Supporting information

Mass-tagged aminated probes for rapid discovery of azaphilic natural products in fungal crude extracts

Victor Flon,[a†] Coralie Pavesi,[†b] Samuel Oger,[a] Stéphane Leleu,[a] Pascal Retailleau,[c] Laurence Jennings [d], Soizic Prado*[b] and Xavier Franck*[a]

Contents

1) General experimental procedure for the obtention of probe 1.

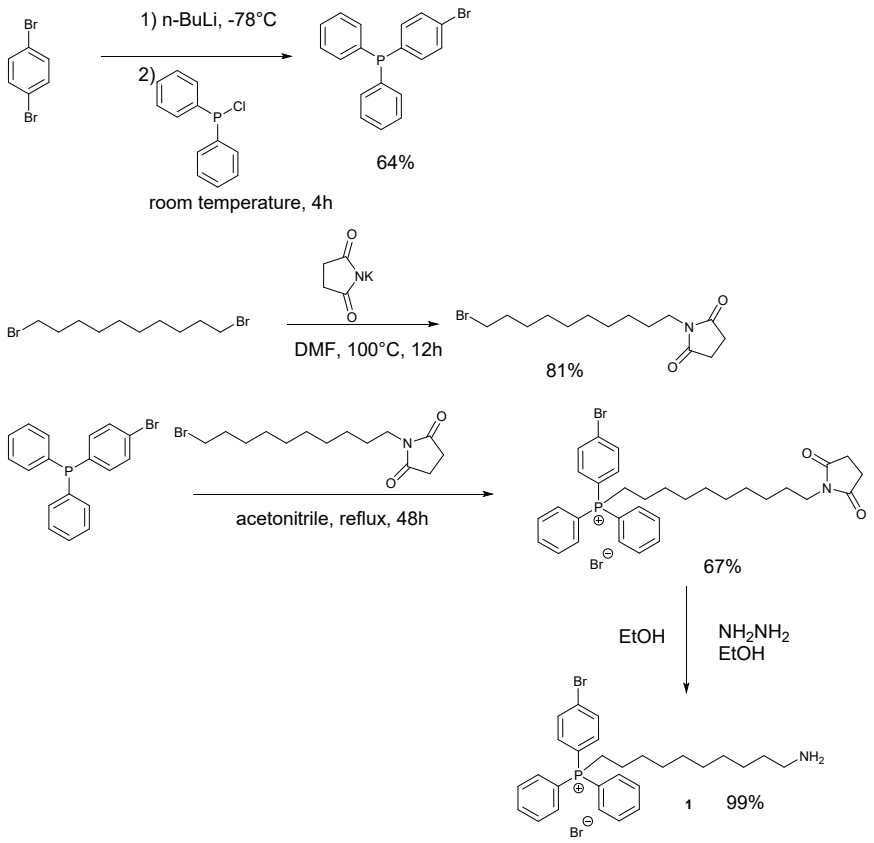
All chemicals were used as received from commercial sources without further purification. Solvents, unless otherwise stated, were purchased in reagent grade or HPLC grade and used as received. Aqueous mobile phases for HPLC were prepared with water that was purified by means of a MilliQ system (purified to 18.2 MΩ cm). All reactions were monitored by thin layer chromatography (TLC) and/or HPLC-MS. TLC were carried out on Merck DC Kieselgel 60 F-254 aluminum sheets. Visualization of spots was performed under a UV lamp at λ = 254 or 365 nm, and/or staining with a $KMnO_4$ solution/K_2CO_3 + 5% NaOH, developed with heat. Flash column chromatography purifications were performed manually on silica gel (40–63 µM) under pressurized air flow.

2) Instruments and Methods for the probe 1.

HPLC-MS analyses were performed with a ThermoScientific UHPLC Vanquish Horizon/Flex with PDA detector coupled with a ThermoScientific ISQ EC Mass Spectrometer. The mass range was *m/z* : 100 to 1200, with unit mass resolution ionization technique by Heated Electrospray Ionization (HESI). Temperature of the column compartment was fixed at 40 °C. A Waters ACQUITY UPLC® BEH C18 column (1.7 µm, 2.1 × 100 mm) was used with a binary solvent system composed of MeCN and 0.1% aq. formic acid (aq. FA, pH 2) as eluents (linear gradient from 5 to 100% MeCN over 9 min and isocratic gradient at 100% MeCN over 3 min) at a flow rate of 0.400 mL/min. High Resolution Mass spectrometry (HRMS) were obtained by using a Waters Micromass LCT Premier XE® equipped with an orthogonal acceleration time-of-flight (oa-TOF) and an electrospray source in positive mode.

^{1}H, ^{13}C, ^{31}P and NMR spectra were recorded on Brüker 300 machine operating at ambient probe temperature. The solvent resonance was used as the internal standard for ^{1}H-NMR (chloroform-d at 7.26 ppm; MeOD at 3.31 ppm) and ^{13}C-NMR (chloroform-d at 77.16 ppm; MeOD at 49.0 ppm). Chemical shifts (δ) were quoted in parts per million (ppm). Coupling constants (J) were quoted in Hertz (Hz). The following abbreviations were used to give the multiplicity of the NMR signals: s: singlet, bs: broad singlet, d: doublet, t: triplet, dd: doublet – doublet.

3) Chemical synthesis of probe 1.



(4-bromophenyl)diphenylphosphine.

Under argon atmosphere, *n*-butyllithium (4.20 mL, 2.50 M, 10.50 mmol, 1.05 eq) was added slowly to a solution of 1,4-dibromobenzene (2.36 g, 10 mmol, 1 eq) in dry THF (50 mL) at -78°C. After 30 mins, chlorodiphenylphosphine (1.80 mL, 10.00 mmol, 1 eq) was added and the resulting solution was stirred at room temperature for 4 h. After completion, the reaction mixture was diluted with water (40 mL) and the aqueous layer was extracted with AcOEt (3 × 50 mL). The organic layers were combined, dried over $MgSO_4$ and filtered through a pad of Celite®. The filtrate was concentrated under reduced pressure and the crude product was purified by chromatography on silica gel in a system: DCM / Cyclohexane (0:4 v/v) to (1:4 v/v), giving the desired product as a white solid (2.17 g, 64%). The ^{1}H NMR data were in accordance with literature data[1]. ^{1}H RMN (300MHz, $CDCl_3$) δ = 7.49-7.45 (m, 2 H), 7.37-7.27 (m, 10 H), 7.20-7.14 (m, 2 H). ^{13}C NMR (75MHz, $CDCl_3$) δ = 136.79, 136.65, 136.63, 135.50, 135.23, 133.98, 133.71, 131.84, 131.75, 129.11, 128.82, 128.73, 123.52. ^{31}P NMR (121MHz, $CDCl_3$) δ = -6.36. IR (neat, cm^{-1}): 1575, 1477, 1436, 1383, 1191, 1117, 1068, 1009.

2-(10-bromodecyl)isoindoline-1,3-dione.

To a solution of 1,10-dibromodecane (10.50 g, 35 mmol, 5 eq) in dry DMF (20 mL) was added potassium phthalimide (1.30 g, 7 mmol, 1 eq) and the reaction mixture was stirred at 100 °C for 12 h. The solvent was evaporated to dryness, water (50 mL) was added and the aqueous phase was extracted with AcOEt (3 x 50 mL). The organic phases were combined, washed with a saturated aqueous solution of NaCl (50 mL), dried over $MgSO_4$ and filtered through a pad of Celite®. The filtrate was concentrated under reduced pressure and the crude product was purified by chromatography on silica gel in a system: AcOEt / Cyclohexane (0:4 v/v) to (1:4 v/v), giving the desired product as a white amorphous solid (2.08 g, 81%). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.85-7.69 (m, 4 H), 3.67 (t, *J* = 7.3 Hz, 2 H), 3.39 (t, *J* = 6.9 Hz, 2 H), 1.88-1.79 (m, 2 H), 1.71-1.62 (m, 2 H), 1.43-1.28 (m, 12 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 168.64, 133.99, 132.33, 123.30, 38.20, 34.19, 32.97, 29.48, 29.46, 29.25, 28.85, 28.72, 28.29, 26.96. IR (neat, cm^{-1}): 2928, 2850, 1713, 1396, 1073. HRMS (ESI+): Calc. for $C_{18}H_{25}BrNO_2$ $[M+H]^+$: 366.1069-368.1048 ; found : 366.1086-368.1063.

4-bromophenyl)(10-(1,3-dioxoisoindolin-2-yl)decyl)diphenylphosphonium bromide.

In a round bottom flask, (4-bromophenyl)diphenylphosphine (800 mg, 2.34 mmol, 1 eq) was solubilized in ACN (10 mL). 2-(10-bromodecyl)isoindoline-1,3-dione (859 mg, 2.34 mmol, 1 eq) was added and the reaction mixture was refluxed for 48 h. The reaction mixture was concentrated under reduced pressure and the resulting residue was purified by chromatography on silica gel in a system: EtOH / DCM (0:9 v/v) to (1:9 v/v), giving the desired product as a colorless oil (1.11 g, 67%). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.86-7.77 (m, 12 H), 7.72-7.66 (m, 6 H), 3.86 (bs, 2 H), 3.63 (t, *J* = 7.3 Hz, 2 H), 1.78 (bs, 2 H), 1.59 (bs, 4 H), 1.21 (m, 10 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 168.58, 135.37, 135.26, 135.22, 134.04, 133.99, 133.88, 133.75, 132.27, 131.02, 130.97, 130.75, 130.58, 123.26, 118.77, 118.27, 117.64, 117.11, 38.11, 30.51, 30.31, 29.38, 29.24, 29.11, 28.63, 26.86, 23.12, 22.76, 22.70, 22.47. ^{31}P NMR (121 MHz, $CDCl_3$) δ = 24.95. IR (neat, cm^{-1}): 3362, 2970, 2927, 1770, 1704, 1482, 1466, 1437, 1397, 1113, 1068, 1046, 1087, 1007. HRMS (ESI+): Calc. for $C_{36}H_{38}BrNO_2P^+$ $[M]^+$: 626.1824 - 628.1803 ; found : 626.1818 - 628.1808.

(4-bromophenyl)(10-(methylamino)decyl)diphenylphosphonium bromide **1**.

To a solution of 4-bromophenyl)(10-(1,3-dioxoisoindolin-2-yl)decyl)diphenylphosphonium bromide (1.1 g, 1.55 mmol, 1 eq) in EtOH (10 mL), hydrazine monohydrate (150 μL, 3.10 mmol, 2 eq) was added at room temperature. The reaction mixture was heated at reflux for 4 h then, it was cooled at 0°C in a bath of ice. The white precipitate was removed by filtration and the filtrate was concentrated under reduced pressure giving the desired product probe **1** as a yellowish amorphous solid (890 mg, quantitative), which was used without further purification. ^{1}H NMR (300 MHz, MeOD) δ 7.98-7.87 (m, 4 H), 7.85-7.67 (m, 10 H), 3.47-3.37 (m, 2 H), 2.91 (t, *J* = 7.4 Hz, 2 H), 1.69-1.51 (m, 6H), 1.40-1.31 (m, 10H). ^{13}C NMR (75 MHz, MeOD) δ = 136.49, 136.43, 136.39, 136.34, 134.92, 134.79, 134.76, 134.00, 131.69, 131.52, 126.54, 120.12, 119.92, 118.97, 118.75, 40.76, 31.75, 31.53, 30.36, 30.19, 29.92, 28.58, 27.46, 23.55, 23.49, 22.91, 22.24. ^{31}P NMR (121 MHz, MeOD) δ = 24.15. IR (neat, cm^{-1}): 3390, 2927, 1627, 1573, 1483, 1387, 1190, 1113, 1069, 1007. HRMS (ESI+): Calc. for $C_{28}H_{36}BrNP^+$ $[M]^+$: 496.1769 - 498.1748 ; found : 496.1766 - 498.1765.

4) NMR spectra

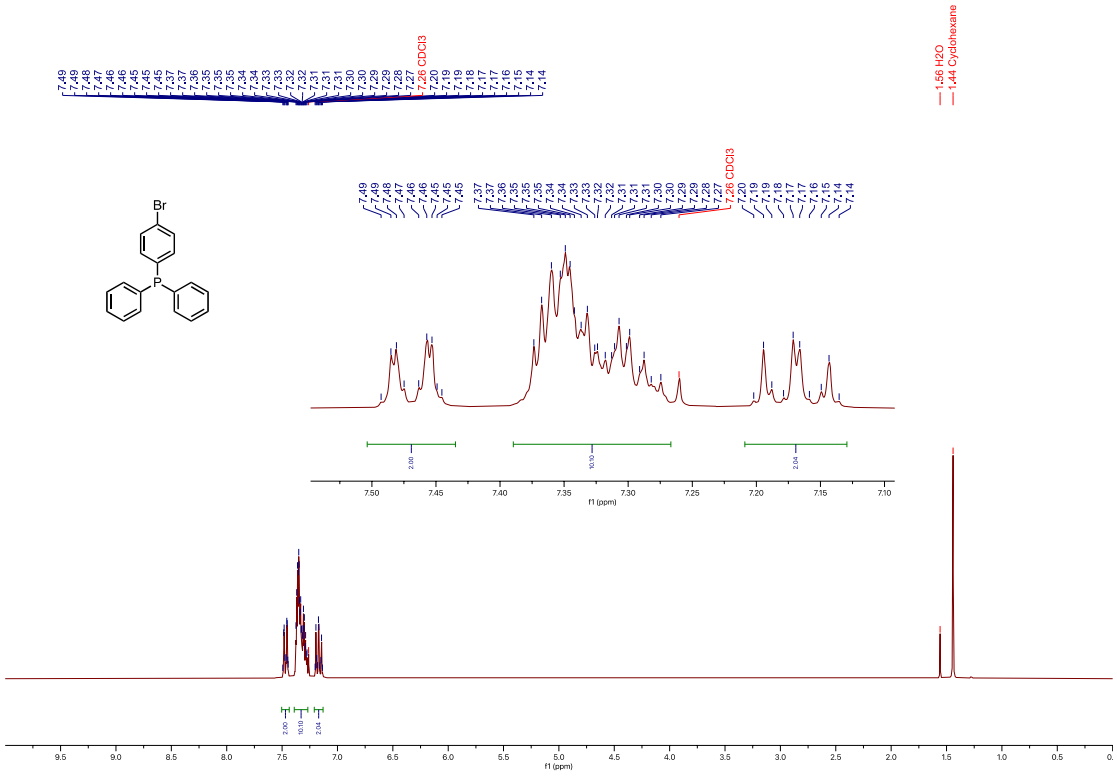


Figure S1 *^{1}H NMR of (4-bromophenyl)diphenylphosphine*

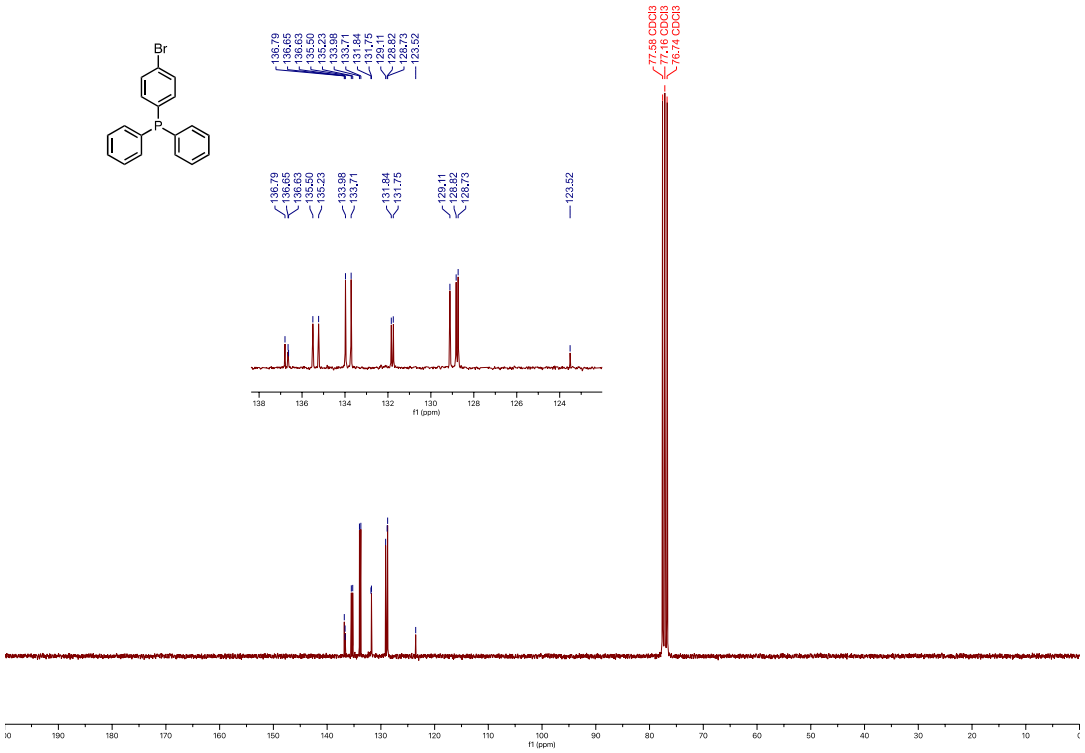


Figure S2 *^{13}C NMR of (4-bromophenyl)diphenylphosphine*

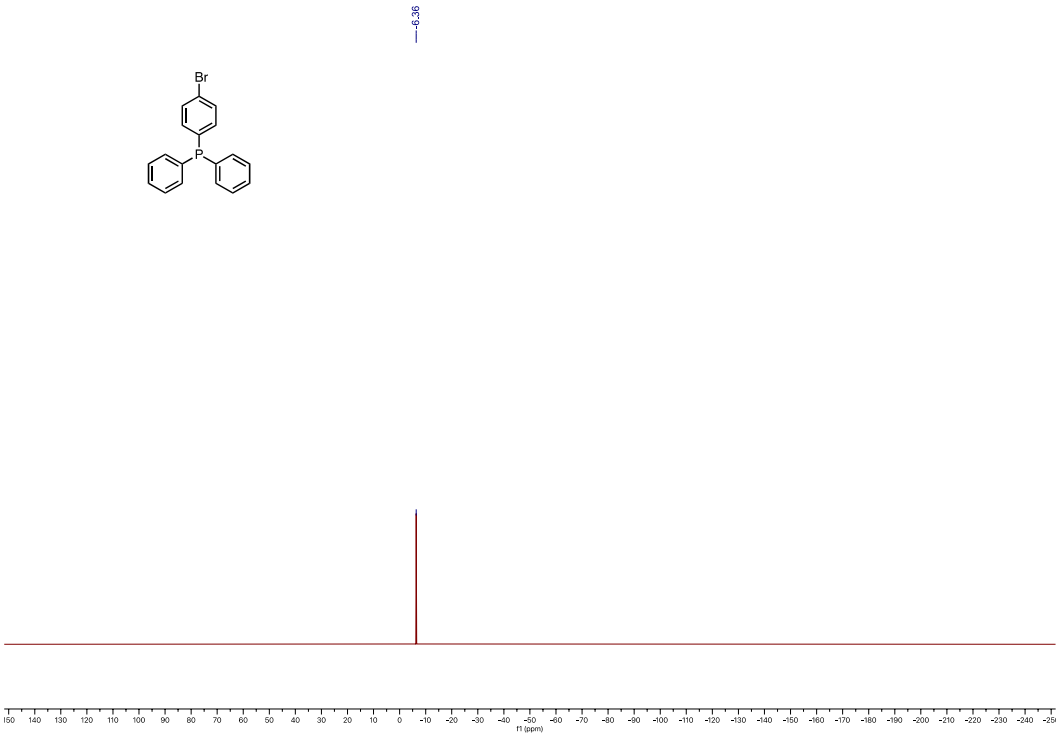


Figure S3 *^{31}P NMR of (4-bromophenyl)diphenylphosphine*

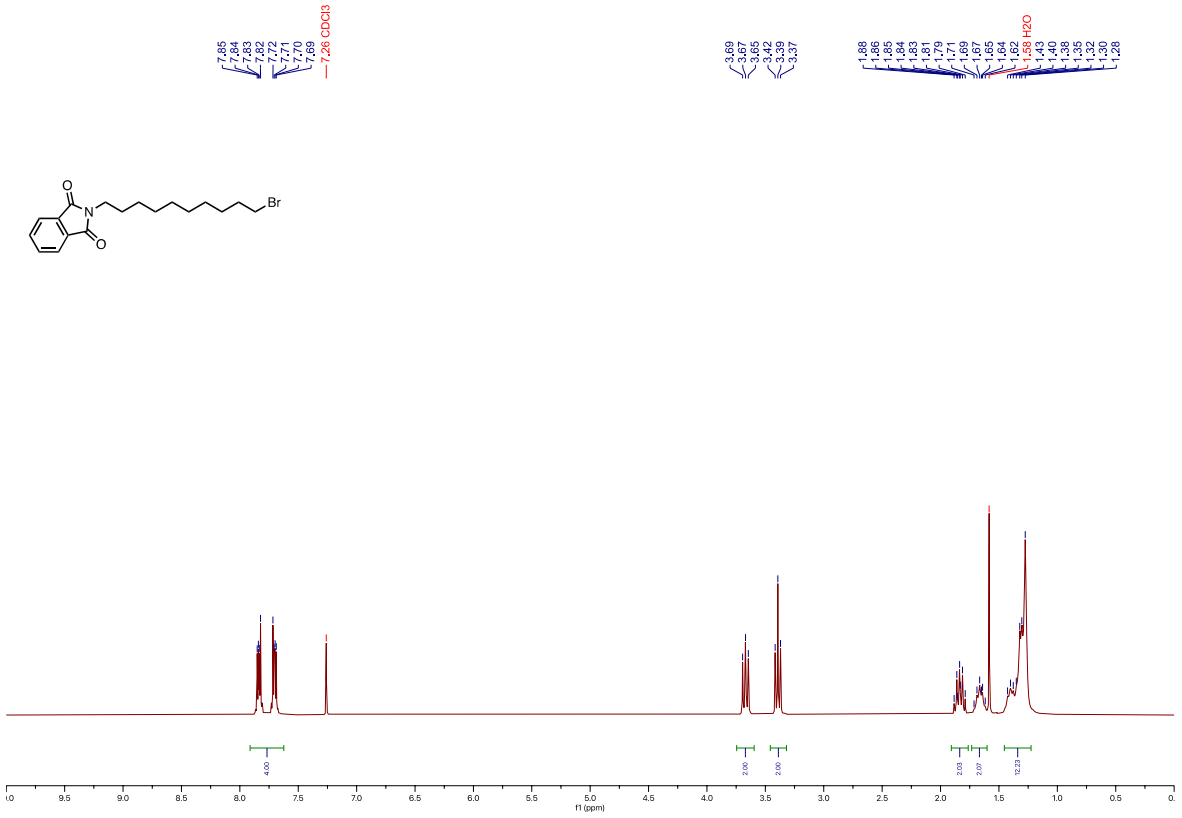


Figure S4 *^{1}H NMR of 2-(10-bromodecyl)isoindoline-1,3-dione*

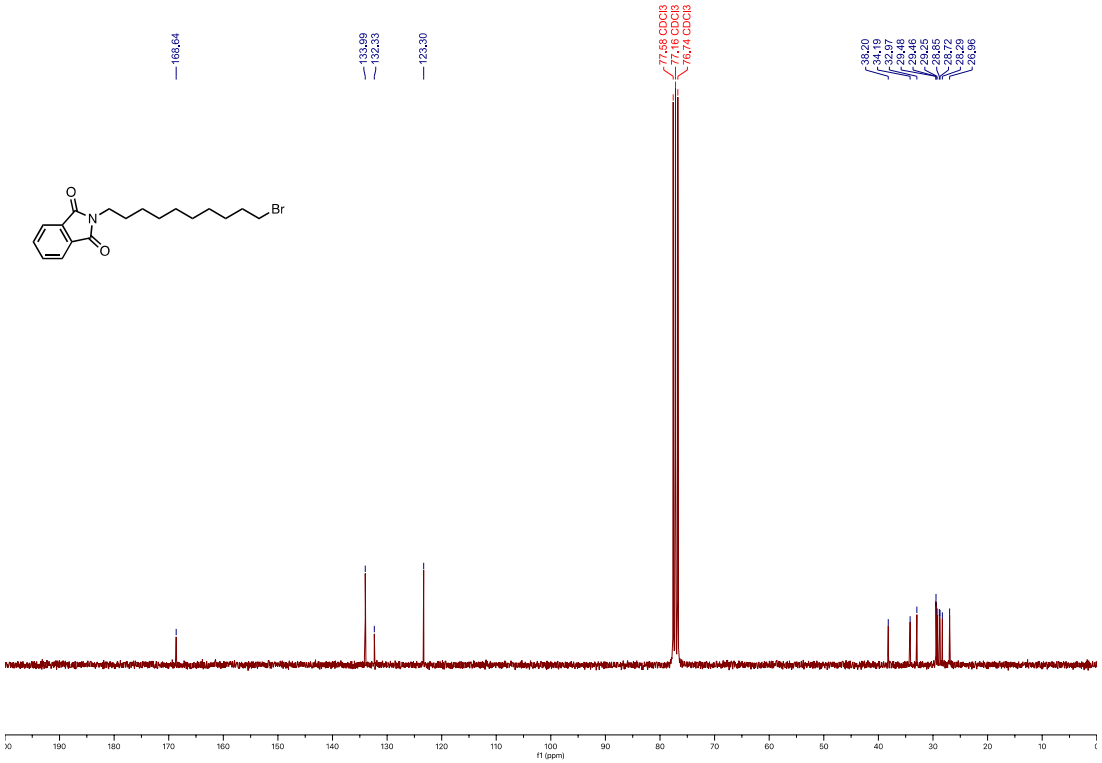


Figure S5 *^{13}C NMR of 2-(10-bromodecyl)isoindoline-1,3-dione*

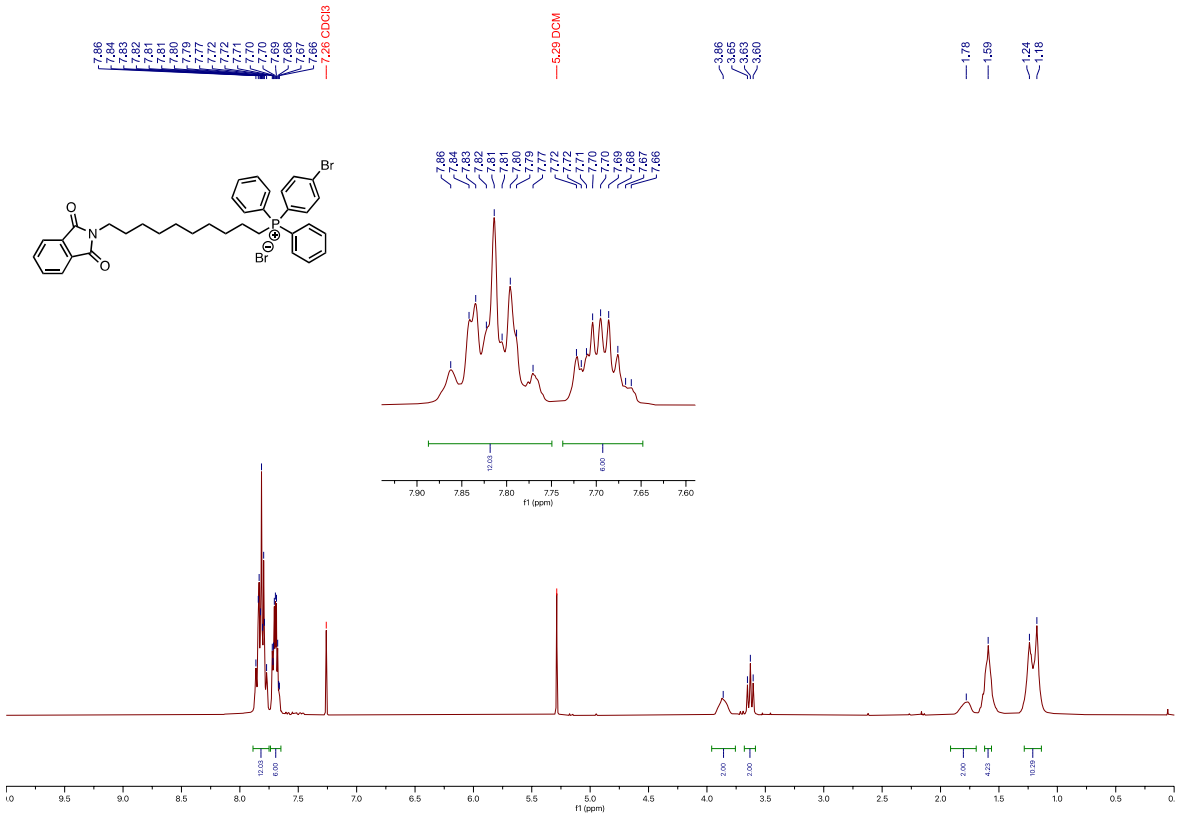


Figure S6 *^{1}H NMR of 4-bromophenyl)(10-(1,3-dioxoisoindolin-2-yl)decyl)diphenylphosphonium bromide hydrate*

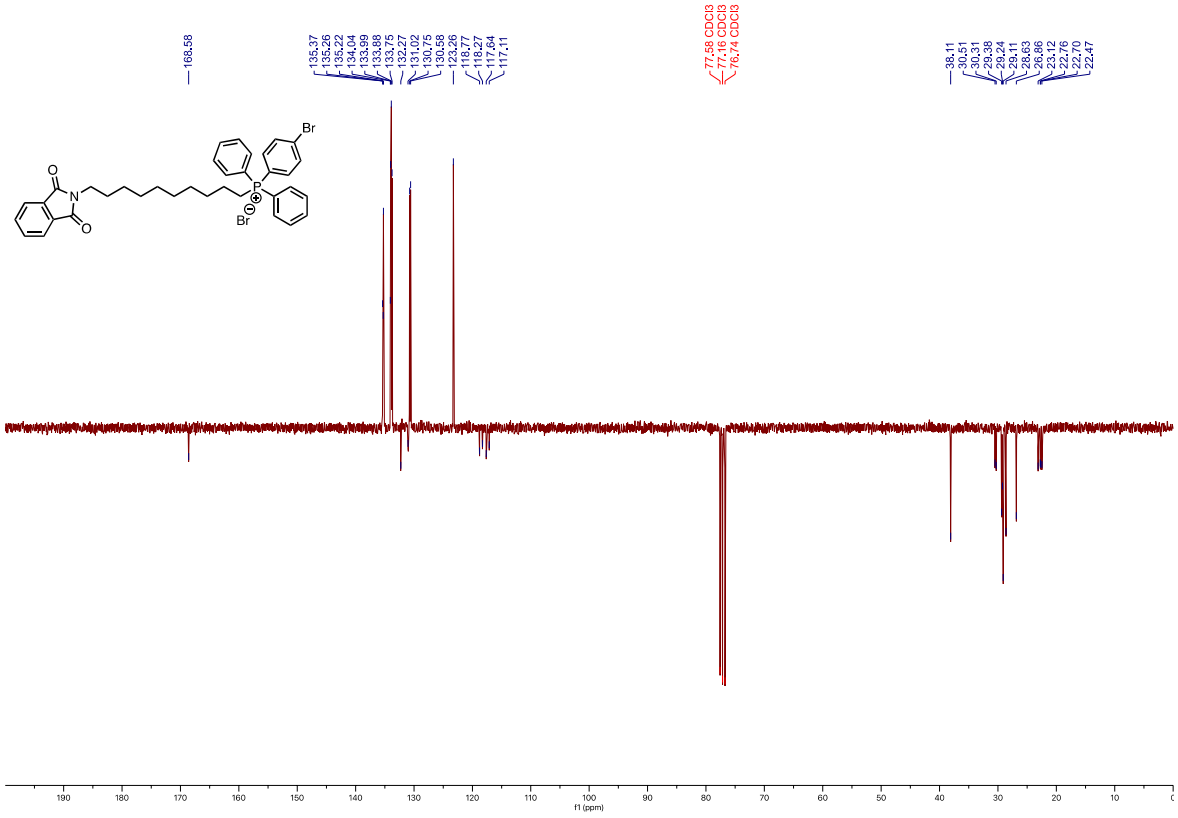


Figure S7 *^{13}C NMR of 4-bromophenyl)(10-(1,3-dioxoisoindolin-2-yl)decyl)diphenylphosphonium bromide hydrate*

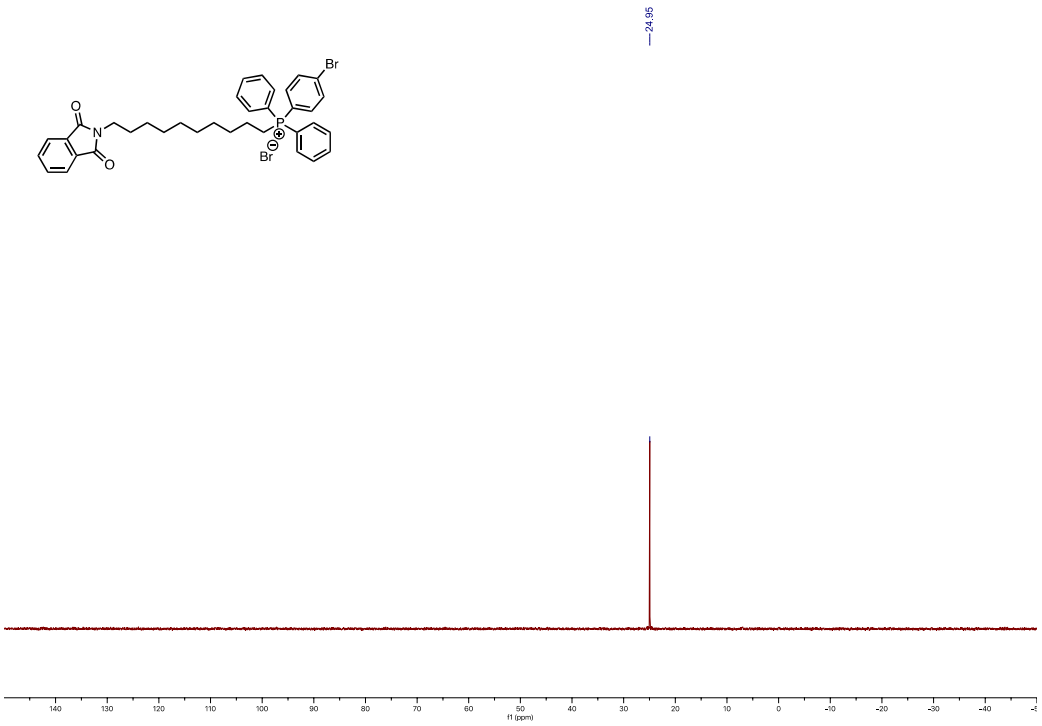


Figure S8 *^{31}P NMR of 4-bromophenyl)(10-(1,3-dioxoisoindolin-2-yl)decyl)diphenylphosphonium bromide hydrate*

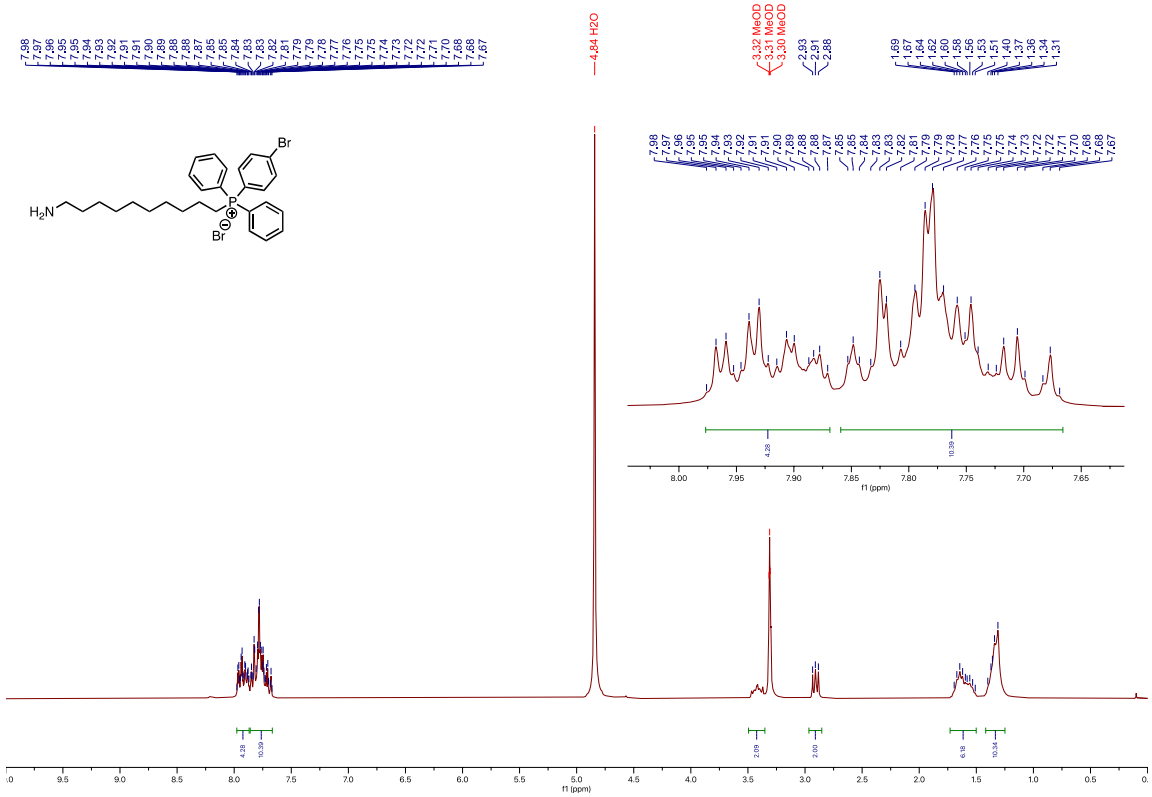


Figure S9 *^{1}H NMR of (4-bromophenyl)(10-(methylamino)decyl)diphenylphosphonium bromide hydrate*

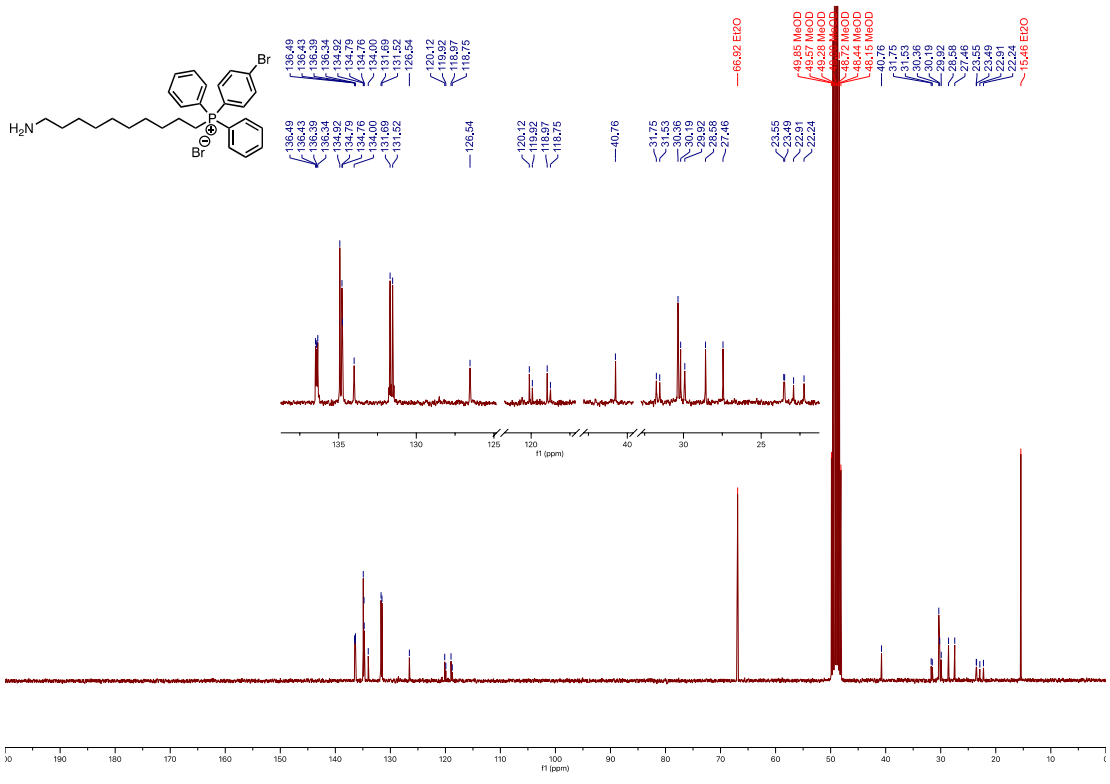


Figure S10 *^{13}C NMR of (4-bromophenyl)(10-(methylamino)decyl)diphenylphosphonium bromide hydrate*

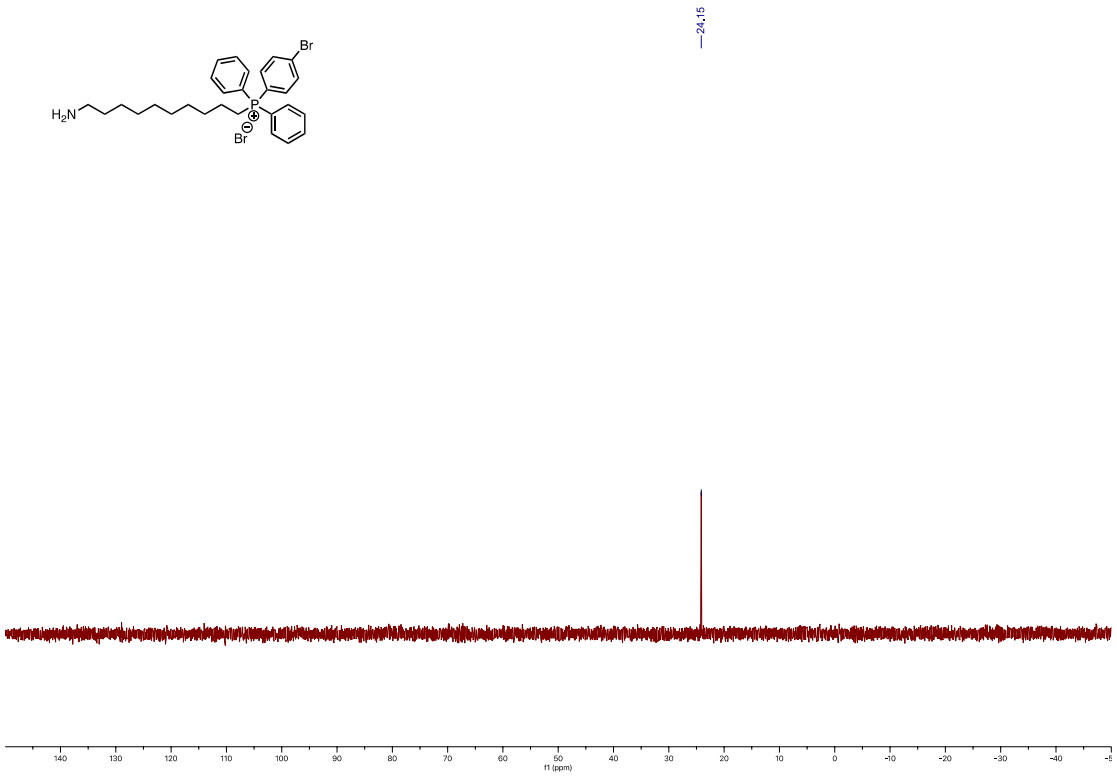


Figure S11 *^{31}P NMR of (4-bromophenyl)(10-(methylamino)decyl)diphenylphosphonium bromide hydrate*

5) General experimental procedure.

High-resolution mass spectra were recorded on a Maxis IITM QTOF mass spectrometer (Bruker, Bellerica, MA, United States) with an electrospray ionization source. 1D and 2D NMR spectra were recorded on Bruker Avance III HD 400 MHz and 600 MHz spectrometers (Wissembourg, France) equipped with a BBFO Plus Smart probe and a triple resonance TCI cryoprobe, respectively (CNRS-MNHN). Preparative HPLC experiments were performed on an Agilent system and an Agilent PrepHT XDB-C18 column (21.2 × 150 mm i.d.; 5 µm; USA). Column chromatography (CC) was performed using 200g of silica gel (Geduran Si 60, 40−63 µm, Merck, Germany and Lichroprep RP-18, 40-63µm, Merck KGaA, Germany). Optical rotations $[\alpha]^{20}_{D}$ were determined using a Anton Paar MCP 150 polarimeter. IR spectra were performed on a PerkinElmer BX FR-IR spectrometer and CD spectra finished Jasco J-810 spectropolarimeter system. UV spectra were recorded on Uvikon 9 X 3 W Bioserv.

The separation occurred onto the C18 Acclaim™ RSLC PolarAdvantage II column (2.1 × 100 mm, 2.2 µm of pore size; Thermo Fisher Scientific, United States) connected to a Dionex Ultimate 3000 HPLC system and coupled to a Maxis II™ QTOF mass spectrometer (Bruker, United States) with an electrospray ionization source. The mobile phases were water (0.1% formic acid) and acetonitrile (0.08% formic acid, solvent B) following a gradient of B at 10 to 100 in 15 min. The flow rate was set at 300 µL min^{-1}. The MS parameters were 3.5 Kv of electrospray voltage, 35 psi of nebulizing gas (N_2) pressure, drying gas (N_2) flow rate of 8 L min^{-1}, and 200°C of drying temperature. For the analysis of the vial with *T. flavus* crude extract mixed with probe 1, the mass spectra were recorded in the range of *m/z* 50-1500 in positive ion mode.

Single-crystal X-ray data for chlorobartaphilone A (4) were collected on a Rigaku mm007 HF rotating anode using CuKα radiation (λ = 1.54187 Å) delivered through Osmic CMF confocal optics, and a Rapid II curved Image Plate detector. The data were recorded at 293 K. Data collection, cell refinement and

data reduction were performed with Fs_process[1] software implemented within the Crystal Clear 2.0[2] suite. Absorption correction using equivalent reflections was performed with the AbsCorr option program[2]. All non-hydrogen atoms were refined anisotropically, and the hydrogen atoms were placed in idealized positions and refined as riding atoms isotropically with fixed individual displacement parameters [U_{iso}(H) = 1.2 U_{eq}(Csp^2 and C_{ar}) or 1.5U_{eq}(Csp^3 or $O_{(hydroxyl)}$)]. The absolute configuration of chlorobartaphilone A (C7 R) was determined unambiguously from the anomalous scattering by chloride at the copper wavelength using established methods[3-5]. X-ray crystallographic data in cif format are available at CCDC 2218370 and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

6) Fungal material.

The strains used for this study were *Talaromyces flavus var. flavus* (CBS 354.72B) and *Bartalinia robillardoides* (CBS 122686) obtained from the CBS collection. Precultures were obtained by seeding 3 cubes of agar covered with the mycelium *Talaromyces flavus var. flavus* or *Bartalinia robillardoides* on Malt Extract Agar (MEA) and incubated 8 days at 25 °C. Precultures were then scratched and sprayed with 100 mL of sterilized water, 1 mL of the mix was thus spread on 100 petri dishes and at 25°C for 10 days. The medium used for the culture was the same as for the preculture.

7) Protocol of the probe addition in *T. flavus* and *B. robillardoides extracts*.

A solution of probe 1 at 10 mg.mL^{-1} in acetonitrile was prepared. 11.25 µL of the solution of probe 1 were added to a LC vial containing 188.75 µL of methanol. Then 50 µL of *Talaromyces flavus* crude extract (or *B. robillardoides* crude extract) at 50 mg.mL^{-1} (in methanol) were added to the LC vial, and 6 µL were injected on the HPLC coupled with Tandem Mass Spectrometry. The separation was carried out using a C18 Acclaim™ RSLC PolarAdvantage II column (2.1 × 100 mm, 2.2 µm pore size; Thermo Fisher Scientific, United States) connected to a Dionex Ultimate 3000 HPLC system. The column was coupled to a Maxis 208 IITM QTOF mass spectrometer (Bruker,United States) equipped with an electrospray ionization source. The flow rate was set at 210 µL.min–1. The MS parameters were 3.5 kV of electrospray voltage, 35 psi of nebulizing gas (N_2)pressure, drying gas (N_2) flow rate of 8 L.min^{-1}, and 200°C of drying temperature. The mobile phases were water (0.1% formic acid) and acetonitrile (0.1% formic acid, solvent B) following a gradient of Solvent B at 5, 50, 90, and 5% for 0, 9, 15, and 21 min, respectively.LC-MS/MS data were analyzed using DataAnalysis (version 4.4 Bruker Daltonik GmbH)

8) Detection of tagged compounds from *B. robillardoides extract*.

Procedure for Haloseeker.

LC-MS/MS data were converted to ".mzXML". The software HaloSeeker was used to detect tagged compounds bearing a bromide. Samples with a crude extract/probe 1 ratio of 4.5% gave the best results and were used for analysis. For the peak picking the m/z tolerance = 5 ppm, s/n= 8, peakwidtch =5, 60 s, prefilter= 3-10 000, the m/z center function =wMean , no baseline check, no integration by CWT, noise= 0, m/z difference = 0.001 . For the pairing tr tolerance= 1 s and m/z tolerance = 0.5 mDa. For the alignment tr and m/z tolerance = 1, the distance function = cor_opt, response= 1, gap init = 0.3, gap extend= 2.4, factor diagonal = 2, no local alignment. For the fragment/adduct, the percentage of the width = 0.75, threshold for EIC correction = 0.75, method for grouping peaks=hcs, multiplier of the standard = 6, p-value threshold = 0.05.

To obtain the Figure 3 the display options were as followed: plot type =Halomap, X axis= RT (min), Y axis = IUPAC m/z, legend scheduling = Cluster ID, m/z range= 600-1500, tr range= 6-8 min, the most intense clusters =inf, pairing and ratio filter = F1.

Table S1 *Overview of HaloSeeker results for probe 1*

	Number of features	Number of clusters	Sum intensities
F1	151	48	96,787,133
filtered	78	21	22,169,715

Procedure for Molecular Networking.

The LC-MS/MS data were preprocessed on MzMine 2.57. The MZmine workflow for probe 1 included the MS^1 detection algorithm with a noise level set to 1.0E3 and MS^2 to 1.0E1. Chromatogram building was performed including a minimum group size of 5, a group intensity threshold and minimum highest intensity of 1.0E1 and a *m/z* tolerance of 0.02. The filtering tool was used to keep only *m/z* = 800-1500. Data were then aligned with a *m/z* tolerance = 0.02, a weight for *m/z* and RT =1 and a retention time tolerance=1.0 min. The single file containing a .csv and a .mgf was analyzed by the Feature-Based-Molecular-Networking (FBMN) of the software Global Natural Products Social Molecular Networking (GNPS). Parameters used were: precursor ion mass tolerance and fragment ion mass tolerance = 0.02 Da, minimum pairs cosinus =0.5, minimum matched fragment ions = 3.

9) Detection of the tagged compounds from *T. flavus extract*.

Prior to MS/MS data processing, raw files of tagged metabolites and probe 1 were converted to the open format mzXML using the DataAnalysis tool "Export Chromatogram Analysis". Then the data were imported into the MZmine 2.57 software. The workflow included the MS^1 detection algorithm with a noise level set to 5.0E2 and MS^2 to 1.0E1. Chromatogram building was performed including a minimum group size of 5, a group intensity threshold and minimum highest intensity of 1.0E1 and a m/z tolerance of 0.02. The filtering tool was used to keep only m/z = 750-850. Data were then deisotoped and filtered with a retention time = 6.6-9.9 min and a height = 1.0E4-1.0E7. The single file containing .csv and .mgf was analyzed by GNPS (with Feature-Based Molecular Networking). Parameters used were: precursor ion mass tolerance and fragment ion mass tolerance = 0.02 Da, minimum pairs cosinus = 0.5, minimum matched fragment ions =3.

10) Extraction and isolation of compounds 2 and 3 from *T. flavus crude extract*.

For large scale culture, the fungus was grown in 3 square Petri dishes (45 mL) of Malt Extract Agar (MEA) at 25°C for 11 days. Then the mycelium was scratched and mixed to 60 mL of sterile water. 60 square Petri dishes were seeded with 1 mL of the water with mycelium and incubated for 11 days à 25°C. The cultivated agar was then cut in squares and extracted three times with ethyl acetate and the solvent was combined and dried to afford a crude extract of 1.215g. The crude extract was subjected to silica gel column chromatography with a dichloromethane-ethyl acetate (DCM- EtOAc) gradient system, 90:10, 30:70, then a DCM-methanol (MeOH) system 90:10, 70:30 and 0:100 to rinse the column yielding 6 fractions (F1-F6). F4 was purified by preparative HPLC at a flow rate of 10 mL/min (ACN-H_2O+0.1%FA, 5:95 to 70:30 in 35 minutes) to yield 9 subfractions. F4F6 yielded the compound **3** (6.1 mg), F4F8 yielded the diazaphilonic acid **2** (44.7 mg). F3 was purified by preparative HPLC at a flow rate of 10 mL/min (ACN-H_2O+0.1%FA, 5:95 to 70:30 in 35 minutes) to yield 8 fractions. F3F4 yielded 6-hydroxy-mitorubrinic acid (2.8 mg), F3F5 mitorubrinol (5.5 mg) and F3F6 mitorubrinic acid (32.2 mg).

11) Extraction and isolation of compounds 4 and 5 from *B. robillardoides crude extracts*.

Precultures of MEA were obtained by seeding 3 cubes of agar covered with mycelium and incubating them 6 days at 25 °C. Precultures were then scratched and sprayed with 30 mL of sterilized water, 1 mL of the mix was thus sprayed on each of 30 erlenmeyers of solid rice medium (50g of rice and 100 mL of water), and incubated at 25°C for 20 days. Then, the 30 erlenmeyers were extracted three times with ethyl acetate by sonication (30 minutes each time). The solvent was evaporated under reduced

pressure to give a crude extract of 17,76 grams which was fractionated over a silica gel column (356 g), eluted successively with DCM, then DCM/EtOAc (9:1), followed by DCM/EtOAc (5:5) and rinsed with MeOH to afford 8 fractions. The fraction 5 (1.08g) was purified by preparative HPLC (10 mL/min, A: water+ 0.1% formic acid, B: acetonitrile, gradient: 5 to 20% for 4 min and 20 to 95% of B for 24 min) yielding 8 fractions. The subfraction F5F3 (4.8 mg) corresponded to chlorobartaphilone A (4). The subfraction F5F6 (10.1 mg) corresponded to 8-11-didehydrochermesinone B. The fraction 6 (1.991 g) was purified by preparative HPLC (10 mL/min, A: water+ 0.1% formic acid, B: acetonitrile, gradient: 5 to 20% for 4 min and 20 to 95% of B for 24 min) yielding 13 fractions. The subfraction F6F10 (80.6 mg) corresponded to chermesinone A. The subfraction F6F7 (249.3 mg) was purified by preparative silica TLC with DCM/MeOH (95:5) yielding 4 subfractions. The subfraction F6F7F3 (4.0 mg) corresponded chloro-hydroxy-chermesinone A (**5**). The subfraction F6F9 (61.6 mg) was purified by a second preparative HPLC (10 mL/min, A:water+ 0.1% formic acid, B: acetonitrile, gradient: 5 to 50% for 4 min, 50 to 60% of B for 14 min and 60 to 95% for 3 min) yielding 5 fractions. The subfraction F6F9F3 corresponded to colletotrichone A.

12) Spectroscopic data

Diazaphilonic acid (2). IR ν_{max}: 3360, 1720, 1640, 1520, 1440, 1320, 1240, 1160, 1080, 1000, 880 cm^{-1}; UV (MeOH): λmax (logε) 216 nm (4.93), 268 nm (4.61), 325 nm (4.62); HRMS (ESI-TOF) *m/z* : 825.1668 $[M+H]^+$ Calcd for $[C_{42}H_{32}O_{18} + H]^+$; Found 825.1663. α_D: -261.5 (*c* 0.54, CH_3OH)

Pavesiflonic acid (3). IR ν_{max}: 3360, 2880, 1760, 1720, 1680, 1618, 1440, 1320, 1240, 1200, 1160, 1080, 840 cm^{-1}; UV (MeOH): λmax (logε) 206 nm (4.29), 265 nm (3.93), 305 nm (3.78); HRMS (ESI-TOF) *m/z* : 811.1874 $C_{42}H_{35}O_{17}$ $[M+H]^+$ Calcd for $[C_{42}H_{34}O_{17} + H]^+$; Found 811.1865. α_D: -95 (*c* 0.24, CH_3OH)

Chlorobartaphilone A (4). IR ν_{max}: 3443, 2106, 1647 cm^{-1}; UV (MeOH): λmax (logε) 348 (2.69), 260 (2.75); HRMS (ESI-TOF) *m/z* : 265.0262 $[M+H]^+$ Calcd for $[C_{13}H_9ClO_4 + H]^+$; Found 265.0263. $[\alpha]_D$ -10 (*c* 0.5, CH_3OH). Crystallographic data: $C_{13}H_9ClO_4$ (M= 264.65 g/mol): monoclinic, space group $P2_{1,a}$ = 5.3067(4) Å, b= 9.1631(7) Å, c= 12.2106(9) Å, α=90°, β= 99.671(7)°, γ= 90°, V= 585.31(8) $Å^3$, Z=2, T= 293(2) K, μ(CuKα)= 2.949 mm^{-1}, F(000)= 272, crystal size = 0.29 x 0.08x0.03 mm^3, ρ_{calc}= 1.502 g/cm^3; out of the 6690 reflections measured (3.67° ≤ θ ≤ 68.2°), 2096 were unique (R_{int} = 0.0438, R_{sigma} =0.058) and were used in all calculations. The final R_1 was 0.0381 (I>2σ(I)), and $_wR_2$ was 0.1159 (all data). Flack parameter (using 520 quotients $\{(I^+)-(I^-)]/[(I^+)+(I^-)]\}$ = 0.016 (9).

Chloro-hydroxy-chermesinone A (5). IR ν_{max}: 3395,2095, 1641, 1015 cm^{-1}; UV (MeOH): λmax (logε) 352 (1.75); HRMS (ESI-TOF) *m/z* : 341.1150 $[M+H]^+$ Calcd for $[C_{17}H_{21}ClO_5 + H]^+$; Found 341.1149. $[\alpha]_D$ + 3 (*c* 0.5, CH_3OH)

13) NMR characterization of compounds (2-5)

Table S2 *2D NMR spectrum (600 MHz) of diazaphilonic acid (**2**) (acetone-d_6) and pavesiflonic acid (**3**) (acetonitrile-d_3)*

Position	Diazaphilonic acid (**2**)		Pavesiflonic acid (**3**)	
	δ_C, type	δ_H, multi (*J* in Hz)	δ_C, type	δ_H, multi (*J* in Hz)
1	154.1, CH	8.18, s	154.4, C	7.99, d (1.1)
2	-		-	
3	159.0, C		160.5, C	
4	111.6, C		114.5, C	
5	142.2, C		143.9, C	
6	105.3, CH	5.60, brs	105.1, CH	5.83, s
7	192.1, C		192.6, C	
8	86.2, C		86.5, C	
9	193.0, C		193.9, C	
10	116.2, C		116.2, C	
11	22.7, CH_3	1.65, s	22.9, CH_3	1.62, s
12	26.3, CH_2	2.92, d (19.2) 3.29, dd (19.2, 7.9)	30.8, CH_2	3.00, dd (19.8, 7.5) 2.59, m
13	38.0, CH	3.65, d (7.7)	28.8, CH	2.66, m
14	173.4, C		70.2, CH_2	4.01, dd (11.5, 1.5) 3.77, dd (11.5, 1.5)
1a	155.5, CH	8.12, s	157.3, CH	7.80, d (1.3)
2a	-		-	
3a	158.6, C		103.5, C	
4a	111.8, CH	6.57, s	36.6, CH_2	3.04, dd (16.5, 2.1) 2.82, d (16.5)
5a	143.2, C		146.7, C	
6a	108.4, CH	5.54, brs	119.4, CH	5.81, t (1.3)
7a	192.4, C		193.8, C	
8a	86.5, C		86.7, C	
9a	193.1, C		192.6, C	
10a	115.8, C		112.7, C	
11a	22.6, CH_3	1.62, s	22.9, CH_3	1.59, s
12a	39.4, C	4.39, s	37.1, CH	3.67, dd (3.2, 1.4)
13a	43.5, CH	3.96, s	39.2, CH	3.61, dd (3.2, 2.3)
14a	172.7, C		172.7, C	
1’	104.7, C		105.1, C	
2’	166.1, C		166.0, C	
3’	101.6, CH	6.21, d (2.2)	101.7, CH	6.21, d (2.4)
4’	163.9, C		163.6, C	
5’	112.6, CH	6.33, m	112.7, CH	6.31, m
6’	144.7, C		145.1, C	
7’	24.0, CH_3	2.58, s	24.0, CH_3	2.58, s
8’	170.3, C		170.6, C	
1a’	104.7, C		104.9, C	
2a’	166.1, C		166.0, C	

3a’	101.6, CH	6.21, d (2.2)	101.7, CH	6.20, d (2.4)
4a’	163.9, C		163.6, C	
5a’	112.6, CH	6.33, m	112.7, CH	6.31, m
6a’	144.7, C		145.2, C	
7a’	24.0, CH_3	2.57, s	24.0, CH_3	2.57, s
8a’	170.3, C		170.5, C	
OH		10.65, brs		10.59, brs
OH		10.71, brs		10.72, brs

Table S3 *NMR Spectroscopic data (600 MHz, acetone-d_6) for chlorobartaphilone A (**4**) and chloro-16-hydroxy-chermesinone A (**5**)*

Position	Chlorobartaphilone A (**4**)			Chloro-16-hydroxy-chermesinone A (**5**)		
	δ_C	δ_H	J(Hz)	δ_C	δ_H	J(Hz)
1	150.9, CH	8.20	d, (*J*= 1.0)	145.2, CH	7.11	d, (*J*= 1.7)
3	160.2, C			164.3, C		
4	108.6, CH	6.40	s	102.7, CH	6.74	brs
5	144.1, C			142.6, C		
6	105.8, CH	5.26	d, (*J*= 1.0)	109.3, C		
7	189.8, C			192.3, C		
8	87.4, C			75.0, C		
9	153.1, C			41.3, CH	3.31	dt (*J*= 9.5, 2.4)
10	111.4, C			120.8, C		
11	115.7, C			38.1, CH_2	3.15	dd (*J*= 18.1, 2.4)
					2.94	dd (*J*= 18.1, 9.5)
12	166.6, C			212.8, C		
13	26.0, CH_3	1.63	s	48.5, CH	2.67	sext (*J*= 7.0)
14	19.4, CH_3	2.25	d (*J*= 1.0)	26.5, CH_2	1.74	dqd (*J*= 14.6, 7.4, 7.0)
					1.39	dqd (*J*= 14.6, 7.4, 7.0)
15				12.0, CH_3	0.88	t (*J*= 7.4)
16				61.2, CH_2	4.42	d (*J*= 6.5)
17				21.4, CH_3	1.11	s
18				16.3, CH_3	1.09	d (*J*= 7.0)
OH					2.82	s

14) NMR spectra of compounds (2-5)

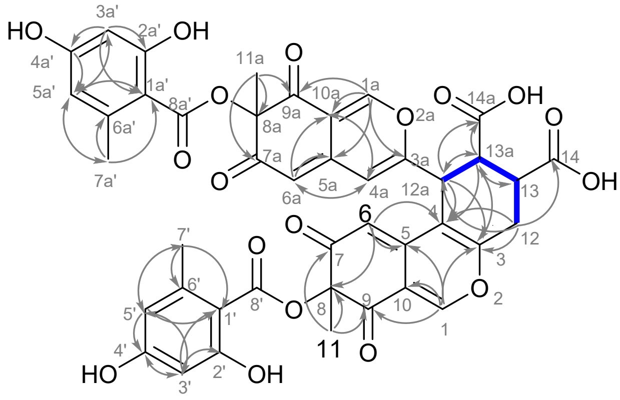


Figure S12 *Key HMBC (arrows) and COSY (blue bold) correlations for diazaphilonic acid (**2**)*

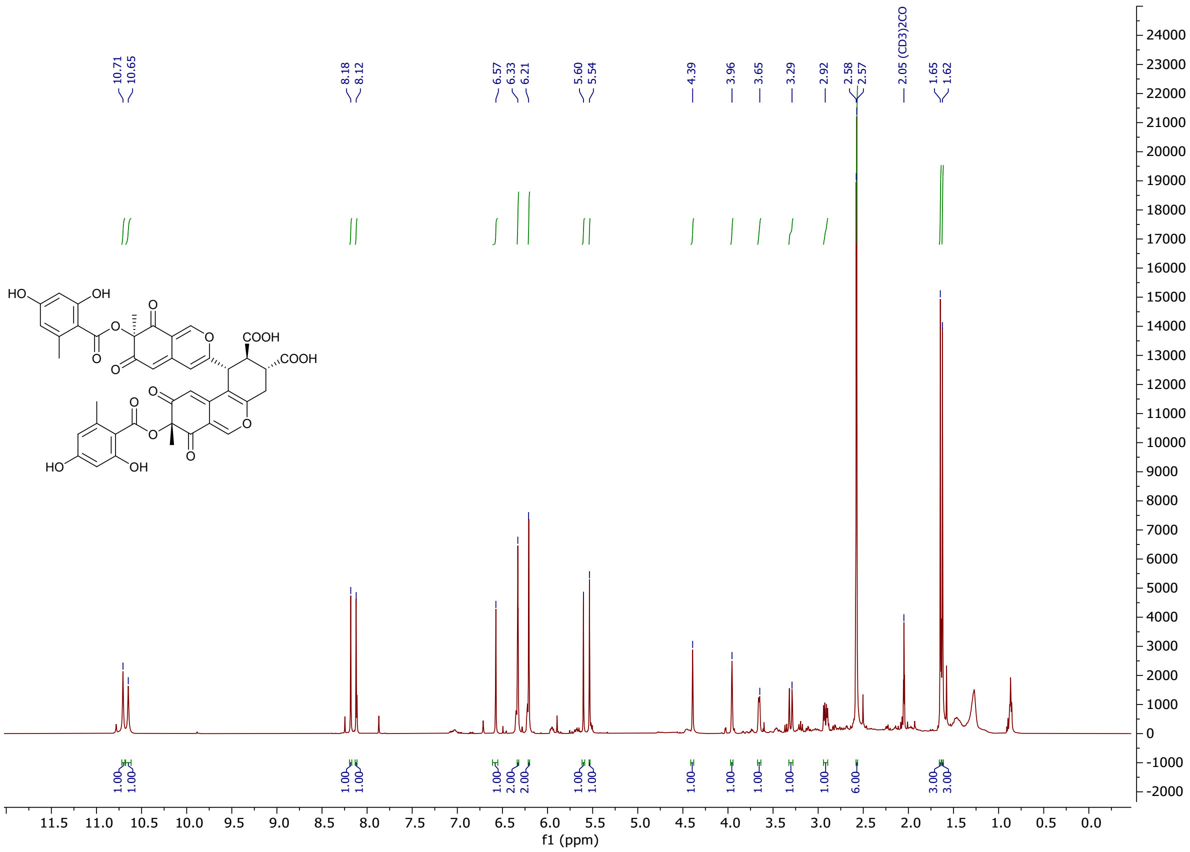


Figure S13 *^{1}H NMR spectrum (600 MHz, acetone-d_6) of diazaphilonic acid (**2**)*

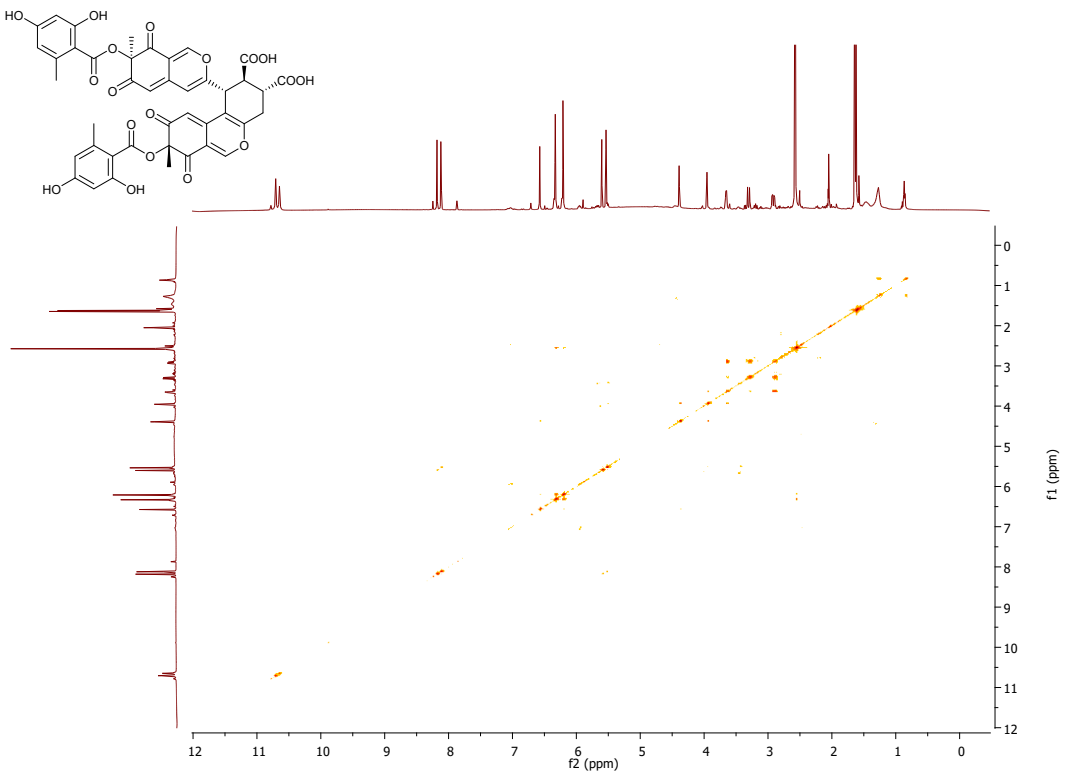


Figure S14 *COSY NMR spectrum (600 MHz, acetone-d_6) of diazaphilonic acid (**2**)*

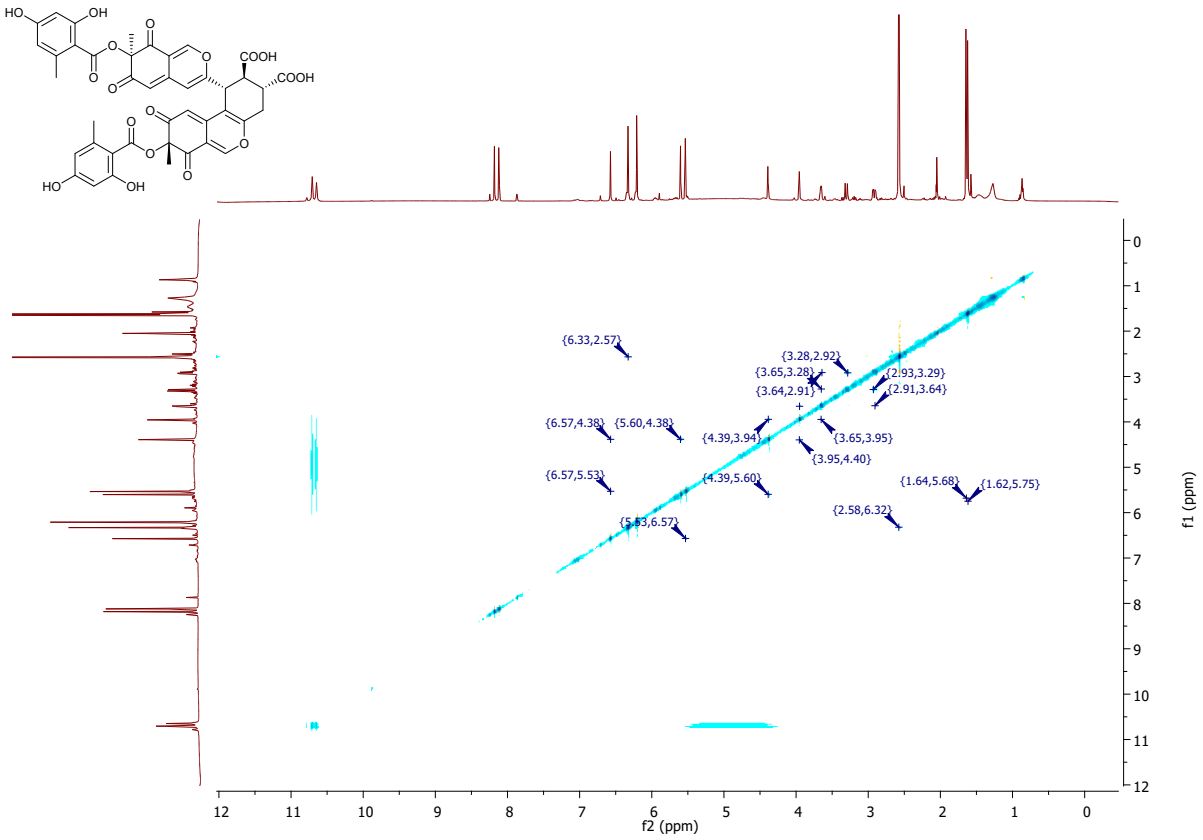


Figure S15*. NOESY NMR spectrum (600 MHz, acetone-d_6) of diazaphilonic acid (**2**)*

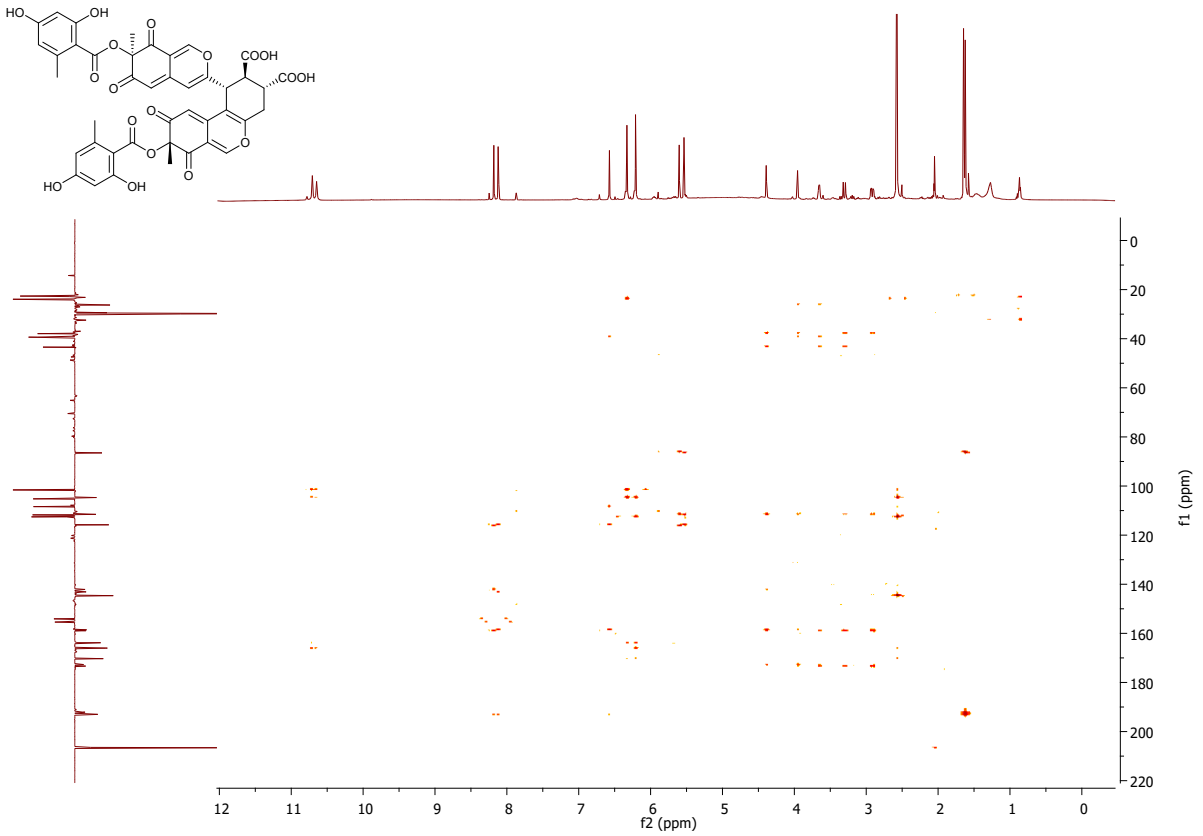


***Figure S16**. HMBC NMR spectrum (600 MHz, acetone-d_6) of diazaphilonic acid (**2**)*

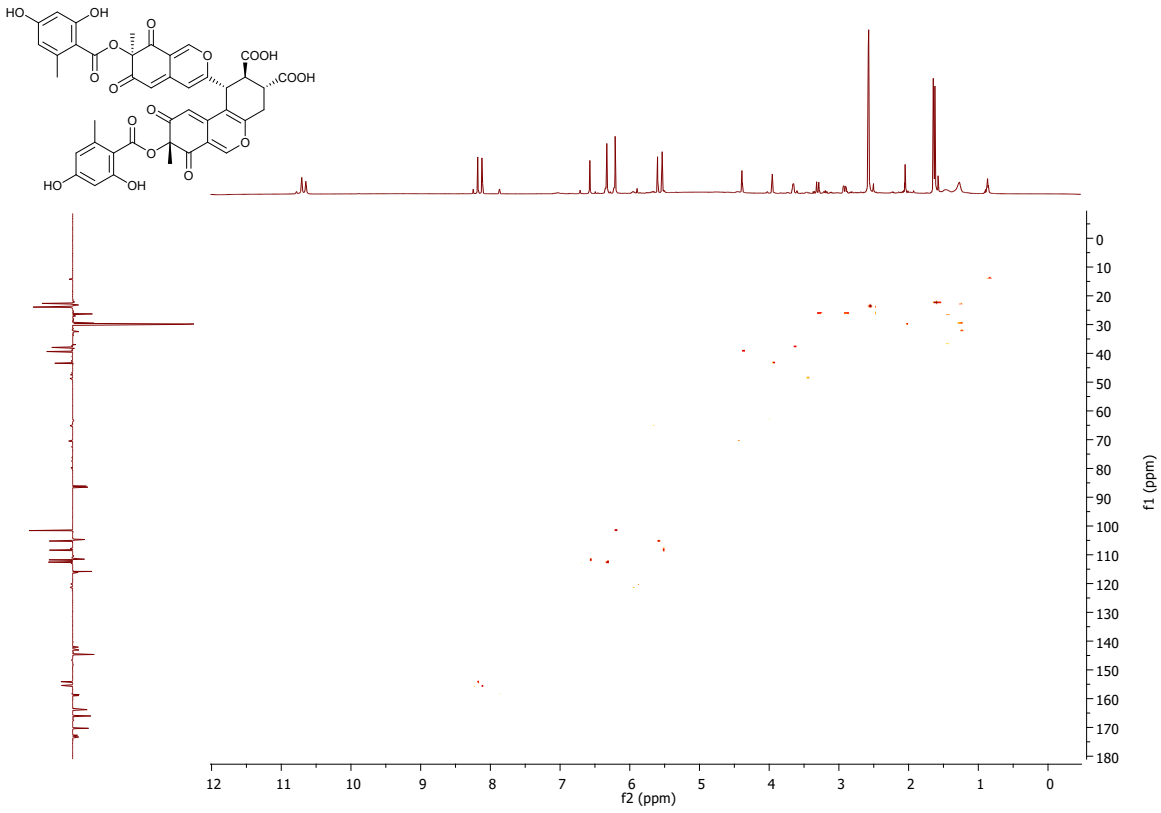


***Figure S17**. HSQC NMR spectrum (600 MHz, acetone-d_6) of diazaphilonic acid (**2**)*

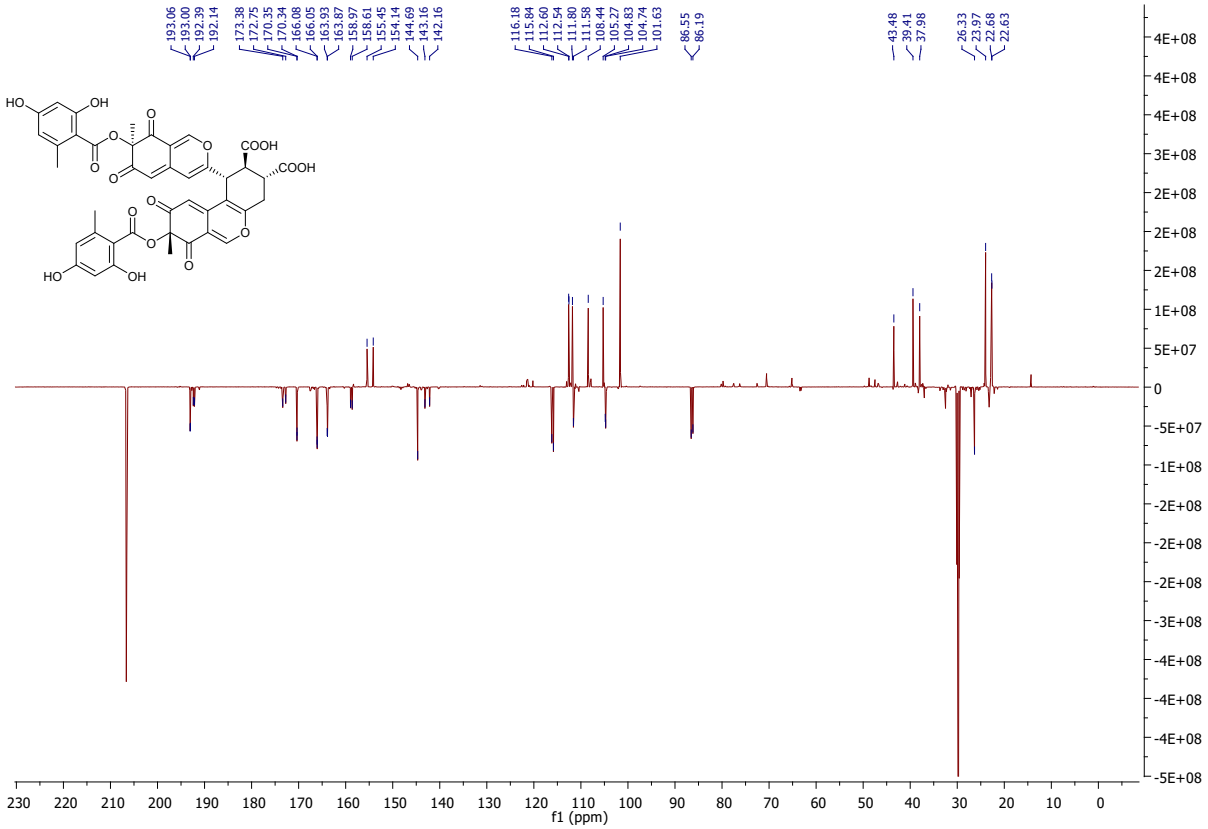


Figure S18. *DEPTQ NMR spectrum (600 MHz, acetone-d_6) of diazaphilonic acid (**2**)*

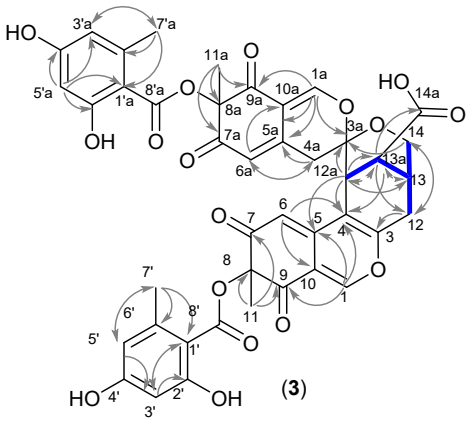


Figure S19. *Key HMBC (grey arrows), COSY (bold) and NOESY (dashed black arrows) correlations for pavesiflonic acid (**3**)*

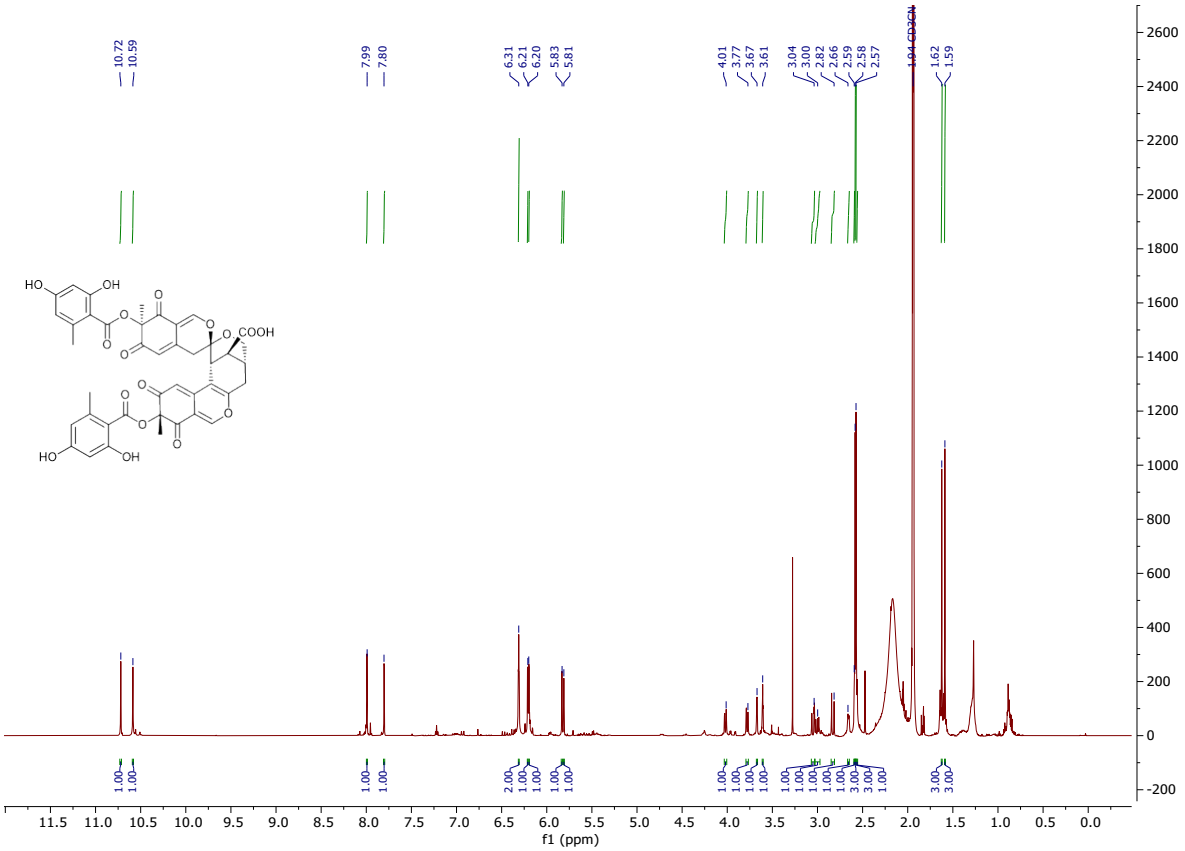


Figure S20. *^{1}H NMR of pavesiflonic acid (**3**) in acetonitrile-d_3 (600MHz)*

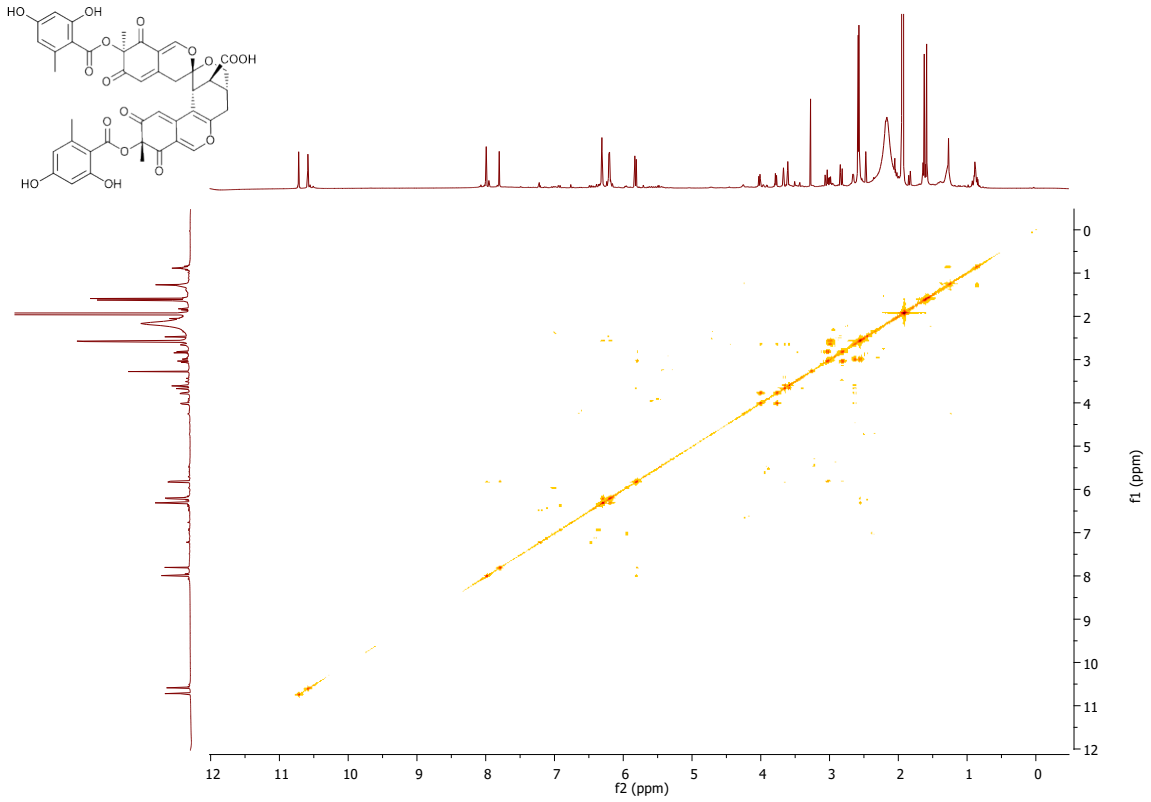


Figure S21. *COSY of pavesiflonic acid (**3**) in acetonitrile-d_3 (600MHz)*

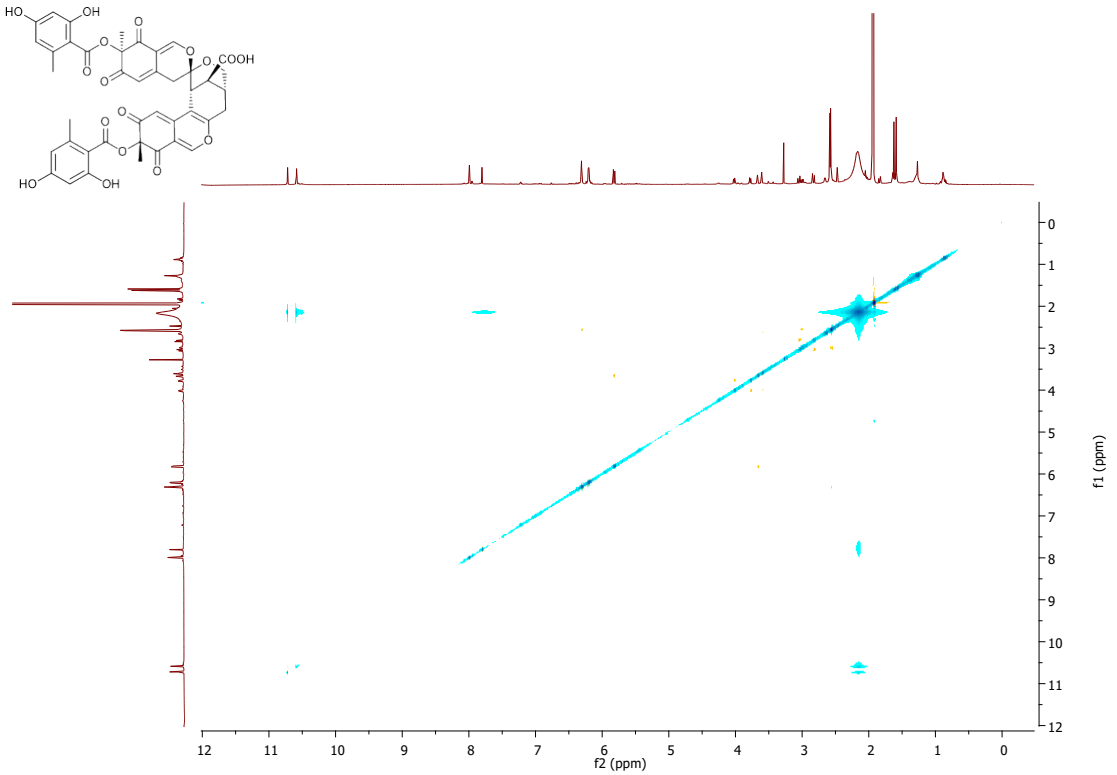


Figure S22. *NOESY of pavesiflonic acid (**3**) in acetonitrile-d_3 (600MHz)*

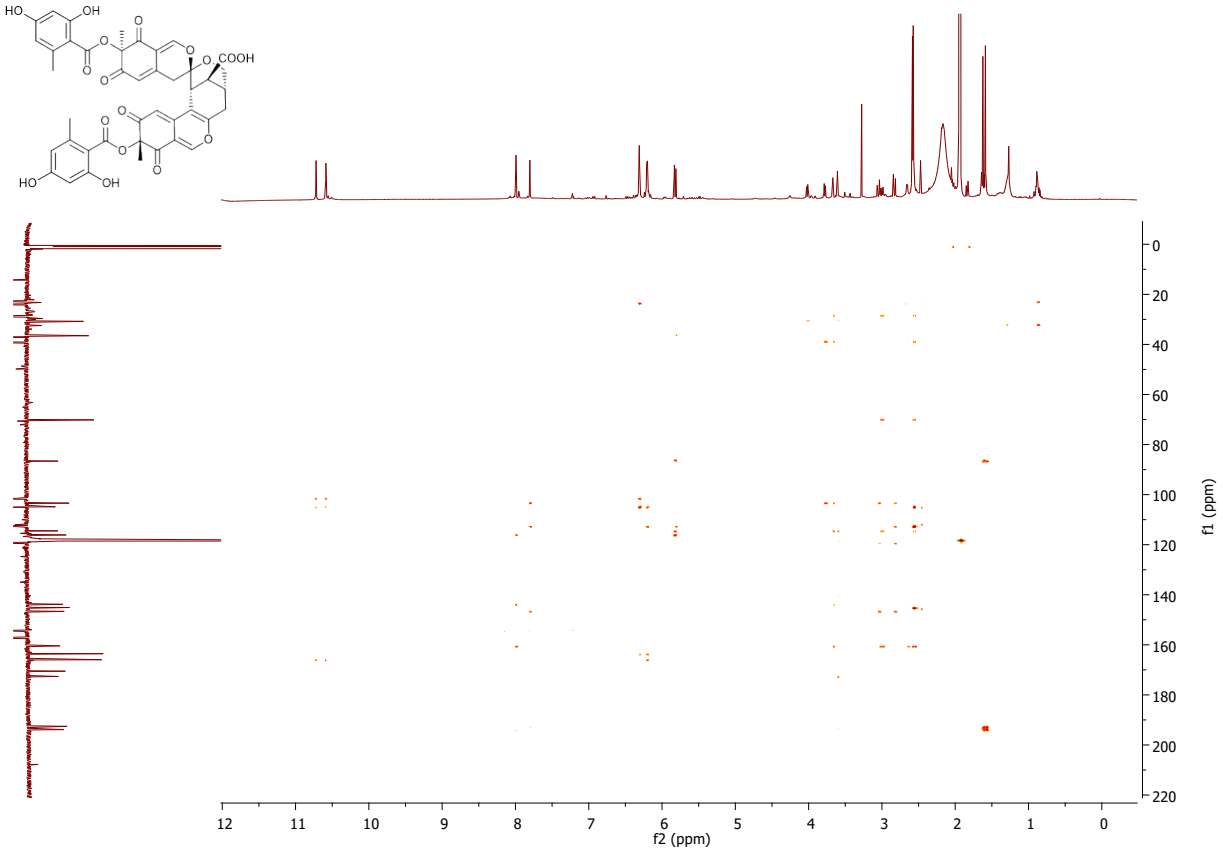


Figure S23. *HMBC of pavesiflonic acid (**3**) in acetonitrile-d_3 (600MHz)*

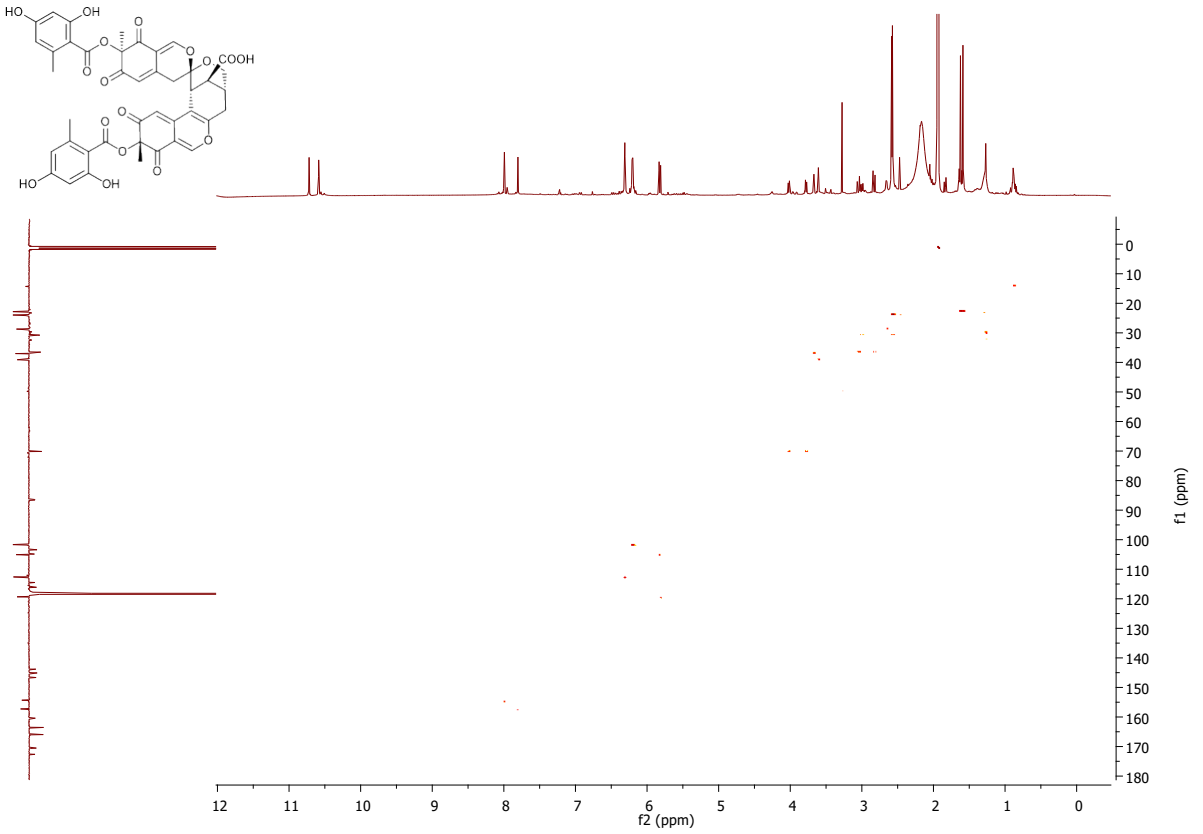


***Figure S24**. HSQC of pavesiflonic acid (**3**) in acetonitrile-d_3 (600MHz)*

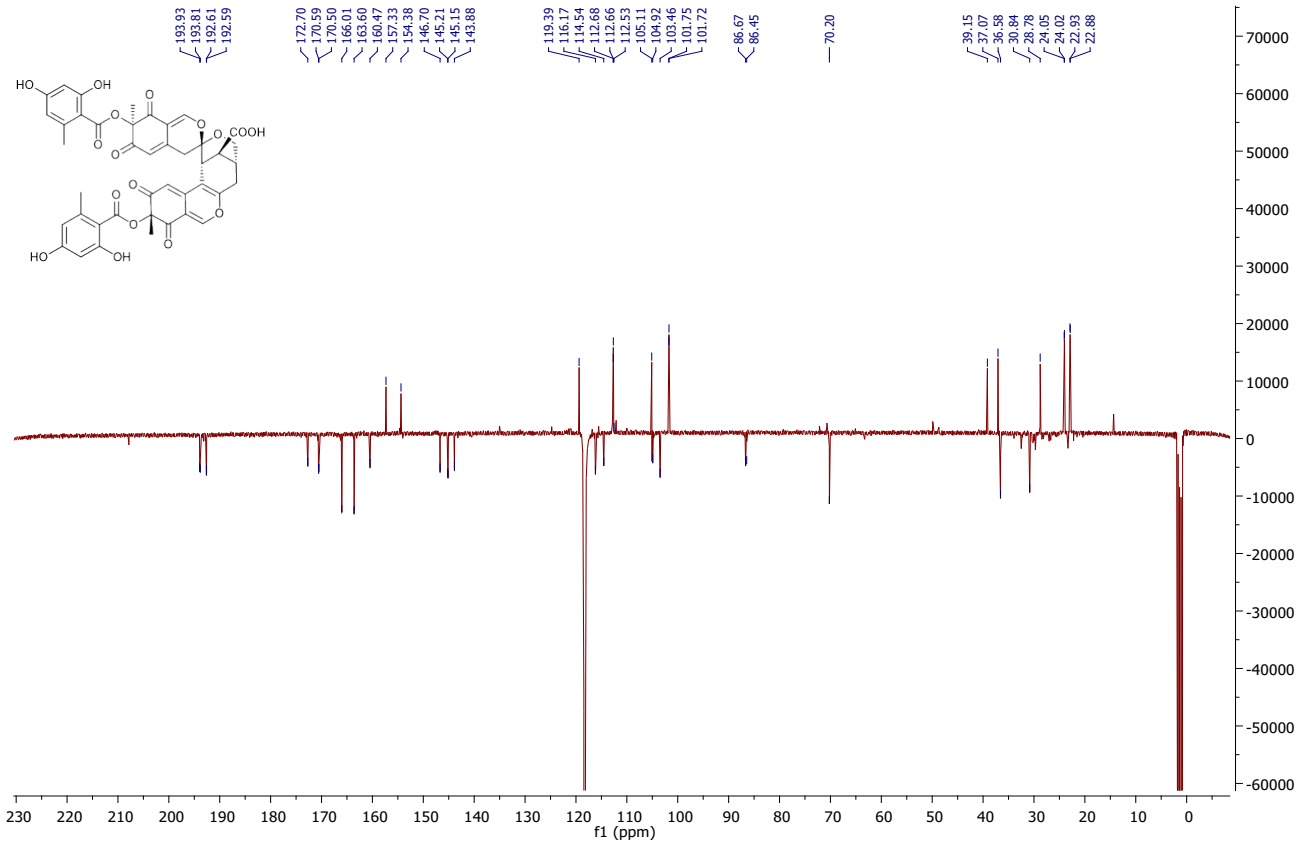


***Figure S25**. DEPT Q of pavesiflonic acid (**3**) in acetonitrile-d_3 (600MHz)*

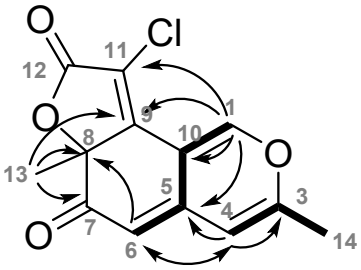


***Figure S26**. COSY correlations (bold bond) and HMBC correlations (arrows) of compound **4**.*

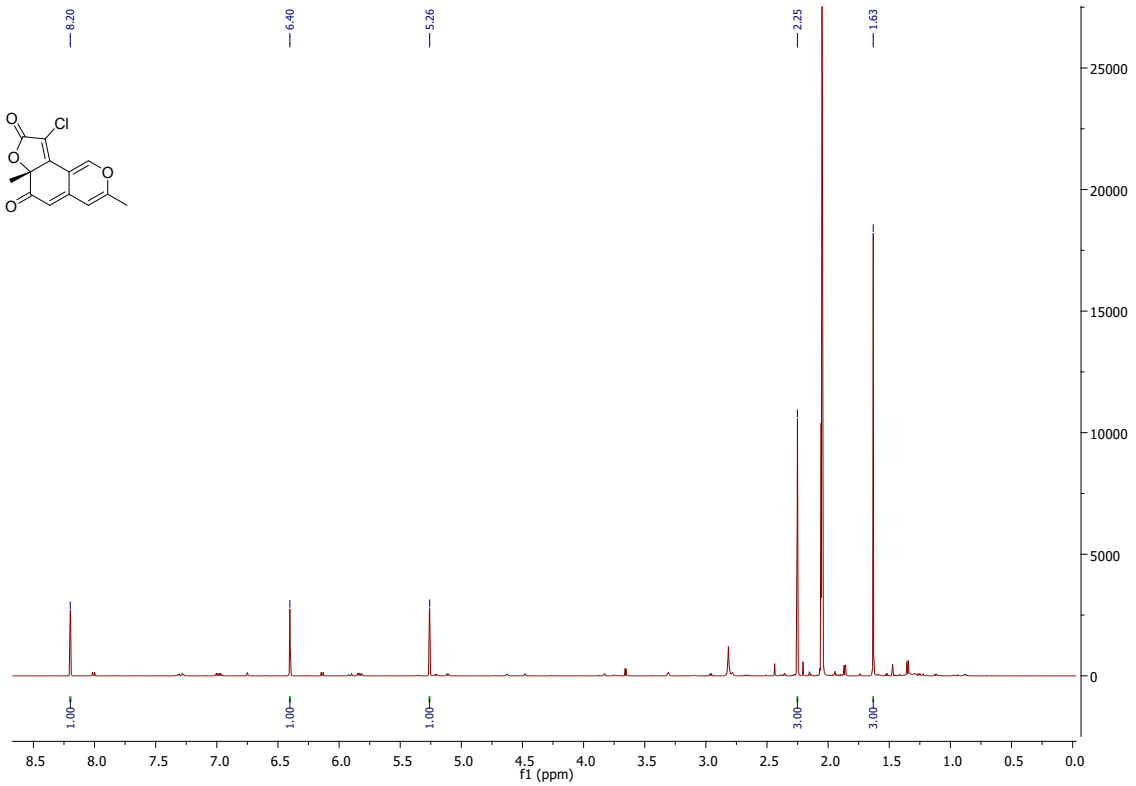


Figure S27. *^{1}H NMR of compound **4** (600 MHz, acetone-d_6)*

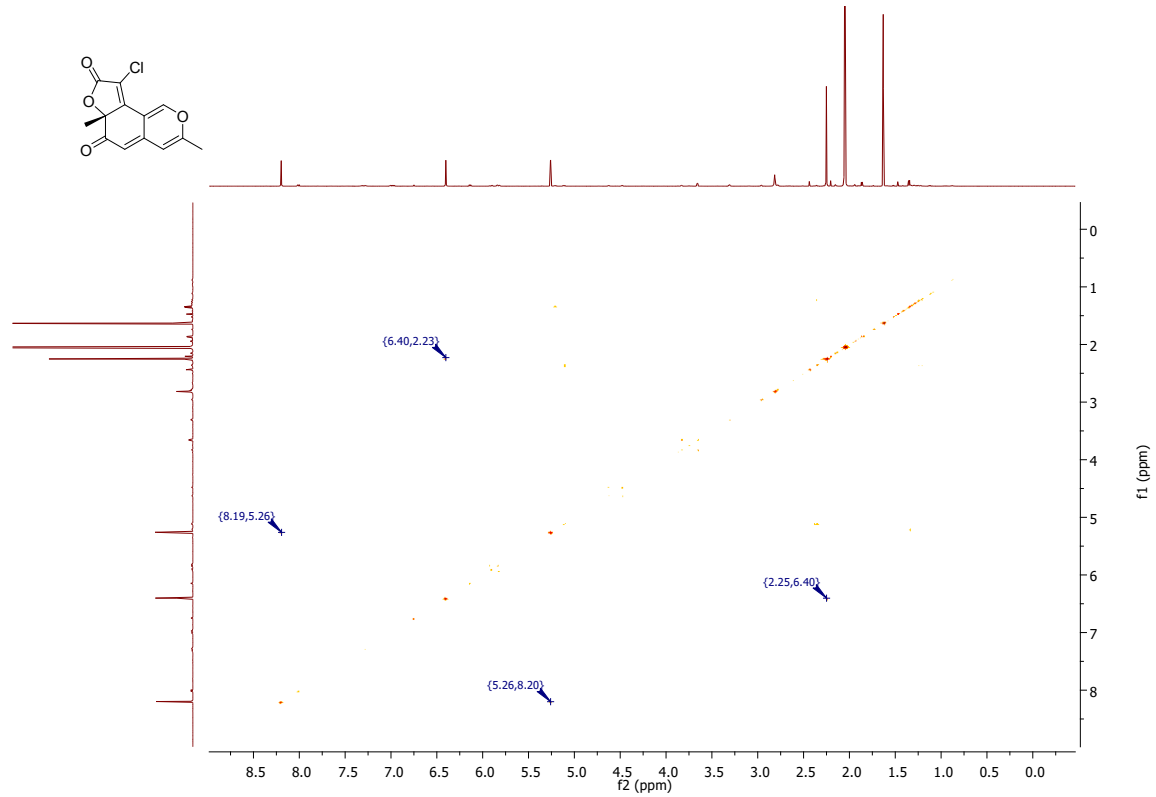


Figure S28*. COSY NMR of compound **4** (600 MHz, acetone-d_6)*

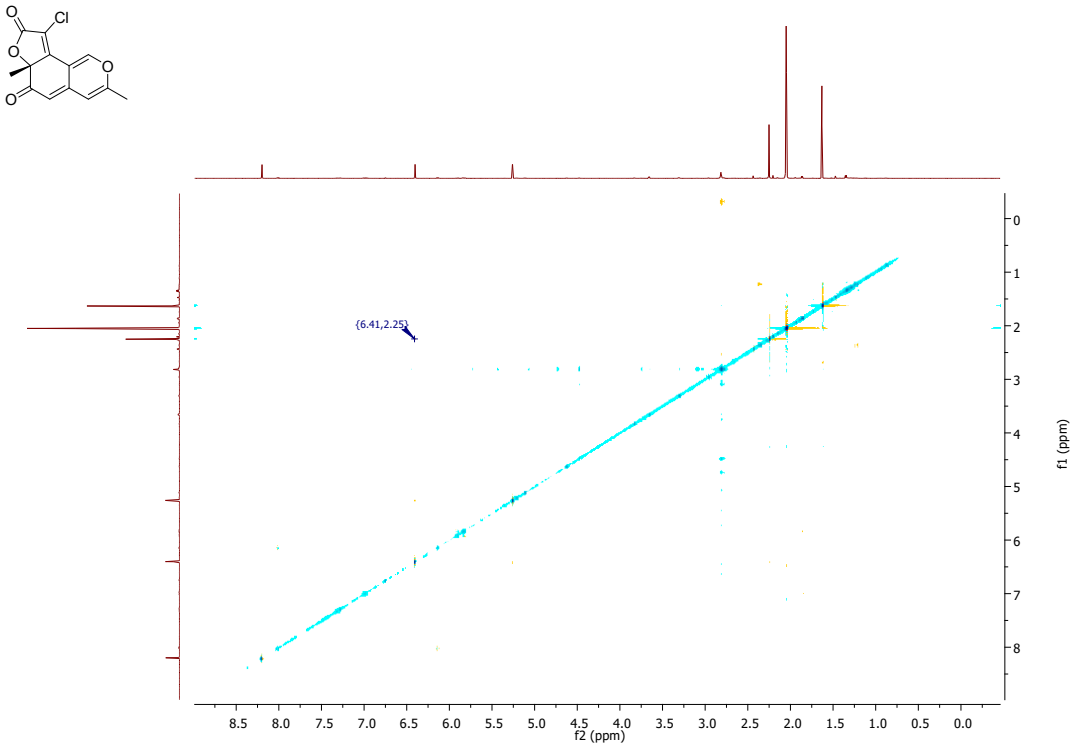


Figure S29. *NOESY NMR of compound* ***4*** *(600 MHz, acetone-d_6)*

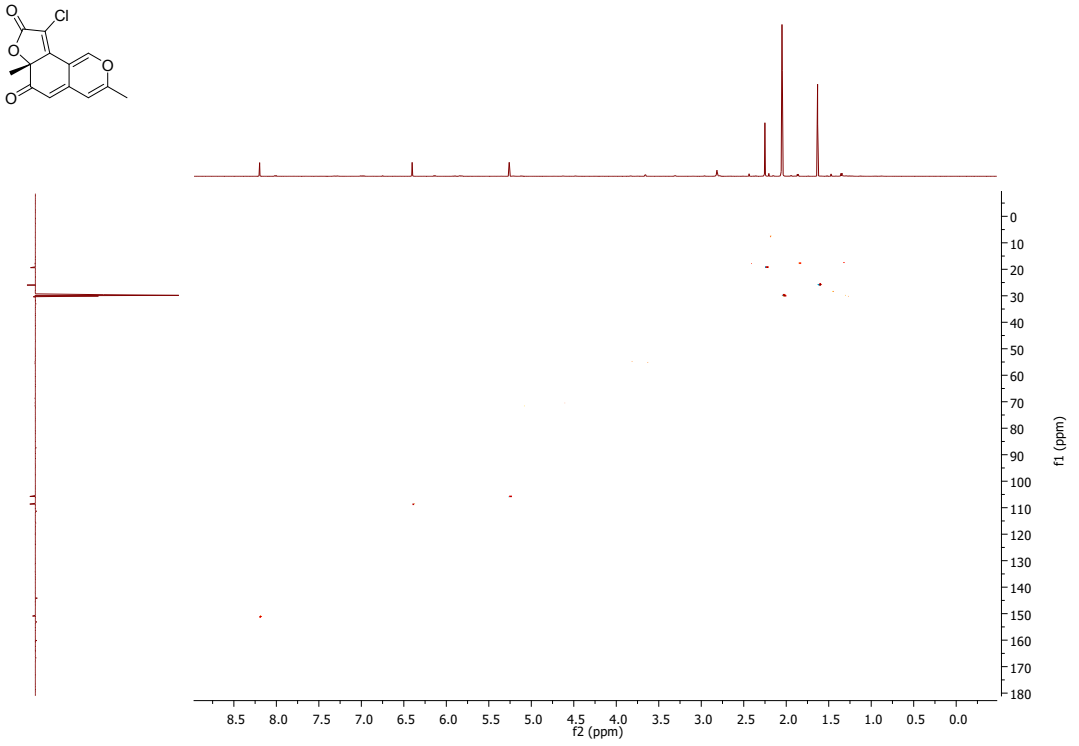


Figure S30. *HSQC NMR of compound* ***4*** *(600 MHz, acetone-d_6)*

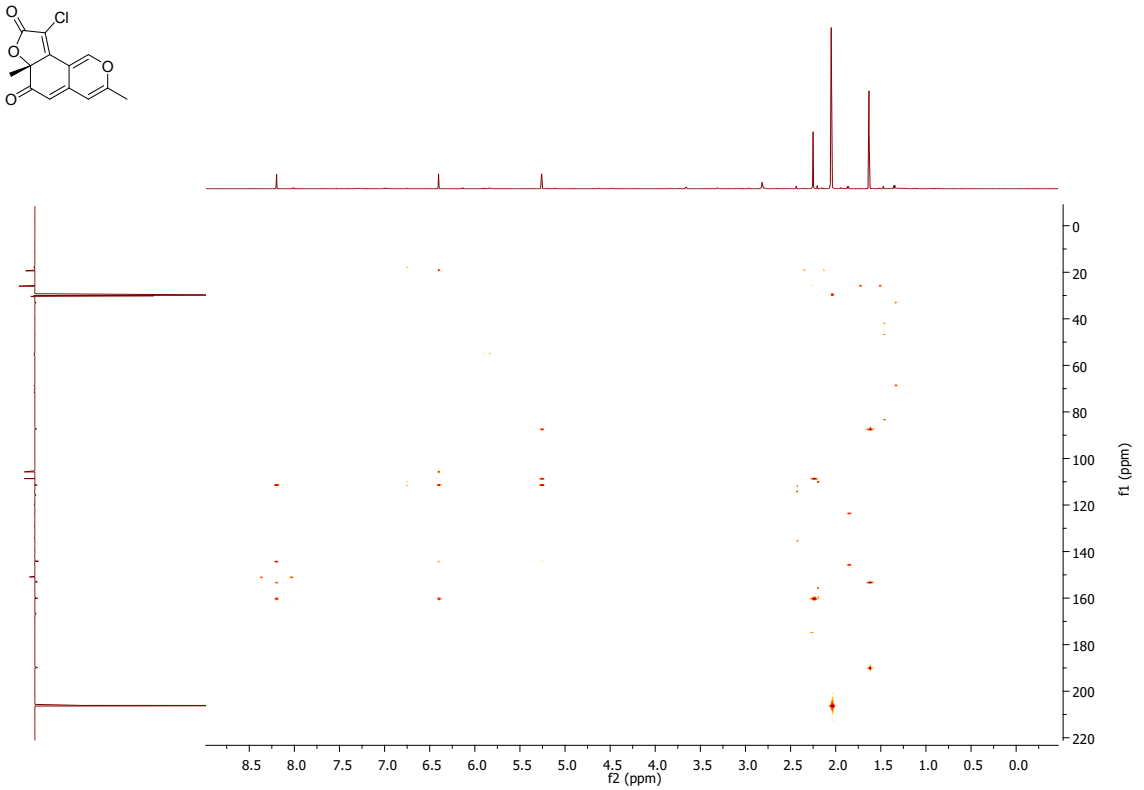


Figure S31. *HMBC NMR of compound* ***4*** *(600 MHz, acetone-d_6)*

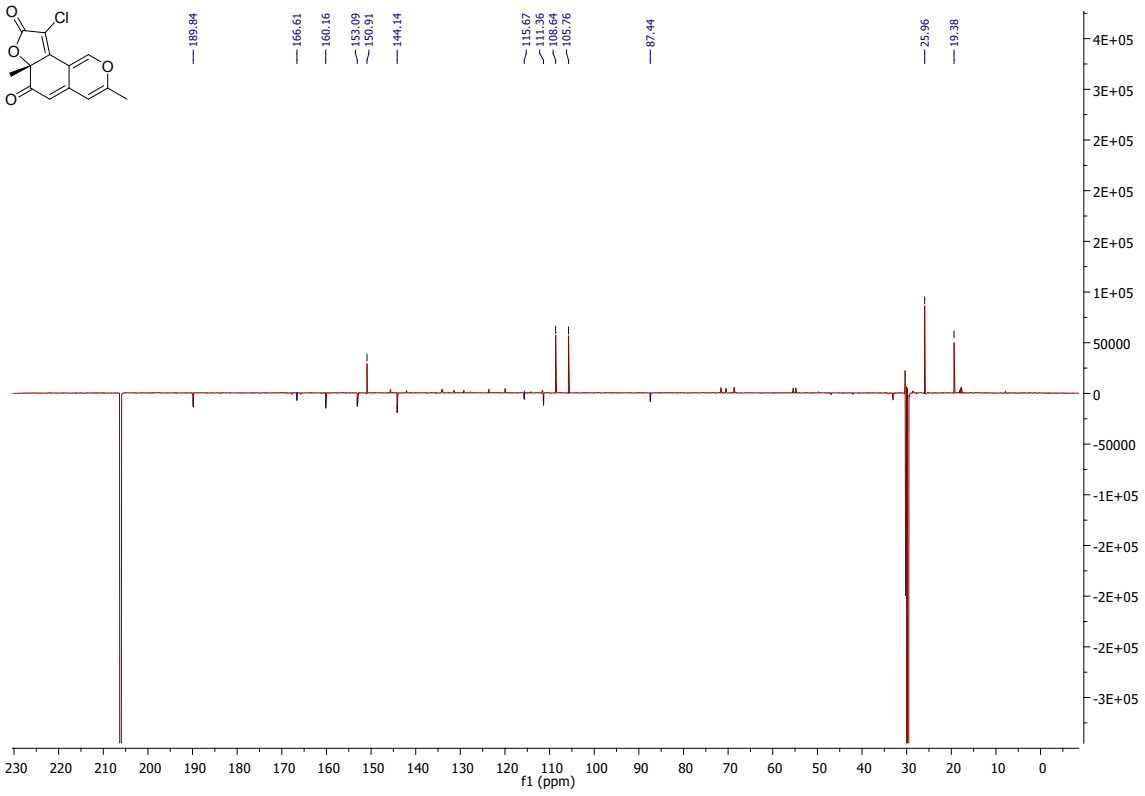


Figure S32. *DEPT Q NMR of compound* ***4*** *(600 MHz, acetone-d_6)*

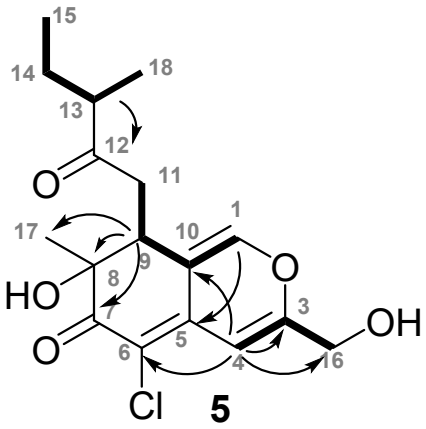


Figure S33. *COSY correlations (bold bond), plain arrows represent HMBC correlations (arrows) of compound* ***5****.*

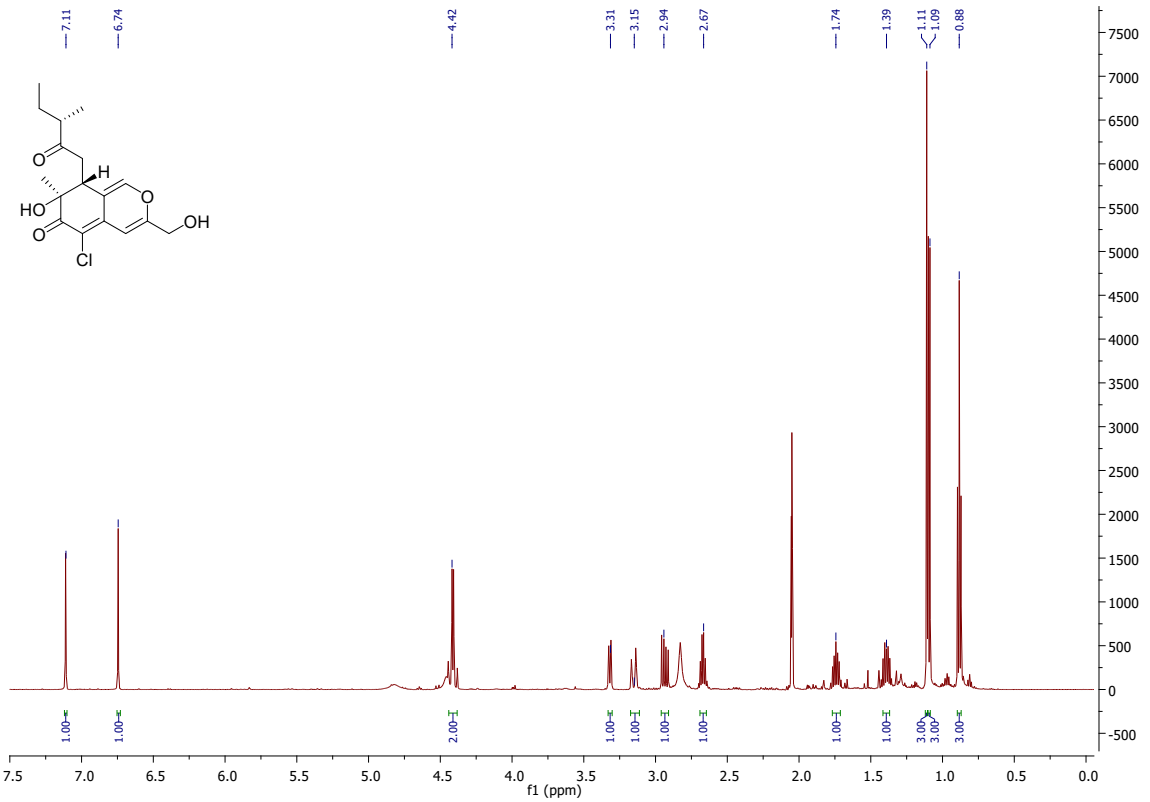


Figure S34. *^{1}H NMR of compound **5** (600 MHz, acetone-d_6)*

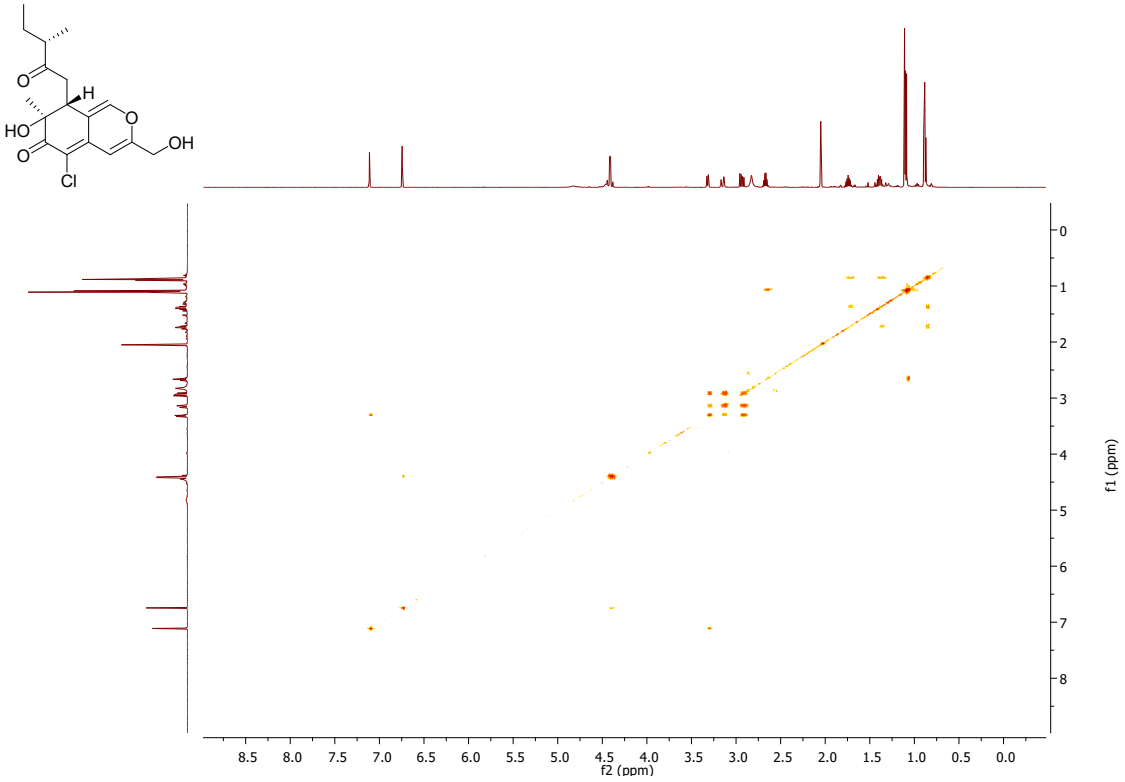


Figure S35. *COSY NMR of compound **5** (600 MHz, acetone-d_6)*

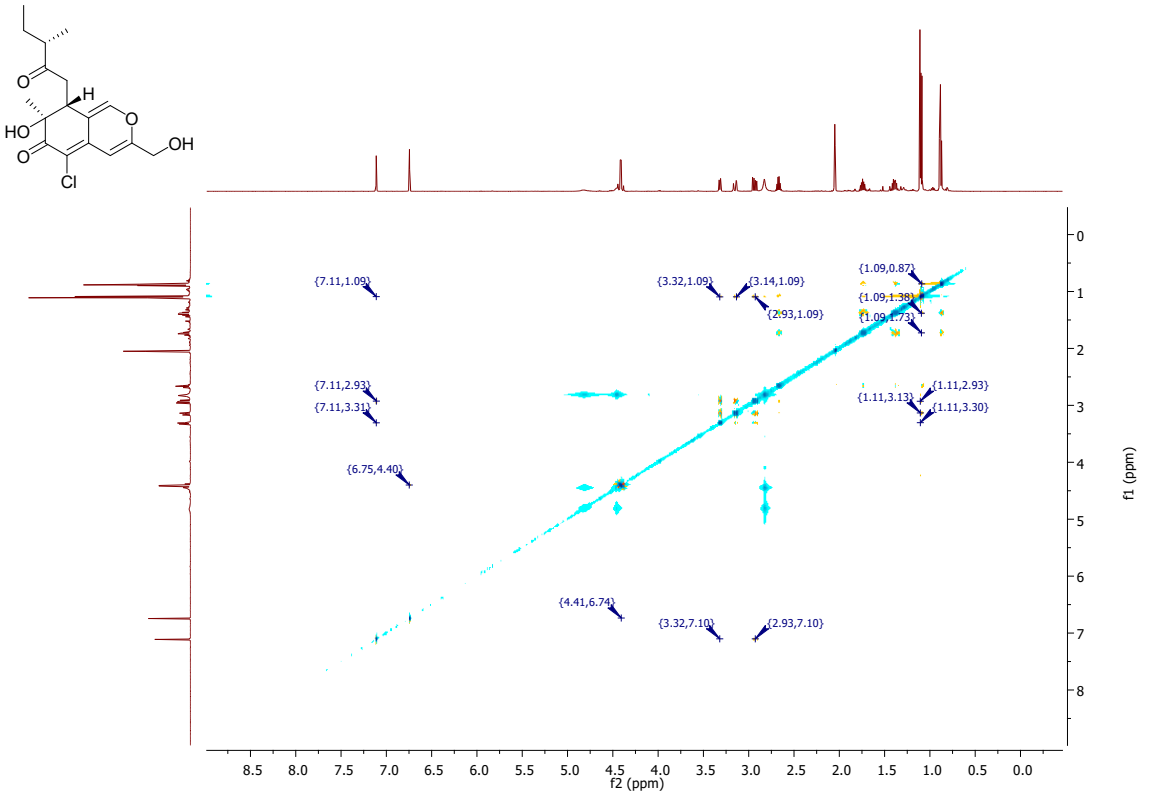


Figure S36. *NOESY NMR of compound* ***5*** *(600 MHz, acetone-d_6)*

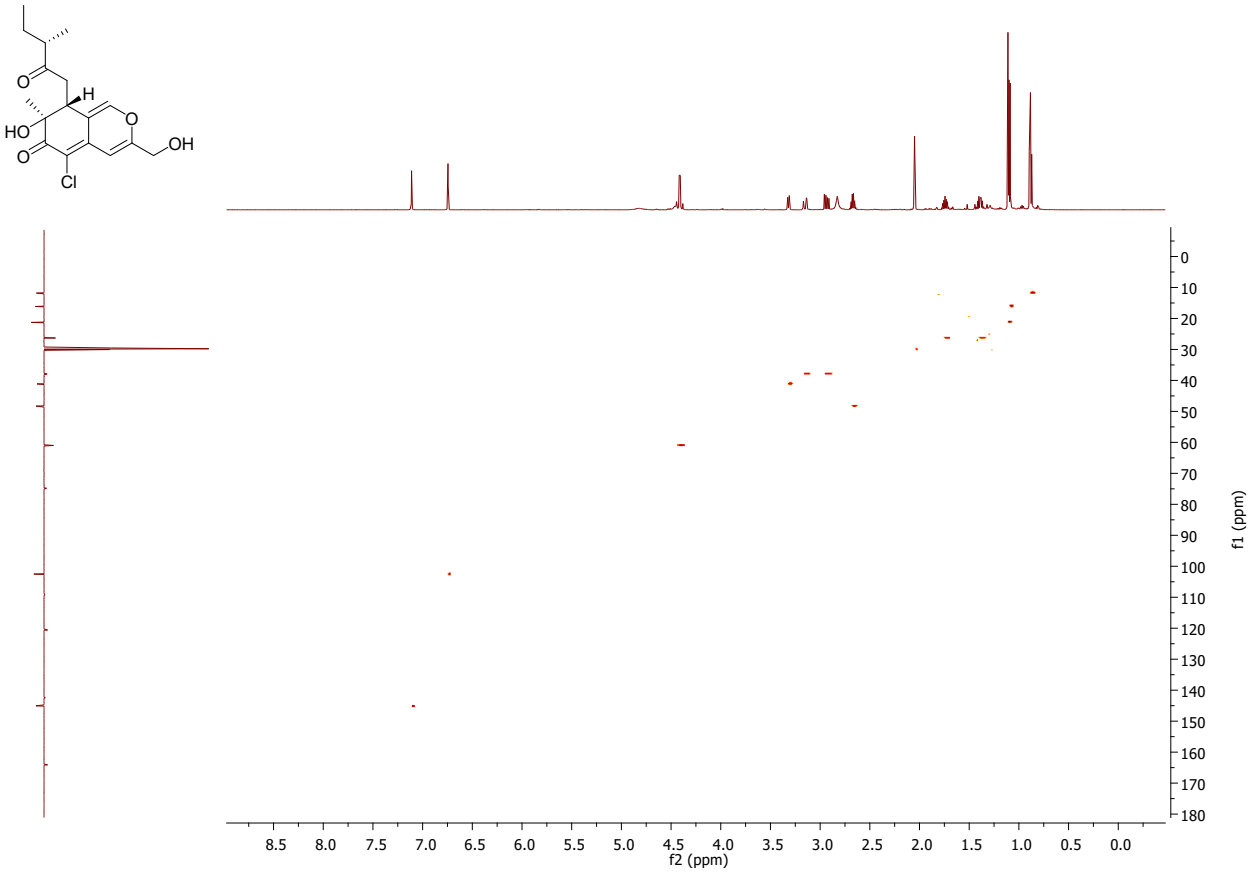


Figure S37. *HSQC NMR of compound* ***5*** *(600 MHz, acetone-d_6)*

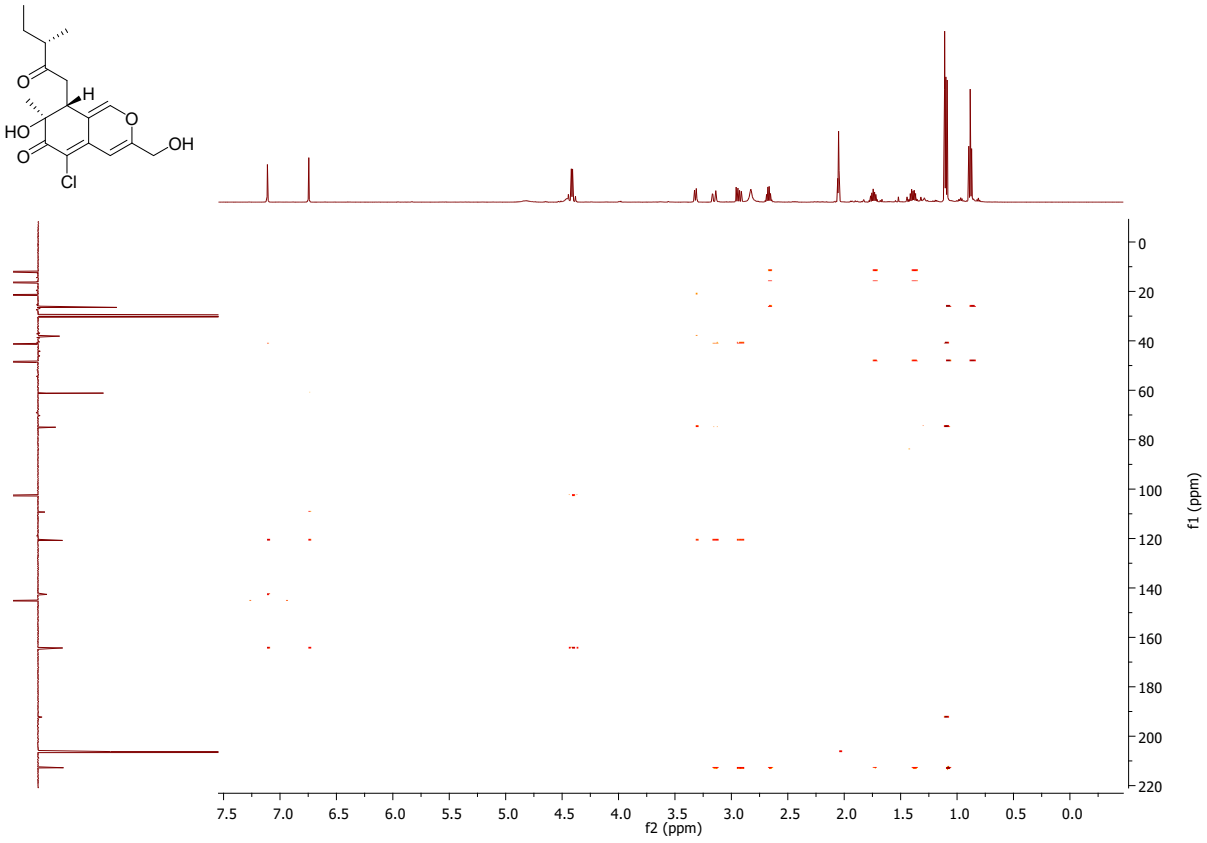


Figure S38. *HMBC NMR of compound* ***5*** *(600 MHz, acetone-d_6)*

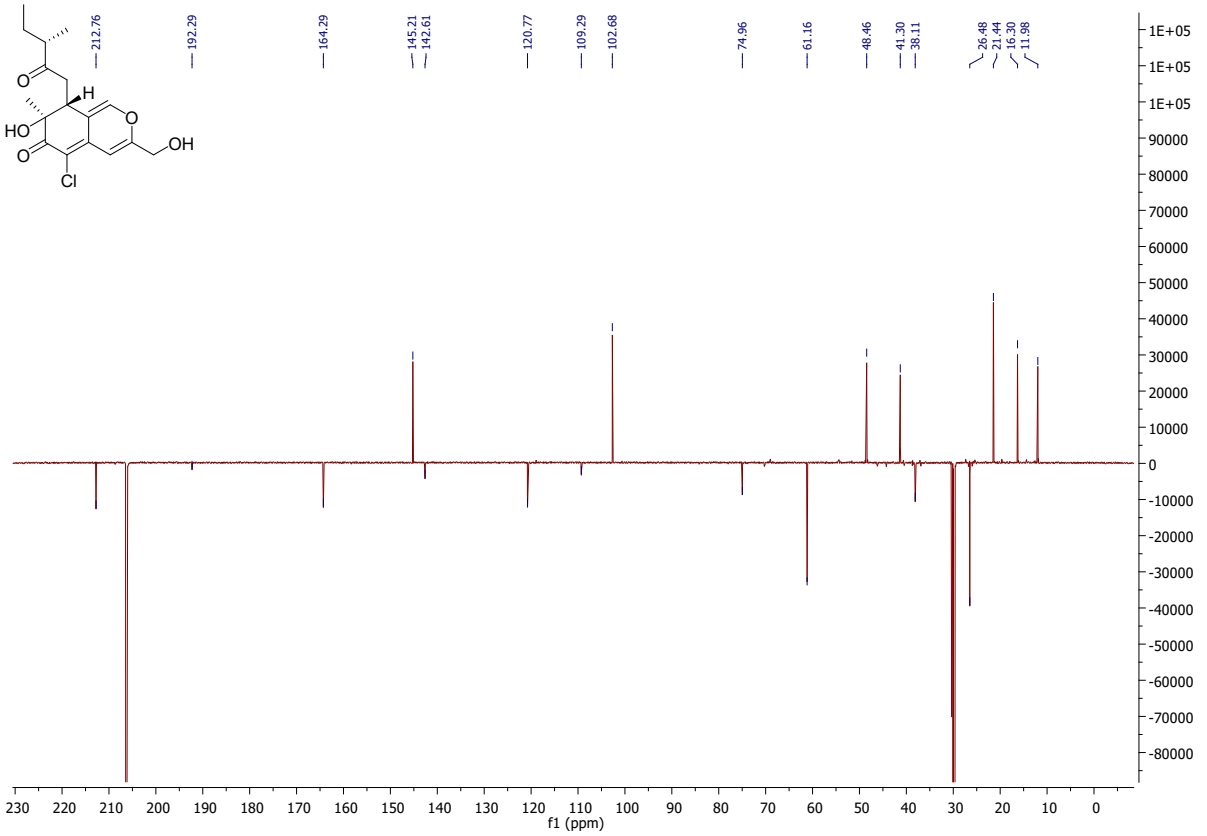


Figure S39. *DEPT Q NMR of compound* ***5*** *(600 MHz, acetone-d_6)*

15) X-ray crystallographic analysis of compound 4

Single-Crystal X-ray diffraction data for chlorobartaphilone A (4) were collected on a Rigaku mm007 HF rotating anode using CuKα radiation (λ = 1.54187 Å) delivered through Osmic CMF confocal optics, and a Rapid II curved Image Plate detector. The data were recorded at 293 K. Data collection, cell refinement and data reduction were performed with *Fs_process*[3] software implemented within the *CrystalClear 2.0*[4] suite. Absorption correction using equivalent reflections was performed with the *Abscor* option program[3]. The structure was readily solved by intrinsic phasing methods (*SHELXT*)[5] and all non-hydrogen atoms were refined anisotropically by full-matrix least-squares methods on F^2 using *SHELXL*[6]. The hydrogen atoms were first placed in idealized positions and refined as riding atoms isotropically with fixed individual displacement parameters. The refinement of the model was continued using the *Transferable aspherical atom model (TAAM)* approach within *Olex2*[7]. The aspherical atomic scattering factors computed by the DiSCaMB library[8] from the multipole model[9] and parametrized using the MATTS2021 data bank[10] were transferred into *NoSpherA2*[11] as a tsc file format. These form factors were utilized during the least-squares refinement against experimental intensities in an iterative cycle until convergence was achieved through *olex2.refine*[12]. The hydrogen atoms were therefore freely refined in an isotropic manner with only soft similar distance restraints for one methyl group. The absolute configuration of chlorobartaphilone A (C8 *R*) was determined unambiguously from the anomalous scattering by chloride at the copper wavelength using established methods[13-15]. A search of the Cambridge Structural Database (Version 5.45)[16] indicated four X-ray structures of azaphilone compounds incorporating an angular lactone moiety (CSD Refcodes URUNEB[17], TEYKAL[18], WUBNOZ[19] and XEXNUN[20]. Of these, the ChaetoviridinA [15] isolated from the crude extract of the fungal strain *Chaetomium elatum* No. 89–1–3–1 was the single example of *8R*-configurated azaphilone but unlike compound 4, a chloride atom is attached to the isochromene moiety and not to the lactone (see figure S40). URUNEB represents the S-form of ChaetoviridinA from the Endophyte *Chaetomium globosum* whereas the 8*S*- Aspersarin D (WUBNOZ) and -trichoflectin (XEXNUN) are non-chlorinated azaphilones (see figure S42).

X-ray crystallographic data in cif format are available at CCDC 2218370 and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

[1]eurjchem.com/index.php/eurjchem/article/downloadSuppFile/1306/896 [Internet]. [accessed on the 9th November 2022]. Available on: https://www.eurjchem.com/index.php/eurjchem/article/downloadSuppFile/1306/896

[2] J. Hubert, J.M. Nuzillard, J.H. Renault. Dereplication strategies in natural product research: How many tools and methodologies behind the same concept? *Phytochem Rev.* **2017**,16, 55-95.

[3] T. Higashi, T. *ABSCOR* and *FS-PROCESS*. 1995; Rigaku Corporation, Tokyo, Japan.

[4] Rigaku. *CrystalClear-SM Expert*. 2009; Rigaku Corporation, Tokyo, Japan.

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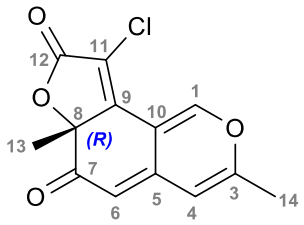
Chlorobartaphilone A (4). IR ν_{max}: 3443, 2106, 1647 cm^{-1}; UV (MeOH): λmax (logε) 348 (2.69), 260 (2.75); HRMS (ESI-TOF) *m/z* : 265.0262 $[M+H]^+$ Calcd for $[C_{13}H_9ClO_4 + H]^+$; Found 265.0263. $[\alpha]_D$ -10 (*c* 0.5, CH_3OH). Crystallographic data: $C_{13}H_9ClO_4$ (M= 264.67 g/mol): monoclinic, space group $P2_1$, a = 5.3067(4) Å, b= 9.1631(7) Å, c= 12.2106(9) Å, α=90°, β= 99.671(7)°, γ= 90°, V= 585.31(8) $Å^3$, Z=2, T= 293(2) K, μ(CuKα)= 2.949 mm^{-1}, F(000)= 272, crystal size = 0.29 x 0.08 x 0.03 mm^3, ρ_{calc}= 1.502 g/cm^3; out of the 6697 reflections measured (3.67° ≤ θ ≤ 68.2°), 2101 were unique (R_{int} = 0.0438, R_{sigma} =0.0581) and 2096 were used in all calculations. The final R_1 was 0.037 (I>2σ(I)), and $_wR_2$ was 0.1016 (all data). Flack parameter (using 542 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$) = 0.020(12)).

Table S4 *Crystal data and structure refinement for chlorobartaphilone A*

Identification code		*Chlorobartaphilone A*
2D-scheme		 **4**
Empirical formula		C_{13} H_9 Cl O_4
Formula weight		264.67
Temperature	(K)	293(2)
Diffractometer		MM007-HF rotating anode Spider
Wavelength	(Å)	1.54187
Crystal system, space group		Monoclinic, $P2_1$
Unit cell dimensions	a (Å) b c α (°) β γ	5.3067(4) 9.1631(7) 12.2106(9) 90 99.671(7) 90
Volume	($Å^3$)	585.31(8)

Z, Calculated density	 Mg/m^3	2, 1.502
Absorption coefficient	mm^{-1}	2.949
F(000)		272
Crystal size	mm	0.29 x 0.08 x 0.03
θ range for data collection	(°)	3.67 to 68.19
Limiting indices		-6 ≤ h ≤ 6, -11 ≤ k ≤ 10, -14 ≤ l ≤ 14
Reflections collected / unique R(int)		6697 / 2101 0.0438
Completeness to θ_{full}	(%)	99.6
Absorption correction		Semi-empirical from equivalents
Max. and min. transmission		1.000 and 0.675
Refinement method		transferable aspherical atom model (TAAM) Full-matrix least-squares on F^2
Data / restraints / parameters		2096 / 4 / 190
Goodness-of-fit on F^2		1.052
Final R indices [$I>2\sigma(I)$]	R1 wR2	0.037, 0.0709
R indices (all data)	 R1 wR2	 0.0759, 0.1016
Absolute structure[$] parameters	Flack [10] Parsons [11] *Hooft* [12] *P2(true)*	0.027(12) 0.020(12) -0.001(13) 1.000

	P3(true) *P3(rac-twin)* *P3(false)*	1.000 0.000 0.000
Largest diff. peak and hole	e.Å^{-3}	0.44 and -0.29
CCDC deposit number		2218370

$ Degree of confidence in configuration assignment from XRD:

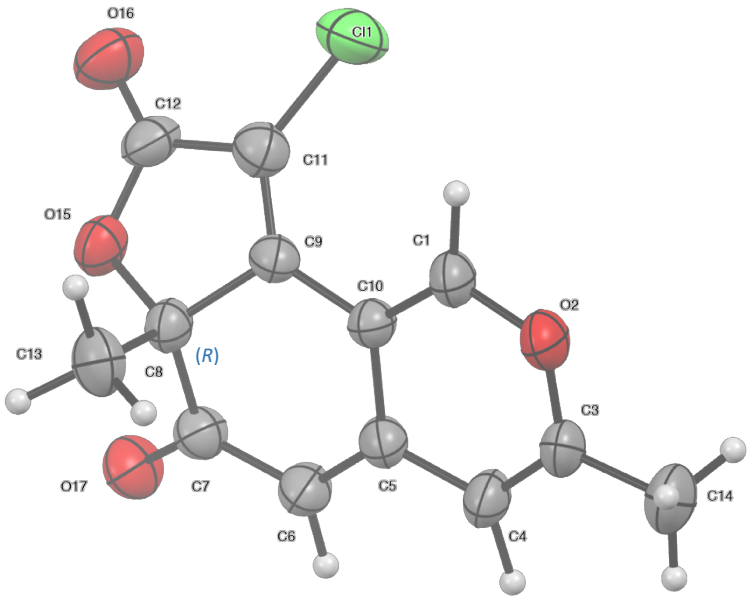


Figure S40. *Ortep view of chlorobartaphilone A. Ellipsoids are drawn at the 50% probability level and H atoms with radius of arbitrary size.*

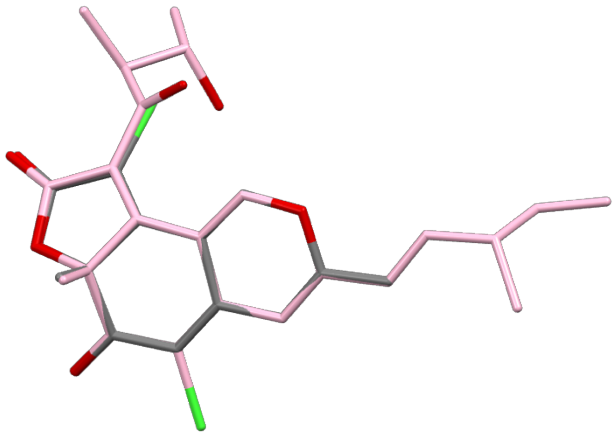


Figure S41. *Overlay over the isochromene moiety between 4 and CSD refcode* TEYKAL *(carbon atoms in pink).*

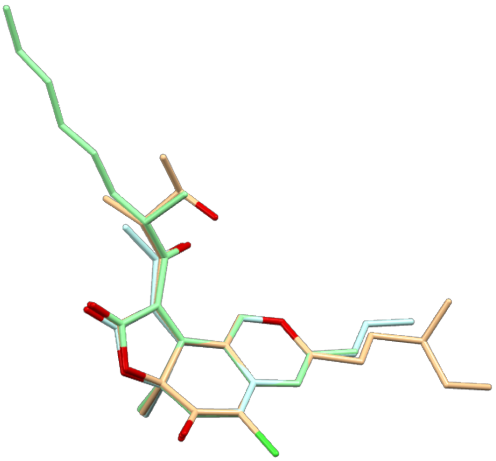


Figure S42. *Overlay between CSD Refcode URUNEB (carbon atoms in ochre), WUBNOZ (carbon atoms in cyan), and XEXNUN (carbon atoms in water green).*

16) Computational Methods.

Conformational analyses of the stereoisomers of compounds **2** and **3** were performed with Schrodinger MacroModel. The conformer generation was performed using the OPLS3 force field with chloroform as the selected solvent. The energy window was set to 5.0 kcal/mol. Due to the flexibility of the molecule, coupling constants were used constrain the torsion angles, NOESY correlations were used to constrain distances and the maximum atom deviation was increased to 1 Å to remove redundant conformers. The conformers generated were further optimized using DFT, at the B3LYP/6-31* level in Gaussian 16, and at the same time, the free energy of each conformer was calculated [1]. The isotropic shielding tensors were then calculated at the mPW1PW91/6-31+G** level. The shielding tensors were compared using DP4+ and were converted to ^{13}C NMR shifts using a linear regression from a test set of molecules. The rotational strength for each conformer was then calculated by using TDDFT in Gaussian 16 at the wB97XD/def2TZVP level for 50 excited states. A polarizable continuum solvation model was used for DFT calculations [2]. The ECD spectra of all conformers were Boltzmann weighted based on the free-energy, combined, and corrected with the experimental UV spectra in the freely available software SpecDis 1.7. [3].

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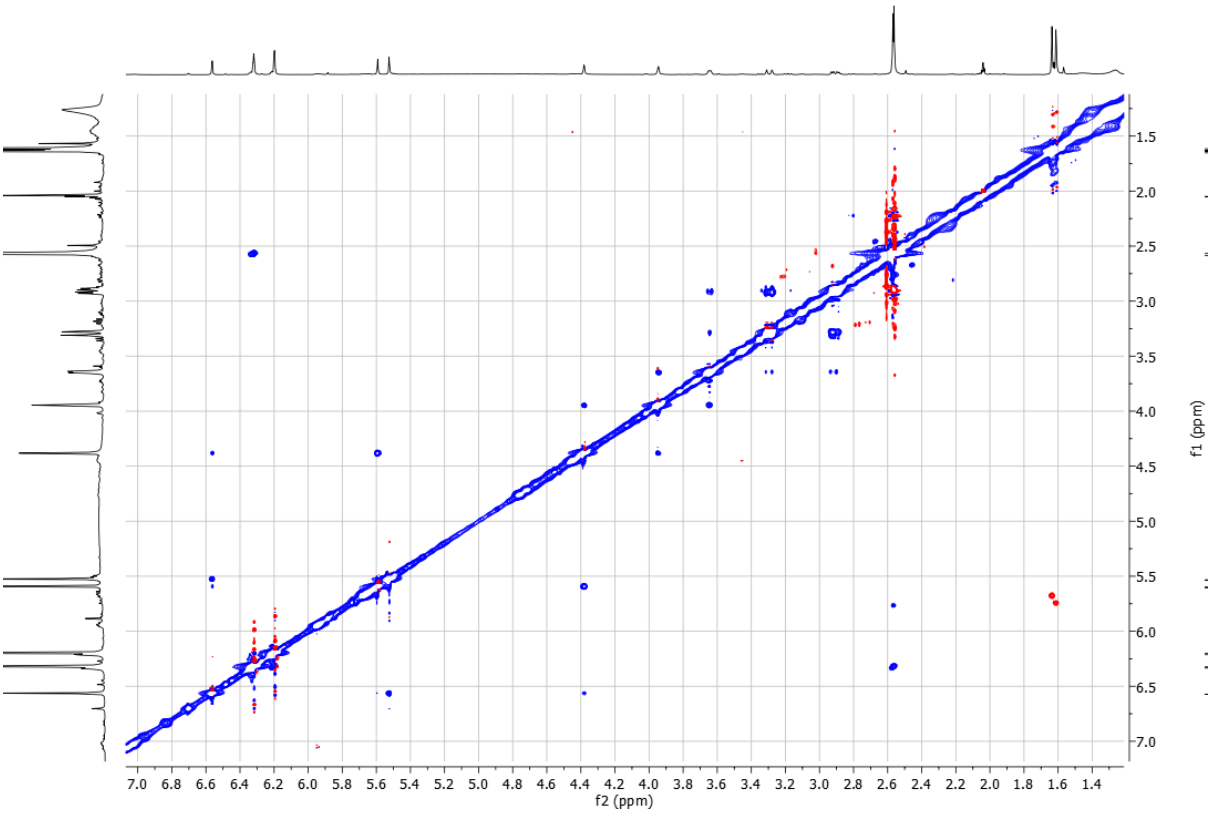


***Figure S43**. NOESY NMR spectra (600 MHz) of diazaphilonic acid (**2**) in acetone-d_6.*

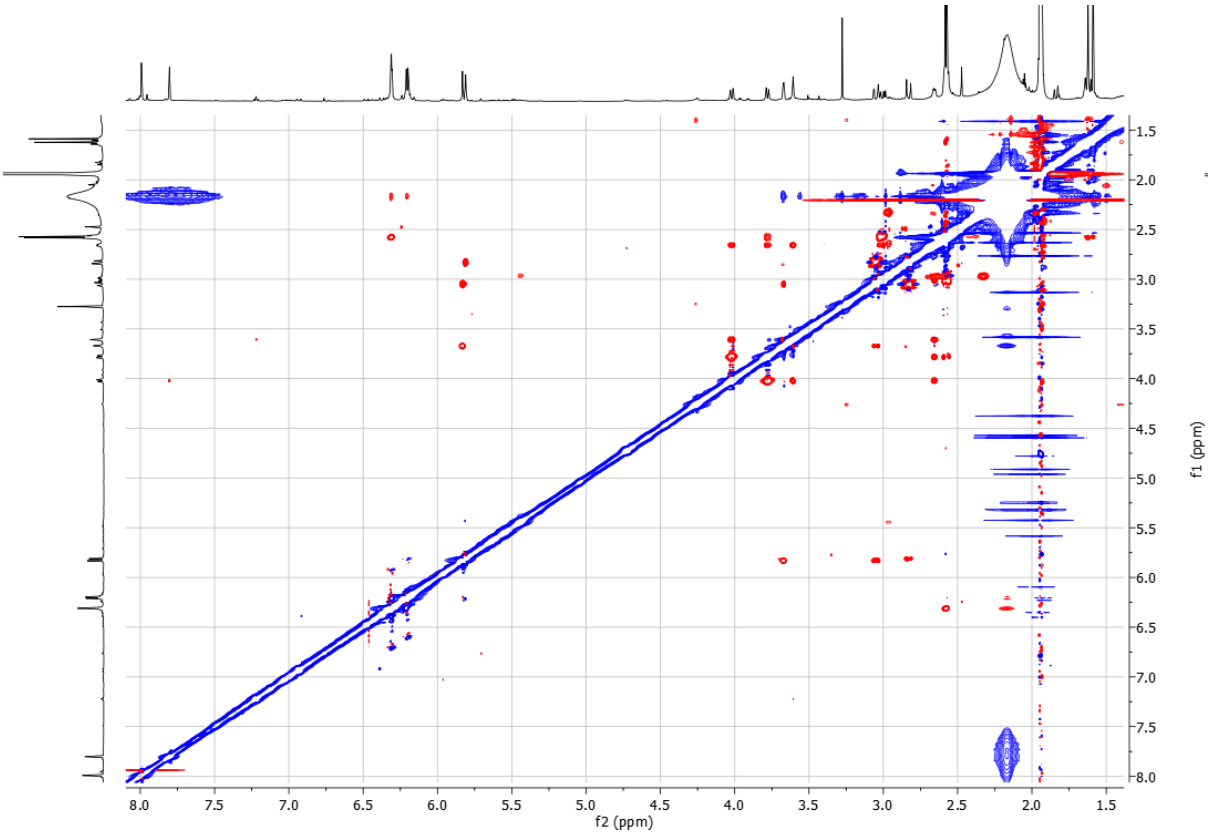


***Figure S44**. NOESY NMR spectra (600 MHz) of pavesiflonic acid (**3**) in acetonitrile-d_3.*

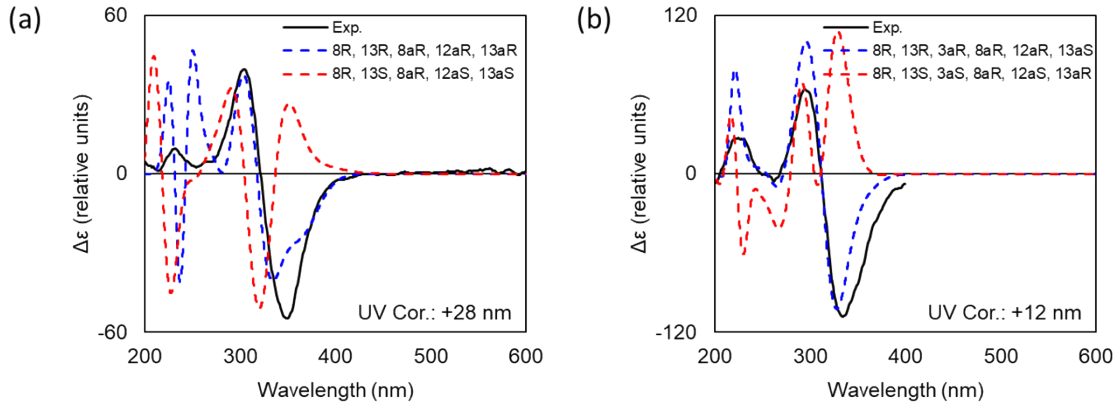


Figure S45. *Comparison of calculated and experimental ECD for the two (8R, 8aR) stereoisomers of (a) diazaphilonic acid (**2**) and (b) pavesiflonic acid (**3**).*

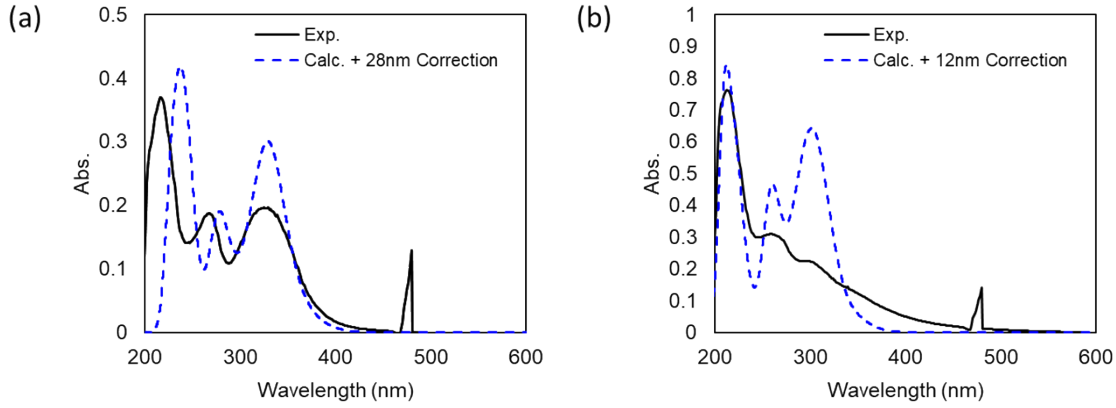


Figure S46. *Comparison of calculated plus correction and experimental UV for (a) diazaphilonic acid (**2**) and (b) pavesiflonic acid (**3**).*

Table S5. *Experimental and calculated ^{13}C NMR shifts for Diazaphilonic acid (Iso1: 8S,13S, 8aS, 12aS, 13aS, Iso2: 8S,13R, 8aS, 12aR, 13aR) and Pavesiflonic acid (Iso1: 8S,13R, 3aR, 8aS, 12aR, 13aS, Iso2: 8S,13S, 3aS, 8aS, 12aS, 13aR). Also displayed is the difference in calculated shift between the two isomers that indicates no large enough differences for a configurational assignment.*

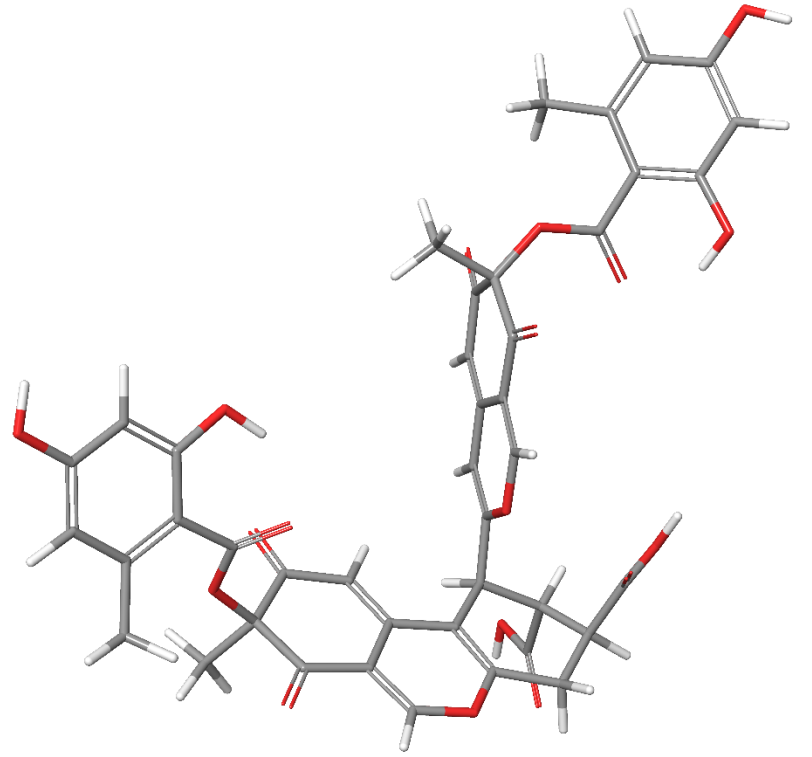
Diazaphilonic acid (2) δ_C				
Pos.	**Exp.**	**Iso 1**	**Iso 2**	**$\Delta_{iso1-iso2}$**
1	154.1	156.27	156.00	0.27
3	159.0	161.13	162.76	-1.63
4	111.6	113.95	112.24	1.71
5	142.2	143.94	143.65	0.29
6	105.3	105.08	104.66	0.42
7	192.1	188.47	189.06	-0.59
8	86.2	83.95	84.32	-0.37
9	193.0	192.92	193.07	-0.15

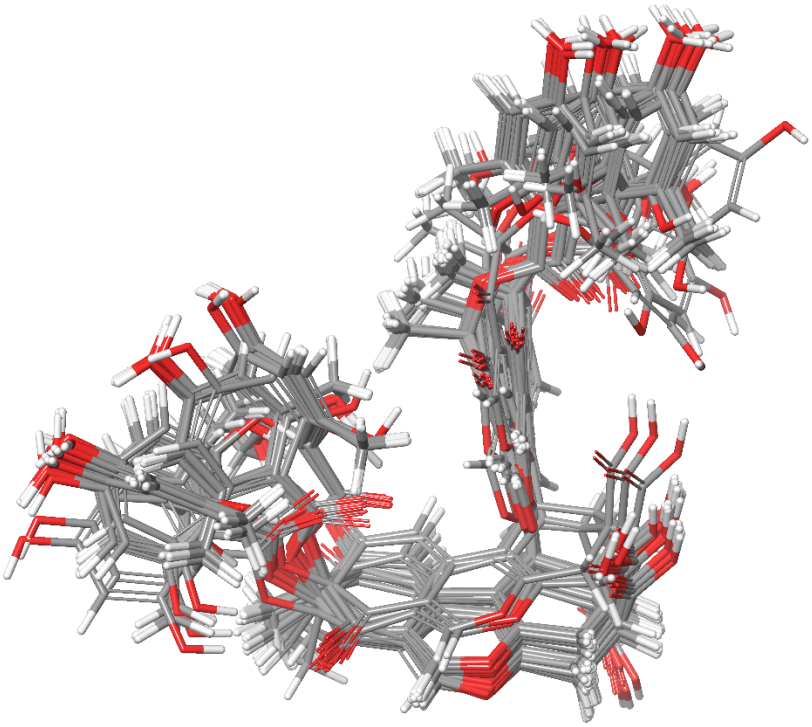
Pavesiflonic acid (3) δ_C				
Pos.	**Exp.**	**Iso 1**	**Iso 2**	**$\Delta_{iso1-iso2}$**
1	154.4	155.46	154.82	0.64
3	160.5	162.86	163.03	-0.17
4	114.5	116.21	116.06	0.15
5	143.9	143.73	143.8	-0.07
6	105.1	105.52	105.91	-0.39
7	192.6	189.41	189.03	0.38
8	86.5	85.38	84.71	0.67
9	193.9	194.42	194.44	-0.02

10	116.2	117.13	116.80	0.33
11	22.7	21.90	22.34	-0.44
12	26.3	24.77	25.77	-1.00
13	38.0	37.34	37.49	-0.15
14	173.4	174.89	175.14	-0.25
1a	155.5	155.66	156.05	-0.39
3a	158.6	161.76	161.76	0.00
4a	111.8	114.52	114.67	-0.15
5a	143.2	144.82	144.97	-0.15
6a	108.4	107.53	107.39	0.14
7a	192.4	188.70	188.85	-0.15
8a	86.5	84.95	84.35	0.60
9a	193.0	193.14	192.75	0.39
10a	115.8	117.58	117.00	0.58
11a	22.6	21.93	22.26	-0.33
12a	39.4	40.77	40.96	-0.19
13a	43.5	46.35	45.99	0.36
14a	172.7	174.49	174.34	0.15
1'	104.7	104.71	104.78	-0.07
2'	166.1	165.60	165.61	-0.01
3'	101.6	99.89	99.69	0.20
4'	163.9	160.98	160.42	0.56
5'	112.6	110.04	109.85	0.19
6'	144.7	147.52	147.71	-0.19
7'	24.0	24.58	24.37	0.21
8'	170.3	169.84	169.93	-0.09
1'a	104.7	104.81	104.68	0.13
2'a	166.1	165.16	165.41	-0.25
3'a	101.6	100.02	99.72	0.30
4'a	163.9	160.83	160.55	0.28
5'a	112.6	109.85	109.91	-0.06
6'a	144.7	147.22	147.73	-0.51
7'a	24.0	24.55	24.57	-0.02
8'a	170.3	169.85	169.83	0.02
MAE		**1.57**	**1.55**	**0.34**
DP4+		**50.49%**	**49.51%**	

10	116.2	116.74	117.07	-0.33
11	22.9	22.02	21.97	0.05
12	30.8	31.37	30.91	0.46
13	28.8	29.34	29.2	0.14
14	70.2	68.96	69.06	-0.10
1a	157.3	158.25	158.02	0.23
3a	103.5	104.16	104.16	0.00
4a	36.6	36.85	36.52	0.33
5a	146.7	149.66	149.51	0.15
6a	119.4	118.1	118.78	-0.68
7a	193.8	192.03	192.16	-0.13
8a	86.7	86.18	86.19	-0.01
9a	192.6	191.24	191.88	-0.64
10a	112.7	112.99	113.98	-0.99
11a	22.9	22.05	22.24	-0.19
12a	37.1	38.67	38.27	0.40
13a	39.2	39.29	39.75	-0.46
14a	172.7	179.93	179.9	0.03
1'	105.1	105.2	105.2	0.00
2'	166	163.95	163.69	0.26
3'	101.7	100.86	100.89	-0.03
4'	163.6	159.5	159.47	0.03
5'	112.7	110.72	110.69	0.03
6'	145.1	146.76	146.66	0.10
7'	24	24.48	24.66	-0.18
8'	170.6	172.15	172.05	0.10
1'a	104.9	105.25	104.95	0.30
2'a	166	164.66	164.45	0.21
3'a	101.7	100.76	101.25	-0.49
4'a	163.6	159.18	159.52	-0.34
5'a	112.7	110.62	110.72	-0.10
6'a	145.2	146.86	146.81	0.05
7'a	24	24.94	24.89	0.05
8'a	170.5	172.22	171.61	0.61
MAE		**1.57**	**1.55**	**0.34**
DP4+		**57.52%**	**42.48%**	

Data S1. Lowest energy conformer 3D structure, all overlaid 3D structures, cartesian coordinates, number of imaginary frequencies, and energy for (8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid conformers.





(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 1

Atom	X	Y	Z	Atom	X	Y	Z
C	1.946572	7.238342	-1.77382	C	3.0126045	-0.778233	-2.2563341
C	0.608001	7.48202	-1.66807	C	3.5684412	-0.0958068	-1.1622126
C	-0.292	6.58461	-0.95507	C	3.2196361	1.2170668	-0.8819043
C	0.211955	5.34674	-0.30324	C	-0.9032281	13.487671	5.4415501
C	1.742656	5.20209	-0.20579	C	-0.5537084	13.440657	6.7826778
C	2.569996	6.055706	-1.20889	C	-0.7612145	12.281555	7.5482384
C	-0.05306	8.621815	-2.27466	C	-1.3027989	11.140746	6.9734106
C	-1.38414	8.81045	-2.17067	C	-1.652515	11.151317	5.6195608
O	-2.18214	7.943639	-1.46202	C	3.8973556	1.87806	0.2979091
C	-1.61384	6.857265	-0.89131	O	0.9002402	1.7383628	-3.7316963
C	-2.17635	9.922211	-2.82516	O	3.4093814	-2.0656049	-2.4422958
C	-3.23191	10.50295	-1.8972	C	-0.6118399	14.770338	4.6944314
C	-4.53845	10.2099	-2.10129	O	-0.3946273	12.337241	8.8563337
C	-5.13006	9.375156	-3.19432	O	-2.1509491	10.006003	5.1292103
C	-4.08675	8.66566	-4.07002	H	2.5929415	7.8993116	-2.3434311
C	-2.7826	9.480834	-4.19605	H	0.5349511	9.3383041	-2.8397016
C	-2.83216	11.36886	-0.78719	H	-2.3360019	6.231173	-0.3825154
C	-3.93536	11.85685	0.028481	H	-1.4504696	10.708476	-3.0508854
C	-5.20543	11.50212	-0.26228	H	-5.7484906	10.031406	-3.8176658
O	-5.53703	10.70831	-1.29898	H	-5.7973714	8.6313152	-2.7468671
C	-1.5377	11.70209	-0.49903	H	-4.5014519	8.5892194	-5.0830917
C	-1.16836	12.53908	0.628918	H	-2.0262002	8.8780163	-4.7099367
C	-2.29091	13.31412	1.368373	H	-6.0644438	11.823178	0.3134649
C	-3.70857	12.73703	1.20549	H	-0.7027067	11.300152	-1.0600464
O	-1.9604	13.42256	2.761798	H	-2.5528383	14.777662	-0.2240476
C	-1.92439	12.25729	3.439109	H	-3.0491432	15.338298	1.3932145
C	-1.48459	12.33226	4.829901	H	-1.3118789	15.196337	0.9800397
C	-2.30384	14.75834	0.842121	H	1.9169215	6.6434469	1.4186228
O	2.112051	3.819969	-0.34391	H	1.6425998	4.9618105	1.9404743
C	1.798318	3.250137	-1.52279	H	3.2454451	5.4650159	1.3187411
C	2.276669	1.884316	-1.72555	H	-2.156951	12.202991	-5.8034547
C	2.164834	5.595915	1.21881	H	-2.7651678	5.7287612	-3.969255
O	-0.53038	4.526632	0.205495	H	1.6872986	-0.6438845	-3.9696198
O	3.732362	5.737921	-1.42582	H	4.287662	-0.6195281	-0.5418432

O	-4.60942	13.06986	1.95448	H	-0.1040521	14.301323	7.2658592
O	-0.0067	12.72017	0.971914	H	-1.4560895	10.225799	7.5387039
C	-3.02719	10.69169	-5.09822	H	4.6782196	1.2207657	0.6908993
C	-3.87938	7.214254	-3.64041	H	4.3498639	2.8331854	0.0165144
O	-4.05142	10.92693	-5.69984	H	3.1877072	2.0898749	1.1036729
O	-1.92911	11.47559	-5.19349	H	0.7836346	2.6843584	-3.459605
O	-2.79934	6.664755	-4.24529	H	2.9649134	-2.4244195	-3.226826
O	-4.61394	6.586682	-2.91338	H	-0.0488899	15.452551	5.3377502
O	1.116984	3.88106	-2.34721	H	-0.0301742	14.582645	3.7873742
O	-2.27799	11.21132	2.872545	H	-1.5323029	15.272691	4.3813292
C	1.755019	1.183112	-2.85748	H	-0.5801087	11.481468	9.2748175
C	2.114774	-0.14509	-3.10434	H	-2.3102884	10.146538	4.1614234

NImag	0
Σ Electronic and thermal Free Energy	-1865701.501
mol Fraction	0.155673243

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 2

Atom	X	Y	Z	Atom	X	Y	Z
C	1.878123	6.905756	-1.68283	C	2.206257	-1.18296	-1.99861
C	0.5663	7.273775	-1.60523	C	2.805802	-0.53273	-0.90797
C	-0.42401	6.477508	-0.89183	C	2.575412	0.812034	-0.65815
C	-0.04707	5.211726	-0.20853	C	-0.4956	13.53449	5.364654
C	1.461961	4.928661	-0.08143	C	-0.17319	13.4823	6.712365
C	2.380487	5.682218	-1.08534	C	-0.49893	12.36273	7.495384
C	0.023163	8.45729	-2.24427	C	-1.13438	11.26535	6.932233
C	-1.28625	8.769803	-2.16726	C	-1.46016	11.28102	5.572476
O	-2.17212	7.994534	-1.45695	C	3.293031	1.431468	0.520625
C	-1.71582	6.872019	-0.85641	O	0.358431	1.487207	-3.55673
C	-1.9618	9.936537	-2.85599	O	2.485286	-2.50486	-2.15375
C	-2.97368	10.63053	-1.95763	C	-0.07522	14.76973	4.599293
C	-4.29832	10.45508	-2.17924	O	-0.14951	12.41056	8.80848
C	-4.94722	9.656552	-3.2668	O	-2.0544	10.17687	5.094626
C	-3.96024	8.836687	-4.11087	H	2.591785	7.49288	-2.25301
C	-2.58451	9.525621	-4.22895	H	0.683786	9.10513	-2.81195
C	-2.51319	11.478	-0.85695	H	-2.50076	6.325407	-0.34899
C	-3.57931	12.08182	-0.07001	H	-1.16284	10.64789	-3.08336
C	-4.87198	11.83989	-0.37649	H	-5.49262	10.35427	-3.91287
O	-5.25912	11.0594	-1.40401	H	-5.68727	8.986348	-2.81738
C	-1.19819	11.69621	-0.55225	H	-4.36419	8.778607	-5.12948
C	-0.77093	12.51803	0.566358	H	-1.87906	8.845571	-4.71831
C	-1.82856	13.4079	1.271465	H	-5.70663	12.25022	0.177997
C	-3.29076	12.96075	1.094348	H	-0.39517	11.20787	-1.09094
O	-1.51154	13.51333	2.66826	H	-1.92881	14.85714	-0.35211
C	-1.59415	12.36351	3.367542	H	-2.39666	15.49341	1.245518
C	-1.17142	12.42549	4.764256	H	-0.67365	15.18374	0.865681
C	-1.69955	14.83632	0.71845	H	1.742902	6.380007	1.51897
O	1.704155	3.515906	-0.1875	H	1.306094	4.741547	2.066805
C	1.357824	2.953937	-1.36102	H	2.958241	5.082469	1.46428
C	1.711198	1.546125	-1.53016	H	-1.68482	12.14612	-5.87482
C	1.896075	5.310313	1.342896	H	-2.91749	5.793157	-3.93296
O	-0.87003	4.473832	0.302059	H	0.925654	-0.9617	-3.73668
O	3.511828	5.254486	-1.27575	H	3.463962	-1.10783	-0.2657
O	-4.16872	13.39015	1.821042	H	0.346305	14.30742	7.187447
O	0.396916	12.59814	0.926363	H	-1.38042	10.37986	7.511505

C	-2.70191	10.7356	-5.15743	H	4.003929	0.713243	0.938964
C	-3.89473	7.381192	-3.65112	H	3.835842	2.3352	0.229374
O	-3.69033	11.05194	-5.78134	H	2.593669	1.723573	1.310111
O	-1.53482	11.4132	-5.24761	H	0.325564	2.4452	-3.30434
O	-2.86061	6.722646	-4.22666	H	2.021738	-2.83695	-2.93901
O	-4.69558	6.838508	-2.92579	H	0.537958	15.41001	5.239794
O	0.75073	3.628268	-2.20876	H	0.501028	14.51123	3.706303
O	-2.03391	11.34342	2.814258	H	-0.94028	15.34825	4.260713
C	1.144614	0.873316	-2.65771	H	-0.41981	11.58401	9.239328
C	1.383932	-0.48705	-2.87358	H	-2.18471	10.3121	4.121751
NImag						0	
Σ Electronic and thermal Free Energy						-1865701.5	
mol Fraction						0.155343476	

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 3

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8650218	7.0938912	-1.4904758	C	2.5288078	-0.9667249	-1.9605241
C	0.5374408	7.4087054	-1.4629628	C	3.054547	-0.3183517	-0.8313787
C	-0.4501651	6.5585534	-0.8106032	C	2.7601478	1.0104431	-0.5639557
C	-0.0528639	5.2932763	-0.1379855	C	-1.0709795	13.465144	5.5819968
C	1.4593737	5.0663113	0.0493296	C	-0.8049169	13.395376	6.9411684
C	2.3895455	5.8776035	-0.8972174	C	-1.1194333	12.246856	7.6859078
C	-0.024408	8.5843251	-2.1003993	C	-1.6861872	11.138585	7.0729514
C	-1.3473469	8.8438034	-2.0745383	C	-1.9536417	11.172018	5.7008489
O	-2.2313909	8.0187533	-1.4202396	C	3.4012325	1.6307186	0.6577048
C	-1.7570067	6.9015599	-0.8237998	O	0.6444595	1.6638621	-3.5421191
C	-2.0385618	9.9986332	-2.7677604	O	2.8667569	-2.2729195	-2.1307749
C	-3.1149257	10.63236	-1.900353	C	-0.6672647	14.73244	4.8613714
C	-4.4207939	10.410515	-2.1833323	O	-0.8288962	12.278813	9.0137521
C	-4.9900467	9.6120812	-3.3146758	O	-2.4826345	10.056665	5.1747436
C	-3.9358485	8.8504874	-4.1316475	H	2.5786268	7.7210988	-2.0163172
C	-2.5848711	9.5948545	-4.1749799	H	0.6337163	9.2700504	-2.6248426
C	-2.7362513	11.472131	-0.76319	H	-2.540669	6.3134628	-0.3629281
C	-3.8583979	12.016186	-0.011326	H	-1.259501	10.745419	-2.9450609
C	-5.1260464	11.731065	-0.3790527	H	-5.534549	10.302466	-3.9693279
O	-5.4372957	10.959359	-1.4385055	H	-5.7214215	8.9036091	-2.9122093
C	-1.4452891	11.734424	-0.3967149	H	-4.2931117	8.7997375	-5.1679548
C	-1.0995391	12.546861	0.7563816	H	-1.8324739	8.9540004	-4.6469957
C	-2.2210863	13.378865	1.4327984	H	-5.999423	12.096039	0.1467496
C	-3.6553616	12.879328	1.1825222	H	-0.6010637	11.289907	-0.9097427
O	-1.9688165	13.46512	2.8440091	H	-2.3090847	14.859212	-0.163195
C	-2.0356341	12.29755	3.5149934	H	-2.8701271	15.440782	1.4252585
C	-1.6760068	12.344559	4.9298512	H	-1.1214188	15.206915	1.1149513
C	-2.1254008	14.823291	0.915721	H	1.6130102	6.4908372	1.6906027
O	1.7620525	3.6668311	-0.0755785	H	1.2186491	4.8246183	2.1842367
C	1.4892871	3.1185051	-1.2746971	H	2.8803288	5.2431355	1.662196
C	1.9055394	1.7297242	-1.457485	H	-1.7200828	12.28461	-5.7249866
C	1.8161461	5.4321821	1.4990493	H	-2.781328	5.8465404	-3.9717247
O	-0.8669921	4.5125563	0.3204106	H	1.3162167	-0.7564147	-3.7480519
O	3.5441587	5.4985872	-1.0467329	H	3.7069738	-0.8816712	-0.1730222
O	-4.5801376	13.257917	1.8787599	H	-0.3393351	14.22913	7.4554533
O	0.0476266	12.664118	1.1688602	H	-1.9216429	10.231535	7.6225006

C	-2.7103426	10.820067	-5.0821619	H	4.1217873	0.9316104	1.0916124
C	-3.8322478	7.3886123	-3.699947	H	3.9193495	2.5613651	0.4093816
O	-3.6830779	11.11222	-5.7415153	H	2.6575711	1.8773254	1.4218254
O	-1.5680708	11.543926	-5.1074384	H	0.5625106	2.6138772	-3.271437
O	-2.7489335	6.7839381	-4.2431748	H	2.4509529	-2.6050484	-2.9423071
O	-4.6413326	6.7989618	-3.0219477	H	-0.1077805	15.38139	5.5410981
O	0.8928186	3.7876352	-2.1340033	H	-0.0435892	14.516343	3.9892168
O	-2.4103942	11.273857	2.9219696	H	-1.5391861	15.284635	4.497399
C	1.4152171	1.0609366	-2.6225314	H	-1.0845427	11.433024	9.4152076
C	1.7176959	-0.2838512	-2.8560058	H	-2.5762898	10.208488	4.2001041
NImag						0	
Σ Electronic and thermal Free Energy						-1865701.501	
mol Fraction						0.155508272	

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 4

Atom	X	Y	Z	Atom	X	Y	Z
C	1.7509996	6.9048093	-1.7042693	C	2.9641264	-0.8140829	-2.2843176
C	0.4395451	7.2780669	-1.5801883	C	1.6201532	-0.5914322	-2.6202021
C	-0.5323421	6.4784794	-0.8487235	C	1.0372958	0.6483843	-2.3980541
C	-0.1419399	5.2096581	-0.1731474	C	-0.9192201	13.501227	5.4755451
C	1.3654592	4.8989255	-0.136514	C	-0.6249298	13.445716	6.8294561
C	2.2334836	5.6550931	-1.1721328	C	-0.9406824	12.312371	7.5967353
C	-0.1138332	8.4643771	-2.1994519	C	-1.537483	11.204839	7.0115861
C	-1.4243899	8.7716861	-2.1004468	C	-1.8340228	11.223789	5.6452369
O	-2.2913027	7.9952181	-1.3742452	C	-0.4132388	0.8512687	-2.773919
C	-1.8229825	6.8740471	-0.7827331	O	4.0226192	2.3882319	-1.0150668
C	-2.1183701	9.9261864	-2.7921367	O	3.465044	-2.0566487	-2.5344007
C	-3.166517	10.584414	-1.9098708	C	-0.5120942	14.752309	4.7289885
C	-4.4808641	10.367401	-2.1549409	O	-0.6208773	12.357958	8.9172761
C	-5.0842405	9.547244	-3.2528843	O	-2.3914476	10.10983	5.1463239
C	-4.0548846	8.7635663	-4.0811899	H	2.4455861	7.4888819	-2.3000767
C	-2.7043664	9.5033076	-4.1775928	H	0.5338898	9.1133099	-2.7804753
C	-2.751202	11.439408	-0.7977047	H	-2.5960283	6.3267954	-0.2581958
C	-3.8487185	12.009632	-0.0294084	H	-1.3359648	10.661133	-3.0016912
C	-5.1277835	11.730243	-0.3602606	H	-5.6442277	10.225162	-3.9073792
O	-5.4728304	10.940102	-1.395805	H	-5.8065368	8.8505247	-2.8149558
C	-1.4487573	11.690972	-0.4663064	H	-4.4407626	8.689396	-5.1057143
C	-1.0657403	12.51717	0.6652168	H	-1.968101	8.8523773	-4.6610204
C	-2.1602051	13.375155	1.3534013	H	-5.9843763	12.114253	0.1793957
C	-3.6069312	12.892763	1.1425751	H	-0.6222387	11.227954	-0.9920696
O	-1.8756879	13.477655	2.7573694	H	-2.2619524	14.833677	-0.2617659
C	-1.9457511	12.320583	3.4462936	H	-2.7799362	15.445799	1.3297866
C	-1.5551707	12.381276	4.8521036	H	-1.0418915	15.1823	0.9852729
C	-2.0552905	14.810441	0.8133529	H	1.7532019	6.3000775	1.4915818
O	1.6070784	3.5000869	-0.3149467	H	1.3156853	4.6496295	2.0048033
C	1.1830466	2.990101	-1.5162382	H	2.9418701	4.9833639	1.3399065
C	1.8022407	1.6859673	-1.7986798	H	-1.8765911	12.168062	-5.7896279
C	1.8800185	5.2346786	1.2739128	H	-2.8826787	5.7668755	-3.8678417
O	-0.9457787	4.5065589	0.4096988	H	4.7900622	0.059135	-1.5069261
O	3.3282282	5.1692923	-1.4688813	H	1.0485257	-1.4062537	-3.0516318
O	-4.5108063	13.29836	1.8508125	H	-0.1357009	14.279012	7.3220664
O	0.0921658	12.624781	1.0491408	H	-1.7747839	10.309098	7.5785886

C	-2.8520579	10.714751	-5.0996882	H	-0.8597489	-0.0970738	-3.086295
C	-3.9396883	7.3119662	-3.6164234	H	-0.9997554	1.2489624	-1.9387198
O	-3.8408694	10.996764	-5.7389554	H	-0.5107707	1.5707592	-3.5927193
O	-1.7103062	11.436889	-5.1644205	H	3.6355344	3.291383	-1.01129
O	-2.8649513	6.6972491	-4.1645625	H	4.39425	-2.0827984	-2.2563085
O	-4.7329672	6.7395293	-2.905835	H	0.0716304	15.401688	5.3875678
O	0.3905786	3.6025648	-2.2126607	H	0.0893644	14.51497	3.8468009
O	-2.3487131	11.294894	2.8753434	H	-1.383216	15.312929	4.3761373
C	3.1720241	1.4600429	-1.4951961	H	-0.8802375	11.521767	9.336116
C	3.7375954	0.2016998	-1.7367066	H	-2.5037184	10.249353	4.1719358

NImag	0
Σ Electronic and thermal Free Energy	-1865699.117
mol Fraction	0.002769472

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 5

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9330793	7.1416736	-1.5508266	C	2.7061205	-0.8960355	-2.2125702
C	0.60127	7.4374467	-1.5317678	C	3.2008266	-0.2745829	-1.0545744
C	-0.3820038	6.5584474	-0.9116604	C	2.8871299	1.0431384	-0.7564528
C	0.025263	5.2824463	-0.2653019	C	-1.9907689	11.413434	5.9322525
C	1.5381172	5.0716969	-0.0647146	C	-1.3832713	11.484906	7.1782135
C	2.4678119	5.9186081	-0.9799078	C	-0.1954614	12.211981	7.348288
C	0.0304715	8.6206564	-2.1474198	C	0.4005499	12.861931	6.2743723
C	-1.2960899	8.8611185	-2.1303454	C	-0.1959481	12.812105	5.0085808
O	-2.1762311	8.0089855	-1.5065467	C	3.4946364	1.633937	0.496518
C	-1.6931097	6.8837568	-0.9314297	O	0.8262826	1.7583845	-3.7589782
C	-1.995779	10.023674	-2.8022729	O	3.061513	-2.1932951	-2.4120045
C	-3.093133	10.616677	-1.9316374	C	-3.268869	10.619125	5.7852898
C	-4.3928084	10.377849	-2.2356297	O	0.3412167	12.233104	8.6007467
C	-4.9335302	9.5994743	-3.3943923	O	0.4912365	13.426741	4.0243858
C	-3.8562426	8.8799307	-4.2193094	H	2.6442466	7.7909805	-2.0526227
C	-2.5188404	9.6494238	-4.2264156	H	0.6849838	9.3274246	-2.6480116
C	-2.7455461	11.430981	-0.769378	H	-2.4738072	6.2745083	-0.4936915
C	-3.8832391	11.933825	-0.0151469	H	-1.2265629	10.786806	-2.950465
C	-5.1413571	11.636014	-0.4060346	H	-5.4835953	10.297494	-4.0361164
O	-5.4246579	10.88742	-1.4887624	H	-5.6557349	8.8670409	-3.0191507
C	-1.4578814	11.699975	-0.3799227	H	-4.2010815	8.8514753	-5.2606263
C	-1.1582894	12.450952	0.8146755	H	-1.7493734	9.0354345	-4.7063832
C	-2.2830429	13.267341	1.4896835	H	-6.0271425	11.971759	0.1184067
C	-3.7116389	12.776853	1.2016327	H	-0.6029267	11.270474	-0.8872921
O	-2.0139412	13.300047	2.892591	H	-2.3593631	14.799862	-0.0639111
C	-2.0742676	12.077024	3.5170498	H	-2.9368737	15.321639	1.540467
C	-1.4175773	12.108868	4.83287	H	-1.1868749	15.114	1.2389765
C	-2.1846761	14.727819	1.0145686	H	1.6528539	6.4575141	1.6127049
O	1.8612504	3.6799491	-0.2201337	H	1.275401	4.7745916	2.0606049
C	1.6108404	3.1583813	-1.4360875	H	2.9372184	5.2278037	1.5691845
C	2.0443702	1.7792129	-1.6478413	H	-1.683108	12.393773	-5.694678
C	1.872593	5.4066992	1.3977405	H	-2.6491822	5.8936199	-4.1266368
O	-0.7834589	4.479479	0.1630239	H	1.5284439	-0.6477054	-4.0184587
O	3.6294457	5.5603223	-1.1243013	H	3.8444579	-0.8500334	-0.3980765
O	-4.6562427	13.159805	1.8663881	H	-1.8160488	10.984579	8.0379648
O	-0.0265101	12.513857	1.3022563	H	1.3411727	13.395869	6.3789959

C	-2.6565216	10.897345	-5.1004331	H	4.2083068	0.9272338	0.9294219
C	-3.7314217	7.4086878	-3.8260879	H	4.0136439	2.5732956	0.2856511
O	-3.6293578	11.193208	-5.7578639	H	2.7311926	1.8566455	1.2483201
O	-1.5252166	11.638416	-5.0966187	H	0.7270238	2.6991479	-3.4628733
O	-2.6310445	6.838686	-4.3717061	H	2.6665345	-2.5067784	-3.241174
O	-4.5383102	6.7873588	-3.1743706	H	-3.6170002	10.276872	6.7639902
O	1.0193902	3.8431618	-2.2867366	H	-4.0667587	11.211172	5.3241842
O	-2.6172229	11.127857	2.9791064	H	-3.1193941	9.7467652	5.1418385
C	1.5847813	1.1380801	-2.8408105	H	1.1519294	12.765988	8.5868017
C	1.9065362	-0.1964021	-3.1054392	H	0.1273323	13.231302	3.1335685

NImag	0
Σ Electronic and thermal Free Energy	-1865698.699
mol Fraction	0.001368293

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 6

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0659578	7.0216148	-1.4590914	C	3.4311179	-0.6447338	-2.3263252
C	0.74452	7.3799129	-1.4672952	C	2.1323206	-0.4106783	-2.8027671
C	-0.2955924	6.5345745	-0.8994055	C	1.5127469	0.8111857	-2.5805038
C	0.029487	5.2314851	-0.2551791	C	-1.4948976	13.181815	5.7202419
C	1.5262186	4.9274813	-0.0614521	C	-1.358286	13.050704	7.0938869
C	2.4988458	5.7462782	-0.9453996	C	-1.7473699	11.873888	7.7546523
C	0.2520548	8.5964925	-2.0792195	C	-2.2596763	10.798498	7.0431151
C	-1.0647918	8.8903893	-2.1158749	C	-2.3966144	10.893788	5.6548169
O	-2.0003129	8.0690184	-1.5397305	C	0.1129678	1.0271627	-3.1100893
C	-1.5899091	6.9185829	-0.961543	O	4.2971189	2.4856114	-0.7651603
C	-1.6881581	10.078528	-2.8177898	O	3.9725574	-1.8681955	-2.5859576
C	-2.8391479	10.679578	-2.0277133	C	-1.0187708	14.475405	5.0971486
C	-4.1136401	10.469659	-2.4354643	O	-1.5827673	11.84574	9.1038344
C	-4.5760959	9.7102106	-3.6402851	O	-2.879628	9.8072646	5.0329731
C	-3.4485272	8.9805399	-4.3858962	H	2.8175812	7.6425473	-1.9366724
C	-2.1049126	9.7319646	-4.2833731	H	0.9546422	9.2810459	-2.5439827
C	-2.56553	11.471998	-0.8287025	H	-2.4116813	6.3380632	-0.5616552
C	-3.7513026	11.991352	-0.1622279	H	-0.8957591	10.828567	-2.8936936
C	-4.9800825	11.724245	-0.6544521	H	-5.064579	10.421344	-4.3164483
O	-5.1935497	10.992622	-1.7657086	H	-5.3358765	8.9858366	-3.3289689
C	-1.3132428	11.71144	-0.3348125	H	-3.7124237	8.9625896	-5.4508344
C	-1.0735896	12.47377	0.8780562	H	-1.3099193	9.113622	-4.7136428
C	-2.2505565	13.284976	1.4816078	H	-5.8978925	12.072078	-0.197199
C	-3.657283	12.807461	1.0775458	H	-0.4259627	11.283771	-0.7862298
O	-2.1314407	13.308593	2.9126491	H	-2.1826285	14.832886	-0.0499807
C	-2.2665035	12.113654	3.5227229	H	-2.8884129	15.35013	1.5025497
C	-2.0415653	12.096035	4.9655069	H	-1.119142	15.116349	1.3478137
C	-2.1013126	14.749344	1.0388436	H	1.7063455	6.2355539	1.6765757
O	1.8037066	3.5424417	-0.2887648	H	1.2325249	4.556105	2.0422715
C	1.5273707	3.0994772	-1.5577721	H	2.9204497	4.9362661	1.5902524
C	2.1907536	1.8170354	-1.8391811	H	-1.1283836	12.488554	-5.6369947
C	1.8703561	5.185035	1.4157126	H	-2.2728977	5.9830258	-4.2055924
O	-0.8277226	4.4919048	0.1902653	H	5.1443817	0.1927306	-1.294674
O	3.6263144	5.2842311	-1.1399397	H	1.6242391	-1.2026653	-3.3426128
O	-4.6417912	13.166984	1.6976963	H	-0.9388783	13.856997	7.6858161
O	0.0308108	12.565674	1.3992041	H	-2.5504171	9.8707012	7.5276963

C	-2.1595639	10.993066	-5.1472453	H	-0.2830113	0.09571	-3.5246932
C	-3.3703519	7.505535	-3.9926245	H	-0.570819	1.3734155	-2.3276169
O	-3.0711699	11.305618	-5.8802039	H	0.101966	1.7915759	-3.8931387
O	-1.0267224	11.723916	-5.0385485	H	3.9013204	3.3849383	-0.7557168
O	-2.2321855	6.9288429	-4.4458508	H	4.8636881	-1.9050627	-2.2038989
O	-4.2334995	6.8893004	-3.4119869	H	-0.5222583	15.08899	5.8542141
O	0.813199	3.7462652	-2.3059447	H	-0.3170411	14.291707	4.278521
O	-2.5885767	11.120094	2.8522547	H	-1.8498126	15.051002	4.6779547
C	3.5189642	1.5816919	-1.392059	H	-1.8790306	10.985736	9.4422568
C	4.1238342	0.342359	-1.6365838	H	-2.8801424	10.001526	4.0614992

NImag	0
Σ Electronic and thermal Free Energy	-1865699.113
mol Fraction	0.002754829

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 7

Atom	X	Y	Z	Atom	X	Y	Z
C	2.063848	7.2293808	-1.7989991	C	3.1083871	-0.7688491	-2.5598098
C	0.7242789	7.473824	-1.7131546	C	3.6347407	-0.1358057	-1.4222189
C	-0.193577	6.5541139	-1.0531132	C	3.2861801	1.1671788	-1.0991238
C	0.2928108	5.2908193	-0.4371669	C	-1.6486979	11.299274	5.8986956
C	1.8205468	5.1369629	-0.3117525	C	-0.984076	11.385936	7.114153
C	2.671751	6.0242639	-1.2642987	C	0.1819121	12.157272	7.2323824
C	0.0796989	8.6380096	-2.2910921	C	0.6992823	12.836887	6.1362992
C	-1.2526307	8.8273723	-2.2079641	C	0.0438447	12.772425	4.9006734
O	-2.0684097	7.9383757	-1.5491088	C	3.9308813	1.7733893	0.1276291
C	-1.515499	6.8290581	-1.0068798	O	1.0567089	1.8209362	-3.9932323
C	-2.027832	9.9663712	-2.8359177	O	3.5025556	-2.0503903	-2.7861721
C	-3.1031467	10.511558	-1.9083902	C	-2.9010125	10.457004	5.8073615
C	-4.4060922	10.225004	-2.1509006	O	0.7780716	12.190809	8.4573661
C	-4.9727253	9.4335026	-3.2881855	O	0.6578534	13.419727	3.8894565
C	-3.9104029	8.7609523	-4.1701973	H	2.724578	7.9084573	-2.3295164
C	-2.6051184	9.581151	-4.2359591	H	0.6817858	9.3723896	-2.8170924
C	-2.7304602	11.331333	-0.7578164	H	-2.2502636	6.1877351	-0.5366542
C	-3.8482443	11.785272	0.0549036	H	-1.2962716	10.759293	-3.0151286
C	-5.111735	11.442038	-0.2769652	H	-5.5797399	10.113715	-3.8968339
O	-5.4189009	10.690126	-1.3508423	H	-5.6472526	8.6715358	-2.8841128
C	-1.4364864	11.647207	-0.4292025	H	-4.3042916	8.7258155	-5.1937634
C	-1.1076967	12.401402	0.7556568	H	-1.8372284	9.000041	-4.7575874
C	-2.2283287	13.169566	1.4912949	H	-5.9829866	11.740254	0.2925674
C	-3.6495869	12.626351	1.2689328	H	-0.5916007	11.25421	-0.9810737
O	-1.8924966	13.203544	2.8796753	H	-2.4385719	14.708056	-0.0439845
C	-1.8756406	11.975105	3.4961504	H	-2.9566464	15.196851	1.5907948
C	-1.1571584	12.023703	4.7786929	H	-1.2167834	15.058517	1.2031595
C	-2.2089266	14.635792	1.0241237	H	1.9641178	6.5162061	1.3688634
O	2.1883221	3.759553	-0.4934599	H	1.6730755	4.8174361	1.8214063
C	1.899151	3.2360227	-1.69994	H	3.2905988	5.33686	1.2536568
C	2.3739436	1.8757764	-1.9431281	H	-1.9468233	12.364595	-5.720818
C	2.2128681	5.4758695	1.1353473	H	-2.5878506	5.8225482	-4.1606464
O	-0.4630432	4.4549101	0.0234597	H	1.8360823	-0.555028	-4.3048895
O	3.8377425	5.7115939	-1.4675554	H	4.3307702	-0.6901165	-0.8019949
O	-4.5744578	12.968362	1.9819851	H	-1.3547115	10.863538	7.9896683
O	0.0433663	12.504583	1.1881496	H	1.6227703	13.406081	6.1995041

C	-2.832529	10.828236	-5.0922447	H	4.6909947	1.0919619	0.5201169
C	-3.7107804	7.2931416	-3.795464	H	4.4030342	2.7331492	-0.1007469
O	-3.8467382	11.090585	-5.699458	H	3.1968939	1.9622684	0.9170865
O	-1.7314059	11.612181	-5.1371757	H	0.9361527	2.7553823	-3.685232
O	-2.6175493	6.7691487	-4.3985587	H	3.0799924	-2.3738427	-3.5977272
O	-4.4607727	6.6372495	-3.1105076	H	-3.1877093	10.095485	6.7989668
O	1.2415708	3.9027271	-2.5156996	H	-3.7425196	11.020461	5.3900825
O	-2.407851	11.009266	2.9774488	H	-2.7495928	9.5950654	5.1504323
C	1.8817123	1.224628	-3.1175189	H	1.566057	12.754826	8.4085526
C	2.2405797	-0.0950039	-3.4076749	H	0.258781	13.215784	3.0157347

NImag	0
Σ Electronic and thermal Free Energy	-1865698.7
mol Fraction	0.001369744

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 8

Atom	X	Y	Z	Atom	X	Y	Z
C	1.7529645	6.7714275	-1.5036975	C	2.6576529	-0.9695281	-2.2856263
C	0.452811	7.1972523	-1.4567395	C	1.3507138	-0.6715941	-2.7003149
C	-0.5994867	6.4196968	-0.8185679	C	0.8106687	0.5858893	-2.4699238
C	-0.3092545	5.1161565	-0.1584579	C	-2.1529358	11.453803	5.947108
C	1.1775049	4.7361037	-0.0340832	C	-1.5927248	11.495064	7.2162907
C	2.1451257	5.4854775	-0.9826696	C	-0.3674254	12.144032	7.4309385
C	-0.0072999	8.423692	-2.0747245	C	0.3129173	12.745105	6.3788596
C	-1.3082101	8.7826033	-2.0569464	C	-0.2340702	12.724614	5.0901779
O	-2.2545759	8.024222	-1.4162478	C	-0.6006993	0.870187	-2.9322008
C	-1.8742976	6.8679334	-0.8281133	O	3.7716891	2.1322901	-0.8285572
C	-1.9057943	9.9829801	-2.7610386	O	3.1175348	-2.2248756	-2.5494309
C	-2.99474	10.653075	-1.9384958	C	-3.4735194	10.743733	5.7524992
C	-4.2948439	10.489067	-2.2871338	O	0.118355	12.139638	8.7039926
C	-4.8396351	9.7234881	-3.45285	O	0.5314975	13.284926	4.1316097
C	-3.7771044	8.9284482	-4.2265524	H	2.5107264	7.3419996	-2.0317638
C	-2.3998756	9.623168	-4.1991876	H	0.7050855	9.060087	-2.5903462
C	-2.6389476	11.457908	-0.7726669	H	-2.7035178	6.3402185	-0.3742036
C	-3.769241	12.042144	-0.0678643	H	-1.0846127	10.694022	-2.8885441
C	-5.0284274	11.818321	-0.5023189	H	-5.3251174	10.440445	-4.1249485
O	-5.3187957	11.072439	-1.5854522	H	-5.6158764	9.040533	-3.0923948
C	-1.3519966	11.646594	-0.3367521	H	-4.0873485	8.8973847	-5.2785717
C	-1.0491571	12.389806	0.8620929	H	-1.651003	8.9615847	-4.6473285
C	-2.142502	13.285922	1.4857945	H	-5.9099634	12.216513	-0.015798
C	-3.5887014	12.888831	1.145212	H	-0.5081988	11.157075	-0.8075953
O	-1.9271559	13.313473	2.8981109	H	-2.0548736	14.805466	-0.0798342
C	-2.0952129	12.10284	3.5273536	H	-2.6586271	15.379521	1.4967203
C	-1.4913562	12.10171	4.8683437	H	-0.9159789	15.052858	1.2665177
C	-1.9278264	14.73198	1.0052094	H	1.5161381	6.0621316	1.666153
O	1.3690529	3.3343196	-0.2481262	H	0.9733524	4.4173486	2.0886351
C	1.0021652	2.8856034	-1.4919317	H	2.6535627	4.6979261	1.5444587
C	1.5795387	1.5644679	-1.782481	H	-1.3642551	12.302192	-5.6604934
C	1.6105621	4.9999674	1.4182373	H	-2.7227392	5.8874967	-4.0176413
O	-1.1795533	4.4338711	0.3486057	H	4.4645397	-0.2117964	-1.3571786
O	3.2357654	4.9612869	-1.2228908	H	0.7733137	-1.44281	-3.1989515
O	-4.5306542	13.343431	1.7670807	H	-2.0916784	11.0308	8.0602553
O	0.0647012	12.383063	1.3927038	H	1.2816785	13.216978	6.5189558

C	-2.4383983	10.866658	-5.0892288	H	-1.0677807	-0.0448001	-3.3075856
C	-3.7454342	7.4609142	-3.799302	H	-1.2232661	1.2672273	-2.1232247
O	-3.3689378	11.205232	-5.7858397	H	-0.6103556	1.6204037	-3.7289039
O	-1.2700413	11.546588	-5.0494116	H	3.4256612	3.051634	-0.8142763
O	-2.6530459	6.824794	-4.283545	H	4.0235809	-2.3054087	-2.2117092
O	-4.6093696	6.8979833	-3.1680317	H	-3.8826279	10.433183	6.718075
O	0.2847637	3.5581336	-2.21418	H	-4.2114671	11.382877	5.2558306
O	-2.679451	11.188024	2.9731172	H	-3.3558271	9.8580385	5.1207714
C	2.9142102	1.2630484	-1.3984676	H	0.9623911	12.617919	8.7207019
C	3.4374962	-0.0114316	-1.6501168	H	0.1910225	13.107554	3.2280393

NImag	0
Σ Electronic and thermal Free Energy	-1865696.387
mol Fraction	2.75E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 9

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8479063	6.8605258	-1.7400326	C	3.0457346	-0.8423481	-2.5050227
C	0.5368563	7.2282524	-1.5991515	C	1.6990747	-0.6093856	-2.8229383
C	-0.4277657	6.4132723	-0.8749338	C	1.1207111	0.6257112	-2.5660124
C	-0.0293776	5.1333034	-0.2251382	C	-1.6957052	11.464783	5.9358327
C	1.4783742	4.8222447	-0.209563	C	-1.0440809	11.548271	7.158439
C	2.3366216	5.6009216	-1.2365741	C	0.163111	12.254084	7.2729929
C	-0.0240787	8.4241234	-2.1933012	C	0.7343735	12.870475	6.1663157
C	-1.3349963	8.7246286	-2.0806417	C	0.0935238	12.808036	4.9230348
O	-2.1947788	7.9335941	-1.3621092	C	-0.3329188	0.8396903	-2.9232899
C	-1.7188354	6.8037642	-0.7924717	O	4.1224795	2.3268937	-1.1701335
C	-2.0381289	9.8871854	-2.7498354	O	3.54163	-2.0794067	-2.789208
C	-3.0914052	10.51924	-1.8539947	C	-2.993522	10.693976	5.8490372
C	-4.4052538	10.292457	-2.1011763	O	0.7429246	12.288737	8.505591
C	-5.0008647	9.4873487	-3.2142039	O	0.7585773	13.388685	3.9035148
C	-3.9645203	8.7298747	-4.0579511	H	2.5369011	7.4570753	-2.329968
C	-2.6222713	9.4857119	-4.1424923	H	0.61762	9.0845702	-2.7680964
C	-2.6858486	11.355245	-0.7269991	H	-2.4865264	6.2457755	-0.2714883
C	-3.7852651	11.898032	0.0554817	H	-1.2622072	10.6324	-2.9467609
C	-5.0620943	11.612131	-0.2797399	H	-5.5676335	10.172623	-3.8550006
O	-5.3989461	10.839112	-1.3298741	H	-5.7159171	8.775522	-2.7888866
C	-1.3796441	11.607348	-0.3920925	H	-4.351461	8.6703545	-5.0829962
C	-1.0215316	12.379736	0.7725862	H	-1.8798963	8.8520725	-4.6391998
C	-2.1044555	13.234604	1.468168	H	-5.9216849	11.97722	0.2681462
C	-3.5526229	12.76871	1.2424228	H	-0.5523004	11.14964	-0.9205952
O	-1.7847647	13.291005	2.8597378	H	-2.2042501	14.734974	-0.115098
C	-1.8497633	12.082769	3.5121914	H	-2.7131954	15.302987	1.4967033
C	-1.1472524	12.126724	4.8034791	H	-0.9797317	15.051422	1.1384421
C	-1.9926879	14.682094	0.9578918	H	1.8824749	6.1860842	1.4458957
O	1.7174721	3.4276455	-0.4224621	H	1.4490998	4.5246736	1.9258299
C	1.2793151	2.9453808	-1.6301622	H	3.0690091	4.8728562	1.2530744
C	1.8932914	1.6475548	-1.9493051	H	-1.8227669	12.187646	-5.7062563
C	2.0067027	5.1258483	1.2029301	H	-2.7599278	5.7422526	-3.8978377
O	-0.8269999	4.4196791	0.3532832	H	4.880525	0.0089784	-1.7241327
O	3.429031	5.1229237	-1.553011	H	1.1218998	-1.4128036	-3.2681266
O	-4.4647856	13.189488	1.9291229	H	-1.456493	11.073769	8.0424844
O	0.1282729	12.430011	1.2172199	H	1.6884636	13.386928	6.227794

C	-2.7843496	10.713742	-5.0400278	H	-0.7843284	-0.1005694	-3.2525645
C	-3.8339086	7.2713017	-3.6190068	H	-0.910624	1.2196321	-2.0738317
O	-3.7792011	11.000786	-5.6674592	H	-0.4367648	1.5774578	-3.724893
O	-1.6484486	11.445555	-5.096217	H	3.7366259	3.229846	-1.1395431
O	-2.7532214	6.6779505	-4.1780339	H	4.473194	-2.1143287	-2.5200794
O	-4.6212832	6.6791552	-2.9181638	H	-3.3141447	10.37834	6.8458906
O	0.4796456	3.5746967	-2.3032587	H	-3.7951129	11.292939	5.4035418
O	-2.4319124	11.135394	3.0131801	H	-2.883635	9.8061235	5.2189432
C	3.2654356	1.4119346	-1.6640664	H	1.5633003	12.804186	8.4533915
C	3.8262813	0.1587836	-1.9407161	H	0.3594342	13.184136	3.0301968

NImag	0
Σ Electronic and thermal Free Energy	-1865696.386
mol Fraction	2.75E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 10

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0141478	7.1450359	-1.7276105	C	2.7608938	-0.9110351	-2.1478283
C	0.6864693	7.4423918	-1.6218778	C	3.3453681	-0.2425194	-1.0600604
C	-0.2471215	6.587015	-0.9004571	C	3.0493582	1.0853229	-0.7897135
C	0.2085376	5.3353356	-0.2395229	C	-0.5712154	13.561018	5.4408546
C	1.7324778	5.1309096	-0.1431334	C	-0.2211852	13.511087	6.781742
C	2.5912203	5.9431073	-1.1542015	C	-0.4731489	12.36746	7.5571736
C	0.0700166	8.6026595	-2.236573	C	-1.0608356	11.244459	6.9926643
C	-1.252354	8.8447269	-2.132152	C	-1.412514	11.257868	5.6393447
O	-2.0828208	8.0158567	-1.4154593	C	3.7549159	1.7282873	0.3837257
C	-1.5570025	6.9123446	-0.836947	O	0.7472002	1.67555	-3.6400379
C	-2.0010382	9.9818293	-2.7942933	O	3.1060123	-2.2145536	-2.324103
C	-3.0308753	10.61146	-1.8693247	C	-0.2304814	14.824907	4.6826902
C	-4.348407	10.368752	-2.0687949	O	-0.1020477	12.419192	8.8641598
C	-4.9747993	9.5492413	-3.1539253	O	-1.9570786	10.129329	5.1592729
C	-3.962171	8.7921616	-4.0258452	H	2.6851896	7.775358	-2.303395
C	-2.6270544	9.5539807	-4.1606018	H	0.6849538	9.290775	-2.808182
C	-2.594912	11.469822	-0.7671006	H	-2.3025056	6.3193978	-0.3221382
C	-3.6762925	12.007842	0.0463278	H	-1.2449256	10.736773	-3.027559
C	-4.9599935	11.701351	-0.2393706	H	-5.5682649	10.224354	-3.7813855
O	-5.3248482	10.912834	-1.2689151	H	-5.6699285	8.835858	-2.69928
C	-1.2876902	11.753711	-0.4837917	H	-4.3817398	8.7242931	-5.0375305
C	-0.883199	12.584448	0.6367018	H	-1.896117	8.9176605	-4.6709267
C	-1.9726572	13.409531	1.3715084	H	-5.8044657	12.060911	0.3351256
C	-3.4124535	12.887969	1.215632	H	-0.4704195	11.314354	-1.0428471
O	-1.6354443	13.516128	2.7634729	H	-2.1791475	14.86925	-0.2325286
C	-1.6444176	12.355924	3.4502892	H	-2.6497802	15.4624	1.3808049
C	-1.1993029	12.424703	4.8397094	H	-0.9203067	15.248096	0.9661775
C	-1.9291397	14.848764	0.8333808	H	1.9665803	6.5770337	1.4694817
O	2.0465777	3.7341947	-0.2707615	H	1.6267712	4.9117699	2.0051275
C	1.7084903	3.1679697	-1.4446428	H	3.2471895	5.3461176	1.3770764
C	2.1320038	1.7827048	-1.6372144	H	-1.8971585	12.23632	-5.7907771
C	2.1724383	5.5189523	1.2776704	H	-2.7577587	5.8060679	-3.9041237
O	-0.5648184	4.5493125	0.2767605	H	1.4387756	-0.7378637	-3.8600863
O	3.7396958	5.5778061	-1.3702837	H	4.04443	-0.7893952	-0.4366339
O	-4.297929	13.262528	1.9632401	H	0.2633208	14.35709	7.2570678
O	0.2853715	12.721919	0.9764218	H	-1.2492901	10.340994	7.5657422

C	-2.8252923	10.766457	-5.0718964	H	4.5099628	1.043768	0.7806693
C	-3.8116649	7.3370352	-3.5852489	H	4.2442608	2.6625449	0.0940403
O	-3.8406753	11.037549	-5.6734075	H	3.0557285	1.9743074	1.1889152
O	-1.6970729	11.505235	-5.1754997	H	0.6686926	2.627548	-3.3753392
O	-2.7552844	6.7405334	-4.1873568	H	2.6462214	-2.5616832	-3.1050522
O	-4.5692537	6.7446854	-2.8523283	H	0.3605013	15.489384	5.3194009
O	1.0512891	3.8188812	-2.2730965	H	0.3414151	14.606772	3.7762286
O	-2.0403671	11.320231	2.8929226	H	-1.13083	15.360966	4.3670151
C	1.5809052	1.0937895	-2.7627097	H	-0.3205878	11.57492	9.2899834
C	1.8872791	-0.2495459	-2.9994834	H	-2.1124673	10.268141	4.1905884

NImag	0
Σ Electronic and thermal Free Energy	-1865701.501
mol Fraction	0.155673243

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 11

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9979187	6.8727062	-1.407304	C	3.0193011	-0.8361831	-2.3492289
C	0.694885	7.2901328	-1.449538	C	1.7467131	-0.5322203	-2.8561777
C	-0.3981616	6.4877924	-0.9197388	C	1.1809847	0.7148818	-2.6311008
C	-0.1505296	5.1660962	-0.2786332	C	-2.5153679	11.298704	5.852798
C	1.3247973	4.7901529	-0.0496198	C	-2.0565226	11.302944	7.1626909
C	2.3578962	5.5733978	-0.8963017	C	-0.8568419	11.951299	7.4928084
C	0.2752001	8.5326721	-2.0641272	C	-0.1009305	12.588807	6.5164759
C	-1.0258196	8.8840468	-2.1375813	C	-0.5452314	12.606024	5.1888495
O	-2.0136117	8.1012695	-1.5965259	C	-0.1919363	1.0061359	-3.1939312
C	-1.6717021	6.9294219	-1.0156833	O	3.9925916	2.2249832	-0.7160222
C	-1.5755743	10.102516	-2.8495459	O	3.5077342	-2.0805273	-2.6138356
C	-2.7307719	10.741039	-2.0950809	C	-3.8111146	10.58811	5.5332718
C	-3.9982313	10.581341	-2.5497922	O	-0.4721505	11.909378	8.7993013
C	-4.4440281	9.8497686	-3.7777448	O	0.2886196	13.20034	4.3111295
C	-3.318131	9.0843219	-4.4891376	H	2.7903327	7.4632208	-1.8567264
C	-1.9525388	9.7848494	-4.3323816	H	1.0208781	9.1884634	-2.5026022
C	-2.4736607	11.510971	-0.8807405	H	-2.5298346	6.3836359	-0.6444003
C	-3.6601759	12.067027	-0.249382	H	-0.7524149	10.821499	-2.8903219
C	-4.8796551	11.850437	-0.7882293	H	-4.8802413	10.584909	-4.4638406
O	-5.0784683	11.137329	-1.9132963	H	-5.2412668	9.1522248	-3.5007269
C	-1.2263347	11.692698	-0.3394323	H	-3.5445552	9.0840651	-5.5627763
C	-1.0241534	12.399611	0.9018272	H	-1.1658826	9.1412005	-4.7400984
C	-2.1698606	13.270109	1.4648699	H	-5.7996355	12.228718	-0.3605563
C	-3.5818181	12.876384	0.999559	H	-0.3444776	11.222598	-0.7573417
O	-2.0661008	13.254503	2.8899097	H	-1.9712763	14.838336	-0.0414828
C	-2.2734762	12.023829	3.4663003	H	-2.7011975	15.359641	1.4996359
C	-1.7764439	11.983755	4.849858	H	-0.943415	15.04936	1.397243
C	-1.9291779	14.731599	1.0474138	H	1.5192405	6.0649812	1.7113242
O	1.5431303	3.3966318	-0.2903029	H	0.9577279	4.405127	2.0399512
C	1.2781389	2.9844615	-1.572069	H	2.6731433	4.7111981	1.6378847
C	1.8863177	1.675772	-1.856131	H	-0.8253929	12.512908	-5.6255617
C	1.640913	5.0114715	1.4395196	H	-2.2607071	6.0438024	-4.2901816
O	-1.0526058	4.463896	0.1375532	H	4.7421302	-0.0982317	-1.2591206
O	3.468069	5.0627062	-1.0657212	H	1.2159214	-1.2906468	-3.4217357
O	-4.5730899	13.30639	1.5591355	H	-2.6163706	10.809691	7.9501205
O	0.0447081	12.382196	1.5178555	H	0.8502109	13.061157	6.7467009

C	-1.9303107	11.054981	-5.184555	H	-0.6209286	0.1010415	-3.6333095
C	-3.3091054	7.6045376	-4.1053095	H	-0.879166	1.3738012	-2.4243391
O	-2.8056351	11.410032	-5.9418817	H	-0.144994	1.7813022	-3.9649879
O	-0.7738692	11.73935	-5.0321059	H	3.6395474	3.1416515	-0.7010173
O	-2.1774012	6.989176	-4.5213011	H	4.3851149	-2.1668115	-2.2085839
O	-4.2156112	7.0180837	-3.5611706	H	-4.292149	10.245214	6.4536898
O	0.6146576	3.6752884	-2.3277975	H	-4.512837	11.238632	5.000198
O	-2.8054876	11.123812	2.839926	H	-3.6374749	9.7233512	4.8856402
C	3.1889218	1.3693827	-1.3776035	H	0.3643066	12.39128	8.8969746
C	3.7397714	0.1058605	-1.6257455	H	0.0211982	13.049853	3.378575

NImag	0
Σ Electronic and thermal Free Energy	-1865696.384
mol Fraction	2.74E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 12

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8402998	6.8475265	-1.7264503	C	2.9586765	-0.8664575	-2.4993537
C	0.5323907	7.2293836	-1.5942248	C	1.6169552	-0.6180438	-2.8263115
C	-0.4463467	6.4236267	-0.8786799	C	1.050374	0.6228064	-2.5708417
C	-0.0667547	5.1380815	-0.2286804	C	-1.7110507	11.477015	5.9341205
C	1.4373359	4.8103508	-0.2029811	C	-1.0677851	11.551729	7.1617002
C	2.3114564	5.5815557	-1.222215	C	0.1458791	12.244607	7.2864565
C	-0.0110461	8.4325514	-2.1899022	C	0.7318808	12.856648	6.1850892
C	-1.3193712	8.7472184	-2.0861385	C	0.0997541	12.802892	4.9369367
O	-2.1929852	7.9642446	-1.3754952	C	-0.3982359	0.8535005	-2.9379799
C	-1.7336147	6.8281535	-0.8047402	O	4.0606075	2.2879794	-1.1500297
C	-2.0048032	9.9187392	-2.7580792	O	3.4429809	-2.1082957	-2.7826744
C	-3.0580312	10.560245	-1.8689005	C	-3.0162138	10.720046	5.836358
C	-4.3723288	10.348389	-2.1266983	O	0.716751	12.271241	8.5234123
C	-4.9680669	9.5522989	-3.2461355	O	0.7785298	13.378163	3.9234135
C	-3.9335621	8.7852175	-4.0834038	H	2.5400409	7.4376413	-2.3101743
C	-2.5825297	9.526573	-4.155997	H	0.6420324	9.0870601	-2.7586433
C	-2.6520832	11.389401	-0.7369796	H	-2.5111265	6.2776167	-0.2904308
C	-3.7515419	11.942565	0.0381709	H	-1.2194097	10.655981	-2.9473362
C	-5.0287813	11.671317	-0.3074794	H	-5.5221642	10.245156	-3.8898553
O	-5.3659312	10.90421	-1.3618516	H	-5.6942783	8.84755	-2.828
C	-1.3458558	11.626553	-0.391467	H	-4.3131385	8.7319727	-5.1115338
C	-0.9883559	12.392834	0.777461	H	-1.8433633	8.8858569	-4.6484099
C	-2.0673285	13.258119	1.4663486	H	-5.8885501	12.04461	0.2345689
C	-3.5186152	12.808217	1.2287422	H	-0.5194689	11.160889	-0.9144926
O	-1.7576558	13.308859	2.8603631	H	-2.1390815	14.762132	-0.115036
C	-1.8404105	12.100308	3.5103625	H	-2.6539605	15.332909	1.4939078
C	-1.1471753	12.134904	4.8069664	H	-0.9206739	15.063255	1.1482061
C	-1.9361645	14.705179	0.9594101	H	1.8446682	6.16625	1.4581942
O	1.6625254	3.413602	-0.417119	H	1.3894987	4.508777	1.9315081
C	1.2277595	2.9386652	-1.6289068	H	3.0179315	4.8403402	1.2710665
C	1.8297055	1.6348109	-1.946467	H	-1.7420313	12.22311	-5.7076186
C	1.9588782	5.1051987	1.2138716	H	-2.7628565	5.7843174	-3.92027
O	-0.876307	4.4321418	0.3425597	H	4.7970928	-0.0369665	-1.703633
O	3.4007666	5.0921759	-1.5318642	H	1.0341703	-1.4141408	-3.2773054
O	-4.4314145	13.237256	1.9094555	H	-1.4917985	11.080226	8.0418542
O	0.1584624	12.429811	1.2309732	H	1.6908481	13.36295	6.2545564

C	-2.7243559	10.758044	-5.05228	H	-0.8576279	-0.0810766	-3.272351
C	-3.8222142	7.3244507	-3.6464669	H	-0.9777479	1.2381495	-2.0918805
O	-3.7109798	11.056675	-5.6872596	H	-0.4882349	1.5939215	-3.7388139
O	-1.5805026	11.478085	-5.0976341	H	3.6845277	3.1950817	-1.1204037
O	-2.7438626	6.7204196	-4.1985439	H	4.3721532	-2.1540204	-2.5069787
O	-4.621194	6.7396134	-2.9526567	H	-3.3476921	10.406422	6.8302961
O	0.4399232	3.5781384	-2.3063822	H	-3.8080555	11.328052	5.3857143
O	-2.4288243	11.159993	3.0054716	H	-2.9109051	9.8319561	5.2058238
C	3.1971118	1.3835244	-1.6520097	H	1.5428702	12.778105	8.4782046
C	3.7461258	0.1248662	-1.9273685	H	0.3837689	13.17924	3.0468203

NImag	0
Σ Electronic and thermal Free Energy	-1865696.388
mol Fraction	2.76E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 13

Atom	X	Y	Z	Atom	X	Y	Z
C	2.031977	7.1184142	-2.0074787	C	2.6773244	-0.9580295	-2.1098177
C	0.7201395	7.4390263	-1.8095537	C	3.356665	-0.2438364	-1.1098023
C	-0.1614424	6.6286468	-0.979168	C	3.0924057	1.098378	-0.8802736
C	0.3323416	5.4007243	-0.301481	C	-0.3769989	13.39234	5.3803781
C	1.856887	5.1807359	-0.3164978	C	-0.013071	13.32089	6.7166976
C	2.6401166	5.934691	-1.4290959	C	-0.3017623	12.184136	7.4892679
C	0.0688843	8.5812796	-2.4215602	C	-0.9408264	11.088796	6.9262038
C	-1.2392122	8.8449052	-2.2258464	C	-1.307646	11.123855	5.5772653
O	-2.0188056	8.0569075	-1.4120695	C	3.8999593	1.7905621	0.1953578
C	-1.4584937	6.9750047	-0.8260088	O	0.5593828	1.5743287	-3.550352
C	-2.0250498	9.9612192	-2.8799289	O	2.9984427	-2.2720069	-2.2511741
C	-3.0265213	10.602899	-1.9306587	C	0.0060248	14.645222	4.6241085
C	-4.3538852	10.419184	-2.120637	O	0.0867136	12.213385	8.7920877
C	-5.01824	9.6423996	-3.2165817	O	-1.9025086	10.020676	5.0977675
C	-4.0403266	8.7907439	-4.0337279	H	2.6614733	7.7140471	-2.6617622
C	-2.6802577	9.508353	-4.2155434	H	0.6446339	9.2395618	-3.0647731
C	-2.5497092	11.433741	-0.8231409	H	-2.1649757	6.4170907	-0.2242193
C	-3.6027178	11.999188	0.0089688	H	-1.2964981	10.729935	-3.1571647
C	-4.8997653	11.747883	-0.2688425	H	-5.5377903	10.352048	-3.8745787
O	-5.3039279	10.989343	-1.3066507	H	-5.7868808	8.9996576	-2.7762932
C	-1.2308666	11.669377	-0.552323	H	-4.4615802	8.6428653	-5.0347629
C	-0.7856524	12.467928	0.5765933	H	-1.9964062	8.8158919	-4.720133
C	-1.8369099	13.324411	1.3302122	H	-5.7244449	12.132418	0.3180066
C	-3.2953652	12.854958	1.1857981	H	-0.4361304	11.215562	-1.1314456
O	-1.481165	13.407585	2.7191534	H	-2.0073817	14.802445	-0.2614756
C	-1.5224522	12.24316	3.3970344	H	-2.4415132	15.399686	1.3610192
C	-1.0577097	12.285774	4.7813609	H	-0.7249089	15.128085	0.9273008
C	-1.7483851	14.765327	0.8017442	H	2.231694	6.6962437	1.2031237
O	2.147128	3.7757505	-0.4032713	H	1.9204358	5.0618296	1.8413396
C	1.7119621	3.1600816	-1.5186253	H	3.4896468	5.4460934	1.0675318
C	2.1098417	1.7630392	-1.6794072	H	-3.5659531	11.253871	-6.7804842
C	2.4120157	5.6279445	1.0454103	H	-2.9272868	5.7868649	-3.685942
O	-0.4057993	4.6479489	0.3076924	H	1.2151539	-0.8541793	-3.710172
O	3.7634239	5.5431466	-1.7194332	H	4.1036341	-0.7668521	-0.5224995
O	-4.1589131	13.250423	1.9482469	H	0.5112233	14.143905	7.1901764
O	0.3896288	12.554197	0.909442	H	-1.1583529	10.190316	7.4968418

C	-2.7922843	10.713716	-5.1548409	H	4.6848353	1.1200164	0.556739
C	-3.9243793	7.3738846	-3.4704372	H	4.3646659	2.7068234	-0.1797531
O	-2.2069662	11.763984	-5.0207965	H	3.2746805	2.0788397	1.0460493
O	-3.5968548	10.459582	-6.2135206	H	0.5109258	2.5390026	-3.3274803
O	-2.9091442	6.6923289	-4.050907	H	2.4717622	-2.65134	-2.9726196
O	-4.6775784	6.8770821	-2.6660481	H	0.6339711	15.280155	5.2555901
O	0.9941118	3.7783127	-2.3212749	H	0.5546672	14.408562	3.7079934
O	-1.962035	11.2262	2.838025	H	-0.8752661	15.2209	4.3248012
C	1.4610853	1.0266608	-2.7194097	H	-0.1604503	11.375954	9.2157333
C	1.7380742	-0.3295579	-2.9154414	H	-2.0620778	10.170749	4.1313931

NImag	0
Σ Electronic and thermal Free Energy	-1865701.096
mol Fraction	0.078477487

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 14

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8287166	7.0454057	-1.5676377	C	2.4413272	-0.9976945	-2.1068423
C	0.5030578	7.3685364	-1.5339279	C	3.0048957	-0.3471946	-0.9959188
C	-0.4866268	6.5262975	-0.8747873	C	2.71601	0.9813861	-0.7121419
C	-0.0944391	5.2602588	-0.2008566	C	-1.0345583	13.460509	5.5010975
C	1.4174754	5.0180864	-0.0284864	C	-0.7633702	13.394793	6.8594778
C	2.3479749	5.825981	-0.9775014	C	-1.0832151	12.251921	7.6105755
C	-0.0541567	8.546338	-2.171083	C	-1.6603889	11.145064	7.0048274
C	-1.3753689	8.8142119	-2.1397226	C	-1.9331581	11.174364	5.633665
O	-2.2612644	7.9965454	-1.4790088	C	3.3999669	1.6016419	0.486173
C	-1.7912878	6.8778882	-0.8821038	O	0.5004468	1.631547	-3.6144541
C	-2.062607	9.9712862	-2.8330878	O	2.710511	-2.3015701	-2.3850603
C	-3.130959	10.614182	-1.9625387	C	-0.6246488	14.721638	4.7731885
C	-4.4394932	10.399617	-2.2388476	O	-0.7871077	12.287615	8.9371319
C	-5.0189266	9.6013365	-3.3650755	O	-2.4721671	10.060505	5.1145996
C	-3.9733134	8.8309173	-4.1847759	H	2.5433836	7.6675734	-2.0979887
C	-2.6179347	9.5666742	-4.2365698	H	0.605765	9.2264245	-2.7005702
C	-2.7417792	11.454881	-0.8296648	H	-2.57644	6.2960132	-0.4159108
C	-3.8569818	12.008443	-0.0744368	H	-1.2797424	10.712682	-3.0162027
C	-5.1280947	11.730117	-0.4354345	H	-5.5623993	10.293099	-4.0191323
O	-5.4490342	10.957062	-1.4909364	H	-5.7526076	8.8984765	-2.956989
C	-1.4474792	11.709881	-0.4697122	H	-4.3356946	8.7794522	-5.2192555
C	-1.0913448	12.523484	0.6793408	H	-1.8717949	8.9196801	-4.710142
C	-2.2044143	13.36527	1.3576063	H	-5.9967308	12.102248	0.0932014
C	-3.6429968	12.874089	1.115643	H	-0.6084666	11.258284	-0.9851026
O	-1.945232	13.455372	2.767332	H	-2.2900706	14.839984	-0.2437196
C	-2.0164564	12.290986	3.4432846	H	-2.8402312	15.431287	1.34495
C	-1.6503489	12.341497	4.8564187	H	-1.0944762	15.184995	1.0277465
C	-2.1017798	14.807054	0.8344916	H	1.5982344	6.4276067	1.622312
O	1.7060862	3.6165343	-0.1681376	H	1.1925786	4.7613182	2.1058805
C	1.4149876	3.0816534	-1.3695372	H	2.8539784	5.1690535	1.5733034
C	1.8289296	1.6947544	-1.5728079	H	-1.7427223	12.245641	-5.7993045
C	1.7901875	5.3687101	1.420654	H	-2.8374445	5.8198067	-4.0241196
O	-0.910868	4.489772	0.2706126	H	1.1777967	-0.8065393	-3.843
O	3.4995296	5.4389331	-1.1330445	H	3.6890053	-0.8933034	-0.3496403
O	-4.5620611	13.260687	1.8150335	H	-0.2896713	14.227418	7.3681524
O	0.058315	12.634289	1.0867027	H	-1.9001584	10.242179	7.5593544

C	-2.739788	10.79006	-5.1467129	H	4.1498112	0.9113785	0.8841549
C	-3.8767087	7.3695801	-3.7493907	H	3.8923514	2.5422401	0.223977
O	-3.713972	11.08708	-5.801696	H	2.6862521	1.8304405	1.2836459
O	-1.5926409	11.505887	-5.1801699	H	0.4316864	2.5812237	-3.3434749
O	-2.8004213	6.7566368	-4.2970342	H	3.3132799	-2.6510894	-1.7098651
O	-4.6856851	6.7873363	-3.0648987	H	-0.0570351	15.36918	5.447503
O	0.8055089	3.7593006	-2.2118737	H	-0.0068291	14.497132	3.8989995
O	-2.4003125	11.26725	2.8562326	H	-1.4940908	15.278916	4.4110285
C	1.3022889	1.0244322	-2.7245789	H	-1.0478217	11.445689	9.3434104
C	1.597575	-0.3173739	-2.9722085	H	-2.5687261	10.208767	4.1396772

NImag	0
Σ Electronic and thermal Free Energy	-1865701.128
mol Fraction	0.082837975

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 15

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0049012	7.1808548	-1.6376474	C	2.6608703	-0.8842763	-2.0439645
C	0.6786286	7.4962883	-1.5774645	C	3.2133021	-0.2252703	-0.9338996
C	-0.29092	6.6524443	-0.8907081	C	2.9249229	1.1059153	-0.671838
C	0.1243877	5.3932619	-0.2172433	C	-2.1206134	11.2671	5.9302597
C	1.6409112	5.1684753	-0.0674827	C	-1.5445495	11.294622	7.1928655
C	2.5451186	5.9700192	-1.0469891	C	-0.3391683	11.979435	7.4083469
C	0.0996356	8.667146	-2.2083636	C	0.3056264	12.630351	6.3636437
C	-1.2226891	8.9256879	-2.1517302	C	-0.258274	12.624414	5.0819503
O	-2.0890327	8.1053412	-1.4683279	C	3.5948055	1.737398	0.5284253
C	-1.5974223	6.995989	-0.8708518	O	0.7371269	1.7308224	-3.6037942
C	-1.9309384	10.073543	-2.8395109	O	2.9953342	-2.1918522	-2.2101832
C	-3.0368862	10.671717	-1.9815288	C	-3.4189346	10.517504	5.733848
C	-4.3345125	10.494145	-2.3281199	O	0.1645384	11.959049	8.6746265
C	-4.8651633	9.7693447	-3.5275938	O	0.4739045	13.235342	4.1285361
C	-3.795821	8.9588569	-4.2685757	H	2.7044338	7.8031466	-2.1877026
C	-2.4282922	9.6853436	-4.2606757	H	0.7440389	9.3511975	-2.7519243
C	-2.696041	11.449664	-0.7915082	H	-2.3671808	6.414665	-0.3789385
C	-3.8372837	11.971593	-0.0555525	H	-1.1782009	10.852869	-2.9958286
C	-5.0932354	11.731406	-0.4896862	H	-5.3118207	10.509618	-4.2050538
O	-5.3711657	11.022708	-1.6006702	H	-5.6743708	9.1055392	-3.2077604
C	-1.4120023	11.669448	-0.36336	H	-4.1002714	8.8595827	-5.3168148
C	-1.1214734	12.380874	0.8578345	H	-1.6877403	9.0184165	-4.7171587
C	-2.2373054	13.218039	1.5214964	H	-5.9812591	12.086469	0.0178806
C	-3.6719643	12.77917	1.1859285	H	-0.5572822	11.232221	-0.8639485
O	-2.0048209	13.212991	2.9313865	H	-2.2224452	14.782647	-0.0016303
C	-2.1187809	11.980029	3.5274827	H	-2.8279916	15.290738	1.5972665
C	-1.4965708	11.964727	4.8605353	H	-1.0777205	15.033518	1.3387322
C	-2.0805415	14.683901	1.0794598	H	1.8370151	6.6100422	1.5545161
O	1.9406908	3.7678587	-0.1860331	H	1.4573075	4.9488906	2.0755419
C	1.6369314	3.2072211	-1.37184	H	3.104102	5.3627395	1.5051637
C	2.0487497	1.8166896	-1.5512612	H	-3.0204453	11.546847	-6.8283578
C	2.0358287	5.5496195	1.3684076	H	-2.7114613	5.9421812	-3.9390294
O	-0.67763	4.6161992	0.2678746	H	1.4051913	-0.6910375	-3.8034601
O	3.6951476	5.589254	-1.2241549	H	3.8815113	-0.7823404	-0.28615
O	-4.6215886	13.174729	1.8361181	H	-2.0157737	10.79192	8.0307509
O	-0.0025787	12.393367	1.3777243	H	1.2596355	13.131508	6.5034357

C	-2.4424918	10.934902	-5.1473368	H	4.3245509	1.0417408	0.9523648
C	-3.7366749	7.5163943	-3.7639763	H	4.1079998	2.6648817	0.2589598
O	-1.8949072	11.982804	-4.8909391	H	2.8693802	1.9924595	1.3071369
O	-3.1073765	10.725565	-6.3075056	H	0.6614675	2.6833141	-3.3399438
O	-2.6576096	6.8643492	-4.2555477	H	2.5603712	-2.5316836	-3.00837
O	-4.5746335	6.982142	-3.0758905	H	-3.8037084	10.167359	6.6959156
O	1.0181734	3.8675913	-2.2222564	H	-4.1850353	11.144028	5.2644348
O	-2.6755572	11.058882	2.956045	H	-3.2801247	9.653715	5.0765995
C	1.5304782	1.1367528	-2.6976316	H	0.9917228	12.465861	8.6921773
C	1.8279148	-0.2100278	-2.925859	H	0.1276646	13.069243	3.2246714

NImag	0
Σ Electronic and thermal Free Energy	-1865698.44
mol Fraction	0.000882147

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 16

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8495525	7.0660144	-1.4876019	C	2.4433424	-0.9750426	-2.0763758
C	0.524619	7.3930219	-1.4645782	C	2.99789	-0.3339788	-0.9554728
C	-0.4740175	6.5493404	-0.820962	C	2.7102386	0.993497	-0.6653384
C	-0.0922932	5.2774431	-0.1520804	C	-1.0634064	13.440235	5.5975214
C	1.4171163	5.0294207	0.0334053	C	-0.8056903	13.364178	6.9579835
C	2.3593263	5.8409783	-0.900832	C	-1.1364958	12.217157	7.6979253
C	-0.0227617	8.5769165	-2.0989552	C	-1.7112634	11.116432	7.0788671
C	-1.3433869	8.8487155	-2.0785423	C	-1.9705323	11.156156	5.7053479
O	-2.2381657	8.0293296	-1.4320886	C	3.3842135	1.6033021	0.5439536
C	-1.7774567	6.9050888	-0.8384714	O	0.5253112	1.6705196	-3.5846765
C	-2.0202764	10.012691	-2.7705458	O	2.7113213	-2.2777897	-2.360973
C	-3.0952063	10.652856	-1.9061138	C	-0.6424001	14.705064	4.8824661
C	-4.4015959	10.444436	-2.1968571	O	-0.8532272	12.242647	9.0275181
C	-4.972346	9.6558829	-3.3343245	O	-2.507983	10.047692	5.1732852
C	-3.9210787	8.8877181	-4.1488614	H	2.5712489	7.6895972	-2.0066497
C	-2.5629441	9.6195175	-4.1822041	H	0.6443412	9.2585631	-2.6173225
C	-2.7146477	11.484352	-0.7635473	H	-2.5688791	6.3224681	-0.3839561
C	-3.8355363	12.036109	-0.0154581	H	-1.233415	10.752928	-2.940763
C	-5.1038746	11.764421	-0.3909908	H	-5.5070063	10.353933	-3.9889569
O	-5.4167563	10.999893	-1.4550738	H	-5.7123289	8.9526541	-2.9384363
C	-1.4231812	11.732701	-0.3890647	H	-4.2732975	8.8444079	-5.1872158
C	-1.0759056	12.537155	0.7690916	H	-1.81421	8.9733966	-4.6528575
C	-2.1930377	13.37764	1.4423034	H	-5.9765337	12.135593	0.1316626
C	-3.6306395	12.892615	1.18281	H	-0.5805157	11.282084	-0.8993286
O	-1.9474416	13.457127	2.8550895	H	-2.2584904	14.863726	-0.1494416
C	-2.0288775	12.288262	3.5221232	H	-2.822373	15.445691	1.4378561
C	-1.6764641	12.327759	4.9390718	H	-1.0743627	15.19614	1.1360297
C	-2.0808737	14.8227	0.9303047	H	2.838279	5.1650079	1.6501879
O	1.7028719	3.6279892	-0.1130859	H	1.5858506	6.4269823	1.6956223
C	1.4221423	3.1022852	-1.3209926	H	1.1705523	4.7586319	2.1636512
C	1.8338474	1.7155404	-1.5297205	H	-1.6640536	12.306361	-5.7177145
C	1.776631	5.3689262	1.4885142	H	-2.7962888	5.8719783	-3.9976412
O	-0.9156443	4.5061665	0.3058654	H	1.1975479	-0.7680239	-3.8234826
O	3.5111959	5.4514978	-1.0477184	H	3.6739383	-0.8866491	-0.3063001
O	-4.5553703	13.277096	1.87587	H	-0.3343075	14.191686	7.4770502
O	0.0700256	12.641578	1.1884802	H	-1.9593116	10.210499	7.6247115

C	-2.6719885	10.849463	-5.0850813	H	4.1279161	0.9079251	0.9445431
C	-3.8333008	7.4231823	-3.7224815	H	3.8820976	2.544107	0.2931512
O	-3.6386712	11.153951	-5.7477116	H	2.6633384	1.8288659	1.3358924
O	-1.5224102	11.561953	-5.1021841	H	0.4567563	2.6185128	-3.3077949
O	-2.7536706	6.8105051	-4.2638225	H	3.3063427	-2.6338264	-1.682321
O	-4.6507306	6.8389112	-3.0498635	H	-0.0792845	15.346021	5.5667654
O	0.8231114	3.7875789	-2.1646407	H	-0.0168584	14.484624	4.01275
O	-2.4101689	11.269889	2.9241806	H	-1.5065022	15.267694	4.5158241
C	1.3165492	1.0548079	-2.6912369	H	-1.1205553	11.398758	9.4253362
C	1.6102053	-0.2861647	-2.945246	H	-2.594378	10.202966	4.1985043

NImag	0
Σ Electronic and thermal Free Energy	-1865701.128
mol Fraction	0.082837975

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 17

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8083409	6.8016919	-1.8350993	C	2.8269875	-0.9701471	-2.2492597
C	0.5130779	7.2103396	-1.6638809	C	1.4769425	-0.72051	-2.543187
C	-0.4474804	6.4475568	-0.8796641	C	0.9305695	0.5413027	-2.3398617
C	-0.0609888	5.1801052	-0.1991453	C	-0.3993719	13.553842	5.3493604
C	1.4395099	4.8368607	-0.2127604	C	-0.051563	13.507337	6.690843
C	2.2820647	5.5497733	-1.2990491	C	-0.3644174	12.392057	7.485323
C	-0.0358663	8.4006811	-2.2796672	C	-1.01275	11.293353	6.9396863
C	-1.332925	8.7432589	-2.1318177	C	-1.3643383	11.303247	5.5863675
O	-2.1885517	8.0002419	-1.3584016	C	-0.5273482	0.7690391	-2.670263
C	-1.7241044	6.8768273	-0.7679487	O	4.0068998	2.2407018	-1.1243384
C	-2.0252749	9.905573	-2.8120827	O	3.3889411	-2.1973919	-2.4404917
C	-3.0193245	10.603099	-1.8979481	C	0.0086882	14.784643	4.5703138
C	-4.3477295	10.417921	-2.0867577	O	0.0102221	12.445526	8.7910364
C	-5.0163233	9.5996351	-3.147714	O	-1.9700679	10.198192	5.125389
C	-4.0421684	8.7770047	-4.0044597	H	2.4921614	7.3576829	-2.4690044
C	-2.6778807	9.4790852	-4.1662758	H	0.603423	9.0239785	-2.8969761
C	-2.5371072	11.461485	-0.8157307	H	-2.4881885	6.3578157	-0.2031191
C	-3.5873539	12.070649	-0.0120321	H	-1.2336747	10.616969	-3.0640714
C	-4.885612	11.821054	-0.2871555	H	-5.5837046	10.283524	-3.7895152
O	-5.2928831	11.026784	-1.2966621	H	-5.7388918	8.9289723	-2.6712781
C	-1.2162246	11.682874	-0.5407413	H	-4.4710418	8.6984252	-5.0114216
C	-0.7662527	12.513322	0.5627485	H	-1.9790021	8.8020644	-4.6689882
C	-1.8092016	13.408783	1.2824716	H	-5.7092994	12.234772	0.2810132
C	-3.2753445	12.962362	1.136648	H	-0.4240214	11.191357	-1.0927964
O	-1.4654206	13.521401	2.6723447	H	-1.9382	14.848961	-0.3471514
C	-1.5374327	12.375332	3.3792352	H	-2.3751757	15.494713	1.255377
C	-1.0885975	12.443212	4.7671728	H	-0.6599759	15.180713	0.8450145
C	-1.688858	14.833813	0.7190253	H	1.9197567	6.2681095	1.3640718
O	1.6447812	3.4293949	-0.3648501	H	1.4684519	4.640289	1.9347747
C	1.1664649	2.8987615	-1.5356411	H	3.0736814	4.9222697	1.1993324
C	1.7436684	1.5718765	-1.8030301	H	-1.8476099	12.098319	-5.8501121
C	2.0155976	5.195293	1.1682281	H	-2.9407333	5.7538165	-3.7912587
O	-0.8585227	4.5038502	0.4228714	H	4.6970264	-0.1441577	-1.5715943
O	3.3510116	5.0312952	-1.630672	H	0.8509724	-1.522493	-2.9295277
O	-4.1389513	13.401053	1.8747811	H	0.4785104	14.333582	7.1520715
O	0.4087021	12.595236	0.8980412	H	-1.2494249	10.411125	7.5277432

C	-2.8313951	10.680759	-5.1001415	H	-1.0724828	1.2109684	-1.8294963
C	-3.946039	7.3297874	-3.5223291	H	-0.6370321	1.4619779	-3.5100876
O	-3.8374302	10.979092	-5.7041874	H	-1.0106819	-0.1768598	-2.9325181
O	-1.6752251	11.372028	-5.2208803	H	3.6390671	3.1511796	-1.1336244
O	-2.9106706	6.6787364	-4.1035006	H	2.7147108	-2.7997633	-2.7917778
O	-4.7245747	6.7886339	-2.7720101	H	0.6347311	15.426915	5.1961809
O	0.3636321	3.5105817	-2.2206954	H	0.5678731	14.520964	3.6680335
O	-1.9898669	11.35363	2.8389306	H	-0.8615689	15.363069	4.2451415
C	3.1204805	1.316717	-1.5431231	H	-0.2524695	11.621349	9.2310787
C	3.6464478	0.0397317	-1.7630993	H	-2.1184909	10.32868	4.1545903

NImag	0
Σ Electronic and thermal Free Energy	-1865698.712
mol Fraction	0.001397618

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 18

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9052839	7.0791592	-1.5933746	C	2.5892016	-0.9457642	-2.3055395
C	0.5766001	7.3888231	-1.5641132	C	3.1300966	-0.3202114	-1.169254
C	-0.4104925	6.5231621	-0.931745	C	2.8293158	0.9993953	-0.8576642
C	-0.0115949	5.2460656	-0.2825999	C	-1.9090373	11.427369	5.9028024
C	1.5009607	5.0145957	-0.101747	C	-1.2900655	11.498995	7.1431148
C	2.4315699	5.8521067	-1.0245172	C	-0.0935232	12.21479	7.2991438
C	0.013339	8.5752913	-2.1801234	C	0.4997596	12.853048	6.2167482
C	-1.3105157	8.8297413	-2.1533341	C	-0.1081357	12.802784	4.9563849
O	-2.1941082	7.9899478	-1.5181247	C	3.4886641	1.5922413	0.3679586
C	-1.7182136	6.8624603	-0.9417236	O	0.6582493	1.7094748	-3.7796945
C	-2.0036274	9.9961712	-2.8253292	O	2.8703105	-2.2407737	-2.6113567
C	-3.0874829	10.604775	-1.9485763	C	-3.1964784	10.645585	5.7709606
C	-4.3920777	10.378181	-2.2407464	O	0.4542189	12.236909	8.5468371
C	-4.9504568	9.6001434	-3.391297	O	0.576716	13.405273	3.9631152
C	-3.887684	8.865039	-4.2212393	H	2.6186418	7.7193586	-2.1036738
C	-2.5422706	9.6201685	-4.2432151	H	0.6710178	9.2726763	-2.6896274
C	-2.7217629	11.42065	-0.7930418	H	-2.5015676	6.2636042	-0.494502
C	-3.8477966	11.938528	-0.0315479	H	-1.2277832	10.750505	-2.9836976
C	-5.1121815	11.652171	-0.4106749	H	-5.4981604	10.300957	-4.0320011
O	-5.4122492	10.901968	-1.4876857	H	-5.6773986	8.8773442	-3.0066344
C	-1.428119	11.678072	-0.4156094	H	-4.2412712	8.8349695	-5.2595601
C	-1.1107401	12.431233	0.7729256	H	-1.7833975	8.9954956	-4.7262544
C	-2.221352	13.262084	1.4536648	H	-5.9900272	11.999371	0.1196314
C	-3.6572362	12.784771	1.1801365	H	-0.5819464	11.237592	-0.9282536
O	-1.9398877	13.298715	2.8540697	H	-2.2956532	14.788029	-0.1065043
C	-2.0067554	12.079393	3.4849457	H	-2.8539913	15.323115	1.5002737
C	-1.3383373	12.111203	4.7949229	H	-1.1088452	15.096372	1.1847513
C	-2.1123889	14.719262	0.9707615	H	1.6540735	6.3889752	1.5813909
O	1.8038488	3.6192829	-0.2697699	H	1.2599564	4.7087564	2.0244034
C	1.5286939	3.1090675	-1.4857095	H	2.921918	5.1433765	1.5157063
C	1.9532149	1.7297303	-1.715606	H	-1.6886532	12.347266	-5.7331122
C	1.8576882	5.3366337	1.358026	H	-2.7124673	5.8660545	-4.125633
O	-0.8247952	4.4573902	0.1634671	H	1.3535763	-0.7181542	-4.0572839
O	3.5882799	5.4806418	-1.1780694	H	3.8056573	-0.8789312	-0.524797
O	-4.5920954	13.179823	1.8515444	H	-1.7205086	11.007615	8.0091764
O	0.0257611	12.484774	1.2506496	H	1.4466077	13.377936	6.3104818

C	-2.6736569	10.865086	-5.1224681	H	4.2316998	0.8938018	0.7643551
C	-3.7751866	7.3945013	-3.821447	H	3.9847555	2.539174	0.137454
O	-3.6489153	11.168706	-5.7726971	H	2.7591707	1.8016456	1.1563907
O	-1.534059	11.593334	-5.1323972	H	0.5779738	2.6513443	-3.4855826
O	-2.6862665	6.809993	-4.3743983	H	3.4635283	-2.6040458	-1.9349517
O	-4.5825557	6.7856079	-3.1586895	H	-3.5393982	10.311515	6.7543166
O	0.9240319	3.8021602	-2.3191317	H	-3.9923151	11.243723	5.3141676
O	-2.5635346	11.132937	2.956488	H	-3.0617548	9.7687821	5.130308
C	1.4490897	1.0850527	-2.8919925	H	1.2697661	12.762013	8.5231689
C	1.7562124	-0.2485348	-3.1678434	H	0.2031944	13.209068	3.0764135

NImag	0
Σ Electronic and thermal Free Energy	-1865698.369
mol Fraction	0.000782541

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 19

Atom	X	Y	Z	Atom	X	Y	Z
C	1.7493678	6.7390297	-1.5040756	C	2.5857109	-1.0128852	-2.2531296
C	0.453047	7.1766024	-1.4591795	C	1.2815452	-0.7051773	-2.6694153
C	-0.6062588	6.4110964	-0.8180425	C	0.7525875	0.557994	-2.4444989
C	-0.3277651	5.1077864	-0.1524357	C	-2.1178542	11.485249	5.9260959
C	1.1555414	4.715074	-0.0261035	C	-1.5578023	11.52644	7.1953563
C	2.1299608	5.4518334	-0.9775904	C	-0.3268633	12.165297	7.4080262
C	0.0039775	8.4045102	-2.0823532	C	0.3592254	12.756232	6.3539333
C	-1.2937031	8.7750178	-2.0664176	C	-0.1874144	12.735647	5.0651124
O	-2.2469112	8.0277314	-1.4228401	C	-0.6561157	0.8527813	-2.9083228
C	-1.8770382	6.8705887	-0.8297817	O	3.7268409	2.0851242	-0.8090014
C	-1.8804388	9.9777075	-2.7756764	O	3.0345321	-2.273362	-2.5114773
C	-2.963692	10.66077	-1.9562908	C	-3.44461	10.786186	5.7336685
C	-4.2650812	10.506904	-2.3047703	O	0.1583466	12.161497	8.6813025
C	-4.8162157	9.7415377	-3.4676333	O	0.5834504	13.285482	4.1047276
C	-3.7605162	8.9338064	-4.2375448	H	2.5122838	7.3006367	-2.0343248
C	-2.3771745	9.6163269	-4.2125199	H	0.7220956	9.0324299	-2.6004075
C	-2.6011863	11.46714	-0.7935972	H	-2.7109922	6.3521556	-0.3738526
C	-3.7264945	12.06423	-0.091604	H	-1.0529679	10.680945	-2.9058018
C	-4.9874654	11.849845	-0.5256418	H	-5.2948536	10.460098	-4.1429257
O	-5.2840599	11.102198	-1.6058658	H	-5.5987652	9.0670922	-3.1048175
C	-1.3127611	11.646175	-0.3579601	H	-4.0706434	8.9010649	-5.2895535
C	-1.0037678	12.391464	0.8380236	H	-1.6340555	8.9462181	-4.657566
C	-2.0893216	13.299753	1.4576945	H	-5.8656002	12.257824	-0.0410837
C	-3.5388761	12.914224	1.118086	H	-0.4731728	11.147326	-0.8265294
O	-1.8742866	13.330945	2.8699833	H	-1.9875058	14.812236	-0.1138921
C	-2.0533765	12.12435	3.5038897	H	-2.5867683	15.397898	1.4601059
C	-1.4500962	12.123067	4.8451299	H	-0.847002	15.054792	1.2319825
C	-1.8615672	14.741929	0.9714904	H	1.5055723	6.0452002	1.668612
O	1.3347112	3.3107655	-0.2342022	H	0.94816	4.4070804	2.0978913
C	0.9641692	2.8600516	-1.4762129	H	2.6308959	4.670476	1.5529167
C	1.5299301	1.5326533	-1.7610194	H	-1.317042	12.27982	-5.6845832
C	1.5906331	4.9812067	1.4251963	H	-2.7332887	5.8845393	-4.0153353
O	-1.2041974	4.4353686	0.3572377	H	4.3990277	-0.267224	-1.3274642
O	3.2159503	4.9169516	-1.2153246	H	0.6974625	-1.4733757	-3.1649173
O	-4.4769728	13.379791	1.7376608	H	-2.0611989	11.069899	8.0408953
O	0.1097938	12.376954	1.3691044	H	1.3320893	13.220006	6.4926365

C	-2.4042295	10.856372	-5.107771	H	-1.1311687	-0.0596238	-3.2799711
C	-3.7420824	7.4678728	-3.8040919	H	-1.2753347	1.2587008	-2.1011849
O	-3.3314275	11.200349	-5.8061831	H	-0.6589848	1.5996946	-3.7081773
O	-1.2298314	11.525959	-5.0703184	H	3.388929	3.0075367	-0.7986235
O	-2.655188	6.8200475	-4.2851723	H	3.939765	-2.3604566	-2.1732032
O	-4.6112294	6.9153125	-3.1708181	H	-3.8568983	10.483136	6.7002712
O	0.252874	3.5358176	-2.2014677	H	-4.1766225	11.429888	5.2341029
O	-2.6455762	11.21263	2.952994	H	-3.3345259	9.8969779	5.1055138
C	2.8618135	1.2210907	-1.3753992	H	1.0066512	12.632216	8.696514
C	3.3738544	-0.059032	-1.6214996	H	0.2417035	13.107735	3.2017073

NImag	0
Σ Electronic and thermal Free Energy	-1865696.386
mol Fraction	2.75E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 20

Atom	X	Y	Z	Atom	X	Y	Z
C	1.7789384	6.8016969	-1.6345298	C	2.5603883	-0.978545	-2.1302486
C	0.4886285	7.2490769	-1.5375697	C	1.2370677	-0.6829664	-2.4911251
C	-0.5392225	6.5122348	-0.8167719	C	0.7221043	0.5898624	-2.2890887
C	-0.2326897	5.2302822	-0.1227681	C	-2.1273103	11.406262	5.9092596
C	1.2537332	4.8354402	-0.0567267	C	-1.5691205	11.419661	7.1800111
C	2.1807289	5.5317482	-1.083243	C	-0.3243942	12.027692	7.4023413
C	0.0137397	8.4594233	-2.1753523	C	0.3771462	12.615114	6.3565294
C	-1.2799352	8.8386361	-2.1059964	C	-0.167192	12.622177	5.0665091
O	-2.2021567	8.117207	-1.3910076	C	-0.7081077	0.8712712	-2.6913472
C	-1.8064546	6.980015	-0.7772397	O	3.7780205	2.1697758	-0.8689306
C	-1.8951475	10.0223	-2.822344	O	2.9937573	-2.2497545	-2.361565
C	-2.970663	10.708416	-1.9934058	C	-3.469224	10.739944	5.7059495
C	-4.272809	10.601263	-2.3516853	O	0.1581439	11.997964	8.6764647
C	-4.8337918	9.8763116	-3.5374676	O	0.6178216	13.165459	4.1140313
C	-3.8044008	8.9922241	-4.2514481	H	2.5160141	7.3403841	-2.2220134
C	-2.3987331	9.6409201	-4.2432477	H	0.7081676	9.0685537	-2.7456098
C	-2.5947799	11.489756	-0.8168437	H	-2.6167932	6.4841617	-0.2578527
C	-3.7088715	12.100731	-0.1086844	H	-1.088444	10.745057	-2.9813958
C	-4.9723737	11.929216	-0.5534317	H	-5.2368378	10.622302	-4.2355176
O	-5.2820463	11.211158	-1.6503411	H	-5.6788128	9.263831	-3.2076966
C	-1.3045905	11.634033	-0.3756342	H	-4.1046638	8.8888354	-5.3004913
C	-0.9833606	12.351735	0.834352	H	-1.6929794	8.9259098	-4.6816465
C	-2.0500175	13.274921	1.4641	H	-5.8420624	12.351811	-0.06627
C	-3.506374	12.925421	1.116085	H	-0.4738178	11.131435	-0.8552245
O	-1.8379147	13.282896	2.8771884	H	-1.9096012	14.803628	-0.0887683
C	-2.0433986	12.072361	3.4947252	H	-2.5019228	15.383273	1.4905649
C	-1.4430314	12.041275	4.8371957	H	-0.7693083	15.00513	1.2636626
C	-1.7895347	14.717691	0.9960697	H	1.6919082	6.2271424	1.5667523
O	1.4186009	3.4235716	-0.2198782	H	1.1533122	4.6086854	2.0853047
C	0.9861212	2.9274457	-1.4238283	H	2.8068613	4.8443432	1.4465331
C	1.5346929	1.5877966	-1.6850322	H	-2.8705016	11.50196	-6.8364063
C	1.7621833	5.1544246	1.3597774	H	-2.8745529	5.9317991	-3.8371159
O	-1.0853324	4.579091	0.45091	H	4.4197246	-0.2033902	-1.3284381
O	3.2509804	4.9821532	-1.356824	H	0.6273049	-1.4679494	-2.9256486
O	-4.4360882	13.399152	1.7421895	H	-2.0845468	10.964744	8.0191647
O	0.1268977	12.301409	1.3698683	H	1.3600333	13.054964	6.5024035

C	-2.3312516	10.87592	-5.147601	H	-1.2024174	-0.0529467	-3.0040775
C	-3.8287064	7.5587591	-3.7169484	H	-1.2849289	1.3085943	-1.869298
O	-1.7120689	11.886866	-4.9063106	H	-0.7509877	1.5881125	-3.517133
O	-3.0119856	10.696296	-6.3031792	H	3.4427324	3.09334	-0.8782803
O	-2.7740625	6.8438221	-4.171913	H	3.9149508	-2.3264469	-2.0666497
O	-4.7051618	7.0838557	-3.0333361	H	-3.8904124	10.434734	6.6680463
O	0.2410765	3.5773428	-2.1386296	H	-4.1852854	11.406135	5.2127681
O	-2.6529607	11.1799	2.9314181	H	-3.3780028	9.8561135	5.0672697
C	2.8841198	1.2871645	-1.3560809	H	1.0169045	12.449036	8.6983456
C	3.3811165	-0.0034061	-1.5776305	H	0.2740883	13.006168	3.2081832

NImag	0
Σ Electronic and thermal Free Energy	-1865696.159
mol Fraction	1.87E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 21

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0749306	7.2771958	-1.9410298	C	3.1798794	-0.7551254	-2.3080176
C	0.7365079	7.5225644	-1.841092	C	3.7226008	-0.0542856	-1.2190838
C	-0.1673709	6.6239185	-1.13616	C	3.3666738	1.261811	-0.9631561
C	0.33149	5.3858923	-0.4811885	C	-1.6224683	11.101242	5.8398982
C	1.8613024	5.2493803	-0.3637874	C	-0.9563399	11.150864	7.0565326
C	2.6945489	6.0953266	-1.3689293	C	0.2114775	11.915969	7.19594
C	0.080498	8.673797	-2.4312568	C	0.7290133	12.626364	6.1196378
C	-1.2494108	8.8676568	-2.3265872	C	0.0720411	12.599548	4.8834671
O	-2.0559919	7.9910089	-1.6379128	C	4.0303361	1.9439515	0.2127054
C	-1.4877519	6.8986807	-1.0771848	O	1.0737054	1.72969	-3.8435009
C	-2.0231487	10.022359	-2.9306809	O	3.5825545	-2.0443705	-2.4705862
C	-3.0925925	10.543585	-1.9826514	C	-2.8766346	10.264539	5.7255752
C	-4.3957299	10.261186	-2.2240504	O	0.8089575	11.912253	8.4206134
C	-4.9667344	9.5118066	-3.3875484	O	0.6864158	13.274842	3.8909954
C	-3.9074654	8.872316	-4.3037005	H	2.725664	7.9381967	-2.5055928
C	-2.6035789	9.6893875	-4.3430783	H	0.6736938	9.40049	-2.977687
C	-2.715056	11.329119	-0.8094064	H	-2.2072464	6.2697802	-0.568329
C	-3.8298574	11.759653	0.0204509	H	-1.2891582	10.818001	-3.0860285
C	-5.0944699	11.422859	-0.3131224	H	-5.5595765	10.223999	-3.9745007
O	-5.4065124	10.698409	-1.4048234	H	-5.6653586	8.7575764	-3.0146558
C	-1.419904	11.63391	-0.4764712	H	-4.320867	8.8875698	-5.3204883
C	-1.0866808	12.352469	0.7296454	H	-1.8464303	9.1046129	-4.8776755
C	-2.2038737	13.101526	1.4900302	H	-5.9628513	11.704123	0.2692673
C	-3.6267469	12.567898	1.2559227	H	-0.5777029	11.255726	-1.0426521
O	-1.8647148	13.094035	2.8780438	H	-2.4139829	14.684148	0.0004765
C	-1.8512411	11.848288	3.4587709	H	-2.9273894	15.126692	1.6498603
C	-1.1307051	11.857185	4.740923	H	-1.1886829	14.9958	1.2543815
C	-2.1821796	14.5806	1.0655446	H	2.0063215	6.7171527	1.2410825
O	2.2409103	3.8687113	-0.4746419	H	1.7377603	5.0415288	1.7851074
C	1.9465275	3.2806791	-1.6509061	H	3.3438611	5.5465501	1.174628
C	2.4305883	1.9127222	-1.8263475	H	-1.9277868	12.513071	-5.7387139
C	2.2636534	5.6685548	1.0598745	H	-4.3749477	5.7896701	-3.4697886
O	-0.4150966	4.5649716	0.0205988	H	1.8712527	-0.6518208	-4.0359625
O	3.8586204	5.7777394	-1.5758207	H	4.4374699	-0.5657029	-0.5835638
O	-4.5494813	12.892472	1.9799065	H	-1.3269903	10.603721	7.9167889
O	0.0652567	12.439876	1.162607	H	1.653807	13.191469	6.1983738

C	-2.8200011	10.96157	-5.1596335	H	4.8105645	1.2965024	0.623041
C	-3.6074306	7.395339	-4.0617819	H	4.4809838	2.8968461	-0.0790125
O	-3.8323648	11.247973	-5.7604427	H	3.3122258	2.1647817	1.0085117
O	-1.7165165	11.742811	-5.1773408	H	0.9490076	2.6805241	-3.5924558
O	-4.6431917	6.7279299	-3.5089968	H	3.1480859	-2.4150415	-3.2551734
O	-2.5823585	6.8475867	-4.4024394	H	-3.1627316	9.8746795	6.706571
O	1.2770528	3.8973649	-2.4934856	H	-3.7175217	10.841817	5.3262641
O	-2.3881272	10.89985	2.9131941	H	-2.7277815	9.4219307	5.0434828
C	1.9218443	1.1929223	-2.9523715	H	1.5985905	12.475116	8.3874375
C	2.2884776	-0.138249	-3.1742827	H	0.2853573	13.098151	3.0123983

NImag	0
Σ Electronic and thermal Free Energy	-1865697.831
mol Fraction	0.000315411

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 22

Atom	X	Y	Z	Atom	X	Y	Z
C	1.6541327	7.4848046	-1.1780213	C	3.7065545	-0.0967695	-0.7469396
C	0.3473766	7.7492166	-1.4855656	C	2.5561972	-0.0329556	-1.5490063
C	-0.7400614	6.8700024	-1.0802251	C	1.8255941	1.1460413	-1.6448554
C	-0.4827544	5.6228084	-0.3064903	C	-1.0496102	11.955581	5.4198386
C	0.9361534	5.4781911	0.2677271	C	-0.6068075	11.448575	6.6318687
C	2.0353593	6.2957236	-0.4553818	C	-0.3983845	10.071391	6.8132268
C	-0.0752306	8.906848	-2.2489996	C	-0.6405593	9.1771248	5.7801159
C	-1.3763645	9.1472656	-2.5112341	C	-1.0963526	9.6550683	4.5484082
O	-2.3626763	8.2920882	-2.0839222	C	0.5932452	1.1756137	-2.520603
C	-2.0151463	7.1787219	-1.402174	O	3.9604814	3.253337	0.5513937
C	-1.9440725	10.35027	-3.2347653	O	4.4426611	-1.2395376	-0.6358407
C	-3.0261432	10.995634	-2.3810668	C	-1.2409513	13.452857	5.326369
C	-4.328906	10.824993	-2.7066668	O	0.0413507	9.6746169	8.0358631
C	-4.8840991	10.159504	-3.9277917	O	-1.3090763	8.7294243	3.5979233
C	-3.8399135	9.3808835	-4.7427481	H	2.4554858	8.1253622	-1.532915
C	-2.4393155	10.028427	-4.6792191	H	0.6706576	9.614004	-2.5970225
C	-2.6557674	11.708565	-1.1579694	H	-2.870452	6.5688981	-1.1393404
C	-3.7789733	12.058289	-0.3008149	H	-1.1125772	11.050476	-3.3451303
C	-5.0447414	11.848785	-0.7229547	H	-5.3344933	10.93581	-4.5580025
O	-5.3489504	11.303673	-1.9179931	H	-5.6881016	9.4818013	-3.6245017
C	-1.3725249	12.008103	-0.7998395	H	-4.1466397	9.4220728	-5.7955469
C	-1.02201	12.624875	0.4660229	H	-1.7071233	9.3535617	-5.1357183
C	-2.1574376	13.12905	1.3984785	H	-5.9224142	12.097336	-0.1394649
C	-3.573515	12.628608	1.0559145	H	-0.524388	11.740615	-1.4178518
O	-1.8392788	12.776701	2.7621494	H	-2.4060545	15.026135	0.3646685
C	-1.7534093	11.454436	3.005193	H	-2.9180539	15.036427	2.0709351
C	-1.3071368	11.055508	4.3370494	H	-1.1748598	15.026808	1.6484311
C	-2.1670035	14.662801	1.36999	H	0.550034	6.9496935	1.8483886
O	1.3558086	4.1117977	0.2819201	H	0.1818802	5.2626091	2.2743822
C	1.446292	3.5209456	-0.9531392	H	1.8799095	5.8126074	2.1842746
C	2.2368346	2.279718	-0.899705	H	-1.3037451	12.699732	-6.0809997
C	0.8837237	5.9123562	1.7448237	H	-2.9082555	6.2982517	-4.7513905
O	-1.3625578	4.8252004	-0.0426958	H	5.0543963	0.9779547	0.5443106
O	3.2037646	5.9178331	-0.3419305	H	2.230428	-0.9145173	-2.0977445
O	-4.4878316	12.768528	1.8490476	H	-0.4102071	12.111205	7.4676582
O	0.138259	12.804958	0.8147051	H	-0.49142	8.1072976	5.8953422

C	-2.4300385	11.292202	-5.5422062	H	0.3673546	0.172496	-2.894749
C	-3.8575534	7.8902335	-4.4101303	H	-0.283718	1.545074	-1.9784699
O	-3.3478863	11.683777	-6.2280479	H	0.7335767	1.8444739	-3.3751943
O	-1.2362972	11.925484	-5.4901545	H	3.517061	4.1050358	0.3448643
O	-2.7967388	7.2467484	-4.9538719	H	4.0353069	-1.928458	-1.1837753
O	-4.7351502	7.3148059	-3.8093534	H	-1.0355435	13.91282	6.296985
O	0.915043	4.0195502	-1.9302491	H	-0.5711311	13.896532	4.5837442
O	-2.0389403	10.653108	2.099268	H	-2.2601842	13.713811	5.0269977
C	3.4252408	2.2140765	-0.1188185	H	0.1500437	8.710136	8.0386208
C	4.1456852	1.0176529	-0.0446869	H	-1.6577084	9.2086126	2.8022437

NImag	0
Σ Electronic and thermal Free Energy	-1865697.131
mol Fraction	9.66E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 23

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9015915	6.902173	-1.8104859	C	2.9695744	-0.8388917	-2.3800405
C	0.6006909	7.2967551	-1.6480048	C	1.6192133	-0.5960069	-2.6738059
C	-0.3597833	6.5170753	-0.8808141	C	1.0641507	0.6544621	-2.4406894
C	0.0320757	5.2468606	-0.2085152	C	-1.8130272	11.324919	5.9377803
C	1.5346302	4.9122126	-0.217723	C	-1.1943259	11.357735	7.1798448
C	2.3809502	5.6480844	-1.2855027	C	0.0341832	12.015226	7.3439248
C	0.0464923	8.488537	-2.2560697	C	0.6594078	12.633289	6.2677995
C	-1.2564262	8.8148617	-2.121411	C	0.0527586	12.621549	5.0059152
O	-2.1124028	8.0548385	-1.3652484	C	-0.3943779	0.8789629	-2.7705538
C	-1.6413433	6.9330667	-0.7768238	O	4.1206678	2.352649	-1.1657481
C	-1.9534582	9.9744444	-2.8013093	O	3.4417003	-2.0909532	-2.6383606
C	-3.013832	10.614131	-1.9175403	C	-3.1352381	10.605182	5.797152
C	-4.3266096	10.455385	-2.2122512	O	0.5793166	12.001872	8.5928451
C	-4.9153653	9.7116933	-3.3726987	O	0.7675206	13.198736	4.0187385
C	-3.8874781	8.8715932	-4.1399413	H	2.5864433	7.4717331	-2.4311157
C	-2.5103254	9.5765907	-4.1975833	H	0.686802	9.1267721	-2.8570058
C	-2.6124956	11.40684	-0.7571016	H	-2.4043966	6.4035132	-0.2204029
C	-3.7142331	11.970313	0.0075387	H	-1.1854444	10.729827	-2.9962847
C	-4.9900854	11.749012	-0.3757086	H	-5.38144	10.442767	-4.0468914
O	-5.3239849	11.021984	-1.459525	H	-5.7181518	9.0649222	-3.0050656
C	-1.3090886	11.602064	-0.3788326	H	-4.234324	8.7586013	-5.1735023
C	-0.958097	12.328959	0.8173108	H	-1.7987448	8.8918019	-4.673214
C	-2.0289089	13.206567	1.5027035	H	-5.8511607	12.134736	0.1553627
C	-3.485303	12.799256	1.2247513	H	-0.4832402	11.134815	-0.9008034
O	-1.7482691	13.219489	2.9037404	H	-2.0264469	14.743675	-0.0482181
C	-1.8742995	12.00006	3.52505	H	-2.5636243	15.294852	1.5607507
C	-1.2082473	11.989913	4.8365082	H	-0.8303718	14.987716	1.2478553
C	-1.8500574	14.659907	1.0290654	H	1.9962457	6.3161619	1.388604
O	1.7478623	3.5085694	-0.3953522	H	1.5494678	4.6759105	1.9255693
C	1.2765072	2.9984941	-1.5787082	H	3.1586016	4.9798619	1.2071496
C	1.8648791	1.6827804	-1.872846	H	-3.182654	11.422924	-6.7567474
C	2.0992848	5.2477071	1.1734476	H	-2.8160026	5.8502917	-3.7847736
O	-0.7642112	4.5603268	0.4036624	H	4.8336413	0.0085276	-1.6672946
O	3.4576569	5.1429631	-1.6139684	H	1.020718	-1.4038109	-3.0813294
O	-4.4015261	13.23334	1.8977351	H	-1.6492768	10.880147	8.0410767
O	0.1782693	12.322262	1.2975684	H	1.6296629	13.112315	6.3675683

C	-2.5372494	10.815568	-5.0986033	H	-0.866057	-0.0636605	-3.0626132
C	-3.8277718	7.4371208	-3.6109552	H	-0.9468618	1.2906245	-1.9190625
O	-1.9493688	11.850666	-4.8827978	H	-0.50687	1.5955373	-3.5899961
O	-3.264933	10.610789	-6.2209249	H	3.7485411	3.2619579	-1.1542863
O	-2.768932	6.7663844	-4.1202316	H	4.3787142	-2.1311618	-2.3896804
O	-4.6497018	6.9256814	-2.8871521	H	-3.4961294	10.280593	6.7772466
O	0.4715031	3.6196721	-2.252877	H	-3.9009441	11.243043	5.3426009
O	-2.4742303	11.085088	2.9881275	H	-3.0397426	9.7274745	5.1507084
C	3.2399198	1.4359802	-1.6122735	H	1.419159	12.487416	8.5748332
C	3.7767893	0.1671094	-1.8640481	H	0.3865406	13.027793	3.130062

NImag	0
Σ Electronic and thermal Free Energy	-1865696.16
mol Fraction	1.87E-05

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 24

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0579111	7.1678649	-1.8448788	C	2.6922373	-0.9090583	-1.9742588
C	0.7409518	7.4896606	-1.6869591	C	3.3398438	-0.2023954	-0.9481771
C	-0.1679188	6.676084	-0.8897887	C	3.0707565	1.1389412	-0.7191419
C	0.3020709	5.4434114	-0.2038863	C	-0.5710421	13.404908	5.4969327
C	1.8259688	5.2207659	-0.1716528	C	-0.2494379	13.325371	6.8436166
C	2.6454495	5.9797509	-1.2543115	C	-0.5645998	12.185071	7.6004427
C	0.1113543	8.6365788	-2.3127637	C	-1.1878069	11.094192	7.0115167
C	-1.2018819	8.9014074	-2.1572745	C	-1.5119411	11.137413	5.6519342
O	-2.0082607	8.1101277	-1.3732913	C	3.8439171	1.8228028	0.3866645
C	-1.4686388	7.0238687	-0.7759998	O	0.6271358	1.6363635	-3.4674765
C	-1.9647589	10.022833	-2.8295213	O	3.0153343	-2.2228057	-2.1131585
C	-2.9945826	10.661088	-1.9087279	C	-0.1618089	14.660999	4.7599468
C	-4.3155811	10.480699	-2.1413983	O	-0.2172628	12.206349	8.9149819
C	-4.9463854	9.710922	-3.261847	O	-2.0935292	10.038119	5.1478338
C	-3.944569	8.8623599	-4.0528263	H	2.7088791	7.7661533	-2.4752923
C	-2.5783007	9.5786609	-4.1876526	H	0.7083561	9.2974961	-2.9335059
C	-2.5515803	11.485061	-0.7822075	H	-2.1948277	6.4637555	-0.2002748
C	-3.6293607	12.047832	0.0194355	H	-1.2265135	10.791698	-3.0793285
C	-4.9174149	11.800298	-0.3004548	H	-5.4443338	10.424942	-3.9317001
O	-5.2898994	11.048128	-1.3546091	H	-5.7291771	9.0668475	-2.8492925
C	-1.2415411	11.716863	-0.4687108	H	-4.3343362	8.7210046	-5.067463
C	-0.8308307	12.508628	0.6778962	H	-1.8800265	8.8878598	-4.6744304
C	-1.9039346	13.362722	1.4028844	H	-5.7595495	12.183072	0.2622638
C	-3.3578675	12.896629	1.2100438	H	-0.4296893	11.264741	-1.0249626
O	-1.5919035	13.437435	2.8028028	H	-2.0220042	14.850031	-0.1848868
C	-1.6561694	12.269237	3.4723391	H	-2.5059128	15.438837	1.4265636
C	-1.2348602	12.303144	4.8707446	H	-0.7769706	15.166679	1.045385
C	-1.7965711	14.80643	0.8857093	H	2.154739	6.7266622	1.368041
O	2.1164976	3.8157604	-0.2574103	H	1.8205764	5.0891404	1.9863813
C	1.7159131	3.2074312	-1.3895985	H	3.4142717	5.474989	1.2651872
C	2.1161238	1.8105427	-1.545861	H	-3.3799662	11.340123	-6.7692482
C	2.3381962	5.6589668	1.2098439	H	-2.8475983	5.8546112	-3.6878321
O	-0.4562809	4.6884999	0.3771781	H	1.2832843	-0.7924106	-3.6208014
O	3.7768493	5.5879726	-1.5109293	H	4.0661601	-0.7305626	-0.3399557
O	-4.244368	13.28937	1.9471433	H	0.2614183	14.14462	7.3378599
O	0.3335711	12.59124	1.0478982	H	-1.4249243	10.193073	7.5700589

C	-2.6589516	10.789527	-5.1230632	H	4.6148766	1.148206	0.7697996
C	-3.8485736	7.4420323	-3.4945399	H	4.3228941	2.7400576	0.0324999
O	-2.076906	11.838203	-4.9644737	H	3.1915552	2.1077261	1.2179155
O	-3.4298496	10.542619	-6.2081856	H	0.5730136	2.5997211	-3.2402059
O	-2.8165386	6.7621653	-4.0466767	H	2.5117823	-2.5966429	-2.8537312
O	-4.6275596	6.9417994	-2.717291	H	0.4476645	15.290877	5.414179
O	1.0252939	3.8318561	-2.2111506	H	0.4144849	14.428018	3.8600109
O	-2.0796503	11.256247	2.8940209	H	-1.0320361	15.240514	4.4366346
C	1.5002374	1.081823	-2.6109591	H	-0.479369	11.367181	9.3260166
C	1.7809795	-0.2737355	-2.8062185	H	-2.2222401	10.193789	4.1777665

NImag	0
Σ Electronic and thermal Free Energy	-1865701.096
mol Fraction	0.078477487

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 25

Atom	X	Y	Z	Atom	X	Y	Z
C	2.8863505	7.051994	-1.6438327	C	1.2456582	-0.2358176	-4.0972115
C	1.6379269	7.3758424	-1.1881626	C	2.5032717	0.1285721	-3.6077926
C	0.9068857	6.5308396	-0.2574193	C	2.6875889	1.3216121	-2.9138576
C	1.4824801	5.2590667	0.2390622	C	-2.1435429	12.415682	6.1986692
C	2.8232404	4.7920388	-0.3787618	C	-1.6359833	12.909972	7.3925125
C	3.4771723	5.7524238	-1.4143727	C	-0.7266382	13.978148	7.3886878
C	0.8767743	8.4999567	-1.6889027	C	-0.3081514	14.551755	6.1942836
C	-0.4345932	8.639854	-1.4022037	C	-0.810773	14.076888	4.9765231
O	-1.0575066	7.8506884	-0.4686132	C	4.0843334	1.6361292	-2.4233164
C	-0.369264	6.8234233	0.0737372	O	-0.7423402	2.6517267	-3.0585047
C	-1.4111838	9.5035255	-2.1746899	O	1.1530348	-1.4240894	-4.7519602
C	-2.6498385	9.8591849	-1.3748263	C	-3.119586	11.261676	6.2396845
C	-3.7899892	9.1534489	-1.5774111	O	-0.2714902	14.406243	8.6003674
C	-4.0103091	8.0198977	-2.5314017	O	-0.299297	14.662825	3.8750909
C	-2.768744	7.6255598	-3.3516076	H	3.405406	7.6951284	-2.3483053
C	-1.7924712	8.8079221	-3.5242632	H	1.3201991	9.151401	-2.4358144
C	-2.6050397	10.927526	-0.3834517	H	-0.9695776	6.2324881	0.7526719
C	-3.8656175	11.179455	0.296412	H	-0.8857904	10.425742	-2.4391521
C	-4.9504542	10.425523	0.012327	H	-4.8262867	8.31054	-3.2027161
O	-4.9483835	9.4311134	-0.8948123	H	-4.3535581	7.1484409	-1.9623709
C	-1.4704669	11.635335	-0.0741596	H	-3.10852	7.3617998	-4.3603722
C	-1.4552423	12.642315	0.9570837	H	-0.8668426	8.4428583	-3.980614
C	-2.8006048	13.191677	1.4845531	H	-5.9113882	10.554716	0.4944177
C	-4.0034958	12.246264	1.326444	H	-0.50901	11.398276	-0.5147341
O	-2.6105121	13.573236	2.8481921	H	-3.2724189	14.301744	-0.335479
C	-2.3243699	12.534856	3.7016423	H	-4.0441467	14.921461	1.1480427
C	-1.7595775	13.019961	4.9710015	H	-2.3022035	15.199891	0.8574778
C	-3.1277101	14.494118	0.7325903	H	4.0569326	5.4245281	1.2853094
O	2.594318	3.5034068	-1.0235467	H	3.3933776	3.7806292	1.4353957
C	1.6785671	3.4856424	-2.0139556	H	4.746147	4.1145955	0.3009734
C	1.5786813	2.1910584	-2.7172608	H	-1.9964223	11.482365	-5.3067424
C	3.8246492	4.5037542	0.7393883	H	-0.5021674	5.2965276	-3.0537899
O	0.9348981	4.5759992	1.0865405	H	-0.8312162	0.332593	-4.3032727
O	4.4756065	5.3564761	-2.0116107	H	3.3384721	-0.5407998	-3.7833875
O	-5.0432588	12.44199	1.9280944	H	-1.9343813	12.482206	8.3437287
O	-0.4154438	13.132498	1.4067605	H	0.4258374	15.352744	6.1703776

C	-2.3759825	9.8227877	-4.5064318	H	4.8078198	0.9905006	-2.92944
C	-2.1103523	6.3387082	-2.8224603	H	4.3651497	2.679138	-2.5890644
O	-3.4098857	9.696598	-5.1242399	H	4.1663132	1.4587019	-1.3455781
O	-1.5685688	10.899767	-4.6506586	H	-1.5514027	2.2109303	-3.3617997
O	-0.9356599	6.1071171	-3.4220381	H	0.2388532	-1.5634106	-5.0451379
O	-2.6230568	5.60013	-2.0078658	H	-3.3891219	11.029734	7.2740231
O	1.0020446	4.4779401	-2.2591774	H	-4.0383289	11.484291	5.6863542
O	-2.535331	11.380346	3.3748321	H	-2.6906981	10.366167	5.7798378
C	0.317543	1.8178693	-3.2436449	H	0.3442637	15.143135	8.4618427
C	0.1494515	0.6068203	-3.9166934	H	-0.5488368	14.193631	3.0486973

NImag	0
Σ Electronic and thermal Free Energy	-1865689.227
mol Fraction	1.53E-10

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 26

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0748947	7.1113234	-1.7959676	C	2.4039468	-1.0477422	-2.2436624
C	0.7525003	7.3983993	-1.6355096	C	1.9993211	-0.5926756	-0.9866196
C	-0.1501355	6.5161297	-0.9059855	C	1.7736129	0.7633896	-0.7546462
C	0.3371713	5.2514524	-0.2980942	C	-1.6753593	11.559448	5.9862548
C	1.8619523	5.031764	-0.2776462	C	-1.0157559	11.704898	7.1989231
C	2.6795501	5.8918805	-1.2838514	C	0.1416749	12.492801	7.2873199
C	0.1052959	8.567154	-2.202378	C	0.6554403	13.130493	6.164718
C	-1.2185285	8.7807556	-2.067995	C	0.0048464	13.006419	4.9309901
O	-2.0200467	7.9252752	-1.3481467	C	1.3365716	1.1797707	0.6333551
C	-1.4620991	6.8203031	-0.8016285	O	2.4974485	2.1097377	-4.0916647
C	-2.0065859	9.9002357	-2.7153085	O	2.6149495	-2.3868669	-2.386327
C	-3.0899098	10.450914	-1.8016665	C	-2.9184375	10.700771	5.9270867
C	-4.3867816	10.128913	-2.0318878	O	0.7337292	12.58501	8.5115361
C	-4.9377085	9.2838809	-3.1383844	O	0.615121	13.616756	3.8949198
C	-3.8617203	8.6196733	-4.0112235	H	2.7238225	7.7624104	-2.3741957
C	-2.5818602	9.4759231	-4.1047948	H	0.6949322	9.2747693	-2.7771022
C	-2.7319609	11.311859	-0.6774598	H	-2.1856632	6.2055812	-0.2814931
C	-3.8583824	11.777442	0.1164724	H	-1.286049	10.698768	-2.9134659
C	-5.1152102	11.398253	-0.2018965	H	-5.5736058	9.9242125	-3.7604898
O	-5.4081363	10.600212	-1.2458446	H	-5.5818145	8.5121892	-2.7038894
C	-1.4427017	11.653503	-0.3555183	H	-4.2612905	8.5470375	-5.0305849
C	-1.1282377	12.453511	0.802575	H	-1.8016213	8.9070489	-4.6213146
C	-2.2616448	13.236447	1.5028568	H	-5.9919089	11.701457	0.3565548
C	-3.6752604	12.666976	1.2976289	H	-0.5916595	11.249555	-0.8901545
O	-1.9318415	13.331456	2.889824	H	-2.4849469	14.708402	-0.0944594
C	-1.9017873	12.129796	3.5563406	H	-3.0156356	15.256819	1.5172685
C	-1.1877663	12.240506	4.837853	H	-1.272649	15.124794	1.1416576
C	-2.2587262	14.682638	0.9765021	H	2.2160815	6.3992657	1.3835642
O	2.1415752	3.6397905	-0.4893088	H	1.8484818	4.7231063	1.864926
C	1.6685464	3.1419224	-1.6634935	H	3.448367	5.133224	1.172474
C	1.9368735	1.6891406	-1.8160817	H	-2.0164206	12.251307	-5.6407309
C	2.3764836	5.3445301	1.1366265	H	-2.4246546	5.7332457	-3.9111629
O	-0.4189719	4.4496129	0.2250578	H	2.8884769	-0.4977287	-4.2786008
O	3.8265927	5.557493	-1.5451675	H	1.8611636	-1.3188085	-0.1925835
O	-4.6068	13.024327	1.9944685	H	-1.3837148	11.216208	8.0948002
O	0.0192337	12.586433	1.2367785	H	1.5727697	13.711551	6.2062046

C	-2.8512076	10.700113	-4.9806757	H	0.9749772	0.3088867	1.1881153
C	-3.6148667	7.1678936	-3.5997391	H	2.1745343	1.6132287	1.1900828
O	-3.8758006	10.921924	-5.5869639	H	0.5478153	1.9360761	0.6135671
O	-1.774441	11.516201	-5.0456205	H	2.8406602	1.6459258	-4.8710181
O	-2.4994758	6.6690404	-4.1809057	H	2.8869988	-2.5734761	-3.2983758
O	-4.3479758	6.5054067	-2.9026402	H	-3.2040583	10.377634	6.9321888
O	1.0870493	3.8489724	-2.4658795	H	-3.7646839	11.237548	5.4848772
O	-2.4203772	11.136765	3.0770743	H	-2.7560964	9.8141137	5.3067337
C	2.3294631	1.2108597	-3.0851437	H	1.5166619	13.153599	8.4400294
C	2.5724565	-0.1487668	-3.2960406	H	0.2226351	13.37024	3.028991

NImag	0
Σ Electronic and thermal Free Energy	-1865687.122
mol Fraction	4.37E-12

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 27

Atom	X	Y	Z	Atom	X	Y	Z
C	1.5668462	7.1955463	-2.5550038	C	2.392645	-0.2110748	-0.1366145
C	0.4360278	7.8209901	-2.0964788	C	1.0397169	0.1153993	0.0418537
C	-0.1446751	7.5443715	-0.7885897	C	0.6121455	1.4295646	-0.0852063
C	0.5340151	6.6319144	0.1629993	C	-1.2839511	11.208437	5.1574868
C	1.9007394	6.0747426	-0.2756058	C	-0.8800309	10.494162	6.2858988
C	2.2219044	6.1737412	-1.7854758	C	-0.448043	9.1672274	6.1840237
C	-0.2886986	8.8007968	-2.8753337	C	-0.4305775	8.5230401	4.9496005
C	-1.4600307	9.3199821	-2.4506612	C	-0.8507967	9.2139064	3.81356
O	-2.0099936	8.9440159	-1.2552382	C	-0.8539014	1.7422999	0.1131759
C	-1.324773	8.1182665	-0.4413826	O	3.8919983	2.9631462	-0.9488876
C	-2.2866944	10.355778	-3.2058913	O	2.7343695	-1.5229783	0.0028562
C	-3.2374203	11.103871	-2.2848168	C	-1.7470449	12.636074	5.3530966
C	-4.5779668	10.977178	-2.4301179	O	-0.0376364	8.4502447	7.2667933
C	-5.298179	10.178687	-3.4718631	O	-0.8366479	8.624552	2.5976241
C	-4.3838199	9.1449023	-4.1362505	H	1.9389745	7.3802997	-3.5579451
C	-2.9975491	9.7419153	-4.4554332	H	0.1153528	9.1260436	-3.8291944
C	-2.6891209	11.889332	-1.1800855	H	-1.816618	7.9927628	0.513705
C	-3.6784615	12.367492	-0.2283745	H	-1.5557064	11.072197	-3.595366
C	-4.9941123	12.220236	-0.4892642	H	-5.6997105	10.853881	-4.2363361
O	-5.4672937	11.598853	-1.5902766	H	-6.1449478	9.6763799	-2.9962609
C	-1.3558329	12.117316	-0.991612	H	-4.8332088	8.8468295	-5.0912647
C	-0.8121927	12.692245	0.2240818	H	-2.3489434	8.9492825	-4.8438203
C	-1.776387	13.199112	1.3336385	H	-5.7816078	12.568294	0.1668722
C	-3.280739	12.968756	1.0710806	H	-0.6084786	11.77764	-1.7000574
O	-1.4131218	12.551765	2.5811511	H	-1.7613346	15.262982	0.6608136
C	-1.7135741	11.226004	2.6436354	H	-2.1623204	15.044221	2.3810437
C	-1.2726679	10.568509	3.8944951	H	-0.4724303	14.836664	1.8088032
C	-1.5271978	14.690787	1.565402	H	2.958737	7.9081847	0.2598908
O	2.0437219	4.7040908	0.1080834	H	2.8132897	6.7112266	1.5731822
C	1.1267854	3.853736	-0.4562682	H	3.9678643	6.4408665	0.2357735
C	1.5597484	2.451375	-0.3679619	H	-2.084227	11.959456	-6.605985
C	2.9860398	6.8410307	0.5017723	H	-3.3954699	6.2125924	-3.2354115
O	0.120816	6.3985481	1.2914062	H	4.3684009	0.5283336	-0.6367388
O	3.0695678	5.4023371	-2.2458168	H	0.3394605	-0.677125	0.2834268
O	-4.1030423	13.311432	1.9052316	H	-0.9067046	10.976223	7.261051
O	0.3944802	12.790276	0.4193495	H	-0.0951443	7.4924465	4.8840683

C	-3.1165305	10.752738	-5.5958712	H	-1.3877882	0.8520099	0.4575717
C	-4.3016922	7.8660188	-3.3038611	H	-1.0061305	2.5402169	0.8478626
O	-4.1150979	10.972808	-6.2441631	H	-1.3130406	2.0875142	-0.8182065
O	-1.9334074	11.358282	-5.8516377	H	3.5446441	3.8501081	-1.1941233
O	-3.3697007	7.0134499	-3.7937508	H	3.6894956	-1.6159167	-0.1404888
O	-5.0006771	7.6011433	-2.3540972	H	-1.9305118	12.829631	6.4143564
O	0.0988082	4.2849755	-0.9524328	H	-0.9917991	13.346302	5.0011941
O	-2.2861254	10.672527	1.719256	H	-2.6636444	12.852296	4.7974885
C	2.9213194	2.1042206	-0.5829187	H	-0.0951289	9.011071	8.0563292
C	3.3242791	0.7687468	-0.4555571	H	-0.4705817	7.720485	2.6206491

NImag	0
Σ Electronic and thermal Free Energy	-1865688.831
mol Fraction	7.85E-11

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 28

Atom	X	Y	Z	Atom	X	Y	Z
C	2.6457835	6.7563791	-2.063192	C	-0.4161444	3.2198448	-3.4821582
C	1.3624682	7.0569673	-1.7057199	C	0.8466145	3.2671882	-4.0777704
C	0.6856807	6.3707485	-0.6148048	C	1.9958634	3.1089829	-3.3039342
C	1.3901801	5.3570283	0.2035322	C	-1.5982799	11.014863	5.9594348
C	2.8775295	5.0959045	-0.100944	C	-0.9699028	11.273084	7.1695943
C	3.4010662	5.6871463	-1.4363708	C	0.0311779	12.252516	7.2553915
C	0.5463762	8.0526771	-2.3731709	C	0.4204928	12.971838	6.1319546
C	-0.7538772	8.2337063	-2.0602234	C	-0.202909	12.736486	4.9006805
O	-1.3656393	7.485033	-1.0811166	C	3.3493424	3.0868992	-3.9743139
C	-0.6246025	6.6074861	-0.3743739	O	0.3594558	2.4211545	-0.0505239
C	-1.6870536	9.2513964	-2.6965528	O	-1.5105563	3.4722475	-4.2875996
C	-2.835307	9.62638	-1.7786424	C	-2.6709728	9.9508118	5.9041909
C	-4.0479375	9.0575461	-1.9807605	O	0.6016713	12.445825	8.4773435
C	-4.4246347	8.060553	-3.0316377	O	0.2873652	13.445257	3.8632753
C	-3.3202295	7.7552115	-4.0620079	H	3.124655	7.2540008	-2.9011046
C	-2.2111741	8.8269622	-4.103065	H	0.9874817	8.6660757	-3.1529631
C	-2.6271683	10.558775	-0.67641	H	-1.1943721	6.1089277	0.3996402
C	-3.8127073	10.82798	0.1218078	H	-1.0797615	10.14543	-2.8655773
C	-4.9811858	10.217051	-0.1723069	H	-5.3153211	8.4445298	-3.5408785
O	-5.1319779	9.3511481	-1.1937475	H	-4.7212242	7.1281629	-2.5362701
C	-1.4151712	11.124149	-0.3717007	H	-3.7830165	7.7721816	-5.0558946
C	-1.2368232	11.981284	0.774952	H	-1.3629213	8.4428997	-4.6787857
C	-2.4845949	12.562328	1.4780054	H	-5.8938591	10.367529	0.3905091
C	-3.7815218	11.757351	1.2863716	H	-0.5102318	10.870544	-0.9118135
O	-2.1678458	12.71738	2.8627819	H	-2.9660902	13.967029	-0.1225954
C	-1.9313206	11.539962	3.531946	H	-3.5735164	14.423276	1.490526
C	-1.2426379	11.772579	4.8100366	H	-1.8359527	14.590731	1.1041028
C	-2.7323978	13.985131	0.9469568	H	3.5042521	6.8568887	1.0436947
O	3.1930853	3.6966964	0.0311737	H	3.3750216	5.3481388	1.986693
C	3.067977	2.7998166	-1.0233151	H	4.7431366	5.5866509	0.855545
C	1.8640932	2.9535545	-1.9018661	H	-2.1712364	11.76106	-5.4346767
C	3.6811426	5.7761472	1.0287326	H	-1.5317036	5.1582598	-4.7778523
O	0.8432394	4.7731728	1.1278364	H	-1.541107	2.8414137	-1.6669999
O	4.4694003	5.2800277	-1.8811256	H	0.9226687	3.4243915	-5.1490978
O	-4.7588916	11.961619	1.9817505	H	-1.2424801	10.726437	8.0660441
O	-0.1271365	12.315123	1.1980842	H	1.2213238	13.705255	6.1711036

C	-2.7199752	10.053663	-4.862653	H	3.2418141	3.2056284	-5.0563095
C	-2.7729205	6.3325797	-3.9500823	H	4.0070555	3.8766624	-3.5984384
O	-3.8087837	10.158468	-5.3808088	H	3.8530056	2.1350377	-3.7771476
O	-1.7820767	11.025985	-4.9234107	H	1.0412754	2.7877386	0.542984
O	-1.7829303	6.1212305	-4.821523	H	-2.2936833	3.6366819	-3.7229223
O	-3.2298485	5.4670928	-3.2198158	H	-2.8920249	9.5831556	6.9101997
O	3.8689427	1.907018	-1.1058549	H	-3.5998932	10.329901	5.4646913
O	-2.2757549	10.472412	3.0547061	H	-2.3567815	9.1059158	5.2838484
C	0.578109	2.7880502	-1.3395817	H	1.2717875	13.143865	8.4056589
C	-0.5650139	2.9387676	-2.1317942	H	-0.062918	13.136762	2.9997816

NImag	0
Σ Electronic and thermal Free Energy	-1865684.231
mol Fraction	3.31E-14

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 29

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9810038	7.2314058	-1.8676203	C	2.8292632	-0.8039633	-2.1684087
C	0.6538634	7.5155572	-1.7212614	C	3.4734533	-0.0882646	-1.1449204
C	-0.2418226	6.6684253	-0.9446247	C	3.162898	1.2404524	-0.8853542
C	0.2529595	5.440938	-0.2671319	C	-0.9104636	13.315817	5.512871
C	1.7815558	5.2526175	-0.2272356	C	-0.6048444	13.231853	6.8630241
C	2.592807	6.0511868	-1.2872894	C	-0.8999271	12.076493	7.6049385
C	0.0010966	8.6526468	-2.3408954	C	-1.4860254	10.975246	6.9975056
C	-1.3207068	8.8799647	-2.1985732	C	-1.7928787	11.022923	5.6340517
O	-2.1143309	8.0581127	-1.4335392	C	3.936766	1.9343467	0.2138159
C	-1.552697	6.9799396	-0.8422128	O	0.6524487	1.6921257	-3.5774965
C	-2.1057922	9.9877831	-2.8677483	O	3.1195806	-2.1085658	-2.4213603
C	-3.1641602	10.586784	-1.9529678	C	-0.5247764	14.589197	4.7930646
C	-4.4767163	10.373011	-2.2045253	O	-0.5709993	12.094317	8.9242939
C	-5.0720582	9.5992002	-3.3414541	O	-2.3381607	9.9135204	5.1118425
C	-4.0374918	8.7876794	-4.1291459	H	2.6225388	7.8552068	-2.4827756
C	-2.6899108	9.5426625	-4.238492	H	0.5872182	9.3366166	-2.9468442
C	-2.758024	11.409352	-0.8116762	H	-2.2701382	6.3937582	-0.2816782
C	-3.86076	11.933465	-0.0178253	H	-1.3860082	10.779491	-3.0994388
C	-5.1374575	11.654534	-0.3568937	H	-5.5812193	10.306994	-4.0094813
O	-5.4759253	10.904482	-1.4239021	H	-5.8417632	8.9290799	-2.9461149
C	-1.4588127	11.672855	-0.4785912	H	-4.4105324	8.6475159	-5.1501963
C	-1.084387	12.462017	0.6821116	H	-1.9669593	8.8769016	-4.7241352
C	-2.1894026	13.279099	1.4017775	H	-5.9967582	12.007781	0.1991441
C	-3.6275334	12.775828	1.185372	H	-0.6279949	11.249245	-1.0292628
O	-1.8973063	13.347824	2.8062215	H	-2.3278112	14.778954	-0.1725308
C	-1.9383237	12.171586	3.4633727	H	-2.8480501	15.337779	1.4382847
C	-1.5364681	12.203034	4.8675886	H	-1.1076221	15.116626	1.0768979
C	-2.1148998	14.730484	0.9004098	H	2.0633073	6.7313363	1.3470756
O	2.104889	3.8564292	-0.3419813	H	1.7620697	5.0736019	1.9268039
C	1.7241489	3.2650751	-1.4905015	H	3.3524971	5.5118835	1.2278552
C	2.1693117	1.885824	-1.6806356	H	-3.5073105	11.31112	-6.8103365
C	2.2728827	5.6718579	1.1673424	H	-2.8633872	5.8064459	-3.7863314
O	-0.4905192	4.6632857	0.3030779	H	1.3963558	-0.7294914	-3.7773202
O	3.7372613	5.6926045	-1.5363429	H	4.2381116	-0.5826903	-0.5492945
O	-4.533568	13.13606	1.9152843	H	-0.122507	14.059501	7.3717221
O	0.0724432	12.57125	1.0686589	H	-1.706697	10.062876	7.5444078

C	-2.792222	10.761703	-5.1611179	H	4.7502919	1.2893431	0.5592078
C	-3.9092597	7.3640653	-3.5856905	H	4.3612858	2.8811524	-0.1314817
O	-2.2413818	11.824048	-4.9831478	H	3.2972197	2.168782	1.0704193
O	-3.5422211	10.506249	-6.258752	H	0.5759908	2.6498521	-3.3387497
O	-2.8527234	6.7191562	-4.1331524	H	3.7983586	-2.4082858	-1.7962194
O	-4.6832146	6.8341712	-2.8232198	H	0.0597814	15.228273	5.4609753
O	1.0141346	3.8870047	-2.2961508	H	0.0686645	14.380014	3.8984416
O	-2.3264608	11.153298	2.8698544	H	-1.4056638	15.149073	4.4640548
C	1.5593436	1.1502796	-2.7482472	H	-0.8169452	11.244867	9.3240345
C	1.8798182	-0.1899859	-2.9717263	H	-2.457908	10.075089	4.1415747

NImag	0
Σ Electronic and thermal Free Energy	-1865700.729
mol Fraction	0.042205142

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 30

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0201907	7.006455	-1.8513502	C	2.6246942	-1.1108499	-2.1002039
C	0.7089696	7.3644649	-1.7441278	C	2.8074378	-0.2131852	-3.1563366
C	-0.2689836	6.5251139	-1.0637818	C	2.4555976	1.1303509	-3.0220087
C	0.1244578	5.2280669	-0.4482409	C	-0.5938192	13.442038	5.4596721
C	1.6362699	4.9573865	-0.33054	C	-0.2872549	13.367672	6.8101403
C	2.5316078	5.7505181	-1.3265838	C	-0.6016549	12.22607	7.5653359
C	0.1500531	8.5712127	-2.3246282	C	-1.2086272	11.128906	6.9712241
C	-1.1630889	8.8616655	-2.2320828	C	-1.5171394	11.166833	5.607809
O	-2.0375878	8.0460951	-1.5533529	C	2.6818779	2.0554844	-4.1966618
C	-1.5645714	6.9019581	-1.0056132	O	1.2113919	1.1156481	0.4302698
C	-1.8581381	10.039759	-2.881101	O	2.9485179	-2.4314258	-2.1975939
C	-2.9007818	10.671339	-1.9725154	C	-0.186284	14.699965	4.7248348
C	-4.2165187	10.462609	-2.216944	O	-0.2698809	12.252575	8.8838481
C	-4.8274533	9.6790138	-3.3370492	O	-2.0831835	10.061744	5.0990267
C	-3.8045428	8.9278935	-4.2028579	H	2.7261016	7.6214625	-2.4017136
C	-2.452697	9.6678599	-4.2775198	H	0.8000919	9.2507656	-2.8670695
C	-2.4799368	11.495296	-0.8388784	H	-2.3411743	6.3224296	-0.5227136
C	-3.5737108	12.045935	-0.0507977	H	-1.0753815	10.780019	-3.0691121
C	-4.8545509	11.774321	-0.3814817	H	-5.3955086	10.378228	-3.9615414
O	-5.2050974	11.012356	-1.4354323	H	-5.5437662	8.9649283	-2.9175596
C	-1.1757225	11.738079	-0.5071066	H	-4.1970818	8.8974381	-5.2271492
C	-0.7877956	12.539056	0.6402951	H	-1.7193521	9.0334872	-4.7866685
C	-1.8798819	13.381956	1.351049	H	-5.7079939	12.143649	0.1732382
C	-3.3265286	12.899987	1.1410424	H	-0.3525559	11.285051	-1.0464113
O	-1.5854618	13.461909	2.7543895	H	-1.997493	14.867209	-0.2383811
C	-1.6459682	12.293769	3.4248748	H	-2.5047995	15.451335	1.3671768
C	-1.2411	12.333699	4.8279286	H	-0.7688211	15.198085	1.0050154
C	-1.7826122	14.82654	0.8345774	H	1.9178068	6.3847553	1.2980727
O	1.8947565	3.5546508	-0.4582834	H	1.4966299	4.7288005	1.8134203
C	1.5560944	3.0238258	-1.6552262	H	3.1392894	5.0923905	1.2065764
C	1.9279076	1.5926425	-1.7931603	H	-1.629021	12.385354	-5.8004343
C	2.0754518	5.3198323	1.0985979	H	-2.6433578	5.9215815	-4.1164699
O	-0.6952128	4.4539987	0.0109202	H	1.9509411	-1.3843124	-0.0809054
O	3.6563472	5.3356279	-1.5733026	H	3.2327754	-0.5641506	-4.0943219
O	-4.2261316	13.285556	1.8659894	H	0.2111091	14.191968	7.3087336
O	0.3715489	12.640455	1.0219654	H	-1.4443087	10.22668	7.5285875

C	-2.6029078	10.911561	-5.1546353	H	3.260485	1.5469117	-4.9738061
C	-3.6933464	7.4576161	-3.8009125	H	1.7318821	2.3864184	-4.6260844
O	-3.5956807	11.221619	-5.7750928	H	3.2205239	2.9607066	-3.8994694
O	-1.458787	11.631571	-5.2039048	H	1.1077302	0.3615512	1.0314359
O	-2.6236396	6.8620461	-4.3788266	H	3.3055822	-2.6022366	-3.0832582
O	-4.488886	6.8575127	-3.115917	H	0.4115672	15.335495	5.3843263
O	1.0343104	3.6961105	-2.5305671	H	0.4010671	14.469724	3.8313622
O	-2.0528982	11.276225	2.8431066	H	-1.0574494	15.272414	4.3915517
C	1.7537869	0.6714781	-0.7346414	H	-0.5292039	11.411672	9.293093
C	2.0937463	-0.6727783	-0.8897189	H	-2.2004943	10.213618	4.1269351

NImag	0
Σ Electronic and thermal Free Energy	-1865691.142
mol Fraction	3.90E-09

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 31

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9279501	7.0441764	-1.8417205	C	2.5767755	-1.0262484	-2.2169287
C	0.6051109	7.3618168	-1.7295366	C	3.1785245	-0.3539048	-1.1411181
C	-0.3379019	6.5206765	-1.0038999	C	2.8981031	0.9792886	-0.8800429
C	0.1021424	5.2643514	-0.3422784	C	-1.8648852	11.490038	5.7794803
C	1.6235384	5.0400548	-0.2506845	C	-1.5153298	11.59352	7.1256244
C	2.4895482	5.8352923	-1.2691321	C	-0.5690143	12.529992	7.5522888
C	0.0040477	8.532314	-2.3393427	C	0.0341749	13.384158	6.6339963
C	-1.3141013	8.7946973	-2.2292296	C	-0.3154512	13.306747	5.2852305
O	-2.1543952	7.9751408	-1.5133853	C	3.6221121	1.6264422	0.2798414
C	-1.64292	6.8651193	-0.936415	O	0.5757584	1.567536	-3.7139884
C	-2.0468501	9.9483221	-2.8807718	O	2.9070081	-2.3349499	-2.384835
C	-3.0663733	10.583184	-1.9485011	C	-2.892634	10.449787	5.3939614
C	-4.3875157	10.367817	-2.1514909	O	-0.1973384	12.652752	8.8569616
C	-5.0277645	9.5756813	-3.2492165	O	0.2859471	14.121809	4.3805412
C	-4.0279247	8.8043806	-4.1231118	H	2.6053376	7.6642054	-2.4212043
C	-2.6786507	9.5423919	-4.2509549	H	0.6275688	9.2138422	-2.9094748
C	-2.6143691	11.415793	-0.8321122	H	-2.3949592	6.2833856	-0.4183663
C	-3.685633	11.953345	-0.0049736	H	-1.279616	10.694359	-3.106448
C	-4.974066	11.675923	-0.2957298	H	-5.6013913	10.270665	-3.8734415
O	-5.3549117	10.916503	-1.3433343	H	-5.7420046	8.8741879	-2.8060652
C	-1.305128	11.677103	-0.5451671	H	-4.4463255	8.748913	-5.1360725
C	-0.8841935	12.486175	0.5896172	H	-1.9591905	8.8963265	-4.7654411
C	-1.960431	13.314046	1.3425965	H	-5.8116708	12.036755	0.2877871
C	-3.4022524	12.796543	1.1876468	H	-0.4933233	11.240151	-1.114303
O	-1.6311403	13.41691	2.731862	H	-2.1474873	14.788515	-0.2565983
C	-1.6420545	12.240502	3.4020166	H	-2.6282634	15.37006	1.3601224
C	-1.2707375	12.36256	4.8320975	H	-0.8983594	15.146283	0.9627063
C	-1.908307	14.756612	0.8116458	H	1.8812324	6.492528	1.3524198
O	1.9193032	3.6386022	-0.3707784	H	1.5231522	4.8345529	1.8991489
C	1.5707349	3.0690461	-1.5397226	H	3.1464438	5.2454584	1.2628454
C	1.9793484	1.6778898	-1.7246398	H	-1.9003033	12.225631	-5.856946
C	2.0735199	5.4309139	1.1662427	H	-2.8773726	5.7969178	-4.0133335
O	-0.6796645	4.4897132	0.1788647	H	1.2405375	-0.8550049	-3.9183896
O	3.6313102	5.4510347	-1.4893771	H	3.8786156	-0.9018686	-0.5197824
O	-4.2796959	13.139256	1.9608166	H	-1.9864657	10.935322	7.852601
O	0.2900683	12.603271	0.9116825	H	0.7725441	14.102685	6.9795884

C	-2.8533505	10.76414	-5.1544832	H	4.3776307	0.940022	0.6726751
C	-3.9038472	7.3449626	-3.6892192	H	4.1135297	2.5554349	-0.0229514
O	-3.8608348	11.05471	-5.7603585	H	2.9344413	1.8829664	1.0916669
O	-1.7135916	11.486582	-5.2470759	H	0.5106581	2.5230128	-3.4581079
O	-2.8575435	6.7320853	-4.2933381	H	2.4363183	-2.6838565	-3.1584448
O	-4.6720999	6.7619585	-2.9598497	H	-3.347156	10.019194	6.2914997
O	0.9168377	3.7205876	-2.3699371	H	-3.6857901	10.872523	4.7704228
O	-1.9763541	11.201945	2.8522629	H	-2.4388938	9.6449731	4.8088648
C	1.4112733	0.9849156	-2.8389547	H	-0.6853215	12.001906	9.3856368
C	1.7018029	-0.3636278	-3.0662988	H	0.9624474	14.644343	4.8392845

NImag	0
Σ Electronic and thermal Free Energy	-1865690.935
mol Fraction	2.75E-09

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 32

Atom	X	Y	Z	Atom	X	Y	Z
C	2.8490133	7.0715859	-1.8475853	C	1.2723817	-0.2798459	-4.1484097
C	1.6167159	7.369654	-1.3341061	C	2.5429652	0.1203684	-3.7249343
C	0.9533621	6.5169366	-0.3606688	C	2.7312221	1.3248948	-3.052216
C	1.5840963	5.2649777	0.1188569	C	-1.9218966	12.394972	6.1819449
C	2.9042717	4.8243465	-0.5597113	C	-1.3691796	12.914441	7.3446348
C	3.4825666	5.7893491	-1.6352467	C	-0.4882516	14.004594	7.2859146
C	0.8042259	8.4695044	-1.8072837	C	-0.1431968	14.575417	6.0669514
C	-0.4946007	8.5803677	-1.4577257	C	-0.6926138	14.075191	4.8799463
O	-1.0512613	7.7861205	-0.4873073	C	4.1420102	1.6786955	-2.6339438
C	-0.3119311	6.7817654	0.0301187	O	-0.7337617	2.5691618	-3.0404365
C	-1.5290132	9.4118202	-2.1891428	O	1.1774693	-1.4769392	-4.7865588
C	-2.7353438	9.7457515	-1.3325323	C	-2.8655701	11.217859	6.2818116
C	-3.8661156	9.0102455	-1.4718626	O	0.0146778	14.456838	8.4696025
C	-4.1046741	7.8613636	-2.4028525	O	-0.2503413	14.661489	3.7491696
C	-2.8955793	7.4888579	-3.279834	H	3.3167884	7.7197044	-2.5827368
C	-1.9587501	8.692822	-3.511641	H	1.1942001	9.1236592	-2.5811593
C	-2.668538	10.825483	-0.3548153	H	-0.8633874	6.1835521	0.743262
C	-3.900094	11.053832	0.3840114	H	-1.0402458	10.343652	-2.4878997
C	-4.9784609	10.270641	0.1609961	H	-4.959857	8.1245264	-3.0355835
O	-4.9961981	9.2669228	-0.7356433	H	-4.3973772	6.9879027	-1.8091752
C	-1.5381501	11.564058	-0.1086667	H	-3.2779892	7.2062413	-4.2680225
C	-1.4974069	12.582229	0.910848	H	-1.0478663	8.3457017	-4.0097373
C	-2.82852	13.104149	1.4988677	H	-5.9174685	10.381535	0.6886967
C	-4.0137294	12.127932	1.409392	H	-0.5938714	11.345852	-0.5938786
O	-2.5812282	13.504818	2.8477877	H	-3.4167679	14.182901	-0.3060525
C	-2.2276443	12.482822	3.6958185	H	-4.1298096	14.799353	1.2078712
C	-1.6136864	12.995214	4.9311704	H	-2.4117194	15.117097	0.8289738
C	-3.2245449	14.390109	0.7517006	H	4.2018259	5.5044624	1.0355956
O	2.6762343	3.5237242	-1.180293	H	3.5875706	3.8465496	1.2336602
C	1.7138358	3.4730847	-2.1242656	H	4.8744205	4.2013509	0.0309258
C	1.6119396	2.169008	-2.8095217	H	-2.3165696	11.34243	-5.3068815
C	3.966091	4.5725346	0.5104759	H	-0.5597586	5.2190644	-3.0726908
O	1.0958626	4.5777943	0.9986617	H	-0.8256249	0.2353931	-4.2573799
O	4.4601369	5.4116018	-2.2771215	H	3.3849986	-0.5302297	-3.9350653
O	-5.0271246	12.304481	2.0599865	H	-1.6098844	12.489734	8.3134079
O	-0.4493363	13.102526	1.3038823	H	0.5683427	15.393973	5.9993506

C	-2.6150004	9.6827213	-4.473152	H	4.8557654	1.0456682	-3.1689739
C	-2.1800971	6.2240662	-2.771981	H	4.3882418	2.7264559	-2.8230739
O	-3.6747389	9.5249844	-5.0376357	H	4.2810426	1.5147557	-1.5599286
O	-1.8425432	10.777333	-4.6674397	H	-1.5454876	2.1054665	-3.2991941
O	-1.030842	6.0149237	-3.4266092	H	0.2537883	-1.6416741	-5.0330625
O	-2.6335667	5.4817917	-1.9262103	H	-3.0776921	10.989899	7.3303041
O	1.0016206	4.4458844	-2.3453322	H	-3.8158791	11.412337	5.772951
O	-2.4253685	11.320101	3.3906161	H	-2.4377981	10.328504	5.8091748
C	0.3362359	1.7595139	-3.2696404	H	0.6042226	15.207123	8.293932
C	0.1656462	0.5376195	-3.9221356	H	-0.5284907	14.177624	2.9405524

NImag	0
Σ Electronic and thermal Free Energy	-1865689.228
mol Fraction	1.54E-10

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 33

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9897681	7.1608957	-1.6324451	C	2.5858054	-0.8846942	-2.1614809
C	0.6653233	7.4855288	-1.5760817	C	3.1678527	-0.2324709	-1.0611729
C	-0.3132559	6.6455742	-0.8977055	C	2.8852583	1.0971147	-0.7757307
C	0.0895299	5.3804236	-0.2281082	C	-2.1400444	11.246861	5.9364598
C	1.6038043	5.1375247	-0.0812508	C	-1.5689575	11.266152	7.2015026
C	2.5180443	5.9420553	-1.0488073	C	-0.3602221	11.942615	7.4243535
C	0.0979081	8.6636817	-2.2035973	C	0.2928964	12.593214	6.3846392
C	-1.222871	8.9313762	-2.1520264	C	-0.265787	12.595418	5.1006316
O	-2.0980021	8.1142524	-1.4762983	C	3.5890308	1.7189198	0.4102319
C	-1.6172952	6.9987449	-0.8817339	O	0.6240071	1.7436871	-3.6435093
C	-1.9198662	10.086974	-2.8382731	O	2.848899	-2.1894757	-2.4411187
C	-3.025965	10.688732	-1.9830417	C	-3.4423223	10.506322	5.7320261
C	-4.3230551	10.520996	-2.3365385	O	0.1382407	11.914515	8.6926092
C	-4.8526292	9.8047635	-3.5416053	O	0.4741274	13.205089	4.1524041
C	-3.7850311	8.9906383	-4.2811085	H	2.6959179	7.7814417	-2.1759643
C	-2.4128287	9.7081199	-4.2635009	H	0.7496837	9.3454408	-2.7411995
C	-2.6857101	11.459296	-0.7881142	H	-2.3934365	6.4208239	-0.395887
C	-3.8269988	11.985215	-0.055104	H	-1.1611465	10.861865	-2.9875825
C	-5.0824305	11.754985	-0.4961624	H	-5.2914134	10.550805	-4.2178809
O	-5.3596534	11.053095	-1.6115829	H	-5.6675076	9.1447373	-3.2284063
C	-1.4022573	11.669026	-0.3530957	H	-4.0850477	8.8980035	-5.3312173
C	-1.1128325	12.373391	0.8723698	H	-1.6745256	9.0382651	-4.7193378
C	-2.2264583	13.214718	1.5344846	H	-5.970549	12.113439	0.0088533
C	-3.6622673	12.785984	1.1908215	H	-0.5480163	11.228592	-0.8516904
O	-2.0002069	13.202821	2.9453661	H	-2.1954551	14.785141	0.0175831
C	-2.1239123	11.968322	3.5362568	H	-2.8048421	15.290673	1.6158284
C	-1.5072763	11.944359	4.8718357	H	-1.0550565	15.023798	1.3638422
C	-2.0588532	14.681313	1.0988804	H	1.8140936	6.5513597	1.5625801
O	1.8887545	3.7353891	-0.222363	H	1.4163263	4.8866247	2.0574855
C	1.5765181	3.197628	-1.4170512	H	3.0682293	5.2920594	1.4947518
C	1.9853857	1.8097315	-1.6237165	H	-2.9799241	11.584548	-6.8259768
C	2.0020333	5.4918973	1.3602213	H	-2.7224922	5.9649531	-3.9622116
O	-0.7197325	4.6110501	0.2572702	H	1.2948374	-0.6957862	-3.8775926
O	3.6661128	5.5533652	-1.2241576	H	3.8614578	-0.7780609	-0.4246657
O	-4.6122685	13.184225	1.8388157	H	-2.0468324	10.763509	8.0356513
O	0.0037364	12.376659	1.3974493	H	1.2494123	13.087935	6.530131

C	-2.4144873	10.961637	-5.1446906	H	4.3437024	1.0281903	0.7981088
C	-3.7376343	7.5455201	-3.7826994	H	4.0790448	2.6579161	0.1380765
O	-1.8614316	12.004828	-4.8808312	H	2.8883454	1.9509993	1.2182266
O	-3.0748603	10.761703	-6.3090045	H	0.5610666	2.6940398	-3.3734227
O	-2.6609819	6.8886606	-4.272873	H	3.4619256	-2.5383431	-1.7748716
O	-4.5819392	7.0141114	-3.1001964	H	-3.8331403	10.154909	6.6911927
O	0.9534656	3.873783	-2.2507416	H	-4.2025381	11.139571	5.2620725
O	-2.6835881	11.052544	2.9591146	H	-3.3064493	9.6442365	5.0719312
C	1.4394486	1.1374532	-2.7653187	H	0.9680628	12.416781	8.7154235
C	1.7290855	-0.2052091	-3.0147282	H	0.1307555	13.044215	3.2464586

NImag	0
Σ Electronic and thermal Free Energy	-1865698.101
mol Fraction	0.000497603

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 34

Atom	X	Y	Z	Atom	X	Y	Z
C	1.7090295	6.7161338	-1.7722772	C	2.5444866	-1.0649301	-2.2308151
C	0.4196815	7.1601591	-1.6451082	C	1.2114141	-0.784899	-2.5668303
C	-0.5896935	6.4194325	-0.9028332	C	0.6889951	0.4852338	-2.3657926
C	-0.2637016	5.1385083	-0.2169452	C	-1.9942524	11.546277	5.7792217
C	1.2262231	4.7531918	-0.1792241	C	-1.6826997	11.633564	7.1357122
C	2.1278295	5.4494412	-1.2282136	C	-0.6939734	12.51091	7.5910211
C	-0.0718328	8.3706991	-2.2689037	C	-0.0091087	13.321785	6.6909648
C	-1.3631841	8.7499309	-2.1649921	C	-0.318755	13.260603	5.3316881
O	-2.2675677	8.0232715	-1.4330757	C	-0.751599	0.7504297	-2.7411501
C	-1.8573761	6.8837757	-0.8353316	O	3.7582915	2.1064241	-1.0238563
C	-1.9950413	9.9423633	-2.8520826	O	2.985195	-2.3344552	-2.4593009
C	-3.0000692	10.654912	-1.9623416	C	-3.0722017	10.570399	5.3636437
C	-4.3253153	10.519406	-2.2040946	O	-0.3578854	12.615838	8.9066572
C	-4.9795806	9.7473376	-3.3081136	O	0.3619592	14.032859	4.4458785
C	-4.0019472	8.9007729	-4.1367971	H	2.4304024	7.2572966	-2.3766814
C	-2.6087617	9.5564894	-4.2361858	H	0.6078592	8.9822275	-2.8539012
C	-2.5299763	11.471884	-0.8424401	H	-2.6560142	6.3826386	-0.3031364
C	-3.5892224	12.089955	-0.0575089	H	-1.1732936	10.632817	-3.0625313
C	-4.8831427	11.891933	-0.3864231	H	-5.4907201	10.463588	-3.9617944
O	-5.2795829	11.141693	-1.4352808	H	-5.7480922	9.0984627	-2.8756725
C	-1.216084	11.649148	-0.5156782	H	-4.3931366	8.848319	-5.1607068
C	-0.7785666	12.441934	0.6244597	H	-1.9149451	8.8618036	-4.7216724
C	-1.8203165	13.348383	1.3341835	H	-5.7135787	12.315002	0.1646122
C	-3.288684	12.929983	1.1333315	H	-0.4171618	11.152765	-1.0538246
O	-1.5322497	13.439154	2.733501	H	-1.8498204	14.81918	-0.2789223
C	-1.6478067	12.271154	3.4086359	H	-2.3446815	15.445384	1.3166742
C	-1.3161674	12.375937	4.8494596	H	-0.6216838	15.099905	0.9812232
C	-1.6503157	14.779471	0.7972027	H	1.6868082	6.1597734	1.4251289
O	1.3979911	3.3414826	-0.3346978	H	1.1710546	4.5408757	1.966037
C	0.9489729	2.8332539	-1.5274565	H	2.8094168	4.7842316	1.2921039
C	1.5045328	1.4958533	-1.7879316	H	-1.625829	12.16882	-5.8467918
C	1.7608939	5.0861124	1.2245229	H	-3.0153343	5.8386572	-3.9208994
O	-1.1008529	4.4818204	0.3734079	H	4.4127869	-0.265416	-1.475098
O	3.1948112	4.9032061	-1.5223715	H	0.6000862	-1.579268	-2.9816892
O	-4.1663833	13.344806	1.8698732	H	-2.2173376	11.009142	7.8483903
O	0.3899735	12.483406	0.9836592	H	0.7611881	13.994222	7.0588911

C	-2.6841189	10.77409	-5.1587609	H	-1.2440589	-0.1808688	-3.0352736
C	-3.9740677	7.4459593	-3.6695672	H	-1.3153634	1.1905387	-1.9115599
O	-3.6533665	11.112531	-5.800772	H	-0.8176954	1.459258	-3.5722838
O	-1.5022578	11.428774	-5.2221915	H	3.4153003	3.0274779	-1.0377376
O	-2.9405376	6.7653259	-4.2200541	H	3.9132988	-2.3989415	-2.18385
O	-4.7981863	6.9232503	-2.9556967	H	-3.580832	10.173056	6.2473593
O	0.186877	3.4711377	-2.2344497	H	-3.817297	11.038878	4.714089
O	-2.0357837	11.255022	2.8517949	H	-2.6513763	9.7361678	4.7954172
C	2.8631084	1.2109104	-1.4844546	H	-0.9020067	11.99869	9.4207774
C	3.3673686	-0.0772214	-1.704298	H	1.0537863	14.514453	4.9261047

NImag	0
Σ Electronic and thermal Free Energy	-1865688.704
mol Fraction	6.33E-11

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 35

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0050366	7.1681471	-1.6463412	C	2.9627743	-0.9081166	-2.0644641
C	0.676197	7.4692835	-1.5966227	C	3.159531	0.0241714	-3.0875645
C	-0.2979168	6.5727694	-0.9874123	C	2.7452154	1.3481533	-2.9380862
C	0.1189575	5.2768717	-0.3850117	C	-1.2360129	13.292833	5.6799292
C	1.6331674	5.0651858	-0.1978008	C	-0.9936532	13.19496	7.0418975
C	2.5424168	5.9206499	-1.1274484	C	-1.2969989	12.021832	7.7519503
C	0.0962659	8.6672746	-2.1746393	C	-1.8274985	10.917204	7.101156
C	-1.230922	8.9012297	-2.1413534	C	-2.0696205	10.978947	5.725265
O	-2.1027245	8.032739	-1.5279591	C	2.9901181	2.3127947	-4.076668
C	-1.6095311	6.8946544	-0.9854311	O	1.3336731	1.1903753	0.4455814
C	-1.942104	10.066855	-2.795398	O	3.3463288	-2.2112981	-2.1779151
C	-3.0541668	10.630701	-1.9253748	C	-0.8455478	14.585337	4.9976983
C	-4.3462138	10.375028	-2.2411491	O	-1.0321536	12.026582	9.0857721
C	-4.8673658	9.5974209	-3.4097626	O	-2.5631164	9.8657878	5.1615056
C	-3.7720861	8.9120823	-4.2408891	H	2.7107214	7.8259664	-2.1450657
C	-2.4505819	9.7084469	-4.228825	H	0.7430797	9.3871125	-2.6666265
C	-2.7250799	11.440465	-0.7518646	H	-2.383918	6.2711617	-0.5567846
C	-3.8787686	11.924578	-0.0067115	H	-1.1829523	10.843304	-2.9252362
C	-5.1290764	11.609849	-0.4084072	H	-5.432658	10.289343	-4.0447934
O	-5.3945759	10.862784	-1.4972988	H	-5.5729183	8.8437674	-3.044809
C	-1.4502858	11.727394	-0.3486622	H	-4.1117183	8.8929246	-5.2841812
C	-1.1537756	12.512504	0.8363447	H	-1.6668761	9.1183829	-4.7157388
C	-2.3142779	13.290653	1.5116212	H	-6.0237477	11.928973	0.1114054
C	-3.727129	12.755705	1.2168924	H	-0.5830532	11.32305	-0.8566956
O	-2.0932763	13.344865	2.929613	H	-2.4157202	14.812014	-0.0444152
C	-2.137607	12.157659	3.5670507	H	-3.0259998	15.331545	1.5474405
C	-1.8044658	12.176442	4.9892769	H	-1.2650961	15.159353	1.2672831
C	-2.2526326	14.751351	1.0366934	H	1.7733657	6.4587619	1.4777012
O	1.9566	3.6781116	-0.3469117	H	1.3974566	4.7737659	1.9300731
C	1.7003125	3.1661146	-1.5721971	H	3.0513072	5.2203534	1.4161367
C	2.1384448	1.7555075	-1.726418	H	-1.6680464	12.497186	-5.6406204
C	1.9854611	5.4068976	1.2602098	H	-2.4908302	5.9545643	-4.1697841
O	-0.6890484	4.4578904	0.0128187	H	2.2021677	-1.2627375	-0.0891155
O	3.6944555	5.5587933	-1.3272613	H	3.6451232	-0.2839337	-4.0112395
O	-4.6769805	13.084578	1.9047341	H	-0.5553514	14.02516	7.5851164
O	-0.0200337	12.650992	1.2785127	H	-2.052478	9.9916194	7.6235432

C	-2.609525	10.967922	-5.0815679	H	3.6273967	1.84923	-4.8358586
C	-3.6189898	7.4374169	-3.8700473	H	2.0494176	2.6159367	-4.5452893
O	-3.5824502	11.253377	-5.7438672	H	3.4747286	3.2310376	-3.7304529
O	-1.4959273	11.735397	-5.0549028	H	1.2323208	0.4168721	1.0219734
O	-2.4978415	6.9016949	-4.4076567	H	3.7535864	-2.34366	-3.0483703
O	-4.4213849	6.7872518	-3.2410233	H	-0.307838	15.226657	5.7018507
O	1.1946732	3.8397157	-2.455962	H	-0.2059051	14.402896	4.1294529
O	-2.472208	11.140339	2.9405123	H	-1.722358	15.130847	4.6352962
C	1.9511782	0.8000345	-0.7010712	H	-1.2760139	11.165254	9.4605945
C	2.3546814	-0.5245982	-0.8718948	H	-2.6384927	10.038651	4.1887722

NImag	0
Σ Electronic and thermal Free Energy	-1865691.14
mol Fraction	3.88E-09

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 36

Atom	X	Y	Z	Atom	X	Y	Z
C	2.8762222	6.8980733	-1.3822632	C	0.8706341	-0.2797771	-3.8444239
C	1.6332959	7.3211226	-0.996795	C	2.1198401	0.0072837	-3.2855722
C	0.7964722	6.5506692	-0.0911308	C	2.3441431	1.192785	-2.5853209
C	1.2501377	5.2499601	0.453646	C	-1.6568402	14.610574	5.4377942
C	2.5824665	4.6748756	-0.0863519	C	-1.4776832	14.856215	6.7910578
C	3.3575335	5.5647966	-1.1012029	C	-1.5828504	13.823873	7.7372468
C	0.9836418	8.4875015	-1.553789	C	-1.8451532	12.521153	7.3380711
C	-0.3259705	8.7306914	-1.3350871	C	-2.0151908	12.238201	5.9791322
O	-1.0499477	8.0089892	-0.420084	C	3.7292488	1.4179672	-2.0182773
C	-0.4688261	6.9439893	0.1710168	O	-0.9795037	2.732316	-2.9302884
C	-1.1960717	9.6488922	-2.1694783	O	0.6198385	-1.4320813	-4.5215627
C	-2.4416832	10.11172	-1.4392472	C	-1.4902477	15.780028	4.4927088
C	-3.6197901	9.4913749	-1.6884729	O	-1.4009876	14.165756	9.0411486
C	-3.8801757	8.3606982	-2.6360534	O	-2.2433212	10.953309	5.6666059
C	-2.6328859	7.8556612	-3.3836125	H	3.4755132	7.4877037	-2.0696464
C	-1.560906	8.9566053	-3.5253899	H	1.5102601	9.0890246	-2.2884036
C	-2.3614948	11.193802	-0.4615154	H	-1.1444039	6.4119362	0.8275955
C	-3.6323581	11.547755	0.1538952	H	-0.5898379	10.523863	-2.4212656
C	-4.7562394	10.87276	-0.1725359	H	-4.6346136	8.7010706	-3.3543822
O	-4.7883345	9.8673524	-1.0677446	H	-4.3200307	7.5295096	-2.0734289
C	-1.200377	11.82729	-0.1122543	H	-2.9399223	7.5964578	-4.4040026
C	-1.1465553	12.880676	0.8843445	H	-0.6445329	8.5128649	-3.9275953
C	-2.4846479	13.507967	1.3604538	H	-5.7260683	11.07996	0.2623239
C	-3.7339672	12.628628	1.1689739	H	-0.2397639	11.527374	-0.5155451
O	-2.3649003	13.901689	2.7366413	H	-2.8116269	14.615038	-0.486954
C	-2.1957439	12.892931	3.6144536	H	-3.6109805	15.306429	0.9481387
C	-1.952869	13.280823	5.0022315	H	-1.8399106	15.469006	0.7343393
C	-2.7038495	14.8164	0.5839607	H	3.7712857	5.2483099	1.6309178
O	2.293887	3.3941042	-0.7227151	H	2.9830133	3.6595689	1.7704055
C	1.4315671	3.4238128	-1.7604261	H	4.4136018	3.8741001	0.7043576
C	1.2854467	2.1298171	-2.4570876	H	-1.469324	11.601917	-5.359479
C	3.5012635	4.3364828	1.0873495	H	-0.5718806	5.3666071	-2.9351528
O	0.6123289	4.6252915	1.2829884	H	-1.1400156	0.3975594	-4.1745078
O	4.3538784	5.0848512	-1.6383408	H	2.9341799	-0.7047872	-3.4009059
O	-4.7710838	12.878909	1.7568982	H	-1.243591	15.854759	7.1440203
O	-0.0969672	13.351126	1.3060926	H	-1.9106952	11.701383	8.0479553

C	-2.0141696	9.992379	-4.5532068	H	4.4370346	0.7227854	-2.4798671
C	-2.1012323	6.5353073	-2.7983162	H	4.087398	2.4387636	-2.1721723
O	-3.0212969	9.9322609	-5.2230349	H	3.7392047	1.2442614	-0.936895
O	-1.1202509	11.002211	-4.672944	H	-1.7923609	2.343969	-3.2906392
O	-0.9221795	6.1997685	-3.3386259	H	1.4228253	-1.976831	-4.529666
O	-2.703839	5.8578035	-1.9924422	H	-1.1231898	16.650646	5.0437475
O	0.8364547	4.4546116	-2.0512735	H	-0.78473	15.548756	3.6895852
O	-2.276686	11.719331	3.2209267	H	-2.436812	16.049432	4.013946
C	0.0323372	1.8311215	-3.0542391	H	-1.4906905	13.371909	9.5921186
C	-0.1768637	0.6313355	-3.7295865	H	-2.2918524	10.896449	4.6785086

NImag	0
Σ Electronic and thermal Free Energy	-1865692.367
mol Fraction	3.09E-08

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 37

Atom	X	Y	Z	Atom	X	Y	Z
C	1.8351746	6.9752083	-1.6573227	C	2.1823574	-1.1919006	-1.9579654
C	0.5217994	7.3319571	-1.5886593	C	1.056867	-0.6283987	-2.5667329
C	-0.4766058	6.489193	-0.9424328	C	0.7754985	0.73094	-2.4322751
C	-0.1008289	5.1895317	-0.3228158	C	-1.9381482	11.472744	5.9667898
C	1.4068715	4.9125958	-0.1648303	C	-1.3236356	11.544751	7.2093713
C	2.3361999	5.7204417	-1.1164555	C	-0.1178725	12.244749	7.3654073
C	-0.0189206	8.5442895	-2.1758311	C	0.4889536	12.866702	6.281078
C	-1.3338192	8.834842	-2.1199186	C	-0.1140699	12.815741	5.0183358
O	-2.2295838	8.0143495	-1.475163	C	-0.4571716	1.2706986	-3.1226316
C	-1.772971	6.8664154	-0.9198635	O	3.6021521	1.7430902	-0.3157679
C	-2.0083017	10.020634	-2.7773764	O	2.4930739	-2.5131691	-2.0746486
C	-3.0878346	10.633215	-1.8987645	C	-3.2354209	10.707444	5.834669
C	-4.3934855	10.41701	-2.1936609	O	0.4249887	12.268457	8.6154185
C	-4.9560575	9.6434903	-3.3455164	O	0.5832732	13.40141	4.0238212
C	-3.8957455	8.9159208	-4.1861126	H	2.5583015	7.5953363	-2.1788709
C	-2.5493043	9.6690127	-4.2004122	H	0.6477376	9.2277293	-2.6927479
C	-2.7178504	11.441903	-0.7398276	H	-2.5636499	6.2854137	-0.4623993
C	-3.8412384	11.9734	0.0162376	H	-1.2226151	10.766886	-2.9251132
C	-5.1071781	11.697556	-0.3657083	H	-5.5096839	10.346358	-3.9787118
O	-5.4113765	10.947589	-1.441562	H	-5.678647	8.9160327	-2.9611054
C	-1.4227472	11.681317	-0.3553379	H	-4.251578	8.8986637	-5.2239925
C	-1.1022969	12.432458	0.8334983	H	-1.7923183	9.0501044	-4.693529
C	-2.2056419	13.28137	1.5041561	H	-5.9830814	12.053938	0.1617182
C	-3.646205	12.821279	1.2258394	H	-0.580388	11.227124	-0.8625258
O	-1.9306986	13.323107	2.90558	H	-2.25203	14.798773	-0.0654352
C	-2.0168056	12.108897	3.5440021	H	-2.8118108	15.350746	1.5351974
C	-1.3532517	12.1405	4.8566346	H	-1.0681426	15.099498	1.2303181
C	-2.0753677	14.73416	1.013175	H	1.6570282	6.3096022	1.4944106
O	1.6525703	3.5087279	-0.3076044	H	1.1994488	4.6528105	1.9715828
C	1.3254191	2.9952704	-1.5150039	H	2.8637836	5.001429	1.4160393
C	1.6273522	1.5491938	-1.6485181	H	-1.6959817	12.418432	-5.6479046
C	1.8068566	5.2458821	1.2824964	H	-2.7051826	5.9211707	-4.1017714
O	-0.9339689	4.413424	0.1106073	H	3.9114923	-0.8511427	-0.7352659
O	3.4753542	5.3222048	-1.3127668	H	0.3905289	-1.2576058	-3.1531345
O	-4.5791962	13.230825	1.8913287	H	-1.7644675	11.065347	8.0769237
O	0.0317987	12.472406	1.3183787	H	1.4428365	13.378658	6.3751503

C	-2.6803429	10.927024	-5.0600853	H	-1.0617596	0.4462688	-3.5131111
C	-3.7844344	7.4404404	-3.8033871	H	-1.0758359	1.864283	-2.4430075
O	-3.6554393	11.241392	-5.7058508	H	-0.186104	1.9315225	-3.9509295
O	-1.5406229	11.655272	-5.0592252	H	4.3606251	1.2074353	-0.0348937
O	-2.687448	6.8655416	-4.3495319	H	1.8230697	-2.9462689	-2.6266237
O	-4.5990245	6.8218418	-3.1584139	H	-3.5874612	10.385549	6.8188916
O	0.7900069	3.6797024	-2.3745849	H	-4.0209259	11.312593	5.3693305
O	-2.5846226	11.166773	3.0199224	H	-3.109298	9.8240145	5.201404
C	2.7617619	0.958635	-1.0375277	H	1.2488741	12.780298	8.5905889
C	3.0373628	-0.4001954	-1.1972055	H	0.2121195	13.202398	3.1365368

NImag	0
Σ Electronic and thermal Free Energy	-1865688.115
mol Fraction	2.34E-11

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 38

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0909782	7.2553079	-1.9193089	C	3.1566726	-0.7831878	-2.2657839
C	0.7531233	7.5078527	-1.8302037	C	3.6945718	-0.0835208	-1.1737051
C	-0.1609371	6.6150354	-1.1310197	C	3.3435875	1.2348142	-0.9225335
C	0.3262811	5.3754029	-0.4703127	C	-1.6454692	11.110863	5.8264456
C	1.8543864	5.231045	-0.3407732	C	-0.9882694	11.158775	7.0479973
C	2.6998828	6.0710801	-1.3406389	C	0.1824078	11.918034	7.1951441
C	0.1078025	8.6616016	-2.4271908	C	0.7116934	12.624212	6.1217861
C	-1.2218479	8.8625906	-2.3331941	C	0.0639276	12.599019	4.8807287
O	-2.0383701	7.9912528	-1.6495368	C	4.0016659	1.9152986	0.2574172
C	-1.4802731	6.8967997	-1.0827624	O	1.0756385	1.7102707	-3.821389
C	-1.9847685	10.020417	-2.945019	O	3.5538219	-2.0747731	-2.4232623
C	-3.0587407	10.548747	-2.0060902	C	-2.9030381	10.280459	5.7038598
C	-4.3614344	10.272731	-2.2570792	O	0.7706228	11.912982	8.4242885
C	-4.9273623	9.5244072	-3.4237357	O	0.6892089	13.26977	3.892002
C	-3.8644296	8.8780417	-4.3307575	H	2.7495629	7.9120231	-2.4797542
C	-2.5560422	9.6882821	-4.3613423	H	0.7090536	9.3843308	-2.9700612
C	-2.6861643	11.334206	-0.8312099	H	-2.2070262	6.2724701	-0.5786183
C	-3.8050584	11.771841	-0.0106344	H	-1.245405	10.811926	-3.0959149
C	-5.0688042	11.441098	-0.3534258	H	-5.5120758	10.238677	-4.0162932
O	-5.3762024	10.716541	-1.4463677	H	-5.6326687	8.7743592	-3.0550005
C	-1.392044	11.63282	-0.4888009	H	-4.2699101	8.8938846	-5.3507205
C	-1.0643813	12.351577	0.7187173	H	-1.7978789	9.0987435	-4.8892248
C	-2.1834984	13.107599	1.4693544	H	-5.9401619	11.727804	0.2218212
C	-3.6072744	12.58098	1.2251281	H	-0.5474877	11.249368	-1.0478854
O	-1.8550344	13.100508	2.8599449	H	-2.3740021	14.688997	-0.0241252
C	-1.8524049	11.855594	3.4426004	H	-2.8977257	15.136708	1.6206159
C	-1.1415447	11.862672	4.7301584	H	-1.1567448	14.99624	1.2386737
C	-2.1508999	14.585885	1.0428396	H	1.9945853	6.7004773	1.2630079
O	2.2275999	3.8482458	-0.446621	H	1.7130007	5.0271145	1.8074002
C	1.9394228	3.2600115	-1.6243312	H	3.3264397	5.5227886	1.2087355
C	2.417675	1.8892879	-1.7939682	H	-1.8550017	12.506372	-5.7558236
C	2.2478159	5.6502724	1.0853643	H	-4.3542068	5.7991645	-3.495718
O	-0.428526	4.5591391	0.0267446	H	1.8621261	-0.6756823	-4.0040478
O	3.8638597	5.7470935	-1.5379303	H	4.4017777	-0.597701	-0.5318714
O	-4.5338628	12.911429	1.9414888	H	-1.3682173	10.614775	7.9061883
O	0.0846451	12.433705	1.1603636	H	1.6387749	13.184655	6.2067014

C	-2.7595836	10.960304	-5.181433	H	4.7753095	1.2644339	0.6747566
C	-3.5739131	7.3999022	-4.0843393	H	4.4595106	2.8653865	-0.0322394
O	-3.7657528	11.250933	-5.7905688	H	3.2785761	2.141086	1.0473013
O	-1.6520418	11.735917	-5.1916576	H	0.954014	2.6621376	-3.5727736
O	-4.6172636	6.7387412	-3.5383902	H	3.1235422	-2.4443805	-3.2106551
O	-2.5491467	6.8463176	-4.4163948	H	-3.1985781	9.893599	6.6832409
O	1.2798331	3.8789345	-2.4730474	H	-3.7378764	10.861422	5.2972778
O	-2.3900003	10.909101	2.8943522	H	-2.7533549	9.4360247	5.0242038
C	1.9139579	1.1704332	-2.9228522	H	1.5634362	12.471638	8.3962574
C	2.2753062	-0.1629829	-3.1399042	H	0.2940256	13.093776	3.0106095

NImag	0
Σ Electronic and thermal Free Energy	-1865697.83
mol Fraction	0.000315077

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 39

Atom	X	Y	Z	Atom	X	Y	Z
C	1.621669	7.483371	-2.0737938	C	2.6055856	0.021339	0.1880047
C	0.3943098	8.0281044	-1.7975027	C	1.2205527	0.2319834	0.0931545
C	-0.3979519	7.6366484	-0.637616	C	0.7102932	1.5132872	-0.0797174
C	0.1306896	6.6719967	0.3531151	C	0.0360893	10.928955	4.4079935
C	1.5948838	6.2424443	0.1677911	C	0.8231506	10.164828	5.2645473
C	2.1868422	6.4515151	-1.2471357	C	0.7329079	8.7694264	5.2850323
C	-0.2284955	9.0289945	-2.6380888	C	-0.1618865	8.1148892	4.4446314
C	-1.4758499	9.482698	-2.3948767	C	-0.9705401	8.8582852	3.5792992
O	-2.2036604	9.0146985	-1.3326709	C	-0.787283	1.6967051	-0.1802436
C	-1.6404679	8.1557361	-0.4663191	O	3.9468979	3.3398532	-0.208128
C	-2.2243095	10.530427	-3.2141632	O	3.1329403	-1.2242498	0.3566611
C	-3.2917585	11.200934	-2.3645075	C	0.2655856	12.425191	4.4356131
C	-4.6045181	10.979438	-2.6100358	O	1.5444068	8.1051709	6.1514596
C	-5.1858135	10.21411	-3.7587349	O	-1.8639075	8.2069332	2.7959419
C	-4.1601673	9.2730656	-4.4011715	H	2.1616052	7.7504091	-2.9768597
C	-2.7824508	9.9522093	-4.5538043	H	0.3200886	9.4257712	-3.4868065
C	-2.8832562	11.946458	-1.1749937	H	-2.283523	7.952833	0.3780347
C	-3.9532267	12.179455	-0.22006	H	-1.4712451	11.272866	-3.4949854
C	-5.2346827	11.95262	-0.5777596	H	-5.5559507	10.916397	-4.5147228
O	-5.5908111	11.454143	-1.7818804	H	-6.0406828	9.6386944	-3.3940624
C	-1.6003491	12.334425	-0.9130705	H	-4.5063023	9.0224924	-5.41129
C	-1.1782235	12.840766	0.3788922	H	-2.0587077	9.2153127	-4.9189469
C	-2.2277213	13.054733	1.5077588	H	-6.0835885	12.13483	0.068908
C	-3.6709811	12.626868	1.1691373	H	-0.7952017	12.179561	-1.6228887
O	-1.772272	12.330542	2.677551	H	-2.5857629	15.154617	1.0888143
C	-1.6707042	10.983264	2.4965025	H	-2.9137153	14.661747	2.7668343
C	-0.8920608	10.278369	3.53722	H	-1.2239169	14.83409	2.1857886
C	-2.2379798	14.529102	1.918528	H	2.386292	8.1214714	0.9508733
O	1.7782475	4.8695964	0.5190146	H	2.0746722	6.8713639	2.1797283
C	1.074637	3.9819368	-0.2562132	H	3.4862889	6.7281507	1.0913171
C	1.6025159	2.6149011	-0.1295128	H	-1.7970432	12.334895	-6.4853534
C	2.4443916	7.0502461	1.1669008	H	-3.1114808	6.3295066	-3.6144333
O	-0.4915833	6.2994171	1.3413109	H	4.5636729	0.9163127	0.1298135
O	3.1573436	5.7617183	-1.573137	H	0.5397235	-0.6144277	0.158804
O	-4.5488705	12.71008	2.0106881	H	1.5384616	10.642687	5.92509
O	-0.0019133	13.083906	0.634201	H	-0.2600266	7.0314899	4.4631035

C	-2.8506131	11.022255	-5.6436169	H	-1.3013268	0.7526103	0.0234927
C	-4.0880537	7.9429742	-3.652906	H	-1.1561932	2.4475127	0.5265089
O	-3.7982577	11.234155	-6.3667713	H	-1.0756187	2.0432231	-1.1773234
O	-1.682734	11.69637	-5.7556707	H	3.5746029	4.2018421	-0.4995913
O	-3.0744159	7.1694299	-4.1112725	H	2.4097766	-1.8700309	0.3863863
O	-4.8543113	7.5788155	-2.7918581	H	1.0921389	12.657243	5.1133725
O	0.1357665	4.3558878	-0.9392128	H	0.5063613	12.812745	3.44166
O	-2.1755044	10.468476	1.5092402	H	-0.6233574	12.962993	4.7774115
C	3.0071177	2.3849342	-0.072235	H	1.3889404	7.1508351	6.0694175
C	3.4937377	1.0846817	0.0964484	H	-1.5244934	7.3145994	2.5829801

NImag	0
Σ Electronic and thermal Free Energy	-1865686.697
mol Fraction	2.13E-12

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 40

Atom	X	Y	Z	Atom	X	Y	Z
C	1.6832087	6.9640638	-1.8324084	C	3.1645848	-0.7611696	-1.8112708
C	0.3675499	7.3314706	-1.7419702	C	1.8288723	-0.6137141	-2.2135962
C	-0.6104981	6.5462548	-1.0047142	C	1.1977545	0.6188338	-2.1133959
C	-0.2236085	5.2992137	-0.2873053	C	-0.7802536	13.069544	5.4637977
C	1.2882146	5.0344392	-0.1764337	C	-0.476575	12.922386	6.8106875
C	2.1706732	5.7478399	-1.2307426	C	-0.8649614	11.777508	7.5279374
C	-0.1804265	8.5088746	-2.3823642	C	-1.5436496	10.744888	6.8985439
C	-1.4886743	8.8268787	-2.2899107	C	-1.8483671	10.854331	5.5403693
O	-2.366801	8.0566792	-1.5683695	C	-0.2420392	0.7425981	-2.5584049
C	-1.9009824	6.9421461	-0.9615933	O	4.0658587	2.569138	-0.7665441
C	-2.1522944	10.022137	-2.9446049	O	3.7159996	-2.0015643	-1.9415342
C	-3.1780041	10.673234	-2.0301535	C	-0.2894288	14.322974	4.773408
C	-4.498255	10.512631	-2.2827117	O	-0.5806626	11.630815	8.8494018
C	-5.1261585	9.7848338	-3.4306441	O	-2.4847417	9.8092758	4.9890142
C	-4.123624	9.0063898	-4.3017899	H	2.3846631	7.5338779	-2.4338922
C	-2.7449437	9.6888133	-4.3520265	H	0.475478	9.1556367	-2.9566093
C	-2.7364948	11.458546	-0.8765168	H	-2.6736877	6.4024253	-0.4289074
C	-3.8159373	12.022158	-0.0778664	H	-1.3479148	10.74235	-3.1188264
C	-5.1032178	11.79976	-0.4192047	H	-5.632691	10.53164	-4.0543038
O	-5.4732773	11.074447	-1.4931643	H	-5.9050345	9.1203218	-3.0462015
C	-1.4269224	11.655361	-0.5366324	H	-4.5205114	9.0183887	-5.3252156
C	-1.019074	12.408875	0.6360208	H	-2.0429331	9.0107567	-4.8505868
C	-2.08616	13.259647	1.3739524	H	-5.9469252	12.182218	0.1414236
C	-3.547631	12.837941	1.136637	H	-0.6152216	11.195779	-1.0875563
O	-1.7983392	13.266756	2.7813065	H	-2.1403689	14.815442	-0.149807
C	-1.9090353	12.072231	3.3982015	H	-2.6380946	15.346439	1.4767974
C	-1.4998976	12.030957	4.7995878	H	-0.909298	15.048355	1.113062
C	-1.9342848	14.720526	0.9214969	H	1.5670486	6.5639909	1.3588264
O	1.5809006	3.63775	-0.2384593	H	1.1668622	4.9395317	1.9758507
C	1.2325949	3.0270507	-1.4187904	H	2.8037301	5.2832339	1.345404
C	1.9043648	1.7258943	-1.5711742	H	-1.7760854	12.373534	-5.8460389
C	1.7373276	5.4911128	1.2238845	H	-4.9111748	6.0203207	-3.3658785
O	-1.0364308	4.5933208	0.2796885	H	4.9294239	0.2349859	-1.0402473
O	3.282834	5.2702404	-1.4700804	H	1.3015589	-1.4794897	-2.599967
O	-4.4395192	13.239967	1.8619462	H	0.0813426	13.705604	7.3197514
O	0.1418344	12.460709	1.0231854	H	-1.8275538	9.8507339	7.4404158

C	-2.82355	10.940646	-5.2232202	H	-0.6444724	-0.2409703	-2.817534
C	-3.9741204	7.5193809	-3.9922705	H	-0.8741547	1.1781844	-1.7769678
O	-3.7928054	11.296713	-5.8568163	H	-0.3302476	1.3989998	-3.429429
O	-1.6494466	11.611035	-5.2497151	H	3.6486171	3.4544737	-0.8564197
O	-5.0865275	6.9772665	-3.4517215	H	4.6339188	-1.9706679	-1.6287957
O	-2.9957457	6.8628035	-4.2729973	H	0.3642946	14.885791	5.4463885
O	0.4603036	3.5590867	-2.1960048	H	0.2659756	14.087033	3.861336
O	-2.3622164	11.102042	2.7719551	H	-1.1197171	14.972209	4.4787639
C	3.2671048	1.5741598	-1.2010968	H	-0.1013051	12.41526	9.1596568
C	3.882651	0.3215731	-1.3189935	H	-2.5862468	10.000888	4.023699

NImag	0
Σ Electronic and thermal Free Energy	-1865697.666
mol Fraction	0.000238909

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 41

Atom	X	Y	Z	Atom	X	Y	Z
C	1.9577843	7.1204746	-1.9981438	C	2.9248404	-0.9394955	-1.9205659
C	0.6357496	7.4325877	-1.8738528	C	3.7800133	-0.0108711	-1.3241752
C	-0.2883729	6.5969722	-1.1207518	C	3.3972199	1.3211186	-1.1686321
C	0.1733929	5.3589705	-0.4367174	C	-0.3322882	13.326913	5.3440146
C	1.6984802	5.1558908	-0.3468591	C	0.0558038	13.230153	6.6718506
C	2.5354001	5.9263245	-1.4075793	C	-0.1925324	12.067294	7.4192779
C	0.0188813	8.5967034	-2.480674	C	-0.8152016	10.971692	6.8386348
C	-1.2971945	8.8563489	-2.3474548	C	-1.205763	11.03237	5.49733
O	-2.1253351	8.0357969	-1.6164338	C	4.3837303	2.2631627	-0.5132517
C	-1.5927434	6.9333292	-1.0386669	O	0.053521	1.1950195	-2.6824211
C	-2.0322915	10.031827	-2.9588079	O	3.3698223	-2.2241198	-2.0270627
C	-3.0266376	10.644732	-1.984695	C	0.0083644	14.607424	4.6142246
C	-4.3505237	10.41762	-2.1518723	O	0.2175899	12.072555	8.7156694
C	-5.0142415	9.6483565	-3.2517146	O	-1.7826962	9.9279371	4.9992676
C	-4.0343817	8.93499	-4.201389	H	2.6242783	7.7313384	-2.5996165
C	-2.6966055	9.6859452	-4.330072	H	0.6309163	9.2801889	-3.0609629
C	-2.5523514	11.46111	-0.8660799	H	-2.326956	6.3519921	-0.4955398
C	-3.6064523	11.981979	-0.0063767	H	-1.2633683	10.778594	-3.175017
C	-4.9001504	11.693098	-0.2634503	H	-5.6144281	10.360769	-3.8308823
O	-5.3011644	10.938843	-1.3054266	H	-5.7168999	8.9353998	-2.8110875
C	-1.2353306	11.7223	-0.608582	H	-4.4971566	8.9442102	-5.1967088
C	-0.7932952	12.512454	0.5271679	H	-1.9963392	9.0489723	-4.8824669
C	-1.8543669	13.324728	1.3161178	H	-5.7244117	12.040544	0.3467475
C	-3.3032048	12.823151	1.1818975	H	-0.4382301	11.291838	-1.2025698
O	-1.4795815	13.382853	2.7014227	H	-2.0862507	14.837507	-0.234402
C	-1.4835002	12.201282	3.350677	H	-2.5077038	15.383251	1.4090332
C	-0.9968586	12.219938	4.7277657	H	-0.7922424	15.164177	0.9419066
C	-1.8087035	14.780022	0.8233056	H	1.9462162	6.6893263	1.1873662
O	2.0057322	3.7583326	-0.399322	H	1.6193194	5.0512161	1.8106737
C	1.6661681	3.1521256	-1.5721064	H	3.2293519	5.4578821	1.1436118
C	2.1271344	1.7418341	-1.6412378	H	-1.9616436	12.433413	-5.8421782
C	2.1530885	5.6233727	1.0469133	H	-4.5741527	5.9033516	-3.2314058
O	-0.5982146	4.5935015	0.1124739	H	0.996871	-1.2640554	-2.8453889
O	3.6796956	5.5565795	-1.6454828	H	4.7548625	-0.3466678	-0.9868893
O	-4.1651405	13.183448	1.9634607	H	0.5688039	14.053026	7.1577809
O	0.3847783	12.627386	0.8411589	H	-1.0012559	10.053814	7.3891548

C	-2.8933122	10.942496	-5.1746667	H	5.3829888	1.8173458	-0.5182629
C	-3.7890982	7.4519219	-3.936781	H	4.4262781	3.2366965	-1.0073915
O	-3.9187259	11.259176	-5.7373057	H	4.1026585	2.4521703	0.5289004
O	-1.7575723	11.670629	-5.2682166	H	-0.4189544	0.4266772	-3.0383348
O	-4.8055639	6.8509038	-3.2803242	H	2.6920428	-2.7620426	-2.4650736
O	-2.8233779	6.8445378	-4.3428355	H	0.6314826	15.241065	5.2517456
O	1.0463334	3.7447429	-2.4339844	H	0.5472669	14.407324	3.6837281
O	-1.9095678	11.188996	2.7729807	H	-0.8911803	15.16915	4.3440496
C	1.2793431	0.7915135	-2.2530027	H	-0.0005611	11.218175	9.1210206
C	1.6709512	-0.5432966	-2.3833557	H	-1.9605366	10.09806	4.0394882

NImag	0
Σ Electronic and thermal Free Energy	-1865688.773
mol Fraction	7.11E-11

(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 42

Atom	X	Y	Z	Atom	X	Y	Z
C	2.0760665	7.1112468	-1.8237901	C	2.3832152	-1.0498252	-2.2339225
C	0.7557916	7.4010492	-1.6512448	C	1.9944699	-0.588006	-0.9743231
C	-0.1403868	6.5241673	-0.9073669	C	1.7737374	0.7695398	-0.7462788
C	0.3517629	5.2633016	-0.2956363	C	-1.6393032	11.631986	5.9725814
C	1.8762326	5.0404051	-0.291809	C	-0.9773318	11.800715	7.1833007
C	2.6840115	5.893345	-1.3119529	C	0.1735185	12.600791	7.2630468
C	0.1041146	8.5670967	-2.2185743	C	0.6823034	13.228458	6.1335533
C	-1.218425	8.7819047	-2.0738864	C	0.0320209	13.080334	4.9047479
O	-2.0138216	7.9310295	-1.3417828	C	1.3543001	1.1934975	0.6448602
C	-1.4512047	6.8296572	-0.792961	O	2.4591935	2.0985209	-4.0982588
C	-2.0120779	9.8969243	-2.7221935	O	2.5903819	-2.3899713	-2.3725613
C	-3.09172	10.44991	-1.8056368	C	-2.8741226	10.760604	5.9271235
C	-4.3891528	10.124962	-2.0279328	O	0.8428264	12.782026	8.4368569
C	-4.9442688	9.2738084	-3.1276358	O	0.6327572	13.679298	3.8569062
C	-3.8713846	8.6063906	-4.0017902	H	2.7198292	7.758122	-2.4124118
C	-2.5936985	9.4646131	-4.1065621	H	0.6888312	9.271003	-2.8028028
C	-2.729352	11.31667	-0.687185	H	-2.1701233	6.2185971	-0.2621924
C	-3.8527085	11.784175	0.1102616	H	-1.2941927	10.695937	-2.9279713
C	-5.1104798	11.401649	-0.2001556	H	-5.5835903	9.9102499	-3.7502177
O	-5.4075071	10.598467	-1.2390193	H	-5.5855373	8.5036513	-2.6862933
C	-1.4392478	11.661614	-0.373142	H	-4.2757446	8.5268305	-5.0187392
C	-1.120382	12.469227	0.7789535	H	-1.8151052	8.8945451	-4.6242283
C	-2.2523952	13.255151	1.4784846	H	-5.9848505	11.706104	0.3612645
C	-3.6648871	12.678721	1.2868743	H	-0.5900677	11.256455	-0.9098473
O	-1.9151563	13.365691	2.8623822	H	-2.4898678	14.710261	-0.1323274
C	-1.8741237	12.172132	3.5412551	H	-3.0130652	15.27338	1.4768817
C	-1.1570376	12.302162	4.8196257	H	-1.2719966	15.143044	1.0927568
C	-2.2575135	14.696077	0.937515	H	2.2533858	6.4155301	1.3579098
O	2.150179	3.6466234	-0.4997287	H	1.8870913	4.7427957	1.85226
C	1.6615455	3.1437935	-1.6653054	H	3.4798256	5.1452465	1.1390273
C	1.9255926	1.6898207	-1.8141006	H	-2.0414254	12.233273	-5.6593459
C	2.4081303	5.3590961	1.1146446	H	-2.4274718	5.7236714	-3.8909542
O	-0.3995631	4.4668834	0.2426605	H	2.8440128	-0.5104971	-4.2772158
O	3.8271465	5.5548103	-1.5847327	H	1.8648205	-1.3100518	-0.1751392
O	-4.5926414	13.033523	1.9901018	H	-1.3575081	11.310575	8.0774433
O	0.0284417	12.606689	1.2069442	H	1.5922425	13.814284	6.1886206

C	-2.8699373	10.683759	-4.9873318	H	0.9976939	0.326024	1.2081461
C	-3.6194211	7.1577015	-3.5825238	H	2.1998126	1.6278971	1.1893103
O	-3.8980001	10.900297	-5.589662	H	0.5668946	1.9513448	0.6309466
O	-1.7951848	11.50159	-5.0617691	H	2.792716	1.6305797	-4.8793508
O	-2.5060836	6.657499	-4.1664065	H	2.8514046	-2.5814388	-3.2868251
O	-4.3473954	6.4981796	-2.8772408	H	-3.1595914	10.451252	6.9370001
O	1.0710112	3.8477939	-2.4637996	H	-3.7248209	11.281167	5.4746291
O	-2.3879947	11.169932	3.0759685	H	-2.7026368	9.8649661	5.3224139
C	2.3020771	1.2047696	-3.0854611	H	0.3937314	12.279577	9.1345167
C	2.5404068	-0.1562583	-3.2926355	H	0.2387142	13.417298	2.9969069

NImag	0
Σ Electronic and thermal Free Energy	-1865686.824
mol Fraction	2.64E-12

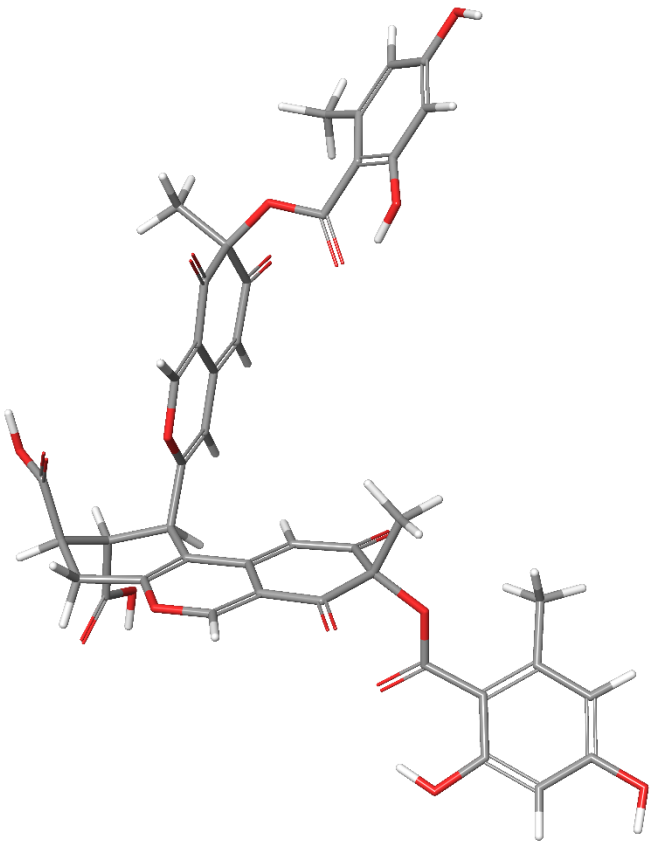
(8*S*, 13*S*, 8a*S*, 12a*S*, 13a*S*)-Diazaphilonic acid (2) - Conformer 43

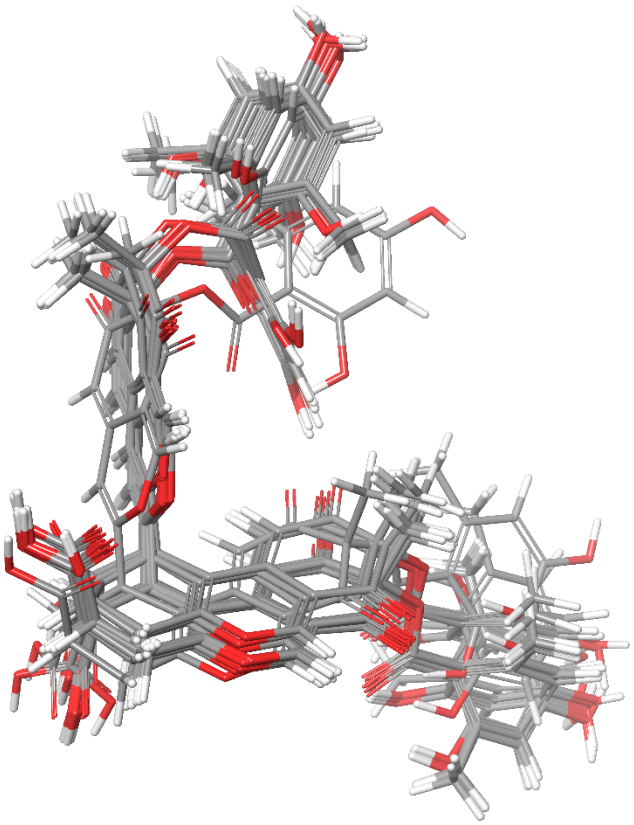
Atom	X	Y	Z	Atom	X	Y	Z
C	2.6971574	6.4159281	-1.1834397	C	1.4170991	1.0030451	-5.182302
C	1.4052814	6.8032004	-0.9425129	C	2.4583471	0.8775858	-4.2509798
C	0.5635453	6.1398103	0.0371197	C	2.4175477	1.5317496	-3.0269638
C	1.0498804	4.9383028	0.7708867	C	-2.0659582	12.159147	6.1548781
C	2.3882186	4.3039966	0.2776715	C	-1.5559065	12.575301	7.3769874
C	3.3041928	5.2682494	-0.5507732	C	-0.5286893	13.529325	7.4295792
C	0.7575778	7.8913168	-1.6411533	C	0.0048288	14.065048	6.2637366
C	-0.5355756	8.2095043	-1.413843	C	-0.4969528	13.667975	5.0182382
O	-1.2706143	7.576757	-0.4504561	C	3.5938083	1.3376026	-2.096051
C	-0.7008493	6.5645718	0.2436253	O	-0.885791	3.191507	-3.4586379
C	-1.3319445	9.2340023	-2.2026303	O	1.5537529	0.3275679	-6.3517594
C	-2.5438374	9.7436007	-1.4480929	C	-3.1706039	11.126951	6.1358572
C	-3.7489275	9.1805404	-1.70502	O	-0.0793421	13.885361	8.6662106
C	-4.0455353	8.0601851	-2.6516239	O	0.1268252	14.203613	3.9494487
C	-2.8799703	7.6567109	-3.5791305	H	3.3213227	6.9668915	-1.8807984
C	-1.7441156	8.7034083	-3.6138124	H	1.3050428	8.4348526	-2.4052376
C	-2.4131992	10.797665	-0.4499247	H	-1.3821825	6.1161094	0.954287
C	-3.6642119	11.195826	0.1763718	H	-0.657996	10.076018	-2.3848156
C	-4.8177829	10.57772	-0.1597642	H	-4.9154223	8.3563257	-3.2473606
O	-4.8954457	9.5917002	-1.0740858	H	-4.3446032	7.1869104	-2.0585975
C	-1.2174507	11.363569	-0.0854945	H	-3.26417	7.601114	-4.6022898
C	-1.1277544	12.358582	0.9539979	H	-0.8586415	8.2575782	-4.0795214
C	-2.4198977	13.061122	1.4304248	H	-5.7765985	10.820031	0.2811023
C	-3.7192118	12.268143	1.209037	H	-0.271979	11.015187	-0.4852262
O	-2.2454445	13.404573	2.806286	H	-2.6759007	14.235863	-0.3921229
C	-2.1241471	12.330486	3.6553147	H	-3.4318712	14.930333	1.066018
C	-1.5617031	12.729882	4.9547197	H	-1.6581261	15.000474	0.8531683
C	-2.5557736	14.399924	0.6837306	H	3.3843405	4.4847939	2.1778294
O	2.1864826	3.1853825	-0.6685839	H	2.5201617	2.9542634	1.9472104
C	1.1313992	3.1436144	-1.4902957	H	4.0730201	3.2604789	1.0938482
C	1.2808303	2.3386775	-2.7082995	H	-1.4983216	11.506539	-5.1803205
C	3.1423147	3.7020045	1.4521599	H	-1.2404327	4.9059072	-4.0445135
O	0.4863211	4.5056645	1.7577423	H	-0.521873	1.890437	-5.594944
O	4.4815517	4.9579891	-0.7050598	H	3.3063946	0.2539884	-4.5121734
O	-4.7543792	12.585352	1.7648292	H	-1.9426424	12.173397	8.3074262
O	-0.0575244	12.719698	1.4512295	H	0.8278276	14.774351	6.2841898

C	-2.1528586	9.8751824	-4.5075558	H	4.2991696	0.6275475	-2.53639
C	-2.3568206	6.2477776	-3.2799498	H	4.1185824	2.278008	-1.9036973
O	-3.2028675	9.9790951	-5.1003098	H	3.2790116	0.9520369	-1.1216605
O	-1.1707661	10.802636	-4.5885498	H	-0.8551196	3.4976226	-2.5068576
O	-1.5036103	5.8420819	-4.2342077	H	0.7743451	0.4844122	-6.9084063
O	-2.6910808	5.5628399	-2.3350895	H	-3.5104432	10.916848	7.1540041
O	0.0980429	3.7761964	-1.2309488	H	-4.0319691	11.461451	5.5477157
O	-2.458294	11.213612	3.3008779	H	-2.8289675	10.192386	5.6805928
C	0.2298032	2.4421803	-3.6694931	H	0.6241296	14.546112	8.5666497
C	0.3030209	1.7852281	-4.8959013	H	-0.1401301	13.777394	3.1057399

NImag	0
Σ Electronic and thermal Free Energy	-1865694.988
mol Fraction	2.59E-06

Data S2. Lowest energy conformer 3D structure, all overlaid 3D structures, cartesian coordinates, number of imaginary frequencies, and energy for (8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid conformers.





(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 1

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.0182255	-4.5273796	-5.2433298	C	-10.413137	-3.331551	-8.2974464
C	-2.9644178	-3.904529	-4.030264	C	-9.9999744	-4.6507734	-8.0492968
C	-4.1180593	-3.8299586	-3.142977	C	-8.8642951	-4.9183669	-7.2998305
C	-5.4168946	-4.4530021	-3.5123159	C	0.1403582	6.0749395	-5.8745651
C	-5.4144464	-5.3535686	-4.7635454	C	0.8378934	7.1145717	-6.4714178
C	-4.2318101	-5.1408602	-5.7515177	C	2.1266424	7.4677903	-6.0397242
C	-1.7792906	-3.2439839	-3.5160769	C	2.7480079	6.7662227	-5.016295
C	-1.7731368	-2.6207479	-2.3202341	C	2.0771799	5.7028529	-4.4045006
O	-2.8998699	-2.5650217	-1.5322266	C	-8.4802156	-6.369969	-7.1159526
C	-4.0274524	-3.1727169	-1.9658872	O	-7.8484401	-1.4061757	-6.6606822
C	-0.5837537	-1.94456	-1.6745764	O	-11.544937	-3.1719433	-9.0340148
C	-0.9355561	-0.5752729	-1.11303	C	-1.2279106	5.7485974	-6.4309682
C	-1.0501936	-0.4103346	0.2262085	O	2.7246844	8.5075706	-6.6804612
C	-0.8324864	-1.4327742	1.297952	O	2.748562	5.0570957	-3.4380004
C	-0.5878895	-2.8537685	0.768511	H	-2.1594098	-4.5342171	-5.9078476
C	0.1090694	-2.85241	-0.6087858	H	-0.8699603	-3.2482975	-4.1087768
C	-1.1458018	0.5556089	-2.019034	H	-4.8477736	-3.07149	-1.2663249
C	-1.4580674	1.8135769	-1.3542167	H	0.146339	-1.8058595	-2.4766108
C	-1.5419107	1.8698758	-0.0080188	H	-1.7005977	-1.4356774	1.9652652
O	-1.3551594	0.8032262	0.7944526	H	0.0298843	-1.1093611	1.8923931
C	-1.0316722	0.4847956	-3.3791557	H	0.1060558	-3.3482316	1.4601532
C	-1.1744054	1.6420825	-4.2462589	H	0.1283687	-3.8724479	-1.0075636
C	-1.7868928	2.9352817	-3.6478424	H	-1.7643743	2.7758681	0.5415515
C	-1.6735444	3.0709979	-2.1190212	H	-0.7718529	-0.4350905	-3.8885468
O	-1.2037145	4.081411	-4.2878791	H	-3.8111823	2.1324181	-3.5704116
C	0.1135356	4.2595252	-4.0668132	H	-3.7160515	3.9100186	-3.6559522
C	0.7487364	5.351293	-4.8009788	H	-3.3764514	2.9155147	-5.1065733
C	-3.2779763	2.976559	-4.0196784	H	-4.4650783	-7.0251571	-3.7393417
O	-6.6558284	-5.2088917	-5.4719879	H	-6.2456644	-7.0067612	-3.6457599
C	-6.9099567	-3.9708926	-5.9420134	H	-5.4244304	-7.4716484	-5.1684384
C	-8.1027582	-3.8283264	-6.7723376	H	3.1441951	-2.1201478	-1.4141349
C	-5.3860016	-6.8167484	-4.2942039	H	-2.5092905	-5.3969995	0.3300953
O	-6.4134905	-4.3455482	-2.8206137	H	-9.9645024	-1.2273717	-8.0141083
O	-4.3431173	-5.5679899	-6.8934936	H	-10.5883	-5.4604013	-8.4674015

O	-1.8435348	4.1455893	-1.5716612	H	0.4006108	7.6719351	-7.2927225
O	-0.9042633	1.6160987	-5.4400168	H	3.7518646	7.0066588	-4.6776086
C	1.5755207	-2.4513902	-0.4281292	H	-9.1255171	-7.0033172	-7.7313419
C	-1.8487107	-3.7105726	0.836889	H	-7.4389191	-6.5480332	-7.3992826
O	2.1271244	-2.2668808	0.6338744	H	-8.5824429	-6.6849557	-6.0727873
O	2.220191	-2.3652485	-1.6124837	H	-7.0318993	-1.723112	-6.1978165
O	-1.6941625	-4.8835133	0.1733233	H	-11.720798	-2.2238885	-9.1441043
O	-2.8479102	-3.445797	1.464303	H	-1.411016	6.3408744	-7.3319924
O	-6.1554096	-3.035114	-5.6342111	H	-1.315395	4.6880707	-6.6837128
O	0.7023657	3.5266147	-3.2564606	H	-2.0198693	5.9674495	-5.7080693
C	-8.5192501	-2.4931718	-7.0719235	H	3.605702	8.6504858	-6.2994324
C	-9.6781771	-2.2567645	-7.8177425	H	2.1738945	4.3091232	-3.1339909

NImag	0
Σ Electronic and thermal Free Energy	-1865700.806
mol Fraction	0.316019856

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 2

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2661341	-4.3209472	-5.1564009	C	-10.833947	-2.8860571	-7.62865
C	-3.1179577	-3.7554674	-3.9232544	C	-10.42605	-4.2206963	-7.4705569
C	-4.2059173	-3.706227	-2.9549335	C	-9.2457482	-4.537768	-6.8152475
C	-5.5374752	-4.2939145	-3.2601289	C	0.0170428	6.2557943	-5.5295167
C	-5.6368326	-5.135788	-4.5477503	C	0.6885493	7.3124943	-6.1262409
C	-4.5221626	-4.893748	-5.6055156	C	2.0099205	7.6279984	-5.7706563
C	-1.8891555	-3.1354536	-3.4640456	C	2.689243	6.8714997	-4.8262374
C	-1.7897157	-2.568096	-2.2447368	C	2.0450104	5.790057	-4.2175439
O	-2.8580387	-2.5334838	-1.3780864	C	-8.8733959	-6.001233	-6.7253148
C	-4.0229713	-3.1052039	-1.758684	O	-8.1311522	-1.072799	-6.0889056
C	-0.5472913	-1.9385603	-1.6541285	O	-12.011267	-2.6775114	-8.2762629
C	-0.8364249	-0.5918908	-1.0084122	C	-1.3918859	5.9740471	-6.0025454
C	-0.8552609	-0.4871493	0.3416219	O	2.5791188	8.6882201	-6.4041221
C	-0.5807622	-1.5606025	1.3484749	O	2.7712419	5.0912935	-3.3308747
C	-0.3974027	-2.9589638	0.7399269	H	-2.4556864	-4.3088048	-5.8790524
C	0.2023841	-2.9037561	-0.6812939	H	-1.0232769	-3.1248171	-4.1185197
C	-1.0900147	0.5821649	-1.8457915	H	-4.7910373	-3.0252038	-0.9995819
C	-1.3345274	1.8123322	-1.1049193	H	0.1277051	-1.7730322	-2.4982313
C	-1.3240124	1.8078291	0.2450075	H	-1.4003045	-1.5823688	2.0742885
O	-1.0999093	0.7029905	0.9837352	H	0.3261619	-1.2766068	1.8948119
C	-1.0714897	0.5724496	-3.2123661	H	0.3343841	-3.4941328	1.3583895
C	-1.2546421	1.7702086	-4.0144936	H	0.1768916	-3.9045638	-1.1258467
C	-1.8026681	3.0426315	-3.3172167	H	-1.4927777	2.6905118	0.8489322
C	-1.5814086	3.1063882	-1.7955309	H	-0.8628876	-0.3264469	-3.77951
O	-1.2463674	4.2090478	-3.944369	H	-3.8297088	2.264155	-3.1344324
C	0.0858232	4.3591733	-3.8083212	H	-3.7113706	4.0423913	-3.1464423
C	0.686521	5.4750952	-4.535182	H	-3.4896144	3.1111893	-4.6605112
C	-3.3150659	3.1208748	-3.5815291	H	-4.6466727	-6.8654108	-3.668835
O	-6.9217334	-4.9418897	-5.1602983	H	-6.4159396	-6.8273587	-3.4500535
C	-7.187237	-3.6801989	-5.5550746	H	-5.7101161	-7.2326336	-5.0458974
C	-8.4320208	-3.4835519	-6.2928971	H	3.1862838	-2.1763985	-1.6632639
C	-5.6002632	-6.6192989	-4.1478958	H	-2.3871597	-5.4527905	0.3231193
O	-6.4817694	-4.205053	-2.4961844	H	-10.332648	-0.803411	-7.2815642
O	-4.7195708	-5.2660598	-6.7550203	H	-11.054904	-5.0021858	-7.8831801
O	-1.6953547	4.1568438	-1.1898894	H	0.2044858	7.913143	-6.8886836
O	-1.0681244	1.7955581	-5.2241495	H	3.7180988	7.0824779	-4.5483974

C	1.6843792	-2.5315077	-0.585838	H	-9.5695001	-6.5965896	-7.3230164
C	-1.6647249	-3.8006717	0.8577832	H	-7.8569752	-6.1792456	-7.0879036
O	2.3113176	-2.4039547	0.4421916	H	-8.9089788	-6.3635186	-5.6931524
O	2.2467456	-2.3994018	-1.8073004	H	-7.289782	-1.421633	-5.6992566
O	-1.576305	-4.9438296	0.1329701	H	-12.178928	-1.7231404	-8.3303399
O	-2.6134642	-3.5513704	1.5648105	H	-1.6273984	6.6099317	-6.8606561
O	-6.3978578	-2.7698045	-5.2587792	H	-1.5144231	4.9276735	-6.2963802
O	0.7172136	3.5818378	-3.0750851	H	-2.1278309	6.1697132	-5.216555
C	-8.8464451	-2.1305596	-6.5014368	H	3.4867707	8.8015065	-6.0798713
C	-10.050197	-1.8444963	-7.1528813	H	2.2067922	4.3378153	-3.0213492

NImag	0
Σ Electronic and thermal Free Energy	-1865700.802
mol Fraction	0.314015801

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 3

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.3511547	-4.3330369	-5.1472921	C	-10.418833	-3.4526657	-8.4460599
C	-3.1972557	-3.7384242	-3.9239046	C	-10.288613	-2.4329078	-7.4912749
C	-4.2898421	-3.6296766	-2.9677417	C	-9.2390113	-2.4506641	-6.5833803
C	-5.6343684	-4.2033796	-3.2568753	C	0.2171931	6.123739	-5.8408603
C	-5.7422216	-5.0627737	-4.5302967	C	0.922149	7.1400185	-6.4682557
C	-4.6270759	-4.8456139	-5.5831619	C	2.2528729	7.4239656	-6.120842
C	-1.9556487	-3.1399115	-3.4777032	C	2.9073543	6.6755376	-5.1527672
C	-1.8487163	-2.533884	-2.2763421	C	2.2287976	5.6343042	-4.5121749
O	-2.9205415	-2.4405207	-1.4231133	C	-9.1287503	-1.332951	-5.5711877
C	-4.0978049	-2.9936821	-1.7907941	O	-7.5638401	-5.5504865	-7.783502
C	-0.5923123	-1.9206734	-1.6980165	O	-11.47401	-3.3638681	-9.3038837
C	-0.8469725	-0.5454427	-1.1001043	C	-1.2001252	5.8737489	-6.3066342
C	-0.8695189	-0.3937966	0.2454149	O	2.8555517	8.4456951	-6.7855185
C	-0.6293211	-1.4393699	1.2896873	O	2.931977	4.9409486	-3.6029862
C	-0.4871136	-2.8626677	0.7301443	H	-2.5396269	-4.3496104	-5.8682531
C	0.1218829	-2.8749192	-0.6882382	H	-1.0856013	-3.1750802	-4.1255909
C	-1.0633341	0.6053827	-1.9791661	H	-4.8677384	-2.8688447	-1.0397187
C	-1.2780085	1.8665817	-1.2826187	H	0.092498	-1.8033096	-2.5423091
C	-1.2743732	1.9084519	0.0666242	H	-1.450463	-1.4112321	2.0134172
O	-1.0841459	0.8238836	0.8444427	H	0.2847913	-1.164222	1.8285145
C	-1.0375778	0.5478689	-3.3442705	H	0.223942	-3.399477	1.3709475
C	-1.1836906	1.7217805	-4.1886654	H	0.0683018	-3.8893816	-1.0980574
C	-1.7007929	3.0318726	-3.5393295	H	-1.421856	2.8156367	0.6389704
C	-1.4858996	3.1421833	-2.0193115	H	-0.8497029	-0.3751134	-3.8791279
O	-1.1095071	4.1604586	-4.2023783	H	-3.7491952	2.3145068	-3.343656
C	0.225832	4.2779827	-4.0637496	H	-3.582775	4.0876014	-3.4150873
C	0.8612783	5.3523612	-4.8225289	H	-3.3775962	3.0996422	-4.8951287
C	-3.2090356	3.1414731	-3.815965	H	-4.7814912	-6.792536	-3.6073497
O	-6.9976414	-4.8667691	-5.1834825	H	-6.5528164	-6.7164486	-3.4073721
C	-7.2222247	-3.582407	-5.6194183	H	-5.8438211	-7.1740486	-4.9834861
C	-8.3114549	-3.5280551	-6.6057224	H	3.1313291	-2.2723341	-1.677411
C	-5.7260491	-6.5403601	-4.1005659	H	-2.5510218	-5.3073904	0.3880884
O	-6.5650882	-4.107715	-2.4788011	H	-9.558195	-5.2654636	-9.267606
O	-4.8651268	-5.1724934	-6.7481874	H	-11.023491	-1.6350754	-7.4769546
O	-1.5742553	4.2154845	-1.4507668	H	0.4575926	7.7326767	-7.2488536
O	-0.9898005	1.6992915	-5.3970438	H	3.9421309	6.862384	-4.8797185

C	1.6143499	-2.5450329	-0.5966745	H	-10.005577	-0.6817394	-5.629214
C	-1.7813501	-3.6592926	0.867561	H	-9.0509113	-1.7150353	-4.5476176
O	2.2395427	-2.4028244	0.4303105	H	-8.2321915	-0.7304108	-5.7457682
O	2.185899	-2.4709863	-1.8186913	H	-6.7517948	-5.4539499	-7.2397093
O	-1.7244612	-4.8298563	0.184216	H	-11.451693	-4.121666	-9.9094113
O	-2.7269695	-3.354469	1.5566278	H	-1.4163688	6.4943156	-7.1808465
O	-6.5551295	-2.6552022	-5.1943064	H	-1.3552042	4.8245147	-6.5737499
O	0.831303	3.5068604	-3.3024195	H	-1.9291682	6.112157	-5.5260831
C	-8.4322296	-4.5356628	-7.6001752	H	3.7662431	8.5402243	-6.4637773
C	-9.4962575	-4.4896901	-8.5092308	H	2.3433876	4.2165654	-3.2699508

NImag	0
Σ Electronic and thermal Free Energy	-1865698.239
mol Fraction	0.004129507

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid – Conformer 4

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2733362	-4.3121147	-5.1640376	C	-10.228403	-3.3963948	-8.6847266
C	-3.1540866	-3.7154356	-3.937783	C	-10.122071	-2.3753309	-7.7283863
C	-4.2753524	-3.5977059	-3.0165083	C	-9.1016922	-2.3974222	-6.7878484
C	-5.6136703	-4.1639671	-3.3462086	C	0.3770406	6.1222774	-5.7695857
C	-5.686961	-5.025774	-4.6204786	C	1.1074501	7.1326863	-6.3770234
C	-4.5381291	-4.818014	-5.6383988	C	2.4288759	7.4085491	-5.9898578
C	-1.923395	-3.1233566	-3.4543332	C	3.0486199	6.657808	-5.0009513
C	-1.8503635	-2.5149803	-2.2516157	C	2.3439961	5.6223642	-4.3793812
O	-2.9477433	-2.4130134	-1.4325564	C	-9.0165561	-1.2781169	-5.7749954
C	-4.1162962	-2.9599629	-1.8355875	O	-7.4087076	-5.5101334	-7.9281943
C	-0.6089121	-1.9079025	-1.6357154	O	-11.255471	-3.3031012	-9.575559
C	-0.8737618	-0.5295669	-1.0494569	C	-1.0271648	5.8809259	-6.277677
C	-0.9372656	-0.3741485	0.294329	O	3.0582297	8.4249444	-6.6377727
C	-0.7358529	-1.4182875	1.348191	O	3.0145666	4.9263441	-3.4478919
C	-0.5852588	-2.8439504	0.7969264	H	-2.4398051	-4.3353982	-5.859249
C	0.0674938	-2.8637648	-0.6017849	H	-1.0337363	-3.1654273	-4.0745868
C	-1.0557309	0.6201302	-1.9377361	H	-4.9085416	-2.8286071	-1.1092362
C	-1.2845232	1.8844387	-1.2513673	H	0.1026567	-1.7968978	-2.458462
C	-1.3226388	1.9299404	0.0972182	H	-1.5787407	-1.3831695	2.0461534
O	-1.1631691	0.8463679	0.8833188	H	0.1629091	-1.1472612	1.9142512
C	-0.9877151	0.558849	-3.3012125	H	0.102151	-3.3834294	1.4608511
C	-1.1004691	1.7313427	-4.1527059	H	0.0203643	-3.8789924	-1.0105161
C	-1.6297591	3.0461772	-3.5230717	H	-1.482496	2.8395087	0.6624116
C	-1.4617475	3.159264	-1.9973704	H	-0.7887088	-0.3666231	-3.8276786
O	-1.0114431	4.169557	-4.1700791	H	-3.6874457	2.3412122	-3.3897013
C	0.3195645	4.2798062	-3.9899092	H	-3.5084727	4.1131336	-3.4602066
C	0.9847587	5.348624	-4.7308115	H	-3.2629954	3.1201336	-4.9307143
C	-3.1279748	3.1638094	-3.846915	H	-4.7662298	-6.7590673	-3.6640688
O	-6.9200936	-4.8236772	-5.3130835	H	-6.5424471	-6.6717334	-3.5197363
C	-7.1231376	-3.5390782	-5.7586199	H	-5.7873476	-7.1374694	-5.0718924
C	-8.1805253	-3.4804685	-6.7787568	H	3.1099763	-2.2821668	-1.4981971
C	-5.6933523	-6.5023767	-4.1871311	H	-2.6528964	-5.2766531	0.3967719
O	-6.5676168	-4.0608889	-2.5977724	H	-9.3535363	-5.2162656	-9.4749895
O	-4.7416819	-5.1463083	-6.8095682	H	-10.852163	-1.5730566	-7.7387848
O	-1.5610401	4.2346314	-1.4345607	H	0.6707361	7.7269084	-7.1723664
O	-0.8690248	1.704496	-5.3543507	H	4.0758035	6.8384281	-4.6968143

C	1.5584457	-2.5428805	-0.4645952	H	-9.8875013	-0.622185	-5.8614929
C	-1.8881765	-3.6320858	0.8959186	H	-8.972557	-1.6583348	-4.7487288
O	2.1522669	-2.4020753	0.5810356	H	-8.1116667	-0.6809247	-5.9229702
O	2.1681657	-2.4752851	-1.6683798	H	-6.6135705	-5.4172365	-7.3593662
O	-1.817366	-4.8048341	0.217659	H	-11.218715	-4.0623463	-10.178566
O	-2.8528967	-3.3194771	1.5543377	H	-1.2129322	6.5019288	-7.1585596
O	-6.4641271	-2.6148452	-5.3148171	H	-1.1809667	4.8324431	-6.5484291
O	0.8963694	3.5069433	-3.2083456	H	-1.7778371	6.1248842	-5.5196569
C	-8.276137	-4.4895932	-7.7744293	H	3.9593391	8.5141281	-6.2886829
C	-9.3107057	-4.4391624	-8.7166529	H	2.4112189	4.2066678	-3.1314101

NImag	0
Σ Electronic and thermal Free Energy	-1865698.245
mol Fraction	0.004173525

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 5

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.9950428	-4.5804942	-5.2048153	C	-10.245523	-3.1402332	-8.4910316
C	-2.9362635	-3.9150923	-4.0146105	C	-9.9041037	-4.4672836	-8.1828488
C	-4.1047656	-3.746833	-3.1602953	C	-8.8015702	-4.7601418	-7.3943218
C	-5.4259426	-4.3149339	-3.5386612	C	-0.1375219	6.0214483	-5.9293616
C	-5.4412379	-5.263646	-4.7534528	C	0.4962572	7.069799	-6.5798151
C	-4.2267564	-5.150556	-5.7192485	C	1.8066073	7.4473211	-6.2446651
C	-1.7308116	-3.2972689	-3.4950724	C	2.5128764	6.7623049	-5.2662298
C	-1.7180088	-2.6339629	-2.3207359	C	1.9072093	5.6907783	-4.6025535
O	-2.8585381	-2.4909391	-1.5634787	C	-8.4938324	-6.2203635	-7.1462111
C	-4.0067585	-3.0506282	-2.0064434	O	-7.6297127	-1.2790698	-6.8610777
C	-0.5047163	-2.0112292	-1.6656096	O	-11.349801	-2.9546662	-9.2626297
C	-0.8033747	-0.6388584	-1.0776852	C	-1.5365165	5.6681979	-6.383621
C	-0.8079297	-0.4620793	0.264139	O	2.3384979	8.4937205	-6.9318247
C	-0.511881	-1.4846466	1.3185727	O	2.6584562	5.0625715	-3.6848482
C	-0.4637968	-2.9168064	0.7763011	H	-2.1229428	-4.656371	-5.8473558
C	0.1648116	-2.9686177	-0.637363	H	-0.8100417	-3.3667821	-4.0658084
C	-1.0687886	0.493269	-1.9695716	H	-4.8387229	-2.8767912	-1.3353239
C	-1.3367649	1.7528881	-1.2879489	H	0.2364332	-1.876528	-2.4600887
C	-1.310391	1.817882	0.0598313	H	-1.2713537	-1.4116438	2.1030277
O	-1.0545985	0.7563609	0.8505355	H	0.449757	-1.2295794	1.7835556
C	-1.0421375	0.4208255	-3.3336209	H	0.177903	-3.5145197	1.4337798
C	-1.2534044	1.5757835	-4.1910531	H	0.07328	-3.994562	-1.0135738
C	-1.8420812	2.8620263	-3.5545793	H	-1.4895332	2.7267856	0.6202114
C	-1.6192749	3.0056526	-2.0389396	H	-0.8046995	-0.4970913	-3.8567773
O	-1.3280051	4.0144192	-4.2397701	H	-3.8411167	2.0249089	-3.3256911
C	-0.0009846	4.2161676	-4.1161907	H	-3.7836182	3.8035336	-3.4244736
C	0.5597813	5.314508	-4.8997813	H	-3.5341346	2.8079995	-4.8924012
C	-3.3571521	2.8758918	-3.8158867	H	-4.6019042	-6.9382479	-3.6417187
O	-6.6570462	-5.0857627	-5.4975378	H	-6.3810226	-6.826985	-3.5929854
C	-6.8368127	-3.8564112	-6.0218498	H	-5.5500968	-7.3930583	-5.0755995
C	-8.0004201	-3.6885906	-6.8881977	H	3.2243453	-3.0124941	0.3995318
C	-5.4981977	-6.7063914	-4.2267998	H	-2.707747	-5.1923522	0.3996629
O	-6.4311884	-4.1291247	-2.8764938	H	-9.7006049	-1.0508335	-8.2753242
O	-4.3345	-5.6166963	-6.8462931	H	-10.521085	-5.2631677	-8.5857798
O	-1.7608207	4.0803486	-1.4835766	H	-0.0092652	7.6147437	-7.3697014
O	-1.0635037	1.5505513	-5.3998059	H	3.5345594	7.0213994	-5.0029704

C	1.6739295	-2.6955986	-0.6130087	H	-9.1535824	-6.845235	-7.7549388
C	-1.8260987	-3.6003077	0.8768964	H	-7.4556358	-6.4589402	-7.3942077
O	2.296697	-2.1564322	-1.4981845	H	-8.6378316	-6.4896211	-6.095184
O	2.2683862	-3.1840802	0.5010611	H	-6.8402831	-1.6164179	-6.3667314
O	-1.8330095	-4.7930545	0.2321999	H	-11.475233	-2.004198	-9.4133945
O	-2.7717584	-3.195072	1.5114468	H	-1.7948719	6.2520963	-7.2716179
O	-6.0440019	-2.9475331	-5.7307431	H	-1.6231251	4.6049159	-6.6247695
O	0.6575455	3.4986851	-3.3474926	H	-2.2778656	5.8772574	-5.6061973
C	-8.3429526	-2.3474977	-7.2485827	H	3.2429448	8.6519591	-6.6176401
C	-9.4704089	-2.0844752	-8.0328487	H	2.1231573	4.3037493	-3.338652

NImag	0
Σ Electronic and thermal Free Energy	-1865699.737
mol Fraction	0.051887123

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 6

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2665843	-4.3107155	-5.1538371	C	-10.82587	-2.8520596	-7.6439572
C	-3.1202176	-3.7485973	-3.9189091	C	-10.421178	-4.1878265	-7.4874115
C	-4.211049	-3.6975583	-2.9539134	C	-9.2430537	-4.508617	-6.829951
C	-5.5436784	-4.2798658	-3.2645656	C	0.1160154	6.1899656	-5.5358672
C	-5.6416179	-5.1189843	-4.5540736	C	0.8071079	7.2337	-6.1374132
C	-4.523284	-4.8778529	-5.6081668	C	2.1188645	7.5604756	-5.7531377
C	-1.8906899	-3.1339258	-3.4545309	C	2.7731044	6.8266926	-4.774997
C	-1.793176	-2.5691658	-2.2338458	C	2.1120037	5.7594703	-4.1637588
O	-2.8641717	-2.53253	-1.3705665	C	-8.874051	-5.9730397	-6.7418189
C	-4.0297938	-3.0995434	-1.7558792	O	-8.1225141	-1.0473964	-6.0949543
C	-0.550701	-1.944465	-1.6383064	O	-12.001319	-2.6397797	-8.2937973
C	-0.8375869	-0.5975355	-0.9920624	C	-1.2781919	5.8950305	-6.0435369
C	-0.8604595	-0.4942608	0.3580982	O	2.7982674	8.5880154	-6.3298557
C	-0.5934803	-1.5699281	1.3645961	O	2.8112169	5.0759642	-3.2439833
C	-0.4124149	-2.9681408	0.7549786	H	-2.4538421	-4.2997972	-5.8739253
C	0.1926459	-2.913011	-0.6640075	H	-1.0226758	-3.1250783	-4.1061962
C	-1.0836916	0.5784085	-1.8287894	H	-4.799939	-3.0184528	-0.9989994
C	-1.3247766	1.8088547	-1.0875046	H	0.1277235	-1.7801281	-2.4798832
C	-1.3190905	1.8027245	0.2624967	H	-1.4158736	-1.5898233	2.0872421
O	-1.1025529	0.6960569	1.0005744	H	0.3122671	-1.2896037	1.9147591
C	-1.0616363	0.5694273	-3.1955299	H	0.315573	-3.5062905	1.3753273
C	-1.234868	1.7685055	-3.9969021	H	0.1659181	-3.9132232	-1.1098326
C	-1.7738954	3.0453903	-3.3008963	H	-1.4859442	2.6854639	0.8668667
C	-1.5639065	3.1047671	-1.7772611	H	-0.8561572	-0.3302592	-3.762512
O	-1.1972538	4.2051993	-3.9226855	H	-3.8115395	2.2923875	-3.1342808
C	0.1360456	4.3374326	-3.7741682	H	-3.6706653	4.0688306	-3.1438208
C	0.7590137	5.4365264	-4.5084266	H	-3.449541	3.1357612	-4.6571997
C	-3.2828092	3.1428249	-3.576973	H	-4.6583363	-6.8527434	-3.6755429
O	-6.9242987	-4.9207228	-5.1698415	H	-6.4281271	-6.8106712	-3.4617897
C	-7.1856642	-3.6578433	-5.5633271	H	-5.7187298	-7.2147592	-5.0563236
C	-8.4282781	-3.4571155	-6.3038374	H	3.1818115	-2.1902301	-1.6339467
C	-5.6099144	-6.6033473	-4.156881	H	-2.408037	-5.4556004	0.3286999
O	-6.4902469	-4.1889379	-2.5036907	H	-10.320895	-0.7711278	-7.2919681
O	-4.7187689	-5.2463318	-6.7592394	H	-11.050774	-4.9672282	-7.9028405
O	-1.6813952	4.1541713	-1.1704734	H	0.3262319	7.8047068	-6.9290056
O	-1.0446859	1.7939352	-5.2063663	H	3.791767	7.0599007	-4.4891377

C	1.675419	-2.545044	-0.5625242	H	-9.5698238	-6.5657806	-7.3424945
C	-1.6827029	-3.8060617	0.8673542	H	-7.8570456	-6.1525246	-7.10203
O	2.2989311	-2.4222822	0.4681389	H	-8.9131617	-6.3372119	-5.7104498
O	2.242243	-2.410819	-1.7816085	H	-7.2829144	-1.3989401	-5.7038326
O	-1.5950984	-4.9487887	0.1417487	H	-12.16703	-1.6849734	-8.3460577
O	-2.6333174	-3.554586	1.5711045	H	-1.484963	6.4980911	-6.9327044
O	-6.394925	-2.7497241	-5.2637332	H	-1.3957828	4.838704	-6.301009
O	0.7485533	3.5610065	-3.025406	H	-2.0382174	6.1228171	-5.2897859
C	-8.8392652	-2.1028779	-6.5109352	H	2.2307282	9.0084933	-6.9950424
C	-10.040923	-1.8130436	-7.1645711	H	2.2423793	4.3251441	-2.940178
NImag						0	
Σ Electronic and thermal Free Energy						-1865700.368	
mol Fraction						0.150924969	

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 7

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.3339428	-4.3803854	-5.1196051	C	-10.290987	-3.3015385	-8.5903512
C	-3.173303	-3.7474225	-3.9162771	C	-10.130488	-2.2520199	-7.6732304
C	-4.2768965	-3.5497247	-2.9874989	C	-9.0996691	-2.2824913	-6.744348
C	-5.6421767	-4.0691237	-3.281458	C	-0.0484483	6.0829738	-5.8787096
C	-5.7679622	-4.97156	-4.5228675	C	0.5929791	7.1127464	-6.5508279
C	-4.6248118	-4.848236	-5.5609604	C	1.9367144	7.4257136	-6.2892172
C	-1.9129952	-3.1921869	-3.4671351	C	2.6674955	6.6935688	-5.3643657
C	-1.7976396	-2.5496127	-2.2853731	C	2.0538296	5.639248	-4.6808629
O	-2.8798045	-2.3727205	-1.4581273	C	-8.9552386	-1.1316721	-5.7744582
C	-4.0759511	-2.8782795	-1.8319682	O	-7.5503004	-5.5013689	-7.7902244
C	-0.5195307	-1.9897284	-1.700664	O	-11.325041	-3.1980637	-9.4720535
C	-0.720878	-0.6142294	-1.0800324	C	-1.4865475	5.8006713	-6.2534761
C	-0.6366418	-0.4563176	0.261498	O	2.4740877	8.4586211	-6.9920627
C	-0.322226	-1.5055795	1.2839119	O	2.8284749	4.9631342	-3.8183005
C	-0.3692691	-2.9308266	0.7233748	H	-2.511443	-4.4624846	-5.8234303
C	0.1684916	-2.9902714	-0.7269905	H	-1.0341706	-3.2897711	-4.096676
C	-0.9889389	0.5403705	-1.9417385	H	-4.8548364	-2.6842577	-1.105059
C	-1.1610853	1.800592	-1.2309853	H	0.1762281	-1.8768305	-2.5384131
C	-1.0508478	1.8456682	0.1132829	H	-1.0289086	-1.4113765	2.1141025
O	-0.793761	0.7631304	0.8751518	H	0.675895	-1.2982954	1.6922141
C	-1.0461504	0.4858261	-3.3055116	H	0.2853035	-3.5642296	1.3330145
C	-1.2564242	1.6608815	-4.135925	H	0.0090326	-4.0060637	-1.108134
C	-1.7506569	2.9619545	-3.4513393	H	-1.1564631	2.7533771	0.6938956
C	-1.4339987	3.0744853	-1.9497279	H	-0.8791977	-0.433616	-3.8527701
O	-1.2270396	4.1007433	-4.1516559	H	-3.7679264	2.2077075	-3.1170089
C	0.1126326	4.2430965	-4.1027696	H	-3.6385342	3.9836298	-3.1967736
C	0.6755069	5.3282233	-4.9026896	H	-3.5175549	3.0001447	-4.6888956
C	-3.2762378	3.0444598	-3.6237254	H	-4.9066713	-6.7067577	-3.5157099
O	-7.0008409	-4.7432994	-5.2075562	H	-6.6757855	-6.5404101	-3.353421
C	-7.1569697	-3.467788	-5.6963426	H	-5.9613675	-7.0918965	-4.8966592
C	-8.2237006	-3.4017886	-6.7062953	H	3.2814881	-3.1739256	0.1188298
C	-5.8293896	-6.4303131	-4.0364962	H	-2.7266278	-5.1061933	0.4635225
O	-6.580808	-3.8999709	-2.5254795	H	-9.5015409	-5.1830515	-9.324114
O	-4.8578079	-5.2087192	-6.7171938	H	-10.827009	-1.4209625	-7.7046451
O	-1.4971171	4.1460151	-1.3743531	H	0.0671055	7.6930766	-7.301223
O	-1.1377888	1.6438362	-5.3537171	H	3.7136043	6.9024736	-5.1587766

C	1.6869522	-2.7830557	-0.7947254	H	-9.7994283	-0.4435322	-5.8750603
C	-1.7509153	-3.5576908	0.9006362	H	-8.913519	-1.4757753	-4.735438
O	2.2760367	-2.2652652	-1.7149799	H	-8.0284785	-0.5785626	-5.9548535
O	2.3268655	-3.3043627	0.2780859	H	-6.7439635	-5.4206584	-7.2352594
O	-1.8489506	-4.7399199	0.2437344	H	-11.326545	-3.9790107	-10.047842
O	-2.6376481	-3.1215412	1.5966294	H	-1.7703494	6.4116606	-7.1150605
O	-6.4558453	-2.5564061	-5.2925395	H	-1.635625	4.7469329	-6.5057464
O	0.7815731	3.4853224	-3.3830993	H	-2.1701801	6.0282122	-5.4297245
C	-8.373239	-4.4410809	-7.663593	H	3.4017806	8.5713384	-6.7303918
C	-9.4171569	-4.3817868	-8.5949597	H	2.2804221	4.2237778	-3.4507693

NImag	0
Σ Electronic and thermal Free Energy	-1865697.333
mol Fraction	0.000894187

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 8

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.9404156	-4.3272139	-5.3107041	C	-10.35355	-3.0251001	-8.2678705
C	-2.8910467	-3.7754224	-4.0638425	C	-9.9283753	-4.3533044	-8.1003892
C	-4.0428474	-3.7679421	-3.1709199	C	-8.7884841	-4.6556578	-7.3710277
C	-5.3346082	-4.3863153	-3.5727046	C	1.7333772	6.2446092	-4.1020487
C	-5.3256188	-5.2105384	-4.8755581	C	2.2679762	7.1745428	-4.9862852
C	-4.147967	-4.9258558	-5.8512075	C	1.8788646	7.1835144	-6.335247
C	-1.7128523	-3.1304074	-3.5146082	C	0.963813	6.2567734	-6.8170428
C	-1.7115871	-2.5780919	-2.2845117	C	0.4059131	5.314864	-5.9471477
O	-2.8364433	-2.5823651	-1.4919686	C	-8.3915937	-6.1123233	-7.2757908
C	-3.9575756	-3.1793097	-1.9578854	O	-7.8020435	-1.1793426	-6.5228221
C	-0.5288695	-1.9262116	-1.602649	O	-11.488366	-2.8315954	-8.9911985
C	-0.8965362	-0.5963866	-0.9609949	C	2.1785859	6.2661398	-2.6571761
C	-1.0106174	-0.5123413	0.38719	O	2.3884033	8.083009	-7.2240896
C	-0.778446	-1.5942468	1.3954603	O	-0.4273318	4.4229086	-6.5187054
C	-0.5164315	-2.9779863	0.7824604	H	-2.0836108	-4.2847627	-5.976518
C	0.1781577	-2.8856786	-0.5928097	H	-0.804958	-3.0893423	-4.1081808
C	-1.1214495	0.5831193	-1.7952276	H	-4.7769907	-3.1299303	-1.2517454
C	-1.4427164	1.796648	-1.058861	H	0.1980935	-1.7320165	-2.3958893
C	-1.5263572	1.7712141	0.2885641	H	-1.6454566	-1.6475937	2.0621094
O	-1.3281514	0.6603802	1.0244221	H	0.0807434	-1.2951878	2.0069724
C	-1.0054892	0.5905264	-3.161223	H	0.1850824	-3.5031607	1.4430662
C	-1.131027	1.8023936	-3.9358421	H	0.2104586	-3.8798532	-1.051431
C	-1.7728495	3.0453172	-3.2808159	H	-1.7581547	2.6404215	0.8910764
C	-1.6791286	3.0972267	-1.7472542	H	-0.7260205	-0.2932461	-3.7210193
O	-1.1870089	4.2036782	-3.8789154	H	-3.7940369	2.2184852	-3.2619928
C	0.1550469	4.3603506	-3.6357052	H	-3.7065926	3.9996554	-3.25435
C	0.7652818	5.3200429	-4.569675	H	-3.356705	3.0883003	-4.7521203
C	-3.263143	3.0878584	-3.6629758	H	-4.3559533	-6.9304765	-3.9556999
O	-6.5701028	-5.0365045	-5.5716649	H	-6.1363633	-6.9363229	-3.8572377
C	-6.8384797	-3.7743061	-5.9636682	H	-5.31472	-7.3004457	-5.4068814
C	-8.034823	-3.5926012	-6.7804769	H	3.2013683	-2.0654983	-1.3580806
C	-5.2805696	-6.6988048	-4.4950191	H	-2.4060522	-5.5155624	0.1968849
O	-6.3292451	-4.3342837	-2.8719725	H	-9.9225161	-0.9379506	-7.8589274
O	-4.2562332	-5.2867757	-7.0158857	H	-10.51085	-5.1413336	-8.5653154
O	-1.8994157	4.1259179	-1.135515	H	2.9913286	7.9043217	-4.6278417
O	-0.7927613	1.879781	-5.1190552	H	0.6923626	6.2407714	-7.8659803

C	1.6393756	-2.4753055	-0.3903623	H	-9.0341245	-6.7131442	-7.9256982
C	-1.7664035	-3.8532643	0.8014936	H	-7.3500683	-6.2642362	-7.5731985
O	2.1892221	-2.343621	0.6803216	H	-8.4868439	-6.4901958	-6.2530435
O	2.2804489	-2.312425	-1.568319	H	-6.9814334	-1.5158823	-6.081848
O	-1.5980298	-4.9828413	0.0702077	H	-11.672408	-1.880201	-9.0448158
O	-2.7675458	-3.6375699	1.444355	H	2.8176715	7.1338717	-2.4682036
O	-6.0916906	-2.852114	-5.600246	H	1.3280825	6.3104358	-1.9686035
O	0.7057069	3.7430802	-2.7403496	H	2.735624	5.3593937	-2.4025686
C	-8.4640104	-2.2454655	-6.9978382	H	3.0186141	8.6576572	-6.7620815
C	-9.6268256	-1.9747485	-7.7256203	H	-0.6710018	3.6913727	-5.9114808

NImag	0
Σ Electronic and thermal Free Energy	-1865697.571
mol Fraction	0.00133644

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 9

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.3078503	-4.4064731	-5.1524528	C	-10.2133	-3.5050152	-8.7804696
C	-3.1701241	-3.7489903	-3.9595161	C	-10.082583	-2.4261855	-7.8932245
C	-4.290399	-3.5340803	-3.0563116	C	-9.068157	-2.4152393	-6.9458248
C	-5.6504982	-4.0557519	-3.3661426	C	0.3023705	6.1987172	-5.6663896
C	-5.7483356	-4.9948744	-4.5817172	C	1.0135231	7.2256596	-6.2688652
C	-4.5884961	-4.8915961	-5.6036011	C	2.3467005	7.4914651	-5.9164106
C	-1.9208511	-3.1801458	-3.4985209	C	2.9973036	6.7142096	-4.968632
C	-1.8267299	-2.5235497	-2.3231897	C	2.3124024	5.6617993	-4.3536139
O	-2.9231571	-2.3316992	-1.5175031	C	-8.9553107	-1.2340871	-6.008682
C	-4.1101558	-2.8454539	-1.9087132	O	-7.4598017	-5.6431765	-7.8648817
C	-0.5567139	-1.9440776	-1.73566	O	-11.23273	-3.4421162	-9.6832258
C	-0.7932228	-0.5829102	-1.1016209	C	-1.1171646	5.9701185	-6.1363575
C	-0.8120914	-0.4673964	0.2466265	O	2.955514	8.5254677	-6.5559323
C	-0.5666584	-1.5432308	1.2590944	O	3.0119401	4.9408002	-3.463316
C	-0.4431431	-2.9556333	0.6575055	H	-2.4728007	-4.5023598	-5.8395093
C	0.1586022	-2.9324729	-0.7589925	H	-1.0301711	-3.2875735	-4.1094942
C	-1.0067931	0.5924819	-1.9483854	H	-4.907239	-2.6397236	-1.2054212
C	-1.2088283	1.8359619	-1.2168203	H	0.123438	-1.8115183	-2.5815344
C	-1.2009485	1.8414626	0.1329788	H	-1.3571383	-1.5090374	2.0140241
O	-1.0173542	0.7345676	0.8812677	H	0.3686982	-1.2964281	1.7760681
C	-0.9902515	0.5699672	-3.3143802	H	0.264959	-3.505233	1.2915474
C	-1.1307577	1.7678952	-4.126251	H	0.073134	-3.9374933	-1.1877745
C	-1.6341421	3.0643625	-3.4394522	H	-1.3400551	2.7341103	0.729772
C	-1.4121094	3.1322986	-1.9179575	H	-0.8143524	-0.3408498	-3.8740148
O	-1.0361647	4.2053692	-4.0744821	H	-3.6875201	2.3584041	-3.2551597
C	0.30052	4.3089	-3.9364326	H	-3.50694	4.1315303	-3.2789227
C	0.9424822	5.3974098	-4.6688378	H	-3.3154746	3.1824909	-4.7860448
C	-3.1424744	3.1936673	-3.7068432	H	-4.8901653	-6.687615	-3.5018978
O	-6.9712959	-4.798497	-5.2938308	H	-6.6635666	-6.5373695	-3.3836102
C	-7.1287783	-3.5423723	-5.8284606	H	-5.910327	-7.1279904	-4.8933756
C	-8.1790701	-3.5209128	-6.8583271	H	3.1663128	-2.3421111	-1.7559087
C	-5.80373	-6.4387662	-4.0515162	H	-3.2440372	-4.158809	1.7104685
O	-6.6067212	-3.857693	-2.6394646	H	-9.3873215	-5.3974695	-9.44222
O	-4.8000361	-5.2824405	-6.7544062	H	-10.788882	-1.6056833	-7.962089
O	-1.4921594	4.1902125	-1.3200283	H	0.5521544	7.8409708	-7.0336637
O	-0.9419998	1.7768823	-5.3353695	H	4.0337741	6.8868077	-4.6926613

C	1.6540398	-2.6288031	-0.6726859	H	-9.8058913	-0.5599961	-6.1447205
C	-1.7009926	-3.8174642	0.6993143	H	-8.9280872	-1.5466355	-4.9592258
O	2.2906517	-2.5302058	0.3532618	H	-8.0321704	-0.6749945	-6.1891781
O	2.2166995	-2.520415	-1.8959778	H	-6.6636679	-5.534645	-7.2993812
O	-2.5207995	-3.50308	1.7255373	H	-11.213931	-4.2406008	-10.234092
O	-1.9185605	-4.7468347	-0.047951	H	-1.3299987	6.6134027	-6.9948366
O	-6.4426088	-2.6106432	-5.4462449	H	-1.2799392	4.9288691	-6.4289029
O	0.901482	3.5137281	-3.1965313	H	-1.8436841	6.1945278	-5.3492986
C	-8.2981255	-4.5906052	-7.7856808	H	3.867552	8.6050876	-6.2339552
C	-9.325988	-4.5732703	-8.7366746	H	2.4192334	4.2117329	-3.148493

NImag	0
Σ Electronic and thermal Free Energy	-1865698.182
mol Fraction	0.003749684

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 10

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.241607	-4.1691411	-5.1987769	C	-10.195217	-2.8862111	-8.6007813
C	-3.0883151	-3.618474	-3.9550271	C	-10.039992	-1.9023271	-7.6126491
C	-4.1947977	-3.4942656	-3.0168431	C	-9.0111946	-1.9938984	-6.6856726
C	-5.5553318	-4.0042269	-3.3483061	C	1.7291443	6.1997602	-4.2189055
C	-5.6727561	-4.8186726	-4.6499937	C	2.1752154	7.1314944	-5.1460361
C	-4.5282914	-4.6160606	-5.6740784	C	1.6221283	7.1712272	-6.4348098
C	-1.8334801	-3.0837062	-3.4668019	C	0.6300826	6.2741038	-6.8109335
C	-1.7255854	-2.5226308	-2.2437098	C	0.1570475	5.3289763	-5.8922681
O	-2.8097919	-2.4125634	-1.4076812	C	-8.872819	-0.9124746	-5.6381709
C	-4.0013321	-2.9021977	-1.8176185	O	-7.4494011	-5.1279942	-7.9487999
C	-0.4531481	-1.9921835	-1.6204575	O	-11.227527	-2.7248019	-9.475495
C	-0.6687118	-0.6649978	-0.9054731	C	2.3495548	6.1841731	-2.840151
C	-0.5813721	-0.5991405	0.4449308	O	2.1137771	8.1129022	-7.2888834
C	-0.2498323	-1.7132499	1.3902797	O	-0.7633528	4.4698582	-6.373978
C	-0.2883916	-3.0966066	0.7331167	H	-2.4173782	-4.1967602	-5.9048443
C	0.2453359	-3.0516782	-0.7190639	H	-0.9530107	-3.1305201	-4.099931
C	-0.9517923	0.5429629	-1.6814297	H	-4.7827236	-2.7653776	-1.0804675
C	-1.1361964	1.7486954	-0.8871454	H	0.2421063	-1.8144036	-2.4472765
C	-1.0239415	1.7009078	0.457148	H	-0.9509508	-1.6824352	2.2298364
O	-0.7513378	0.5711837	1.1396675	H	0.7496167	-1.5246229	1.8042837
C	-1.0063105	0.5793155	-3.0502614	H	0.3725166	-3.7656222	1.2959661
C	-1.1967663	1.8123494	-3.7781545	H	0.0920429	-4.0398651	-1.1689709
C	-1.7241144	3.0524398	-3.023354	H	-1.1406003	2.5644188	1.0996836
C	-1.4361501	3.0680183	-1.5133295	H	-0.8166656	-0.2963128	-3.6580918
O	-1.1939229	4.2120566	-3.6680851	H	-3.7442459	2.2628563	-2.76579
C	0.1718352	4.3410308	-3.5861308	H	-3.6181298	4.0414779	-2.7329047
C	0.6842116	5.3037429	-4.5734271	H	-3.4798623	3.1579345	-4.2811383
C	-3.2495421	3.1311049	-3.2128544	H	-4.8035715	-6.615195	-3.7646247
O	-6.9052537	-4.5496123	-5.3204288	H	-6.5739485	-6.4707048	-3.59582
C	-7.067231	-3.2432329	-5.7178328	H	-5.8527996	-6.9085902	-5.1720146
C	-8.1316937	-3.1106687	-6.7231427	H	3.3626365	-3.2700426	0.1034336
C	-5.7267129	-6.3081869	-4.2672638	H	-2.6314283	-5.2661182	0.332209
O	-6.495552	-3.896648	-2.5831985	H	-9.3981465	-4.7099546	-9.4613309
O	-4.7557507	-4.8979977	-6.8527545	H	-10.739018	-1.0731521	-7.5881485
O	-1.5623194	4.0847724	-0.8566878	H	2.9531025	7.8430084	-4.8901533
O	-1.0064069	1.9097097	-4.9923089	H	0.2187088	6.2640016	-7.8166603

C	1.7621952	-2.8285231	-0.7765913	H	-9.7193731	-0.222109	-5.6927346
C	-1.6658005	-3.7429431	0.8699427	H	-8.8317222	-1.3274972	-4.625368
O	2.3434341	-2.2431846	-1.660578	H	-7.9479161	-0.3447094	-5.7780084
O	2.4093405	-3.417909	0.2554984	H	-6.6450932	-5.0835555	-7.3872474
O	-1.7565436	-4.8797673	0.1368987	H	-11.225493	-3.4636532	-10.104403
O	-2.5544013	-3.3581611	1.5932536	H	3.032706	7.0302328	-2.7225335
O	-6.3713508	-2.3597216	-5.2479226	H	1.5920351	6.2413589	-2.0510342
O	0.8120094	3.6990614	-2.7717479	H	2.9057948	5.2575664	-2.6687497
C	-8.2760322	-4.0815169	-7.7506633	H	1.6510227	8.0386175	-8.1384512
C	-9.3179921	-3.9609606	-8.6781569	H	-0.946983	3.72972	-5.7554212

NImag	0
Σ Electronic and thermal Free Energy	-1865694.711
mol Fraction	1.06E-05

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 11

Atom	X	Y	Z	Atom	X	Y	Z
C	-4.1177479	-5.1894493	-4.897772	C	-4.281031	-1.2626846	-6.6229911
C	-3.8917917	-4.2784368	-3.9090151	C	-4.6089789	-2.4067904	-7.3725828
C	-4.9693618	-3.7384386	-3.0928611	C	-5.7840189	-3.1088987	-7.1340939
C	-6.388828	-4.057462	-3.3903641	C	-1.3857975	6.0647874	-5.6606073
C	-6.6757208	-5.1537806	-4.4436381	C	-0.8510274	7.1069484	-6.401515
C	-5.4447786	-5.661779	-5.2509075	C	0.5355294	7.2300359	-6.5917728
C	-2.5848721	-3.7422918	-3.5849643	C	1.4096549	6.2990886	-6.0495554
C	-2.3998888	-2.8904987	-2.5559788	C	0.9027088	5.2312635	-5.3031433
O	-3.4436399	-2.4784975	-1.7614318	C	-6.182728	-4.216785	-8.085245
C	-4.6949693	-2.8850466	-2.0809757	O	-7.2422724	-0.8888354	-4.5581201
C	-1.0564786	-2.3135522	-2.1401425	O	-3.0869417	-0.6831906	-6.8675569
C	-1.169189	-0.9969489	-1.3850998	C	-2.8917855	6.0140235	-5.5302467
C	-0.8342132	-0.9420137	-0.071253	O	0.9599331	8.2889801	-7.3291141
C	-0.3651011	-2.0655222	0.7980322	O	1.8090309	4.3677728	-4.8207144
C	-0.5014399	-3.4377871	0.1316819	H	-3.2989948	-5.5820028	-5.4934615
C	-0.1873324	-3.3649722	-1.3769727	H	-1.728779	-4.026626	-4.1893203
C	-1.6125165	0.2120563	-2.0773489	H	-5.4508242	-2.445262	-1.4429523
C	-1.5783944	1.4212652	-1.2720098	H	-0.5283096	-2.1080362	-3.077173
C	-1.2046016	1.3678111	0.0253491	H	-0.9384307	-2.0437378	1.7300074
O	-0.8577261	0.2274128	0.6457165	H	0.6853589	-1.886163	1.0539817
C	-2.014701	0.2481545	-3.3891591	H	0.2397209	-4.1111145	0.5787012
C	-2.4315053	1.4649256	-4.0411984	H	-0.3837142	-4.3411499	-1.8329006
C	-2.6394567	2.7460141	-3.2018989	H	-1.1566691	2.2340304	0.6733088
C	-1.9330439	2.7496111	-1.8367103	H	-2.0216141	-0.6397729	-4.0112689
O	-2.2440102	3.8979226	-3.961783	H	-4.5473418	2.0762741	-2.382078
C	-0.9299004	3.9632717	-4.2648866	H	-4.3166434	3.843517	-2.3962927
C	-0.5051164	5.0960906	-5.0792403	H	-4.6637565	2.9663808	-3.9175675
C	-4.1480829	2.9192697	-2.9552127	H	-6.5123251	-6.7834242	-2.9969705
O	-7.752802	-4.7295053	-5.3125971	H	-8.139037	-6.0572898	-3.1389768
C	-7.8692116	-3.4026577	-5.6677885	H	-7.5075564	-7.1320676	-4.4301057
C	-6.6503442	-2.6747178	-6.0954353	H	2.5793781	-2.8350977	-2.9421065
C	-7.2502971	-6.3679728	-3.6929557	H	-2.8754148	-5.6077233	0.0431103
O	-7.3070506	-3.510287	-2.8019052	H	-5.000255	0.1719724	-5.1623353
O	-5.6308517	-6.4938582	-6.1317701	H	-3.9315237	-2.7167774	-8.1621318
O	-1.7664719	3.7856763	-1.2200242	H	-1.498384	7.849433	-6.8551932
O	-2.7274262	1.5265822	-5.2405351	H	2.4847787	6.3653371	-6.1900129

C	1.3083424	-3.1156565	-1.5806833	H	-5.3045993	-4.7500498	-8.4600454
C	-1.8562732	-4.0733404	0.4336703	H	-6.8506623	-4.9501127	-7.6340938
O	2.1438793	-3.095468	-0.7046107	H	-6.6982669	-3.7759815	-8.9489867
O	1.6131556	-2.9652351	-2.888448	H	-8.1010558	-1.3511699	-4.6306128
O	-2.0148567	-5.2405304	-0.2353717	H	-2.9685507	0.1260122	-6.3145426
O	-2.680063	-3.6433879	1.2071587	H	-3.3404432	6.819062	-6.1186662
O	-8.9630913	-2.8802047	-5.5700299	H	-3.2946115	5.0598633	-5.8820037
O	-0.1677351	3.0820491	-3.8342299	H	-3.2112753	6.1276733	-4.4899733
C	-6.38729	-1.4342753	-5.4572125	H	1.9279595	8.264707	-7.3950436
C	-5.1905235	-0.7566608	-5.688009	H	1.3118166	3.659058	-4.3390309

NImag	0
Σ Electronic and thermal Free Energy	-1865686.958
mol Fraction	2.18E-11

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 12

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.383484	-4.3896643	-5.2176239	C	-10.868773	-2.3496527	-7.4986235
C	-3.1451331	-3.8025452	-4.009122	C	-10.576176	-3.7109929	-7.3139425
C	-4.1918285	-3.628454	-3.0101736	C	-9.4083108	-4.1152906	-6.6851293
C	-5.5788572	-4.1071006	-3.2536049	C	1.7893088	5.937615	-4.8209756
C	-5.7952636	-4.9737291	-4.5099652	C	2.1788307	6.8468846	-5.7977464
C	-4.6991681	-4.8632525	-5.6084338	C	1.5433441	6.8667666	-7.0494422
C	-1.85259	-3.2792899	-3.6078858	C	0.5234485	5.9713042	-7.3428545
C	-1.6625291	-2.6897306	-2.4099152	C	0.1081903	5.0506206	-6.3757839
O	-2.6946529	-2.5343776	-1.5125733	C	-9.1645503	-5.6033696	-6.5638523
C	-3.9177897	-3.009022	-1.8412563	O	-7.9684204	-0.7460552	-6.092175
C	-0.3462658	-2.1701196	-1.8745032	O	-12.042911	-2.0536135	-8.1170452
C	-0.4946629	-0.8209888	-1.1835275	C	2.4999035	5.9459033	-3.4863409
C	-0.3301822	-0.7234933	0.1576443	O	1.9064987	7.7467746	-8.0256743
C	0.0319415	-1.8203122	1.1119782	O	-0.8469356	4.1867172	-6.7730372
C	-0.0694869	-3.2185395	0.4942052	H	-2.6000839	-4.4705538	-5.9652468
C	0.3828445	-3.2197465	-0.9862412	H	-1.0115456	-3.3616788	-4.2893072
C	-0.7987303	0.3732128	-1.972981	H	-4.6524925	-2.8348583	-1.0649602
C	-0.9139668	1.601916	-1.2007961	H	0.3036493	-2.0271708	-2.7438273
C	-0.7263074	1.58498	0.1358622	H	-0.6207448	-1.7542476	1.9877894
O	-0.4378693	0.4672668	0.8308876	H	1.0562978	-1.6419904	1.4653707
C	-0.9311742	0.3771798	-3.3369332	H	0.6093738	-3.8865155	1.0365775
C	-1.1430705	1.5953525	-4.0838979	H	0.1866805	-4.2155461	-1.4012838
C	-1.6056901	2.8620702	-3.3304777	H	-0.7893473	2.4664863	0.7612581
C	-1.2227168	2.9113668	-1.8427294	H	-0.7941247	-0.5170147	-3.9316322
O	-1.1045194	3.9977995	-4.0376643	H	-3.6147291	2.1074859	-2.9238262
C	0.2641319	4.110796	-4.0496714	H	-3.4656806	3.8844576	-2.9474662
C	0.7198204	5.0464184	-5.0902971	H	-3.4368541	2.9590334	-4.4767006
C	-3.139231	2.9567808	-3.4248257	H	-4.9339978	-6.7595418	-3.6078439
O	-7.0773725	-4.6827734	-5.0887916	H	-6.6845753	-6.5560483	-3.3358374
C	-7.2425791	-3.4129306	-5.5122233	H	-6.0715731	-7.0687501	-4.9390941
C	-8.4877951	-3.1248376	-6.2178788	H	3.5357121	-3.491566	-0.3357534
C	-5.8774694	-6.4423468	-4.0647016	H	-2.4728805	-5.347508	0.2776778
O	-6.483949	-3.9160356	-2.4613388	H	-10.173663	-0.3119342	-7.2270345
O	-4.9662191	-5.2519965	-6.7381456	H	-11.284791	-4.4434674	-7.6851356
O	-1.283602	3.9480187	-1.2080492	H	2.9811882	7.5515574	-5.5879854
O	-1.0237528	1.6600313	-5.3090403	H	0.0594227	5.9622092	-8.3220456

C	1.8978091	-3.0278276	-1.1310918	H	-9.9297495	-6.1494857	-7.1228472
C	-1.44866	-3.8336337	0.7244643	H	-8.1802435	-5.8812602	-6.9514233
O	2.4414195	-2.4645543	-2.052608	H	-9.1986381	-5.9337149	-5.5209628
O	2.5898353	-3.6184264	-0.1286812	H	-7.1482224	-1.1575748	-5.7194199
O	-1.6019253	-4.9854868	0.0265179	H	-12.126068	-1.0898616	-8.1955542
O	-2.2868302	-3.4146386	1.4880049	H	3.1919065	6.7914619	-3.4284326
O	-6.3659378	-2.5699691	-5.2656506	H	1.7968124	6.020263	-2.64993
O	0.9514815	3.4801002	-3.2655594	H	3.064181	5.0207882	-3.3345664
C	-8.7870644	-1.7459679	-6.4529538	H	2.6329873	8.2981927	-7.6955794
C	-9.9809688	-1.370404	-7.0764741	H	-0.9935661	3.4633441	-6.126058

NImag	0
Σ Electronic and thermal Free Energy	-1865696.728
mol Fraction	0.000321416

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 13

Atom	X	Y	Z	Atom	X	Y	Z
C	-4.3943289	-5.1753384	-4.8714591	C	-4.5107582	-1.2523542	-6.6043421
C	-4.0479263	-4.2745303	-3.9085824	C	-4.9524241	-2.3809333	-7.3181441
C	-5.0305132	-3.6836606	-3.0117303	C	-6.1362217	-3.0256241	-6.9810725
C	-6.4824811	-3.9365781	-3.1932472	C	1.1403213	5.1346143	-5.6351263
C	-6.9033178	-5.0198612	-4.2145302	C	1.5127298	6.1409306	-6.5127017
C	-5.7658601	-5.5858545	-5.1149276	C	0.5486079	6.8570872	-7.2387021
C	-2.6958002	-3.799438	-3.6927901	C	-0.8021315	6.576479	-7.0851665
C	-2.3898379	-2.9555234	-2.6864359	C	-1.2091762	5.5762939	-6.1972383
O	-3.3463887	-2.4940167	-1.8131987	C	-6.6628667	-4.115185	-7.8902008
C	-4.6367991	-2.8423797	-2.0295483	O	-7.2728507	-0.7338441	-4.3076998
C	-0.992245	-2.4410772	-2.3824264	O	-3.3143497	-0.730954	-6.9484033
C	-0.9831173	-1.1178071	-1.6304525	C	2.238929	4.4093339	-4.8919221
C	-0.5415539	-1.0738571	-0.3477692	O	1.0033493	7.8211298	-8.0815949
C	-0.0564497	-2.2149491	0.4891986	O	-2.5409065	5.3779511	-6.1402962
C	-0.3106595	-3.5816534	-0.1534619	H	-3.6449972	-5.6064779	-5.5286652
C	-0.1153973	-3.5298391	-1.6828865	H	-1.9048773	-4.124341	-4.3620189
C	-1.4231984	0.1079525	-2.2936492	H	-5.3179528	-2.3668487	-1.3354991
C	-1.2681135	1.3172422	-1.503546	H	-0.5310683	-2.2639616	-3.3597424
C	-0.796125	1.2507101	-0.2391901	H	-0.5503329	-2.162475	1.4644133
O	-0.4538458	0.097571	0.3596583	H	1.0186263	-2.0845329	0.6575301
C	-1.9287041	0.1565491	-3.5697277	H	0.4311714	-4.2879168	0.2382144
C	-2.3320859	1.3888222	-4.1958705	H	-0.3937787	-4.4972174	-2.1141707
C	-2.4011957	2.6863355	-3.3607158	H	-0.6577603	2.115965	0.396879
C	-1.606719	2.6598525	-2.0448473	H	-2.0282618	-0.7331065	-4.1812593
O	-1.9675332	3.7949985	-4.1653469	H	-4.2850098	2.1720126	-2.3922465
C	-0.6330798	3.7558954	-4.5360333	H	-3.9399922	3.9177582	-2.478946
C	-0.2467327	4.8341204	-5.449867	H	-4.4575748	3.0213496	-3.9418448
C	-3.8733732	2.9697323	-3.019063	H	-6.7006756	-6.6533067	-2.7772137
O	-8.0256239	-4.5467631	-4.9967682	H	-8.2979928	-5.8520676	-2.7925753
C	-8.1072136	-3.2165536	-5.349116	H	-7.8225342	-6.9570316	-4.1244561
C	-6.8936703	-2.5486248	-5.8780793	H	2.5382767	-3.1401384	-3.4690138
C	-7.4718484	-6.2047612	-3.4141567	H	-2.7850837	-5.6349061	-0.0359113
O	-7.3243047	-3.3460755	-2.5364197	H	-5.039892	0.2174909	-5.0981562
O	-6.0601708	-6.4097141	-5.9737134	H	-4.3569324	-2.7243899	-8.1582844
O	-1.3664413	3.6870724	-1.4379198	H	2.5582823	6.3920483	-6.6544383
O	-2.7162919	1.4656869	-5.3703708	H	-1.5677091	7.1115698	-7.639847

C	1.3691592	-3.3529942	-2.0076623	H	-5.8442789	-4.6906619	-8.3314277
C	-1.6655644	-4.1502801	0.2607922	H	-7.3261018	-4.8147375	-7.3820873
O	2.2723445	-3.3671269	-1.2013699	H	-7.2251455	-3.652103	-8.7121091
O	1.5745702	-3.2250405	-3.336981	H	-8.1560183	-1.1540107	-4.3080799
O	-1.9332604	-5.3104386	-0.3852903	H	-3.1137494	0.0736212	-6.4129373
O	-2.4027783	-3.67865	1.0949671	H	3.2025294	4.8831375	-5.1004882
O	-9.1634243	-2.6420477	-5.1664133	H	2.0727474	4.4155109	-3.8105377
O	0.0791159	2.8751725	-4.0832706	H	2.2935496	3.3572	-5.1861871
C	-6.5209137	-1.3211098	-5.2703197	H	0.2480525	8.2406659	-8.5237307
C	-5.3160618	-0.7019194	-5.6014303	H	-2.7302489	4.67694	-5.4869159

NImag	0
Σ Electronic and thermal Free Energy	-1865684.171
mol Fraction	1.96E-13

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 14

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.0625015	-4.3255161	-5.3304456	C	-10.564422	-3.1067007	-8.0542033
C	-2.9623492	-3.7882478	-4.0803637	C	-9.7879488	-4.24145	-8.3025753
C	-4.0794397	-3.7886739	-3.1459404	C	-8.6221737	-4.491951	-7.5754219
C	-5.3835445	-4.4098163	-3.5026268	C	0.0471614	6.2882811	-5.4664906
C	-5.4356975	-5.2076059	-4.8222605	C	0.7136245	7.371049	-6.0209221
C	-4.295261	-4.9028843	-5.8345763	C	2.0000278	7.7317432	-5.5886808
C	-1.7623005	-3.1525952	-3.5696348	C	2.650744	6.9951055	-4.6090489
C	-1.7156147	-2.6074468	-2.3371546	C	2.0118052	5.8882495	-4.0417602
O	-2.8113404	-2.6129639	-1.5057227	C	-7.842269	-5.7452218	-7.9095266
C	-3.9493689	-3.2079489	-1.9334568	O	-8.6207033	-1.5472033	-5.384258
C	-0.5084597	-1.9611149	-1.6939993	O	-11.711113	-2.8394376	-8.7402838
C	-0.849215	-0.6258327	-1.0498923	C	-1.3205526	5.9571985	-6.0215226
C	-0.9326374	-0.5359618	0.2986577	O	2.5666583	8.8147878	-6.1852305
C	-0.6824528	-1.6139967	1.3070091	O	2.7106084	5.2104636	-3.1174839
C	-0.4377235	-3.0018668	0.6953956	H	-2.2328874	-4.2761956	-6.0294296
C	0.2198888	-2.9195562	-0.6987207	H	-0.8764746	-3.1096949	-4.1954914
C	-1.0863129	0.5520314	-1.8867927	H	-4.7420323	-3.1631627	-1.1972803
C	-1.3967684	1.7676134	-1.1463174	H	0.1962945	-1.7765117	-2.509171
C	-1.4490683	1.7487628	0.2025522	H	-1.53522	-1.6623253	1.992162
O	-1.2317952	0.6422466	0.9404744	H	0.1901356	-1.3149576	1.8993466
C	-0.9969109	0.5589394	-3.2506066	H	0.2810664	-3.5234282	1.3402025
C	-1.1647473	1.7622529	-4.0474835	H	0.234897	-3.916124	-1.1531176
C	-1.7860168	3.0095799	-3.3666197	H	-1.667905	2.6206332	0.8061224
C	-1.6446865	3.0622317	-1.8350698	H	-0.7387615	-0.3281968	-3.8157742
O	-1.2344805	4.1992601	-3.9530329	H	-3.7943833	2.1668513	-3.2972412
C	0.0836943	4.3881535	-3.7483088	H	-3.7310989	3.9483644	-3.2835986
C	0.685658	5.5276825	-4.43717	H	-3.4034832	3.0426173	-4.7940831
C	-3.2847105	3.0446349	-3.7074946	H	-4.4332821	-6.9528607	-3.9825716
O	-6.7092995	-5.010512	-5.4502894	H	-6.2083371	-6.9510735	-3.8077729
C	-6.9576963	-3.7185067	-5.8091266	H	-5.4570458	-7.2861758	-5.3980947
C	-8.2135248	-3.5666107	-6.583999	H	3.2263274	-2.1200772	-1.545829
C	-5.3789942	-6.704252	-4.4761081	H	-2.3475732	-5.5379232	0.1708027
O	-6.3424827	-4.3824568	-2.7523137	H	-10.794735	-1.3166392	-6.8912072
O	-4.4406242	-5.2331873	-7.0064497	H	-10.09239	-4.9407226	-9.0786947
O	-1.8192844	4.1022521	-1.2256493	H	0.253253	7.9571926	-6.8089193
O	-0.9096043	1.8098551	-5.2438753	H	3.6539651	7.2408794	-4.2722716

C	1.6877042	-2.5160647	-0.5370874	H	-8.1546856	-6.1302749	-8.8852894
C	-1.6864782	-3.8769853	0.7548449	H	-6.7629156	-5.5772024	-7.9250456
O	2.2673095	-2.3815656	0.5176269	H	-8.027442	-6.5259061	-7.1631591
O	2.2993299	-2.3630586	-1.7322902	H	-9.2828424	-0.8411598	-5.321154
O	-1.5416175	-5.0081912	0.0207956	H	-11.86273	-3.5476388	-9.3857834
O	-2.6665175	-3.6610258	1.4295142	H	-1.526578	6.5837622	-6.8939991
O	-6.1973214	-2.8225626	-5.4939301	H	-1.3889499	4.9068536	-6.3186946
O	0.7011244	3.6259679	-2.9880945	H	-2.1082102	6.1279407	-5.2811241
C	-9.0077172	-2.415948	-6.354837	H	3.4495223	8.9581991	-5.8087218
C	-10.179139	-2.1926264	-7.0767105	H	2.1573153	4.4346268	-2.845196

NImag	0
Σ Electronic and thermal Free Energy	-1865689.919
mol Fraction	3.24E-09

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 15

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.3339863	-4.3641288	-5.1279749	C	-10.28636	-3.2424732	-8.5963147
C	-3.1721038	-3.7402747	-3.9200346	C	-10.123976	-2.1995755	-7.6719874
C	-4.2757378	-3.5451989	-2.9907678	C	-9.0937351	-2.2387445	-6.7427776
C	-5.6426471	-4.0573833	-3.2896408	C	0.0322516	6.0330714	-5.8482134
C	-5.7703699	-4.9510535	-4.5371548	C	0.688062	7.0566565	-6.5197642
C	-4.626109	-4.8242112	-5.5736425	C	2.023072	7.3853589	-6.2284235
C	-1.9102715	-3.1924649	-3.4661608	C	2.7350423	6.6734624	-5.2748622
C	-1.7936122	-2.5583998	-2.2799259	C	2.1097405	5.6263043	-4.5948518
O	-2.8757499	-2.3838672	-1.4521197	C	-8.947293	-1.0950448	-5.7647785
C	-4.0733108	-2.8826595	-1.8303373	O	-7.5509238	-5.4536944	-7.8097956
C	-0.5142388	-2.0059554	-1.691016	O	-11.319718	-3.1306818	-9.4778417
C	-0.7120588	-0.633911	-1.0616055	C	-1.3928472	5.7336592	-6.2581585
C	-0.6273671	-0.4847789	0.2809784	O	2.6686717	8.3936047	-6.8741859
C	-0.315642	-1.541344	1.2966504	O	2.8633216	4.9632854	-3.7038023
C	-0.3665196	-2.9628337	0.7270461	H	-2.5111685	-4.4441482	-5.8316648
C	0.1709607	-3.0146053	-0.7236649	H	-1.0313446	-3.2884999	-4.0957953
C	-0.9765977	0.5269365	-1.9157988	H	-4.8520677	-2.6910769	-1.1026389
C	-1.1454445	1.782983	-1.1971531	H	0.1822037	-1.889656	-2.5277391
C	-1.0354684	1.8191074	0.1474556	H	-1.0219474	-1.4504531	2.1275293
O	-0.7812951	0.7310697	0.9022453	H	0.68308	-1.3392792	1.7060355
C	-1.0336955	0.4808092	-3.280097	H	0.2863362	-3.6018317	1.3326717
C	-1.2379963	1.6615341	-4.1030341	H	0.0085103	-4.0274483	-1.1113448
C	-1.7245487	2.961834	-3.4116825	H	-1.1388563	2.723333	0.7338729
C	-1.4155884	3.0621375	-1.9074169	H	-0.8695799	-0.4359185	-3.8327054
O	-1.1847905	4.0993862	-4.1023228	H	-3.7507404	2.2258396	-3.0932022
C	0.1563494	4.227885	-4.042054	H	-3.6031242	4.000654	-3.1614784
C	0.7360823	5.302811	-4.8442142	H	-3.4840338	3.0246618	-4.6590186
C	-3.2479543	3.0605647	-3.5923677	H	-4.9150228	-6.6955452	-3.5410105
O	-7.0021559	-4.7145518	-5.2210918	H	-6.6837341	-6.5249862	-3.3788882
C	-7.1542214	-3.4355801	-5.7018233	H	-5.9698354	-7.0682922	-4.9252498
C	-8.2202512	-3.3601626	-6.7119589	H	3.2838339	-3.2065481	0.1218539
C	-5.836513	-6.4128442	-4.0606079	H	-2.72958	-5.1302921	0.453745
O	-6.581526	-3.8896081	-2.5336659	H	-9.5007429	-5.1207509	-9.3424015
O	-4.8594996	-5.1756319	-6.7326043	H	-10.818711	-1.3668339	-7.6979947
O	-1.4831738	4.1291754	-1.3242422	H	0.1601964	7.6097548	-7.2939468
O	-1.1178727	1.6519895	-5.3211279	H	3.7710214	6.9074777	-5.0609798

C	1.6900547	-2.8113022	-0.7910722	H	-9.7897985	-0.4042317	-5.8611235
C	-1.7498284	-3.5870798	0.9003242	H	-8.9071481	-1.4465193	-4.7281645
O	2.2800058	-2.2941839	-1.7111313	H	-8.019072	-0.5429072	-5.9406014
O	2.3289239	-3.3349956	0.2811159	H	-6.7447912	-5.378741	-7.2536619
O	-1.8509534	-4.7649995	0.2361535	H	-11.323078	-3.9080403	-10.058455
O	-2.6356856	-3.1526608	1.5985313	H	-1.6533415	6.3150013	-7.147678
O	-6.4507015	-2.5287252	-5.2920479	H	-1.5312124	4.671862	-6.4803723
O	0.8110691	3.4689245	-3.31194	H	-2.1022262	5.985186	-5.4636957
C	-8.3716044	-4.3925392	-7.6763707	H	2.0620429	8.7985602	-7.5140036
C	-9.4149412	-4.3246024	-8.6078296	H	2.3139567	4.2216197	-3.3464572

NImag	0
Σ Electronic and thermal Free Energy	-1865696.967
mol Fraction	0.000481403

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 16

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.9074598	-4.3881068	-5.2746198	C	-10.171721	-2.8080786	-8.4571644
C	-2.8561782	-3.7949371	-4.0468132	C	-9.8186957	-4.1495156	-8.236027
C	-4.0260249	-3.6934047	-3.1837148	C	-8.7132063	-4.483672	-7.4685648
C	-5.3399157	-4.2565632	-3.5945335	C	1.5143937	6.2415279	-4.2602499
C	-5.3459104	-5.1271426	-4.8666717	C	1.9619047	7.1800798	-5.1829851
C	-4.1329034	-4.9410757	-5.8228489	C	1.4841059	7.1682719	-6.5030354
C	-1.6580426	-3.1940377	-3.4910805	C	0.566509	6.2123004	-6.9181004
C	-1.65345	-2.6015204	-2.2795736	C	0.0953974	5.2608091	-6.0081382
O	-2.7952097	-2.5172512	-1.5154478	C	-8.3927972	-5.9542554	-7.3161533
C	-3.936586	-3.0656123	-1.9908061	O	-7.5715599	-1.0345212	-6.7092272
C	-0.4479265	-2.0037032	-1.5877949	O	-11.277879	-2.5824292	-9.2149135
C	-0.7645727	-0.6711471	-0.9217277	C	2.0546398	6.2856435	-2.8487161
C	-0.7715286	-0.5722788	0.4293822	O	1.9072773	8.0759738	-7.4284215
C	-0.4599626	-1.6503866	1.4220991	O	-0.7472863	4.3410642	-6.5183805
C	-0.3967902	-3.0481476	0.7981927	H	-2.0350281	-4.4147695	-5.9206481
C	0.2321062	-3.0112438	-0.6157971	H	-0.73652	-3.2189058	-4.0643668
C	-1.0448957	0.5067076	-1.7438471	H	-4.7701896	-2.9429824	-1.3104952
C	-1.3309793	1.7206477	-0.9930039	H	0.2929381	-1.8144659	-2.3712904
C	-1.3072004	1.7067944	0.356588	H	-1.2174452	-1.6311829	2.2115662
O	-1.0356732	0.6048994	1.0829848	H	0.5003371	-1.4104035	1.8977295
C	-1.0098684	0.5112603	-3.1137727	H	0.2515166	-3.6757481	1.4203132
C	-1.205611	1.7185491	-3.8824801	H	0.1513856	-4.014646	-1.0505776
C	-1.8357836	2.9487386	-3.1927607	H	-1.5017232	2.5784674	0.9685456
C	-1.6411992	3.0122767	-1.6694178	H	-0.7450346	-0.3686437	-3.6861919
O	-1.3248004	4.1182963	-3.8347163	H	-3.8277144	2.0667207	-3.0338171
C	0.0252002	4.3171783	-3.6793854	H	-3.7894747	3.8496697	-3.0411301
C	0.5444696	5.2865229	-4.6574772	H	-3.5158154	2.9379581	-4.5543065
C	-3.3492576	2.9474978	-3.4739379	H	-4.4902881	-6.8609196	-3.8633416
O	-6.5634126	-4.913735	-5.5985132	H	-6.2703269	-6.7696302	-3.8079435
C	-6.7554228	-3.654138	-6.0408383	H	-5.4347741	-7.2326339	-5.3233771
C	-7.9208329	-3.4403591	-6.8938393	H	3.2927699	-3.0883851	0.415749
C	-5.3889786	-6.6008043	-4.4326956	H	-2.6166427	-5.3222865	0.2919616
O	-6.3453829	-4.1275377	-2.9194299	H	-9.6447254	-0.7325082	-8.1057438
O	-4.2347966	-5.3385691	-6.9762316	H	-10.429144	-4.9226671	-8.6899303
O	-1.8445536	4.0388572	-1.0481659	H	2.6863742	7.9324799	-4.8774037
O	-0.9420836	1.7986106	-5.08396	H	0.2271094	6.1805745	-7.9466998

C	1.7382627	-2.7236376	-0.5746227	H	-9.0481449	-6.5438208	-7.9635963
C	-1.7522256	-3.7500161	0.8587356	H	-7.3530247	-6.1674841	-7.5801661
O	2.3536738	-2.1217319	-1.4237135	H	-8.5329884	-6.2925288	-6.2847335
O	2.3385861	-3.2756886	0.5058259	H	-6.7788074	-1.3961205	-6.2382579
O	-1.7460962	-4.9047202	0.1488016	H	-11.411393	-1.6253198	-9.3044408
O	-2.7021467	-3.3893882	1.5134668	H	2.6794376	7.1727056	-2.7074903
O	-5.970416	-2.7593661	-5.6900966	H	1.2513565	6.3099702	-2.1046851
O	0.6500977	3.7257749	-2.8163817	H	2.6536037	5.3969129	-2.6280628
C	-8.2754187	-2.0815406	-7.1658257	H	2.5514543	8.6699639	-7.0124589
C	-9.4055537	-1.7777243	-7.9311618	H	-0.925978	3.6057021	-5.8933463

NImag	0
Σ Electronic and thermal Free Energy	-1865696.729
mol Fraction	0.000322098

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 17

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2023899	-4.2041094	-5.1892554	C	-10.141195	-3.0055777	-8.6695463
C	-3.0622239	-3.6399274	-3.9502479	C	-9.9883734	-2.0016253	-7.7000393
C	-4.178481	-3.5064061	-3.02477	C	-8.9622874	-2.0708408	-6.765085
C	-5.5360378	-4.0177575	-3.3662281	C	1.7015024	6.2041184	-4.223943
C	-5.6380301	-4.8509236	-4.6570449	C	2.1465138	7.134677	-5.1527558
C	-4.4837401	-4.659063	-5.6724192	C	1.598616	7.1666169	-6.4439574
C	-1.8128765	-3.0987736	-3.4547183	C	0.6127773	6.2629286	-6.8207401
C	-1.7173877	-2.527078	-2.2355869	C	0.1408643	5.3188487	-5.9004407
O	-2.80971	-2.4111098	-1.4107312	C	-8.8305039	-0.967058	-5.7402763
C	-3.9971528	-2.9038214	-1.828926	O	-7.393033	-5.2232684	-7.9627543
C	-0.451188	-1.9903586	-1.6047986	O	-11.13751	-2.9615537	-9.5985947
C	-0.6760215	-0.6617035	-0.8953987	C	2.3163899	6.1968864	-2.842653
C	-0.5953859	-0.590664	0.4551741	O	2.08897	8.107538	-7.2995723
C	-0.2643356	-1.7002913	1.4059326	O	-0.7731685	4.4531717	-6.3826285
C	-0.2983253	-3.0858809	0.7534456	H	-2.3710289	-4.239088	-5.8865795
C	0.2442846	-3.0450846	-0.6955454	H	-0.9262394	-3.1501077	-4.078849
C	-0.9608411	0.5422649	-1.6768791	H	-4.7861463	-2.760281	-1.1012087
C	-1.1547367	1.7498589	-0.8877032	H	0.249358	-1.812627	-2.4272
C	-1.0481887	1.7073845	0.4572565	H	-0.9681706	-1.6676244	2.2431182
O	-0.7734645	0.5814205	1.1449524	H	0.7335092	-1.5083616	1.8223187
C	-1.0090943	0.5735392	-3.0461197	H	0.3592056	-3.7529283	1.3225471
C	-1.2026871	1.8029714	-3.7791646	H	0.095891	-4.0352114	-1.1427894
C	-1.7399312	3.0428877	-3.0310177	H	-1.1717489	2.5726263	1.0961673
C	-1.4587411	3.0653581	-1.5198088	H	-0.8122779	-0.3033143	-3.6499095
O	-1.2134387	4.2030892	-3.6776173	H	-3.7567463	2.2431334	-2.7793358
C	0.1513229	4.339704	-3.5905009	H	-3.6405379	4.0225685	-2.7522632
C	0.6626814	5.301351	-4.5793468	H	-3.4906545	3.1342922	-4.2967596
C	-3.2649216	3.1125223	-3.2273743	H	-4.7715523	-6.6316772	-3.7375355
O	-6.864771	-4.5961695	-5.3432173	H	-6.5441298	-6.4913322	-3.5884554
C	-7.0265818	-3.2980466	-5.764738	H	-5.8058329	-6.9485885	-5.1509587
C	-8.0847171	-3.185534	-6.7795566	H	3.3567525	-3.2583688	0.1455671
C	-5.6907062	-6.335114	-4.2535497	H	-2.6388299	-5.2566072	0.3443161
O	-6.4859891	-3.8957231	-2.6153926	H	-9.3581871	-4.8336113	-9.4969453
O	-4.6987253	-4.9559138	-6.8493609	H	-10.68081	-1.1624353	-7.6778678
O	-1.5931961	4.0838153	-0.8674276	H	2.9197021	7.8511309	-4.8964182
O	-1.007732	1.8972514	-4.9928497	H	0.2057773	6.2467611	-7.8281664

C	1.7609456	-2.818829	-0.7439483	H	-9.6800561	-0.2810132	-5.8085245
C	-1.6767391	-3.7315377	0.883212	H	-8.7880842	-1.3603551	-4.7190954
O	2.3464227	-2.2314447	-1.6237659	H	-7.9083051	-0.3977789	-5.8909869
O	2.4027826	-3.4079643	0.2915941	H	-6.5926524	-5.1628921	-7.3981353
O	-1.7624708	-4.8711147	0.1539788	H	-11.660317	-2.1563154	-9.4601139
O	-2.5703626	-3.3436065	1.5986311	H	2.9945635	7.0469877	-2.7253978
O	-6.3373018	-2.4038551	-5.3051446	H	1.5554001	6.2528995	-2.0567983
O	0.7914523	3.7041734	-2.7710782	H	2.8768486	5.273887	-2.6656287
C	-8.226003	-4.1773856	-7.7917908	H	1.6307837	8.0271058	-8.1510544
C	-9.2634302	-4.0802468	-8.7238742	H	-0.9545847	3.7137924	-5.7624697

NImag	0
Σ Electronic and thermal Free Energy	-1865694.384
mol Fraction	6.13E-06

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 18

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2899048	-4.4986101	-5.2016314	C	-10.749311	-3.0758096	-7.9952242
C	-3.1765707	-3.8848289	-3.988021	C	-10.364876	-4.4073826	-7.7678853
C	-4.2968966	-3.7811249	-3.0618145	C	-9.2120208	-4.7107262	-7.0593325
C	-5.625448	-4.3631788	-3.3899121	C	0.2210903	5.9418252	-5.9260645
C	-5.6917422	-5.2566388	-4.6444543	C	0.942778	6.9515609	-6.5493317
C	-4.5378016	-5.0726211	-5.6713574	C	2.2452575	7.2816103	-6.1373127
C	-1.9555873	-3.2627266	-3.5111594	C	2.8596523	6.584477	-5.1078737
C	-1.8905729	-2.6464868	-2.3134294	C	2.1673685	5.5513995	-4.4729535
O	-2.9879904	-2.5618129	-1.4875125	C	-8.8625364	-6.1734667	-6.8958512
C	-4.1470937	-3.1334671	-1.8854391	O	-8.0767105	-1.231902	-6.4391003
C	-0.6606841	-2.008826	-1.7056317	O	-11.900938	-2.8805562	-8.6914087
C	-0.9527248	-0.6323643	-1.1275293	C	-1.1595101	5.6390652	-6.4653476
C	-1.0171524	-0.4703573	0.2154998	O	2.9542976	8.2763454	-6.7354846
C	-0.7942184	-1.5038857	1.2754518	O	2.8291142	4.9015206	-3.5024798
C	-0.6098108	-2.9289769	0.7327557	H	-2.454609	-4.5270196	-5.8949349
C	0.040429	-2.9415306	-0.6671338	H	-1.0672523	-3.2907506	-4.1342717
C	-1.1589808	0.5085427	-2.0215884	H	-4.939958	-3.0119548	-1.1579994
C	-1.4096433	1.7723061	-1.3421095	H	0.0459122	-1.8878879	-2.5312285
C	-1.446751	1.8247117	0.006391	H	-1.6391537	-1.484218	1.9716082
O	-1.2660573	0.7490594	0.798012	H	0.0968505	-1.2089265	1.8416996
C	-1.0937113	0.4400423	-3.3852543	H	0.0920272	-3.4469276	1.3987574
C	-1.227992	1.6048541	-4.242679	H	0.0164823	-3.9598353	-1.0700883
C	-1.7744296	2.9160034	-3.6200002	H	-1.622791	2.734443	0.5665102
C	-1.6123256	3.0393414	-2.0943507	H	-0.880445	-0.4853772	-3.9060622
O	-1.1652377	4.0419847	-4.2721984	H	-3.8247257	2.1911912	-3.4869733
C	0.16407	4.167272	-4.0865944	H	-3.6635567	3.9640614	-3.5684348
C	0.8224687	5.2272948	-4.8469281	H	-3.4049504	2.9640627	-5.0323081
C	-3.2725979	3.0163321	-3.9485676	H	-4.7563505	-6.9600593	-3.6605807
O	-6.9518885	-5.0728206	-5.3092384	H	-6.5314643	-6.8914206	-3.5060715
C	-7.1865444	-3.8257362	-5.765031	H	-5.7762517	-7.3714432	-5.0579369
C	-8.4026686	-3.6453209	-6.5532118	H	3.0668188	-2.2915786	-1.5708655
C	-5.6892851	-6.7225554	-4.1826985	H	-2.6189982	-5.4125984	0.3501208
O	-6.5946775	-4.2298462	-2.6646466	H	-10.232507	-0.9865665	-7.7175421
O	-4.7006722	-5.4889349	-6.8111393	H	-10.989626	-5.1979492	-8.1692919
O	-1.7372769	4.1151861	-1.537401	H	0.4938581	7.4924514	-7.3798803
O	-0.999363	1.575865	-5.4453859	H	3.8712733	6.8197298	-4.7995676

C	1.5233211	-2.5842918	-0.5340542	H	-9.5455889	-6.7850402	-7.4922325
C	-1.8924396	-3.7485282	0.8402458	H	-7.8367336	-6.3785787	-7.2151137
O	2.1152337	-2.4229295	0.5098338	H	-8.9383534	-6.4917343	-5.8514272
O	2.1299589	-2.5090146	-1.7389699	H	-7.2539668	-1.5742637	-6.0062401
O	-1.7948162	-4.9225393	0.167805	H	-12.054157	-1.9273605	-8.7903309
O	-2.8620275	-3.4572033	1.5014605	H	-1.331066	6.2051587	-7.3857612
O	-6.3956719	-2.9132016	-5.4795671	H	-1.280778	4.5738231	-6.6809554
O	0.7436476	3.4179935	-3.2857694	H	-1.9405013	5.9067614	-5.7469724
C	-8.791607	-2.2974417	-6.8319759	H	2.4130342	8.6732027	-7.4361351
C	-9.9684549	-2.0246266	-7.5361311	H	2.2424108	4.1702746	-3.1852175

NImag	0
Σ Electronic and thermal Free Energy	-1865700.372
mol Fraction	0.151727215

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 19

Atom	X	Y	Z	Atom	X	Y	Z
C	-4.0851506	-5.2717209	-4.8596236	C	-4.2301793	-1.4762734	-6.7887743
C	-3.8830171	-4.3220721	-3.9026066	C	-4.556622	-2.6490154	-7.4939208
C	-4.9803391	-3.7537275	-3.1332432	C	-5.7371304	-3.3351981	-7.2380486
C	-6.3919293	-4.0916385	-3.4475688	C	-1.3862967	5.8514204	-6.1478409
C	-6.651303	-5.237063	-4.4543637	C	-0.8511813	6.8530167	-6.942585
C	-5.4024224	-5.7663087	-5.219382	C	0.5367541	6.9796991	-7.119749
C	-2.5841252	-3.7734387	-3.5665852	C	1.4119143	6.0929201	-6.5097294
C	-2.4230279	-2.8861765	-2.5636979	C	0.9048249	5.0661806	-5.7075131
O	-3.4880168	-2.4399823	-1.8158892	C	-6.1315209	-4.4828645	-8.1424347
C	-4.7313455	-2.8585668	-2.1515238	O	-7.212955	-1.0006312	-4.7753191
C	-1.0893161	-2.3169614	-2.1152521	O	-3.0307111	-0.9142539	-7.0436669
C	-1.1989264	-0.9515697	-1.4473847	C	-2.8935449	5.791127	-6.0371769
C	-0.8575443	-0.8062165	-0.1427787	O	0.9617526	7.99692	-7.9137661
C	-0.3904511	-1.8738654	0.7982253	O	1.8128357	4.2438915	-5.1614237
C	-0.6286389	-3.2808942	0.2489768	H	-3.2527172	-5.6839983	-5.4220743
C	-0.2902923	-3.3425424	-1.2598858	H	-1.7135921	-4.0822494	-4.1372916
C	-1.6255439	0.2151585	-2.2209969	H	-5.5032033	-2.3922225	-1.5525639
C	-1.5963856	1.4730221	-1.4927744	H	-0.4962166	-2.176834	-3.0264859
C	-1.2208377	1.5048693	-0.1955919	H	-0.9114288	-1.748319	1.751988
O	-0.8704267	0.4075516	0.4965909	H	0.6794639	-1.7247567	0.9963609
C	-2.0074048	0.1723518	-3.5383216	H	0.0372887	-3.9820794	0.7640415
C	-2.4114235	1.3485524	-4.2694493	H	-0.5269467	-4.3501127	-1.6201928
C	-2.6417669	2.6745351	-3.5096713	H	-1.1726731	2.4116508	0.394129
C	-1.9521358	2.7635018	-2.1393286	H	-2.000896	-0.7506591	-4.1066404
O	-2.2480065	3.7838188	-4.3304662	H	-4.5536117	2.0342036	-2.675049
C	-0.9300955	3.8437905	-4.620206	H	-4.3387801	3.7999505	-2.7884019
C	-0.5047804	4.9296676	-5.496047	H	-4.6594499	2.8336964	-4.2603723
C	-4.1549785	2.8467023	-3.2910072	H	-6.4887226	-6.7979587	-2.933248
O	-7.7214032	-4.8654751	-5.3544366	H	-8.1221655	-6.0995081	-3.1299921
C	-7.8367015	-3.5593321	-5.7812252	H	-7.4595797	-7.223136	-4.3623595
C	-6.6120822	-2.8529807	-6.2280883	H	2.8899018	-3.7235973	-0.8767301
C	-7.2218181	-6.4234516	-3.6570589	H	-3.2008161	-5.2161561	0.2645743
O	-7.3246125	-3.5228724	-2.9039349	H	-4.9577013	0.0224981	-5.3985969
O	-5.5663265	-6.6354069	-6.0683002	H	-3.8717586	-2.9957594	-8.2614484
O	-1.7997433	3.8351475	-1.582511	H	-1.4992397	7.5592208	-7.4500269
O	-2.6815038	1.3404711	-5.4760671	H	2.488284	6.1619817	-6.6388986

C	1.2103299	-3.1692667	-1.5154713	H	-5.2509581	-5.026747	-8.4954963
C	-2.0399813	-3.7667883	0.5748835	H	-6.7949526	-5.2002173	-7.659802
O	1.6966631	-2.5522589	-2.4346142	H	-6.6505121	-4.0810656	-9.0230085
O	1.9580632	-3.8422473	-0.609804	H	-8.0728211	-1.4620227	-4.836804
O	-2.3082259	-4.9493165	-0.0271957	H	-2.9072886	-0.0931095	-6.5102565
O	-2.8164643	-3.2157722	1.3196483	H	-3.3416065	6.5528452	-6.6811465
O	-8.9328859	-3.0359909	-5.7266254	H	-3.2803336	4.8123008	-6.3350017
O	-0.1661953	2.9983354	-4.126918	H	-3.2306067	5.9651572	-5.010879
C	-6.3503187	-1.5878785	-5.6409197	H	1.9307829	7.9779759	-7.9648775
C	-5.1475752	-0.9264665	-5.8866104	H	1.3175577	3.5569686	-4.6473923

NImag	0
Σ Electronic and thermal Free Energy	-1865686.219
mol Fraction	6.24E-12

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 20

Atom	X	Y	Z	Atom	X	Y	Z
C	-4.2289212	-4.8662469	-4.9457838	C	-4.3586392	-1.1695486	-6.8283691
C	-3.9570056	-4.0913202	-3.8586442	C	-4.7410842	-2.1354039	-7.771543
C	-4.9806806	-3.7225481	-2.8892554	C	-5.8615296	-2.9389776	-7.5728136
C	-6.4070446	-4.1224723	-3.0797448	C	-1.4020517	6.0204762	-5.6689032
C	-6.745396	-5.0050783	-4.3081097	C	-0.8723381	7.0370387	-6.4475167
C	-5.5659193	-5.3302723	-5.2697154	C	0.5084777	7.1236691	-6.693295
C	-2.6411329	-3.5612201	-3.5582977	C	1.3812216	6.1815783	-6.1683432
C	-2.399019	-2.8465962	-2.4414973	C	0.8791085	5.1389587	-5.3841913
O	-3.3880572	-2.5780582	-1.5238265	C	-6.269308	-3.9306714	-8.6348758
C	-4.6461049	-3.0126901	-1.7900744	O	-7.0460201	-1.6464229	-4.3664498
C	-1.0446629	-2.290809	-2.045418	O	-3.2449771	-0.4485423	-7.0807963
C	-1.1309157	-0.9668283	-1.2984263	C	-2.9025513	6.008375	-5.4795136
C	-0.7574233	-0.8993507	0.0046619	O	0.9277882	8.159422	-7.464843
C	-0.2718248	-2.016515	0.8728071	O	1.7835471	4.2632187	-4.9210453
C	-0.4512547	-3.3958631	0.2311318	H	-3.4474526	-5.1365144	-5.6494696
C	-0.180552	-3.3507471	-1.2866384	H	-1.8265829	-3.7364574	-4.2545215
C	-1.5907205	0.2366132	-1.9890091	H	-5.3537295	-2.725095	-1.0224317
C	-1.5208127	1.4558667	-1.2020011	H	-0.5271913	-2.0990628	-2.9909384
C	-1.1069904	1.4150573	0.0840154	H	-0.8109005	-1.9753542	1.8243521
O	-0.7527376	0.2792146	0.7075628	H	0.7894696	-1.8482842	1.088805
C	-2.0405046	0.2581772	-3.2862156	H	0.2953843	-4.0716966	0.6659258
C	-2.4795951	1.4655504	-3.9397052	H	-0.4111115	-4.327897	-1.724222
C	-2.6344934	2.7651026	-3.1151706	H	-1.0303646	2.2887261	0.7191853
C	-1.8813297	2.779405	-1.7741255	H	-2.0746537	-0.6390516	-3.8927922
O	-2.24597	3.8961051	-3.9087592	H	-4.5192829	2.154508	-2.2054057
C	-0.9409461	3.9312893	-4.2570183	H	-4.2622161	3.9149584	-2.2812663
C	-0.5221201	5.0404935	-5.1048649	H	-4.6781998	3.0028706	-3.7645117
C	-4.129435	2.9730682	-2.8198136	H	-6.4734307	-6.8456305	-3.1549937
O	-7.880622	-4.4717674	-5.0131201	H	-8.1202327	-6.1611498	-3.1162162
C	-7.8192934	-3.6525826	-6.1197075	H	-7.5194884	-6.9897743	-4.5908688
C	-6.5946415	-2.8219299	-6.3655873	H	2.555189	-2.905767	-2.9322456
C	-7.2500024	-6.3492127	-3.7488522	H	-2.882246	-5.5055944	0.2234567
O	-7.2615681	-3.8366753	-2.2624986	H	-4.8894041	-0.1967504	-4.9705028
O	-5.7950897	-6.0300348	-6.2516301	H	-4.149122	-2.2319077	-8.6759785
O	-1.6851098	3.8225852	-1.1786003	H	-1.519133	7.7873388	-6.8889267
O	-2.8360083	1.5077723	-5.1228474	H	2.4513479	6.2199615	-6.350827

C	1.3146095	-3.138553	-1.5344353	H	-5.6096301	-3.8565944	-9.5041613
C	-1.8004977	-4.0103937	0.5964849	H	-6.2264385	-4.9561204	-8.2516069
O	2.1739857	-3.127157	-0.6815135	H	-7.2991849	-3.747787	-8.9563926
O	1.5877463	-3.0104781	-2.8515876	H	-6.7311275	-0.8910944	-3.8471845
O	-2.0353882	-5.1461329	-0.1031882	H	-3.0931342	0.2206248	-6.3751202
O	-2.5547144	-3.5941312	1.4446649	H	-3.3542354	6.8174964	-6.0598825
O	-8.7907917	-3.630046	-6.8351126	H	-3.3417313	5.0606534	-5.8042678
O	-0.1831361	3.0416819	-3.8358484	H	-3.1781882	6.1417564	-4.429067
C	-6.2429631	-1.804953	-5.4654697	H	1.8915587	8.111055	-7.5691521
C	-5.1354014	-0.9849394	-5.6775824	H	1.2904812	3.5748202	-4.4073145

NImag	0
Σ Electronic and thermal Free Energy	-1865682.671
mol Fraction	1.56E-14

(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 21

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.10899	-4.3613845	-5.3100842	C	-10.642146	-3.3735106	-8.2529868
C	-3.0074191	-3.7521429	-4.0947402	C	-9.4805648	-2.7184469	-8.669943
C	-4.14915	-3.618384	-3.2001997	C	-8.3028568	-2.818792	-7.933093
C	-5.4853268	-4.1615581	-3.5658459	C	0.2664829	6.3066295	-5.4708286
C	-5.5321715	-5.0877954	-4.7958092	C	0.9632907	7.3708598	-6.023714
C	-4.3618749	-4.9075182	-5.8071396	C	2.2663873	7.6832178	-5.6039218
C	-1.7859983	-3.157109	-3.5851785	C	2.9026552	6.916051	-4.6383508
C	-1.7358098	-2.551227	-2.3822972	C	2.232615	5.826829	-4.0728486
O	-2.8524167	-2.4365211	-1.5835426	C	-7.0770916	-2.0916191	-8.4381026
C	-4.0143057	-2.9754722	-2.0214347	O	-9.440001	-5.00156	-5.2041975
C	-0.5017628	-1.9463733	-1.7467286	O	-11.757399	-3.2206948	-9.0219113
C	-0.8009722	-0.6058492	-1.0945355	C	-1.1184249	6.0283193	-6.0120209
C	-0.8826773	-0.5241117	0.2537627	O	2.8628941	8.7514054	-6.1979625
C	-0.6532485	-1.6169784	1.2516269	O	2.9182834	5.1176891	-3.1624202
C	-0.442638	-3.008653	0.6260426	H	-2.2608374	-4.4087733	-5.9866866
C	0.2139158	-2.9278966	-0.764142	H	-0.882293	-3.2040613	-4.1847945
C	-1.0121569	0.5834758	-1.9220678	H	-4.8304209	-2.8278119	-1.3254372
C	-1.2828422	1.8022752	-1.1711845	H	0.1998436	-1.7769893	-2.5679183
C	-1.3338662	1.7748021	0.1775624	H	-1.4853328	-1.6307952	1.9611918
O	-1.1503501	0.6561961	0.9071115	H	0.2416744	-1.3485982	1.8262275
C	-0.9354127	0.5953913	-3.2864194	H	0.2642918	-3.5408495	1.275954
C	-1.0770404	1.8080865	-4.0747339	H	0.1861968	-3.9251817	-1.2179099
C	-1.6514853	3.070457	-3.3799413	H	-1.5255302	2.6484351	0.7878158
C	-1.4949095	3.1087708	-1.8495341	H	-0.7097091	-0.2964052	-3.858421
O	-1.067451	4.2456238	-3.9640329	H	-3.6851299	2.2923635	-3.2970199
C	0.2579809	4.3906807	-3.7698609	H	-3.5647268	4.0707308	-3.2730762
C	0.890441	5.5151597	-4.4558207	H	-3.2798094	3.1649658	-4.7920654
C	-3.1512762	3.1560093	-3.7066324	H	-4.577386	-6.7549325	-3.7578864
O	-6.7857102	-4.9467693	-5.472156	H	-6.35728	-6.7078769	-3.6280617
C	-7.0157791	-3.7111997	-5.9767632	H	-5.5792984	-7.21051	-5.1579859
C	-8.2748231	-3.6128423	-6.7571844	H	3.2326829	-2.1952138	-1.6216131
C	-5.5072709	-6.5424931	-4.2956037	H	-3.2469421	-4.3396242	1.5052082
O	-6.4742146	-3.9652115	-2.8823039	H	-11.540266	-4.6525763	-6.7595317
O	-4.5048278	-5.3079006	-6.9546295	H	-9.5139281	-2.1320309	-9.5818705
O	-1.6316228	4.1495926	-1.2318247	H	0.514174	7.9796821	-6.8009275
O	-0.8357813	1.8549535	-5.2739067	H	3.9175407	7.1242968	-4.3113865

C	1.6903906	-2.5663219	-0.6096575	H	-7.262118	-1.6928296	-9.439716
C	-1.6584081	-3.9296329	0.5976658	H	-6.8075035	-1.2653111	-7.7742077
O	2.2807384	-2.4625462	0.4434	H	-6.2047745	-2.7511912	-8.4812932
O	2.298257	-2.4094451	-1.8059679	H	-10.334811	-5.334959	-5.0354343
O	-2.5596936	-3.648722	1.5643701	H	-12.486425	-3.7292501	-8.6338829
O	-1.779154	-4.8756273	-0.1501766	H	-1.3138753	6.671528	-6.8747481
O	-6.2206283	-2.7996738	-5.8173671	H	-1.2260089	4.9844352	-6.3201653
O	0.8568235	3.6029615	-3.0208081	H	-1.8906489	6.216907	-5.2598088
C	-9.4557239	-4.2705716	-6.3519611	H	3.754771	8.8607833	-5.8313917
C	-10.634853	-4.146228	-7.0930806	H	2.3418008	4.3591333	-2.8896147

NImag	0
Σ Electronic and thermal Free Energy	-1865689.647
mol Fraction	2.05E-09

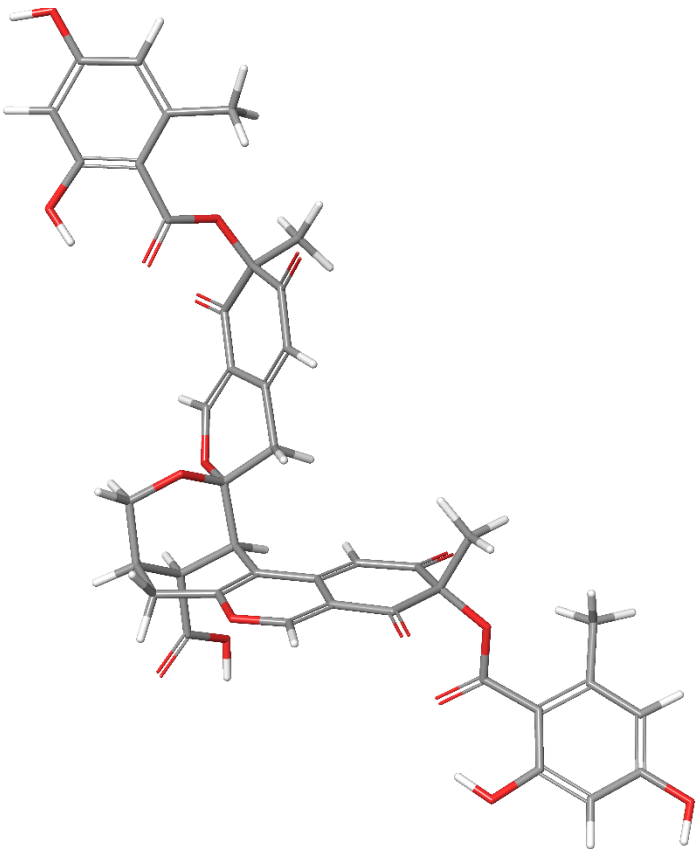
(8*S*, 13*R*, 8a*S*, 12a*R*, 13a*R*)-Diazaphilonic acid - Conformer 22

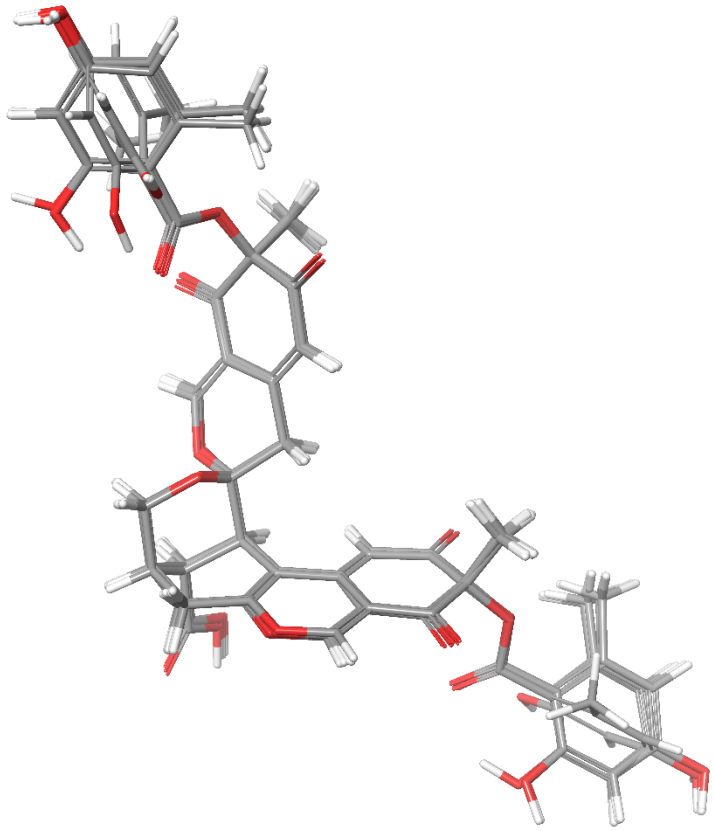
Atom	X	Y	Z	Atom	X	Y	Z
C	-10.476301	-3.1462007	-8.3122657	C	-2.9975887	-4.2473392	-5.2899997
C	-9.3222636	-2.4308819	-8.6425171	C	-2.9386068	-3.6855452	-4.0495903
C	-8.1569664	-2.57312	-7.8935346	C	-4.1017655	-3.6205364	-3.1737911
C	2.0790992	6.1418501	-4.1451274	C	-5.4139477	-4.1875154	-3.5902341
C	2.6661134	7.0316289	-5.0343313	C	-5.41811	-5.0462392	-4.8704133
C	2.2983758	7.0280426	-6.3882385	C	-4.2254513	-4.8009956	-5.8402205
C	1.3527714	6.1291286	-6.8660201	C	-1.7424864	-3.0818615	-3.4906593
C	0.7399824	5.2260619	-5.9883695	C	-1.7365064	-2.5154079	-2.2674503
C	-6.9416776	-1.7733352	-8.3054714	O	-2.8713605	-2.4638059	-1.4905363
O	-9.2985764	-5.0224932	-5.4009687	C	-4.0102793	-3.0201825	-1.9676339
O	-11.57908	-2.9469062	-9.0874259	C	-0.5378933	-1.9035629	-1.5761064
C	2.4999653	6.1724174	-2.6931557	C	-0.8612294	-0.5526721	-0.9548972
O	2.9203748	7.9299332	-7.199462	C	-0.9916875	-0.4484635	0.3904146
O	-0.11982	4.360493	-6.5616731	C	-0.8177903	-1.5269021	1.4140268
H	-2.1335887	-4.2460715	-5.9480444	C	-0.6023318	-2.927	0.8202338
H	-0.8253116	-3.0846537	-4.0713769	C	0.1159662	-2.8778148	-0.5449907
H	-4.8376626	-2.9266947	-1.2755297	C	-1.0286298	0.6247318	-1.8052153
H	0.2075069	-1.7478496	-2.360648	C	-1.3140502	1.8580468	-1.0874381
H	-1.6961947	-1.5381625	2.0676825	C	-1.4174943	1.8518192	0.2589227
H	0.0434355	-1.2552168	2.0353818	O	-1.2723065	0.7432888	1.0099122
H	0.0674259	-3.4720684	1.4974832	C	-0.8927645	0.6113978	-3.1696206
H	0.1156041	-3.8775657	-0.9924617	C	-0.9613693	1.8173756	-3.9591104
H	-1.6245288	2.7363893	0.8479561	C	-1.5650813	3.0912582	-3.328018
H	-0.6404915	-0.2894835	-3.7147625	C	-1.4927809	3.157927	-1.7938326
H	-3.6159683	2.3409213	-3.3313084	O	-0.9267654	4.2193923	-3.9303279
H	-3.4614888	4.1177069	-3.3415527	C	0.4172329	4.3268263	-3.6688163
H	-3.1240106	3.1763643	-4.8237825	C	1.0787151	5.2453943	-4.6091252
H	-4.4736625	-6.7638204	-3.9089119	C	-3.046825	3.1852006	-3.7333777
H	-6.2567302	-6.7335809	-3.8132613	O	-6.6556725	-4.8771522	-5.5696604
H	-5.4431615	-7.144964	-5.352322	C	-6.8874738	-3.6136186	-6.0000487
H	3.1803736	-2.1848754	-1.270586	C	-8.1320885	-3.4721112	-6.7945017
H	-2.5873274	-5.3888024	0.2254576	C	-5.3943481	-6.5262071	-4.4524934
H	-11.372671	-4.5762163	-6.9618587	O	-6.4176924	-4.0612612	-2.9124782
H	-9.3521459	-1.7632988	-9.4969019	O	-4.3285831	-5.1579039	-7.0058711
H	3.41268	7.7434257	-4.6984054	O	-1.6858076	4.2011718	-1.1976498
H	1.0848638	6.0854633	-7.9182422	O	-0.6036215	1.8685472	-5.1386211

H	-7.1200867	-1.2887637	-9.2697206	C	1.5888533	-2.5231563	-0.3241059
H	-6.7051114	-1.0051863	-7.5637685	C	-1.8867879	-3.7511486	0.8296156
H	-6.0515773	-2.4040697	-8.3918939	O	2.1276652	-2.401623	0.7535097
H	-10.190821	-5.3828809	-5.2806846	O	2.2540193	-2.3980299	-1.4934139
H	-12.30464	-3.502826	-8.7629736	O	-1.7549276	-4.8924535	0.1095682
H	3.1746652	7.0139417	-2.5116377	O	-2.8859689	-3.490174	1.4587289
H	1.6404331	6.2696683	-2.0211538	O	-6.1008262	-2.7101088	-5.7655477
H	3.0102817	5.2465168	-2.410865	O	0.9294555	3.7022017	-2.7561947
H	2.5778761	7.8291424	-8.1016438	C	-9.3062356	-4.189171	-6.4763847
H	-0.4010562	3.6463669	-5.9485616	C	-10.473098	-4.0220274	-7.2282551

NImag	0
Σ Electronic and thermal Free Energy	-1865687.124
mol Fraction	2.88E-11

Data S3. Lowest energy conformer 3D structure, all overlaid 3D structures, cartesian coordinates, number of imaginary frequencies, and energy for (8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid conformers.





(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 1

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.5559794	-8.9522551	-0.3367636	C	-18.276353	-5.1756033	6.8350881
C	-8.566997	-7.9202476	-0.6908413	C	-2.6678509	-9.7460143	1.0212856
C	-8.754332	-6.7193865	0.1145277	C	-1.3165928	-10.021554	0.8753228
C	-7.9804035	-6.4865963	1.2184525	C	-0.5683984	-9.458841	-0.1715685
C	-6.9295934	-7.3871077	1.6569226	C	-1.1600884	-8.5902662	-1.0776047
C	-6.8712732	-8.8063549	1.0337798	C	-2.5176228	-8.2809724	-0.9491283
C	-9.2968415	-8.1146372	-1.810825	C	-17.361649	-5.3798945	8.0223291
O	-10.222509	-7.2442953	-2.2572842	C	-3.3799681	-10.375802	2.1979101
C	-10.447897	-6.0959391	-1.5371299	O	0.7468577	-9.7973089	-0.2358392
C	-9.7862679	-5.8106102	-0.3872602	O	-3.0152371	-7.4185577	-1.849098
C	-11.435677	-5.215408	-2.2401143	O	-21.871771	-4.7948995	6.4146293
C	-11.718812	-3.8887948	-1.5031086	O	-18.456439	-4.8932446	3.1387782
C	-10.476971	-3.419185	-0.7258754	H	-8.0632768	-5.573402	1.7964295
C	-10.137843	-4.5114241	0.3202637	H	-9.1918851	-8.983031	-2.4490941
C	-11.366825	-4.6805551	1.2614853	H	-12.365716	-5.7766202	-2.3992722
O	-12.543373	-4.9409714	0.555789	H	-11.02489	-5.0035073	-3.2340953
C	-9.3022596	-3.0927643	-1.6348026	H	-11.998405	-3.1337316	-2.2452179
C	-12.864848	-4.0185947	-0.4970031	H	-10.710487	-2.4934109	-0.1854826
O	-8.1806825	-2.8378129	-0.9253367	H	-9.2960515	-4.1749835	0.9269226
O	-9.3467668	-3.0297711	-2.8439556	H	-13.764238	-4.4300167	-0.9616194
O	-11.473169	-3.3785675	1.9308537	H	-13.114057	-3.0393208	-0.0691685
C	-12.274287	-3.3033597	3.0068006	H	-7.4780993	-2.6314852	-1.5710815
C	-12.762507	-4.3660731	3.6939942	H	-12.511129	-2.2818198	3.2869523
C	-12.360782	-5.7118964	3.3267434	H	-10.285397	-5.6759075	2.8260815
C	-11.246511	-5.7885404	2.3091154	H	-11.238379	-6.7567989	1.8047429
C	-13.722188	-4.1192971	4.7908647	H	-12.623978	-7.8122871	3.5908864
C	-14.134174	-5.3474822	5.6323439	H	-12.240337	-5.4347742	6.7072819
C	-13.927013	-6.7225841	4.9455697	H	-13.475376	-4.3904527	7.4538287
C	-12.904311	-6.809552	3.9009639	H	-13.616924	-6.1717811	7.5610563
O	-15.49991	-5.2170926	6.0571289	H	-7.4586999	-10.804175	1.6133774
C	-13.307744	-5.334933	6.9291308	H	-7.0450126	-9.7214695	2.9792892
O	-5.5029309	-9.2354436	0.9473754	H	-8.6010076	-9.5407661	2.136023
C	-7.5419303	-9.787912	2.007977	H	-20.842838	-4.7117898	3.9132959
O	-6.1415236	-7.1060535	2.5515817	H	-20.006376	-5.1236702	8.113029

O	-7.3344878	-9.9179055	-1.045353	H	-0.8083782	-10.675278	1.5758607
O	-14.540323	-7.6964449	5.3524259	H	-0.5994594	-8.1273294	-1.8848119
O	-14.125288	-3.0075959	5.0888953	H	-17.956627	-5.4712144	8.9354364
C	-16.415472	-5.1850675	5.0683087	H	-16.753532	-6.2821385	7.9102483
C	-17.815372	-5.1059431	5.4821773	H	-16.666243	-4.5441419	8.1446716
O	-16.037747	-5.2091559	3.8869241	H	-3.905731	-9.6263144	2.7963627
C	-4.7258353	-8.5224092	0.1080611	H	-4.1298786	-11.103546	1.8728647
C	-3.3075961	-8.8713125	0.087098	H	-2.6554521	-10.889607	2.8360482
O	-5.240749	-7.6451838	-0.6032732	H	1.1545853	-9.3452888	-0.9916735
C	-18.782324	-4.9478208	4.4391049	H	-3.9644057	-7.2631359	-1.6103511
C	-20.144399	-4.835623	4.7361604	H	-22.410918	-4.682368	5.6155924
C	-20.563312	-4.8939664	6.057232	H	-17.473173	-5.011855	3.0802572
C	-19.634448	-5.0689381	7.0956676				

NImag	0
Σ Electronic and thermal Free Energy	-1819235.386
mol Fraction	0.500795215

(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 2

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.6063742	-9.0007768	-0.1942116	C	-18.181059	-4.6938255	6.895505
C	-8.6196105	-7.9898181	-0.5990285	C	-2.6975596	-9.7260929	1.1270703
C	-8.787687	-6.7365227	0.126763	C	-1.3502525	-10.017738	0.9759806
C	-7.9929906	-6.4338679	1.1985241	C	-0.6190029	-9.530813	-0.1197427
C	-6.9379213	-7.308149	1.6779377	C	-1.2236618	-8.7223883	-1.0717213
C	-6.8964071	-8.7664144	1.1509718	C	-2.5774335	-8.3982153	-0.940245
C	-9.3703245	-8.2554565	-1.6902143	C	-17.245924	-4.821697	8.0775026
O	-10.30051	-7.4124397	-2.1778126	C	-3.3906569	-10.271383	2.3560768
C	-10.508391	-6.2170732	-1.532808	O	0.6935488	-9.8795422	-0.1844254
C	-9.8250009	-5.8583605	-0.4167129	O	-3.0879635	-7.5960276	-1.8874442
C	-11.505236	-5.3808291	-2.2759165	O	-21.78195	-4.3241943	6.5138657
C	-11.769817	-4.0061618	-1.6251281	O	-18.426533	-4.661709	3.1923118
C	-10.512333	-3.4916641	-0.9034496	H	-8.0618382	-5.4834189	1.7150113
C	-10.158672	-4.5127143	0.2077556	H	-9.2802896	-9.1653733	-2.2702615
C	-11.371149	-4.6117773	1.179874	H	-12.440189	-5.9467126	-2.3803389
O	-12.561239	-4.9131029	0.5142799	H	-11.111631	-5.2384527	-3.2890547
C	-9.3529232	-3.233197	-1.8529776	H	-12.059782	-3.3013573	-2.4113795
C	-12.898023	-4.06204	-0.592405	H	-10.732441	-2.5304328	-0.4226159
O	-8.2177531	-2.9368442	-1.1822802	H	-9.3047544	-4.1405118	0.7753243
O	-9.4189596	-3.2514801	-3.0626484	H	-13.807262	-4.4991791	-1.0122097
O	-11.460312	-3.2671631	1.7616956	H	-13.135613	-3.0549152	-0.2271933
C	-12.241633	-3.11554	2.8441408	H	-7.5261052	-2.7780576	-1.8527992
C	-12.721552	-4.1270442	3.6099591	H	-12.469379	-2.0762491	3.058909
C	-12.331795	-5.4965856	3.3272335	H	-10.265637	-5.5050983	2.7886143
C	-11.236348	-5.6473136	2.2975196	H	-11.241143	-6.6473626	1.8595004
C	-13.660305	-3.8020266	4.7045586	H	-12.598457	-7.5730407	3.7370484
C	-14.061939	-4.9686216	5.6340719	H	-12.14942	-4.9931436	6.6787773
C	-13.87259	-6.3878865	5.0380016	H	-13.366676	-3.8945367	7.3749425
C	-12.869209	-6.5502653	3.9837028	H	-13.513343	-5.6638611	7.6044952
O	-15.419281	-4.8028497	6.0731749	H	-7.4809983	-10.717638	1.8743165
C	-13.212255	-4.8730586	6.9122393	H	-7.0384319	-9.5475112	3.1565331
O	-5.5315261	-9.2073237	1.0693262	H	-8.6087369	-9.4160897	2.3308473
C	-7.5531212	-9.6766996	2.2009216	H	-20.797883	-4.4160779	3.9948182
O	-6.1327519	-6.9715371	2.5375057	H	-19.887572	-4.5464848	8.1973868
O	-7.4015033	-10.013084	-0.8398895	H	-0.8319427	-10.625243	1.7099327
O	-14.482294	-7.3289699	5.5203996	H	-0.6759826	-8.317868	-1.918251

O	-14.053659	-2.6707373	4.9340025	H	-17.8247	-4.8474844	9.005112
C	-16.352358	-4.8326742	5.1007847	H	-16.643667	-5.7327336	8.016409
C	-17.744244	-4.7184439	5.5330427	H	-16.544965	-3.9833079	8.1302712
O	-15.996055	-4.9383708	3.917226	H	-3.9027283	-9.4806062	2.9117254
C	-4.7670164	-8.5565013	0.1700553	H	-4.1490144	-11.015726	2.0943652
C	-3.3507489	-8.9132184	0.1474488	H	-2.6566514	-10.744484	3.0145272
O	-5.2913125	-7.7266175	-0.5895941	H	1.0892527	-9.4816682	-0.9762384
C	-18.729186	-4.626424	4.4989065	H	-4.0320174	-7.419956	-1.6428184
C	-20.085248	-4.4874211	4.8117172	H	-22.334959	-4.2633478	5.7187018
C	-20.480541	-4.4539469	6.1409099	H	-17.444917	-4.7888048	3.1245587
C	-19.533816	-4.562815	7.1722318				

NImag	0
Σ Electronic and thermal Free Energy	-1819235.384
mol Fraction	0.499204781

(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 3

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.5845824	-8.9076987	-0.4248791	C	-18.293879	-5.2411684	6.8491454
C	-8.5849715	-7.8551147	-0.7511358	C	-2.6444673	-9.2385484	1.2000038
C	-8.7687035	-6.6824083	0.0938258	C	-1.2852774	-9.541264	1.1313881
C	-7.9989982	-6.495459	1.2088457	C	-0.5986556	-9.4943836	-0.0838423
C	-6.9488493	-7.412498	1.6132215	C	-1.2639798	-9.1283335	-1.2530203
C	-6.8914315	-8.8117096	0.9471294	C	-2.6213112	-8.802145	-1.1991062
C	-9.3093205	-8.0048277	-1.8808839	C	-17.379516	-5.4886198	8.0284093
O	-10.226341	-7.1115175	-2.3029315	C	-3.3131518	-9.313919	2.5556111
C	-10.44621	-5.9875398	-1.5449539	O	0.7260646	-9.8142719	-0.0672112
C	-9.789962	-5.7481753	-0.3816792	O	-3.293467	-8.4576234	-2.3297802
C	-11.421015	-5.0730877	-2.2230214	O	-21.885608	-4.8072269	6.4471922
C	-11.692038	-3.7673986	-1.4447161	O	-18.477012	-4.8499214	3.1630662
C	-10.449059	-3.339623	-0.6454946	H	-8.0770048	-5.6024772	1.8183337
C	-10.131487	-4.4694759	0.3665497	H	-9.2067551	-8.8511326	-2.5483275
C	-11.367972	-4.6544259	1.2939142	H	-12.356989	-5.6176358	-2.4040281
O	-12.544187	-4.8745521	0.5743002	H	-11.003479	-4.8338646	-3.2079179
C	-9.2638098	-3.0024444	-1.536966	H	-11.957322	-2.9849723	-2.1634109
C	-12.845928	-3.9144123	-0.4501284	H	-10.673313	-2.4278111	-0.0779334
O	-8.1402375	-2.8002654	-0.8144316	H	-9.2897304	-4.1641565	0.9894447
O	-9.302581	-2.8907004	-2.7429011	H	-13.747776	-4.2982317	-0.9333109
O	-11.461869	-3.3738364	2.0071183	H	-13.084758	-2.946143	0.0077932
C	-12.265265	-3.3252636	3.0820832	H	-7.4280924	-2.5927035	-1.449141
C	-12.769281	-4.4043152	3.7317956	H	-12.490255	-2.3109874	3.3964889
C	-12.383759	-5.7420368	3.3202344	H	-10.3065	-5.7177629	2.8270376
C	-11.267351	-5.7988328	2.3037229	H	-11.270417	-6.7492017	1.7663891
C	-13.728496	-4.1823217	4.8339461	H	-12.674813	-7.8465659	3.5122268
C	-14.156215	-5.4328978	5.6335608	H	-12.263118	-5.5809526	6.7030794
C	-13.966885	-6.7865649	4.9005252	H	-13.484239	-4.5469585	7.4860708
C	-12.943154	-6.8514509	3.8556371	H	-13.648546	-6.3289541	7.5325989
O	-15.51987	-5.2990465	6.0642463	H	-7.4803498	-10.825031	1.4614563
C	-13.329001	-5.4750518	6.9292596	H	-7.0582791	-9.7922829	2.8617247
O	-5.5295513	-9.2430489	0.8303239	H	-8.6193219	-9.5798454	2.0346893
C	-7.5611056	-9.8231986	1.8916409	H	-20.85982	-4.6638273	3.9473481
O	-6.1635413	-7.1507	2.5185331	H	-20.020878	-5.2052101	8.1318274
O	-7.3804834	-9.8569824	-1.1602968	H	-0.7361425	-9.8156842	2.0257788
O	-14.594273	-7.7651091	5.2734668	H	-0.7347809	-9.0931696	-2.2047782

O	-14.119792	-3.0765096	5.1679214	H	-17.973719	-5.5955016	8.940354
C	-16.436146	-5.2229203	5.0787831	H	-16.783934	-6.3957951	7.8915458
C	-17.834488	-5.1385507	5.4978824	H	-16.672498	-4.665849	8.1704444
O	-16.061098	-5.2140977	3.8964553	H	-4.0078698	-8.488495	2.7282586
C	-4.765563	-8.4651863	0.0126005	H	-3.8944746	-10.238193	2.6481884
C	-3.3344817	-8.857521	0.0197265	H	-2.5550527	-9.3113873	3.3445572
O	-5.2576987	-7.5620785	-0.6377153	H	1.0862795	-9.7369312	-0.9644143
C	-18.801241	-4.9387139	4.4618754	H	-2.6873002	-8.5211175	-3.0840693
C	-20.161481	-4.8195489	4.7648761	H	-22.424452	-4.6657672	5.6525748
C	-20.578792	-4.9110936	6.0845268	H	-17.495016	-4.97704	3.0992874
C	-19.650246	-5.1262	7.1155828				

NImag	0
Σ Electronic and thermal Free Energy	-1819223.957
mol Fraction	2.06E-09

(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 4

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.6058059	-8.9332143	-0.4879834	C	-18.233047	-5.2093071	6.8978591
C	-8.6221506	-7.8967426	-0.8056681	C	-3.1326888	-10.474986	-0.29806
C	-8.7978684	-6.7148054	0.0307148	C	-1.8137299	-10.895033	-0.4639166
C	-8.016625	-6.5156989	1.1335881	C	-0.7681419	-9.9706185	-0.5200751
C	-6.9733228	-7.4391511	1.5520105	C	-1.0317508	-8.6047858	-0.4261826
C	-6.9209418	-8.8401329	0.8865495	C	-2.3504805	-8.1667325	-0.2805489
C	-9.3603119	-8.0600478	-1.9249859	C	-17.301836	-5.4546566	8.0643562
O	-10.287182	-7.1761553	-2.3430535	C	-4.2105346	-11.536495	-0.2487104
C	-10.498971	-6.0421519	-1.5946021	O	0.4940288	-10.462038	-0.6731307
C	-9.8273549	-5.787774	-0.4441871	O	-2.6325849	-6.8410071	-0.1737816
C	-11.484265	-5.1381565	-2.2711396	O	-21.829531	-4.7701979	6.547078
C	-11.745825	-3.8226754	-1.5062087	O	-18.470147	-4.8362797	3.2129704
C	-10.492991	-3.3837785	-0.728834	H	-8.0910284	-5.6183925	1.7372196
C	-10.160683	-4.5005329	0.2928948	H	-9.2620435	-8.9113927	-2.5867406
C	-11.384606	-4.6754117	1.2387724	H	-12.422194	-5.685754	-2.4318461
O	-12.570442	-4.904327	0.5379415	H	-11.08095	-4.9115185	-3.2649199
C	-9.32006	-3.0570061	-1.64019	H	-12.021212	-3.0497018	-2.2313016
C	-12.886373	-3.9575311	-0.4946078	H	-10.710779	-2.4650659	-0.1699267
O	-8.1869115	-2.8451725	-0.9354644	H	-9.3110548	-4.1867826	0.9007322
O	-9.3749437	-2.9603644	-2.8467969	H	-13.794226	-4.3480572	-0.9608829
O	-11.469655	-3.3867052	1.9385143	H	-13.119877	-2.9835762	-0.046039
C	-12.258249	-3.3263034	3.0237916	H	-7.4835899	-2.6463228	-1.5826498
C	-12.75307	-4.3981352	3.6922933	H	-12.479154	-2.3086291	3.3300167
C	-12.373015	-5.7403119	3.2902585	H	-10.3025	-5.7208094	2.7699406
C	-11.269963	-5.8082028	2.2600715	H	-11.279392	-6.7645018	1.733444
C	-13.697119	-4.1639636	4.8049351	H	-12.66172	-7.8425781	3.5088205
C	-14.113594	-5.4057699	5.6238327	H	-12.20507	-5.542931	6.6670444
C	-13.935073	-6.7672156	4.9026385	H	-13.414455	-4.5001871	7.4566668
C	-12.925421	-6.8437581	3.8449697	H	-13.578243	-6.2815083	7.5248864
O	-15.470799	-5.2672546	6.0728137	H	-8.6559899	-9.5728858	1.9884689
C	-13.2675	-5.4342853	6.907694	H	-7.5506241	-10.845035	1.4088043
O	-5.5634315	-9.2860352	0.7790471	H	-7.0898751	-9.8144673	2.7984064
C	-7.6049612	-9.8394637	1.8345612	H	-20.840656	-4.641165	4.0316238
O	-6.203827	-7.1914322	2.4703952	H	-19.940904	-5.1650055	8.2057014
O	-7.3743086	-9.8647843	-1.2414961	H	-1.5779849	-11.949908	-0.556165
O	-14.558099	-7.7412497	5.2942975	H	-0.2202218	-7.8790097	-0.4678029

O	-14.083684	-3.0545193	5.132318	H	-17.883	-5.5610455	8.98473
C	-16.401519	-5.2008119	5.1003528	H	-16.70752	-6.3614729	7.9199335
C	-17.793501	-5.1132252	5.5395604	H	-16.593577	-4.6311543	8.19565
O	-16.044185	-5.2024069	3.91255	H	-3.8237246	-12.480004	-0.6451452
C	-4.7984564	-8.5577577	-0.0819205	H	-4.5371146	-11.71004	0.7824937
C	-3.4171882	-9.0889635	-0.2056859	H	-5.100376	-11.254614	-0.8171512
O	-5.2483541	-7.5903959	-0.6656832	H	1.1238364	-9.7250919	-0.7037252
C	-18.775171	-4.917354	4.5169642	H	-1.8003716	-6.3432925	-0.175723
C	-20.130533	-4.7939437	4.8395008	H	-22.37976	-4.6313056	5.7598448
C	-20.528404	-4.8783156	6.1656238	H	-17.489656	-4.9669395	3.1350114
C	-19.585138	-5.0907316	7.1837964				

NImag	0
Σ Electronic and thermal Free Energy	-1819223.533
mol Fraction	1.00E-09

(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 5

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.566636	-8.9584674	-0.2905989	C	-18.108828	-3.7741601	6.4576093
C	-8.5669564	-7.9264406	-0.6731474	C	-2.6909994	-9.7584464	1.11955
C	-8.7465369	-6.7048615	0.1023267	C	-1.3416961	-10.051608	0.9897018
C	-7.9735119	-6.451537	1.202476	C	-0.5831971	-9.5309421	-0.0713188
C	-6.931387	-7.3496136	1.6651722	C	-1.1619631	-8.6866306	-1.0081601
C	-6.8855475	-8.7847899	1.0784191	C	-2.5169498	-8.3600202	-0.8965773
C	-9.2946325	-8.1413922	-1.7908268	C	-17.051038	-2.9467903	7.1557394
O	-10.210828	-7.2741906	-2.2616096	C	-3.4149624	-10.341182	2.3131026
C	-10.429349	-6.1070414	-1.5695245	O	0.7291387	-9.8840089	-0.1180795
C	-9.7693976	-5.7999557	-0.4243079	O	-3.0018819	-7.522054	-1.826169
C	-11.407242	-5.2355265	-2.2970786	O	-21.741054	-4.0475492	6.6368078
C	-11.683641	-3.8903322	-1.5919311	O	-18.540795	-6.3538136	3.883605
C	-10.441104	-3.412092	-0.8209515	H	-8.0509	-5.5240649	1.7579356
C	-10.113764	-4.4822398	0.2516339	H	-9.195011	-9.0259285	-2.4074253
C	-11.348051	-4.6203075	1.1914785	H	-12.340855	-5.7932748	-2.4471672
O	-12.522186	-4.8910467	0.485452	H	-10.990487	-5.0497482	-3.2938331
C	-9.2608625	-3.1148339	-1.73242	H	-11.954885	-3.1505295	-2.3523238
C	-12.83426	-3.989851	-0.5873321	H	-10.669988	-2.4727476	-0.3024943
O	-8.1399433	-2.8510342	-1.024825	H	-9.2718369	-4.1378472	0.8535713
O	-9.2997063	-3.0794399	-2.9430095	H	-13.735064	-4.4049262	-1.0458925
O	-11.448329	-3.3022615	1.8274277	H	-13.078165	-2.9997407	-0.1820082
C	-12.257853	-3.1945955	2.8957142	H	-7.4339661	-2.6648584	-1.6729331
C	-12.756157	-4.2366024	3.6061653	H	-12.491456	-2.1647516	3.1460238
C	-12.362091	-5.5942692	3.2735799	H	-10.282042	-5.582616	2.7864172
C	-11.240728	-5.7030585	2.2666248	H	-11.235419	-6.6836441	1.7865234
C	-13.72713	-3.9595557	4.6847279	H	-12.647438	-7.6840469	3.586428
C	-14.147695	-5.1575234	5.5631068	H	-13.647754	-5.9281477	7.5139856
C	-13.943558	-6.5518613	4.9136336	H	-12.251812	-5.2499004	6.6415594
C	-12.920962	-6.6712637	3.8690399	H	-13.463997	-4.1557947	7.3548107
O	-15.507662	-5.0003027	5.9821728	H	-7.495976	-10.761032	1.7061967
C	-13.317074	-5.1185572	6.8578914	H	-7.0768445	-9.6481509	3.0459446
O	-5.5213066	-9.2300254	1.0089224	H	-8.6272711	-9.4730108	2.191547
C	-7.5703363	-9.7342171	2.0744199	H	-20.975381	-5.8079067	4.7557105
O	-6.1413739	-7.0533483	2.5533353	H	-19.698305	-2.83683	7.5780541
O	-7.3513172	-9.9432549	-0.9744676	H	-0.8431905	-10.686411	1.7142201
O	-14.544059	-7.5177904	5.3547478	H	-0.5928546	-8.255455	-1.8269537

O	-14.136183	-2.8357557	4.9346379	H	-16.277251	-2.5924707	6.4702839
C	-16.413871	-4.9573215	4.9646176	H	-17.513853	-2.0833025	7.6429879
C	-17.798801	-4.7197404	5.447996	H	-16.542794	-3.5381858	7.9254409
O	-16.07556	-5.0996458	3.8062334	H	-3.9394246	-9.5672662	2.880809
C	-4.7328662	-8.5467305	0.1558917	H	-4.1678155	-11.074999	2.0091705
C	-3.3176	-8.9091523	0.1538052	H	-2.6981136	-10.836816	2.9738964
O	-5.234653	-7.6847468	-0.5827168	H	1.1445226	-9.4605796	-0.8861812
C	-18.851235	-5.4366923	4.8379759	H	-3.9500159	-7.3483804	-1.5959565
C	-20.177794	-5.2352298	5.2279877	H	-22.356897	-4.6099098	6.1417258
C	-20.467493	-4.2981033	6.2187959	H	-19.352821	-6.8070239	3.6089534
C	-19.439454	-3.5697276	6.821226				

NImag	0
Σ Electronic and thermal Free Energy	-1819223.244
mol Fraction	6.16E-10

(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 6

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.5580554	-8.9533049	-0.3308973	C	-18.272474	-5.8413241	6.5892147
C	-8.5672083	-7.9236992	-0.6997648	C	-2.6071848	-9.1841859	1.281353
C	-8.7549477	-6.7145381	0.0912985	C	-1.2472899	-9.4857088	1.2199438
C	-7.9793295	-6.4701096	1.191125	C	-0.5682186	-9.498787	-0.000285
C	-6.9190727	-7.3591894	1.6295921	C	-1.2418804	-9.1951679	-1.1824915
C	-6.8580206	-8.7883897	1.030981	C	-2.6000195	-8.8709225	-1.1368396
C	-9.2962621	-8.130261	-1.8175187	C	-17.357216	-6.741149	7.3911008
O	-10.221621	-7.2639055	-2.2752521	C	-3.2678309	-9.1925162	2.6429249
C	-10.447048	-6.1083606	-1.5674836	O	0.7578664	-9.8131843	0.0242803
C	-9.7867974	-5.8113061	-0.4198719	O	-3.2803101	-8.5868114	-2.2794493
C	-11.432863	-5.2336971	-2.2810251	O	-21.817073	-4.987091	6.6873016
C	-11.712986	-3.8975214	-1.5600114	O	-18.308942	-3.5242152	3.7411635
C	-10.470502	-3.4232283	-0.7865354	H	-8.0609499	-5.5506913	1.759387
C	-10.136952	-4.5041306	0.2728871	H	-9.1909676	-9.005774	-2.4457193
C	-11.368062	-4.6593946	1.2133949	H	-12.364523	-5.7942179	-2.4331751
O	-12.543505	-4.9254648	0.5073943	H	-11.021603	-5.0348161	-3.2775135
C	-9.2930216	-3.1136575	-1.6977859	H	-11.988912	-3.1501031	-2.3112668
C	-12.860802	-4.0127906	-0.5538548	H	-10.701371	-2.4898971	-0.2579833
O	-8.1677597	-2.8691301	-0.9908379	H	-9.2954419	-4.1633012	0.8773512
O	-9.3380448	-3.0547667	-2.9073668	H	-13.761303	-4.4254326	-1.015298
O	-11.472444	-3.3504771	1.8675155	H	-13.107023	-3.0283555	-0.1361425
C	-12.274029	-3.2619234	2.9434237	H	-7.4612449	-2.6827887	-1.6382433
C	-12.765892	-4.3153407	3.6409787	H	-12.50792	-2.2369722	3.2130309
C	-12.369331	-5.6652434	3.2865605	H	-10.292377	-5.6422668	2.7899065
C	-11.253052	-5.7569461	2.2724876	H	-11.247285	-6.7302834	1.777935
C	-13.721168	-4.0542894	4.7401797	H	-12.647192	-7.7615193	3.5685371
C	-14.150365	-5.2734745	5.5878004	H	-12.253914	-5.3698701	6.6644106
C	-13.952469	-6.650284	4.9030534	H	-13.486284	-4.3167005	7.4047021
C	-12.920917	-6.7541979	3.8695031	H	-13.635991	-6.0956755	7.5198293
O	-15.510716	-5.1232979	6.0085719	H	-7.4352767	-10.77717	1.6448985
C	-13.321317	-5.2637959	6.884008	H	-7.0098325	-9.6764653	2.9913417
O	-5.4947996	-9.2190774	0.9276947	H	-8.5764126	-9.510365	2.1642493
C	-7.5180378	-9.7561146	2.0268327	H	-20.792564	-3.5869782	4.634715
O	-6.1278526	-7.0494066	2.5144618	H	-19.984487	-6.3878395	7.7846449
O	-7.3512632	-9.9345817	-1.0223898	H	-0.6918778	-9.7122937	2.1238186
O	-14.57768	-7.623679	5.2990887	H	-0.7185877	-9.2070796	-2.138101

O	-14.101044	-2.9347328	5.0383938	H	-17.950517	-7.4589482	7.9655608
C	-16.420256	-5.1128589	4.9929517	H	-16.650804	-7.2880983	6.762142
C	-17.821781	-5.0742116	5.484504	H	-16.759901	-6.153633	8.0973684
O	-16.071029	-5.1301989	3.8290096	H	-3.9655191	-8.362447	2.7768884
C	-4.7381948	-8.4789238	0.0693545	H	-3.8442728	-10.113387	2.7863014
C	-3.3055216	-8.866151	0.0875603	H	-2.5053552	-9.1460676	3.4262884
O	-5.2362821	-7.6097334	-0.6211742	H	1.1120747	-9.7803395	-0.8780174
C	-18.752503	-4.2737098	4.7859372	H	-2.6782713	-8.6859362	-3.0331797
C	-20.092625	-4.2214193	5.1777245	H	-22.34024	-4.3980297	6.1216944
C	-20.521623	-4.9861427	6.2615842	H	-19.047279	-2.993988	3.4035524
C	-19.617363	-5.7931831	6.9548969				

NImag	0
Σ Electronic and thermal Free Energy	-1819211.98
mol Fraction	3.34E-18

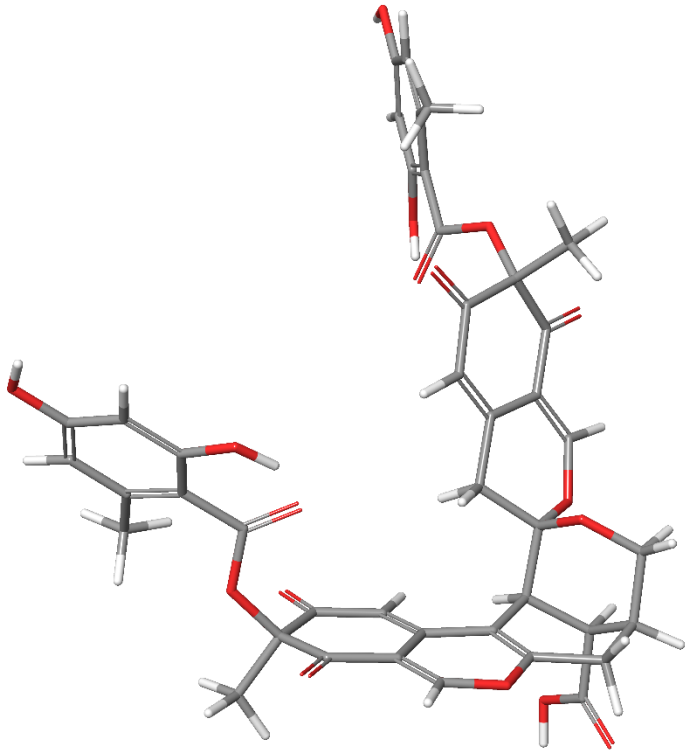
(8*S*, 13*R*, 3a*R*, 8a*S*, 12a*R*, 13a*S*)- Pavesiflonic acid - Conformer 7

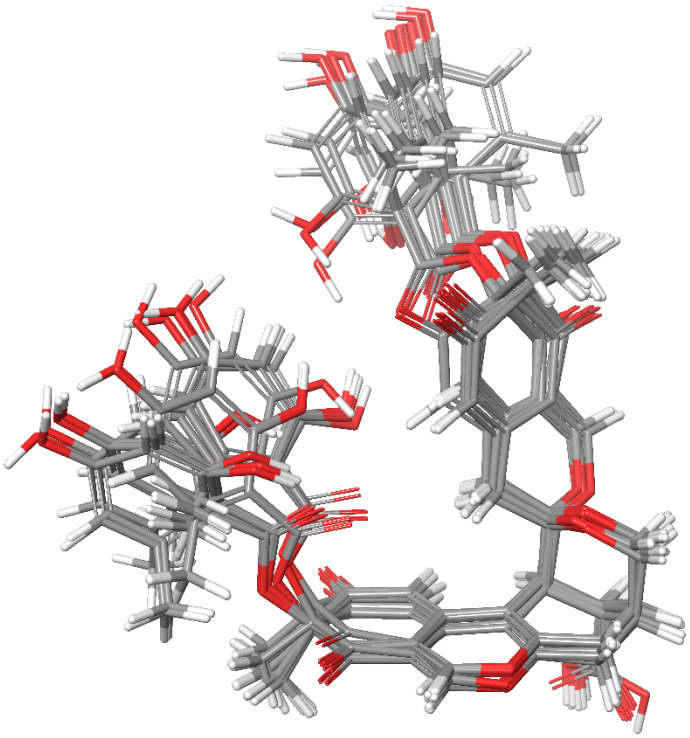
Atom	X	Y	Z	Atom	X	Y	Z
C	-7.5917875	-8.9140614	-0.380791	C	-18.112215	-3.8330331	6.5091381
C	-8.582197	-7.8618373	-0.7365497	C	-2.6645919	-9.2542928	1.2850052
C	-8.7600464	-6.6676217	0.0791147	C	-1.3081542	-9.5728437	1.2339951
C	-7.9928184	-6.4594855	1.1921688	C	-0.6129774	-9.5654882	0.0228323
C	-6.9516582	-7.374634	1.6225868	C	-1.2666057	-9.2240763	-1.1603055
C	-6.9050018	-8.7906873	0.9921071	C	-2.6208046	-8.8825788	-1.1245354
C	-9.3030601	-8.0329891	-1.8655237	C	-17.042004	-3.0417924	7.2298921
O	-10.211008	-7.1431036	-2.3129607	C	-3.3432105	-9.2864903	2.6373571
C	-10.425491	-5.9994571	-1.5827741	O	0.708356	-9.8984232	0.0570644
C	-9.7722207	-5.7373386	-0.4227607	O	-3.2818025	-8.5616069	-2.2686993
C	-11.39044	-5.0943352	-2.2868823	O	-21.747408	-4.0656782	6.6899378
C	-11.655768	-3.7688433	-1.5407494	O	-18.583094	-6.3247324	3.8568587
C	-10.413063	-3.3312795	-0.7462744	H	-8.0666359	-5.5516192	1.779705
C	-10.107785	-4.439116	0.2937074	H	-9.2043998	-8.8960306	-2.5117987
C	-11.350148	-4.5931451	1.2193933	H	-12.329527	-5.6363665	-2.459097
O	-12.523207	-4.824347	0.4978467	H	-10.966653	-4.881549	-3.275202
C	-9.2217948	-3.0230742	-1.639917	H	-11.912275	-3.0016696	-2.2788509
C	-12.814877	-3.8854711	-0.5479438	H	-10.633394	-2.4050919	-0.2009255
O	-8.0997706	-2.8112434	-0.9174315	H	-9.2666326	-4.1249873	0.9129845
O	-9.253877	-2.9393809	-2.8484356	H	-13.717544	-4.2736795	-1.0260364
O	-11.438753	-3.2952583	1.8991453	H	-13.048956	-2.9055964	-0.1128612
C	-12.25069	-3.213729	2.9671014	H	-7.3839426	-2.623596	-1.5541441
C	-12.764832	-4.2726039	3.6407242	H	-12.472464	-2.1901179	3.2516042
C	-12.386946	-5.6233003	3.2638801	H	-10.305036	-5.6237667	2.7851422
C	-11.263072	-5.712795	2.2578884	H	-11.268677	-6.6764017	1.744601
C	-13.735154	-4.0193842	4.7253196	H	-12.700413	-7.7185586	3.5049397
C	-14.171631	-5.2408132	5.5626747	H	-13.680778	-6.0841024	7.4856426
C	-13.985883	-6.6148865	4.8661508	H	-12.276502	-5.3948883	6.6354634
C	-12.961866	-6.712491	3.8209626	H	-13.473755	-4.3099161	7.3869447
O	-15.529046	-5.0798907	5.9886187	H	-7.5183518	-10.784079	1.5537439
C	-13.339778	-5.2569884	6.8572498	H	-7.0932475	-9.7206276	2.9298867
O	-5.5471693	-9.2392898	0.894365	H	-8.6471514	-9.5127039	2.0885727
C	-7.5908727	-9.7708297	1.957918	H	-21.008645	-5.7757332	4.7525194
O	-6.1664251	-7.0972125	2.5233906	H	-19.686814	-2.911083	7.6629776
O	-7.3912899	-9.8820738	-1.0925424	H	-0.7679843	-9.8288786	2.1392397
O	-14.601572	-7.5864867	5.2726769	H	-0.7307306	-9.2199306	-2.1089808

O	-14.131455	-2.8996303	5.011824	H	-16.264492	-2.6775032	6.5539479
C	-16.435908	-4.9898785	4.974937	H	-17.492115	-2.1872919	7.7441906
C	-17.816804	-4.7502084	5.4695677	H	-16.540626	-3.6632379	7.9801864
O	-16.102093	-5.0968197	3.8115935	H	-4.0309069	-8.4500241	2.7827651
C	-4.7694556	-8.4903445	0.0629131	H	-3.9343376	-10.202243	2.7505549
C	-3.3425978	-8.8978734	0.0902728	H	-2.5905461	-9.2701747	3.431347
O	-5.2466329	-7.5984924	-0.6133496	H	1.0751027	-9.8482993	-0.8394124
C	-18.879707	-5.434198	4.8403579	H	-2.6709202	-8.6502354	-3.016601
C	-20.202669	-5.2282642	5.2402319	H	-22.371294	-4.6044983	6.1790099
C	-20.477958	-4.3190726	6.2607306	H	-19.401515	-6.7580456	3.5694084
C	-19.439294	-3.623097	6.8827722				

NImag	0
Σ Electronic and thermal Free Energy	-1819211.801
mol Fraction	2.47E-18

Data S4. Lowest energy conformer 3D structure, all overlaid 3D structures, cartesian coordinates, number of imaginary frequencies, and energy for (8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid conformers.





(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 1

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.4350631	-8.9606827	0.9892467	C	-5.8429939	-1.2427826	8.2931802
C	-2.4863633	-9.8833183	1.4913629	C	0.8253062	-4.4900824	1.8484776
C	-2.5973905	-10.193734	2.9101207	C	1.1562349	-3.1625144	2.0703561
C	-1.6112009	-9.8590198	3.7910926	C	0.3809532	-2.3513211	2.9168008
C	-0.4409146	-9.0872866	3.414587	C	-0.7582866	-2.8499156	3.5305292
C	-0.2408646	-8.6893541	1.9237422	C	-1.1338987	-4.1766236	3.3023308
C	-3.3614659	-10.420606	0.6121123	C	-7.2673971	-1.6430015	8.60898
O	-4.3793901	-11.231008	0.9755342	C	1.7202006	-5.2836312	0.9222888
C	-4.669247	-11.343835	2.3174782	O	0.7988339	-1.0693018	3.0900075
C	-3.8601568	-10.832581	3.2751071	O	-2.2544824	-4.5804282	3.9218629
C	-5.9291917	-12.122851	2.5521105	O	-3.7226457	1.599794	9.1134511
C	-6.380044	-12.139701	4.0315625	O	-2.6934477	-2.3004291	6.6310259
C	-5.1738112	-12.120897	4.9862886	H	-1.6742705	-10.103313	4.8456966
C	-4.3729543	-10.829669	4.7020906	H	-3.3197412	-10.2539	-0.457193
C	-5.2974448	-9.5884514	4.9130479	H	-5.7487727	-13.15073	2.214195
O	-6.5130167	-9.6989727	4.2262123	H	-6.7244261	-11.71818	1.9133771
C	-4.3180319	-13.372743	4.8799329	H	-6.9736857	-13.043902	4.2022153
C	-7.2393449	-10.924353	4.3886216	H	-5.5301003	-12.081099	6.0242288
O	-3.1857497	-13.267118	5.612047	H	-3.549544	-10.748749	5.4113492
O	-4.6037369	-14.368232	4.2511143	H	-7.6087349	-11.00777	5.4194132
O	-5.548318	-9.569641	6.3551694	H	-8.0994288	-10.828789	3.7207206
C	-5.9434154	-8.4094648	6.9130051	H	-2.7045659	-14.110029	5.5070903
C	-6.0001495	-7.2102395	6.2812469	H	-6.2337906	-8.5273192	7.9520425
C	-5.5226715	-7.0930452	4.9157647	H	-4.5832436	-8.2657065	3.3733649
C	-4.6901631	-8.2598443	4.4582442	H	-3.684687	-8.1620138	4.8850372
C	-6.5135681	-6.0296267	7.0057804	H	-5.3355158	-5.9122468	3.1511341
C	-6.9553136	-4.8331525	6.1336852	H	-8.8312272	-5.7633461	5.5462606
C	-6.3812242	-4.793233	4.6880099	H	-8.9127716	-4.8114247	7.0502105
C	-5.717638	-5.9869335	4.1651996	H	-8.8155519	-3.9859018	5.4614244
O	-6.6305384	-3.5997823	6.8087282	H	1.8348008	-9.2389696	2.0168712
C	-8.4870332	-4.8504349	6.0440384	H	0.7866702	-10.528756	1.3826174
O	0.1251024	-7.2938016	1.8529653	H	1.1753979	-9.1287093	0.3515763
C	0.9743514	-9.4494815	1.3770064	H	-2.1642379	-0.0654486	7.6621355
O	0.4154963	-8.7488909	4.221676	H	-6.0422947	0.5902918	9.4045408

O	-1.4677133	-8.4844587	-0.1317812	H	2.0273263	-2.72455	1.5949723
O	-6.5417009	-3.7824505	4.0221584	H	-1.3713114	-2.249842	4.1976895
O	-6.670077	-5.9967279	8.2153399	H	-7.6916707	-0.9531499	9.3441593
C	-5.3125713	-3.3329552	6.9100268	H	-7.895984	-1.6213935	7.71325
C	-4.9538344	-2.0546456	7.5256892	H	-7.3250044	-2.6595519	9.0082184
O	-4.4861068	-4.137765	6.4635692	H	1.1502047	-5.7905166	0.1383937
C	-0.7670883	-6.4271678	2.3770536	H	2.4462569	-4.616731	0.448654
C	-0.3402307	-5.0345382	2.4753997	H	2.268551	-6.0598987	1.4649477
O	-1.865955	-6.8493338	2.7740934	H	0.1826241	-0.6171408	3.6884459
C	-3.6123837	-1.605354	7.3243549	H	-2.4247582	-5.5147303	3.650059
C	-3.1902962	-0.3755887	7.8399153	H	-2.79521	1.7841082	8.8956117
C	-4.0755366	0.4005174	8.5755339	H	-3.0917293	-3.1724033	6.37917
C	-5.3888773	-0.0363483	8.8071099				

NImag	0
Σ Electronic and thermal Free Energy	-1819230.846
mol Fraction	0.000174106

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 2

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.9543728	-9.458964	1.0443388	C	-6.9715152	-0.9055068	8.7654366
C	-2.2288527	-9.9833655	1.6045567	C	2.2734487	-5.4584775	1.1368253
C	-2.529875	-9.910476	3.0291639	C	2.8484109	-4.2576179	0.7497731
C	-1.6248901	-9.3910476	3.9130152	C	2.0582768	-3.1746775	0.3300125
C	-0.3436849	-8.8410662	3.5088558	C	0.6741788	-3.2715907	0.3137729
C	0.142955	-9.0840266	2.0563314	C	0.063164	-4.4639853	0.7131274
C	-3.1123574	-10.534754	0.7447757	C	-8.259872	-0.9912728	7.9773487
O	-4.2952546	-11.056338	1.1247388	C	3.2045614	-6.5545294	1.6060601
C	-4.6509115	-10.9816	2.4499447	O	2.7156146	-2.0431179	-0.0381155
C	-3.8522925	-10.421734	3.3931713	O	-1.2784218	-4.4773899	0.6910865
C	-5.9673449	-11.658028	2.6831781	O	-5.5935618	1.4610766	11.163613
C	-6.4336131	-11.613532	4.1534729	O	-3.6723305	-2.4849709	9.3925499
C	-5.2294665	-11.633929	5.1107774	H	-1.8369983	-9.308394	4.9725474
C	-4.3766515	-10.372555	4.8196056	H	-2.9416841	-10.609313	-0.3218907
C	-5.2686339	-9.1181133	5.0630946	H	-5.854898	-12.700863	2.3641575
O	-6.4528647	-9.1626796	4.3170858	H	-6.7214626	-11.209246	2.0236043
C	-4.427493	-12.921899	5.0208429	H	-7.0711105	-12.483906	4.3413371
C	-7.2426065	-10.351973	4.4652519	H	-5.5834143	-11.570034	6.1472056
O	-3.2972101	-12.858336	5.7607992	H	-3.5458344	-10.332917	5.5253488
O	-4.7518414	-13.911714	4.4015927	H	-7.6529865	-10.402125	5.481977
O	-5.5900651	-9.1915006	6.4901432	H	-8.0720444	-10.225276	3.7647437
C	-6.1199545	-8.0931112	7.0583427	H	-2.8554008	-13.724254	5.6713091
C	-6.1461665	-6.859511	6.4971913	H	-6.5448688	-8.2886613	8.0376035
C	-5.4671255	-6.6212194	5.2361135	H	-4.4280287	-7.6993377	3.6763278
C	-4.6158088	-7.7709513	4.749459	H	-3.6442728	-7.726331	5.2567062
C	-6.8528156	-5.7719988	7.2096188	H	-4.9489129	-5.2443279	3.6921511
C	-7.1377566	-4.4991733	6.3840638	H	-9.2668355	-4.7120352	6.6907184
C	-6.1944821	-4.2629055	5.1753723	H	-8.8151577	-3.6910987	5.2910996
C	-5.4993403	-5.4214983	4.6118643	H	-8.6799556	-5.4625904	5.1842234
O	-7.1325857	-3.343367	7.2355529	H	0.7171719	-11.153438	2.4167361
C	-8.5764434	-4.5998016	5.8501876	H	1.5786957	-10.363513	1.0714434
O	0.8597491	-7.9262843	1.5960054	H	1.9825885	-9.9534876	2.7685797
C	1.1778624	-10.219297	2.0783822	H	-3.6856148	-0.4305469	10.842418
O	0.3992592	-8.2496688	4.2827955	H	-7.6002354	0.9323982	9.6907667
O	-0.7395356	-9.4147836	-0.1538091	H	3.9250882	-4.1286993	0.7734834
O	-6.1130797	-3.1446502	4.6923454	H	0.0400663	-2.4421159	0.0138401

O	-7.290866	-5.8869165	8.3413535	H	-8.0690892	-1.0753142	6.9036258
C	-5.9582359	-3.073804	7.8412766	H	-8.8497305	-1.8676519	8.2623542
C	-5.9184612	-1.8693135	8.6689164	H	-8.8623872	-0.0961577	8.156299
O	-5.0001278	-3.8454166	7.6855783	H	3.2090493	-7.4029019	0.9145745
C	0.1205356	-6.8073258	1.4587619	H	4.2241808	-6.1658493	1.6802498
C	0.8491993	-5.5923083	1.1071606	H	2.9051597	-6.944736	2.5829868
O	-1.1106951	-6.8675559	1.6089073	H	2.0669549	-1.3677559	-0.2932044
C	-4.7263142	-1.6566898	9.4312666	H	-1.5681502	-5.3546225	1.0471332
C	-4.6060102	-0.5494471	10.277621	H	-4.7407523	1.4733882	11.626616
C	-5.647781	0.3620753	10.363723	H	-3.8830874	-3.197141	8.7354071
C	-6.817254	0.1865643	9.6064917				

NImag	0
Σ Electronic and thermal Free Energy	-1819235.305
mol Fraction	0.325815679

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 3

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.2663905	-9.4125113	0.7355493	C	-6.8750741	-1.2333719	9.1413272
C	-2.4741247	-9.989356	1.3850069	C	1.8381169	-5.314748	0.6652502
C	-2.6581323	-9.9585897	2.8309145	C	2.3433325	-4.0877837	0.2630163
C	-1.6988459	-9.4311065	3.6503767	C	1.4895014	-3.021218	-0.0635937
C	-0.4724827	-8.8315873	3.1564558	C	0.1122503	-3.1615593	0.0306026
C	-0.1007085	-9.0260308	1.6632646	C	-0.4281069	-4.3814678	0.4482714
C	-3.4091868	-10.5484	0.5869174	C	-8.2211695	-1.3419673	8.4597744
O	-4.5407061	-11.115455	1.0493116	C	2.8368765	-6.3909828	1.0294982
C	-4.787265	-11.082591	2.400731	O	2.0803914	-1.8613357	-0.4554692
C	-3.9300938	-10.51966	3.2891461	O	-1.7659646	-4.4368784	0.5354671
C	-6.05922	-11.805488	2.7240014	O	-5.3745257	1.1201948	11.477961
C	-6.4029955	-11.8098	4.2283137	O	-3.4894922	-2.7206966	9.4548249
C	-5.1234884	-11.81414	5.0825329	H	-1.8247734	-9.3794239	4.725507
C	-4.335567	-10.520016	4.7546516	H	-3.325307	-10.59314	-0.4917045
C	-5.2410878	-9.3004165	5.1026429	H	-5.9428414	-12.836578	2.3701266
O	-6.4812933	-9.3652339	4.4557654	H	-6.8784208	-11.36561	2.140427
C	-4.2939221	-13.073651	4.8939296	H	-6.9965608	-12.704072	4.4455637
C	-7.2204014	-10.582059	4.6378162	H	-5.3919753	-11.785437	6.1458418
O	-3.1084173	-12.991395	5.5396144	H	-3.4506067	-10.470346	5.3904763
O	-4.6391357	-14.058695	4.2783631	H	-7.5433301	-10.668648	5.6832198
O	-5.4405972	-9.4168372	6.5490813	H	-8.1084774	-10.465523	4.0113486
C	-5.9539297	-8.3491934	7.1867956	H	-2.6500938	-13.840592	5.3918947
C	-6.0632937	-7.1044539	6.6614146	H	-6.2901118	-8.5805762	8.192377
C	-5.4986073	-6.8157378	5.3552902	H	-4.5608033	-7.8240862	3.6883085
C	-4.6568008	-7.9263683	4.7710488	H	-3.6483259	-7.8626907	5.1977757
C	-6.7404293	-6.0566285	7.4571163	H	-5.1514292	-5.3878403	3.8096938
C	-7.1305887	-4.7748096	6.6906083	H	-8.7373977	-5.7590809	5.597191
C	-6.2981828	-4.4809096	5.4149795	H	-9.2196197	-5.0624526	7.1654639
C	-5.61813	-5.603578	4.7667085	H	-8.9161734	-3.9957202	5.7600132
O	-7.0893876	-3.6393368	7.5680257	H	1.816541	-9.852764	2.2000912
C	-8.6049193	-4.9089611	6.2742249	H	0.5624979	-11.083873	1.9230853
O	0.5408638	-7.836005	1.1751093	H	1.2859073	-10.236766	0.5319968
C	0.9657077	-10.128195	1.5717396	H	-3.4440032	-0.7016803	10.952886
O	0.3140865	-8.2347222	3.8815446	H	-7.479632	0.5617407	10.161848
O	-1.15273	-9.3345644	-0.4746855	H	3.4140042	-3.9253399	0.2022852
O	-6.2902113	-3.3497457	4.9557931	H	-0.5687829	-2.3460142	-0.195606

O	-7.0794252	-6.211413	8.6177401	H	-8.8332863	-0.4709388	8.7105666
C	-5.8774143	-3.3463659	8.0819186	H	-8.1175748	-1.3949752	7.3722019
C	-5.8052849	-2.1606069	8.9340441	H	-8.7589107	-2.2431072	8.7695808
O	-4.9128622	-4.0831837	7.8283503	H	2.8102259	-7.222758	0.3186156
C	-0.240017	-6.7381505	1.1271981	H	3.8470539	-5.9717621	1.030642
C	0.4208592	-5.4929635	0.7482996	H	2.6301911	-6.812784	2.0172536
O	-1.452319	-6.8406839	1.3759644	H	1.3931471	-1.2012417	-0.6396287
C	-4.5609562	-1.9276047	9.6011149	H	-1.9991897	-5.3306089	0.8919677
C	-4.4040877	-0.8368603	10.462757	H	-4.4870132	1.1490951	11.869488
C	-5.4619406	0.0387163	10.6574	H	-3.7325023	-3.4238443	8.7991183
C	-6.6843661	-0.1565827	9.9945327				

NImag	0
Σ Electronic and thermal Free Energy	-1819235.3
mol Fraction	0.323063694

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 4

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.2889943	-9.2143536	0.8619252	C	-5.5870962	-1.1964449	8.3296867
C	-2.400106	-10.059542	1.3822394	C	0.1917107	-4.531711	2.1551396
C	-2.5203845	-10.349144	2.8035611	C	0.3825649	-3.23432	2.6292164
C	-1.4904499	-10.116899	3.6678203	C	-0.2562222	-2.798279	3.7965638
C	-0.2477572	-9.4894938	3.2641163	C	-1.0776579	-3.6723905	4.50431
C	-0.1107563	-8.9158678	1.8198268	C	-1.3431612	-4.9443774	4.0015388
C	-3.3181739	-10.546099	0.5199777	C	-6.791412	-1.9384899	8.8667755
O	-4.3931285	-11.275433	0.9060424	C	0.9169663	-4.9508185	0.8950131
C	-4.679492	-11.340988	2.2488703	O	-0.0478417	-1.5219092	4.2147986
C	-3.8259777	-10.873914	3.1905885	O	-2.1853735	-5.7700231	4.6811753
C	-5.9882749	-12.025481	2.513265	O	-3.9519859	1.9663392	9.0849287
C	-6.4105412	-12.007507	4.0023335	O	-2.7616556	-1.3719795	5.9278346
C	-5.1894201	-12.049197	4.9372411	H	-1.5486988	-10.384398	4.7173057
C	-4.3197601	-10.810923	4.6225263	H	-3.2768949	-10.398479	-0.5518425
C	-5.1629343	-9.5123606	4.8243171	H	-5.8885717	-13.06453	2.1761399
O	-6.4056744	-9.5615337	4.1837201	H	-6.7663481	-11.567826	1.8891878
C	-4.4094143	-13.349567	4.8295496	H	-7.0506985	-12.875755	4.1907603
C	-7.1934863	-10.74504	4.3687348	H	-5.5259944	-11.979582	5.9804468
O	-3.2549513	-13.29902	5.5321696	H	-3.4829303	-10.764861	5.3187955
O	-4.7681791	-14.335502	4.2236278	H	-7.5455207	-10.802646	5.407631
O	-5.369878	-9.4474584	6.2816045	H	-8.0609295	-10.605369	3.7182542
C	-5.6485261	-8.2551104	6.8278318	H	-2.822596	-14.167603	5.4242888
C	-5.6626912	-7.0680548	6.1664079	H	-5.8874685	-8.3280268	7.8844761
C	-5.2451095	-7.0124588	4.7762223	H	-4.4161022	-8.2658058	3.236673
C	-4.4939747	-8.2333279	4.3221065	H	-3.4707496	-8.1680949	4.7093019
C	-6.0372537	-5.8334146	6.8778164	H	-5.0433073	-5.8878681	2.9813155
C	-6.5305022	-4.6816584	5.9777669	H	-8.38582	-5.6963431	5.4647336
C	-6.0070752	-4.6832227	4.5113631	H	-8.4731094	-4.6964749	6.9379675
C	-5.4082365	-5.9138414	4.0031958	H	-8.4344929	-3.9229254	5.3219324
O	-6.2436851	-3.4185994	6.6133051	H	2.0167693	-9.1853453	1.8495127
C	-8.0651466	-4.7564632	5.9251925	H	1.1416409	-10.509311	1.048995
O	0.0767825	-7.4799195	1.9720767	H	1.3181386	-8.9502783	0.2100318
C	1.1833977	-9.4230339	1.1854787	H	-2.4657304	0.8398714	7.1263958
O	0.6977291	-9.3504435	4.03199	H	-5.8876366	0.433982	9.7030329
O	-1.2569524	-8.8295011	-0.2943346	H	1.0197088	-2.5394198	2.0922854
O	-6.1682774	-3.6817262	3.831617	H	-1.4918287	-3.3846901	5.4628625

O	-6.0395981	-5.7171229	8.0933639	H	-7.1162538	-1.4844377	9.8072622
C	-4.9730445	-2.9972902	6.6216691	H	-7.627488	-1.8950905	8.1606813
C	-4.7486234	-1.7127488	7.2972171	H	-6.5808181	-2.9971158	9.0405014
O	-4.0747192	-3.6409534	6.0573134	H	0.259318	-5.4728234	0.1929533
C	-1.0182667	-6.7739012	2.3608178	H	1.3342241	-4.0756998	0.3886569
C	-0.7022693	-5.4026865	2.829358	H	1.7385264	-5.6369173	1.1266127
O	-2.1307849	-7.2733574	2.3478701	H	-0.6981337	-1.3097913	4.9091366
C	-3.6100847	-0.9548347	6.8995115	H	-2.7170134	-5.2305925	5.2938457
C	-3.3328477	0.2847971	7.4730265	H	-3.1610429	2.3830664	8.7073282
C	-4.1672494	0.7723855	8.473786	H	-3.0599567	-2.2659643	5.6410102
C	-5.2764887	0.0295335	8.903375				

NImag	0
Σ Electronic and thermal Free Energy	-1819222.12
mol Fraction	6.88E-11

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 5

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.9956945	-9.4784692	0.9871689	C	-6.9096386	-0.9275804	8.7928584
C	-2.2637665	-10.001887	1.5626698	C	2.2372961	-5.481092	1.044879
C	-2.5469859	-9.9300523	2.9909807	C	2.8088622	-4.2804516	0.6521323
C	-1.6305494	-9.4124031	3.8640073	C	2.0149132	-3.1964051	0.2425576
C	-0.3539123	-8.8632972	3.4444638	C	0.6306216	-3.2919573	0.2424786
C	0.1144405	-9.1054821	1.9858187	C	0.0231743	-4.4840933	0.6479854
C	-3.1585395	-10.551361	0.713386	C	-8.2081409	-1.0119928	8.0214626
O	-4.3372598	-11.071919	1.1074814	C	3.1727565	-6.5784069	1.5023784
C	-4.6762299	-10.998316	2.4371106	O	2.6689902	-2.0651589	-0.1323075
C	-3.8653033	-10.440324	3.3708928	O	-1.3185991	-4.4962001	0.6417224
C	-5.9903343	-11.673671	2.6860433	O	-5.499883	1.4359441	11.175521
C	-6.4380732	-11.630504	4.1621242	O	-3.6032815	-2.5090003	9.3757247
C	-5.2220276	-11.65313	5.1042341	H	-1.8293768	-9.3305119	4.9261725
C	-4.3717365	-10.392237	4.8038358	H	-3.0011894	-10.625084	-0.3553849
C	-5.2594135	-9.1372502	5.0598508	H	-5.8829869	-12.716223	2.3643628
O	-6.4529568	-9.1798428	4.3288157	H	-6.7522093	-11.223304	2.0365373
C	-4.4224835	-12.941751	5.0027497	H	-7.0739489	-12.500532	4.3569479
C	-7.241909	-10.368576	4.4855027	H	-5.5629011	-11.590088	6.1450842
O	-3.2828196	-12.880041	5.7283239	H	-3.5321048	-10.354161	5.4991522
O	-4.7556143	-13.930585	4.3866046	H	-7.6395395	-10.419523	5.5072389
O	-5.5629349	-9.2119663	6.4908579	H	-8.0799339	-10.240259	3.7955959
C	-6.0846657	-8.1137457	7.066846	H	-2.8429969	-13.746269	5.6322908
C	-6.1168415	-6.8795024	6.5074122	H	-6.4974146	-8.3099653	8.0511663
C	-5.4534625	-6.6403861	5.2381769	H	-4.4348462	-7.7176449	3.6643296
C	-4.6093232	-7.7903246	4.7396329	H	-3.6315139	-7.7471648	5.2348062
C	-6.8135164	-5.7921703	7.2298473	H	-4.9534233	-5.2621713	3.6893848
C	-7.1077445	-4.5182112	6.4093146	H	-9.2329963	-4.7299649	6.7421584
C	-6.1794393	-4.281379	5.1892043	H	-8.7980187	-3.7078273	5.3381175
C	-5.4924264	-5.4399403	4.6157245	H	-8.6653878	-5.4793044	5.2276873
O	-7.0911396	-3.3633371	7.2618763	H	1.961883	-9.9774307	2.6744352
C	-8.5530328	-4.6172958	5.8932308	H	0.6909355	-11.175791	2.3373289
O	0.826667	-7.9480234	1.5177462	H	1.5364887	-10.385584	0.9821037
C	1.1483682	-10.241836	1.9940754	H	-3.597008	-0.4561267	10.827773
O	0.3991149	-8.2732182	4.2096079	H	-7.5256396	0.9095461	9.7282222
O	-0.795578	-9.4335979	-0.2134951	H	3.885864	-4.1525716	0.6634329
O	-6.103071	-3.1626388	4.7064786	H	-0.0061632	-2.4616106	-0.0492745

O	-7.2373522	-5.9079096	8.3669036	H	-8.0313263	-1.0945699	6.945233
C	-5.9091187	-3.0951664	7.8532185	H	-8.7944367	-1.88866	8.3128579
C	-5.8583007	-1.8916902	8.681715	H	-8.8080841	-0.1170105	8.2094736
O	-4.9534877	-3.867106	7.6845723	H	3.1687473	-7.4260405	0.8099719
C	0.0870232	-6.8281335	1.3908282	H	4.1934727	-6.1906337	1.5654198
C	0.81268	-5.6135164	1.0317427	H	2.8840952	-6.9694222	2.4822099
O	-1.1423406	-6.8872087	1.5558835	H	2.0180219	-1.3889161	-0.3790465
C	-4.6563388	-1.6803428	9.428877	H	-1.60499	-5.3733131	1.0007337
C	-4.5246638	-0.574046	10.274771	H	-4.6411337	1.447472	11.627433
C	-5.5648628	0.3377966	10.375263	H	-3.8226643	-3.2202986	8.7204732
C	-6.7440926	0.1635213	9.63303				

NImag	0
Σ Electronic and thermal Free Energy	-1819235.304
mol Fraction	0.325125493

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 6

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.9469616	-9.4277089	1.311586	C	-5.6975811	-0.8294594	8.0652988
C	-2.1069354	-10.229466	1.7796404	C	0.4748825	-4.9611565	0.6951748
C	-2.4513376	-10.319022	3.1927619	C	0.6317117	-3.6274007	0.315526
C	-1.6070085	-9.8398294	4.1516731	C	-0.1149911	-2.6106174	0.9204604
C	-0.4185307	-9.0586519	3.8503954	C	-1.0362497	-2.9104176	1.9197133
C	0.0341855	-8.8927096	2.3740096	C	-1.2156144	-4.2386744	2.3066706
C	-2.8694384	-10.852058	0.8548969	C	-6.777499	-0.6004842	7.0310033
O	-3.9909931	-11.539537	1.1564001	C	1.3078045	-5.9985052	-0.0278172
C	-4.4786546	-11.456462	2.4404652	O	0.0225979	-1.3010097	0.5692744
C	-3.779912	-10.880778	3.4489381	O	-2.06548	-4.5624945	3.3021991
C	-5.8313548	-12.093424	2.5463531	O	-4.2702245	1.169272	10.751851
C	-6.5096296	-11.856809	3.9111339	O	-3.1390888	-3.2006033	9.3323744
C	-5.4698219	-11.868131	5.0452962	H	-1.8337087	-9.9222082	5.2090491
C	-4.4854221	-10.704821	4.7873586	H	-2.6515712	-10.84711	-0.2057124
C	-5.2863704	-9.3644432	4.7742335	H	-5.7120306	-13.170523	2.3778611
O	-6.3441539	-9.3954039	3.8585072	H	-6.4623104	-11.716512	1.7314321
C	-4.7756053	-13.211929	5.1969061	H	-7.2460366	-12.65085	4.0746561
C	-7.2415762	-10.510968	3.9760627	H	-5.9705327	-11.678287	6.003603
O	-3.7502394	-13.147924	6.0766469	H	-3.7617541	-10.654915	5.6019902
O	-5.1001556	-14.23907	4.6417994	H	-7.8078545	-10.433836	4.9133069
O	-5.8380363	-9.2367039	6.1293465	H	-7.9386989	-10.396087	3.1420516
C	-6.2623188	-8.0218793	6.5196302	H	-3.3754022	-14.047444	6.1344117
C	-5.9860285	-6.8491991	5.8913282	H	-6.8595294	-8.0591428	7.4253853
C	-5.0914709	-6.8410173	4.7558878	H	-4.1285293	-8.1873423	3.3903232
C	-4.4302294	-8.1506659	4.4369481	H	-3.5092003	-8.2000657	5.0282768
C	-6.5423013	-5.5859377	6.4205851	H	-3.96678	-5.7595606	3.3244155
C	-6.2729788	-4.3077043	5.577546	H	-7.7075201	-4.8536719	4.0311766
C	-5.0582385	-4.3985697	4.6259549	H	-8.3915198	-3.9316202	5.3950126
C	-4.7066259	-5.711449	4.1157098	H	-7.3891901	-3.1074109	4.164356
O	-6.1428854	-3.1691883	6.4397847	H	2.0902347	-9.1872547	2.9189769
C	-7.528258	-4.03204	4.7314516	H	1.2746658	-10.679682	2.3986363
O	0.3072298	-7.4984324	2.1064778	H	1.7420216	-9.4666238	1.1807479
C	1.3803171	-9.6069422	2.2023282	H	-2.9072345	-1.168211	10.791938
O	0.2570134	-8.533484	4.726514	H	-6.0001226	1.1360634	8.8863917
O	-0.7363562	-9.230214	0.1253287	H	1.339297	-3.376778	-0.4722841
O	-4.4590009	-3.3730004	4.2986816	H	-1.5950388	-2.1125382	2.398561

O	-7.2506611	-5.5225947	7.4100001	H	-6.3974099	-0.740889	6.0150031
C	-5.1155675	-3.2139525	7.3142626	H	-7.6103382	-1.2989792	7.1552651
C	-4.9376235	-2.0380085	8.1645507	H	-7.1644104	0.4185706	7.1205904
O	-4.4013903	-4.2256668	7.3641265	H	0.7178008	-6.8666734	-0.333686
C	-0.7849653	-6.6871671	2.0733772	H	1.7642296	-5.5571679	-0.9191822
C	-0.4688313	-5.2864114	1.7011043	H	2.1103778	-6.3745014	0.6153129
O	-1.8982858	-7.1319053	2.3076146	H	0.7027794	-1.2307558	-0.1188477
C	-3.9190808	-2.122905	9.1665739	H	-2.6806922	-3.8336533	3.5363998
C	-3.6878772	-1.058429	10.04443	H	-3.5587829	0.9727317	11.381973
C	-4.4458806	0.0974252	9.9330242	H	-3.3930884	-3.8579899	8.6346011
C	-5.4388884	0.2098849	8.9464113				

NImag	0
Σ Electronic and thermal Free Energy	-1819227.052
mol Fraction	2.86E-07

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 7

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1629804	-9.2036157	1.069948	C	-5.2063355	-0.7028233	6.8045841
C	-2.2690637	-10.082874	1.5382936	C	-0.0477724	-4.4311549	1.7853587
C	-2.4834435	-10.330365	2.9566339	C	0.0380943	-3.0590475	2.0106455
C	-1.539742	-10.003627	3.8861489	C	-0.6656647	-2.4648684	3.0636568
C	-0.3209841	-9.2892281	3.5598609	C	-1.4618026	-3.2331089	3.9095806
C	-0.0789952	-8.8068845	2.0979911	C	-1.5724011	-4.6097706	3.6886766
C	-3.1019959	-10.631469	0.6277923	C	-6.3817077	-0.6953236	5.8514448
O	-4.1760233	-11.387003	0.9577098	C	0.7281814	-5.0206052	0.6272117
C	-4.5576135	-11.424321	2.2785123	O	-0.5322298	-1.1159801	3.2209844
C	-3.7898822	-10.904599	3.2653995	O	-2.3063762	-5.3884315	4.5128825
C	-5.8665561	-12.133657	2.4636969	O	-3.3574898	1.826682	8.6661327
C	-6.4040783	-12.07572	3.9133509	O	-2.7579289	-2.9351569	8.3936093
C	-5.2567091	-12.069433	4.9379389	H	-1.6683176	-10.227383	4.9395506
C	-4.3877877	-10.822706	4.6565608	H	-2.9861243	-10.514332	-0.442354
C	-5.2684552	-9.5374557	4.7695148	H	-5.7188863	-13.180593	2.171717
O	-6.4513254	-9.6236846	4.0252274	H	-6.602364	-11.714843	1.7654587
C	-4.4500603	-13.357591	4.9271406	H	-7.0445939	-12.948309	4.0796536
C	-7.2322352	-10.815824	4.1786938	H	-5.6717219	-11.977457	5.9505811
O	-3.3546706	-13.268176	5.7157225	H	-3.604797	-10.746897	5.4106485
O	-4.7439276	-14.366495	4.3237123	H	-7.666835	-10.852233	5.1867962
O	-5.5993226	-9.4601093	6.1991012	H	-8.0461359	-10.709988	3.4564813
C	-5.9297374	-8.2639328	6.7116035	H	-2.9032631	-14.132273	5.6658667
C	-5.8807385	-7.0782807	6.0509943	H	-6.2619032	-8.3318433	7.7428403
C	-5.3507272	-7.0286655	4.7024813	H	-4.4325674	-8.2945497	3.2248454
C	-4.5801839	-8.2555552	4.3028444	H	-3.583271	-8.1845268	4.7532262
C	-6.3099698	-5.845791	6.7390869	H	-4.9677435	-5.9053719	2.9376329
C	-6.5982497	-4.6279115	5.8310387	H	-8.5800474	-4.4095571	6.6588418
C	-5.955375	-4.6625186	4.4162105	H	-8.354994	-3.6470761	5.0522891
C	-5.4206421	-5.9242502	3.923571	H	-8.520997	-5.4132504	5.1876763
O	-6.1970165	-3.4134621	6.5034319	H	2.0448993	-9.0079218	2.3216861
C	-8.1209616	-4.5163562	5.6722893	H	1.2734228	-10.416974	1.5596922
O	0.0581386	-7.3607386	2.1432858	H	1.4820904	-8.9212258	0.6175773
C	1.2763672	-9.3225481	1.6126021	H	-2.1665873	-0.5103873	9.2544014
O	0.5265225	-9.0182089	4.4031956	H	-5.2848019	1.4399147	7.0408928
O	-1.064654	-8.8526097	-0.0940765	H	0.6415829	-2.4284731	1.3662691
O	-5.9350903	-3.6296935	3.7573033	H	-2.0009741	-2.7816015	4.7394284

O	-6.5143066	-5.7762819	7.9395945	H	-6.2304202	-1.3599543	4.9969976
C	-4.8674447	-3.2228748	6.6262791	H	-7.2924484	-1.0335274	6.3576439
C	-4.5131428	-1.88929	7.1660146	H	-6.5557833	0.3203163	5.4841701
O	-4.066414	-4.092607	6.3112883	H	0.1331854	-5.7334279	0.0481975
C	-1.0863192	-6.6713422	2.3959689	H	1.0651608	-4.2262675	-0.0452615
C	-0.8728246	-5.2223839	2.6204122	H	1.6101408	-5.5641168	0.9829701
O	-2.1661734	-7.2378893	2.4357959	H	-1.1041247	-0.8272985	3.9495321
C	-3.4083369	-1.7942562	8.0448273	H	-2.7738485	-4.844419	5.1787867
C	-3.0102617	-0.5614036	8.5672138	H	-2.5989183	1.7479074	9.2656287
C	-3.6996579	0.594192	8.2012065	H	-2.073564	-2.7218931	9.0470622
C	-4.7813632	0.5203009	7.3192841				

NImag	0
Σ Electronic and thermal Free Energy	-1819215.677
mol Fraction	1.29E-15

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 8

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.9900681	-9.4383175	0.9762459	C	-6.5195453	-0.7342565	8.3225511
C	-2.2553471	-9.9683493	1.5513903	C	2.2455806	-5.4420443	1.0570725
C	-2.5350812	-9.9076596	2.98099	C	2.8183722	-4.2403547	0.668972
C	-1.6183518	-9.3920822	3.855131	C	2.025511	-3.1555055	0.2596845
C	-0.3438289	-8.8380491	3.4361269	C	0.6412695	-3.2510139	0.2557628
C	0.1217449	-9.0712487	1.9749969	C	0.0326261	-4.4440989	0.6569829
C	-3.1509753	-10.513596	0.7002519	C	-7.3161762	-0.6354468	7.0394897
O	-4.3265884	-11.041156	1.0934186	C	3.179495	-6.5404951	1.5151342
C	-4.6607622	-10.981841	2.4252368	O	2.6804687	-2.0230375	-0.1108452
C	-3.8495269	-10.427822	3.3611815	O	-1.3090243	-4.4559587	0.6476047
C	-5.9693471	-11.668339	2.6724937	O	-5.6423084	1.5588063	11.020007
C	-6.4108166	-11.644258	4.1508539	O	-4.5343571	-3.0710489	10.341462
C	-5.1902564	-11.668169	5.0871429	H	-1.8154689	-9.3167274	4.9180623
C	-4.3502506	-10.397866	4.7966335	H	-2.9963583	-10.578025	-0.369523
C	-5.2464661	-9.1525243	5.0710705	H	-5.8565337	-12.706518	2.3387185
O	-6.441539	-9.196491	4.3407939	H	-6.7370198	-11.215727	2.0314196
C	-4.3822873	-12.949824	4.9685829	H	-7.0395572	-12.520915	4.3391438
C	-7.2218665	-10.391063	4.4903714	H	-5.526746	-11.618098	6.1300854
O	-3.2401248	-12.888511	5.6906174	H	-3.507889	-10.361188	5.488716
O	-4.7102941	-13.934525	4.3429213	H	-7.6142564	-10.45461	5.5134289
O	-5.5450864	-9.2474038	6.499867	H	-8.0641982	-10.26244	3.8056994
C	-6.0767908	-8.159551	7.0902834	H	-2.795174	-13.750654	5.5825432
C	-6.1190578	-6.9193906	6.5467738	H	-6.487793	-8.3718051	8.0718407
C	-5.4597383	-6.6602273	5.2803552	H	-4.4378493	-7.7097699	3.6895658
C	-4.6081416	-7.7969336	4.764538	H	-3.6293692	-7.7513031	5.2576427
C	-6.8270266	-5.8462027	7.2824021	H	-4.9731001	-5.2569275	3.7500814
C	-7.1212802	-4.5545656	6.4880086	H	-9.2437399	-4.7635705	6.8243894
C	-6.1934262	-4.303708	5.2710679	H	-8.8132008	-3.7234625	5.4335251
C	-5.5090282	-5.4518245	4.6747772	H	-8.6882025	-5.4939462	5.2955302
O	-7.0975858	-3.4222269	7.3639451	H	1.9699336	-9.9481426	2.6553393
C	-8.5682702	-4.6422111	5.9731881	H	0.697997	-11.143902	2.3128033
O	0.8338596	-7.9114419	1.512692	H	1.5418061	-10.34569	0.9611375
C	1.1552856	-10.208046	1.9745847	H	-4.4931332	-0.7844294	11.661107
O	0.4109408	-8.2520773	4.2028329	H	-6.8851388	1.3388483	8.7992635
O	-0.7927395	-9.3846446	-0.2246101	H	3.8953415	-4.1124624	0.6838935
O	-6.1077267	-3.1790974	4.7985163	H	0.0052486	-2.4198266	-0.0353017

O	-7.264038	-5.9909985	8.4108773	H	-6.837234	-1.1573437	6.2075976
C	-5.8809417	-3.1727232	7.9280496	H	-8.3073286	-1.0857643	7.1641981
C	-5.870512	-1.9261273	8.7353728	H	-7.4538467	0.4152643	6.766902
O	-4.9400071	-3.9231737	7.7592099	H	4.1995028	-6.1520433	1.5856077
C	0.0945541	-6.7906115	1.3923599	H	2.8855109	-6.9361718	2.4914964
C	0.8212126	-5.5744715	1.0393987	H	3.1802391	-7.3850706	0.8189678
O	-1.1345739	-6.849526	1.5569602	H	2.029697	-1.3467331	-0.3578742
C	-5.1346127	-1.9188707	9.9413858	H	-1.5967719	-5.3330084	1.0057272
C	-5.0537184	-0.7662289	10.726957	H	-5.1047648	1.42103	11.815428
C	-5.6916027	0.3990337	10.304368	H	-4.1057013	-2.9190102	11.197845
C	-6.4126047	0.4126276	9.1086203				

NImag	0
Σ Electronic and thermal Free Energy	-1819223.235
mol Fraction	4.53E-10

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 9

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.2455804	-9.3821563	0.7419603	C	-6.9292566	-1.2453836	9.1857986
C	-2.4395446	-9.9659664	1.4104569	C	1.8001718	-5.2346616	0.6266063
C	-2.6123763	-9.9151198	2.8572993	C	2.29475	-4.0120392	0.1920857
C	-1.6615266	-9.3483515	3.6592362	C	1.4345634	-2.9783186	-0.2170847
C	-0.4560249	-8.7252789	3.1437925	C	0.0582893	-3.142318	-0.1700974
C	-0.084266	-8.9530877	1.6559111	C	-0.4706984	-4.3528902	0.2816219
C	-3.3697615	-10.554176	0.6283516	C	-8.2691284	-1.3717031	8.495077
O	-4.4872294	-11.135101	1.1086264	C	2.8044349	-6.2713409	1.080135
C	-4.7172804	-11.091458	2.4636386	O	1.9117744	-1.7825605	-0.6552718
C	-3.8656157	-10.500778	3.3369629	O	-1.8095055	-4.4366609	0.3265672
C	-5.9661656	-11.846676	2.809301	O	-5.4705318	1.1336993	11.523127
C	-6.3008938	-11.828035	4.3140547	O	-3.5273834	-2.6898535	9.5219188
C	-5.0078423	-11.800376	5.1557872	H	-1.7788061	-9.2847639	4.7344021
C	-4.2487808	-10.50112	4.8091411	H	-3.2931955	-10.613884	-0.4500542
C	-5.1661037	-9.2938747	5.1632643	H	-5.8260565	-12.882167	2.4704493
O	-6.4097505	-9.3784477	4.5213632	H	-6.8025255	-11.448757	2.2200686
C	-4.1070266	-13.01813	5.0123412	H	-6.8866827	-12.72039	4.5557491
C	-7.1302588	-10.602607	4.7122321	H	-5.2883897	-11.77345	6.2167064
O	-4.8225678	-14.165547	4.9053313	H	-3.3505169	-10.44264	5.4253784
O	-2.8977804	-13.002598	5.0360966	H	-7.451232	-10.687686	5.7584312
O	-5.3579225	-9.4123637	6.6103854	H	-8.0209502	-10.504166	4.086074
C	-5.8883583	-8.3534969	7.2492282	H	-4.1706857	-14.891819	4.8737095
C	-6.0227372	-7.1117693	6.7229371	H	-6.2163661	-8.5900233	8.2563015
C	-5.467676	-6.8141923	5.4145305	H	-4.5159174	-7.8066847	3.7457038
C	-4.6076933	-7.9100612	4.8286952	H	-3.5996597	-7.8279672	5.2530931
C	-6.7171843	-6.0762513	7.5199566	H	-5.1512974	-5.3811589	3.8669902
C	-7.132329	-4.8021665	6.7539483	H	-9.2145135	-5.1266495	7.234887
C	-6.3088699	-4.4941312	5.4757785	H	-8.9341244	-4.0558858	5.8276788
C	-5.6109306	-5.6048009	4.8256093	H	-8.7242685	-5.8158735	5.6657452
O	-7.1089443	-3.6653248	7.6301208	H	1.8462187	-9.7377677	2.2101447
C	-8.6051759	-4.9629644	6.3417703	H	0.6091317	-10.993111	1.9718339
O	0.5378238	-7.7665358	1.1359603	H	1.3168135	-10.174801	0.5548305
C	0.9976561	-10.042343	1.5921995	H	-3.5149793	-0.6658289	11.014292
O	0.3138854	-8.0828612	3.8477284	H	-7.5608448	0.5464139	10.195786
O	-1.1375263	-9.3314889	-0.4702848	H	3.3701644	-3.8470398	0.1773673
O	-6.3223771	-3.3631113	5.0165962	H	-0.6104526	-2.3411275	-0.4609512

O	-7.0513052	-6.2373144	8.6811742	H	-8.8910142	-0.5043303	8.7342665
C	-5.9010745	-3.3507297	8.1410257	H	-8.1566492	-1.4324658	7.4087972
C	-5.8474281	-2.1605899	8.9883693	H	-8.8010258	-2.275221	8.8081066
O	-4.9251394	-4.0730392	7.8896589	H	2.84415	-7.121499	0.3919096
C	-0.2601322	-6.6823248	1.0601298	H	3.8018674	-5.8244381	1.1308663
C	0.3877836	-5.4364334	0.6586938	H	2.5495593	-6.6736766	2.0645437
O	-1.4722475	-6.7962226	1.2993713	H	2.8814156	-1.7989929	-0.625982
C	-4.609438	-1.9098136	9.6605754	H	-2.0371442	-5.3137801	0.7224438
C	-4.4707622	-0.8146617	10.519726	H	-4.5851944	1.1751881	11.918413
C	-5.5403109	0.0485624	10.705611	H	-3.7573321	-3.3962627	8.8650932
C	-6.756403	-0.1634254	10.036288				

NImag	0
Σ Electronic and thermal Free Energy	-1819233.804
mol Fraction	0.025820741

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 10

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1389492	-9.2904514	1.0690251	C	-5.431842	-1.5400446	8.5628026
C	-2.2744545	-10.135441	1.5310536	C	0.1669339	-4.5524237	2.036913
C	-2.500081	-10.381879	2.9477233	C	0.3005262	-3.2010861	2.3637043
C	-1.5482334	-10.091513	3.8815157	C	-0.4512513	-2.6433033	3.4034604
C	-0.3007642	-9.4280992	3.5596258	C	-1.3441634	-3.4184152	4.1292194
C	-0.0472477	-8.9313494	2.1039649	C	-1.5111907	-4.7622777	3.7985357
C	-3.1199482	-10.657123	0.6164143	C	-6.5412424	-2.3946607	9.1358595
O	-4.2149408	-11.384818	0.9405491	C	1.0050806	-5.1011484	0.9023384
C	-4.5988751	-11.421041	2.2604794	O	-0.349133	-1.3209759	3.7565659
C	-3.8213951	-10.922885	3.2509372	O	-2.3672548	-5.52977	4.5106024
C	-5.9200081	-12.108502	2.4417858	O	-3.8284997	1.6050796	9.4756556
C	-6.4520608	-12.0599	3.8941696	O	-3.0886906	-1.3489188	5.7521058
C	-5.3022281	-12.077518	4.9158896	H	-1.6856069	-10.319462	4.9328303
C	-4.4174381	-10.839932	4.6424271	H	-2.9980258	-10.539312	-0.45297
C	-5.2803152	-9.5437031	4.7653766	H	-5.791257	-13.153994	2.1359981
O	-6.4682548	-9.6099764	4.0271506	H	-6.6508647	-11.668439	1.7514106
C	-4.5121085	-13.375663	4.8917139	H	-7.1023813	-12.926539	4.0532701
C	-7.2636034	-10.792825	4.1748958	H	-5.7136619	-11.988755	5.930284
O	-3.4152969	-13.3079	5.6803832	H	-3.6330128	-10.779323	5.3962532
O	-4.8190417	-14.374491	4.2781134	H	-7.6934826	-10.832483	5.1849335
O	-5.6008642	-9.4694007	6.1977003	H	-8.0797874	-10.670592	3.4578501
C	-5.9110199	-8.2712787	6.719254	H	-2.9745635	-14.176944	5.6217805
C	-5.8632415	-7.0860658	6.0582822	H	-6.2272056	-8.3402046	7.7553972
C	-5.3490768	-7.0387232	4.7016842	H	-4.430709	-8.304957	3.2235093
C	-4.5797696	-8.2668107	4.3014818	H	-3.5837983	-8.2034282	4.7550049
C	-6.2641955	-5.8469561	6.7490276	H	-5.002492	-5.9174303	2.928451
C	-6.6253468	-4.6561448	5.8348154	H	-8.5154136	-5.5362264	5.2070506
C	-6.01378	-4.6854859	4.4040833	H	-8.6140327	-4.540136	6.6822836
C	-5.4383928	-5.9379392	3.9220331	H	-8.4301718	-3.7625351	5.0786639
O	-6.2850297	-3.4147699	6.4840257	H	2.0715861	-9.1806713	2.326171
C	-8.1551713	-4.623671	5.6932709	H	1.2711211	-10.558498	1.5383172
O	0.1203351	-7.4883989	2.1793256	H	1.5120543	-9.0516605	0.6228796
C	1.2974087	-9.4655517	1.6108003	H	-2.6284985	0.8167832	7.2001962
O	0.5627602	-9.2069862	4.4015239	H	-5.609581	-0.0932494	10.154121
O	-1.0208946	-8.9447214	-0.0945788	H	0.99079	-2.5789896	1.7971775
O	-6.0723202	-3.6731622	3.7232056	H	-1.9248892	-2.9815247	4.9322094

O	-6.3855719	-5.7609173	7.9617914	H	-6.713783	-2.1299686	10.183276
C	-4.969339	-3.1637404	6.6570162	H	-7.4754792	-2.2280107	8.58741
C	-4.7231599	-1.8911264	7.3861958	H	-6.3303999	-3.4647037	9.0731752
O	-4.104941	-3.9283549	6.255002	H	0.4229269	-5.7348611	0.226704
C	-1.01039	-6.7761627	2.4325221	H	1.4362367	-4.2822911	0.3182783
C	-0.7579914	-5.3503835	2.7501096	H	1.8254953	-5.718647	1.2828835
O	-2.1077252	-7.3078943	2.4131665	H	0.298312	-0.8922654	3.1752505
C	-3.7130155	-1.0241612	6.9140127	H	-2.8676065	-4.9677856	5.1357959
C	-3.4000431	0.1552899	7.5913234	H	-3.1107578	2.0972847	9.0474398
C	-4.0907057	0.4757224	8.7599303	H	-2.4055434	-0.6960257	5.528251
C	-5.0954545	-0.3681193	9.2392752				

NImag	0
Σ Electronic and thermal Free Energy	-1819216.215
mol Fraction	3.20E-15

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 11

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.9862314	-9.4214363	1.2358036	C	-5.0764314	-0.7773	7.644743
C	-2.130377	-10.234326	1.7239796	C	0.3723379	-4.9206464	0.6355002
C	-2.4447042	-10.333504	3.1434643	C	0.5062397	-3.5816693	0.273731
C	-1.5833182	-9.8543832	4.0870657	C	-0.2315077	-2.585098	0.920193
C	-0.402746	-9.0694315	3.7651611	C	-1.1184751	-2.9134298	1.9426887
C	0.01441	-8.8864389	2.2799546	C	-1.2754093	-4.2521017	2.3130204
C	-2.906641	-10.858743	0.8121627	C	-5.5024541	-0.5183394	6.2156798
O	-4.0158511	-11.557638	1.1333753	C	1.1919104	-5.9394829	-0.1277673
C	-4.4773594	-11.484813	2.427659	O	-0.0384663	-1.2999443	0.5082779
C	-3.7633101	-10.906945	3.4240892	O	-2.0889296	-4.599291	3.3305734
C	-5.8210097	-12.136136	2.5589291	O	-4.2360692	1.3016435	10.520462
C	-6.4729236	-11.912816	3.9387157	O	-4.3217918	-3.4787077	10.012525
C	-5.4094654	-11.917721	5.0508643	H	-1.7871466	-9.9435766	5.1485545
C	-4.4426754	-10.743175	4.7774016	H	-2.710927	-10.846602	-0.2526923
C	-5.2578857	-9.4112828	4.7865852	H	-5.6940898	-13.211138	2.3826931
O	-6.3335374	-9.4505895	3.8911842	H	-6.472909	-11.762082	1.7593079
C	-4.6986049	-13.25478	5.1822737	H	-7.1972969	-12.715373	4.1141058
C	-7.2170737	-10.574857	4.0244598	H	-5.8919957	-11.736688	6.020159
O	-3.6551236	-13.18391	6.0401103	H	-3.7028912	-10.688689	5.5770967
O	-5.0243615	-14.283382	4.6304262	H	-7.7636549	-10.506691	4.97405
O	-5.783128	-9.2948684	6.1518927	H	-7.9333626	-10.464603	3.2061547
C	-6.2158888	-8.0857091	6.5536788	H	-3.2699138	-14.079752	6.0849971
C	-5.9653504	-6.9083238	5.9244862	H	-6.7964971	-8.132972	7.4695789
C	-5.0923745	-6.8867915	4.7741622	H	-4.141472	-8.2165187	3.3834828
C	-4.4223397	-8.1870412	4.4361587	H	-3.4889988	-8.2269667	5.0087565
C	-6.5315807	-5.6524664	6.4640976	H	-4.0077381	-5.787335	3.3269487
C	-6.2780368	-4.3607374	5.6340498	H	-7.7433116	-4.8920943	4.1073665
C	-5.0794717	-4.4447523	4.6628322	H	-8.3963952	-3.9814803	5.4946403
C	-4.7327034	-5.7495114	4.1322969	H	-7.419974	-3.1472092	4.2513508
O	-6.1350156	-3.2396985	6.5108071	H	2.0849934	-9.165826	2.7747588
C	-7.5479153	-4.0775189	4.8118085	H	1.2725465	-10.660881	2.256765
O	0.2678726	-7.4866727	2.0202	H	1.6996354	-9.4298779	1.0419568
C	1.3630958	-9.5850404	2.0699433	H	-3.9516914	-1.2370735	11.355802
O	0.2935526	-8.5530247	4.6302714	H	-4.956683	1.3352946	8.0709296
O	-0.8027591	-9.2160759	0.046463	H	1.1804224	-3.2908992	-0.5248766
O	-4.4786415	-3.4183203	4.3293976	H	-1.6786208	-2.1430969	2.4691142

O	-7.2427735	-5.6078376	7.4521007	H	-5.0034418	-1.1827407	5.5061931
C	-5.0632804	-3.3134395	7.3537607	H	-6.5791313	-0.6821003	6.0961168
C	-4.8914285	-2.0829667	8.1676424	H	-5.2857929	0.5194675	5.9446666
O	-4.3622934	-4.3044372	7.3990096	H	0.6001694	-6.8076606	-0.4308782
C	-0.8326867	-6.6866767	2.0193393	H	1.6190909	-5.4789218	-1.0234477
C	-0.5387265	-5.2764355	1.6647474	H	2.0152059	-6.3191652	0.4865439
O	-1.9371278	-7.1464192	2.2667271	H	-0.6056082	-0.7113535	1.0307902
C	-4.4748028	-2.2253895	9.5106094	H	-2.7215345	-3.8902007	3.5806741
C	-4.2594188	-1.1060226	10.318871	H	-3.9526277	1.0574054	11.41529
C	-4.4393592	0.1700777	9.7878851	H	-4.0714696	-3.4133749	10.947089
C	-4.8390473	0.3291599	8.4591949				

NImag	0
Σ Electronic and thermal Free Energy	-1819214.92
mol Fraction	3.58E-16

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 12

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1574427	-9.1752784	1.1072444	C	-5.308322	-0.723358	6.8192198
C	-2.2692577	-10.05692	1.5560606	C	0.0439077	-4.4404056	1.9037646
C	-2.4944537	-10.321483	2.9696474	C	0.1754237	-3.0759817	2.1636259
C	-1.5570108	-10.009643	3.9105552	C	-0.5161392	-2.4786954	3.2238386
C	-0.3327384	-9.2976582	3.6019625	C	-1.3586438	-3.2316415	4.0358757
C	-0.0766551	-8.8021911	2.1470568	C	-1.5195098	-4.5952751	3.7786208
C	-3.0967031	-10.59291	0.6329067	C	-6.5322071	-0.7291045	5.9290294
O	-4.1737515	-11.350937	0.9457232	C	0.8179443	-5.0282501	0.7433024
C	-4.5654478	-11.403276	2.2634413	O	-0.3957749	-1.149225	3.5091507
C	-3.8043455	-10.896062	3.2617712	O	-2.3030183	-5.3623277	4.564804
C	-5.8763605	-12.11324	2.4310676	O	-3.4096968	1.8354748	8.5876891
C	-6.4254839	-12.068769	3.8769369	O	-2.7032197	-2.9026069	8.227952
C	-5.2866854	-12.073831	4.9110677	H	-1.6950556	-10.2455	4.960066
C	-4.4131466	-10.826168	4.6485989	H	-2.9728455	-10.462946	-0.4348841
C	-5.2920359	-9.5400047	4.7652919	H	-5.7271753	-13.157447	2.1301365
O	-6.4686643	-9.6186155	4.0091323	H	-6.6062471	-11.686945	1.7311492
C	-4.4821029	-13.363154	4.8953697	H	-7.0685717	-12.941973	4.0295255
C	-7.2532825	-10.809702	4.1473855	H	-5.7100804	-11.990069	5.9209397
O	-3.3942066	-13.283537	5.6953926	H	-3.6364258	-10.758845	5.4098858
O	-4.7713524	-14.365589	4.2789678	H	-7.6948513	-10.853949	5.1521574
O	-5.6338172	-9.4733242	6.1913745	H	-8.0620368	-10.696267	3.4205166
C	-5.9707157	-8.2796236	6.7087075	H	-2.944065	-14.148034	5.6414076
C	-5.9200076	-7.0911729	6.0544407	H	-6.3103322	-8.3544821	7.7369486
C	-5.3810883	-7.0340845	4.70942	H	-4.4373212	-8.2877483	3.2376496
C	-4.5988944	-8.254863	4.3138682	H	-3.6087466	-8.1842107	4.7789398
C	-6.3615587	-5.8629284	6.7434151	H	-5.0062644	-5.9050728	2.946101
C	-6.6613776	-4.6472446	5.836763	H	-8.6373707	-4.4345101	6.6792199
C	-6.0279048	-4.6796197	4.4168833	H	-8.4277845	-3.6768279	5.0680104
C	-5.4615426	-5.930905	3.930847	H	-8.5857266	-5.4431346	5.2113467
O	-6.2598026	-3.4303383	6.5029511	H	2.0432025	-9.0321608	2.3820951
C	-8.185568	-4.5426918	5.6894905	H	1.2593769	-10.423407	1.600335
O	0.0776197	-7.359358	2.2090147	H	1.4927753	-8.920763	0.6752044
C	1.2755204	-9.3297066	1.6647115	H	-2.1243314	-0.4742608	9.0719364
O	0.5102487	-9.0400734	4.4540454	H	-5.4214902	1.4144191	7.0776948
O	-1.0509046	-8.8059102	-0.050477	H	0.8199842	-2.469304	1.5303538
O	-6.0417441	-3.6533205	3.7483701	H	-1.8844172	-2.76121	4.8601785

O	-6.5694377	-5.7985	7.9436281	H	-6.4011405	-1.3653461	5.0499745
C	-4.9274327	-3.2357374	6.610047	H	-7.4060003	-1.1093837	6.4688368
C	-4.5686019	-1.8978718	7.1295416	H	-6.7537055	0.2898332	5.5982988
O	-4.1351699	-4.1147848	6.2971103	H	0.2149739	-5.7218851	0.1500707
C	-1.0596062	-6.6571185	2.4649674	H	1.174754	-4.2315666	0.0832545
C	-0.8193978	-5.2154021	2.7100555	H	1.6873564	-5.5924051	1.0976365
O	-2.1468788	-7.2087437	2.4931752	H	0.2073081	-0.7466484	2.8648949
C	-3.4097562	-1.7794502	7.9341137	H	-2.7760877	-4.8141675	5.2247948
C	-3.0111841	-0.5415451	8.4429951	H	-2.6024219	1.7720351	9.1217903
C	-3.7497803	0.5988039	8.1323257	H	-1.9712063	-2.6672882	8.819317
C	-4.8827443	0.5046336	7.3196245				

NImag	0
Σ Electronic and thermal Free Energy	-1819215.709
mol Fraction	1.36E-15

(8*S*, 13*S*, 3a*S*, 8a*S*, 12a*S*, 13a*R*)- Pavesiflonic acid (3) - Conformer 13

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.9834799	-9.3929513	1.2505487	C	-5.1118706	-0.7905808	7.6912914
C	-2.1263735	-10.209974	1.7338831	C	0.36768	-4.8973238	0.656663
C	-2.4444865	-10.312693	3.1523355	C	0.4995906	-3.5563837	0.2928271
C	-1.5878619	-9.8316191	4.099387	C	-0.2498273	-2.5586647	0.9254958
C	-0.4096037	-9.0415984	3.7824258	C	-1.1484399	-2.8847445	1.936995
C	0.0115575	-8.8555938	2.2987845	C	-1.3027327	-4.2206933	2.308722
C	-2.8984174	-10.83467	0.8185841	C	-5.5320853	-0.5247558	6.2618565
O	-4.0062194	-11.537391	1.1351204	C	1.2009241	-5.9138735	-0.0949523
C	-4.4709539	-11.470017	2.428751	O	-0.1363183	-1.2422822	0.5899666
C	-3.7613287	-10.8923	3.4284327	O	-2.1289034	-4.5711658	3.3142025
C	-5.812298	-12.126952	2.5548889	O	-4.2809218	1.2741244	10.580398
C	-6.4678593	-11.911136	3.9341381	O	-4.3667419	-3.5037544	10.049208
C	-5.4064785	-11.915775	5.0482572	H	-1.7947779	-9.9232351	5.1600294
C	-4.4439555	-10.736206	4.7809781	H	-2.6998012	-10.819552	-0.2456994
C	-5.2649417	-9.4077432	4.7940218	H	-5.6808305	-13.200796	2.3749458
O	-6.3379002	-9.4485108	3.8949513	H	-6.4639584	-11.752378	1.7553062
C	-4.6904735	-13.250338	5.1763845	H	-7.1893652	-12.717207	4.1052126
C	-7.2173794	-10.576309	4.0229584	H	-5.8914735	-11.739928	6.0172532
O	-3.6495944	-13.178551	6.0373807	H	-3.7059242	-10.681819	5.5822991
O	-5.0098526	-14.278131	4.6192348	H	-7.7659576	-10.513492	4.9717586
O	-5.7937285	-9.2999445	6.1577262	H	-7.9326571	-10.46627	3.2037134
C	-6.2333646	-8.0938845	6.5637826	H	-3.2609449	-14.073021	6.0797481
C	-5.9861029	-6.9129623	5.9406652	H	-6.8164301	-8.1481104	7.4776715
C	-5.1107044	-6.8825564	4.7920591	H	-4.1496985	-8.2024771	3.3987818
C	-4.4337495	-8.1784637	4.4507661	H	-3.5022651	-8.2169278	5.0264532
C	-6.5598047	-5.6619322	6.4843785	H	-4.0300312	-5.7711147	3.3504151
C	-6.3096614	-4.3650903	5.6617858	H	-7.7724414	-4.8910842	4.1309745
C	-5.1103898	-4.4395385	4.6900754	H	-8.4290093	-3.990704	5.5233023
C	-4.7557981	-5.7412929	4.1554224	H	-7.4535613	-3.1462958	4.2859075
O	-6.1698366	-3.2486259	6.5450137	H	2.0813389	-9.1282805	2.8006143
C	-7.5797387	-4.0802926	4.8405652	H	1.2756267	-10.625724	2.2794483
O	0.2609393	-7.454764	2.0407451	H	1.7029947	-9.3934041	1.0662601
C	1.3633057	-9.5495758	2.0930815	H	-4.0006054	-1.2685797	11.404339
O	0.282472	-8.5235504	4.6499628	H	-4.9919486	1.3197819	8.1277644
O	-0.795877	-9.1856179	0.062006	H	1.1891193	-3.2851538	-0.5041691
O	-4.5156724	-3.4095438	4.3597408	H	-1.7095557	-2.1014815	2.4367277

O	-7.2744371	-5.6260109	7.4703279	H	-5.030076	-1.1852863	5.5509481
C	-5.0989675	-3.3252125	7.388647	H	-6.6083562	-0.687821	6.1373605
C	-4.929385	-2.0987408	8.2089376	H	-5.3139394	0.5140702	5.9964125
O	-4.3971761	-4.3159423	7.4299542	H	0.6172028	-6.7864594	-0.4003635
C	-0.843402	-6.6592446	2.0327092	H	1.6342012	-5.4554305	-0.9892732
C	-0.552801	-5.2491505	1.6745895	H	2.0206718	-6.2865747	0.5281718
O	-1.9467365	-7.1228222	2.2761052	H	0.5293711	-1.1540443	-0.11013
C	-4.5174227	-2.2477787	9.5524851	H	-2.7489886	-3.8546627	3.5732084
C	-4.3045075	-1.1324749	10.366895	H	-3.9989407	1.0248851	11.474286
C	-4.4820034	0.1462255	9.8412387	H	-4.1186828	-3.4423664	10.984621
C	-4.8769314	0.311838	8.5120428				

NImag	0
Σ Electronic and thermal Free Energy	-1819214.941
mol Fraction	3.71E-16