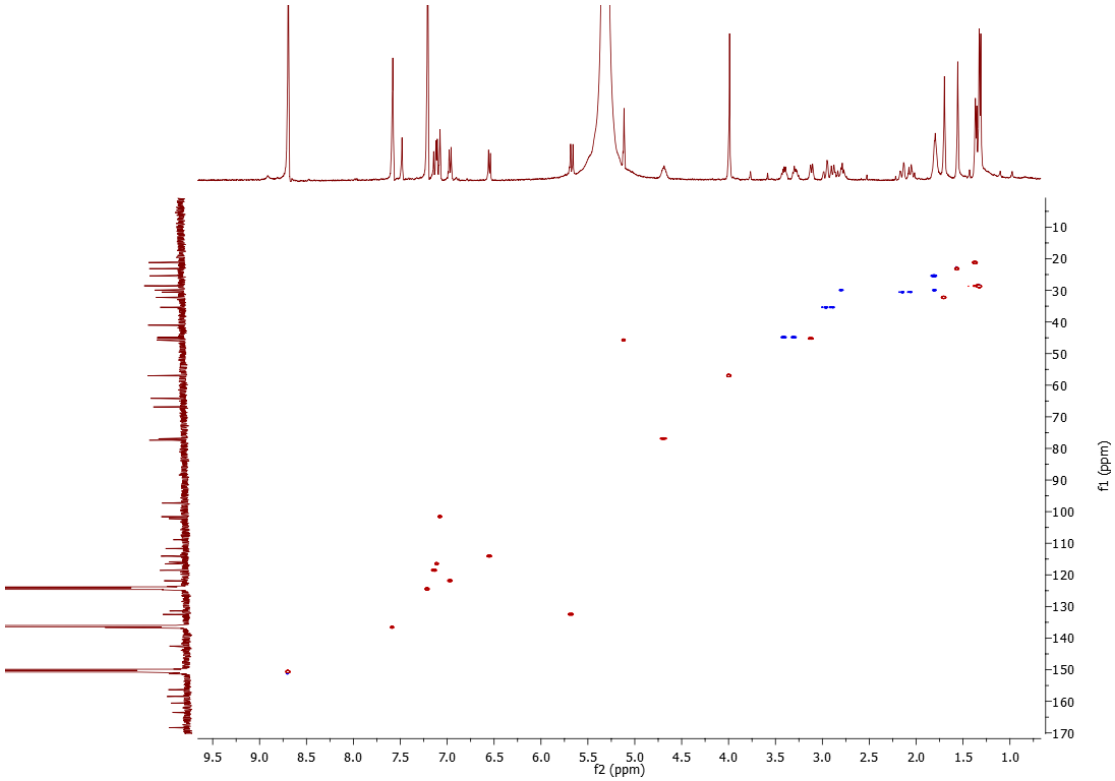
S51: ^{1}H NMR spectrum (400MHz) of **2** in pyridine-d_5



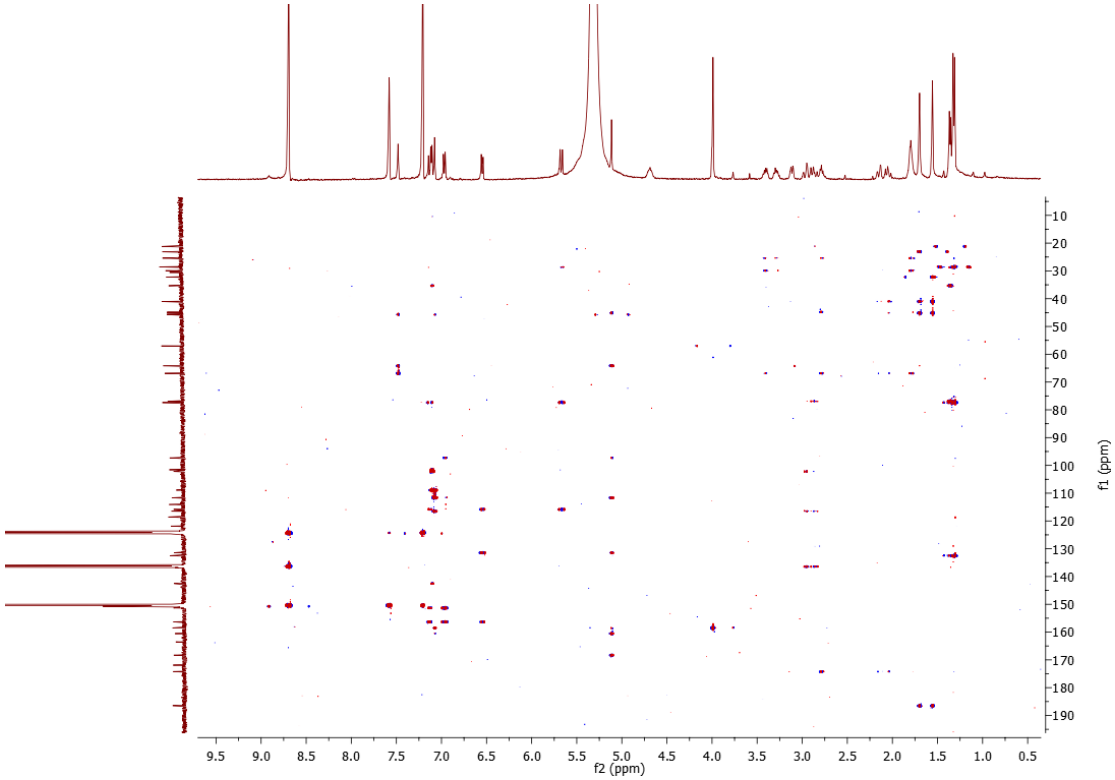
S52: ^{13}C NMR spectrum (100MHz) of **2** in pyridine-d_5



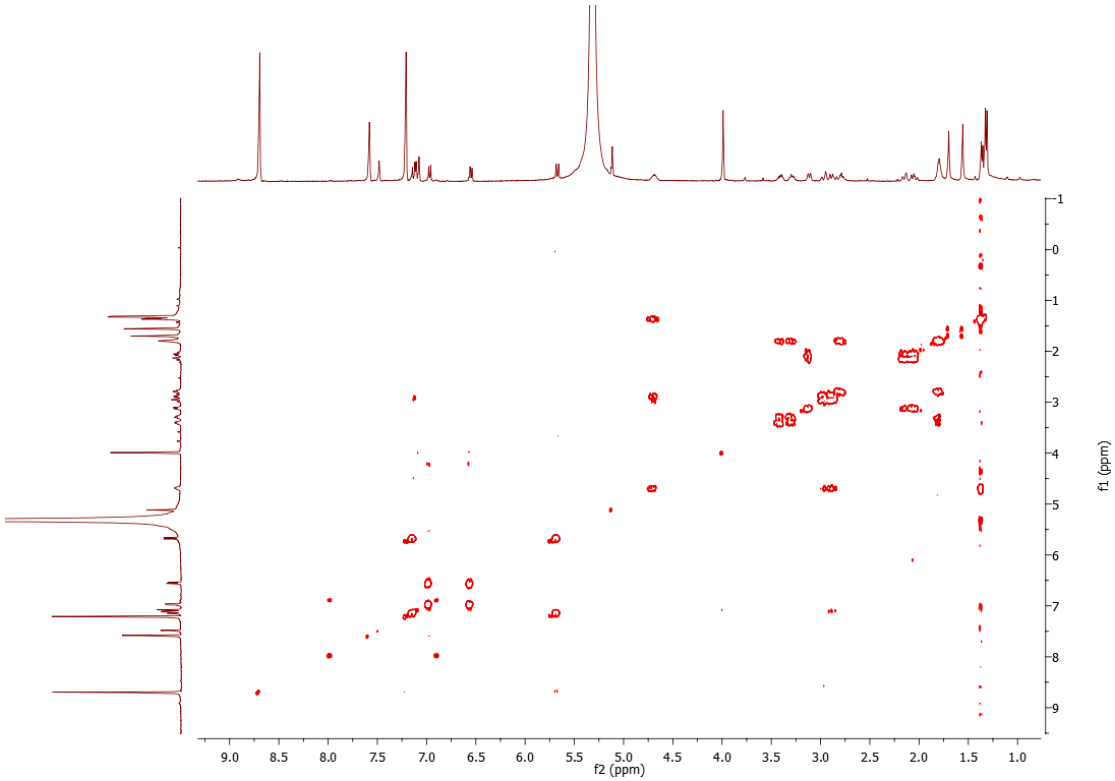
S53: HSQC spectrum of **2** in pyridine-d_5



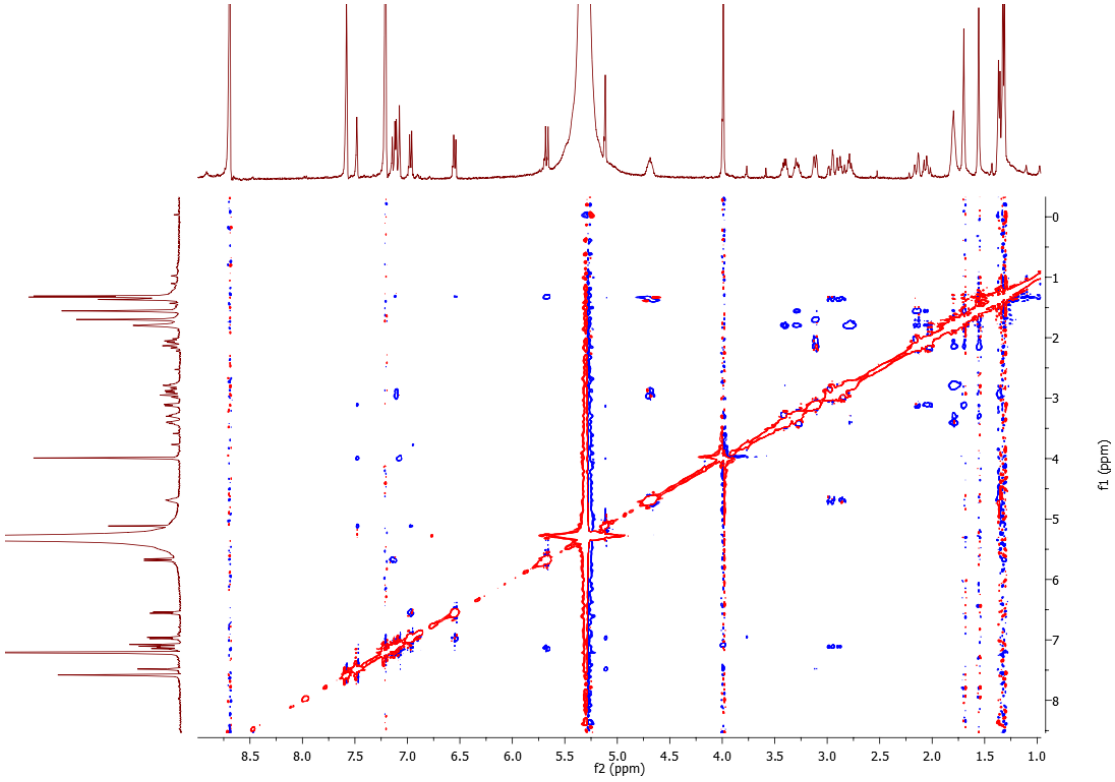
S54: HMBC spectrum of **2** in pyridine-d_5



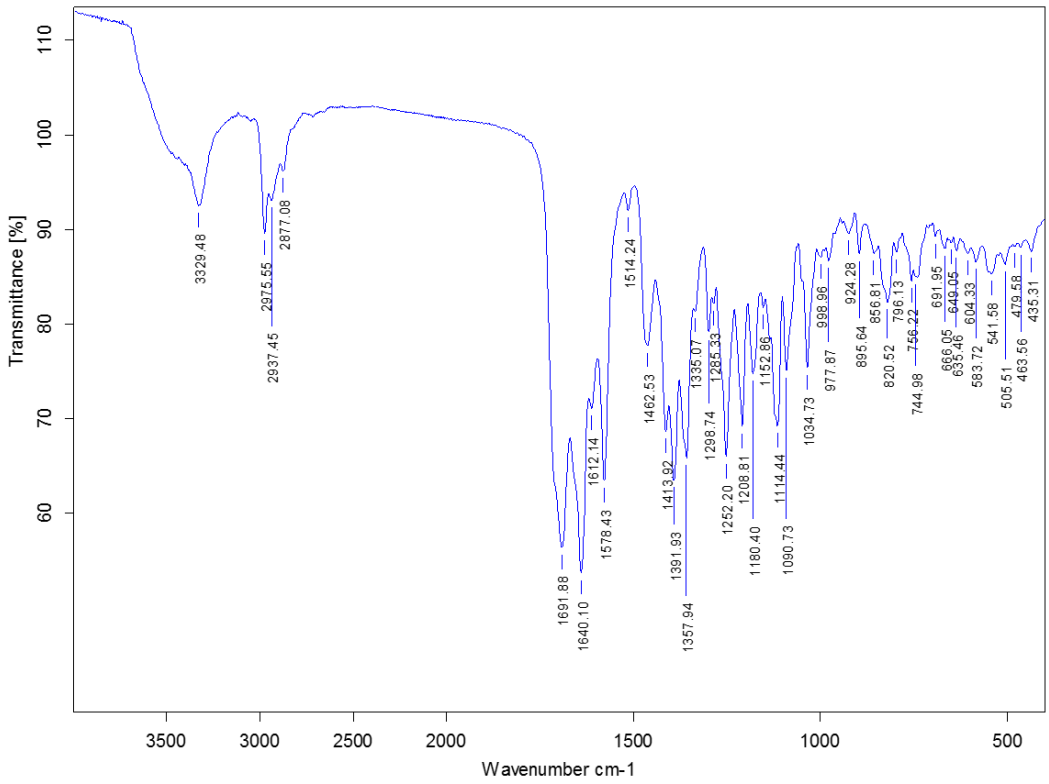
S55: ^{1}H-^{1}H COSY spectrum of **2** in pyridine-d_5



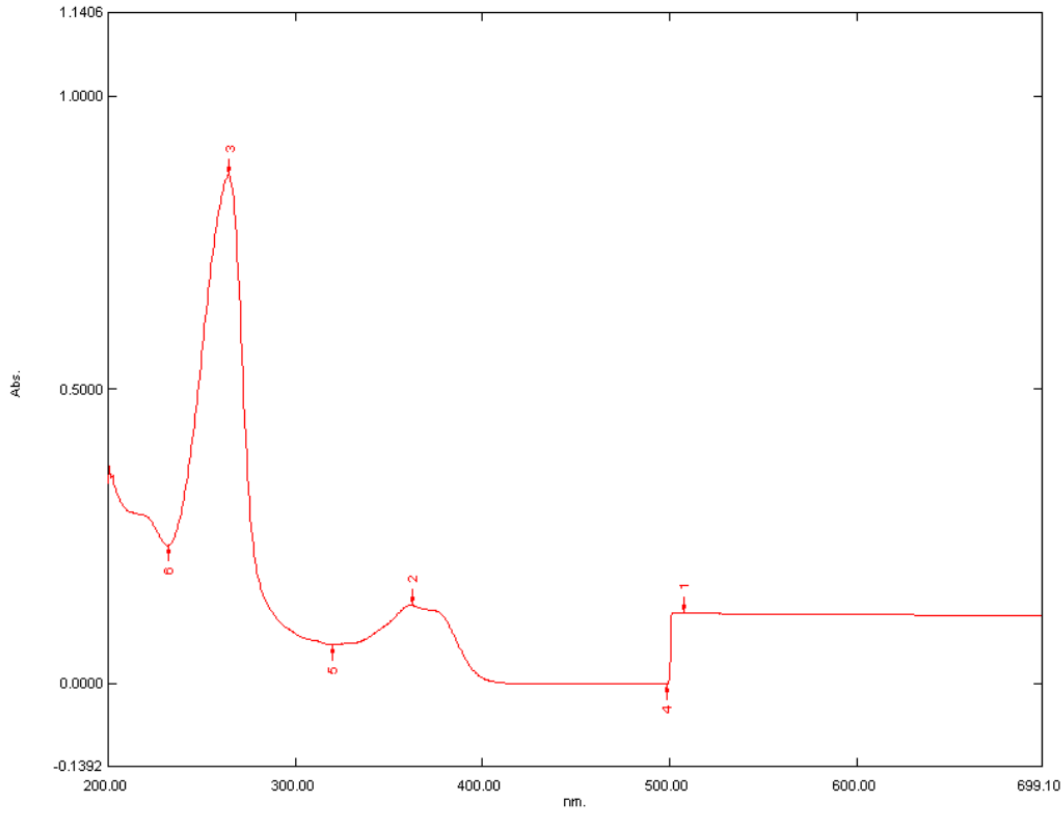
S56: NOESY spectrum of **2** in pyridine-d_5



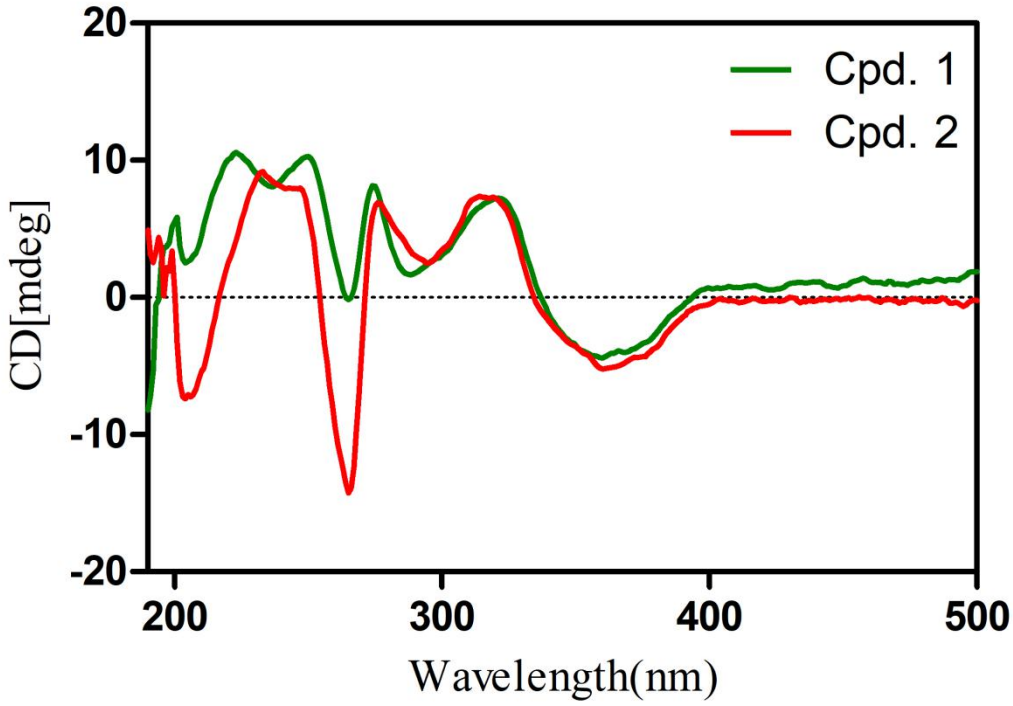
S57: IR spectrum of **2**



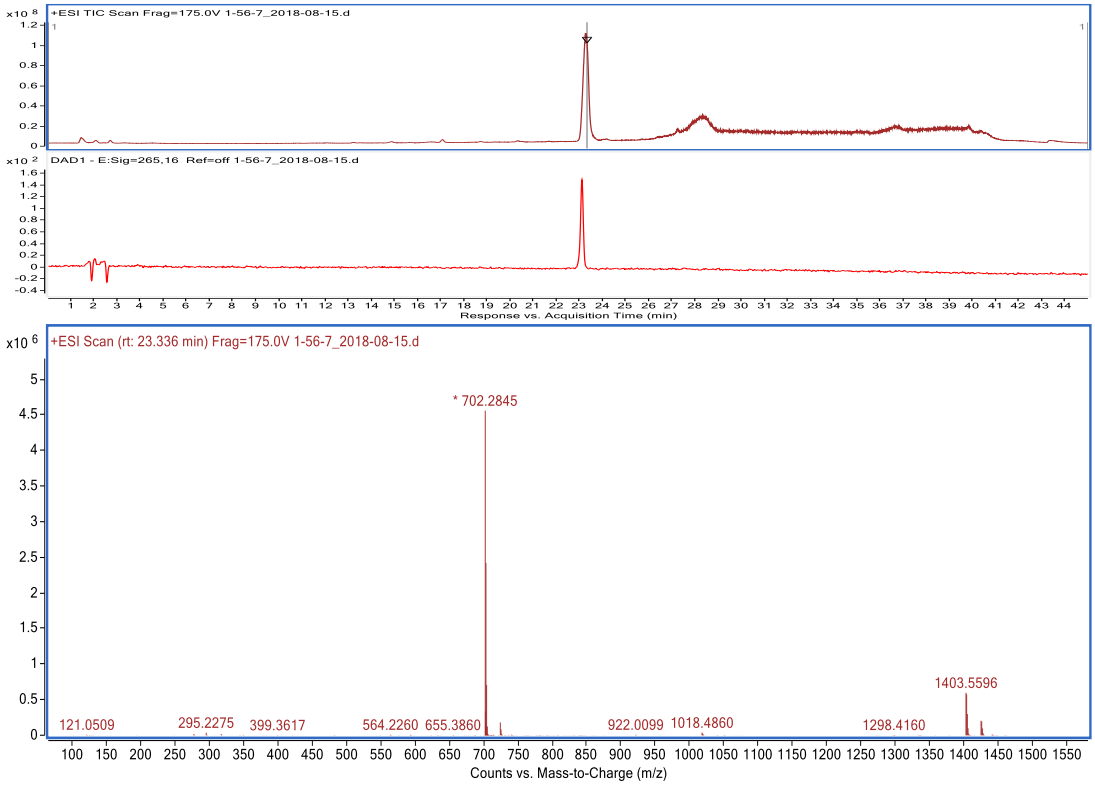
S58: UV spectrum of **2**



S59: CD spectrum of **1** and **2**

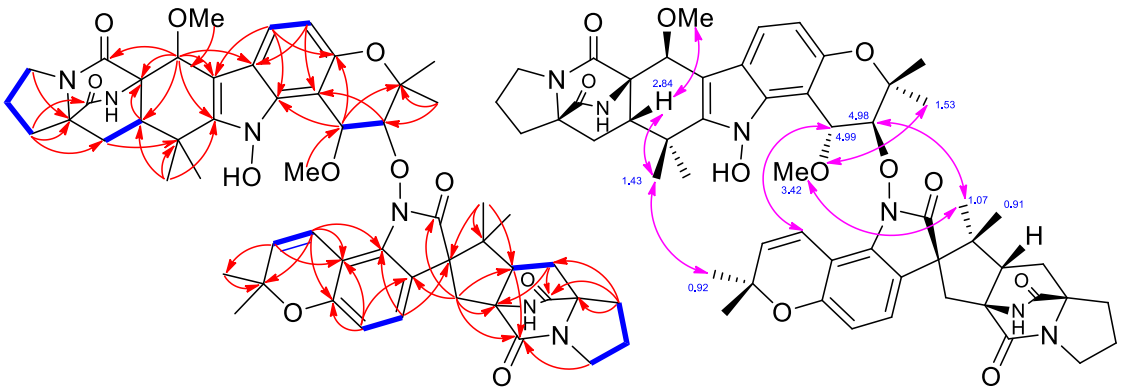


S60: (+)-HR-MS spectrum of **2**

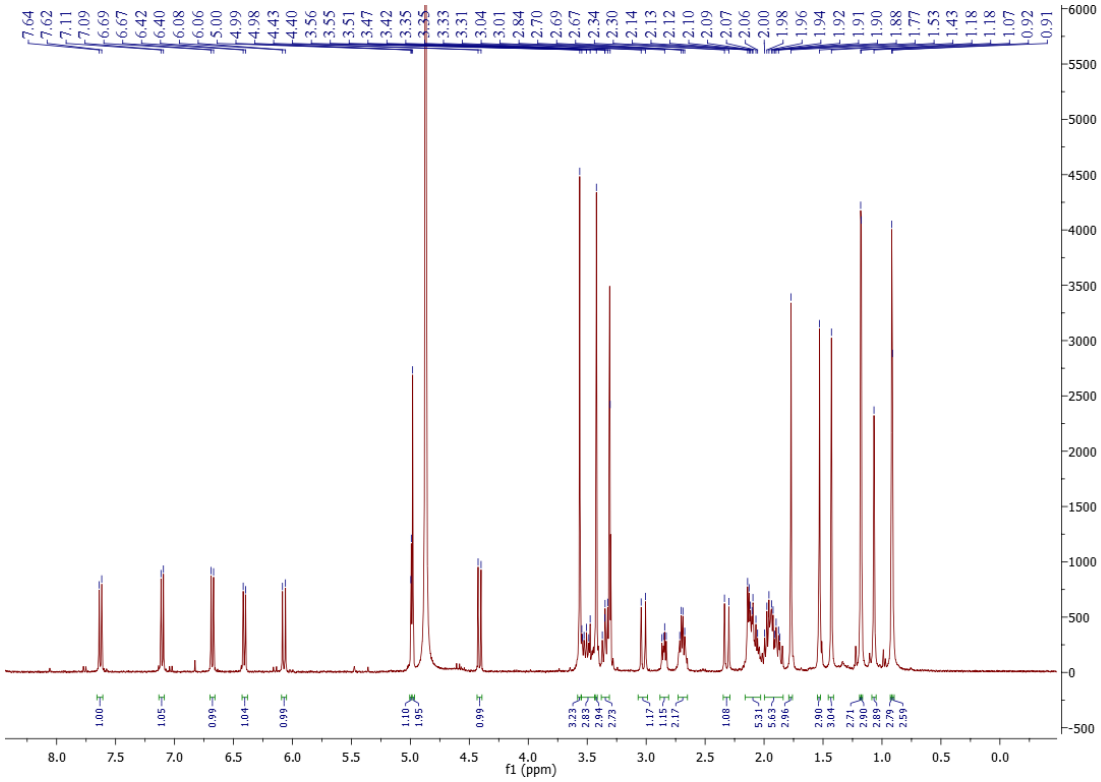


For compound 3

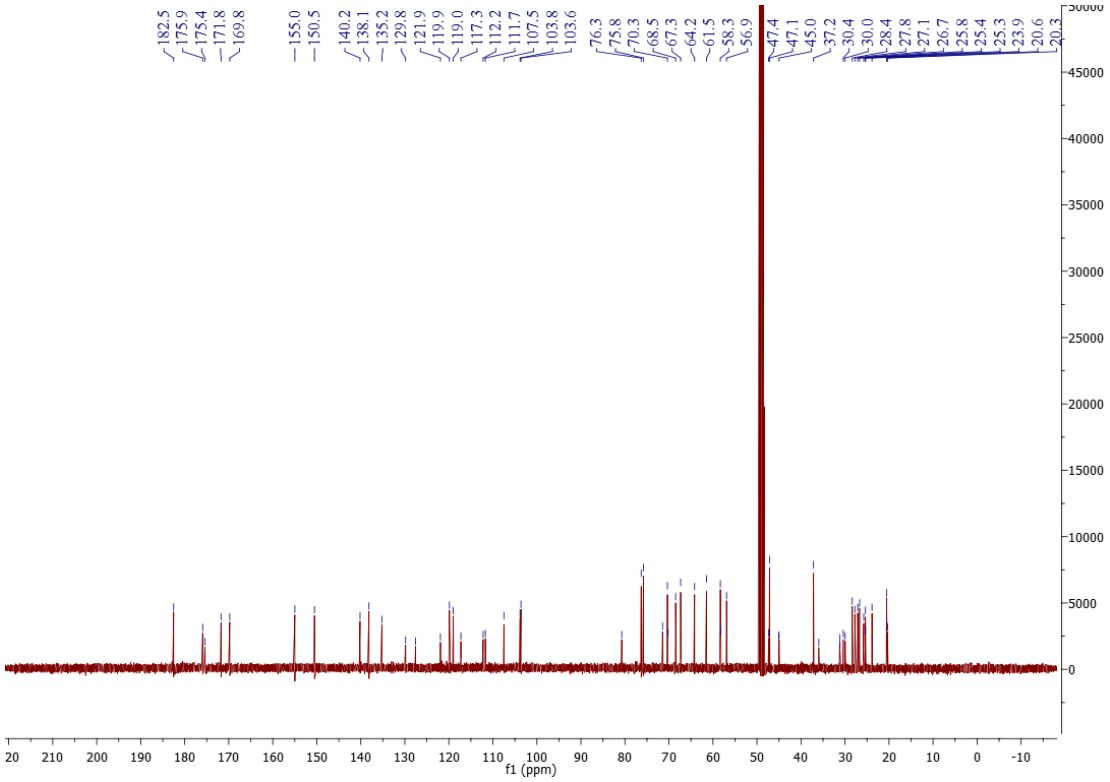
S61: Key 2D NMR correlations of **3**



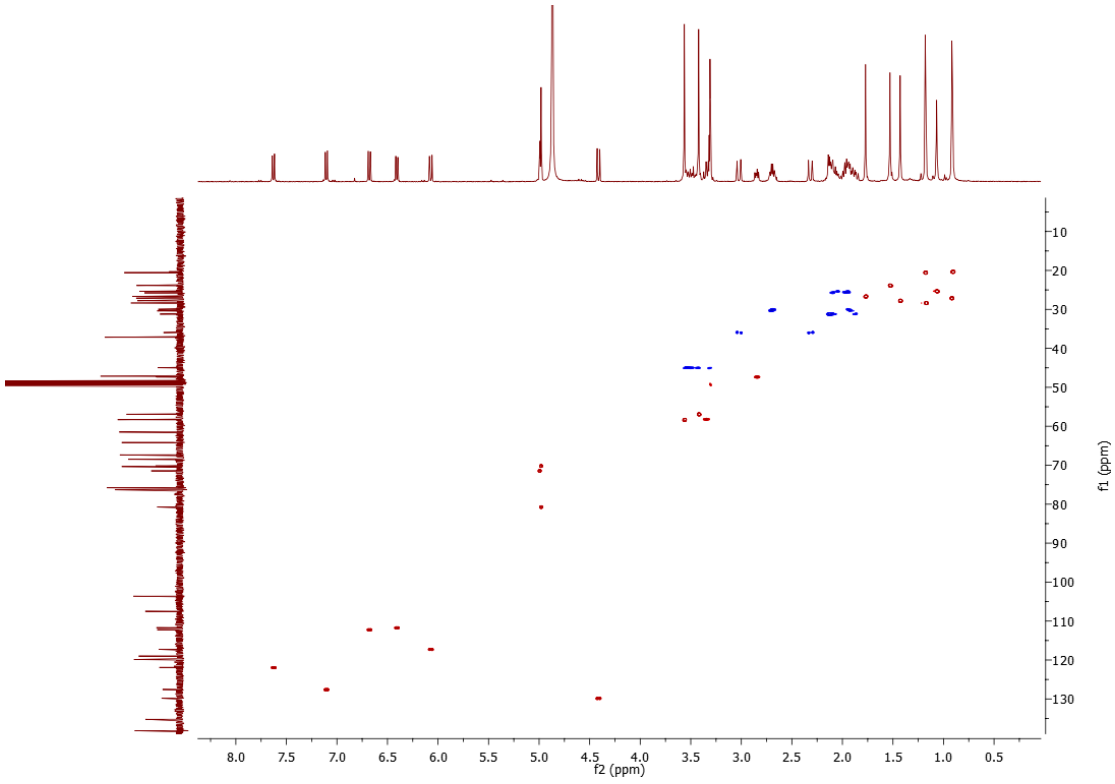
S62: ^{1}H NMR spectrum (400MHz) of **3** in CD_3OD



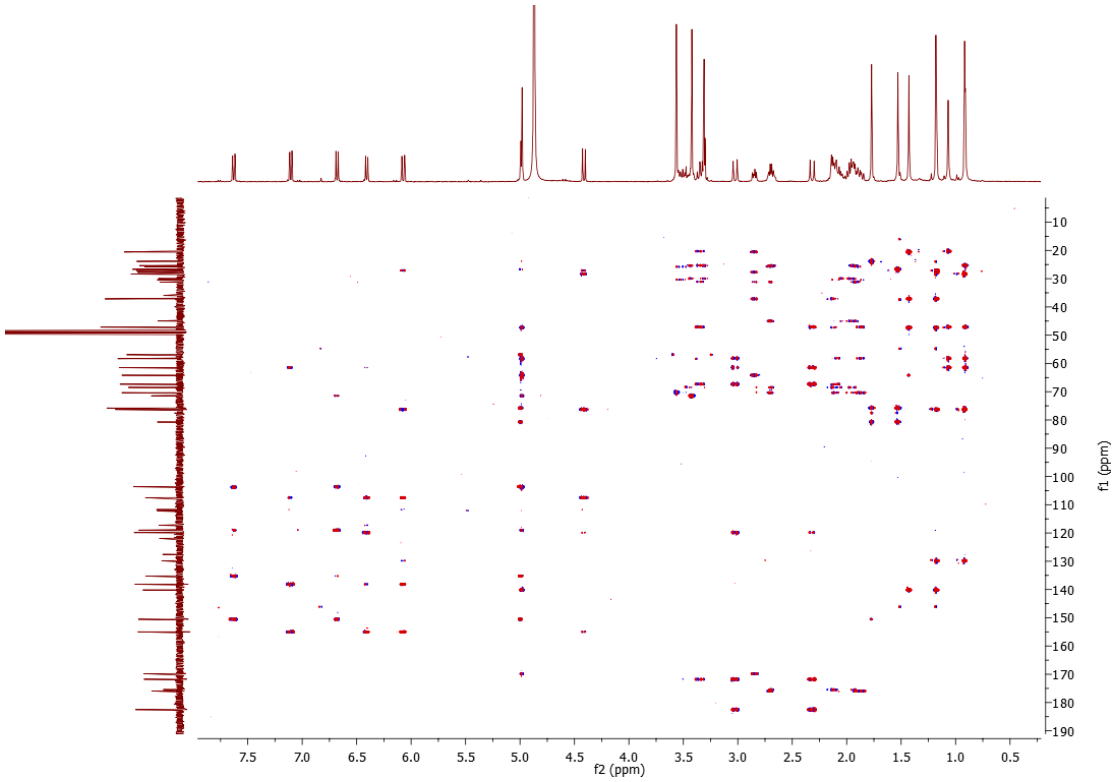
S63: ^{13}C NMR spectrum (100MHz) of **3** in CD_3OD



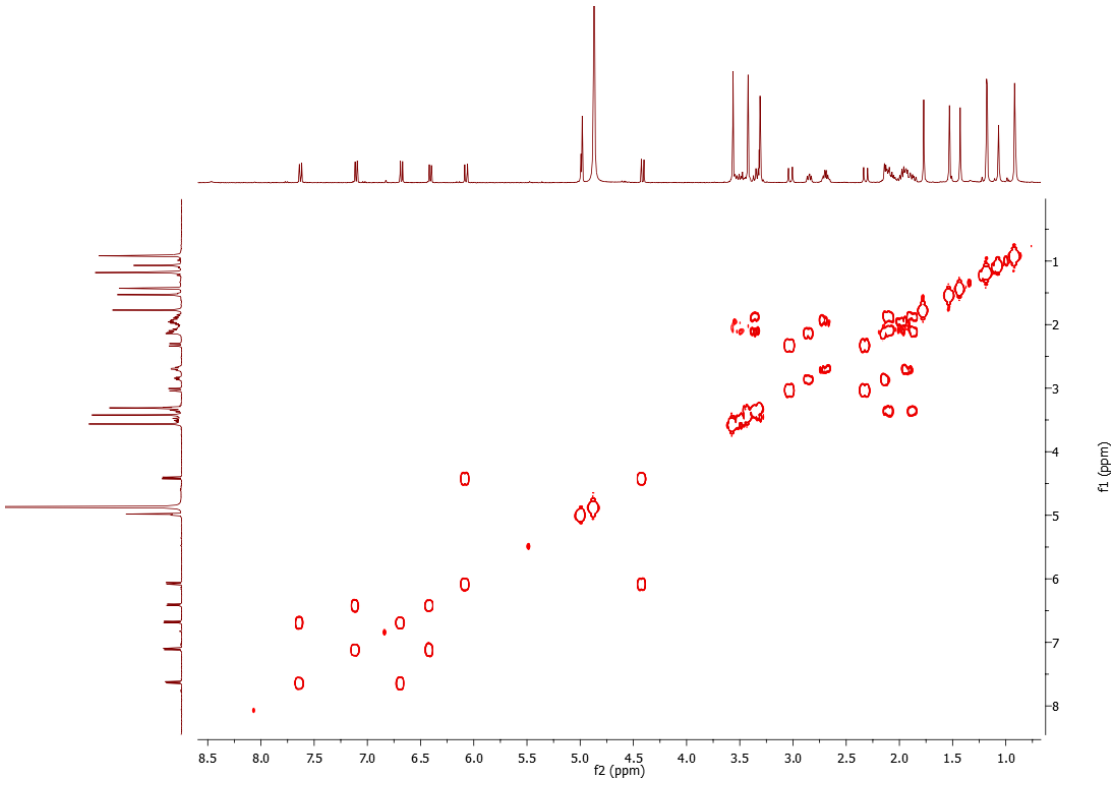
S64: HSQC spectrum of **3** in CD_3OD



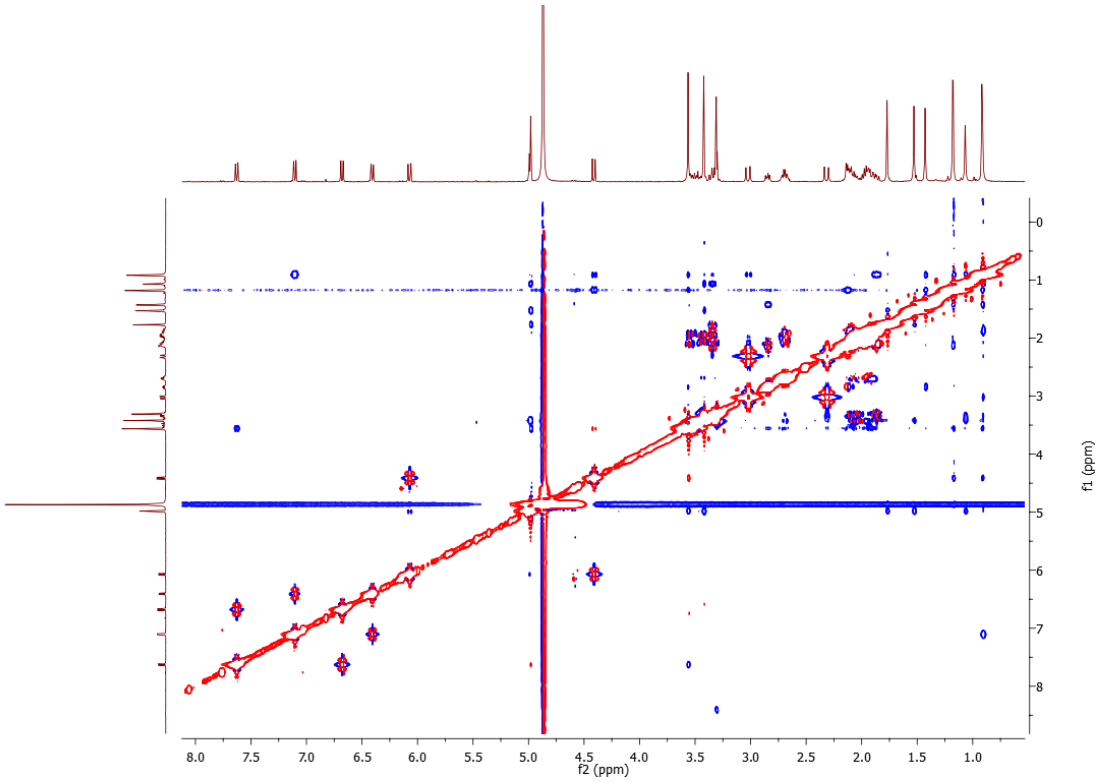
S65: HMBC spectrum of **3** in CD_3OD



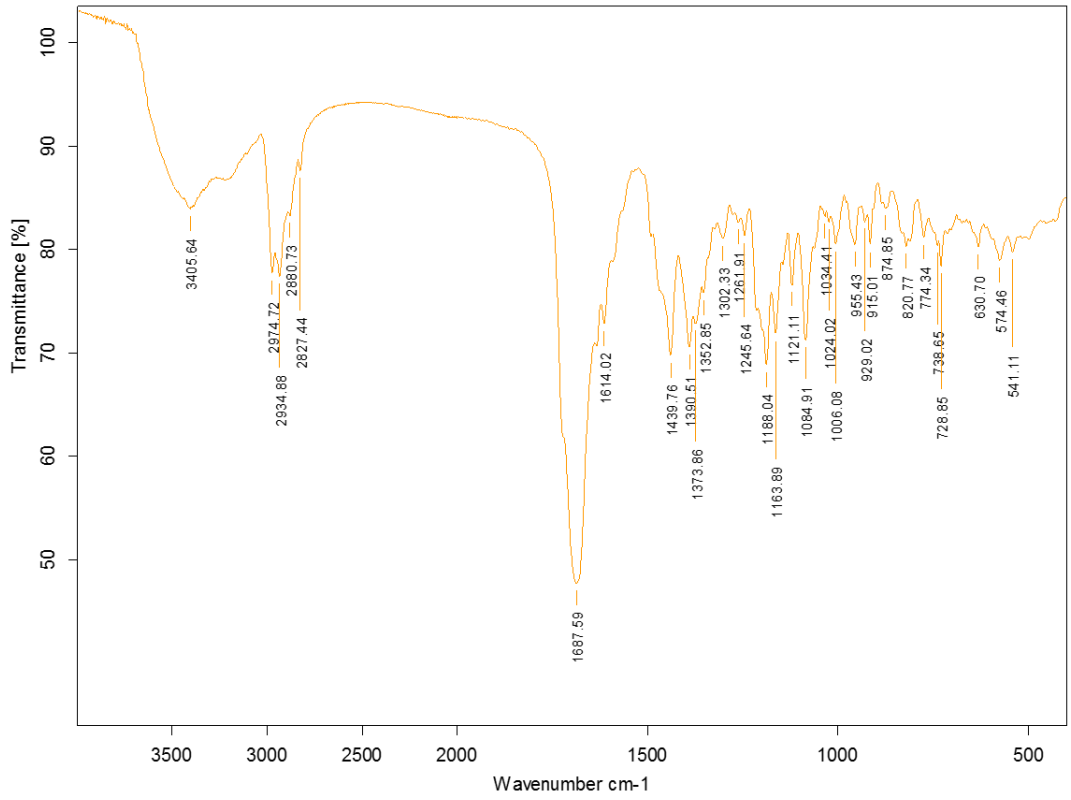
S66: ^{1}H-^{1}H COSY spectrum of **3** in CD_3OD



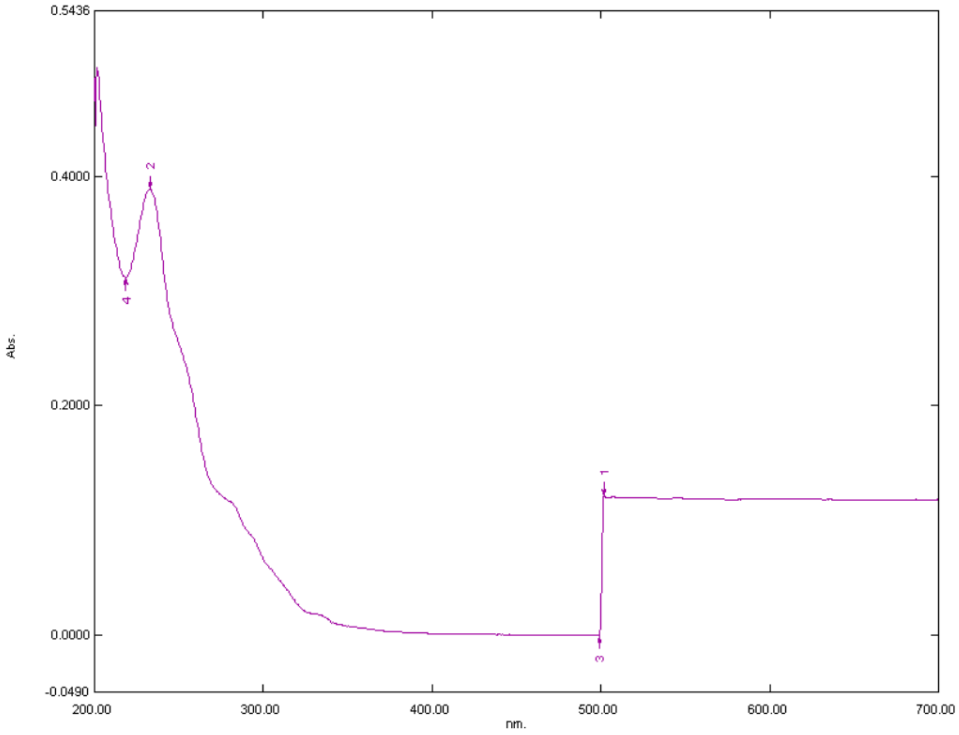
S67: NOESY spectrum of **3** in CD_3OD



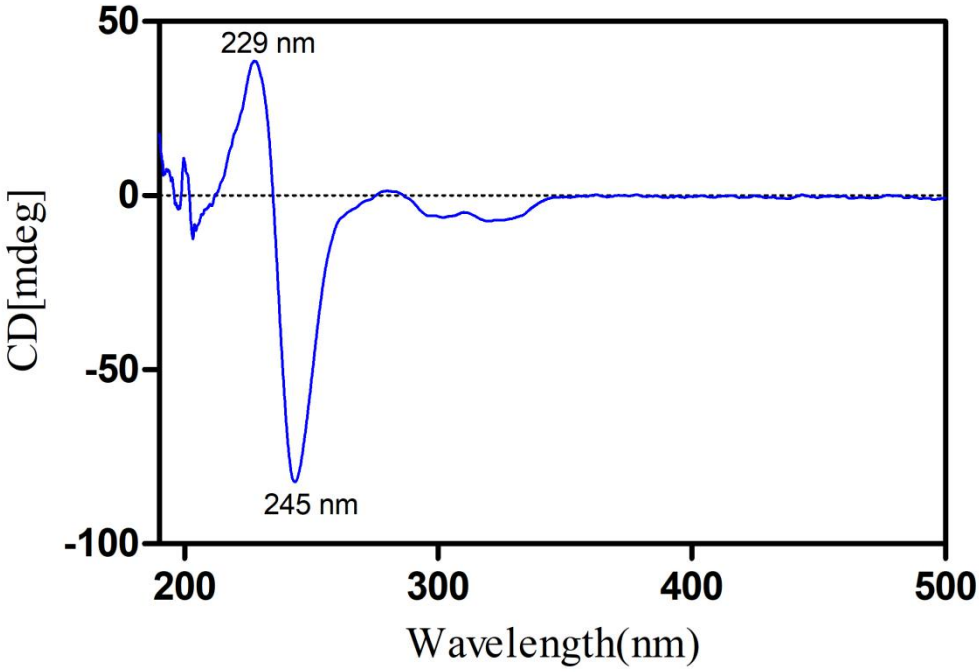
S68: IR spectrum of **3**



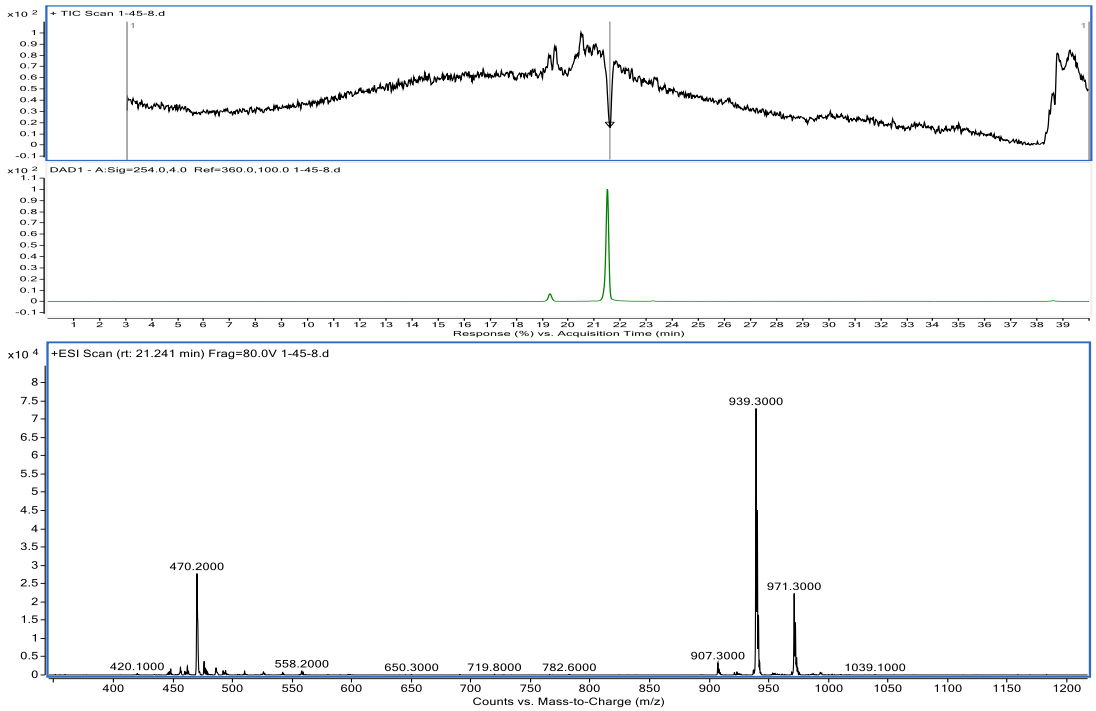
S69: UV spectrum of **3**



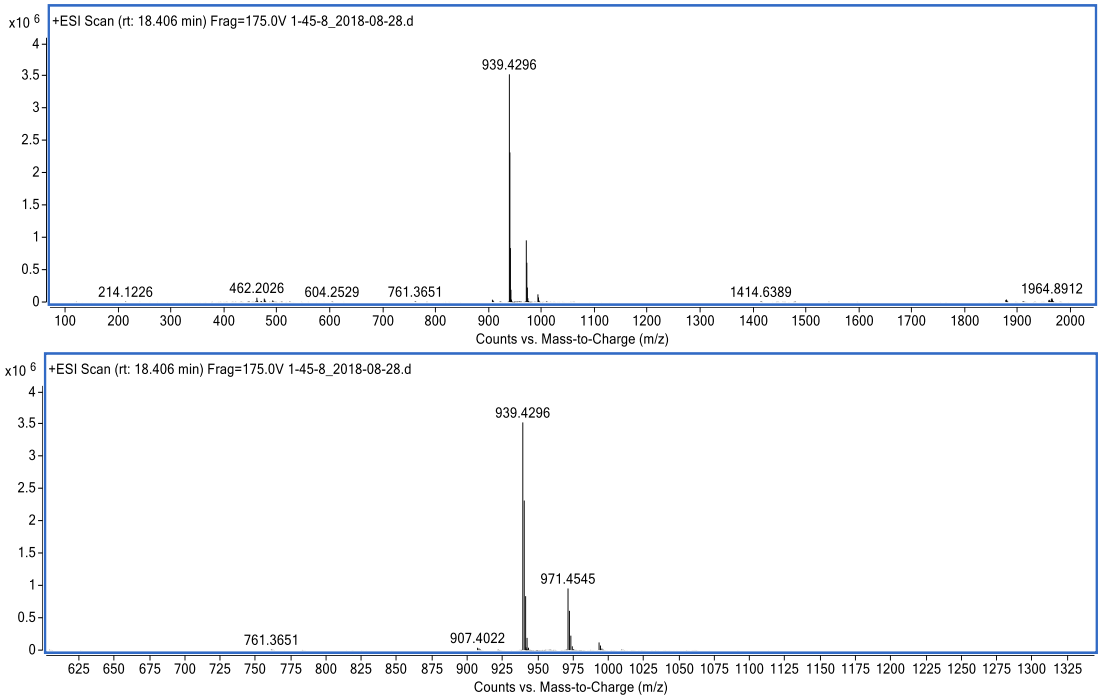
S70: CD spectrum of **3**



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

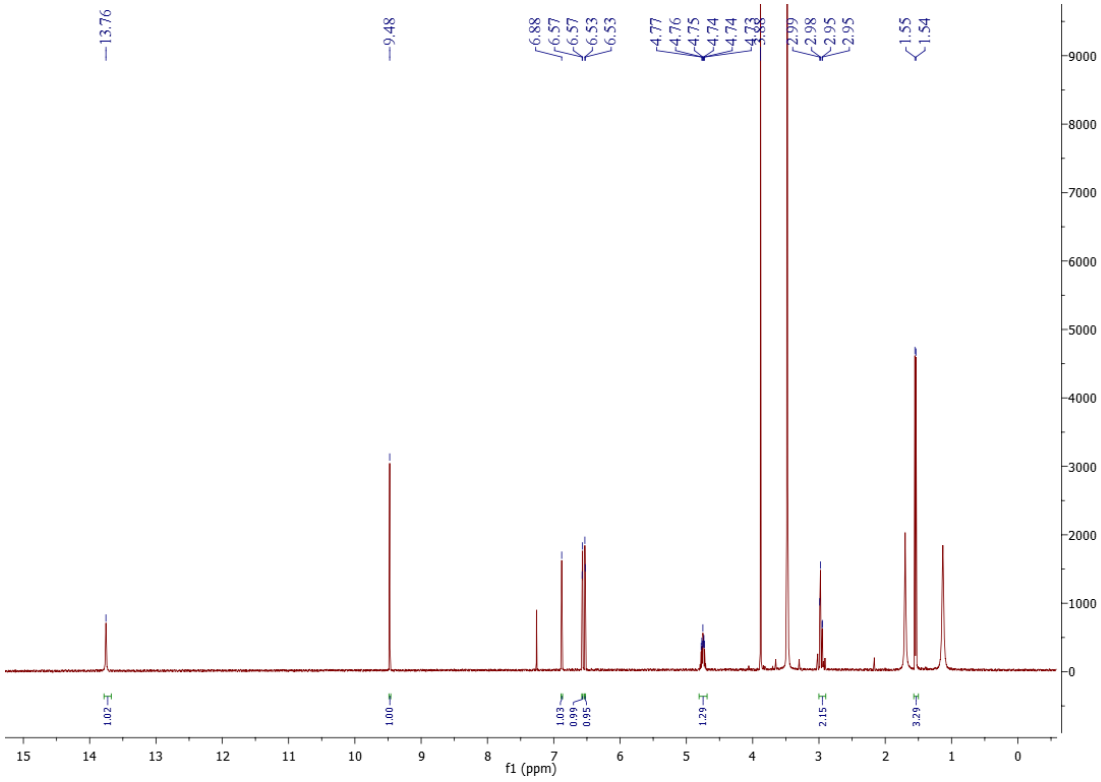


S72: (+)-HR-MS spectrum of **3**

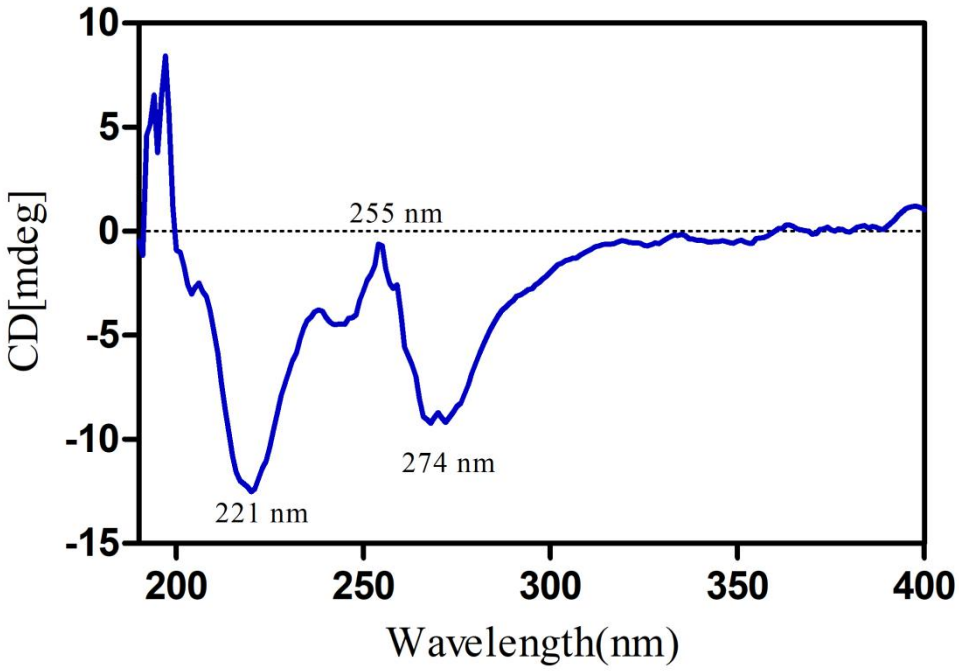


For compound 4

S73: ^{1}H NMR spectrum (400MHz) of **4** in CCl_3D

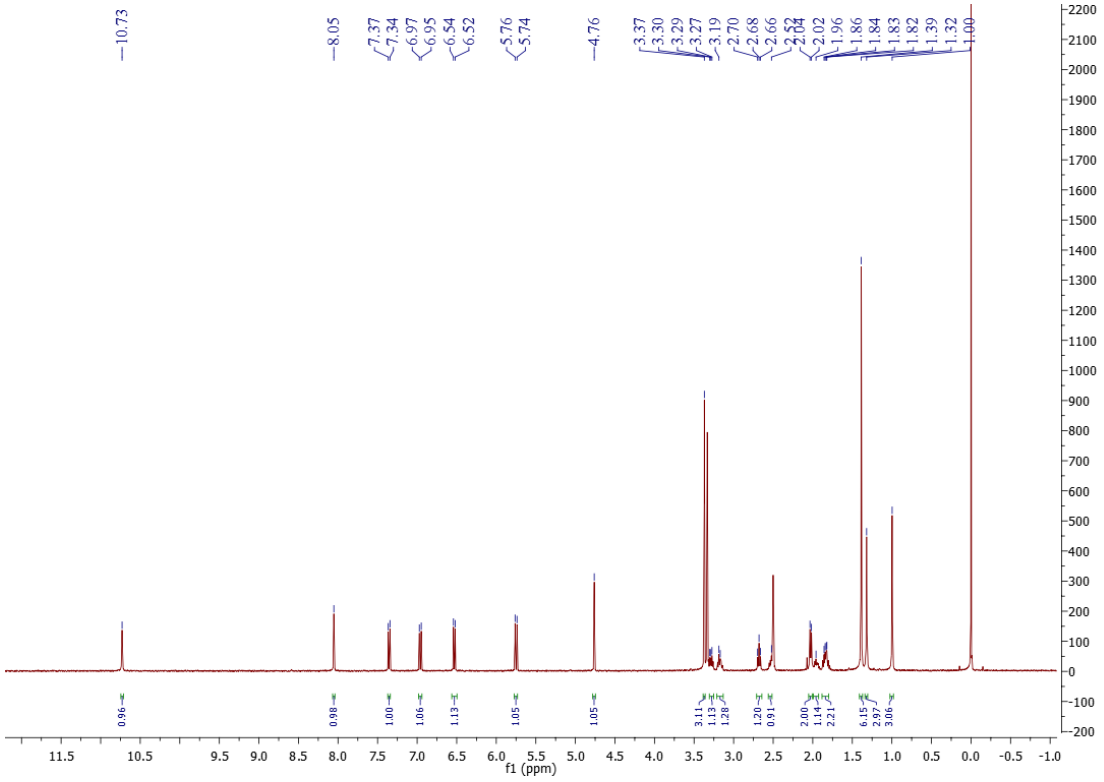


S74: CD spectrum of **4**

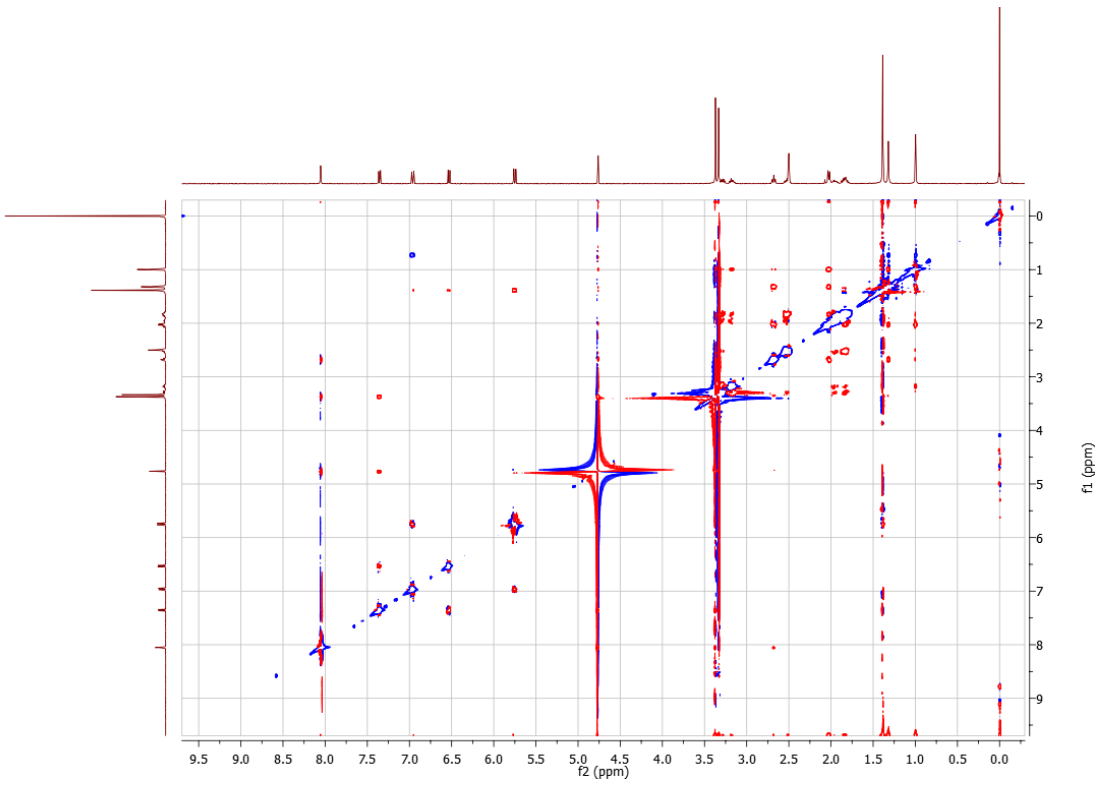


For compound 5

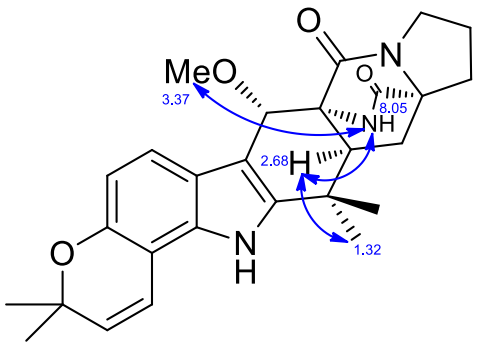
S75: ^{1}H NMR spectrum (400MHz) of **5** in DMSO-d_6



S76: ROESY spectrum of **5** in DMSO-d_6

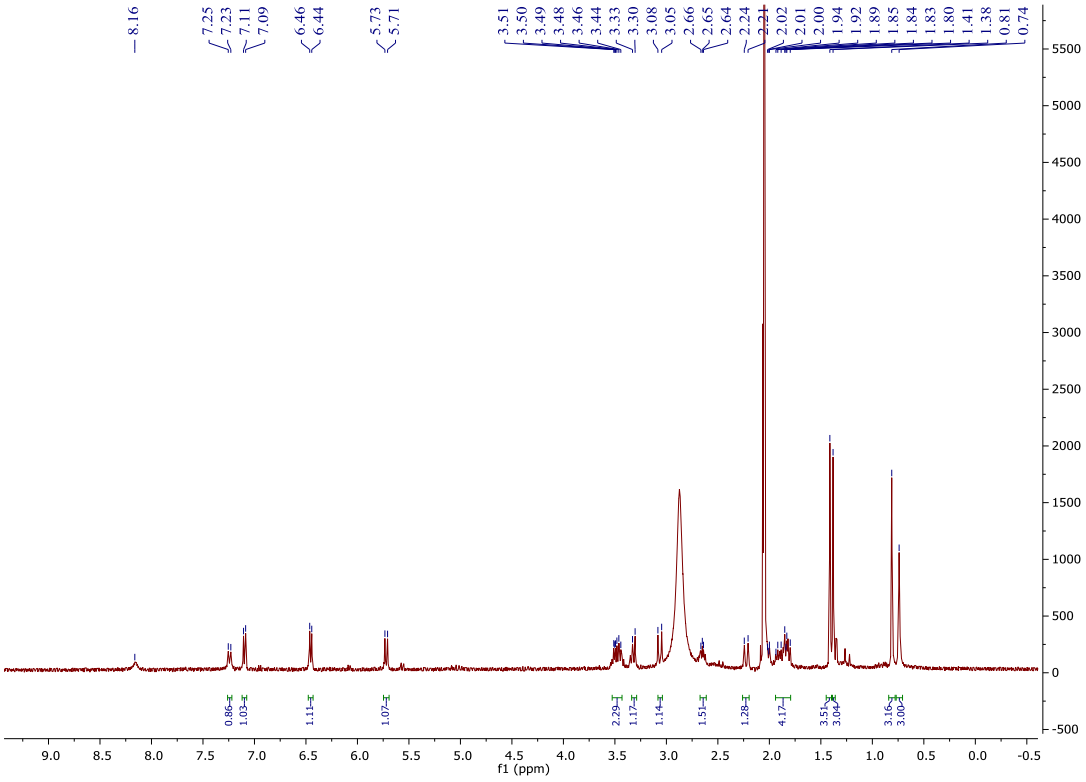


S77: Key ROESY correlations for compound **5**

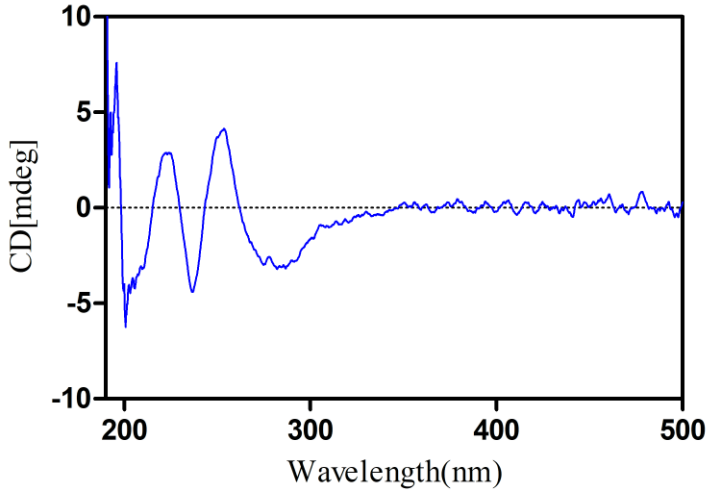


For compound 6

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



S79: CD spectrum of **6**



References

[1] Bruker AXS APEX3, Bruker AXS, Madison, Wisconsin, **2015**.

[2] G. M. Sheldrick, *Acta Cryst.* **2015**. *A71*, 3-8.

[3] G. M. Sheldrick, *Acta Cryst.* **2015**, C*71*, 3-8.

[4] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339-341.

[5] Accelrys DS Visualizer v2.0.1, Accelrys Software. Inc., **2007**.

[6] K. A. U. Zaman, Z. Hu, X. Wu, S. Hou, J. Saito, T. P. Kondratyuk, J. M. Pezzuto, S.Cao, *J Nat Prod*. **2020**, *83*, 730-737.

[7] S. Andrews, FastQC. *Babraham Bioinformatics,* **2010**. https://doi.org/citeulike-article-id:11583827.

[8] A. Bankevich, S. Nurk, D. Antipov, A. A. Gurevich, M. Dvorkin, A. S. Kulikov, V. M. Lesin, S. I. Nikolenko, S. Pham, A. D. Prjibelski, A. V. Pyshkin, A. V. Sirotkin, N. Vyahhi, G. Tesler, M. A. Alekseyev, P. A. Pevzner, *J Comput Biol.* **2012** ,*19*, 455-477.

[9] B. J. Walker, T. Abeel, T. Shea, M. Priest, A. Abouelliel, S. Sakthikumar, C. A. Cuomo, Q. Zeng, J. Wortman, S. K. Young, A. M. Earl, *PLoS One*. **2014**, *9*, e112963.

[10] K. Blin, T. Wolf, M. G. Chevrette, X. Lu, C. J. Schwalen, S. A. Kautsar, H. G. Suarez Duran, E. L. C. de Los Santos, H. U. Kim, M. Nave, J. S. Dickschat, D. A. Mitchell, E. Shelest, R. Breitling, E. Takano, S. Y. Lee, T. Weber, M. H. Medema, *Nucleic Acids Res*. **2017**, *45*, W36-W41.

[11] S. F. Altschul, W. Gish, W. Miller, E. W. Myers, D. J. Lipman, *J Mol Biol*. **1990**, *215*, 403-410.

[12] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Gaussian, Inc.: Wallingford, CT, **2009**.

[13] Spartan'14; Wavefunction: Irvine, CA.

[14] MacroModel Schrodinger release 2018-3; Schrodinger LLC: New York, **2018**.

[15] a) R. J. Ditchfield, *Chem. Phys.* **1972**, *56*, 5688. b) R. Ditchfield, *Mol. Phys.* **1974**, *27*, 789. c) C. M. Rohlfing, L. C. Allen, R. Ditchfield, *Chem. Phys.* **1984**, *87*, 9. d) K. Wolinski, J. F. Hinton, P. Pulay, *J. Am. Chem. Soc.* **1990**, *112*, 8251.

[16] a) N. Grimblat, A. M. Sarotti, *Chem. Eur. J.* **2016**, *22*, 12246. b) M. W. Lodewyk, M. R. Siebert, D. J. Tantillo, *Chem. Rev.* **2012**, *112*, 1839.

[17] N. Grimblat, M. M. Zanardi, A. M. Sarotti, *J. Org. Chem.* **2015**, *80*, 12526.

[18] X.C. Li, D. Ferreira, Y. Ding, *Curr. Org. Chem.* **2010**, *14*, 1678–1697.

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
O 4.418267 -5.250591 -1.591011
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
C -1.098664 0.458888 -0.102816
O -0.046611 -0.411537 -0.679407
C -1.898266 1.163836 -1.170015
C -1.426118 2.434724 -1.847813
C -0.961016 3.357201 -0.652891
C 0.136016 2.741198 0.281238
C 1.519925 2.780925 -0.460084
N 1.790590 4.072355 -0.786866
C 0.835235 5.123929 -0.376195
C -0.508411 4.793237 -1.056412
O 2.496278 -4.666802 -2.513120
H 5.949127 -4.127252 1.214309
H 4.692533 -5.364783 1.112098
H 6.002615 -3.970910 -1.268607
H 4.558836 -2.389699 2.349705
H 3.421490 -0.459907 3.230511
H -0.984895 1.624688 1.714009
H -1.841471 3.457657 -0.006361
H -0.349402 4.872255 -2.135792
H -1.268816 5.532529 -0.784345
C -2.130064 -0.460043 0.532862
C -4.331870 -2.049952 1.113670
C -3.291123 -0.394227 -0.224018
C -2.061668 -1.337381 1.607146
C -3.178380 -2.128799 1.896688
C -4.434303 -1.154784 0.016405
H -1.165044 -1.420466 2.211506
H -3.171561 -2.821515 2.731752
N -3.109229 0.621686 -1.254979
O -4.058399 0.907874 -2.046693
O -5.389003 -2.817127 1.489982
C -5.710292 -1.089986 -0.691014
H -5.860480 -0.286970 -1.399485
C -6.650529 -2.010604 -0.438846
H -7.610945 -1.980300 -0.947799
C -6.416567 -3.162310 0.510474
C -5.948607 -4.413652 -0.250881
H -5.017608 -4.209973 -0.789028
H -6.703810 -4.720908 -0.982960
H -5.779706 -5.241596 0.446595
C -7.660051 -3.457767 1.352745
H -7.971622 -2.565009 1.903228
H -7.447531 -4.255327 2.071606
H -8.486455 -3.779814 0.710124
C -2.553833 3.180690 -2.596171
H -2.148465 4.097904 -3.036227
H -3.381324 3.450324 -1.933787
H -2.964891 2.567836 -3.397227
C -0.309413 2.095651 -2.867111
H 0.144450 3.009234 -3.268131
H -0.750771 1.548528 -3.706646
H 0.479985 1.472454 -2.445239
O 2.266727 1.842398 -0.702167
C 3.065298 4.599348 -1.274002
H 3.112288 4.534959 -2.369461
H 3.891660 4.008508 -0.869426

C 3.032970 6.058979 -0.786253
H 3.630901 6.723117 -1.416966
H 3.421217 6.118909 0.235941
C 1.532712 6.425096 -0.783436
H 1.203656 6.724980 -1.785464
H 1.298923 7.228304 -0.081434
C 0.698436 4.954359 1.152673
N 0.261542 3.684610 1.419197
H 0.463860 3.294199 2.335095
O 0.978534 5.797000 1.991539
C 6.532088 -6.014416 -0.819738
H 7.454330 -5.752338 -0.290023
H 6.784209 -6.267856 -1.853598
H 6.094379 -6.898697 -0.344324
O 1.214167 -2.579632 -1.689388
H 1.459731 -3.376202 -2.238077
O 1.506520 1.508281 3.227855
C 2.415212 1.631140 4.318084
H 3.441089 1.783332 3.962276
H 2.379206 0.745420 4.963723
H 2.090132 2.506879 4.881775
SCF Energy (PCM/mPW1PW91/6-31+G**)= -2426.72976841
Number of imaginary frequencies = 0

1a_c02
B3LYP/6-31G* Geometry
C 1.614978 6.644941 0.115000
C 1.685827 4.349464 -0.859012
O 3.086270 6.114559 -1.768443
C 2.575743 4.869775 -1.897761
C 3.010818 6.804042 -0.489743
C 1.226173 5.190411 0.198706
C 0.434293 4.684334 1.194233
C 0.027796 3.316312 1.194078
C 0.460068 2.462427 0.122556
C 1.284999 2.999773 -0.914766
C 0.016156 1.117722 0.177560
C -0.782262 0.642836 1.199966
C -1.207876 1.492083 2.232128
C -0.790074 2.815261 2.237776
C -1.150542 -0.786295 0.885727
C -0.003205 -1.134773 -0.097303
O 0.313229 0.160180 -0.744781
C -0.304670 -2.209500 -1.111941
C -1.665458 -2.370881 -1.759205
C -2.678962 -2.296970 -0.549002
C -2.588348 -0.997558 0.322523
C -3.240130 0.193204 -0.467332
N -4.525002 -0.141903 -0.757804
C -5.047430 -1.438057 -0.275686
C -4.174624 -2.535112 -0.917690
O 2.889969 4.231750 -2.905463
H 0.897133 7.177925 -0.524580
H 1.580363 7.121772 1.100910
H 3.173862 7.850308 -0.763228
H 0.087539 5.330198 1.997056
H -1.089087 3.496580 3.025394
H -1.071081 -1.448597 1.754360
H -2.374563 -3.100926 0.132539
H -4.331704 -2.478004 -1.998552
H -4.503454 -3.527548 -0.592501
C 1.282995 -1.633542 0.541917
C 3.684362 -2.893665 1.141743
C 1.723014 -2.735311 -0.177954
C 2.055203 -1.146869 1.588553
C 3.259274 -1.793153 1.888582
C 2.912107 -3.418086 0.072110
H 1.744682 -0.281968 2.164438
H 3.888468 -1.452671 2.704344
N 0.713522 -3.061299 -1.179849
O 0.860162 -4.072175 -1.932508
O 4.840883 -3.494263 1.528513
C 3.407735 -4.614983 -0.601852
H 2.745763 -5.122845 -1.289586
C 4.650185 -5.047224 -0.347525
H 5.041026 -5.937629 -0.834155
C 5.590955 -4.305048 0.572614

C 6.512899 -3.368132 -0.225592
H 5.923675 -2.638500 -0.789795
H 7.117660 -3.940374 -0.938088
H 7.185684 -2.830823 0.451982
C 6.399184 -5.269346 1.444237
H 5.730634 -5.913285 2.023382
H 7.033604 -4.709196 2.138516
H 7.040163 -5.900707 0.819615
C -1.856721 -3.745757 -2.438862
H -2.868189 -3.804248 -2.854338
H -1.721992 -4.575003 -1.738461
H -1.143660 -3.885981 -3.250251
C -1.864238 -1.267213 -2.828625
H -2.887005 -1.282635 -3.222404
H -1.184364 -1.458894 -3.665278
H -1.651885 -0.265859 -2.452270
O -2.726005 1.261168 -0.770839
C -5.561796 0.748310 -1.279653
H -5.536655 0.761895 -2.377655
H -5.387080 1.769321 -0.929507
C -6.855327 0.108064 -0.743657
H -7.720191 0.321448 -1.378348
H -7.069345 0.486049 0.261621
C -6.528374 -1.399330 -0.663486
H -6.669880 -1.880582 -1.638467
H -7.137971 -1.920898 0.077516
C -4.811493 -1.413602 1.249966
N -3.474362 -1.239919 1.487571
H -3.196864 -0.845139 2.381591
O -5.678546 -1.488971 2.107087
C 4.149683 6.337095 0.413614
H 4.194469 6.961012 1.313551
H 5.104687 6.420866 -0.113425
H 4.013722 5.296439 0.724629
O 1.657227 2.194968 -1.907704
H 2.186922 2.755708 -2.541503
O -2.026344 0.919209 3.168035
C -2.510686 1.736793 4.229421
H -3.097080 2.579043 3.843552
H -1.685003 2.116354 4.843328
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