Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supporting Information:

Development of an Asymmetric Formal Synthesis of (-)-Quinagolide via Enzymatic Resolution and Stereoselective Iminium Ion Reduction

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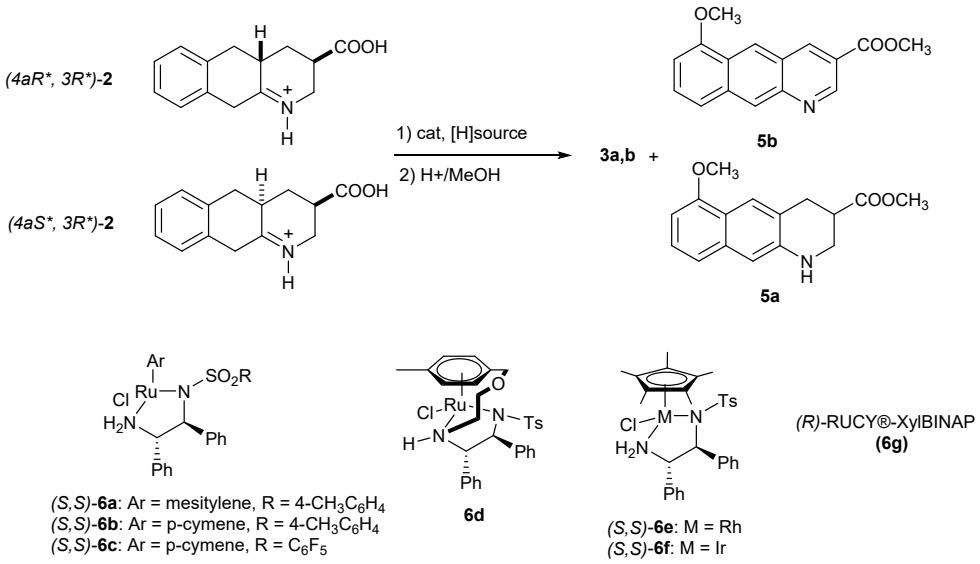
Summary:

Materials and Methods:

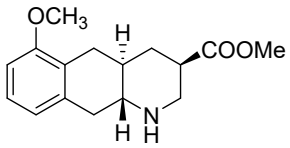
All reagents were purchased from commercially available sources. Solvents for extraction and chromatography were distilled before use. Anhydrous MeOH was obtained by distillation on Mg turnings. Protease from Bacillus licheniformis (P4860 >2.4 U/g) has been purchased by Sigma-Aldrich. A particular kind of $NaBH_4$ powder (>98% purity) purchased by Sigma-Aldrich was used for entry 13 of Table 1. Analytical TLC were performed on silica gel on TLC Al foils (Sigma-Aldrich) with detection by exposure to ultraviolet light (254 nm) and/or by immersion in an acidic staining solution of vanillin in EtOH. Merck silica gel 60 (230-400 mesh) was used for flash chromatography. Semipreparative TLC were performed on Merck PLC silica gel 60. Molecular sieves AW-300 (Alfa Aesar), 4 Å (SigmaAldrich) used were activated under vacuum by heating with a drying pistol. All compounds have been characterized using one-dimensional and bidimensional NMR spectroscopic techniques, respectively 1H, 13C and HSQC, HMBC, NOESY/ROESY and COSY. NMR spectra were recorded on Bruker Avance II 400 spectrometer, dissolving the compounds in appropriate deuterated solvents. ^{1}H NMR spectra were recorded on Bruker Avance II 400 MHz spectrometer. Chemical shifts are reported in ppm downfield from tetramethylsilane with the solvent resonance as the internal standard (Chloroform-d: δ 7.26). Signal patterns are indicated as follows: br s, broad singlet; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Coupling constants (*J*) are given in hertz (Hz). ^{13}C NMR spectra were recorded at 101 MHz with complete proton decoupling. Chemical shifts are reported in ppm downfield from tetramethylsilane with the solvent resonance as the internal standard (Chloroform-d: δ 77.16). Melting points were determined on a Kofler apparatus and are uncorrected. HRESIMS were acquired in positive ion mode with Orbitrap high-resolution mass spectrometer (Thermo, San Jose, CA, USA), equipped with H-ESI source. Analytical high performance liquid chromatography (HPLC) was performed on a Waters 600E equipped with Varian Prostar 325 detector using a Daicel® Chiralpak AD-H (250 X 4.6 mm) columns with detection at 220 nm.

Screening of reductive reaction conditions of ([3R, 4aS,R)-(2).

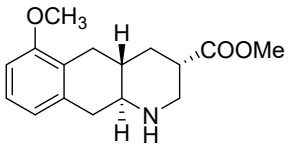


Scheme S-1. Screening conditions for asymmetric reduction of cyclic iminium ion **(2)**.

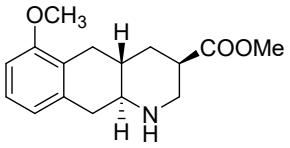
Table S-1. Screening of reductive reaction conditions of **([3R, 4aS,R)-(2)**.



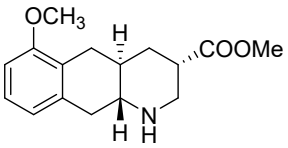
3a



ent-3a



3b



ent-3b

entry[a]	catalyst	[H] source	Yield[b]	ee[c]
1	**6a**	$HCOONH_4$	**3a** (28%), **3b** (11%), **5a** (25%), **5b** (8%)	**3a** (28%), **3b**(15%)
2	**6b**	$HCOONH_4$	**3a** (38%), **3b** (11%), **5a** (19%), **5b** (6%)	**3a** (32%), **3b** (12%)
3	**6c**	$HCOONH_4$	**3a** (31%), **3b** (13%), **5a** (26%), **5b** (1%)	**3a** (44%), **3b** (10%)
4	**6d**	$HCOONH_4$	**3a** (25%), **3b** (14%), **5a** (16%), **5b** (3%)	**3a** (46%), **3b** (40%)
5	**6g**	$HCOONH_4$	**3a** (<5%), **3b** (<5%), **5a** (45%), **5b** (9%)	Nd
6	**6e**	$HCOONH_4$	complex	mixture
7	**6f**	$HCOONH_4$	complex	mixture
8	**6b**	HCOONa	**3a** (29%), **3b** (19%), **5a** (8%), **5b** (3%)	**3a** (25%), **3b**(10%)
9[d]	**6b**	H_2	**3a (***ent*-**3a)** (28%), **3b (***ent*-**3b)** (11%)	**3a** (rac), **3b** (rac)
10[e]	(*S*)-CBS	BH_3	**3a** (33%), **3b** (57%)	**3a** (4%), **3b** (2%)
11[f]	-	$NaBH_4$	**3a (***ent*-**3a)** (48%), **3b (***ent*-**3b)** (32%)	N/A
12[g]	-	$NaBH_4$	**3a (***ent*-**3a)** (47%), **3b (***ent*-**3b)** (30%)	N/A
13[h]	-	$NaBH_4$	**3a (***ent*-**3a)** (72%), **3b (***ent*-**3b)** (8%)	N/A
14[i]	-	$NaBH_4$	**3a (***ent*-**3a)** (66%), **3b (***ent*-**3b)** (14%)	N/A
15[j]	-	$NaBH_4$	**3a (***ent*-**3a)** (49%), **3b (***ent*-**3b)** (16%)	N/A
16[k]	-	$LiBH_4$	**3a (***ent*-**3a)** (68%), **3b (***ent*-**3b)** (12%)	N/A

a) Unless noted otherwise, all ATH (asymmetric transfer hydrogenation) reactions were carried out in MeOH with 6.0 equiv. of $HCOONH_4$ or HCOONa at 60 °C for 3.5 hours. b) NMR yield using 1-bromo-3-chlorobenzene as internal standard. c) Values determined by HPLC on Daicel Chiralcel AD-H on the corresponding acetamide. d) Reaction carried out at 2 bar of H_2 at 60 °C in MeOH for 15h. e) Reaction carried out in THF with methyl ester of compound 2 at 0° C for 1h. f) Technical grade NaBH4. g) $NaBH_4$ (granules >99.99% purity) in anhydrous MeOH. h) $NaBH_4$ powder (>98% purity), Aldrich SKU 452882. i) Conditions g + $MgCl_2$ (20 mol%). j) Conditions g + LiCl (20 mol%). k) LiBH4 (1.5 equiv) in anhydrous MeOH. N/A = not applicable.

General procedure for the screening of catalysts for ATH:

Method A: (2) (0,30 mmol) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH (1.5 mL), catalyst (2 mol%) was added. After stirring for 5 minutes, [H] source (6.0 eq) was added and the reaction mixture was heated to 60°C. The reaction was stirred at the same temperature until complete conversion of **2**, then is cooled to r.t. and a solution of H_2SO_4 in MeOH (2.64M, 0.5 mL) was dropwise added. The mixture was refluxed for 3.5h, then cooled again to r.t. and quenched with water (3 mL), Na_2CO_3 was added to reach pH>7. The biphasic mixture was extracted with DCM (10 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvents were evaporated under reduced pressure affording the desired product as a dark brown oil.

Method B: (2) (1.7mmol) was added in a round-bottomed flask in argon atmosphere, RuCl[(S,S)-TsDPEN](*p*-cymene) (2 mol%, 0.02 mmol), and MeOH (18mL) were then added. After stirring at r.t. for 10 minutes, the mixture was transferred in an autoclave and 2 bar of H_2 at 60°C were added for 18h. After cooling to r.t., the mixture was concentrated under reduced pressure and a solution of H_2SO_4 in MeOH (2.64M, 3 mL) was dropwise added, the mixture was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature, MeOH was partially evaporated under reduced pressure, and the mixture was quenched with water (18 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM (20 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvent were evaporated under reduced pressure affording the desired product as a dark brown oil.

Entry 10: Step 1) In a round-bottomed flask in argon atmosphere DCC (3.4 mmol, 703 mg) and DMAP (0.31 mmol, 38 mg) are added to a solution of DCM (18 mL) and MeOH (1.25 mL, 10 eq), then compound **(2)** (3.1 mmol, 1 g) is added. The reaction mixture is stirred a r.t. for 2h, then filtered under vacuum on silica gel pad and washed with 40 mL of a solution of DCM:MeOH=9:1. The crude brown solid is solubilized in Et_2O and $CHCl_3$ and then is filtered under vacuum, a dark yellow solid is obtained (crude 1.24 mmol, 339.8 mg). Step 2) Methyl ester of compound **(2)** (93 mg, 0.3 mmol) was dissolved in dry THF (3.3 mL), CBS in toluene (10 mol%, 0.03 mmol, 8.3 mg, 9 *m*L) was added at 0°C, and the mixture was stirred for 10 minutes, BH_3 (1.1 eq, 0.33 mmol, 29 *m*L) was added and the mixture was stirred for 1h. MeOH (3 mL) and the reaction is stirred for further 30 minutes, $NaHCO_{3\,(sat)}$ is added to pH>7 and then extracted with AcOEt (10 mLx3), the organic phase is washed with Brine (10 mL), the organic phase is dried over Na_2SO_4, the filtered, and the organic solvents are evaporated under reduced pressure, the crude is a brown sticky oil (crude 83 mg).

Screening of conditions for the reduction of (2) with metal borohydride:

General procedure: (2) (1.0 eq) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH. The solution was cooled to -75°C, the metal borohydride (1.5 eq) was mixed with the additive 20 mol% and the mixture was portion-wise added. The reaction was left under vigorous stirring for 2h at -70°C, then the cooling bath was removed and a solution of H_2SO_4 in MeOH (0.64 M) was dropwise added to the mixture at -20°C, the reaction was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature and then was quenched with water (3 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM. The organic phase was dried over Na_2SO_4, filtered, and then the solvents were evaporated under reduced pressure affording the desired product as a dark yellow oil.

Entry 11: **(2)** (100 mg, 0.34 mmol) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH (2 mL). The solution was cooled to -75°C, and technical grade $NaBH_4$ (1.5 eq, 0.51 mmol, 19.2 mg) was portion-wise added. The reaction was left under vigorous stirring for 2h at -70°C, then the cooling bath was removed and a solution of H_2SO_4 in MeOH (0.5 mL, 0.64 M) was dropwise added to the mixture at -20°C, the reaction was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature and then was quenched with water (3 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM (10 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvents were evaporated under reduced pressure affording the desired product as a dark yellow oil (crude 72.3 mg, dr: 60/40).

Entry 12: **(2)** (100 mg, 0.34 mmol) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH (2 mL). The solution was cooled to -75°C, $NaBH_4$ (99.99% purity)(1.5 eq, 0.51 mmol, 19.2 mg) was portion-wise added. The reaction was left under vigorous stirring for 2h at -70°C, then the cooling bath was removed and a solution of H_2SO_4 in MeOH (0.5 mL, 0.64 M) was dropwise added to the mixture at -20°C, the reaction was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature and then was quenched with water (3 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM (10 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvents were

evaporated under reduced pressure affording the desired product as a dark yellow oil (crude 79 mg, dr: 60/40).

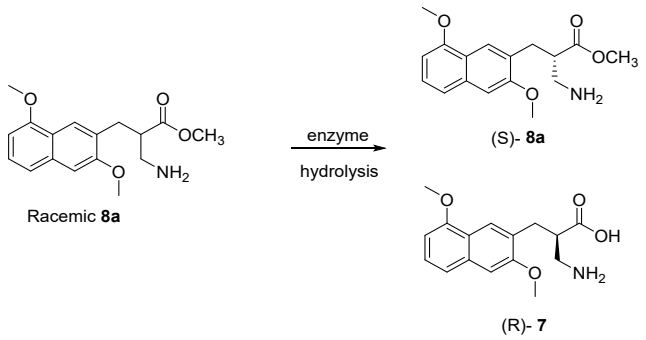
Entry 13: **(2)** (100 mg, 0.34 mmol) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH (2 mL). The solution was cooled to -75°C, $NaBH_4$ (98% purity, Aldrich SKU 452882.)(1.5 eq, 0.51 mmol, 19.2 mg) was portion-wise added. The reaction was left under vigorous stirring for 2h at -70°C, then the cooling bath was removed and a solution of H_2SO_4 in MeOH (0.5 mL, 0.64 M) was dropwise added to the mixture at -20°C, the reaction was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature and then was quenched with water (3 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM (10 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvents were evaporated under reduced pressure affording the desired product as a dark yellow oil (crude 76 mg, dr: 90/10).

Entry 14: **(2)** (100 mg, 0.34 mmol) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH (2 mL). The solution was cooled to -75°C, $NaBH_4$ (99.99% purity)(1.5 eq, 0.51 mmol, 19.2 mg) was mixed with dry $MgCl_2$ (20 mol%, 6.47 mg) and portion-wise added. The reaction was left under vigorous stirring for 2h at -70°C, then the cooling bath was removed and a solution of H_2SO_4 in MeOH (0.5 mL, 0.64 M) was dropwise added to the mixture at -20°C, the reaction was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature and then was quenched with water (3 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM (10 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvents were evaporated under reduced pressure affording the desired product as a dark yellow oil (crude 82 mg, dr: 80/20).

Entry 15: **(2)** (200 mg, 0.68 mmol) was added in a Schlenk-tube in argon atmosphere and dissolved in HPLC grade MeOH (4 mL). The solution was cooled to -75°C, $NaBH_4$ (99.99% purity)(1.5 eq, 1.02 mmol, 38.5 mg) was mixed with dry LiCl (20 mol%, 5.7 mg) was portion-wise added. The reaction was left under vigorous stirring for 2h at -70°C, then the cooling bath was removed and a solution of H_2SO_4 in MeOH (0.5 mL, 0.64 M) was dropwise added to the mixture at -20°C, the reaction was then refluxed for 3.5h. The mixture was allowed to cool down to room temperature and then was quenched with water (3 mL), Na_2CO_3 was added to reach pH>7 and then the biphasic mixture was extracted with DCM (10 mLx3). The organic phase was dried over Na_2SO_4, filtered, and then the solvents were evaporated under reduced pressure affording the desired product as a dark yellow oil (crude 112 mg, dr: 80/20).

Screening of enzymes for the enzymatic kinetic resolution of (8a)

Table S-2. Screening of enzymes for the enzymatic kinetic resolution of **(8a)**.



Entry	Enzyme	Solvent	Temp. (°C)	Time	Conversion[a]	ee% (starting material)[b]	E[c]
1	*Protease from bacillus amiloliquefaciens*	Phosphate buffer pH=7	37	5 days	10%	1.7%	nd
2	*Protease from bacillus species*	Phosphate buffer pH=7	40	21 hours	49%	52.6%	12
3	*Protease type XIII aspergillus saitoi*	Phosphate buffer pH=7	37	48 hours	<5%	0.2%	nd
4	*Lipase B Candida antarctica*	*n*-Hexane/H_2O	45	48 hours	<5%	2.1%	nd
5	*Lipase A Candida antarctica*	CH_3CN/H_2O	45	5 days	<5%	0.8%	nd
6	*Lipase B Candida antarctica*	Acetone/H_2O	37	24 hours	46%	0.1%	nd
7	*Lipase A Candida antarctica*	CH_3CN/H_2O	37	18 hours	58%	0%	nd
8	*Trypsin tpck treated from bovine pancreas*	Phosphate buffer pH=7	r.t.	3 days	14%	0.7%	nd
9	*Protease from bacillus streptomices griseus*	Carbonate buffer pH=9.7	r.t.	52 hours	40%	0.3%	nd
10	*Alcalase from bacillus licheniformis*[d]	Phosphate buffer pH=7	37	24 hours	47%	73.6%	23.6
11	*Protease from bacillus licheniformis*[e]	Phosphate buffer pH=7	37	24 hours	49%	98.2%	>300
12	*Protease from bacillus amiloliquefaciens*	Phosphate buffer pH=9	60	5 days	18%	1.2%	nd
13	*Protease from bovine pancreas Type I*	Phosphate buffer pH=7	37	7h	50%	90.3%	60.7
14	*Lipase from Candida rugosa (powder)*	Phosphate buffer pH=7/Acetone (5:1)	r.t.	72h	<10%	n.d	nd
15	***Protease from bacillus licheniformis*** [e]	**Phosphate buffer pH=7**	**37**	**48h**	**50%**	**>99%**	**>300**

a)Conversion calculated using HPLC on Luna C8 stationary phase. b) Enantiomeric excess calculated on the acetamide of unreacted **8a** using Daicel Chiralcel AD-H column (eluant heptane/IPA 88/12, retention times were 17.5' (major) 18.5 (minor). c) Stereoselectivity

factor evaluated using ln[(0-c)(1-ee)]/ln[(0-c)(1+ee)]. d) ALCALASE enzyme, Bacillus licheniformis, Merck-Aldrich 126741. e) Protease from Bacillus licheniformis > 2.4U/g, Aldrich P 4860. (r.t. = room temperature; n.d. = not determined).

Entry 1: Protease from bacillus amiloliquefaciens[1] (WO 2005/085462)

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer pH=7 (4mL) at 37°C obtaining a white suspension, protease from bacillus amiloliquefaciens (8.4mL) was added slowly. The mixture was left to react at 37°C and sampled several times for 5 days, the maximum conversion was 10% circa. The reaction was filtered and the filtered solution (showing pH=6.5) was basified to pH=9.3, then was extracted with DCM, dried over Na_2SO_4, and the solvent was evaporated affording (**8a**) (31.4mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (8.2mg).

Entry 2: Protease from bacillus species[1] (WO 2005/085462)

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer pH=7 (4mL) at 37°C obtaining a white suspension, protease from bacillus species (0.42mL) was added slowly. The mixture was left to react at 40°C and sampled several times for 21 hours, the maximum conversion was 49% circa. The reaction was filtered and the filtered solution (showing pH=7.15) was basified to pH=9.7, then was extracted with DCM, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (44.1mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (38.2mg).

Entry 3: Protease type XIII aspergillus Saitoi[1] (WO 2005/085462)

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer pH=7 (5mL) at 37°C obtaining a white suspension, protease from bacillus species (100mg) was added slowly. The mixture was left to react at 37°C and sampled several times for 48 hours, the maximum conversion was <5%. The reaction was filtered and the filtered solution (showing pH=7.2) was basified to pH=9.3, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (38.3mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (2.2mg).

Entry 4: Lipase B Candida Antarctica[2].

Racemic **(8a)** (100mg, 0.33mmol) was suspended in hexane (2.06mL), H_2O (0.5 eq, 2.97 µL) was added and then Lipase B Candida antarctica (33mg) was added. The reaction was left to react at 45°C for 12 hours and sampled several times, because of the lack of solubility of the starting material in the solvent, 20% acetone was added to the mixture, the maximum conversion after 48 hours was <5%. The reaction was filtered and the filtered solution was dried, affording **(8a)** in a rather complicated crude mixture (98.2mg).

Entry 5: Lipase A Candida Antarctica[2].

Racemic **(8a)** (100mg, 0.33mmol) was suspended in CH_3CN (2.0mL), H_2O (0.5 eq, 2.97 µL) was added and then Lipase A Candida antarctica (33mg) was added. The reaction was left to react at 45°C for 5 days and sampled several times, the maximum conversion was <5%. %. The reaction was filtered and the filtered solution was dried, affording a complicated crude mixture (103. 2mg).

Entry 6: Lipase B Candida Antarctica[3].

Racemic **(8a)** (67mg, 0.17mmol) was solubilized in acetone (1.4mL), H_2O (10.5mL) was added and then Lipase B Candida antarctica (17.0mg) was added. The mixture was stirred for 24 hours at 37°C and sampled various times, the maximum conversion was 46%. The reaction was filtered and the filtered solution (showing pH=7.4) was basified to pH=10.3, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (42.8mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (39.4mg).

Entry 7: Lipase A Candida Antarctica[3].

Racemic **(8a)** (67mg, 0.17mmol) was solubilized in CH_3CN (1.4mL), H_2O (10.5mL) was added and then Lipase A Candida antarctica (17.0mg) was added. The mixture was stirred for 18 hours at 37°C and sampled various times, the maximum conversion was 58%. The reaction was filtered and the filtered solution (showing pH=7.4) was basified to pH=10.3, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (41.3mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (36.4mg).

Entry 8: Trypsin tpck treated from bovine pancreas[4] (DE 3919029)

Racemic **(8a)** (152.7mg, 0.5mmol) was suspended in phosphate buffer pH=7 (3.2mL) at r.t. obtaining a white suspension, Trypsin tpck treated from bovine pancreas (33mg) was added. The mixture was left to react at r.t. and sampled several times for 3 days, the maximum conversion was 14%. The reaction was filtered and the filtered solution (showing pH=8.2) was basified to pH=10.1, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (42.1mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (31.2mg).

Entry 9: Protease from bacillus streptomices griseus[5].

Racemic **(8a)** (100mg, 0.33mmol) was suspended in carbonate buffer (22mL) pH=7 at r.t. obtaining a white suspension, Protease from bacillus streptomices griseus (15mg) was added. The mixture was left to react at r.t. and sampled several times for 52 hours, the maximum conversion was 40%. The reaction was filtered and the filtered solution (showing pH=8.1) was basified to pH=10.2, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (39.2mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (28.1mg).

Entry 10: Alcalase from bacillus licheniformis[6].

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer (2mL) pH=7 at 37°C obtaining a white suspension, Alcalase from bacillus licheniformis (111 mg of solution that corresponds to 10 mg of pure enzyme) was added. The mixture was left to react at 37°C and sampled several times for 24 hours, the maximum conversion was 47%. The reaction was filtered and the filtered solution (showing pH=7.4) was basified to pH=9.5, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (36.2mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (29.5mg).

Entry 11: Protease from bacillus licheniformis[1] (WO 2005/085462)

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer (3.9mL) pH=7 at 37°C obtaining a white suspension, Protease from bacillus licheniformis (1.4 mL) was added. The mixture was left to react at 37°C and sampled several times for 24 hours, the maximum conversion was 49%. The reaction was filtered and the filtered solution (showing pH=7.4) was basified to pH=10.1, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (37.6mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (28.7mg).

Entry 12: Protease from bacillus amiloliquefaciens[1,7] (WO 2005/085462).

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer pH=9 (4mL) at 60°C obtaining a white suspension, protease from bovine pancreas type I (8.4mL) was added in portions. The mixture was left to react at 60°C and sampled after 6h, the maximum conversion was 50% circa. The reaction was filtered and the filtered solution (showing pH=7.3) was basified to pH=9.4, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (36.2mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (39.8mg).

Entry 13: Protease from bovine pancreas Type I[1] (WO 2005/085462).

Racemic **(8a)** (100mg, 0.33mmol) was suspended in phosphate buffer pH=7 (5mL) at 37°C obtaining a white suspension, protease from bovine pancreas type I (100mg) was added in portions. The mixture was left to react at 37°C and sampled after 6h, the maximum conversion was 50% circa. The reaction was filtered and the filtered solution (showing pH=7.3) was basified to pH=9.4, then was extracted with AcOEt, dried over Na_2SO_4, and the solvent was evaporated affording **(8a)** (36.2mg). From the filtration a white solid was recovered from the filter, NMR analysis showed to be **(7)** (39.8mg).

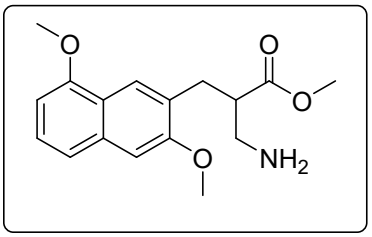
Entry 14: Lipase from Candida Rugosa

Racemic **(8a)** (150mg, 0.5mmol) was suspended in acetone (0.2mL), then phosphate buffer pH=7 (1.1 mL) was added and then Lipase from Candida Rugosa (19mg) was added. The reaction was left to react at room temperature for 72 hours and conversions determined by HPLC was <10%.

Entry 15: reported in optimized synthesis of the intermediates.

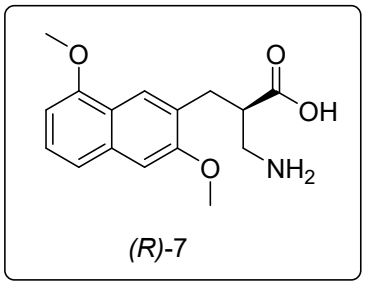
Optimized synthesis of the intermediates:

Methyl 3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoate (8a).



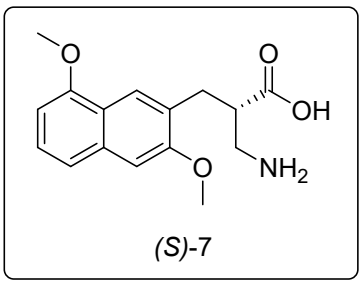
3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid (10.0 g, 34.6 mmol) was suspended in MeOH (158.9 mL), a solution of H_2SO_4 (6.06 mL, 3.3 eq.) in MeOH (37.2 mL) was dropwise added. The obtained solution was refluxed for 3.5h, then MeOH was partially evaporated, water (80 mL) was added, and the mixture was basified to pH>7 using Na_2CO_3. The ester was extracted using AcOEt (3 x 30 mL), the organic phase was washed with brine (2 x 20 mL), dried with Na_2SO_4 and the organic solvent was evaporated affording the title compound as a yellow oil (9.8 g, 32.1 mmol, yield 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.33–7.27 (m, 2H), 7.05 (s, 1H), 6.67 (dd, *J* = 6.1, 2.5 Hz, 1H), 3.96 (s, 3H), 3.92 (s, 3H), 3.66 (s, 3H), 3.10 (dd, *J* = 13.2, 5.9 Hz, 1H), 3.00 (dd, *J* = 13.2, 6.5 Hz, 1H), 2.96–2.83 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 156.8, 155.4, 135.1, 128.0, 126.2, 123.8, 120.4, 119.0 105.0, 102.2, 55.5, 55.4, 51.6, 49.2, 43.5, 31.1. m/z HRMS ESI-MS calcd for $C_{17}H_{21}NO_4$: 303.1471; found [M+H] : 304.1549

***(R)*-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid *(R)*-7.**



Racemic compound **(8a)** (5.0 g, 16.38 mmol) was suspended in phosphate buffer pH=7 (195 mL) at 37°C and stirred for 10 minutes. Protease from Bacillus licheniformis (>2.4 U/g, 140 mL) was portion-wise added, and the mixture was left to react for 48h under vigorous stirring. The obtained suspension was filtered under vacuum affording a filtered dark yellow solution and a solid cake. The filtered solution was basified using Na_2CO_3 to pH=9 and extracted with AcOEt (3 x 25 mL). The organic phase was washed with brine (2 x 20 mL) and dried with Na_2SO_4. The organic solvent was evaporated affording ***(S)*-8** (2.2 g, 7.2 mmol, yield 44%, ee > 99%, Daicel AD-H column, eluent heptane/IPA 88:12). The solid cake was suspended in a mixture of EtOH/H_2O (1:1) (300 mL), LiOH*H_2O was added to pH=11 and the mixture was stirred overnight at 60°C. The suspension was filtered under vacuum, obtaining a brown slime and a filtered solution. The filtered solution was heated to 60°C and a solution of AcOH (1:1) in EtOH/H_2O (1:1) was dropwise added to pH=9-9.5. The mixture was stirred for 30 minutes, then AcOH in EtOH/H_2O was added to pH=8-8.5, and the mixture was cooled to room temperature. The pH was adjusted to pH=8-8.5, then the suspension was filtered under vacuum affording ***(R)*-7** as a white solid [1.97g, 6.80 mmol, total yield 39%, single enantiomer (73% yield), ee= 97.4%, $[\alpha]_D$= -38.4, 1.2 mg in 1 mL MeOH]. ^{1}H NMR (400 MHz, MeOD) δ 8.03 (s, 1H), 7.33–7.25 (m, 2H), 7.18 (s, 1H), 6.73 (dd, *J* = 6.1, 2.5 Hz, 1H), 3.97 (s, 6H), 3.10 (dd, *J* = 13.2, 5.9 Hz, 1H), 3.02-2.94 (m, 1H), 2.93–2.81 (m, 3H). ^{13}C NMR (101 MHz, MeOD) δ 169.2, 156.6, 155.2, 135.4, 135.2, 127.8, 125.9, 123.5, 120.3, 118.6, 104.8, 101.8, 54.4, 44.9, 40.6, 31.4. m/z HRMS ESI-MS calcd for $C_{16}H_{19}NO_4$: 289.1314; found [M+HCOO]: 334.1296.

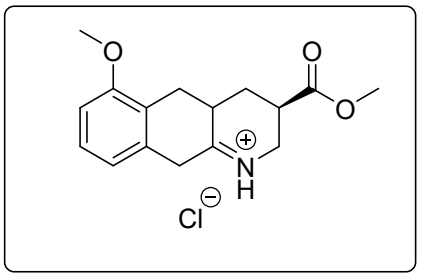
***(S)*-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid [(*S*)-7].**



Methyl *(S)*-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoate **[(*S*)-8a]** (1.53 g, 5.0 mmol) was dissolved in a mixture of EtOH/H_2O (1:1) (28.0 mL) and LiOH*H_2O was added (4.3 eq, 902.15 mg), the reaction mixture was refluxed for 3h. The mixture was cooled to 60°C, and AcOH (1:1) in EtOH/H_2O (1:1) was dropwise added to pH=9-9.5. The mixture was stirred for 30 minutes, then AcOH in EtOH/H_2O was added to pH=8-8.5, and the mixture was cooled to room temperature. The pH was adjusted to pH=8-8.5, then the suspension was filtered under vacuum affording title

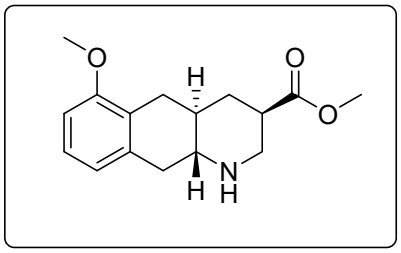
compound as a white solid (1.17 g, 4.0 mmol, yield 80%). ^{1}H NMR (400 MHz, MeOD) δ 8.03 (s, 1H), 7.33–7.25 (m, 2H), 7.18 (s, 1H), 6.73 (dd, *J* = 6.1, 2.5 Hz, 1H), 3.97 (s, 6H), 3.10 (dd, *J* = 13.2, 5.9 Hz, 1H), 3.02-2.94 (m, 1H), 2.93–2.81 (m, 3H). ^{13}C NMR (101 MHz, MeOD) δ 169.2, 156.6, 155.2, 135.4, 135.2, 127.8, 125.9, 123.5, 120.3, 118.6, 104.8, 101.8, 54.4, 44.9, 40.6, 31.4. m/z HRMS ESI-MS calcd for $C_{16}H_{19}NO_4$: 289.1314; found [M+HCOO] : 334.1293.

***(3R, 4aS,R)*-3-carboxy-6-methoxy-2,3,4,4a,5,10-hexahydrobenzo[g]quinolin-1-ium chloride *(3R, 4aS,R)*-(2).**



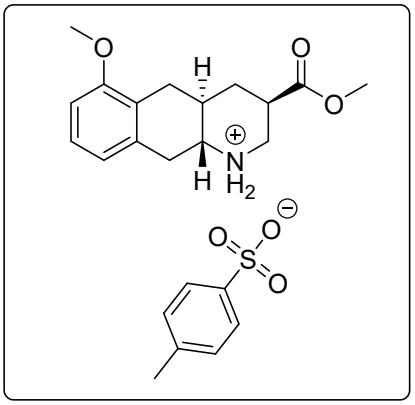
(R)-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid **[*(R)*-7]** (1.83 g, 6.34 mmol) was suspended in dry THF (18,33 mL, 10 Vol.) in argon atmosphere using mechanical stirring; dry t-BuOH (2.4 eq, 13.2 mmol, 1.45 mL) was added and the mixture was cooled to -70°C. NH_3 (9.17 mL, 5 Vol.) was condensed in a trap at -50°C then added to the reaction mixture. Lithium wires (5.2 eq, 32.97 mmol, 227.48 mg) in oil were dried and portion-wise added, after the addition, the mixture turned from white to dark green and after 2-3 minutes it turned dark blue. The reaction mixture is left to react at -70°C for 2.5h (if during this time there is a loss of color, extra lithium has to be added). NH_3 was evaporated overnight at room temperature, then the reaction was quenched with water (13.0 mL). The organic solvents were evaporated at 50°C and 100mbar, and the aqueous phase was dropwise added to a solution of concentrated HCl (4.6 mL) at 0°C. The obtained suspension was left to stir for 4.0h, then it was filtered under vacuum, and washed with HCl 2N (2 mL) and water (2 mL x 2) affording title compound as a beige solid after drying for 48h at 50°C under vacuum (780 mg, 2.64 mmol, yield 42%). ^{1}H NMR (400 MHz, MeOD) δ 7.23 (t, *J* = 8.0 Hz, 1H), 6.87 (dd, *J* = 8.2, 4.0 Hz, 1H), 6.83–6.77 (m, 1H), 4.02–3.93 (m, 2H), 3.94–3.75 (m, 4H), 3.50 (t, *J* = 16.5 Hz, 1H), 3.20–3.09 (m, 1H), 2.66 (d, *J* = 16.4 Hz, 1H), 2.59–2.47 (m, 1H), 2.38 (dd, *J* = 14.0, 7.7 Hz, 1H), 2.07 (dd, *J* = 14.0, 4.4 Hz, 1H), 1.79 (dd, *J* = 13.6, 11.9 Hz, 1H). ^{13}C NMR (101 MHz, MeOD) δ 193.8, 174.6, 158.0, 132.3, 129.4, 123.8, 121.1, 110.0, 56.1, 46.8, 46.8, 37.4, 35.9, 29.9, 28.2, 26.7. m/z HRMS ESI-MS calcd for $C_{16}H_{20}ClNO_3$: 309.1132; found [M+H]: 310.1210

Methyl *(3R,4aR,10aR)*-6-methoxy-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinoline-3-carboxylate [(*3R,4aR,10aR*-3a)].



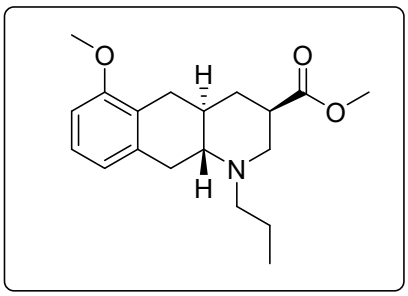
Iminium chloride **(*3R, 4aS,R)*-(2)** (700 mg, 2.36 mmol) was solubilized in dry MeOH (14 mL) in argon atmosphere and cooled to -70°C, and $LiBH_4$ (77.8 mg, 3.57 mmol) was portion-wise added. After 2.0h the mixture was heated to -20°C and a solution of H_2SO_4 in MeOH (2.64 M, 2.4 mL) was dropwise added. The reaction mixture was refluxed for 3.5h. Once cooled to room temperature, MeOH was partially evaporated and water (14 mL) was added. Na_2CO_3 was added to pH>7, and the biphasic mixture was extracted with AcOEt (15 mL x 3). The organic phase was dried with Na_2SO_4 and the solvents were evaporated to afford the title compound as dark yellow oil (403 mg, 1.47 mmol, yield 62%, dr = 5.7). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (t, *J* = 7.8 Hz, 1H), 6.69 (dd, *J* = 17.2, 7.9 Hz, 2H), 3.81 (s, 3H), 3.69 (s, 3H), 3.40–3.34 (m, 1H), 3.01–2.78 (m, 3H), 2.67–2.54 (m, 2H), 2.29–2.23 (m, 1H), 2.22–2.12 (m, 1H), 1.45–1.36 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 155.4, 143.0, 135.1, 125.8, 122.3, 121.7, 119.2, 118.1, 107.0, 100.4, 55.4, 52.1, 43.8, 38.6, 30.5. m/z HRMS ESI-MS calcd for $C_{16}H_{21}NO_3$: 275.1521; found [M+H]: 276.1599

***(3R,4aR,10aR)*-6-methoxy-3-(methoxycarbonyl)-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinolin-1-ium 4-methylbenzenesulfonate [*(3R,4aR,10aR)*-4)].**



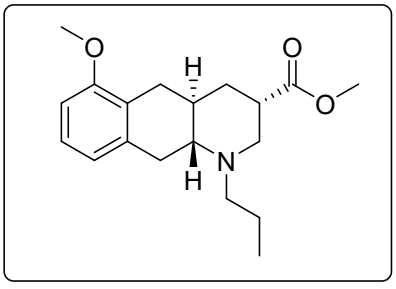
***(3R,4aR,10aR)*-(3a)** (550 mg, 2.0 mmol) was solubilized in AcOEt (3.0 mL) at 70°C, and a solution of p-toluene sulphonic acid (378 mg, 2.19 mmol) in AcOEt (3.30 mL) was dropwise added. The obtained suspension was cooled to 0°C for 3.0h and filtered under vacuum. The afforded purple solid was washed using cold AcOEt (3 mL) affording a light pink powder that was dried under vacuum (695 mg, 1.55 mmol, yield 78%, dr >10). ^{1}H NMR (400 MHz, MeOD) δ 7.70 – 7.65 (m, 2H), 7.22 – 7.17 (m, 2H), 7.12 (t, J = 8.0 Hz, 1H), 6.77 (d, J = 8.2 Hz, 1H), 6.69 (d, J = 7.7 Hz, 1H), 3.80 (s, 3H), 3.74 (s, 3H), 3.65 (ddd, J = 12.7, 4.0, 1.9 Hz, 1H), 3.22 – 3.06 (m, 4H), 2.97 (tt, J = 12.5, 3.8 Hz, 1H), 2.84 (dd, J = 15.3, 11.1 Hz, 1H), 2.34 (s, 3H), 2.30 – 2.19 (m, 1H), 1.90 (ddd, J = 11.5, 5.5, 3.8 Hz, 1H), 1.51 (q, J = 12.7 Hz, 1H).^{13}C NMR (101 MHz, MeOD) δ 171.5, 156.9, 140.4, 132.7, 128.5, 126.9, 125.5, 122.6, 120.4, 107.6, 55.9, 54.4, 51.4, 48.2, 48.0, 47.8, 47.6, 47.4, 47.2, 47.0, 44.4, 38.6, 34.1, 32.5, 32.1, 29.0, 19.9. (Banziger, M.; Cercus, J.; Stampfer, W.; Sunay U.; *Organic Process Research & Development* **2000**, *4*, 460-466)

Methyl *(3R,4aR,10aR)*-6-methoxy-1-propyl-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinoline-3-carboxylate [*(3R,4aR,10aR)*-10].



***(3R,4aR,10aR)*-(9)** (675 mg, 1.5 mmol) was suspended in DMF (6.5 mL), K_2CO_3 (384 mg, 3.0 mmol) was added in argon atmosphere. 1-Iodopropane (364 mL, 637.5 mg, 3.75 mmol) was dropwise added at 50°C, and the reaction mixture was left to stir for 4.0h. Toluene (14.5 mL) was added, then water (12.9 mL) was added to the mixture at 0°C. The biphasic mixture was extracted with toluene (15 mL x 3), dried with Na_2SO_4, and the organic solvents were evaporated affording title compound as a brown sticky oil (457 mg, 1.44 mmol, yield 96%, dr >10). ^{1}H NMR (400 MHz, $CHCl_3$) δ 7.11 (t, *J* = 7.9 Hz, 1H), 6.73 (d, *J* = 7.7 Hz, 1H), 6.66 (d, *J* = 8.1 Hz, 1H), 3.81 (s, 3H), 3.70 (s, 3H), 3.27 (bd, *J* = 11.5 Hz, 1H), 3.17 (dd, *J* = 16.1, 5.0 Hz, 1H), 2.98 (dd, *J* = 17.6, 5.1 Hz, 1H), 2.87–2.56 (m, 4H), 2.44 (t, *J* = 11.7 Hz, 1H), 2.30–2.14 (m, 3H), 1.61–1.51 (m, 2H), 1.37–1.22 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 156.8, 136.3, 126.5, 124.2, 121.4, 107.1, 60.5, 55.3, 55.2, 54.2, 51.8, 41.6, 36.8, 34.7, 30.6, 30.4, 17.6, 12.1. m/z HRMS ESI-MS calcd for $C_{19}H_{27}NO_3$: 317.1991; found [M+H]: 318.2069

Methyl *(3S,4aR,10aR)*-6-methoxy-1-propyl-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinoline-3-carboxylate [*(3S,4aR,10aR)*-11)].



In a Schlenk at -50°C, LDA (0.85 mL, 1.7 mmol, 2M in THF) was added in argon atmosphere, a solution of ***(3R,4aR,10aR)*-10** (250 mg, 0.79 mmol) in THF (1.95 mL, 0.4M) was dropwise added, and the mixture was left to react for 40 minutes. Freshly distilled TMSCl (0.2 mL, 170 mg, 1.56 mmol) was dropwise added and the mixture was left to react for 1.0 h. The mixture was then slowly dropwise added to a solution of HCl 15% (2.44 mL) at -30°C and left to stir for 15 minutes. A saturated solution of Na_2CO_3 was added at -10°C and then the mixture was left to stir at room temperature for 1.0h. The biphasic mixture was extracted with toluene (10 mL x 3), the organic phase was dried with Na_2SO_4, and the solvents were evaporated affording crude **[*(3S,4aR,10aR)*-11]** as a brown sticky oil (210 mg). The solid was purified by flash chromatography (Hex/AcOEt: 8/2) affording a light yellow solid (105 mg, 0.32 mmol, yield 41%). A simple crystallization from MeOH afforded the title compound as single stereoisomer. $[\alpha]_D$= -137 (c = 0.5, $CHCl_3$). The comparison of the sign of the optical rotatory power reported

in the literature (S. P. Chavan, A. L. Kadam, R. G. Gonnade, Org. Lett. 2019, 21, 9089-9094) established the absolute configuration of the final product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (t, *J* = 7.9 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 1H), 6.64 (d, *J* = 8.1 Hz, 1H), 3.81 (s, 3H), 3.69 (s, 3H), 3.45 (dt, *J* = 11.4, 2.4 Hz, 1H), 3.11 (dd, *J* = 16.1, 5.0 Hz, 1H), 2.96 (dd, *J* = 17.3, 5.0 Hz, 1H), 2.78–2.57 (m, 3H), 2.41–2.29 (m, 3H), 2.20–2.06 (m, 2H), 1.92–1.80 (m, 1H), 1.48 (q, *J* = 7.4 Hz, 2H), 1.32–1.27 (m, 1H), 0.88 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 156.5, 136.6, 125.9, 125.4, 121.1, 106.6, 61.3, 55.0, 54.3, 53.4, 51.4, 39.8, 34.6, 34.0, 32.2, 30.5, 18.0, 11.7. m/z HRMS ESI-MS calcd for $C_{19}H_{27}NO_3$: 317.1991; found [M+H]: 318.2068.

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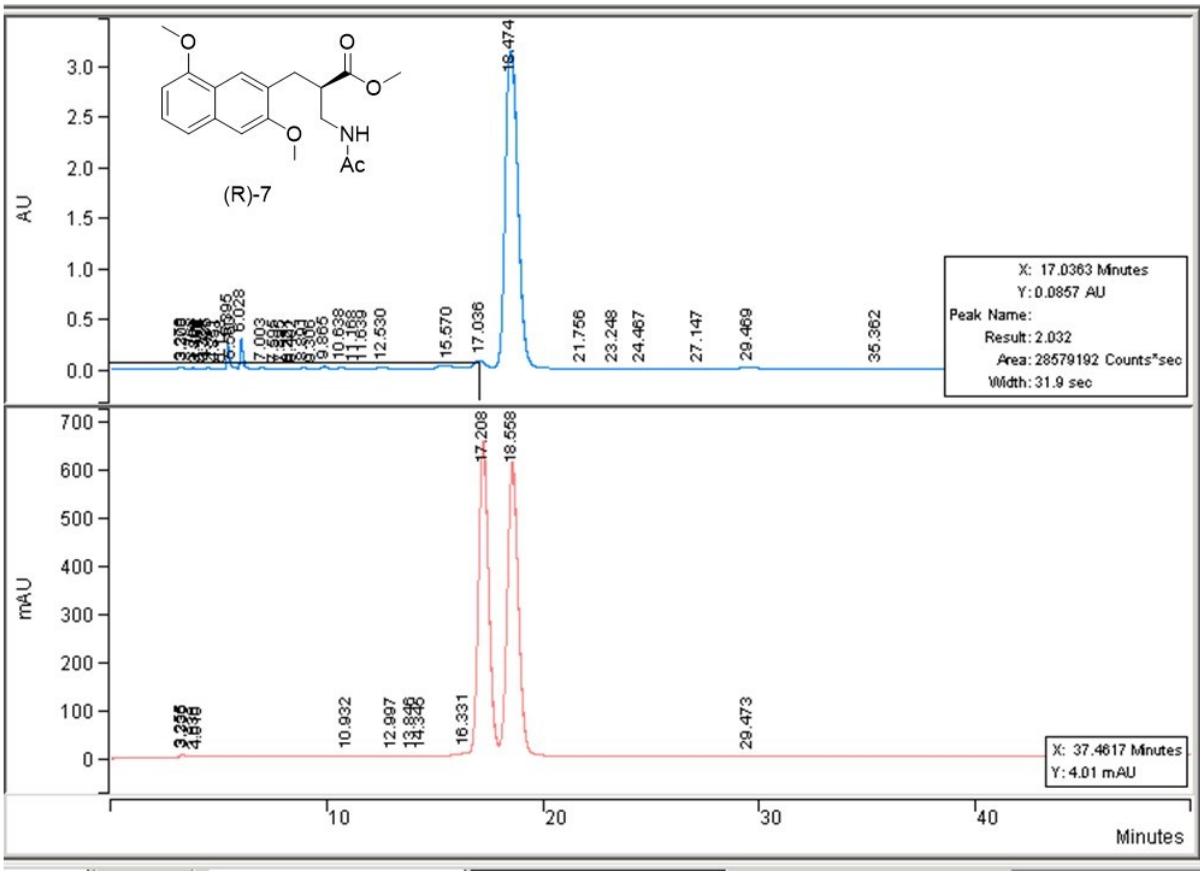
CSP-HPLC traces:



Calculation Type: Percent

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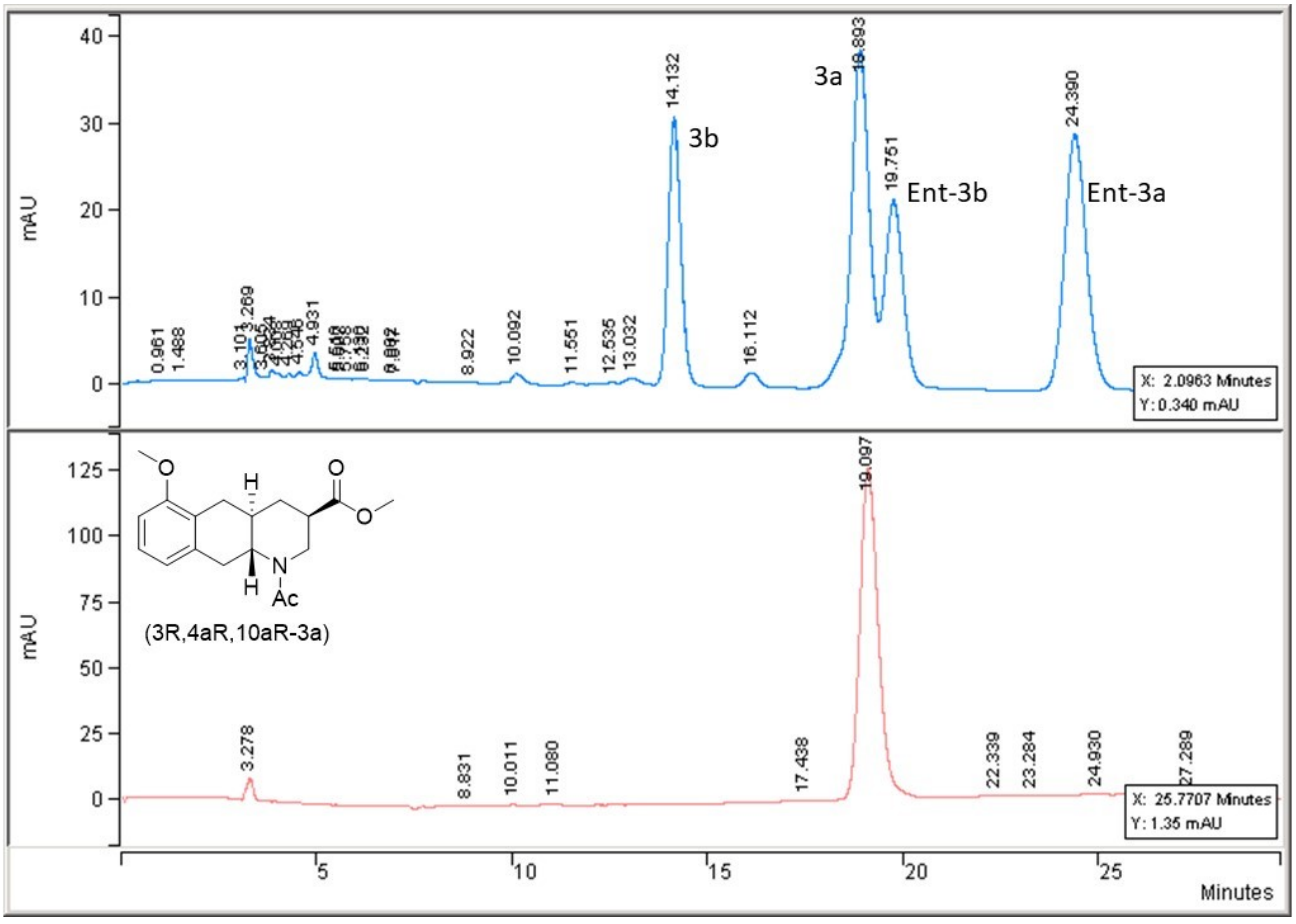
2		0.0740	3.308	0.000	1041277	VV	12.8	
3		0.0452	3.768	0.000	636030	VV	10.5	
4		0.0212	3.898	0.000	297471	VV	0.0	
5		0.0266	4.106	0.000	374441	VV	8.4	
6		0.0067	4.335	0.000	93770	VV	0.0	
7		0.0692	4.485	0.000	973759	VV	8.0	
8		0.0088	4.851	0.000	123556	VV	0.0	
9		0.0168	5.128	0.000	236255	VV	17.2	
10		1.2639	5.395	0.000	17773310	VV	6.4	
11		0.1685	5.560	0.000	2369319	VV	9.9	
12		1.8992	6.028	0.000	26706590	VP	7.1	
13		0.1188	7.003	0.000	1671200	TF	0.0	
14		0.0255	7.595	0.000	358938	TF	0.0	
15		0.0069	7.895	0.000	97115	TF	0.0	
16		0.0130	8.221	0.000	182432	TF	0.0	
17		0.0079	8.402	0.000	111044	TF	0.0	
18		0.0642	8.891	0.000	902570	TF	0.0	
19		0.0217	9.306	0.000	304857	TF	0.0	
20		0.2346	9.865	0.000	3299401	TF	0.0	
21		0.1091	10.638	0.000	1534566	TF	0.0	
22		0.0060	11.168	0.000	84808	TF	0.0	
23		0.0101	11.639	0.000	142183	TF	0.0	
24		0.2369	12.530	0.000	3330881	TF	0.0	
25		1.1167	15.570	0.000	15703240	BV	53.3	
26		2.0324	17.036	0.000	28579192	VV	31.9	
27		91.2999	18.474	0.000	1283852544	VB	38.0	
28		0.0426	21.756	0.000	599205	BB	29.3	
29		0.0137	23.248	0.000	192253	BV	25.9	
30		0.1499	24.467	0.000	2107657	VP	51.8	
31		0.1604	27.147	0.000	2255091	PV	42.4	
32		0.5965	29.469	0.000	8388104	VB	50.7	
33		0.0217	35.362	0.000	305512	BB	42.6	
	Totals:	99.9999		0.000	1406193116			

(R)-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid ***(R)*-7**

Figure S-1. Values determined by HPLC on Daicel Chiralcel AD-H on the corresponding methyl ester and acetamides. Comparison of ***(R)*-7** with the racemic mixture.

Methyl *(3R,4aR,10aR)*-6-methoxy-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinoline-3-carboxylate



Instrument : Sample Rate : 5.00 Hz
Channel : 2 = 220 nm Run Time : 29.713 min

** LC Workstation Multi Instrument Version 6.20 ** 00469-2188-EA8-20F5 **

Run Mode : Analysis
Peak Measurement: Peak Area
Calculation Type: Percent

Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		2.2665	3.278	0.000	1016438	PB	9.7	
2		0.1330	8.831	0.000	59641	BB	13.7	
3		0.1674	10.011	0.000	75076	BV	15.3	
4		0.3385	11.080	0.000	151811	VB	48.2	
5		0.2013	17.438	0.000	90268	PV	0.0	
6		95.3776	19.097	0.000	42773080	VB	30.1	
7		0.7021	22.339	0.000	314858	TF	0.0	
8		0.1327	23.284	0.000	59489	TF	0.0	
9		0.4982	24.930	0.000	223413	TF	0.0	
10		0.1828	27.289	0.000	81971	BB	12.3	
Totals:		100.0001		0.000	44846045			

[*(3R,4aR,10aR-3a)*].

Figure S-2. Values determined by HPLC on Daicel Chiralcel AD-H on [(*3R,4aR,10aR)*-3a] acetamide, acetylation was performed on the tosyl salt [(3R,4aR,10aR)-4)] of the product of entry 16 of Table S-1. Comparison of **[*(3R,4aR,10aR)*-3a]** with the racemic mixture.

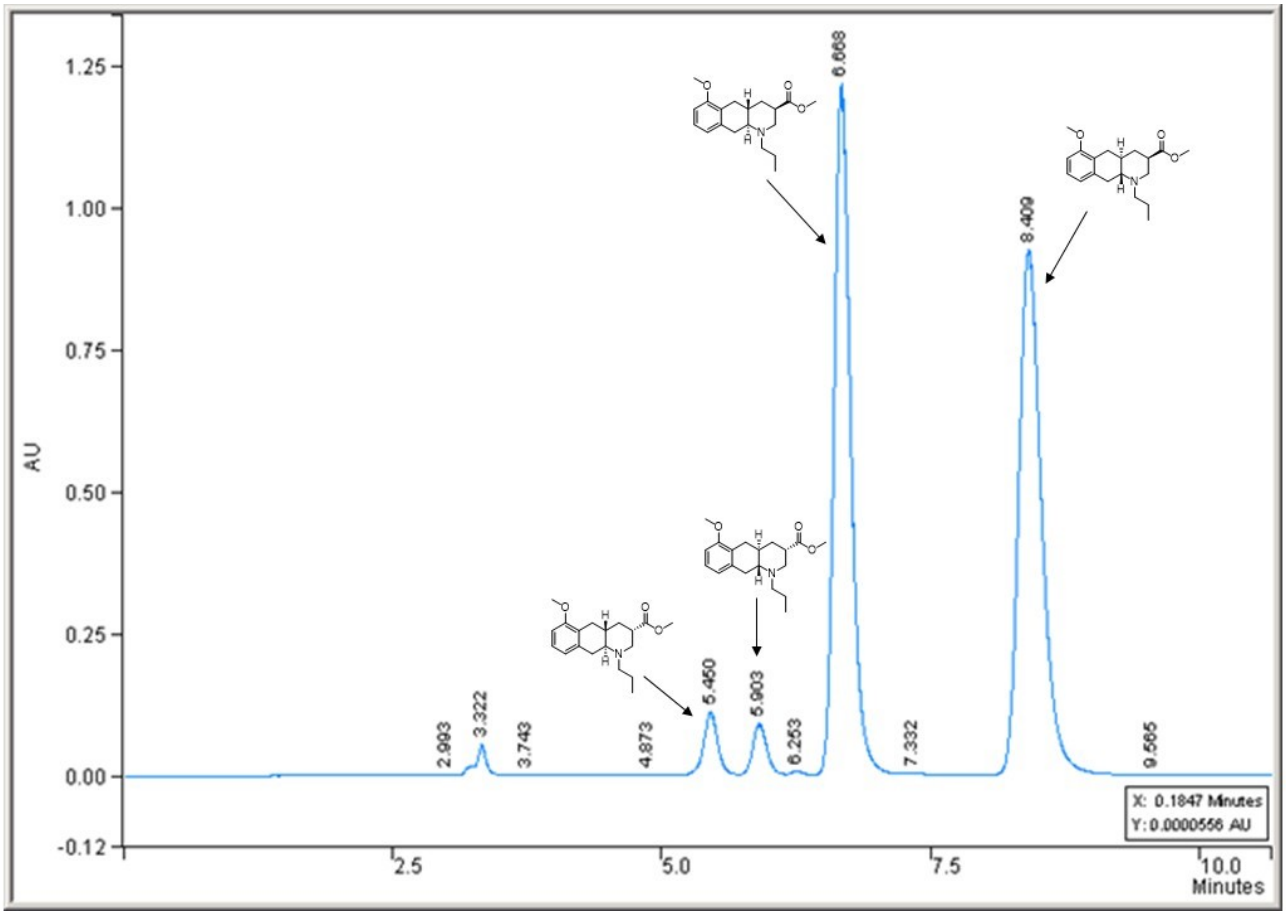
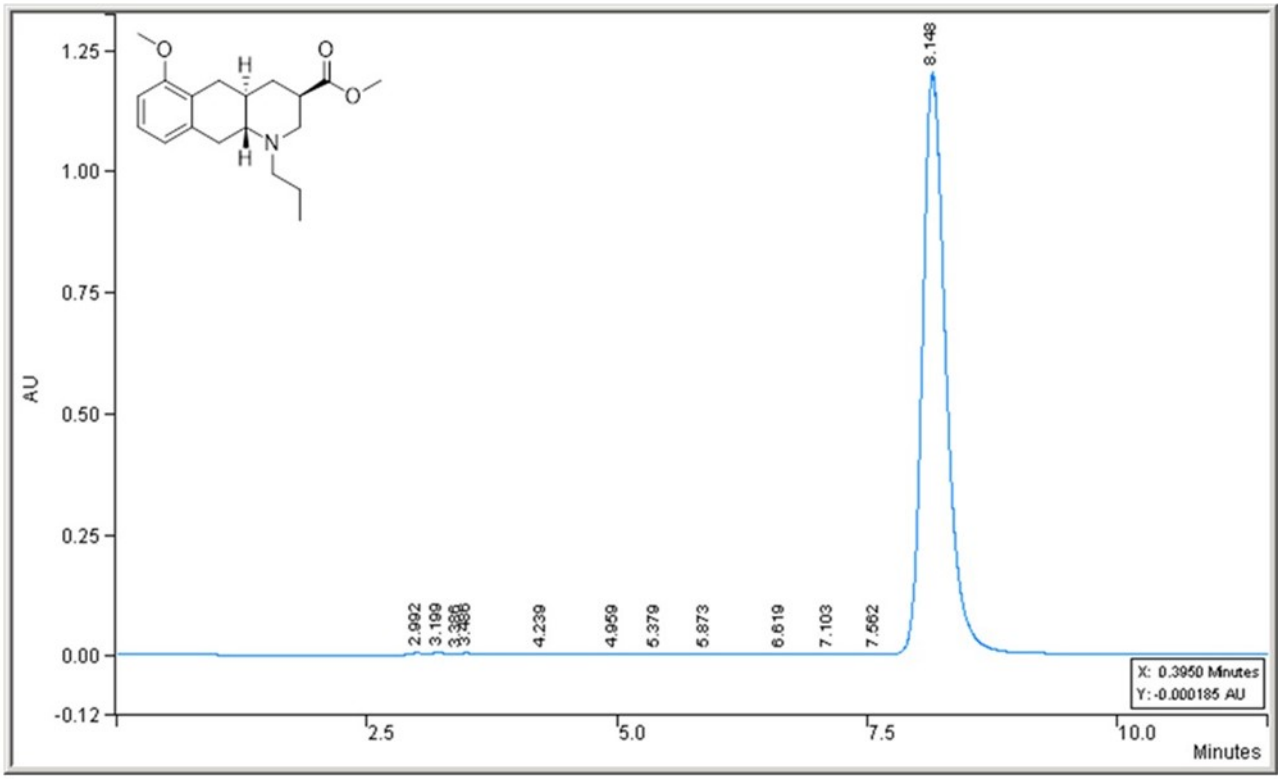


Figure S-3. Racemic mixture of compound **10** and **11.**

Methyl *(3R,4aR,10aR)*-6-methoxy-1-propyl-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinoline-3-carboxylate



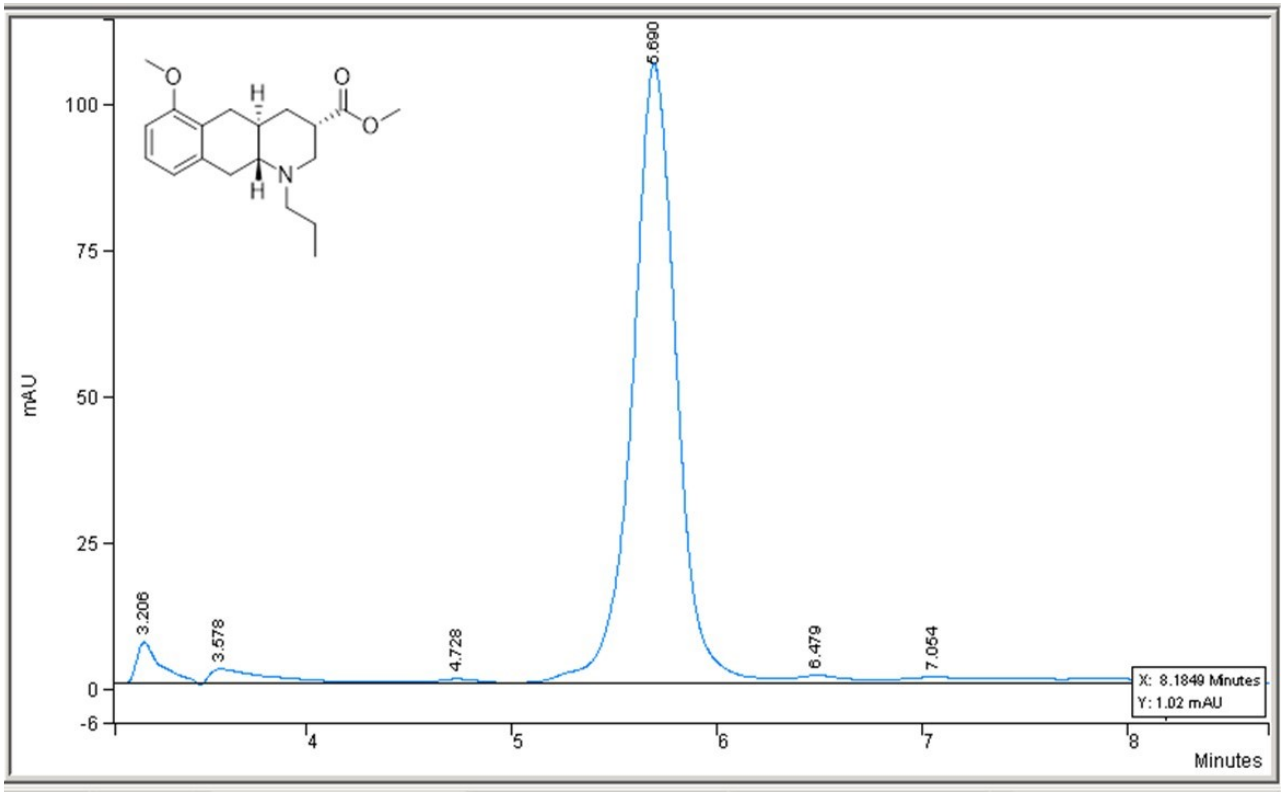
Run Mode : Analysis
Peak Measurement: Peak Area
Calculation Type: Percent

Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.1768	2.992	0.000	352661	PV	6.9	
2		0.2724	3.199	0.000	543344	VV	0.0	
3		0.0338	3.386	0.000	67514	VV	0.0	
4		0.3240	3.486	0.000	646262	VV	22.5	
5		0.0638	4.239	0.000	127217	VV	0.0	
6		0.0338	4.959	0.000	67507	VV	0.0	
7		0.1239	5.379	0.000	247124	VV	25.0	
8		0.0517	5.873	0.000	103189	VV	0.0	
9		0.1779	6.619	0.000	354924	VV	39.6	
10		0.0358	7.103	0.000	71406	VV	0.0	
11		0.0346	7.562	0.000	69115	VV	0.0	
12		98.6715	8.148	0.000	196843424	VB	14.5	
	Totals:	100.0000		0.000	199493687			

[*(3R,4aR,10aR)*-10].

Figure S-4. Values determined by HPLC on Daicel Chiralcel AD-H on **[*(3R,4aR,10aR)*-10].**

Methyl (3S,4aR,10aR)-6-methoxy-1-propyl-1,2,3,4,4a,5,10,10a-octahydrobenzo[g]quinoline-3-carboxylate **[*(3S,4aR,10aR)*-11)].**



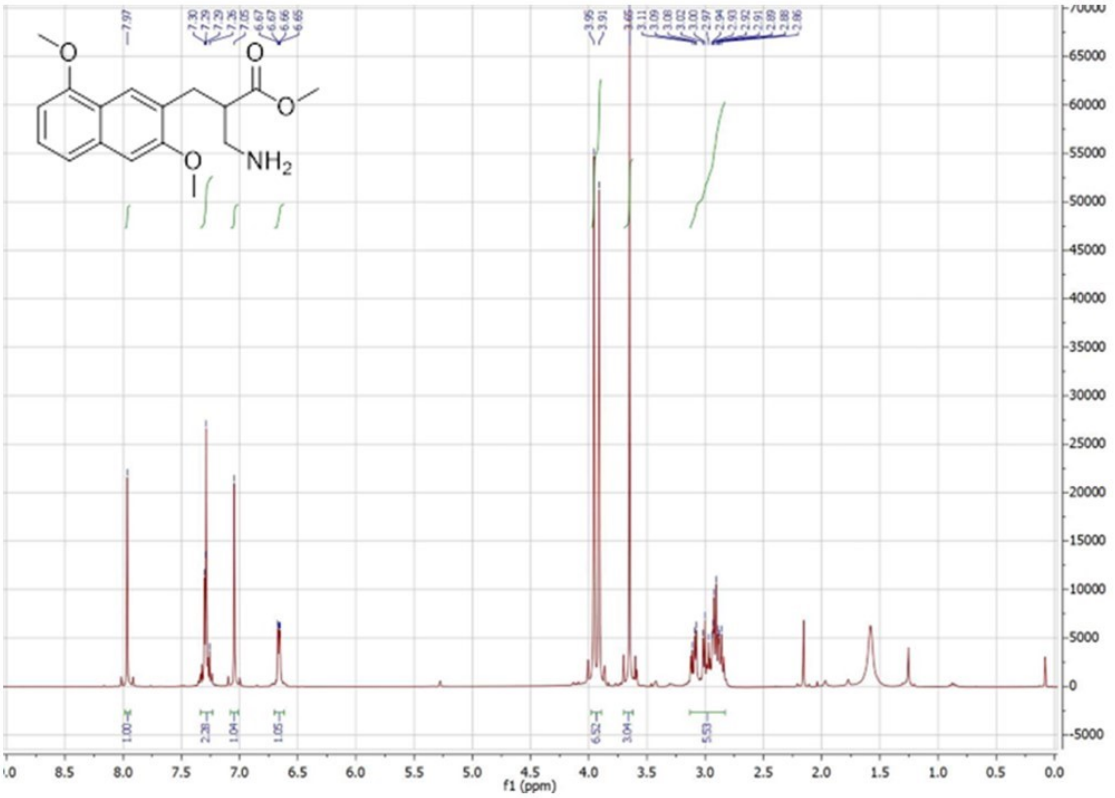
Run Mode : Analysis
Peak Measurement: Peak Area
Calculation Type: Percent

Peak No.	Peak Name	Result (%)	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		3.5268	3.206	0.000	629902	VP	6.4	
2		2.7402	3.578	0.000	489408	PB	19.3	
3		0.4144	4.728	0.000	74013	BP	10.6	
4		92.2550	5.690	0.000	16477101	PB	12.8	
5		0.3579	6.479	0.000	63919	TS	0.0	
6		0.7058	7.054	0.000	126052	TF	0.0	
	Totals:	100.0001		0.000	17860395			

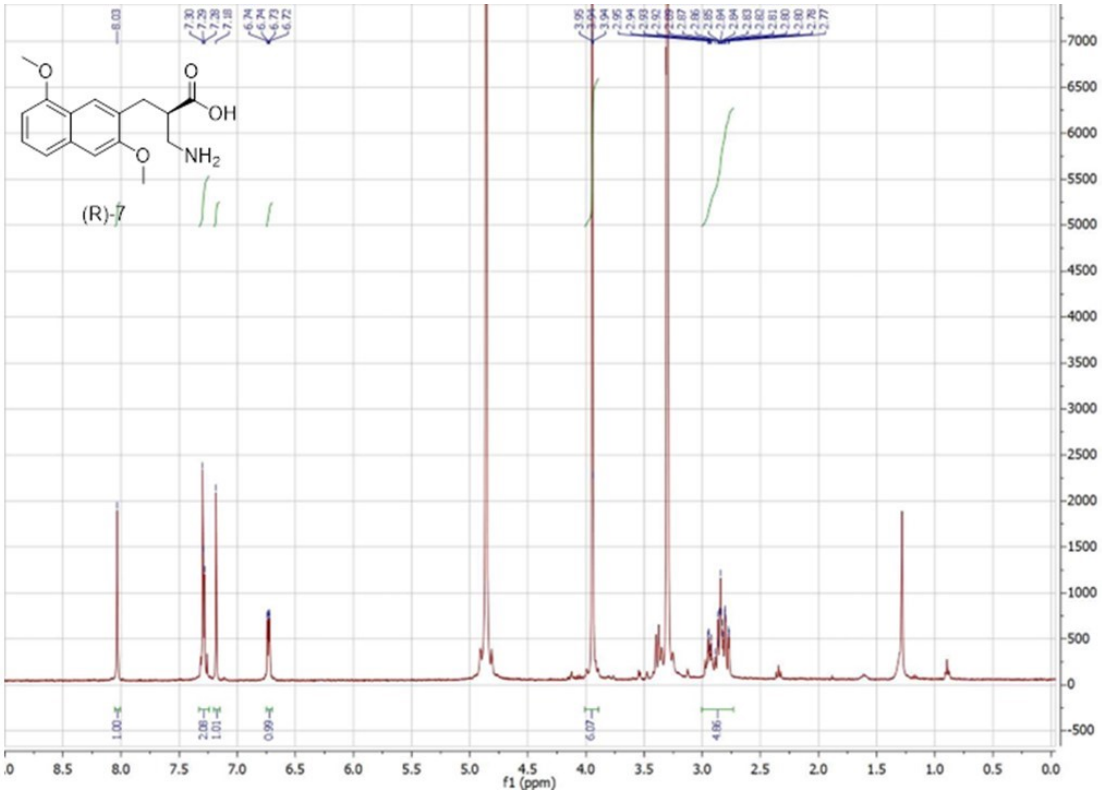
Figure S-4. Values determined by HPLC on Daicel Ciralcel AD-H on [***(3S,4aR,10aR)*-11**)] after chromatographic purification (Hex/AcOEt:7/3) and crystallization in MeOH.

Copies of ^{1}H NMR and ^{13}C NMR spectra:

Methyl 3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoate **(8a)**.

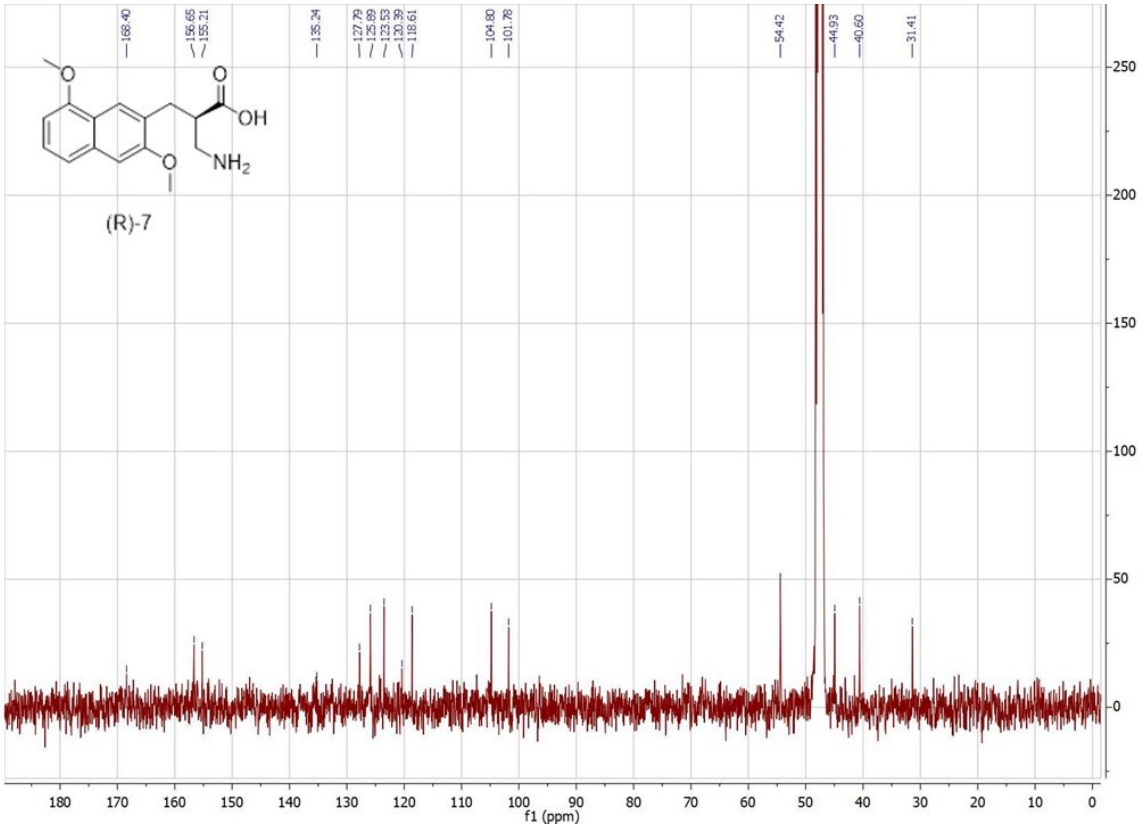


^{1}H NMR of **8a** (400 MHz, $CDCl_3$)

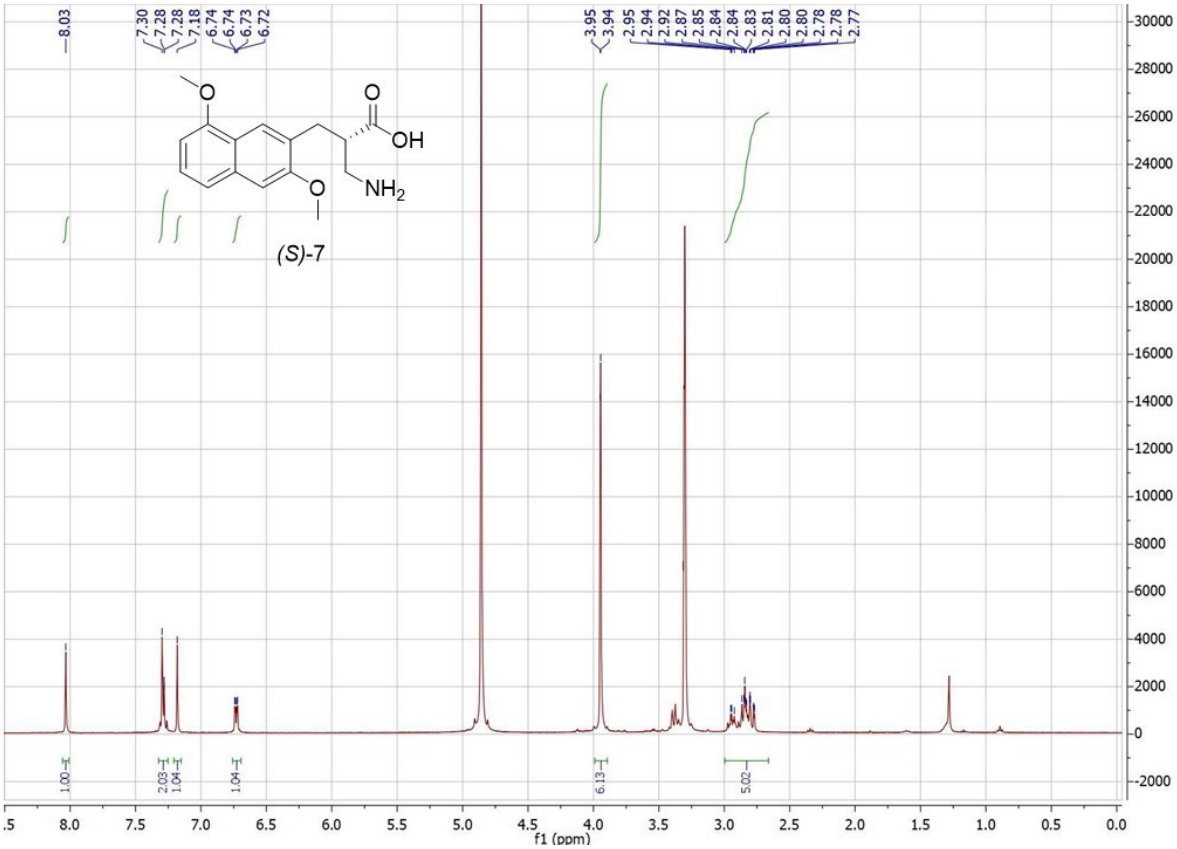


(R)-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid *(R)*-**7.**

^{1}H NMR of ***(R)*-7** (400 MHz, MeOD)

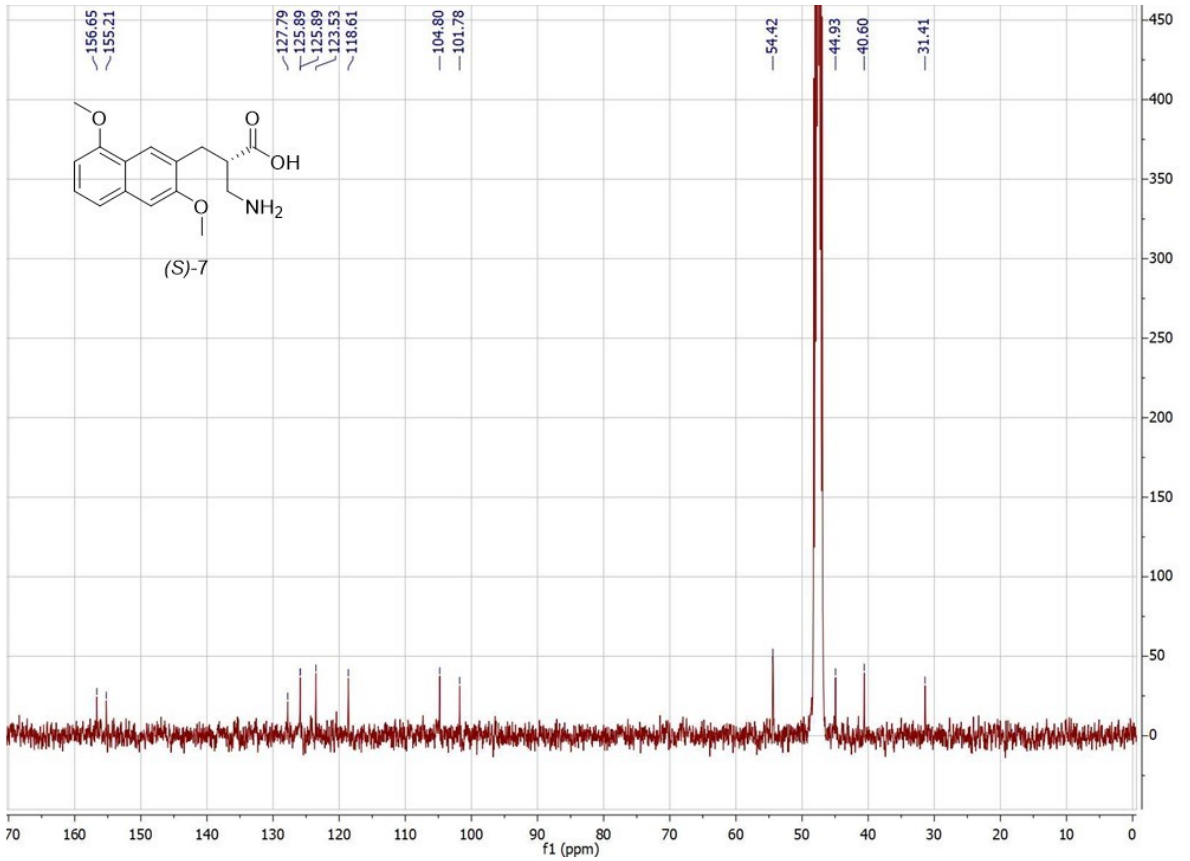


^{13}C NMR of ***(R)*-7** (101 MHz, MeOD)



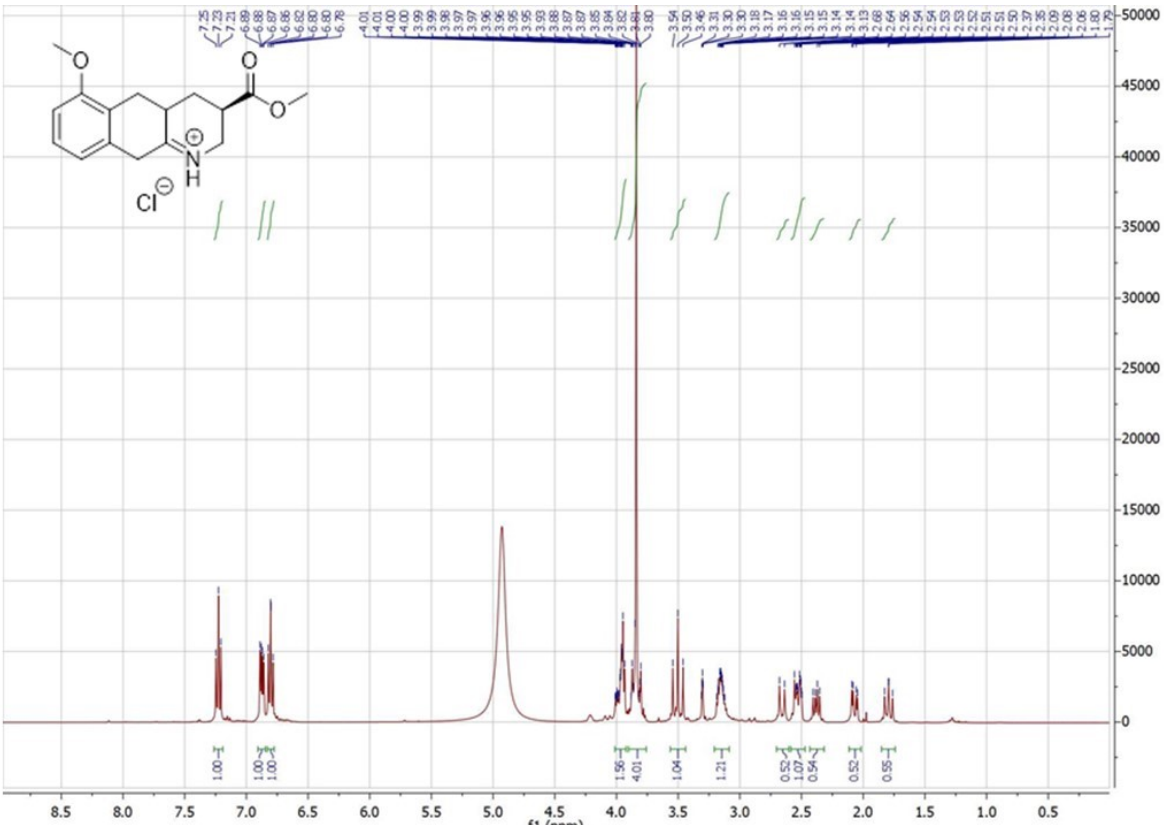
(S)-3-amino-2-((3,8-dimethoxynaphthalen-2-yl)methyl)propanoic acid *(S)*-**7**

^{1}H NMR of ***(S)*-7** (400 MHz, MeOD)

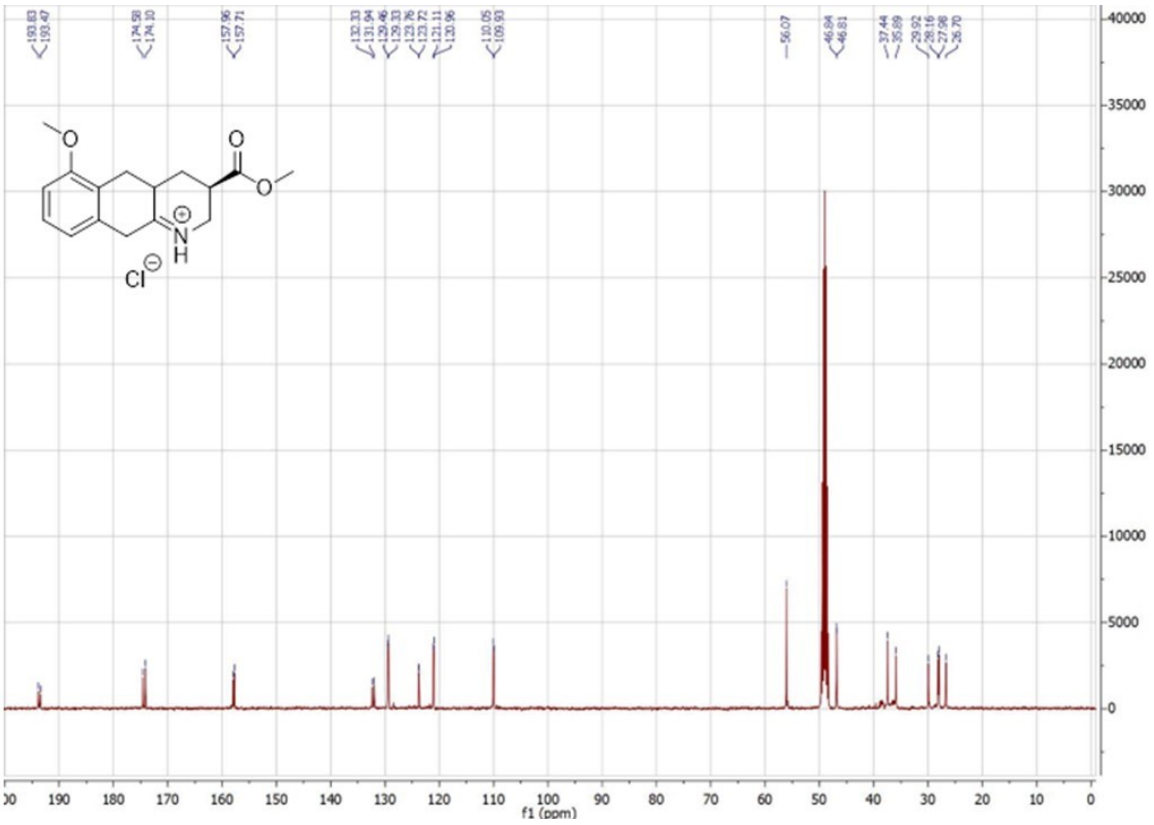


^{13}C NMR of ***(S)*-7** (101 MHz, MeOD)

(3R, 4aS,R)-3-carboxy-6-methoxy-2,3,4,4ª,5,10-hexahydrobenzo[g]quinolin-1-ium chloride ***(3R, 4aS,R)*-(2)**.

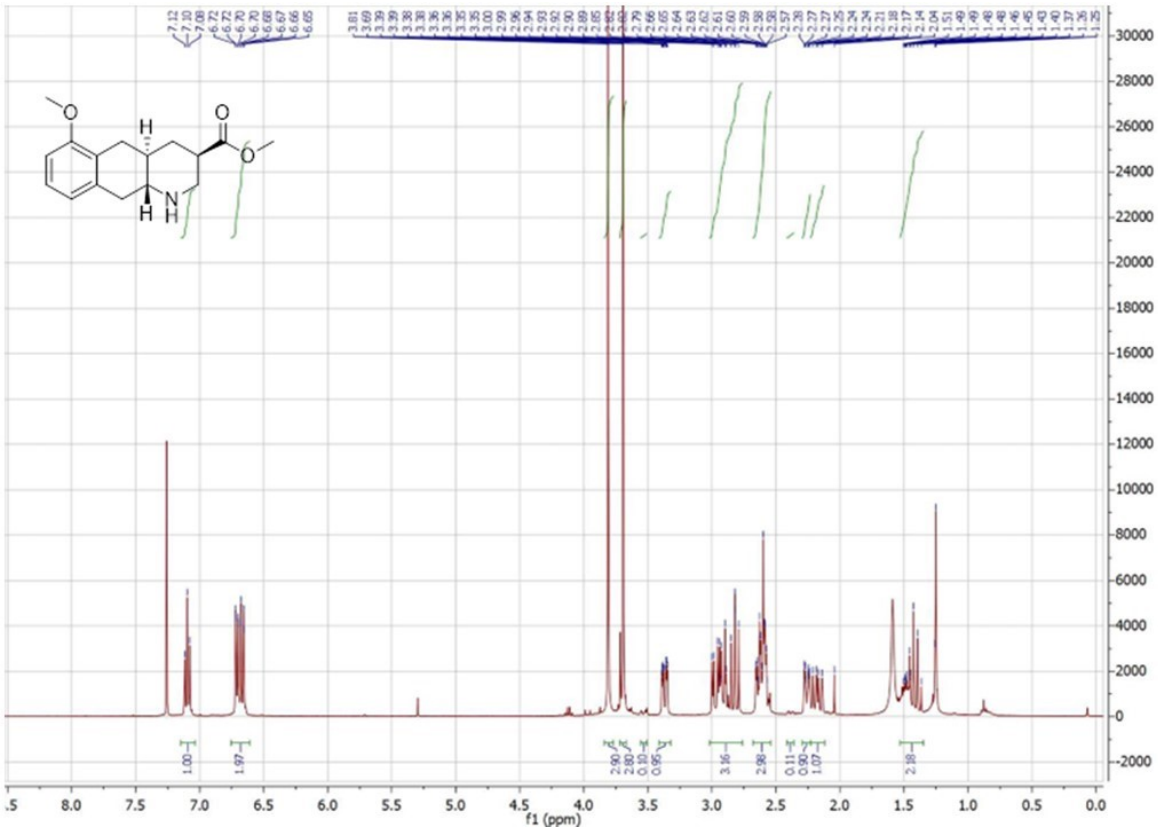


^{1}H NMR of ***(3R, 4aS,R)*-(2)** (400 MHz, MeOD)



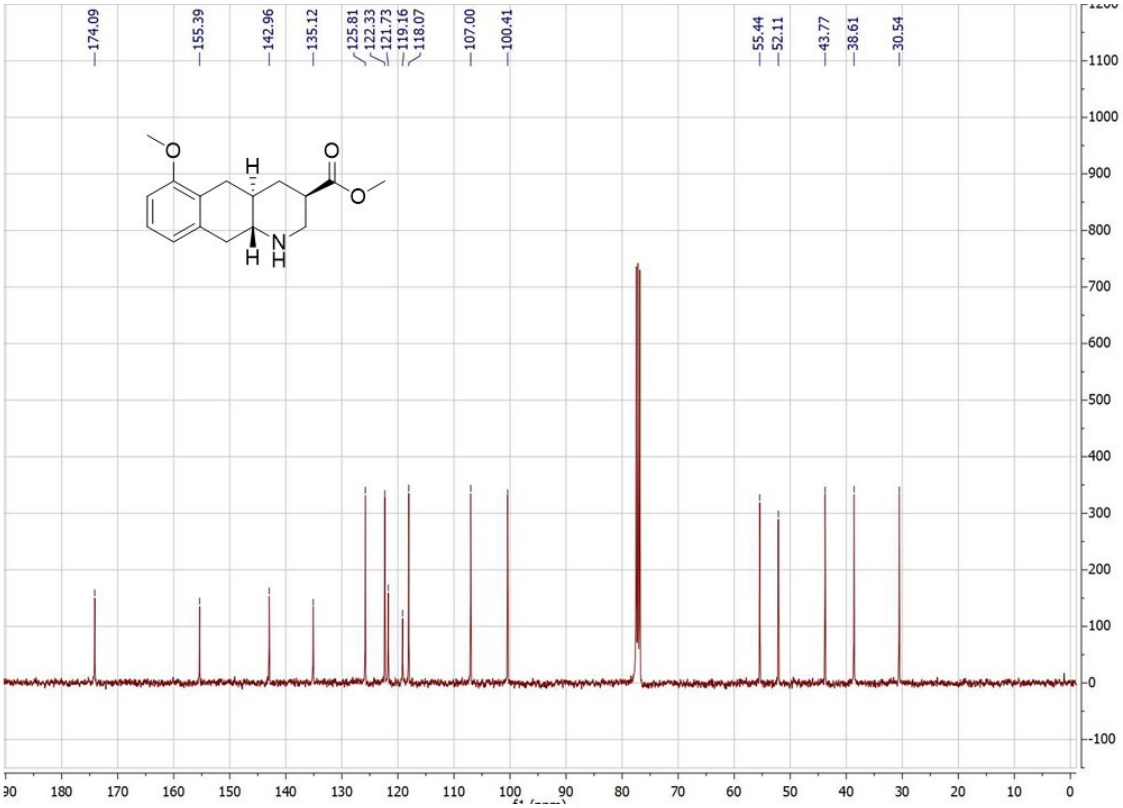
^{13}C NMR of ***(3R, 4aS,R)*-(2)** (101 MHz, MeOD)

Methyl *(3R,4aR,10aR)*-6-methoxy-1,2,3,4,4ª,5,10,10ª-octahydrobenzo[g]quinoline-3-carboxylate



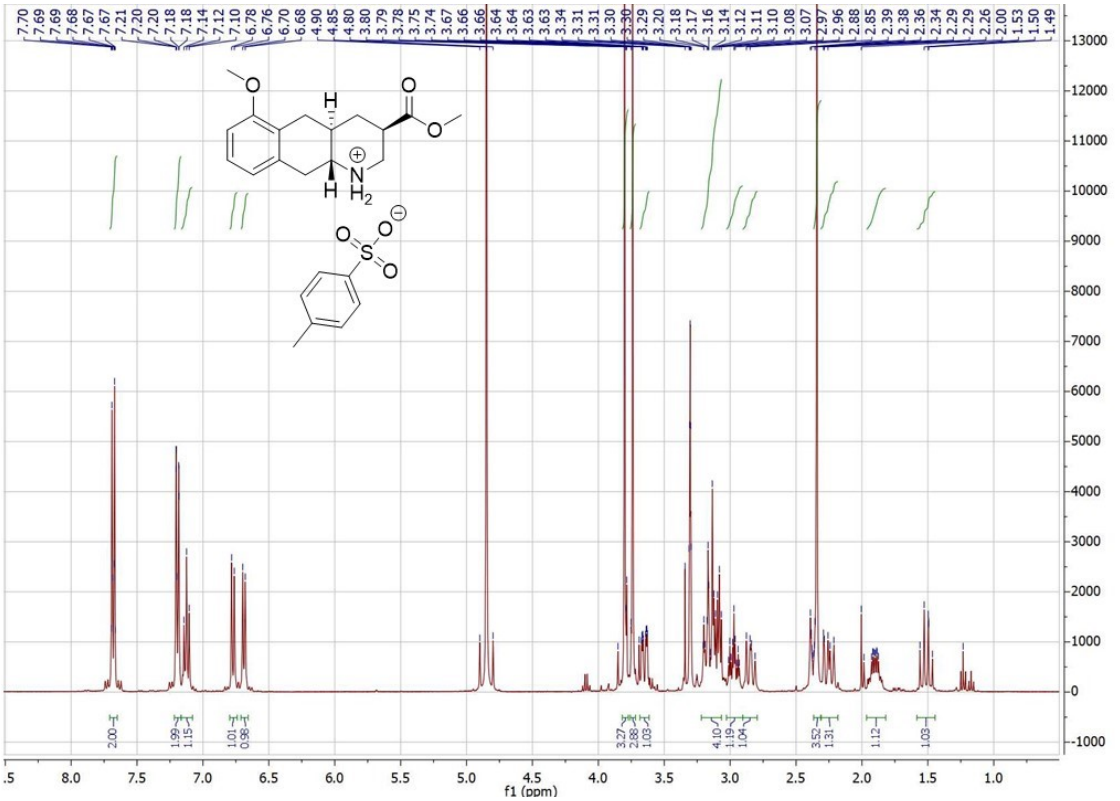
[(*3R,4aR,10aR)*-3a].

^{1}H NMR of **[*(3R,4aR,10aR)*-3a]** (400 MHz, $CDCl_3$)

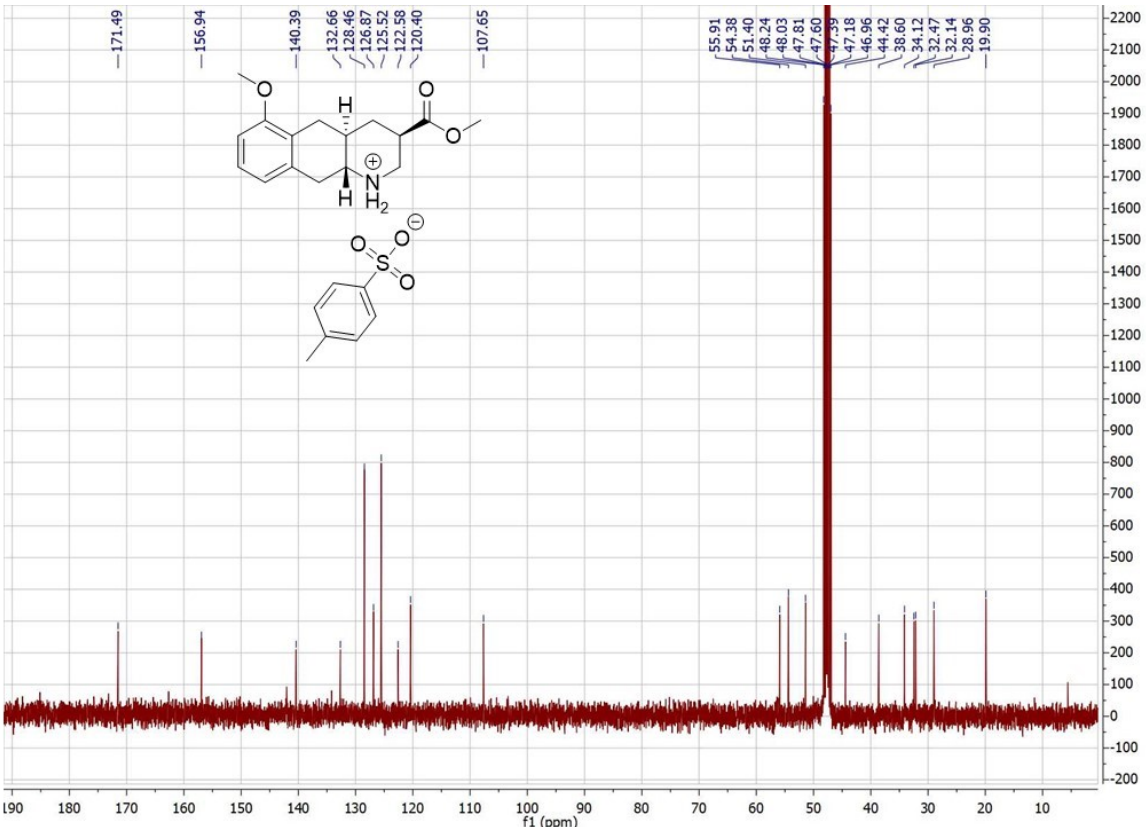


^{13}C NMR of **[*(3R,4aR,10aR)*-3a]** (101 MHz, $CDCl_3$)

(3R,4aR,10aR)-6-methoxy-3-(methoxycarbonyl)-1,2,3,4,4ª,5,10,10ª-octahydrobenzo[g]quinolin-1-ium 4-methylbenzenesulfonate **[*(3R,4aR,10aR)*-4]**.

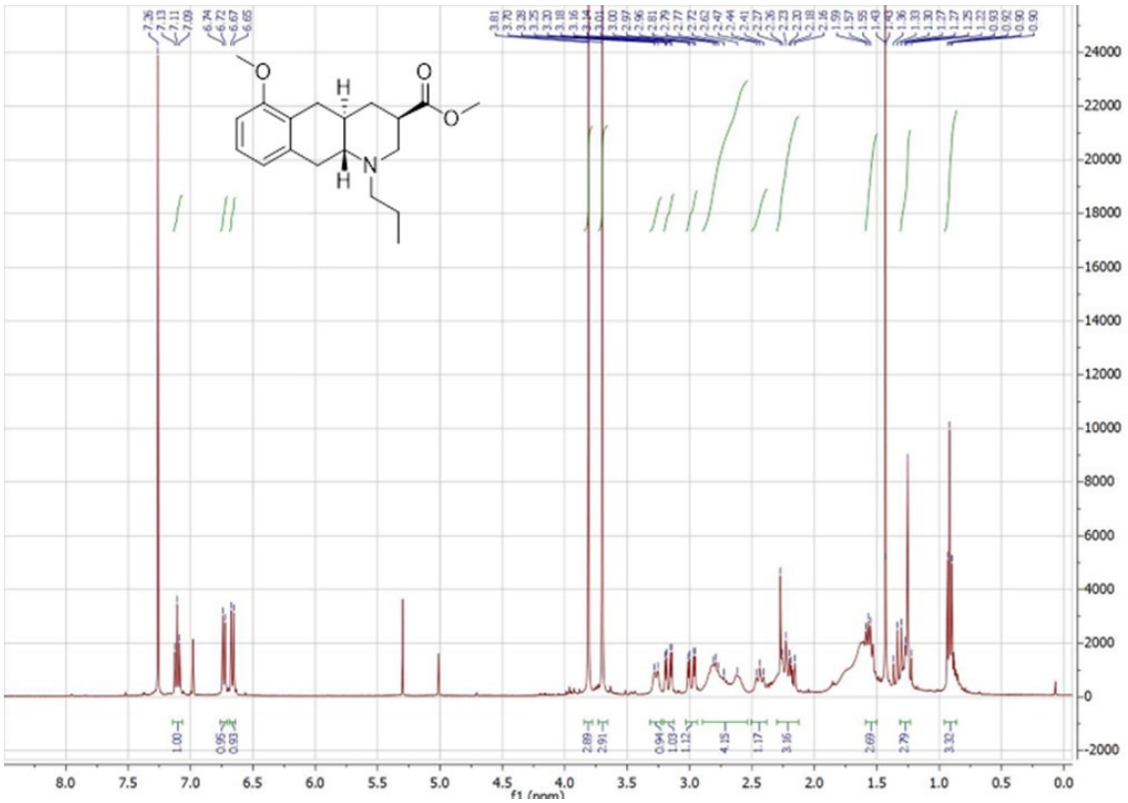


^{1}H NMR of **[*(3R,4aR,10aR)*-4]** (400 MHz, MeOD)

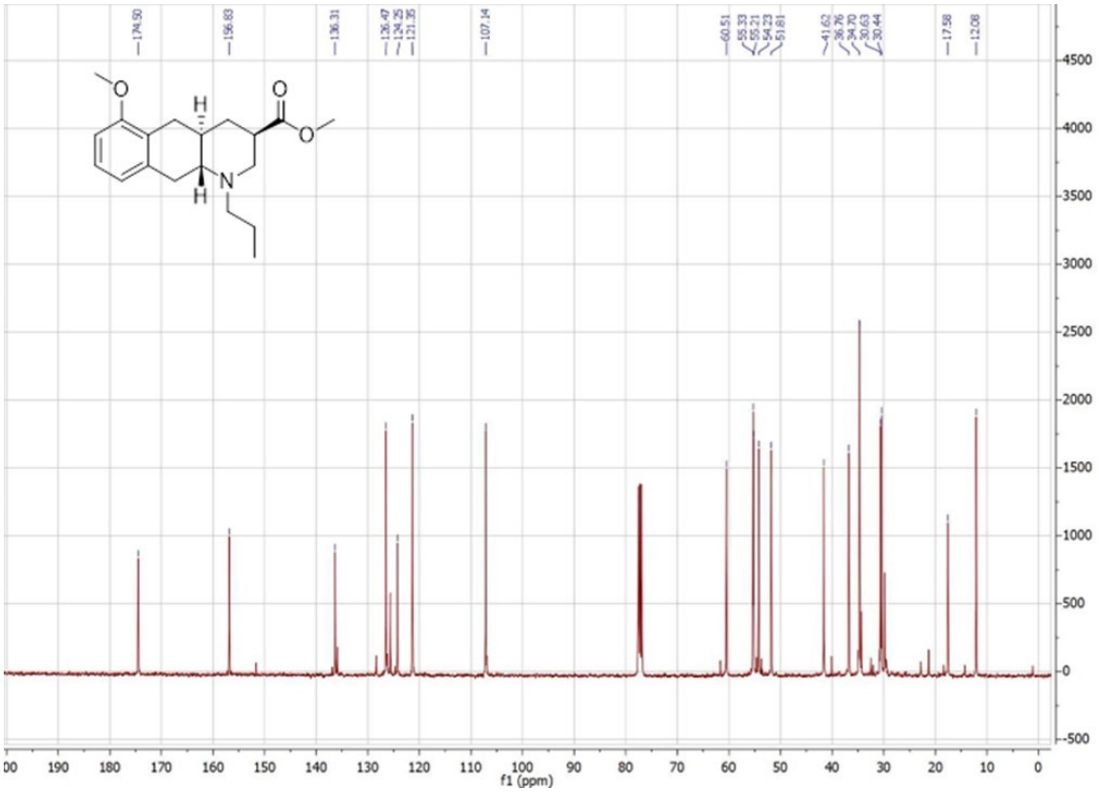


^{13}C NMR of **[*(3R,4aR,10aR)*-4]** (101 MHz, MeOD)

Methyl *(3R,4aR,10aR)*-6-methoxy-1-propyl-1,2,3,4,4ª,5,10,10ª-octahydrobenzo[g]quinoline-3-carboxylate **[*(3R,4aR,10aR)*-10]**.

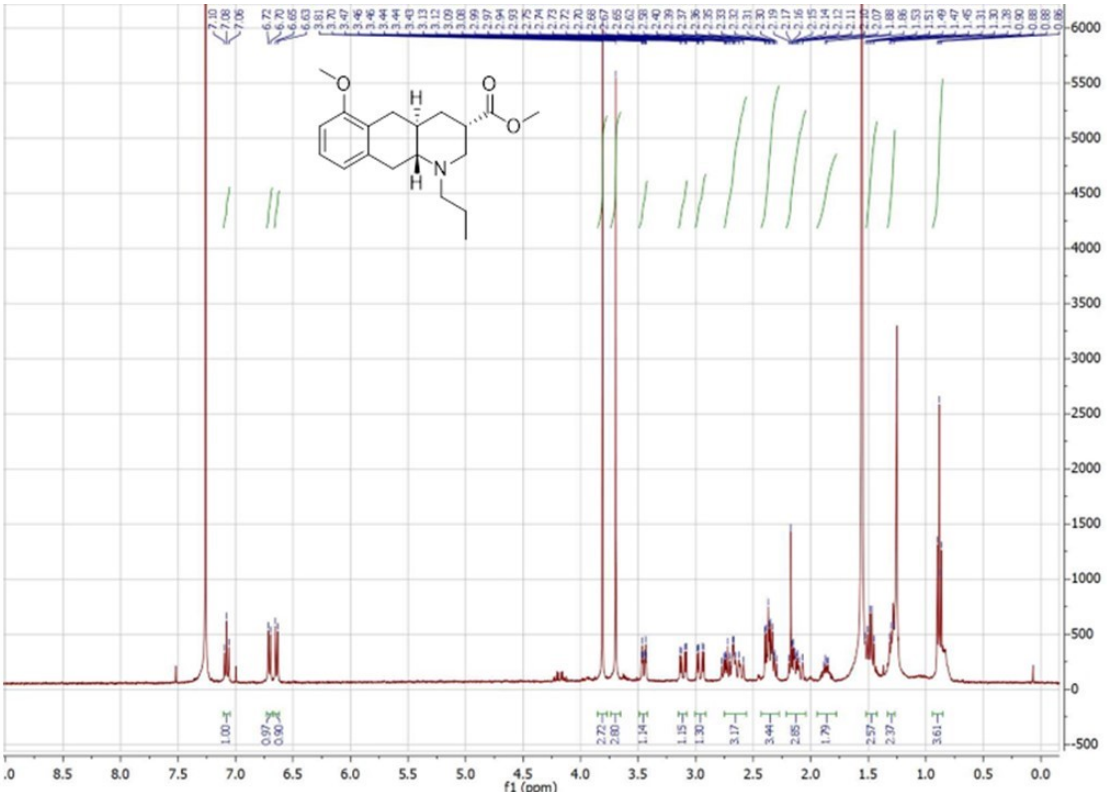


^{1}H NMR of **[*(3R,4aR,10aR)*-10]** (400 MHz, $CDCl_3$)



^{13}C NMR of **[*(3R,4aR,10aR)*-10]** (101 MHz, $CDCl_3$)

Methyl *(3S,4aR,10aR)*-6-methoxy-1-propyl-1,2,3,4,4ª,5,10,10ª-octahydrobenzo[g]quinoline-3-carboxylate



[*(3S,4aR,10aR)*-11].

^{1}H NMR of **[*(3S,4aR,10aR)*-11]** (400 MHz, $CDCl_3$)

^{13}C NMR of **[*(3S,4aR,10aR)*-11]** (101 MHz, $CDCl_3$)

Computational section:

The Conformational space was investigated with the Conformer-Rotamer Ensemble Sampling Tool CREST[8], which combines semiempirical tight-binding methods xTB[9] with a meta-dynamics driven search algorithm. Calculation was performed using Hamiltonian GFN2-xTB[10] and implicit solvation model GBSA[11,12] (solvent=methanol). The Conformer energy range was fixed at 6 kcal/mol.
All obtained structures were further optimized at the DFT-D3 level with the Gaussian 16 package[13], employing the functional PW6B95D3[14] and def2-SVP basis set.[15] Solvent (methanol) was simulated by PCM model.[16] Berny analytical gradient optimization routines were applied for optimization of the minima on the PES.[17]. After removing doubles, only the structures inside an energy range of 6.00 Kcal/mol were considered for analytical frequency calculations (T = 298.15 K and 1 atm pressure) to verify that minima had no imaginary frequencies. Free Energies, obtained by frequency calculation, were corrected with the single point energy obtained using the larger basis def2-QZVPP,[15] solvent (methanol) was also included (PCM model).

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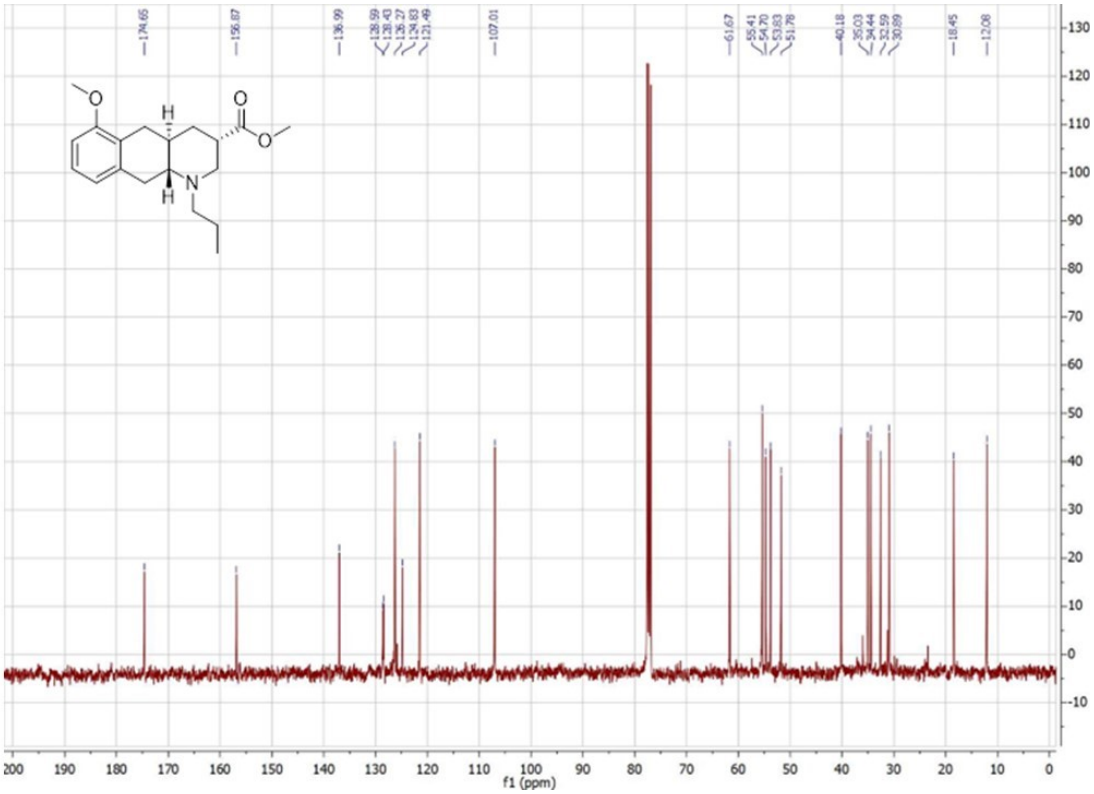

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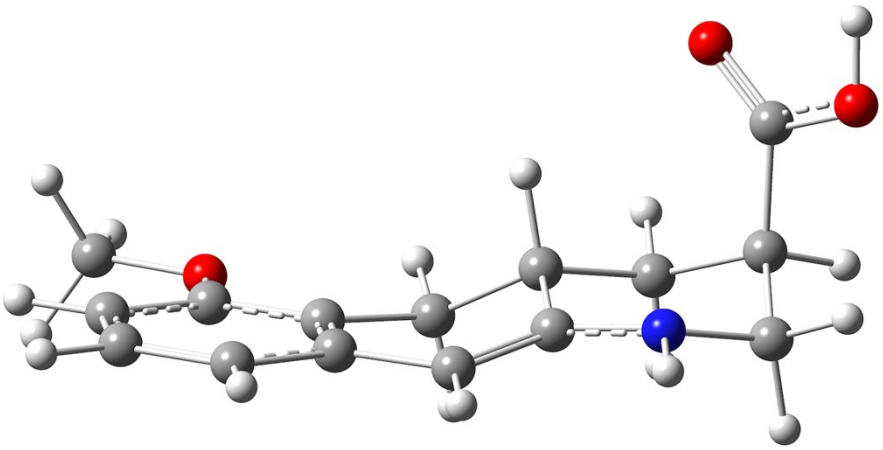
Table S-3. Conformers of enamine D (def2-SVP Electronic Energy (EE), def2-SVP Gibbs Energy (GE); def2-QZVPP Electronic Energy (EE), Corrected G Energy (corr-GE).



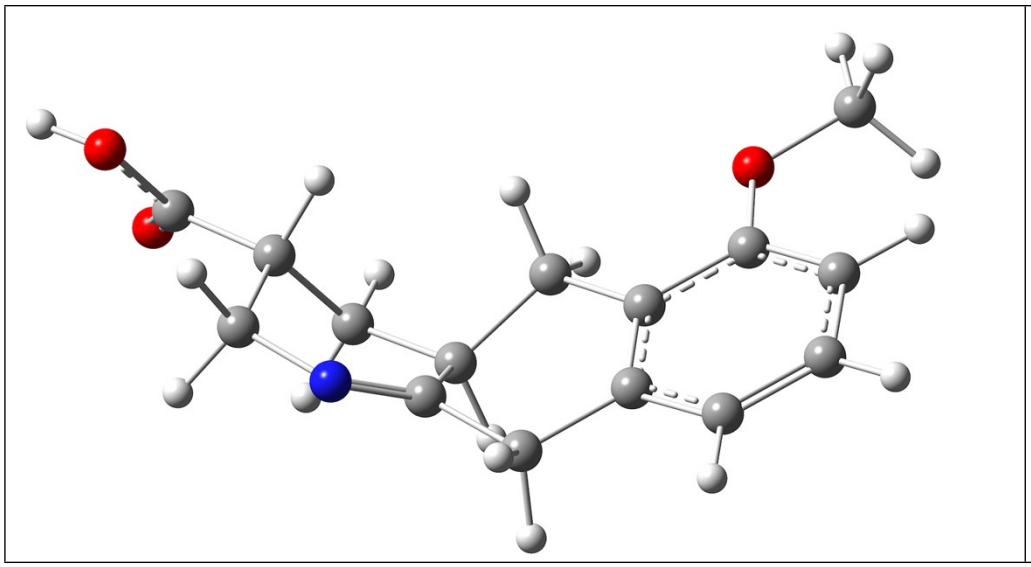
CONFORMER 1

ENAMINE D

CONFORMER	EE-DEF2SVP(Eh)	GE-DEF2SVP(Eh)	EE-DEFQZVPP(Eh)	corr-GE-DEF2QZVPP(Eh)
conf1	-862.7649041370	-862.5061430000	-863.7671553560	-863.5083942190[a]
conf2	-862.7646417610	-862.5059180000	-863.7667481460	-863.5080243850
conf3	-862.7594918160	-862.5018590000	-863.7627406490	-863.5051078330
conf4	-862.7581920870	-862.5010920000	-863.7614687140	-863.5043686270
conf5	-862.7596438490	-862.5024390000	-863.7631773330	-863.5059724840
conf6	-862.7564511200	-862.4992720000	-863.7605802540	-863.5034011340
conf7	-862.7579044090	-862.4998250000	-863.7621031700	-863.5040237610
conf8	-862.7563414820	-862.4988620000	-863.7601721340	-863.5026926520
conf9	-862.7543461800	-862.4967950000	-863.7592683210	-863.5017171410
conf10	-862.7662609110	-862.5056280000	-863.7694909020	-863.5088579910
conf11	-862.7590837990	-862.5009520000	-863.7625570770	-863.5044252780
conf12	-862.7546532560	-862.4969840000	-863.7593460690	-863.5016768130

[a]Most Stable Conformer. Conformer conf10 with intramolecular H-bond between nitrogen and carboxylic group was not considered as more stable conformer because reasonably not present in protic solvent (methanol) and basic environment.

Table S-4. Conformers of imine *cis*-2: def2-SVP Electronic Energy (EE), def2-SVP Gibbs Energy (GE); def2-QZVPP Electronic Energy (EE), Corrected G Energy (corr-GE).



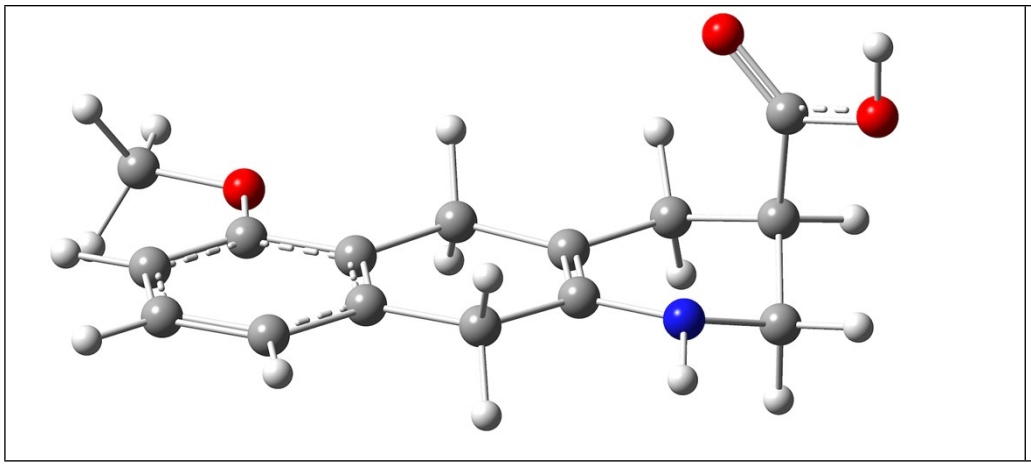
CONFORMER 1

IMINE CIS 2

CONFORMER	EE-DEF2SVP(Eh)	GE-DEF2SVP(Eh)	EE-DEFQZVPP(Eh)	corr-GE-DEF2QZVPP(Eh)
conf1	-862.756363358	-862.499159000	-863.762742110	-863.505537752[a]
conf2	-862.755966034	-862.498930000	-863.761034397	-863.503998363
conf3	-862.754929470	-862.497990000	-863.761893338	-863.504953868
conf4	-862.756520786	-862.499582000	-863.761804729	-863.504865943
conf5	-862.755926729	-862.498989000	-863.761046404	-863.504108675
conf6	-862.754253800	-862.496295000	-863.759471002	-863.501512202
conf7	-862.754323843	-862.497135000	-863.761121828	-863.503932985
conf8	-862.754084319	-862.497672000	-863.759902244	-863.503489925
conf9	-862.754005890	-862.496802000	-863.760957551	-863.503753661
conf10	-862.754084314	-862.497718000	-863.759902822	-863.503536508
conf11	-862.755929194	-862.499474000	-863.761016760	-863.504561566
conf12	-862.752183864	-862.495816000	-863.759926921	-863.503559057
conf13	-862.752767366	-862.495243000	-863.758550385	-863.501026019
conf14	-862.751844743	-862.494977000	-863.759747901	-863.502880158
conf15	-862.751409234	-862.494093000	-863.759112983	-863.501796749
conf16	-862.750506564	-862.494328000	-863.757044762	-863.500866198
conf17	-862.751449354	-862.494544000	-863.758125334	-863.501219980
conf18	-862.750926408	-862.493603000	-863.757822996	-863.500499588
conf19	-862.748698954	-862.490697000	-863.755412178	-863.497410224
conf20	-862.750897929	-862.493226000	-863.757800862	-863.500128933

[a]Most Stable Conformer.

Table S-5. Conformers of enamine E: def2-SVP Electronic Energy (EE), def2-SVP Gibbs Energy (GE); def2-QZVPP Electronic Energy (EE), Corrected G Energy (corr-GE).



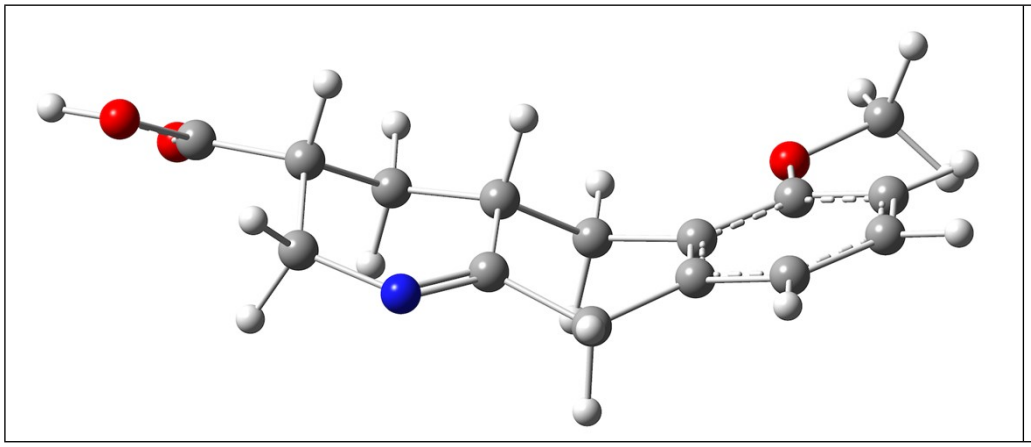
CONFORMER 2

ENAMINE E

CONFORMER	EE-DEF2SVP(Eh)	GE-DEF2SVP(Eh)	EE-DEFQZVPP(Eh)	corr-GE-DEF2QZVPP(Eh)
conf1	-862.763748460	-862.505171000	-863.768032389	-863.509454929
conf2	-862.760024957	-862.503326000	-863.764093996	-863.507395039[a]
conf3	-862.759647187	-862.502218000	-863.764640522	-863.507211335
conf4	-862.759384025	-862.503200000	-863.763219899	-863.507035874
conf5	-862.758727010	-862.503181000	-863.762527277	-863.506981267
conf6	-862.758709376	-862.502682000	-863.762659871	-863.506632495
conf7	-862.758334427	-862.501925000	-863.763439082	-863.507029655
conf8	-862.757449729	-862.501789000	-863.762802668	-863.507141939
conf9	-862.756679750	-862.500671000	-863.762499236	-863.506490486
conf10	-862.756482340	-862.500028000	-863.762327183	-863.505872843
conf11	-862.754663893	-862.498169000	-863.759752889	-863.503257996

[a]Most Stable Conformer. Conformer conf1 with intramolecular H-bond between nitrogen and carboxylic group was not considered as more stable conformer because reasonably not present in protic solvent (methanol) and basic environment.

Table S-6. Conformers of imine *trans*-2: def2-SVP Electronic Energy (EE), def2-SVP Gibbs Energy (GE); def2-QZVPP Electronic Energy (EE), Corrected G Energy (corr-GE).



CONFORMER 1

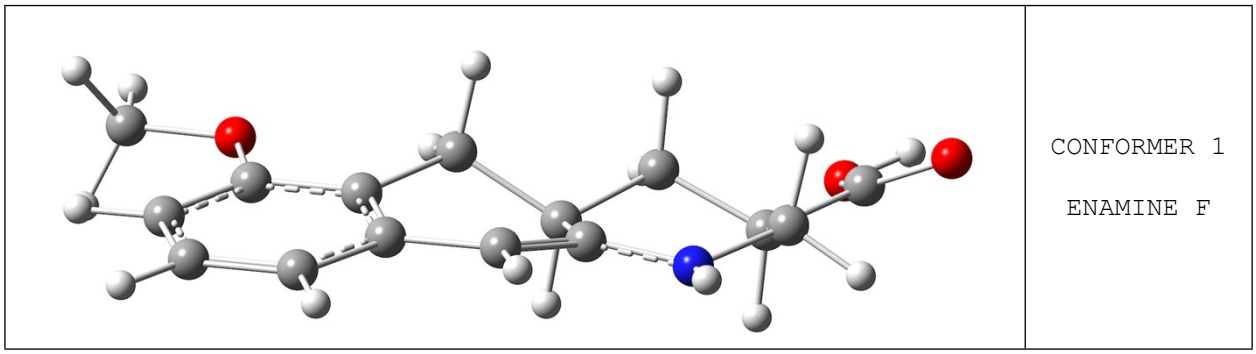
IMINE TRANS 2

CONFORMER	EE-DEF2SVP(Eh)	GE-DEF2SVP(Eh)	EE-DEFQZVPP(Eh)	corr-GE-DEF2QZVPP(Eh)
conf1	-862.755447425	-862.499205000	-863.761827821	-863.505585396[a]
conf2	-862.753984482	-862.497638000	-863.760960586	-863.504614104

conf3	-862.753817507	-862.496851000	-863.760302357	-863.503335850
conf4	-862.753753135	-862.496547000	-863.759893025	-863.502686890
conf5	-862.752336192	-862.495325000	-863.759406635	-863.502395443
conf6	-862.755900337	-862.497379000	-863.761541013	-863.503019676
conf7	-862.755313528	-862.497927000	-863.761090124	-863.503703596
conf8	-862.755843730	-862.497931000	-863.760945244	-863.503032514
conf9	-862.754099765	-862.495365000	-863.759681801	-863.500947036
conf10	-862.753607597	-862.495509000	-863.758864937	-863.500766340
conf11	-862.754462843	-862.497502000	-863.758992334	-863.502031491
conf12	-862.754369116	-862.496719000	-863.759683190	-863.502033074
conf13	-862.753967755	-862.495576000	-863.760881555	-863.502489800
conf14	-862.752988678	-862.494620000	-863.760014008	-863.501645330
conf15	-862.750470178	-862.494143000	-863.758093771	-863.501766593
conf16	-862.750477186	-862.493467000	-863.757988930	-863.500978744
conf17	-862.750664761	-862.493976000	-863.758516807	-863.501828046
conf18	-862.748808696	-862.491171000	-863.756463120	-863.498825424
conf19	-862.748870289	-862.492017000	-863.756449266	-863.499595977

[a]Most Stable Conformer.

Table S-7. Conformers of enamine F Summary: def2-SVP Electronic Energy (EE), def2-SVP Gibbs Energy (GE); def2-QZVPP Electronic Energy (EE), Corrected G Energy (corr-GE).



CONFORMER	EE-DEF2SVP(Eh)	GE-DEF2SVP(Eh)	EE-DEFQZVPP(Eh)	corr-GE(Eh)
conf1	-862.763828747	-862.505903000	-863.767081470	-863.509155723[a]
conf2	-862.761768993	-862.503956000	-863.765917096	-863.508104103
conf3	-862.763517129	-862.505998000	-863.766754242	-863.509235113
conf4	-862.759723534	-862.501688000	-863.761355383	-863.503319849
conf5	-862.760650701	-862.502794000	-863.761871832	-863.504015131
conf6	-862.759698676	-862.502190000	-863.763111838	-863.505603162
conf7	-862.757841158	-862.499382000	-863.760857950	-863.502398792
conf8	-862.757730192	-862.499917000	-863.760449483	-863.502636291
conf9	-862.755022032	-862.496745000	-863.758782048	-863.500505016
conf10	-862.761008961	-862.500751000	-863.765363088	-863.505105127
conf11	-862.758885210	-862.500907000	-863.763497846	-863.505519636

[a]Most Stable Conformer.

CARTESIAN COORDINADATES and THERMOCHEMICAL DATA

CONFORMERS of ENAMINE D

CONFORMER 1

CARTESIAN COORDINATES

C	-0.6393240578	-0.7851853985	0.7992706276
C	0.7394475607	-0.3853967870	0.2946351358
C	-0.1502304035	1.9279506936	0.2157007499
H	-0.6525270373	-0.6650105866	1.8971137317
H	-0.8152700987	-1.8475339666	0.6036323861
H	-0.0051724505	3.0079286153	0.1775827965
H	0.8066612200	-0.6359665519	-0.7768571193
C	1.8364952328	-1.1671408930	1.0102696833
C	3.2615688632	0.8600512196	1.1083493463
C	3.2191668039	-0.6082984126	0.7182358816
H	1.7786538546	-2.2209683708	0.7178458409
H	1.6703589500	-1.1190446944	2.0949908654
H	4.2236087952	1.3021467472	0.8356386092
H	3.1613730069	0.9315288034	2.2045273400
H	3.9716227587	-1.1394877717	1.3189574743
C	0.9237098403	1.1123367644	0.3680859342
N	2.2121704993	1.5789352847	0.4193844260
C	-1.7364786931	0.0469225340	0.2091847617
C	-1.4815627039	1.4066648117	-0.0326889075
C	-3.0140323147	-0.4738333241	-0.0284331683
C	-2.5187387472	2.2283312855	-0.5044545837
H	-2.3238377099	3.2835382232	-0.6888274531
C	-3.7754022367	1.6950924762	-0.7418506153
H	-4.5747181190	2.3345771856	-1.1132537132
C	-4.0374471987	0.3452567230	-0.5144228049
H	-5.0285222760	-0.0542640560	-0.7061063222
H	2.2979821212	2.5857837628	0.4510986925
C	3.6229472530	-0.8348905639	-0.7226037046
O	3.0660332088	-1.5815451673	-1.4868672115
O	4.7080554700	-0.1403837505	-1.0632423588
H	4.9197804843	-0.3540296139	-1.9843996753
O	-3.1826036055	-1.7882351716	0.2521008401
C	-4.4355610670	-2.3748824369	0.0168509482
H	-4.3482128737	-3.4281251596	0.2954961816
H	-5.2231640628	-1.9077053826	0.6251676008
H	-4.7230878646	-2.3069199495	-1.0420914156

Electronic Energy (RPW6B95D3/def2-SVP)= -862.764904137 (Hartree/Particle)

Dipole Moment= 3.6004 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302773 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.462131
Sum of electronic and thermal Energies= -862.446041
Sum of electronic and thermal Enthalpies= -862.445096
Sum of electronic and thermal Free Energies= -862.506143

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.767155356 (Hartree/Particle)
Corrected Free Energy= -863.508394219 (Hartree/Particle)

CONFORMER 2

CARTESIAN COORDINATES

C	-0.6012309631	-0.7592644654	0.8246618332
C	0.7763079174	-0.3467070090	0.3270943340
C	-0.1476547708	1.9514784550	0.2041991433
H	-0.6249633330	-0.6214452962	1.9201483196
H	-0.7587060295	-1.8273066018	0.6451040316
H	-0.0187905747	3.0328198119	0.1509915181
H	0.8562096558	-0.6198969977	-0.7399611073
C	1.8792562556	-1.0861329033	1.0732382337

C	3.3093829759	0.9408557226	1.0690927428
C	3.2549017199	-0.5344344306	0.7249286280
H	1.8199721308	-2.1563323011	0.8518529784
H	1.7284839787	-0.9696063233	2.1551409075
H	4.2494216313	1.3720109091	0.7130025538
H	3.2826698728	1.0476767087	2.1662530929
H	4.0155907396	-1.0591031839	1.3214153345
C	0.9392375046	1.1547738283	0.3756635542
N	2.2161223066	1.6412182394	0.4315953143
C	-1.7052893534	0.0465931310	0.2121683345
C	-1.4680983781	1.4065643028	-0.0471906116
C	-2.9721965584	-0.4977509892	-0.0285236528
C	-2.5146567152	2.2047017842	-0.5392366321
H	-2.3349720790	3.2601144187	-0.7373600483
C	-3.7607534480	1.6483384323	-0.7791139136
H	-4.5666422314	2.2700636624	-1.1661986067
C	-4.0042239112	0.2979146588	-0.5348753566
H	-4.9872888678	-0.1196166104	-0.7292266003
H	2.2931453211	2.6488196232	0.4362204324
C	3.6637443656	-0.7602554022	-0.7164398385
O	4.3870696737	-0.0321861094	-1.3458625697
O	3.1700815310	-1.8919175780	-1.2201345394
H	3.5039370238	-1.9844711790	-2.1253336701
O	-3.1221244452	-1.8105228668	0.2701534045
C	-4.3635468086	-2.4208514160	0.0342238860
H	-4.6426728281	-2.3761087501	-1.0282006933
H	-4.2622353708	-3.4675877143	0.3320383631
H	-5.1638383453	-1.9557188713	0.6273353229

Electronic Energy (RPW6B95D3/def2-SVP)= -862.764641761 (Hartree/Particle)

Dipole Moment= 2.8048 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302743 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.461899
Sum of electronic and thermal Energies= -862.445800
Sum of electronic and thermal Enthalpies= -862.444856
Sum of electronic and thermal Free Energies= -862.505918

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.766748146 (Hartree/Particle)
Corrected Free Energy= -863.508024385 (Hartree/Particle)

CONFORMER 3

CARTESIAN COORDINATES

C	-0.5590269005	-0.7066571406	0.7146546107
C	0.7898381272	-0.1421859937	0.2935042768
C	-0.2909998285	2.0977855875	0.4040452162
H	-0.5953618653	-0.7247001687	1.8181480082
H	-0.6462612214	-1.7477320437	0.3891120706
H	-0.2338475214	3.1832322066	0.4821728597
H	0.9401703458	-0.3382302056	-0.7827677068
C	1.9349903931	-0.7826877267	1.0653151490
C	3.2595516208	1.2108604082	0.2331439988
C	3.2972398575	-0.2912002425	0.5506483660
H	1.8825852325	-1.8758252013	1.0047512170
H	1.8383069598	-0.5144843686	2.1244223338
H	3.3096869035	1.3365802286	-0.8588202238
H	4.1378108638	1.7057222746	0.6576426593
H	4.0482361119	-0.5113845510	1.3161501838
C	0.8379904447	1.3523875027	0.4919366631
N	2.0797540154	1.8507245317	0.7809716160

C	-1.7185253556	0.0991730990	0.2089601612
C	-1.5775358001	1.4935412064	0.1109649535
C	-2.9505984219	-0.4967601652	-0.0846503575
C	-2.6813933280	2.2699822350	-0.2788377313
H	-2.5747574259	3.3509911526	-0.3529024627
C	-3.8912312591	1.6628461756	-0.5748992966
H	-4.7418609964	2.2696709326	-0.8814538246
C	-4.0408129442	0.2801780232	-0.4881108340
H	-4.9965468500	-0.1779584993	-0.7230316798
H	2.1392655357	2.8582006062	0.8386187487
C	3.6659343551	-1.1027694392	-0.6682935856
O	3.5208717968	-0.7614659808	-1.8151865012
O	4.1373420202	-2.3027848062	-0.3305194847
H	4.2999941169	-2.8005116274	-1.1459367429
O	-3.0095059221	-1.8424266704	0.0603180858
C	-4.2123984359	-2.5027711157	-0.2334486546
H	-4.0385346045	-3.5676772306	-0.0592455708
H	-5.0312547385	-2.1624347568	0.4163382359
H	-4.5112306631	-2.3551532332	-1.2810784157

Electronic Energy (RPW6B95D3/def2-SVP)= -862.759491816 (Hartree/Particle)

Dipole Moment= 3.1734 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302788 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.456704
Sum of electronic and thermal Energies= -862.440455
Sum of electronic and thermal Enthalpies= -862.439511
Sum of electronic and thermal Free Energies= -862.501859

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762740649 (Hartree/Particle)
Corrected Free Energy= -863.505107833 (Hartree/Particle)

CONFORMER 4

CARTESIAN COORDINATES

C	-0.5631577209	-0.7059816778	0.0532874161
C	0.5578012049	-0.0194459802	-0.7151015121
C	-0.3464367828	2.0950780271	0.1993575360
H	-0.2250185380	-0.8867609127	1.0895114035
H	-0.7656173819	-1.6879210853	-0.3849817557
H	-0.2382872053	3.1381180232	0.4966833573
H	0.2107909726	0.1074452576	-1.7530900977
C	1.8448779576	-0.8546858567	-0.7477487593
C	3.2152318409	1.1233433471	-0.1508057205
C	2.8849241224	-0.3070985279	0.2228529593
H	2.2796190002	-0.8477149794	-1.7555080986
H	1.6161848111	-1.8982437860	-0.5077880465
H	3.7558886456	1.1217862400	-1.1105076267
H	3.8963375578	1.5603482366	0.5884775257
H	2.4568066923	-0.3294606265	1.2377925324
C	0.7492798570	1.3847829934	-0.1828634687
N	2.0053544833	1.9122076173	-0.2171664634
C	-1.8105895324	0.1252392532	0.0703396058
C	-1.6767160581	1.5219146390	0.1612104201
C	-3.0845410043	-0.4540924210	0.0600557574
C	-2.8329262655	2.3167699806	0.2455638838
H	-2.7339069175	3.3983721630	0.3218111505
C	-4.0865621798	1.7272245273	0.2257927100
H	-4.9786158105	2.3489655346	0.2860340750
C	-4.2303231125	0.3440904602	0.1280782367
H	-5.2214573206	-0.0985475704	0.1142398817

H	2.0889383874	2.8722090051	0.0835860984
C	4.1307523734	-1.1501149196	0.2701581838
O	5.2486774554	-0.7409785238	0.0848428785
O	3.8639737449	-2.4250122926	0.5499600455
H	4.7031454304	-2.9092051259	0.5688748700
O	-3.1227221266	-1.8068946768	-0.0053903762
C	-4.3707892945	-2.4476597916	-0.0332337227
H	-4.9529374736	-2.2420848893	0.8764076807
H	-4.9648500732	-2.1421263304	-0.9064171907
H	-4.1733964568	-3.5209195349	-0.0946033283

Electronic Energy (RPW6B95D3/def2-SVP)= -862.758192087 (Hartree/Particle)

Dipole Moment= 2.1275 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302091 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.456101
Sum of electronic and thermal Energies= -862.439634
Sum of electronic and thermal Enthalpies= -862.438690
Sum of electronic and thermal Free Energies= -862.501092

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761468714 (Hartree/Particle)
Corrected Free Energy= -863.504368627 (Hartree/Particle)

CONFORMER 5

CARTESIAN COORDINATES

C	-0.6385297493	-0.7501094023	0.5792429151
C	0.7098479198	-0.1689095970	0.1759245260
C	-0.3453005705	2.0699606031	0.4792194502
H	-0.6426385385	-0.8678724176	1.6772672464
H	-0.7488058883	-1.7575629411	0.1667029433
H	-0.2686408065	3.1484068923	0.6161073397
H	0.8480374662	-0.3007289403	-0.9119477038
C	1.8480874648	-0.8857527243	0.8965584339
C	3.1442075521	1.1068501927	0.0201590411
C	3.2244084449	-0.3498182166	0.5122652004
H	1.8044702639	-1.9593000807	0.6866421754
H	1.6956494550	-0.7570465052	1.9747078405
H	3.0356950262	1.1193126079	-1.0777279196
H	4.0722097597	1.6370978981	0.2469555477
H	3.8781307532	-0.3767275496	1.3946537878
C	0.7770456953	1.3113179130	0.4561297680
N	2.0451481039	1.7902266422	0.6620616218
C	-1.8060712842	0.1066763780	0.1902398992
C	-1.6527651932	1.5025646997	0.2052021561
C	-3.0572934428	-0.4510023861	-0.0982699377
C	-2.7625279312	2.3195877479	-0.0666279971
H	-2.6451888935	3.4019502230	-0.0536601703
C	-3.9918176791	1.7509134276	-0.3588893405
H	-4.8474858292	2.3891915933	-0.5738183696
C	-4.1544891394	0.3672539877	-0.3840925288
H	-5.1254727335	-0.0604757026	-0.6136810141
H	2.1323437875	2.7959086199	0.7129396195
C	3.9143994643	-1.2125072977	-0.5173357850
O	3.5447720234	-2.2936803589	-0.8963512662
O	5.0255226148	-0.6313941476	-0.9731530827
H	5.4293135634	-1.2239106131	-1.6249384884
O	-3.1261541876	-1.8035271681	-0.0669017663
C	-4.3471201381	-2.4268773479	-0.3669409890
H	-4.6877073986	-2.1843320341	-1.3836914453
H	-4.1771416471	-3.5042107034	-0.2957427361

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  H   -5.1345959882   -2.1408941920    0.3448410340


 Electronic Energy (RPW6B95D3/def2-SVP)=          -862.759643849 (Hartree/Particle)

 Dipole Moment=                    3.3368 (Debye)
 Number of imaginary frequencies   0


 THERMOCHEMICAL DATA  (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

 Zero-point correction=                           0.302341 (Hartree/Particle)
 Sum of electronic and zero-point Energies=          -862.457303
 Sum of electronic and thermal Energies=             -862.440980
 Sum of electronic and thermal Enthalpies=           -862.440036
 Sum of electronic and thermal Free Energies=        -862.502439

 Electronic Energy SP (RPW6B95D3/def2-QZVPP)=     -863.763177333 (Hartree/Particle)
 Corrected Free Energy=                           -863.505972484 (Hartree/Particle)

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  CONFORMER 6

  CARTESIAN COORDINATES

   C   -0.5868082516   -0.7229219335   -0.0286396774
   C    0.5586880852    0.0242700158   -0.6980027931
   C   -0.3468598354    2.0444090578    0.4105886452
   H   -0.2735521262   -1.0124478610    0.9904828000
   H   -0.7888774524   -1.6524452892   -0.5694203926
   H   -0.2349380828    3.0501697478    0.8153812014
   H    0.2411570205    0.2563694842   -1.7272781403
   C    1.8396981307   -0.8169677000   -0.7813723516
   C    3.2095899089    1.0748001746    0.0119594824
   C    2.8567178342   -0.3843537837    0.2711343928
   H    2.3094344119   -0.7116840420   -1.7665739285
   H    1.5887492533   -1.8776378449   -0.6618906033
   H    3.7408859211    1.1413271427   -0.9499772949
   H    3.8940255209    1.4478074576    0.7836616548
   H    2.4206072915   -0.4815803677    1.2726589776
   C    0.7491873400    1.3659851772   -0.0238613555
   N    2.0102984302    1.8815217055    0.0197774193
   C   -1.8264183332    0.1163430476    0.0472890903
   C   -1.6815407942    1.4939043524    0.2873808395
   C   -3.1052332085   -0.4439470811   -0.0503307908
   C   -2.8315232386    2.2891168095    0.4313444225
   H   -2.7239055103    3.3554723803    0.6230502766
   C   -4.0899146540    1.7194985046    0.3239144222
   H   -4.9771886424    2.3417185169    0.4311771269
   C   -4.2445058713    0.3560923467    0.0778848468
   H   -5.2392483678   -0.0710707131   -0.0027035513
   H    2.0984092654    2.7968176786    0.4364580769
   C    4.0744256112   -1.2675247189    0.2591928173
   O    4.4108092061   -1.9951724807    1.1571178370
   O    4.7544796466   -1.1711503881   -0.8857987610
   H    5.5155138197   -1.7689494925   -0.8336403857
   O   -3.1546830533   -1.7817315545   -0.2586957148
   C   -4.4077857257   -2.4015498633   -0.3798062658
   H   -4.9797563846   -1.9988941055   -1.2279864432
   H   -4.2190625901   -3.4645694007   -0.5500070022
   H   -5.0076427342   -2.2862329476    0.5342269708


 Electronic Energy (RPW6B95D3/def2-SVP)=          -862.756451120 (Hartree/Particle)

 Dipole Moment=                    2.9350 (Debye)
 Number of imaginary frequencies   0
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THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302272 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454179
Sum of electronic and thermal Energies= -862.437680
Sum of electronic and thermal Enthalpies= -862.436736
Sum of electronic and thermal Free Energies= -862.499272

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760580254 (Hartree/Particle)
Corrected Free Energy= -863.503401134 (Hartree/Particle)

CONFORMER 7

CARTESIAN COORDINATES

C	-0.5967522263	-0.7461894383	0.5618057776
C	0.7594250401	-0.1525420714	0.2054628881
C	-0.2985750706	2.0760733888	0.5716576717
H	-0.6232962080	-0.9063546557	1.6541765516
H	-0.7011626750	-1.7365607142	0.1082241497
H	-0.2223458172	3.1484401326	0.7500556835
H	0.9279061502	-0.2510395583	-0.8800555803
C	1.8809560229	-0.8909940589	0.9300152968
C	3.1923677761	1.1152302137	0.1350795201
C	3.2819473468	-0.3534737026	0.5908698562
H	1.8153931142	-1.9645985982	0.7178134324
H	1.7179320547	-0.7753961302	2.0084812761
H	3.0840463316	1.1469554031	-0.9615299766
H	4.1169363358	1.6432835364	0.3833533197
H	3.9198309321	-0.4225469642	1.4757082145
C	0.8223498872	1.3159798965	0.5400349089
N	2.0882027654	1.7807598191	0.7873114912
C	-1.7555618980	0.1272518586	0.1833577530
C	-1.6016610741	1.5214297410	0.2535650951
C	-3.0016746768	-0.4174765873	-0.1485876238
C	-2.7059131852	2.3494406723	-0.0070638130
H	-2.5881991393	3.4303932550	0.0487635910
C	-3.9301919119	1.7937165408	-0.3423845213
H	-4.7815043854	2.4407748932	-0.5481475479
C	-4.0931306497	0.4122736602	-0.4228452268
H	-5.0600571368	-0.0054867478	-0.6856125914
H	2.1804239290	2.7827418295	0.8816679953
C	3.9604466965	-1.1829363358	-0.4675839172
O	5.0407991814	-1.7029053473	-0.3606498706
O	3.2187313311	-1.2870726979	-1.5751409458
H	3.7051224634	-1.8303382151	-2.2133862867
O	-3.0719486794	-1.7701267087	-0.1697833199
C	-4.2878981069	-2.3798478365	-0.5148790367
H	-4.6105466795	-2.0978613367	-1.5272898692
H	-4.1199607448	-3.4593581303	-0.4823038104
H	-5.0874988734	-2.1204481392	0.1935487431

Electronic Energy (RPW6B95D3/def2-SVP)= -862.757904409 (Hartree/Particle)

Dipole Moment= 1.3539 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302717 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.455187
Sum of electronic and thermal Energies= -862.438908
Sum of electronic and thermal Enthalpies= -862.437964
Sum of electronic and thermal Free Energies= -862.499825

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762103170 (Hartree/Particle)

Corrected Free Energy= -863.504023761 (Hartree/Particle)

CONFORMER 8

CARTESIAN COORDINATES

C	-0.7761036003	-0.5382105767	-1.1568604022
C	0.6587058327	-0.0734873449	-0.9268451034
C	-0.2896433442	2.1008122923	-0.1443624277
H	-0.8414484130	-1.6227696237	-1.0178775106
H	-1.0335254151	-0.3595376163	-2.2127075997
H	-0.1527567527	3.1361287881	0.1672789715
H	1.2012787666	-0.2281159777	-1.8685467833
C	1.4224795603	-0.8528449438	0.1533573447
C	3.1213647522	0.8756288672	-0.5968065517
C	2.7806494923	-0.2024997650	0.4527022369
H	1.5760288748	-1.8841342258	-0.1826795225
H	0.8157106120	-0.8960080478	1.0660102303
H	3.2891164059	0.3954581579	-1.5711665811
H	4.0492284198	1.3867236373	-0.3301900038
H	2.7487496422	0.3176081193	1.4198182762
C	0.7690829822	1.3861982960	-0.5933788058
N	2.0567235028	1.8519765195	-0.6837512126
C	-1.8035507641	0.1554205515	-0.3100689205
C	-1.5762370445	1.4771562771	0.1066223836
C	-3.0233410770	-0.4642171177	-0.0131581837
C	-2.5841382792	2.1580795157	0.8098350761
H	-2.4082516904	3.1823259204	1.1346264180
C	-3.7835445214	1.5277484197	1.0990616604
H	-4.5582678502	2.0610071092	1.6478729783
C	-4.0172678020	0.2137541104	0.6992285815
H	-4.9634867793	-0.2644485279	0.9322664782
H	2.2383379386	2.7336328255	-0.2246815878
C	3.8987237201	-1.2086263679	0.5697422263
O	3.8019228785	-2.3981066299	0.4107307301
O	5.0562531452	-0.6167134962	0.8721643802
H	5.7383546027	-1.3028554634	0.9237612589
O	-3.1684905292	-1.7313550261	-0.4701172357
C	-4.3566963420	-2.4224027707	-0.1874511965
H	-4.5182176981	-2.5259291801	0.8950390107
H	-5.2314610160	-1.9219287394	-0.6266171752
H	-4.2561629753	-3.4168630004	-0.6296908748

Electronic Energy (RPW6B95D3/def2-SVP)= -862.756341482 (Hartree/Particle)

Dipole Moment= 3.1084 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302479 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.453862
Sum of electronic and thermal Energies= -862.437531
Sum of electronic and thermal Enthalpies= -862.436587
Sum of electronic and thermal Free Energies= -862.498862

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760172134 (Hartree/Particle)
Corrected Free Energy= -863.502692652 (Hartree/Particle)

CONFORMER 9

CARTESIAN COORDINATES

C	-0.7431812108	-0.4294275558	-1.2182307853
C	0.6863314027	0.0216685737	-0.9345450112

C	-0.2805049256	2.1139103426	0.0261473247
H	-0.8038485496	-1.5223051884	-1.1747660960
H	-0.9916172293	-0.1611154890	-2.2570689873
H	-0.1532218572	3.1200271700	0.4250828289
H	1.2399596771	-0.0463382254	-1.8797429424
C	1.4441312573	-0.8498139899	0.0787246883
C	3.1353746048	0.9454160909	-0.4818888072
C	2.7771751808	-0.1871712853	0.5000829517
H	1.6292756392	-1.8295628336	-0.3764343928
H	0.8188974436	-1.0135236748	0.9644541555
H	3.3179067426	0.5152754997	-1.4754711755
H	4.0585645676	1.4467827941	-0.1770572396
H	2.6746783776	0.2594639670	1.4937991540
C	0.7851925545	1.4471993623	-0.4755094038
N	2.0711616576	1.9264881760	-0.5238528288
C	-1.7818398078	0.1828920761	-0.3234066923
C	-1.5656173687	1.4635774183	0.2104667917
C	-3.0010186560	-0.4659728369	-0.0940940139
C	-2.5828511502	2.0750086049	0.9620599659
H	-2.4151675962	3.0672701668	1.3776971801
C	-3.7813555569	1.4160294159	1.1835616174
H	-4.5635283728	1.8949758898	1.7705248082
C	-4.0045736793	0.1418062370	0.6665442063
H	-4.9502066257	-0.3595579516	0.8475316065
H	2.2421588915	2.7697683795	0.0062875873
C	3.9032030986	-1.1779056330	0.6075720577
O	4.5381172282	-1.4095187333	1.6041444205
O	4.1492530195	-1.7812853637	-0.5593409236
H	4.8870636763	-2.3957120226	-0.4291050030
O	-3.1356632611	-1.6879433468	-0.6631591537
C	-4.3240402768	-2.4052696326	-0.4564497500
H	-4.2142524283	-3.3562152516	-0.9839516474
H	-4.4971176340	-2.6050080175	0.6106291972
H	-5.1959131406	-1.8707810885	-0.8597625427

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754346180 (Hartree/Particle)

Dipole Moment= 2.1996 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302639 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.451708
Sum of electronic and thermal Energies= -862.435356
Sum of electronic and thermal Enthalpies= -862.434412
Sum of electronic and thermal Free Energies= -862.496795

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759268321 (Hartree/Particle)
Corrected Free Energy= -863.501717141 (Hartree/Particle)

CONFORMER 10

CARTESIAN COORDINATES

C	-0.6283037259	-0.8206611728	0.7133028133
C	0.7606865237	-0.4054960313	0.2452584515
C	-0.1193765388	1.9196926653	0.2478664005
H	-0.6444120859	-0.7720657266	1.8158961340
H	-0.8138662046	-1.8665639215	0.4509617277
H	0.0386588359	2.9983146644	0.2422708158
H	0.8608224632	-0.6462510137	-0.8283578598
C	1.8354232550	-1.1805850731	1.0050825828
C	3.2499788478	0.8477515732	1.1423558846
C	3.2446037342	-0.6284654398	0.7750252818
H	1.7901099245	-2.2411429242	0.7322675462

H	1.6254746311	-1.1169134586	2.0816657702
H	4.2269997881	1.3029079740	0.9480945555
H	3.0449823575	0.9477854397	2.2192061782
H	3.9429591627	-1.1667304933	1.4232089966
C	0.9387529085	1.0899974604	0.3434144703
N	2.2564477572	1.5479713000	0.3330644260
C	-1.7228717812	0.0552103449	0.1848699414
C	-1.4671742790	1.4231408284	0.0138232922
C	-3.0096157080	-0.4425253842	-0.0566104424
C	-2.5006689072	2.2800691383	-0.3915581656
H	-2.2981836533	3.3417272268	-0.5208522697
C	-3.7662665754	1.7701957471	-0.6350692182
H	-4.5674413158	2.4340341195	-0.9552450394
C	-4.0327343830	0.4120786428	-0.4766021695
H	-5.0307670283	0.0310958825	-0.6703394700
H	2.3307594733	2.5570084891	0.3904672232
C	3.7065506864	-0.9135018144	-0.6460003348
O	4.2500553767	-1.9430625448	-0.9541921536
O	3.4470012972	0.0209460126	-1.5552928864
H	2.9877549576	0.7801020998	-1.1191378113
O	-3.1833728491	-1.7672579647	0.1532116712
C	-4.4443369045	-2.3336324762	-0.0939065911
H	-4.3584810953	-3.4007658770	0.1253140651
H	-5.2184235629	-1.8959963890	0.5521644618
H	-4.7469127163	-2.2059423919	-1.1428923944

Electronic Energy (RPW6B95D3/def2-SVP)= -862.766260911 (Hartree/Particle)

Dipole Moment= 6.0110 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.303709 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.462552
Sum of electronic and thermal Energies= -862.446901
Sum of electronic and thermal Enthalpies= -862.445957
Sum of electronic and thermal Free Energies= -862.505628

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.769490902 (Hartree/Particle)
Corrected Free Energy= -863.508857991 (Hartree/Particle)

CONFORMER 11

CARTESIAN COORDINATES

C	-0.5813993109	-0.7591329520	0.8259794169
C	0.7971304018	-0.3440750641	0.3336105199
C	-0.1325227923	1.9489577780	0.1881161732
H	-0.6112417751	-0.6143587132	1.9202248012
H	-0.7344900836	-1.8287246281	0.6517304594
H	-0.0072166442	3.0303256375	0.1300068133
H	0.8856306403	-0.6271197769	-0.7310075771
C	1.8985450863	-1.0638448687	1.1002658239
C	3.3257987327	0.9541571384	1.0771697225
C	3.2789060457	-0.5235838333	0.7414000279
H	1.8137321439	-2.1488511238	0.9460523037
H	1.7495429923	-0.9174393448	2.1784022380
H	4.2641912189	1.3853520781	0.7179231166
H	3.2994043098	1.0656674186	2.1737803957
H	4.0376900318	-1.0423434392	1.3453494555
C	0.9563625761	1.1583522940	0.3724893626
N	2.2309257581	1.6478716251	0.4368101307
C	-1.6841466060	0.0393094315	0.2017161944
C	-1.4499020101	1.3979438241	-0.0660116473
C	-2.9480085972	-0.5111266852	-0.0407985330

C	-2.4965821677	2.1895667253	-0.5677558995
H	-2.3193014840	3.2441376016	-0.7721135103
C	-3.7399638050	1.6276250774	-0.8086808368
H	-4.5462588341	2.2442622155	-1.2028867936
C	-3.9802308763	0.2781348618	-0.5564970780
H	-4.9612188590	-0.1437179110	-0.7519298735
H	2.3076746566	2.6553342391	0.4299745118
C	3.6883596299	-0.7540261905	-0.7066187794
O	4.3334678041	0.0257577328	-1.3523151643
O	3.3273855782	-1.9220603551	-1.2475799831
H	2.8347581058	-2.4607971929	-0.6166049181
O	-3.0944743026	-1.8222508988	0.2655546916
C	-4.3324880320	-2.4388541873	0.0268311418
H	-5.1370183761	-1.9747426862	0.6148996057
H	-4.6071021629	-2.3991455618	-1.0369154436
H	-4.2279197590	-3.4839467083	0.3291248983

Electronic Energy (RPW6B95D3/def2-SVP)= -862.759083799 (Hartree/Particle)

Dipole Moment= 5.3720 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302490 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.456594
Sum of electronic and thermal Energies= -862.440417
Sum of electronic and thermal Enthalpies= -862.439473
Sum of electronic and thermal Free Energies= -862.500952

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762557077 (Hartree/Particle)
Corrected Free Energy= -863.504425278 (Hartree/Particle)

CONFORMER 12

CARTESIAN COORDINATES

C	-0.5619678041	-0.7029931652	0.6964989874
C	0.7829073535	-0.1296014078	0.2743413072
C	-0.3094996437	2.1044829612	0.3919846681
H	-0.5953000796	-0.7262206751	1.7999567021
H	-0.6448315785	-1.7430053267	0.3664355381
H	-0.2574572798	3.1900660761	0.4711656073
H	0.9360542063	-0.3255808712	-0.8014127098
C	1.9307756940	-0.7635104837	1.0482666979
C	3.2371058432	1.2282368623	0.1898645622
C	3.2922424200	-0.2675980715	0.5315412241
H	1.8731017860	-1.8574748918	0.9921320617
H	1.8333110811	-0.4931576027	2.1065004510
H	3.2600526918	1.3309024634	-0.9052592255
H	4.1223300217	1.7354645094	0.5837098766
H	4.0419802977	-0.4490832740	1.3117729078
C	0.8232022863	1.3650557818	0.4737290174
N	2.0658413480	1.8677121137	0.7549690156
C	-1.7273672895	0.0988081439	0.1980777592
C	-1.5944336455	1.4940198636	0.1034907504
C	-2.9575928411	-0.5029710030	-0.0914700079
C	-2.7038239579	2.2657836642	-0.2793019239
H	-2.6031075110	3.3474970649	-0.3509866997
C	-3.9117559260	1.6530220431	-0.5717052282
H	-4.7669178305	2.2560892301	-0.8729477233
C	-4.0535952447	0.2694101582	-0.4878154444
H	-5.0079537129	-0.1931735989	-0.7195852721
H	2.1240839847	2.8755005249	0.8084211842
C	3.6757246379	-1.0960043891	-0.6801013370
O	3.5195031900	-0.7578403392	-1.8230291401

O	4.1621562422	-2.3115176771	-0.4118002640
H	4.2632990693	-2.4443733341	0.5389372415
O	-3.0085254760	-1.8491389156	0.0502649515
C	-4.2087132772	-2.5156757878	-0.2409224291
H	-4.5126440848	-2.3661594071	-1.2867859747
H	-4.0276650650	-3.5801037039	-0.0712374940
H	-5.0268436785	-2.1826615667	0.4135290722

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754653256 (Hartree/Particle)

Dipole Moment= 5.0728 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302640 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452013
Sum of electronic and thermal Energies= -862.435734
Sum of electronic and thermal Enthalpies= -862.434789
Sum of electronic and thermal Free Energies= -862.496984

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759346069 (Hartree/Particle)
Corrected Free Energy= -863.501676813 (Hartree/Particle)

CONFORMERS of IMINE CIS-2

CONFORMER 1

CARTESIAN COORDINATES

C	-0.4466039886	0.6929335868	0.4338342835
C	0.6160410448	-0.2498594752	1.0020642593
C	-0.6645914991	-2.2681117428	0.2280143673
H	-0.0715846501	1.1642262074	-0.4883843842
H	-0.6141189172	1.5205550442	1.1338021333
H	-0.6495352334	-3.0537022525	-0.5349173899
H	-0.7326006769	-2.7765385503	1.2033907251
H	0.2778173134	-0.5447405749	2.0062590852
C	1.9929290140	0.3893982450	1.1036402056
C	2.8276596139	-1.2181701951	-0.6070490353
C	2.7185134398	0.2595391638	-0.2206042961
H	2.5872593633	-0.1105401841	1.8787749841
H	1.9101967631	1.4407055110	1.4025201038
H	3.5647574158	-1.7211144431	0.0392551098
H	3.2181520674	-1.3061202346	-1.6280200149
H	2.1442394918	0.7611446944	-1.0149570285
C	0.6285990264	-1.5128945709	0.1788578143
N	1.5871072869	-1.9520112237	-0.5289582150
C	-1.7545795331	0.0108380426	0.1480702929
C	-1.8709142704	-1.3767528768	0.0542130943
C	-2.9018313306	0.8062183022	-0.0436864886
C	-3.1172189917	-1.9574345633	-0.2112822697
H	-3.1961495239	-3.0407437656	-0.2850818942
C	-4.2368377450	-1.1623890375	-0.3845404919
H	-5.2034250447	-1.6181168001	-0.5914142542
C	-4.1403055663	0.2259693081	-0.3037039776
H	-5.0242399579	0.8397459438	-0.4477392035
C	4.0688032676	0.9199319745	-0.1981845856
O	4.5561375078	1.4768440615	0.7524294323
O	4.6955766875	0.8153075792	-1.3719579321
H	5.5594797953	1.2460174127	-1.2884366808
O	-2.7007121942	2.1393982092	0.0415646006
C	-3.7971823356	3.0029490680	-0.1190658863
H	-3.4158219547	4.0203563720	-0.0033504687

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  H   -4.2495484452    2.8994379659   -1.1152770744
  H   -4.5698165483    2.8195209250    0.6407264861


 Electronic Energy (RPW6B95D3/def2-SVP)=          -862.756363358 (Hartree/Particle)

 Dipole Moment=                    2.9024 (Debye)
 Number of imaginary frequencies   0


 THERMOCHEMICAL DATA  (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

 Zero-point correction=                          0.301807 (Hartree/Particle)
 Sum of electronic and zero-point Energies=          -862.454557
 Sum of electronic and thermal Energies=             -862.438337
 Sum of electronic and thermal Enthalpies=           -862.437393
 Sum of electronic and thermal Free Energies=        -862.499159

 Electronic Energy SP (RPW6B95D3/def2-QZVPP)=     -863.762742110 (Hartree/Particle)
 Corrected Free Energy=                           -863.505537752 (Hartree/Particle)

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  CONFORMER 2

  CARTESIAN COORDINATES

   C   -0.5685640241    0.6825609182   -1.1002232776
   C    0.7643711845    0.2039769416   -0.5268705331
   C   -0.4485194358   -2.0601879653   -0.4267588485
   H   -0.6328492375    0.4013298034   -2.1635053582
   H   -0.6204953547    1.7745226166   -1.0619766952
   H   -0.6926205876   -2.4428286727   -1.4315596123
   H   -0.2823720147   -2.9477795984    0.1928328802
   H    0.7625453400    0.4804101592    0.5392094295
   C    1.9787454956    0.8438856058   -1.1776144156
   C    3.1828514776   -1.3335055236   -0.9764285188
   C    3.2456673949    0.1682296292   -0.6813576557
   H    1.9997996001    1.9169580575   -0.9598292428
   H    1.9188072299    0.7277083242   -2.2679634428
   H    3.9474301229   -1.8617640547   -0.3945249691
   H    3.4511908677   -1.4974753354   -2.0301552515
   H    4.1243842941    0.5685185984   -1.2077438877
   C    0.8536646600   -1.3027047288   -0.5713719301
   N    1.9121560671   -1.9791676818   -0.7548688699
   C   -1.7027287480    0.0848307829   -0.3233516474
   C   -1.6139020986   -1.2525988450    0.0655903191
   C   -2.8174315326    0.8453185686    0.0672005805
   C   -2.6211939022   -1.8266844612    0.8452296685
   H   -2.5417740781   -2.8693309656    1.1479362307
   C   -3.7169898730   -1.0660885849    1.2249791274
   H   -4.5042595340   -1.5093702342    1.8321222304
   C   -3.8258289862    0.2681358589    0.8400674933
   H   -4.6906314678    0.8482504222    1.1475878564
   C    3.5046647077    0.4861015193    0.7738803194
   O    2.9162416932    1.3171463764    1.4196691578
   O    4.5049232365   -0.2343624640    1.2823635686
   H    4.6310554355    0.0420221317    2.2025203561
   O   -2.8372496843    2.1312255147   -0.3477393041
   C   -3.9098042752    2.9521237292    0.0372913194
   H   -3.7181089277    3.9403045398   -0.3879014879
   H   -4.8669479829    2.5746379547   -0.3492640369
   H   -3.9803768330    3.0384662479    1.1308049229


 Electronic Energy (RPW6B95D3/def2-SVP)=          -862.755966034 (Hartree/Particle)

 Dipole Moment=                    1.8282 (Debye)
 Number of imaginary frequencies   0
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THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301791 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454175
Sum of electronic and thermal Energies= -862.438012
Sum of electronic and thermal Enthalpies= -862.437068
Sum of electronic and thermal Free Energies= -862.498930

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761034397 (Hartree/Particle)
Corrected Free Energy= -863.503998363 (Hartree/Particle)

CONFORMER 3

CARTESIAN COORDINATES

C	-0.4391886127	0.6858063113	0.4093600121
C	0.6200127889	-0.2629783256	0.9735287435
C	-0.6786289183	-2.2749480244	0.2136801013
H	-0.0669818084	1.1503211681	-0.5172466641
H	-0.5955395073	1.5170754359	1.1075381318
H	-0.6734190082	-3.0614298649	-0.5484860087
H	-0.7439585241	-2.7820247804	1.1899164762
H	0.2881750804	-0.5523998619	1.9814792772
C	2.0031071773	0.3633754623	1.0680907689
C	2.8164162872	-1.2488435605	-0.6377168019
C	2.7180173160	0.2353363856	-0.2734510515
H	2.5991362221	-0.1507558170	1.8317176644
H	1.9231385630	1.4136340802	1.3744463873
H	3.5521013429	-1.7382179107	0.0184234114
H	3.2051253254	-1.3572993799	-1.6587683582
H	2.1455749061	0.7535399006	-1.0518241418
C	0.6190068585	-1.5286805072	0.1554725186
N	1.5721190582	-1.9756972041	-0.5542940279
C	-1.7538597580	0.0113969836	0.1357029930
C	-1.8799767925	-1.3756718263	0.0464845969
C	-2.8973251589	0.8137324831	-0.0500296892
C	-3.1318750452	-1.9490321059	-0.2081956827
H	-3.2182745918	-3.0319946775	-0.2783705456
C	-4.2475039287	-1.1472473629	-0.3755306430
H	-5.2185097699	-1.5972198843	-0.5740748396
C	-4.1413665131	0.2406289749	-0.2993230432
H	-5.0224347975	0.8595524425	-0.4386146082
C	4.0748043247	0.8802868086	-0.2690555378
O	4.4466830925	1.7267071352	-1.0413615616
O	4.8583826200	0.3984608127	0.7003053387
H	5.7155743407	0.8462065486	0.6408646136
O	-2.6870920536	2.1457585704	0.0298813130
C	-3.7785030685	3.0162900206	-0.1273971477
H	-3.3891029794	4.0314700497	-0.0191964708
H	-4.2383233956	2.9113161895	-1.1200301811
H	-4.5472197654	2.8421651551	0.6385287641

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754929470 (Hartree/Particle)

Dipole Moment= 3.7474 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301859 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.453070
Sum of electronic and thermal Energies= -862.436793
Sum of electronic and thermal Enthalpies= -862.435849
Sum of electronic and thermal Free Energies= -862.497990

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761893338 (Hartree/Particle)
Corrected Free Energy= -863.504953868 (Hartree/Particle)

CONFORMER 4

CARTESIAN COORDINATES

C	-0.5334845860	1.0344717852	-0.4427693888
C	0.8226661985	0.4656732032	-0.0254603952
C	-0.2024328675	-1.8433516077	0.1289871017
H	-0.5452941338	1.1700088211	-1.5361269048
H	-0.6507649228	2.0407913274	-0.0240308866
H	-0.2605993925	-2.7619165175	-0.4661573200
H	0.1085215896	-2.1601950175	1.1380260948
H	0.8660290742	0.4770263541	1.0741641953
C	1.9747660780	1.2979484558	-0.5793589469
C	2.9419080388	-0.7633694669	-1.5681922464
C	3.2375835007	0.4675468048	-0.7099518629
H	2.1432716894	2.1734824910	0.0569411473
H	1.7102646629	1.6693864659	-1.5777658154
H	3.8187589095	-1.4208552671	-1.5954399148
H	2.7699526686	-0.4429849971	-2.6061169540
H	4.0320767221	1.0432613239	-1.2046839285
C	0.9014161213	-0.9867593102	-0.4211939823
N	1.8066163762	-1.5385317515	-1.1227105293
C	-1.6980648873	0.1814689622	-0.0340422252
C	-1.5499451305	-1.1789367598	0.2310827758
C	-2.9789022744	0.7613751129	0.0584429179
C	-2.6622673520	-1.9454028058	0.6005283777
H	-2.5352784499	-3.0069553532	0.8063907819
C	-3.9119540466	-1.3595453924	0.6991182108
H	-4.7748360596	-1.9577830568	0.9860849235
C	-4.0827565334	-0.0022343417	0.4290290286
H	-5.0695753085	0.4440364563	0.5053513018
C	3.7928186669	0.0823924167	0.6412341765
O	3.3545915644	0.4447766830	1.7043451298
O	4.8616398754	-0.7091119114	0.5410788744
H	5.1679286450	-0.9095525593	1.4382272526
O	-3.0433907635	2.0782217822	-0.2375480644
C	-4.2817144365	2.7349537968	-0.1467181087
H	-5.0177553134	2.3063723164	-0.8413363990
H	-4.6896302889	2.6885116063	0.8728155610
H	-4.1041642589	3.7795323990	-0.4138646812

Electronic Energy (RPW6B95D3/def2-SVP)= -862.756520786 (Hartree/Particle)

Dipole Moment= 2.2983 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301730 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454791
Sum of electronic and thermal Energies= -862.438594
Sum of electronic and thermal Enthalpies= -862.437650
Sum of electronic and thermal Free Energies= -862.499582

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761804729 (Hartree/Particle)
Corrected Free Energy= -863.504865943 (Hartree/Particle)

CONFORMER 5

CARTESIAN COORDINATES

C	-0.5033424837	0.5110660895	-1.2000156737

C	0.8143034888	0.0789153285	-0.5584100530
C	-0.4616088988	-2.1263843146	-0.2073849835
H	-0.5685718353	0.0910223145	-2.2162633984
H	-0.5277988106	1.5992099094	-1.3077832011
H	-0.7058493204	-2.5949864050	-1.1752102454
H	-0.3315626317	-2.9542874420	0.4971851829
H	0.8112584055	0.5000226760	0.4616281502
C	2.0520555409	0.5801771832	-1.2794885864
C	3.2060770496	-1.5567433642	-0.7252099868
C	3.2844499569	-0.0386175246	-0.6307140180
H	2.0964713434	1.6732687203	-1.2534227538
H	2.0167326511	0.2757525901	-2.3341125489
H	3.9228911919	-2.0040378318	-0.0262250210
H	3.5217979148	-1.8762876933	-1.7286065991
H	4.1895248416	0.3051567923	-1.1527410324
C	0.8652513813	-1.4254681489	-0.4036238159
N	1.9094355946	-2.1432147228	-0.4744844530
C	-1.6544520743	0.0472674784	-0.3592021439
C	-1.6045009290	-1.2367910849	0.1855711504
C	-2.7437991105	0.8825930022	-0.0622186231
C	-2.6260374097	-1.6844394797	1.0266209062
H	-2.5771006579	-2.6857897906	1.4507094037
C	-3.6973845007	-0.8511214300	1.3124460176
H	-4.4961996711	-1.1953499071	1.9668890635
C	-3.7669538188	0.4310119519	0.7726380813
H	-4.6131516991	1.0689997135	1.0090105669
C	3.4692949563	0.4088230434	0.8044097066
O	3.8642603598	-0.2885974268	1.7035214301
O	3.1696413848	1.6973166559	0.9795305248
H	3.3358839193	1.9163409416	1.9088328133
O	-2.7253157771	2.1105826155	-0.6257612764
C	-3.7718787127	3.0035555264	-0.3428160122
H	-4.7409018003	2.6113277515	-0.6820981373
H	-3.8366664270	3.2227751113	0.7323278374
H	-3.5518855741	3.9273399344	-0.8834217725

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755926729 (Hartree/Particle)

Dipole Moment= 5.2292 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301807 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454119
Sum of electronic and thermal Energies= -862.437976
Sum of electronic and thermal Enthalpies= -862.437032
Sum of electronic and thermal Free Energies= -862.498989

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761046404 (Hartree/Particle)
Corrected Free Energy= -863.504108675 (Hartree/Particle)

CONFORMER 6

CARTESIAN COORDINATES

C	-0.4858867869	0.6862838596	1.1910867998
C	0.8662582388	0.1752304319	0.6599439133
C	-0.3719431644	-2.0377583227	0.7520465036
H	-0.5345264551	1.7751119647	1.0994502090
H	-0.5479403681	0.4663501058	2.2668139566
H	-0.3391169133	-3.0699454962	0.3947003589
H	-0.2918182950	-2.0397418371	1.8505126750
H	1.5674619551	0.1649584430	1.5063453856
C	1.4724402934	1.0561165790	-0.4224024807
C	2.4692535879	-0.9994860224	-1.4574565812

C	2.7511598460	0.4178067634	-0.9394878781
H	1.6771005399	2.0551908451	-0.0235885037
H	0.7611163761	1.1661346511	-1.2521237831
H	3.4000272746	-1.5781084385	-1.4927960419
H	2.1296768237	-0.9319663152	-2.5008256009
H	3.1494536510	0.9967453121	-1.7854834792
C	0.7663607751	-1.2494941936	0.1623207788
N	1.4748062834	-1.7706544361	-0.7524608221
C	-1.6627584011	0.0470235198	0.5159929594
C	-1.6354310817	-1.3366868813	0.3285946531
C	-2.7886856224	0.7755959924	0.1029603899
C	-2.7076082784	-1.9947857762	-0.2741157761
H	-2.6686943707	-3.0718218042	-0.4255368722
C	-3.8159208347	-1.2627744441	-0.6773539853
H	-4.6595960454	-1.7659352733	-1.1463987308
C	-3.8653615787	0.1173320400	-0.4955671933
H	-4.7415463721	0.6701316931	-0.8207413786
C	3.8510145771	0.4798742513	0.0966345886
O	3.8090894140	1.1174596168	1.1192737512
O	4.9249553407	-0.2267194499	-0.2579312760
H	5.5942245676	-0.1158221929	0.4340288744
O	-2.7549936849	2.1080008992	0.3239180830
C	-3.8434581888	2.8926788009	-0.0913793684
H	-3.6045310811	3.9260991777	0.1712232152
H	-3.9998887790	2.8244826326	-1.1771950700
H	-4.7717180492	2.5982273702	0.4181830029

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754253800 (Hartree/Particle)

Dipole Moment= 2.3219 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302268 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.451986
Sum of electronic and thermal Energies= -862.436025
Sum of electronic and thermal Enthalpies= -862.435081
Sum of electronic and thermal Free Energies= -862.496295

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759471002 (Hartree/Particle)
Corrected Free Energy= -863.501512202 (Hartree/Particle)

CONFORMER 7

CARTESIAN COORDINATES

C	-0.6752533719	0.2315844895	1.5698908739
C	0.6963985376	-0.2514101634	1.0960673561
C	-0.6874896042	-2.3354224336	0.5418940351
H	-0.6531919242	1.3065298296	1.7692495682
H	-0.9174702257	-0.2616953077	2.5228645494
H	-0.6381040018	-3.2576821514	-0.0429763043
H	-0.9031701147	-2.6089520848	1.5881450916
H	1.3742557471	-0.3112913348	1.9620797457
C	1.3335058242	0.7026086352	0.0758984855
C	2.8339633834	-1.3364276098	-0.0696070537
C	2.5190208016	0.0622497734	-0.6452595309
H	1.6616762410	1.6122140244	0.5890544419
H	0.5662702102	0.9966028841	-0.6503121520
H	3.2298472210	-1.2216637650	0.9534855620
H	3.6181037214	-1.8119656876	-0.6665041510
H	2.2833101438	-0.0974500741	-1.7052733409
C	0.6386526634	-1.6338866081	0.5023096650
N	1.6501319366	-2.1650318670	-0.0576650160
C	-1.7363974199	-0.1015641672	0.5625611006

C	-1.7542639455	-1.3979702058	0.0437156559
C	-2.6905880042	0.8293905936	0.1239720037
C	-2.7059222523	-1.7711491024	-0.9052958175
H	-2.7046313445	-2.7822310354	-1.3079293415
C	-3.6473047890	-0.8425944815	-1.3276082119
H	-4.3956788965	-1.1233818918	-2.0664882270
C	-3.6473425013	0.4552181466	-0.8221974485
H	-4.3903882356	1.1667563427	-1.1694866495
C	3.7584454362	0.9208443765	-0.6169612982
O	3.8976662938	1.9466760394	-0.0012455380
O	4.7324745473	0.3956741268	-1.3630948715
H	5.5073214744	0.9727633088	-1.2903954842
O	-2.6158503493	2.0644556606	0.6655494343
C	-3.5289775177	3.0461412197	0.2463525058
H	-3.2851480774	3.9578790189	0.7970144955
H	-3.4437247217	3.2433975799	-0.8315751114
H	-4.5650538569	2.7567280891	0.4716266059

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754323843 (Hartree/Particle)

Dipole Moment= 2.2796 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302165 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452159
Sum of electronic and thermal Energies= -862.436046
Sum of electronic and thermal Enthalpies= -862.435101
Sum of electronic and thermal Free Energies= -862.497135

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761121828 (Hartree/Particle)
Corrected Free Energy= -863.503932985 (Hartree/Particle)

CONFORMER 8

CARTESIAN COORDINATES

C	-0.4486109763	0.7880798770	1.0897845000
C	0.8932113938	0.1950286195	0.6226447486
C	-0.3856972550	-1.9687895994	0.9822555261
H	-0.4774627290	1.8601581187	0.8752302010
H	-0.5137125971	0.6915579832	2.1832007758
H	-0.3717409778	-3.0372823813	0.7538461555
H	-0.3107673741	-1.8386978236	2.0733576993
H	1.5955580643	0.2776399020	1.4672876479
C	1.4958385415	0.9122132466	-0.5748888553
C	2.4977861491	-1.2664411725	-1.3073467826
C	2.7844355881	0.1980705615	-0.9903174200
H	1.6978995536	1.9623844626	-0.3375801743
H	0.7870339391	0.8932637884	-1.4139153225
H	3.4210609352	-1.8518488403	-1.2117868798
H	2.1982440597	-1.3527334934	-2.3616030403
H	3.2015021902	0.6943016893	-1.8757369005
C	0.7723245051	-1.2821371037	0.3092843640
N	1.4732604575	-1.9235411759	-0.5305644717
C	-1.6347632177	0.0956851954	0.4874331754
C	-1.6330320175	-1.3007063158	0.4679618941
C	-2.7429203477	0.7908171189	-0.0202134164
C	-2.7142348305	-2.0061407199	-0.0601826442
H	-2.6956437639	-3.0940707909	-0.0809492870
C	-3.8053289237	-1.3070634139	-0.5578431802
H	-4.6559012498	-1.8469588667	-0.9701141346
C	-3.8286929859	0.0855336552	-0.5440906519
H	-4.6916598784	0.6116117175	-0.9409588161
C	3.8108767477	0.3350315884	0.1074613102

O	4.2082544510	-0.5621812042	0.8072927221
O	4.2263437573	1.5948144367	0.2475395955
H	4.8561469409	1.6211464092	0.9835708386
O	-2.6836103161	2.1391243836	0.0383860063
C	-3.7533019612	2.8888048574	-0.4782667395
H	-3.4943208007	3.9415466057	-0.3417541786
H	-3.9050861586	2.6915057258	-1.5488490623
H	-4.6902352098	2.6774177533	0.0560291361

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754084319 (Hartree/Particle)

Dipole Moment= 5.1855 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301927 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452157
Sum of electronic and thermal Energies= -862.436004
Sum of electronic and thermal Enthalpies= -862.435060
Sum of electronic and thermal Free Energies= -862.497672

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759902244 (Hartree/Particle)
Corrected Free Energy= -863.503489925 (Hartree/Particle)

CONFORMER 9

CARTESIAN COORDINATES

C	-0.6268272062	0.8189286913	-0.8006026600
C	0.6223045857	0.1843001410	-0.1959010829
C	-0.6216893560	-1.9581471572	-0.8723981768
H	-0.5556954255	0.7543879268	-1.8983573067
H	-0.6745880426	1.8827231593	-0.5527679995
H	-0.5869328409	-1.8392857389	-1.9690945244
H	-0.6071162176	-3.0314569323	-0.6635922924
H	0.6107682298	0.3834871576	0.8888792841
C	1.9290289259	0.7585288976	-0.7553227141
C	2.7406290108	-1.2641829481	0.5406011472
C	3.1303565922	-0.1276429871	-0.4274187149
H	2.0896590261	1.7622313387	-0.3484748699
H	1.8302114572	0.8636514905	-1.8419941758
H	2.4911130316	-0.8280120386	1.5227829438
H	3.5975615971	-1.9274905211	0.6929148416
H	3.4993379360	-0.6232610629	-1.3347067773
C	0.6182071054	-1.3159592326	-0.3193892930
N	1.6148779526	-2.0199122801	0.0402286935
C	-1.8634359281	0.1091257347	-0.3361246307
C	-1.8633717360	-1.2869017792	-0.3552644567
C	-2.9991609001	0.7919095582	0.1266828592
C	-2.9766458065	-2.0031602810	0.0856712705
H	-2.9623812488	-3.0913368412	0.0717678899
C	-4.0944670232	-1.3167695798	0.5388215111
H	-4.9683174400	-1.8663765473	0.8840406744
C	-4.1156844357	0.0755972882	0.5631461899
H	-4.9997168932	0.5931081790	0.9233054151
C	4.2977981269	0.6482356962	0.1287433427
O	4.2949202095	1.8138592090	0.4321907333
O	5.3748859380	-0.1266973052	0.2713557238
H	6.0829445852	0.4141173059	0.6519930334
O	-2.9333351575	2.1410470008	0.1157151185
C	-4.0310198874	2.8786609501	0.5889972991
H	-3.7609882983	3.9339932400	0.5033810047
H	-4.9334093093	2.6895786779	-0.0092914343
H	-4.2498855345	2.6477471498	1.6410921380

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754005890 (Hartree/Particle)

Dipole Moment= 2.1147 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301898 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452108
Sum of electronic and thermal Energies= -862.435913
Sum of electronic and thermal Enthalpies= -862.434969
Sum of electronic and thermal Free Energies= -862.496802

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760957551 (Hartree/Particle)
Corrected Free Energy= -863.503753661 (Hartree/Particle)

CONFORMER 10

CARTESIAN COORDINATES

C	-0.4217337881	0.7643952989	1.1019565678
C	0.9097703355	0.1737466473	0.6033199340
C	-0.3752468191	-1.9900973922	0.9403052432
H	-0.4480099538	1.8405908584	0.9087600557
H	-0.4710729700	0.6468282563	2.1941348712
H	-0.3704242615	-3.0540322736	0.6911856611
H	-0.2834076690	-1.8814803306	2.0324607665
H	1.6250835764	0.2364542560	1.4387509737
C	1.4982870175	0.9109171646	-0.5890742334
C	2.4773738760	-1.2581744582	-1.3785131800
C	2.7766772460	0.1983603973	-1.0374356773
H	1.7095088572	1.9552468517	-0.3346121998
H	0.7769570026	0.9117993815	-1.4175726169
H	3.3988031832	-1.8500444993	-1.3083703198
H	2.1614907301	-1.3223116460	-2.4295747931
H	3.1833006447	0.7095641846	-1.9192000907
C	0.7762687207	-1.2964402208	0.2633525984
N	1.4611058906	-1.9250078132	-0.5991795471
C	-1.6203971490	0.0898943948	0.5040766233
C	-1.6264681352	-1.3058583372	0.4576584896
C	-2.7321515084	0.8003638059	0.0264390814
C	-2.7191328528	-1.9954098798	-0.0678481221
H	-2.7067188868	-3.0828147302	-0.1098707313
C	-3.8136804372	-1.2812697535	-0.5356593745
H	-4.6731447957	-1.8087455829	-0.9455587026
C	-3.8293331298	0.1108970332	-0.4947285571
H	-4.6952162874	0.6489567587	-0.8685093374
C	3.8201173235	0.3085739914	0.0472702634
O	4.2241650237	-0.6044437853	0.7224063084
O	4.2431360807	1.5635156624	0.2067978644
H	4.8841807545	1.5721331464	0.9334815489
O	-2.6647117132	2.1469723216	0.1100996460
C	-3.7378786503	2.9119515305	-0.3760161669
H	-4.6679302995	2.6950363789	0.1679991813
H	-3.4712511211	3.9605234032	-0.2231091681
H	-3.9065420414	2.7361888030	-1.4478241219

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754084314 (Hartree/Particle)

Dipole Moment= 5.1864 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301926 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452159
Sum of electronic and thermal Energies= -862.436004
Sum of electronic and thermal Enthalpies= -862.435060
Sum of electronic and thermal Free Energies= -862.497718

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759902822 (Hartree/Particle)
Corrected Free Energy= -863.503536508 (Hartree/Particle)

CONFORMER 11

CARTESIAN COORDINATES

C	-0.5034891264	0.9173851554	-0.6417103284
C	0.8372680665	0.3748668379	-0.1494328913
C	-0.2585444153	-1.8948525347	0.2057661986
H	-0.5083005534	0.9061635001	-1.7433841999
H	-0.5945790458	1.9724458749	-0.3601462811
H	-0.3490395235	-2.8353463484	-0.3507020474
H	0.0267793807	-2.1873237430	1.2292708138
H	0.8788522789	0.5346761287	0.9411618345
C	2.0034014563	1.0967970405	-0.8088776262
C	3.0380903612	-1.0867205460	-1.3543929887
C	3.2701333503	0.2630298561	-0.6928674325
H	2.1343186188	2.0905295235	-0.3694530318
H	1.7875845380	1.2397615023	-1.8757403427
H	3.8868837845	-1.7498928256	-1.1501707510
H	3.0018021186	-0.9595476449	-2.4457808192
H	4.0997471195	0.7780109009	-1.1991093387
C	0.8978003388	-1.1191051081	-0.3624142639
N	1.8349551471	-1.7662644515	-0.9258021802
C	-1.6887012117	0.1553616321	-0.1292998340
C	-1.5792078863	-1.1756809206	0.2673826653
C	-2.9466105953	0.7876841990	-0.0695454333
C	-2.7078276544	-1.8617898416	0.7334613139
H	-2.6115123327	-2.9011246278	1.0432662956
C	-3.9348918866	-1.2253705918	0.7966059349
H	-4.8103500664	-1.7613931120	1.1586442016
C	-4.0664697156	0.1038181993	0.3962589970
H	-5.0355748786	0.5906865060	0.4471367141
C	3.7299733883	0.0838774245	0.7390352738
O	4.2456265671	-0.9104250163	1.1818750228
O	3.5282388481	1.1749630384	1.4805918548
H	3.8719035732	0.9964253546	2.3690140225
O	-2.9750572254	2.0707972755	-0.4923360408
C	-4.1890820208	2.7754371599	-0.4403042669
H	-4.5736347602	2.8419509590	0.5871845879
H	-3.9845328341	3.7825074606	-0.8117451534
H	-4.9549781287	2.3070833787	-1.0743342699

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755929194 (Hartree/Particle)

Dipole Moment= 5.3555 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301598 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454331
Sum of electronic and thermal Energies= -862.438115
Sum of electronic and thermal Enthalpies= -862.437171
Sum of electronic and thermal Free Energies= -862.499474

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761016760 (Hartree/Particle)
Corrected Free Energy= -863.504561566 (Hartree/Particle)

CONFORMER 12

CARTESIAN COORDINATES

C	-0.6664936685	0.3576614332	1.4955125561
C	0.7004828936	-0.1758005535	1.0650204076
C	-0.6983089527	-2.2912897995	0.6979642214
H	-0.6374269418	1.4460223559	1.5976732886
H	-0.9074775246	-0.0463089610	2.4899578081
H	-0.6546328176	-3.2603528254	0.1938735397
H	-0.9152103512	-2.4740610358	1.7636454011
H	1.3849078273	-0.1515671335	1.9273777227
C	1.3355793245	0.6694233196	-0.0483547946
C	2.8320059534	-1.3760186223	0.0240187187
C	2.5441636468	-0.0364474524	-0.6895432222
H	1.6250925427	1.6385616822	0.3709750707
H	0.5758319409	0.8627400308	-0.8147559737
H	3.2125366285	-1.1585632691	1.0348946076
H	3.6217988504	-1.9168415136	-0.5090470271
H	2.3384538740	-0.2638710708	-1.7392606399
C	0.6332064608	-1.6060551821	0.6013373229
N	1.6425729043	-2.1927974022	0.0950426186
C	-1.7340666156	-0.0577174586	0.5261833057
C	-1.7610096112	-1.3944057261	0.1228543448
C	-2.6862488481	0.8365549066	0.0133984647
C	-2.7204645780	-1.8439400895	-0.7844593989
H	-2.7266498428	-2.8863828522	-1.0970042855
C	-3.6601727044	-0.9509043480	-1.2804740744
H	-4.4146819905	-1.2913780291	-1.9873327558
C	-3.6510626775	0.3860894085	-0.8904239577
H	-4.3934960408	1.0678553114	-1.2941132010
C	3.7919321031	0.8038325656	-0.6880839987
O	4.4883401174	1.0186482577	-1.6467608380
O	4.0790237193	1.2749567918	0.5294394993
H	4.8992654322	1.7867110291	0.4664986418
O	-2.6016876867	2.1137604096	0.4444256898
C	-3.5126916613	3.0605473458	-0.0526660022
H	-3.2577330098	4.0160498292	0.4120560877
H	-3.4365981687	3.1601043731	-1.1446114544
H	-4.5483299789	2.8001490251	0.2072665567

Electronic Energy (RPW6B95D3/def2-SVP)= -862.752183864 (Hartree/Particle)

Dipole Moment= 4.8682 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302145 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.450039
Sum of electronic and thermal Energies= -862.433849
Sum of electronic and thermal Enthalpies= -862.432905
Sum of electronic and thermal Free Energies= -862.495816

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759926921 (Hartree/Particle)
Corrected Free Energy= -863.503559057 (Hartree/Particle)

CONFORMER 13

CARTESIAN COORDINATES

C	-0.4614820590	0.6966811683	1.1642459707
C	0.8882429842	0.1601158113	0.6522941102
C	-0.3812593686	-2.0347395859	0.7623214641
H	-0.4941637655	1.7848268944	1.0587736223

H	-0.5356016332	0.4906218307	2.2417899865
H	-0.3602343608	-3.0720402497	0.4192744447
H	-0.3114292493	-2.0234287026	1.8614336996
H	1.5772590231	0.1441887289	1.5109632011
C	1.5068292135	1.0108123253	-0.4455518914
C	2.4987136672	-1.0660244491	-1.4309398433
C	2.7972571726	0.3486446877	-0.9365914354
H	1.7144892598	2.0239981199	-0.0830339245
H	0.8055860504	1.0981164875	-1.2867495638
H	3.4167662587	-1.6670496150	-1.4386943809
H	2.1795119238	-1.0086855342	-2.4818088927
H	3.2134294066	0.9431700714	-1.7580129088
C	0.7747733544	-1.2722028869	0.1730314389
N	1.4799974516	-1.8130591955	-0.7316399137
C	-1.6399497359	0.0646683052	0.4852206370
C	-1.6304305771	-1.3217086960	0.3173255049
C	-2.7503042894	0.8040281508	0.0498851946
C	-2.7059296868	-1.9724606538	-0.2872574614
H	-2.6812621601	-3.0519147519	-0.4234160491
C	-3.7991089017	-1.2300900995	-0.7122743561
H	-4.6452017137	-1.7274733213	-1.1830743833
C	-3.8301803233	0.1530112639	-0.5507184489
H	-4.6946037686	0.7138769123	-0.8930151052
C	3.8242233307	0.4267208043	0.1680908077
O	4.4127281060	1.4337643330	0.4699639877
O	3.9943060296	-0.7264017025	0.8188922163
H	4.6423363631	-0.5777380901	1.5243398751
O	-2.6989392537	2.1386471975	0.2523395562
C	-3.7707177304	2.9337200762	-0.1862692927
H	-4.7088675530	2.6606332518	0.3170102513
H	-3.5188160429	3.9670116019	0.0643514950
H	-3.9161731174	2.8522501575	-1.2726950358

Electronic Energy (RPW6B95D3/def2-SVP)= -862.752767366 (Hartree/Particle)

Dipole Moment= 2.5892 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302064 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.450703
Sum of electronic and thermal Energies= -862.434634
Sum of electronic and thermal Enthalpies= -862.433689
Sum of electronic and thermal Free Energies= -862.495243

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758550385 (Hartree/Particle)
Corrected Free Energy= -863.501026019 (Hartree/Particle)

CONFORMER 14

CARTESIAN COORDINATES

C	-0.5863556203	0.7068149015	-0.9072434361
C	0.6405531641	0.1327392488	-0.2043024420
C	-0.6122455536	-2.0606894750	-0.6637393192
H	-0.4908345504	0.5181730327	-1.9886453205
H	-0.6276687307	1.7921259680	-0.7816042510
H	-0.5502897214	-2.0680476563	-1.7656353586
H	-0.6150113416	-3.1032110594	-0.3337275970
H	0.6084891457	0.4544471321	0.8499396306
C	1.9667421026	0.6314525417	-0.7924835198
C	2.7220587562	-1.2350317293	0.7411715049
C	3.1551946889	-0.2442964531	-0.3574875546
H	2.1165528469	1.6715421238	-0.4848205337
H	1.8942929332	0.6276624558	-1.8860251271

H	2.4578127868	-0.6637314877	1.6459640013
H	3.5613677734	-1.8878483430	1.0061292457
H	3.5149634760	-0.8386094929	-1.2024716985
C	0.6215810990	-1.3710499789	-0.1563779078
N	1.6008524878	-2.0375754930	0.3077168027
C	-1.8415721308	0.0653653767	-0.3954351822
C	-1.8577029048	-1.3238315445	-0.2567181349
C	-2.9791777362	0.8067804026	-0.0400411095
C	-2.9892629065	-1.9751684032	0.2353576039
H	-2.9876526879	-3.0580016767	0.3448510026
C	-4.1087777097	-1.2314419775	0.5811923878
H	-4.9967631100	-1.7302885211	0.9652319931
C	-4.1137984884	0.1548499552	0.4476804546
H	-4.9994077568	0.7181557729	0.7259121625
C	4.3397063906	0.5533974253	0.1152423984
O	5.4668999864	0.4330575199	-0.2913970520
O	4.0131930605	1.4124359961	1.0855842225
H	4.8188468456	1.8769518726	1.3572372003
O	-2.8969598244	2.1453457467	-0.2014060977
C	-3.9962761923	2.9417835808	0.1596501640
H	-4.2415472220	2.8329954621	1.2255419697
H	-3.7118669313	3.9781963875	-0.0376695025
H	-4.8870676382	2.6947995070	-0.4348744583

Electronic Energy (RPW6B95D3/def2-SVP)= -862.751844743 (Hartree/Particle)

Dipole Moment= 5.3757 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301975 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.449870
Sum of electronic and thermal Energies= -862.433614
Sum of electronic and thermal Enthalpies= -862.432670
Sum of electronic and thermal Free Energies= -862.494977

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759747901 (Hartree/Particle)
Corrected Free Energy= -863.502880158 (Hartree/Particle)

CONFORMER 15

CARTESIAN COORDINATES

C	-0.4488676157	0.7009738190	0.4370023957
C	0.6197450378	-0.2403493840	0.9970038028
C	-0.6591730812	-2.2606764988	0.2255906505
H	-0.0802343288	1.1771221352	-0.4853116492
H	-0.6156907942	1.5253910066	1.1408418777
H	-0.6454396688	-3.0450772618	-0.5385078595
H	-0.7197393839	-2.7703866397	1.2007203345
H	0.2887312196	-0.5385309290	2.0024911027
C	1.9958378396	0.4007106199	1.0928758632
C	2.8232109597	-1.1974369353	-0.6257474557
C	2.7160547108	0.2825265975	-0.2358004514
H	2.5983339306	-0.1015599568	1.8595690233
H	1.9129971291	1.4502290867	1.3977871351
H	3.5651922988	-1.6969852567	0.0170001312
H	3.2055695123	-1.3014531461	-1.6507382006
H	2.1327398247	0.7913422005	-1.0196497923
C	0.6303756584	-1.5007179682	0.1710186088
N	1.5858037810	-1.9339837082	-0.5447118728
C	-1.7558789076	0.0152945110	0.1551201707
C	-1.8687790282	-1.3723842132	0.0592191018
C	-2.9059820219	0.8078054331	-0.0312942959
C	-3.1143106763	-1.9563563783	-0.2022276313

H	-3.1904021110	-3.0397463494	-0.2774662670
C	-4.2367825251	-1.1641355380	-0.3697710428
H	-5.2029039653	-1.6222581466	-0.5734339851
C	-4.1437802985	0.2243487952	-0.2874111068
H	-5.0299986129	0.8357752953	-0.4272363536
C	4.0786631513	0.9308183053	-0.2020645992
O	4.5996528827	1.3663112211	0.7890245667
O	4.7302335722	0.9805344303	-1.3707112039
H	4.1888060212	0.6313901593	-2.0892017447
O	-2.7079510755	2.1412739571	0.0546132466
C	-3.8068954265	3.0023767161	-0.1030721669
H	-4.5769394977	2.8172826985	0.6589021265
H	-3.4274786996	4.0206291761	0.0114303360
H	-4.2616907837	2.8975978124	-1.0980318150

Electronic Energy (RPW6B95D3/def2-SVP)= -862.751409234 (Hartree/Particle)

Dipole Moment= 5.5065 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301750 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.449659
Sum of electronic and thermal Energies= -862.433412
Sum of electronic and thermal Enthalpies= -862.432468
Sum of electronic and thermal Free Energies= -862.494093

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759112983 (Hartree/Particle)
Corrected Free Energy= -863.501796749 (Hartree/Particle)

CONFORMER 16

CARTESIAN COORDINATES

C	-0.5644670870	0.6677172992	-1.0870904569
C	0.7663487436	0.1944524663	-0.5048738893
C	-0.4434787360	-2.0665368533	-0.3384722724
H	-0.6269470740	0.3759374383	-2.1476070535
H	-0.6142509226	1.7601894373	-1.0609075352
H	-0.6895617409	-2.5084091672	-1.3178140166
H	-0.2671066175	-2.9170484411	0.3289323337
H	0.7630872003	0.4789456959	0.5585142019
C	1.9798203042	0.8318318272	-1.1597643040
C	3.1680250322	-1.3499177180	-0.9961769289
C	3.2529615009	0.1505193683	-0.6865878849
H	2.0080975340	1.9029027275	-0.9335108342
H	1.9093689531	0.7265109862	-2.2505502914
H	3.9482894055	-1.9131238086	-0.4637111558
H	3.3973560219	-1.4992763614	-2.0609494440
H	4.1199326567	0.5501063393	-1.2336439853
C	0.8528305366	-1.3108521248	-0.5320496059
N	1.9059984164	-1.9919011663	-0.7311338125
C	-1.7021902382	0.0825231516	-0.3059057351
C	-1.6133014727	-1.2439651679	0.1183549593
C	-2.8233987482	0.8491372521	0.0539502514
C	-2.6272735658	-1.8003753240	0.9025886944
H	-2.5479026732	-2.8345179396	1.2332071355
C	-3.7290117703	-1.0340637835	1.2516175073
H	-4.5208776198	-1.4641619028	1.8622261792
C	-3.8378506612	0.2894670138	0.8313304399
H	-4.7071269566	0.8749413444	1.1151510060
C	3.5372180778	0.4548685813	0.7731929353
O	2.8863543286	1.2015793186	1.4548356608
O	4.6124583951	-0.1420149290	1.2985792638
H	5.0696982905	-0.6828810319	0.6432876530

O	-2.8424751020	2.1237787859	-0.3941860944
C	-3.9196241423	2.9518838713	-0.0383117643
H	-3.9998565654	3.0639173330	1.0521863089
H	-3.7256514988	3.9299458152	-0.4852731179
H	-4.8727122589	2.5635216917	-0.4240789501

Electronic Energy (RPW6B95D3/def2-SVP)= -862.750506564 (Hartree/Particle)

Dipole Moment= 3.7130 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301628 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.448878
Sum of electronic and thermal Energies= -862.432632
Sum of electronic and thermal Enthalpies= -862.431688
Sum of electronic and thermal Free Energies= -862.494328

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.757044762 (Hartree/Particle)
Corrected Free Energy= -863.500866198 (Hartree/Particle)

CONFORMER 17

CARTESIAN COORDINATES

C	-0.5313625035	1.0393259848	-0.4318067801
C	0.8243707186	0.4770513408	-0.0035808959
C	-0.1868235856	-1.8310559096	0.1783221435
H	-0.5391086621	1.1684789842	-1.5259245758
H	-0.6546018365	2.0474766706	-0.0190748398
H	-0.2377728230	-2.7637333633	-0.3947945117
H	0.1277099699	-2.1187892913	1.1949163429
H	0.8587026156	0.4888727364	1.0956189116
C	1.9800697124	1.3110660391	-0.5489432478
C	2.9104876061	-0.7365237506	-1.5877619948
C	3.2378825912	0.4774800573	-0.7125564606
H	2.1634496635	2.1697574475	0.1056278956
H	1.7109750998	1.7086465476	-1.5358244882
H	3.7794687846	-1.4017837263	-1.6901898568
H	2.6966610231	-0.3877144970	-2.6084123815
H	4.0198340012	1.0637335607	-1.2163544479
C	0.9049564341	-0.9754944009	-0.3936863664
N	1.7989578482	-1.5249516625	-1.1115614620
C	-1.6934026118	0.1829635027	-0.0215112643
C	-1.5392832523	-1.1731743445	0.2626168559
C	-2.9783718740	0.7560407992	0.0538205149
C	-2.6495787947	-1.9415560677	0.6337133766
H	-2.5177889990	-2.9995651642	0.8541209212
C	-3.9034572724	-1.3619734922	0.7153317418
H	-4.7648515868	-1.9616726693	1.0036683171
C	-4.0803691453	-0.0094605447	0.4261112735
H	-5.0704069696	0.4317170540	0.4891589296
C	3.8110953540	0.0598349553	0.6281765400
O	3.3296453401	0.3412964823	1.6933365663
O	4.9339504646	-0.6661473426	0.5857782236
H	5.2316792533	-0.8011189109	-0.3221746933
O	-3.0482131225	2.0684188584	-0.2597181962
C	-4.2910183421	2.7190415405	-0.1867247030
H	-5.0189829272	2.2776538336	-0.8818133230
H	-4.7066499553	2.6825915432	0.8300724960
H	-4.1172964136	3.7612691516	-0.4652784686

Electronic Energy (RPW6B95D3/def2-SVP)= -862.751449354 (Hartree/Particle)

Dipole Moment= 4.8096 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301622 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.449827
Sum of electronic and thermal Energies= -862.433596
Sum of electronic and thermal Enthalpies= -862.432652
Sum of electronic and thermal Free Energies= -862.494544

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758125334 (Hartree/Particle)
Corrected Free Energy= -863.501219980 (Hartree/Particle)

CONFORMER 18

CARTESIAN COORDINATES

C	-0.5036151084	0.5050182372	-1.1846760440
C	0.8116766858	0.0570406878	-0.5487798406
C	-0.4768939323	-2.1429936803	-0.2213437463
H	-0.5726729734	0.0959769540	-2.2050502474
H	-0.5215839851	1.5944505904	-1.2808663546
H	-0.7245790813	-2.5972004021	-1.1951448091
H	-0.3520719965	-2.9804276152	0.4727187628
H	0.8120708791	0.4640499990	0.4769097029
C	2.0477700397	0.5541564359	-1.2753202930
C	3.1954736490	-1.5880191336	-0.7148924880
C	3.2927157825	-0.0691266478	-0.6387725686
H	2.0848909854	1.6506419148	-1.2600077155
H	2.0059864221	0.2559646976	-2.3311961820
H	3.8969001508	-2.0353532313	0.0003530462
H	3.5278503201	-1.9197857122	-1.7090855511
H	4.1892664156	0.2648879408	-1.1796580834
C	0.8541244424	-1.4479715235	-0.4070096117
N	1.8953134150	-2.1682320386	-0.4805106397
C	-1.6560002556	0.0396711709	-0.3465417292
C	-1.6133715826	-1.2507248158	0.1835976110
C	-2.7390743642	0.8788940339	-0.0383002318
C	-2.6359205759	-1.7010200045	1.0218419030
H	-2.5925257819	-2.7071840613	1.4349059508
C	-3.7010627447	-0.8638465294	1.3190552809
H	-4.5007178110	-1.2099165635	1.9714805160
C	-3.7634559230	0.4246363308	0.7935830576
H	-4.6049971957	1.0653429323	1.0389121381
C	3.4274963987	0.4013720401	0.7954903804
O	3.2977349441	-0.3044795053	1.7591756230
O	3.6751605533	1.7066223884	0.9577849423
H	3.7793662051	2.1493785690	0.1065110049
O	-2.7134178600	2.1127275049	-0.5883649891
C	-3.7536242418	3.0093422896	-0.2932566926
H	-4.7256853212	2.6269843282	-0.6350973050
H	-3.8150292917	3.2161200659	0.7845219600
H	-3.5285812537	3.9378221807	-0.8235990789

Electronic Energy (RPW6B95D3/def2-SVP)= -862.750926408 (Hartree/Particle)

Dipole Moment= 6.9750 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301753 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.449173
Sum of electronic and thermal Energies= -862.432979

Sum of electronic and thermal Enthalpies= -862.432035
Sum of electronic and thermal Free Energies= -862.493603

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.757822996 (Hartree/Particle)
Corrected Free Energy= -863.500499588 (Hartree/Particle)

CONFORMER 19

CARTESIAN COORDINATES

C	-0.4905471174	0.7004070704	1.1850756281
C	0.8659970883	0.1778838381	0.6742313554
C	-0.3711540175	-2.0318691804	0.7753688402
H	-0.5380915836	1.7870581935	1.0698094001
H	-0.5599224500	0.5046983774	2.2649339306
H	-0.3366381276	-3.0670355135	0.4270735063
H	-0.2887435833	-2.0231201884	1.8735031274
H	1.5540977312	0.1566280412	1.5302704942
C	1.4964610334	1.0595894620	-0.3930876465
C	2.4481239937	-0.9951804316	-1.4571133275
C	2.7659917709	0.4104636326	-0.9209145897
H	1.7187076844	2.0488219941	0.0205254815
H	0.7913757131	1.1964229352	-1.2241112179
H	3.3584053124	-1.6064559507	-1.5400143902
H	2.0840300323	-0.8998148736	-2.4897426411
H	3.1611047985	0.9965042866	-1.7642525385
C	0.7620030717	-1.2444425083	0.1766320589
N	1.4649171128	-1.7680862545	-0.7413537750
C	-1.6651064031	0.0490065145	0.5170346959
C	-1.6363208037	-1.3367899404	0.3464015896
C	-2.7929572953	0.7704862933	0.0963843500
C	-2.7080831571	-2.0040416478	-0.2468021918
H	-2.6674298390	-3.0827629828	-0.3849391000
C	-3.8181248709	-1.2789178893	-0.6573841808
H	-4.6616619687	-1.7891641327	-1.1188961179
C	-3.8692738780	0.1032169602	-0.4926509582
H	-4.7466839549	0.6506751105	-0.8234571099
C	3.8744575097	0.4356587569	0.1165627196
O	3.7924374371	0.9679316205	1.1917476650
O	5.0215493130	-0.1567327670	-0.2334870649
H	4.9795974578	-0.5083544432	-1.1311066454
O	-2.7612426221	2.1054584770	0.3007599958
C	-3.8506408763	2.8833884293	-0.1248796387
H	-4.7785470356	2.5945322636	0.3884561304
H	-3.6129048225	3.9204171689	0.1241189198
H	-4.0068351200	2.8006588832	-1.2097047496

Electronic Energy (RPW6B95D3/def2-SVP)= -862.748698954 (Hartree/Particle)

Dipole Moment= 4.8919 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302126 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.446573
Sum of electronic and thermal Energies= -862.430573
Sum of electronic and thermal Enthalpies= -862.429629
Sum of electronic and thermal Free Energies= -862.490697

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.755412178 (Hartree/Particle)
Corrected Free Energy= -863.497410224 (Hartree/Particle)

CONFORMER 20

CARTESIAN COORDINATES

C	-0.4963815453	0.7342812680	-1.0686321613
C	0.8206679357	0.2250332311	-0.4859961711
C	-0.4014447477	-2.0346037149	-0.4209433736
H	-0.5372388842	0.4947280530	-2.1427295977
H	-0.5386992572	1.8244245601	-0.9900854986
H	-0.6321764049	-2.4541366751	-1.4136093243
H	-0.2344497008	-2.9011076521	0.2280059485
H	0.7815654254	0.4436106959	0.5954802321
C	2.0518584681	0.8855080294	-1.0794005212
C	3.2214570352	-1.3059877864	-1.0541598274
C	3.3161556570	0.1532908831	-0.6243483256
H	2.0935768034	1.9433777772	-0.7969866504
H	2.0031117533	0.8427269078	-2.1755617665
H	4.0148800705	-1.9027924647	-0.5834614708
H	3.4166693551	-1.3725966431	-2.1338427168
H	4.1912839497	0.6187750067	-1.0895474421
C	0.8976245637	-1.2805398027	-0.5826525805
N	1.9524663214	-1.9607761515	-0.8004309386
C	-1.6519963291	0.1204651728	-0.3374437003
C	-1.5767168292	-1.2209343031	0.0388225107
C	-2.7800229574	0.8771205248	0.0226115861
C	-2.6102463011	-1.8025838217	0.7777736037
H	-2.5417736571	-2.8485392046	1.0713585723
C	-3.7175682366	-1.0456286153	1.1290277953
H	-4.5244377414	-1.4952345261	1.7048593351
C	-3.8135678219	0.2927143375	0.7550728995
H	-4.6877455222	0.8705313593	1.0395252494
C	3.5094032137	0.3474128323	0.8681195215
O	4.0299874422	1.3231897769	1.3381357552
O	3.0364812701	-0.6067355100	1.6802828324
H	2.6271518272	-1.3309500461	1.1845888955
O	-2.7849614109	2.1660903548	-0.3806707260
C	-3.8717668502	2.9836531723	-0.0282848677
H	-3.6664703007	3.9743498462	-0.4409068303
H	-4.8138307703	2.6067701739	-0.4505172751
H	-3.9801005989	3.0633449982	1.0625128311

Electronic Energy (RPW6B95D3/def2-SVP)= -862.750897929 (Hartree/Particle)

Dipole Moment= 5.5164 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301932 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.448966
Sum of electronic and thermal Energies= -862.432864
Sum of electronic and thermal Enthalpies= -862.431919
Sum of electronic and thermal Free Energies= -862.493226

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.757800862 (Hartree/Particle)
Corrected Free Energy= -863.500128933 (Hartree/Particle)

CONFORMERS of ENAMINE E

CONFORMER 1

CARTESIAN COORDINATES

C	0.5684730	-0.9602740	-0.3603060
C	-0.7852780	-0.3507190	-0.5213670
C	0.0734870	1.9518870	-0.0410230

H	0.8236100	-1.5437330	-1.2602260
H	0.5412610	-1.7201100	0.4385490
H	0.0793100	2.7565110	-0.7937260
H	-0.2014220	2.4510180	0.9020310
C	-1.9048820	-1.2998400	-0.8380250
C	-3.2582840	0.7484230	-1.2352960
C	-3.2885640	-0.6630680	-0.6634240
H	-1.8282180	-2.1955300	-0.2055330
H	-1.8043790	-1.6622340	-1.8720210
H	-4.2365610	1.2339640	-1.1503090
H	-3.0008330	0.6921890	-2.3040950
H	-4.0264410	-1.2631700	-1.2040600
C	-0.9932780	0.9681490	-0.3896580
C	1.6738140	0.0084470	-0.0759250
C	1.4539060	1.3734740	0.0777340
C	2.9852680	-0.4920040	0.0455860
C	2.5303670	2.2291110	0.3468060
H	2.3483030	3.2961550	0.4641460
C	3.8132710	1.7237150	0.4622870
H	4.6466090	2.3919850	0.6713520
C	4.0539340	0.3581600	0.3128620
H	5.0644480	-0.0280500	0.4057640
C	-3.7167140	-0.7299390	0.7974970
O	-4.2171670	-1.7204670	1.2697560
O	-3.4886280	0.3420230	1.5418780
H	-3.0324090	1.0311330	0.9870310
O	3.1074360	-1.8279260	-0.1144080
C	4.3824620	-2.4081490	-0.0095380
H	4.2544930	-3.4812740	-0.1707040
H	5.0704860	-2.0097730	-0.7684090
H	4.8201130	-2.2432920	0.9850570
N	-2.2833370	1.5273960	-0.4876900
H	-2.2760290	2.5091560	-0.7380850

Electronic Energy (RPW6B95D3/def2-SVP)= -862.763748460 (Hartree/Particle)

Dipole Moment= 7.5973 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302662 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.461086
Sum of electronic and thermal Energies= -862.445114
Sum of electronic and thermal Enthalpies= -862.444170
Sum of electronic and thermal Free Energies= -862.505171

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.768032389 (Hartree/Particle)
Corrected Free Energy= -863.509454929 (Hartree/Particle)

CONFORMER 2

CARTESIAN COORDINATES

C	0.6062700	-0.9624260	-0.3770360
C	-0.7583630	-0.3843760	-0.5584330
C	0.0290890	1.9272660	-0.0195120
H	0.8931840	-1.5430700	-1.2699530
H	0.5887580	-1.7208220	0.4251230
H	0.0158910	2.7541620	-0.7479210
H	-0.2642570	2.3919990	0.9355840
C	-1.8568610	-1.3602530	-0.8754810
C	-3.2677690	0.6649000	-1.2273020
C	-3.2336150	-0.7510350	-0.6586230
H	-1.7491520	-2.2470030	-0.2361930
H	-1.7715330	-1.7199780	-1.9118640

H	-4.2606980	1.1062080	-1.0998500
H	-3.0551410	0.6075380	-2.3089710
H	-4.0083410	-1.3484920	-1.1572480
C	-1.0137110	0.9268760	-0.4004880
C	1.6855780	0.0312660	-0.0786040
C	1.4254420	1.3875490	0.0907920
C	3.0113800	-0.4310510	0.0411940
C	2.4763830	2.2711680	0.3721760
H	2.2624280	3.3310300	0.5014010
C	3.7733890	1.8033160	0.4850660
H	4.5863760	2.4933740	0.7036440
C	4.0543550	0.4469180	0.3209230
H	5.0757270	0.0899340	0.4122720
C	-3.5941020	-0.7226740	0.8101730
O	-2.9395280	-1.1964130	1.7029390
O	-4.7628570	-0.1140620	1.0254740
H	-4.9323710	-0.1315150	1.9790230
O	3.1747600	-1.7616450	-0.1324610
C	4.4661090	-2.3037090	-0.0304460
H	4.3715460	-3.3785230	-0.2036230
H	5.1441600	-1.8766670	-0.7828440
H	4.8967130	-2.1369300	0.9670320
N	-2.2960800	1.4569350	-0.5158640
H	-2.3211790	2.4447520	-0.7285730

Electronic Energy (RPW6B95D3/def2-SVP)= -862.760024957 (Hartree/Particle)

Dipole Moment= 2.4147 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301663 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.458362
Sum of electronic and thermal Energies= -862.441923
Sum of electronic and thermal Enthalpies= -862.440979
Sum of electronic and thermal Free Energies= -862.503326

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.764093996 (Hartree/Particle)
Corrected Free Energy= -863.507395039 (Hartree/Particle)

CONFORMER 3

CARTESIAN COORDINATES

C	0.5641550	-0.9240920	-0.5703280
C	-0.8104840	-0.3412610	-0.6292020
C	0.0326990	1.9731600	-0.1731270
H	0.8256770	-1.3729240	-1.5445900
H	0.5806890	-1.7828350	0.1198690
H	0.0657860	2.7082480	-0.9932180
H	-0.2606870	2.5521900	0.7154210
C	-1.9381360	-1.2897790	-0.9425810
C	-3.3807570	0.7390180	-1.1019790
C	-3.3019950	-0.6999280	-0.5844000
H	-1.7871460	-2.2387760	-0.4068630
H	-1.9320980	-1.5553030	-2.0102110
H	-4.3430650	1.1884610	-0.8348530
H	-3.3212230	0.7072790	-2.2026190
H	-4.1070150	-1.2762450	-1.0492730
C	-1.0456550	0.9829430	-0.4732830
C	1.6415660	0.0348140	-0.1687680
C	1.4010760	1.3904420	0.0307900
C	2.9463230	-0.4635300	0.0180110
C	2.4486050	2.2376070	0.4162390
H	2.2497540	3.2967920	0.5713090

C	3.7243740	1.7338150	0.5976270
H	4.5352000	2.3952410	0.8972870
C	3.9864000	0.3783280	0.4000130
H	4.9912670	-0.0066260	0.5449220
C	-3.5973880	-0.7236450	0.9043780
O	-4.7064850	-0.8695110	1.3501670
O	-2.5610860	-0.5526810	1.7229490
H	-1.7497460	-0.3809070	1.2036880
O	3.0920380	-1.7889030	-0.1997810
C	4.3596660	-2.3682960	-0.0246500
H	4.7190360	-2.2479840	1.0070190
H	4.2523380	-3.4332800	-0.2442950
H	5.1005520	-1.9325930	-0.7096340
N	-2.3156760	1.5133720	-0.5215050
H	-2.3880090	2.5168420	-0.5925580

Electronic Energy (RPW6B95D3/def2-SVP)= -862.759647187 (Hartree/Particle)

Dipole Moment= 6.9596 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301877 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457770
Sum of electronic and thermal Energies= -862.441394
Sum of electronic and thermal Enthalpies= -862.440449
Sum of electronic and thermal Free Energies= -862.502218

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.764640522 (Hartree/Particle)
Corrected Free Energy= -863.507211335 (Hartree/Particle)

CONFORMER 4

CARTESIAN COORDINATES

C	0.5473740	-0.9207530	-0.5581400
C	-0.8259720	-0.3487460	-0.6933350
C	-0.0472800	1.9544530	-0.1046460
H	0.8528140	-1.4125600	-1.4981230
H	0.5341220	-1.7493310	0.1695420
H	-0.0265260	2.7726280	-0.8403620
H	-0.3741570	2.4318570	0.8342150
C	-1.9351510	-1.3143810	-0.9988140
C	-3.4183410	0.6647540	-1.1661040
C	-3.2750240	-0.7271410	-0.5655650
H	-1.7541090	-2.2612100	-0.4753280
H	-1.9786940	-1.5626340	-2.0700350
H	-4.3615660	1.1244330	-0.8589430
H	-3.4403040	0.5640890	-2.2606780
H	-4.0948520	-1.3710830	-0.9126990
C	-1.0851380	0.9627020	-0.5240260
C	1.6075770	0.0559460	-0.1532860
C	1.3370430	1.4019600	0.0727960
C	2.9255870	-0.4144810	0.0126930
C	2.3699640	2.2662690	0.4611930
H	2.1482560	3.3180490	0.6355200
C	3.6590150	1.7902870	0.6211010
H	4.4576130	2.4655790	0.9230240
C	3.9504430	0.4444970	0.3979680
H	4.9654910	0.0808840	0.5261930
C	-3.3961200	-0.6511740	0.9393550
O	-3.8029120	0.3063660	1.5495280
O	-3.0255120	-1.7785800	1.5479290
H	-3.1453850	-1.6507500	2.5009650
O	3.0998400	-1.7335390	-0.2261410

C	4.3840040	-2.2831400	-0.0817150
H	5.1024870	-1.8176370	-0.7711430
H	4.7581530	-2.1709030	0.9457210
H	4.3001970	-3.3468770	-0.3174910
N	-2.3301740	1.5306970	-0.7675940
H	-2.5915450	2.2302860	-0.0845890

Electronic Energy (RPW6B95D3/def2-SVP)= -862.759384025 (Hartree/Particle)

Dipole Moment= 1.9644 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301494 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457890
Sum of electronic and thermal Energies= -862.441352
Sum of electronic and thermal Enthalpies= -862.440408
Sum of electronic and thermal Free Energies= -862.503200

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.763219899 (Hartree/Particle)
Corrected Free Energy= -863.507035874 (Hartree/Particle)

CONFORMER 5

CARTESIAN COORDINATES

C	0.5887260	-0.9549260	-0.4966920
C	-0.7912220	-0.4041380	-0.6521190
C	-0.0383810	1.9258800	-0.1347620
H	0.8970440	-1.4815360	-1.4165410
H	0.5844800	-1.7533540	0.2640910
H	-0.0325290	2.7233100	-0.8931610
H	-0.3664750	2.4253410	0.7921960
C	-1.8846410	-1.4011890	-0.9184790
C	-3.3635110	0.5614980	-1.2302790
C	-3.2429190	-0.8104240	-0.5719260
H	-1.7117640	-2.2972260	-0.3088890
H	-1.8833280	-1.7350150	-1.9667580
H	-4.3331930	1.0199550	-1.0226170
H	-3.2952500	0.4166530	-2.3184600
H	-4.0487380	-1.4611000	-0.9408460
C	-1.0638000	0.9085800	-0.5218140
C	1.6399080	0.0476780	-0.1334710
C	1.3540410	1.3970870	0.0499420
C	2.9650700	-0.4002680	0.0372570
C	2.3786430	2.2869620	0.4005990
H	2.1447430	3.3411340	0.5413440
C	3.6748310	1.8329670	0.5655610
H	4.4671640	2.5278970	0.8379650
C	3.9817500	0.4841380	0.3851700
H	5.0025110	0.1384250	0.5171410
C	-3.4199000	-0.7489820	0.9303560
O	-2.9169490	-1.5094510	1.7176820
O	-4.2345250	0.2368030	1.3151350
H	-4.3189120	0.1891740	2.2792720
O	3.1541700	-1.7243470	-0.1588370
C	4.4462410	-2.2533540	-0.0084110
H	5.1533210	-1.8004460	-0.7177390
H	4.8272280	-2.1053170	1.0119460
H	4.3738400	-3.3247720	-0.2108710
N	-2.3171710	1.4512100	-0.7874520
H	-2.6105330	2.1653180	-0.1333360

Electronic Energy (RPW6B95D3/def2-SVP)= -862.758727010 (Hartree/Particle)

Dipole Moment= 1.5552 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301447 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457280
Sum of electronic and thermal Energies= -862.440726
Sum of electronic and thermal Enthalpies= -862.439781
Sum of electronic and thermal Free Energies= -862.503181

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762527277 (Hartree/Particle)
Corrected Free Energy= -863.506981267 (Hartree/Particle)

CONFORMER 6

CARTESIAN COORDINATES

C	0.5780790	-0.9353780	-0.4297400
C	-0.7823100	-0.3434740	-0.5946050
C	0.0196170	1.9488880	0.0012230
H	0.8649410	-1.4873260	-1.3408310
H	0.5541010	-1.7202990	0.3464000
H	0.0163750	2.7866480	-0.7148230
H	-0.2731220	2.4018860	0.9619880
C	-1.8884180	-1.2968100	-0.9496400
C	-3.3102130	0.7356930	-1.1895440
C	-3.2606050	-0.6977940	-0.6710570
H	-1.7661530	-2.2314250	-0.3874920
H	-1.8300180	-1.5795710	-2.0118790
H	-4.2972540	1.1677230	-0.9977270
H	-3.1471620	0.7182060	-2.2807280
H	-4.0401500	-1.2795130	-1.1807900
C	-1.0310920	0.9644300	-0.3997650
C	1.6619240	0.0415960	-0.0951400
C	1.4107920	1.3949470	0.1082140
C	2.9829980	-0.4344450	0.0234430
C	2.4664850	2.2622730	0.4210370
H	2.2599510	3.3200920	0.5764440
C	3.7589390	1.7811820	0.5315090
H	4.5755010	2.4588370	0.7742340
C	4.0305490	0.4273240	0.3343410
H	5.0482420	0.0596190	0.4243650
C	-3.6665860	-0.6841040	0.7886520
O	-4.6533750	-0.1261620	1.1989670
O	-2.8463590	-1.3610560	1.5905790
H	-3.2011590	-1.2986750	2.4902460
O	3.1372880	-1.7613790	-0.1833980
C	4.4230600	-2.3166360	-0.0815470
H	4.3215460	-3.3861200	-0.2816610
H	5.1123130	-1.8772140	-0.8164190
H	4.8446140	-2.1775310	0.9240210
N	-2.3093810	1.5041140	-0.4927010
H	-2.3366320	2.4984840	-0.6699100

Electronic Energy (RPW6B95D3/def2-SVP)= -862.758709376 (Hartree/Particle)

Dipole Moment= 2.5001 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301694 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457016

Sum of electronic and thermal Energies= -862.440525
Sum of electronic and thermal Enthalpies= -862.439581
Sum of electronic and thermal Free Energies= -862.502682

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762659871 (Hartree/Particle)
Corrected Free Energy= -863.506632495 (Hartree/Particle)

CONFORMER 7

CARTESIAN COORDINATES

C	-0.6188280	0.8480350	0.0399090
C	0.6585590	0.0749520	0.0285000
C	-0.5364500	-2.1173990	-0.1097380
H	-0.6399730	1.5589420	-0.8042850
H	-0.6559610	1.5059670	0.9251080
H	-0.4855410	-2.7248070	-1.0272730
H	-0.5138700	-2.8512370	0.7123090
C	1.9218930	0.8857110	0.0655710
C	3.0854290	-1.3159250	0.3289350
C	3.1368490	0.0480370	-0.3353350
H	2.0744680	1.3153560	1.0696970
H	1.8355160	1.7476200	-0.6101850
H	3.1359100	-1.1764630	1.4238450
H	3.9581800	-1.9104970	0.0400430
H	3.0996740	-0.1009930	-1.4251900
C	0.6924030	-1.2692510	-0.0328790
C	-1.8647200	0.0193340	0.0023470
C	-1.8377260	-1.3699730	-0.0705100
C	-3.1092470	0.6792470	0.0355610
C	-3.0394260	-2.0906090	-0.1075020
H	-3.0084430	-3.1776610	-0.1634880
C	-4.2541630	-1.4290430	-0.0730690
H	-5.1846020	-1.9932660	-0.1020600
C	-4.3017160	-0.0367710	-0.0013140
H	-5.2602440	0.4727350	0.0244290
C	4.4344160	0.7483790	-0.0443490
O	5.3570410	0.2738430	0.5693830
O	4.4656010	1.9827160	-0.5483710
H	5.3237320	2.3731240	-0.3246070
O	-3.0430880	2.0275960	0.1029690
C	-4.2392720	2.7623970	0.1398140
H	-3.9598130	3.8174820	0.1929510
H	-4.8435770	2.5955470	-0.7630370
H	-4.8439700	2.5057280	1.0210820
N	1.8801770	-1.9871930	-0.0868610
H	1.8028260	-2.9431930	0.2311840

Electronic Energy (RPW6B95D3/def2-SVP)= -862.758334427 (Hartree/Particle)

Dipole Moment= 2.0544 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301534 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.456801
Sum of electronic and thermal Energies= -862.440181
Sum of electronic and thermal Enthalpies= -862.439236
Sum of electronic and thermal Free Energies= -862.501925

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.763439082 (Hartree/Particle)
Corrected Free Energy= -863.507029655 (Hartree/Particle)

CONFORMER 8

CARTESIAN COORDINATES

C	-0.6542670	0.8671590	0.1092600
C	0.6395400	0.1199780	0.1171540
C	-0.5165940	-2.0998340	0.0537490
H	-0.6647960	1.5846470	-0.7279970
H	-0.7279750	1.5158220	0.9996060
H	-0.4186530	-2.7683060	-0.8177820
H	-0.5156950	-2.7751920	0.9228630
C	1.8888270	0.9508410	0.0814130
C	3.1017600	-1.1855200	0.4638810
C	3.0948350	0.1284230	-0.3332370
H	2.0933580	1.4226300	1.0549360
H	1.7496450	1.7860710	-0.6200570
H	3.2243130	-0.9345640	1.5297930
H	3.9543050	-1.8075250	0.1763490
H	3.0282480	-0.1390950	-1.3970350
C	0.6941310	-1.2250040	0.1289110
C	-1.8826610	0.0152960	0.0236930
C	-1.8289980	-1.3745860	-0.0174610
C	-3.1379490	0.6537390	-0.0254190
C	-3.0146230	-2.1165010	-0.1096720
H	-2.9624880	-3.2037430	-0.1411750
C	-4.2399760	-1.4760060	-0.1587560
H	-5.1577940	-2.0568620	-0.2305470
C	-4.3144370	-0.0836800	-0.1166510
H	-5.2811250	0.4092680	-0.1555140
C	4.3875370	0.8706300	-0.1441760
O	4.5228410	1.9040140	0.4607260
O	5.4135870	0.2319340	-0.7127300
H	6.2177430	0.7412240	-0.5320610
O	-3.0983690	2.0041540	0.0209140
C	-4.3069110	2.7179600	-0.0237200
H	-4.0488300	3.7786260	0.0263010
H	-4.8557390	2.5250090	-0.9563100
H	-4.9566310	2.4654350	0.8261580
N	1.8847200	-1.9270860	0.2721950
H	1.9633210	-2.7520200	-0.3080060

Electronic Energy (RPW6B95D3/def2-SVP)= -862.757449729 (Hartree/Particle)

Dipole Moment= 2.5963 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301280 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.456170
Sum of electronic and thermal Energies= -862.439428
Sum of electronic and thermal Enthalpies= -862.438484
Sum of electronic and thermal Free Energies= -862.501789

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762802668 (Hartree/Particle)
Corrected Free Energy= -863.507141939 (Hartree/Particle)

CONFORMER 9

CARTESIAN COORDINATES

C	0.6235180	-0.8612900	-0.0114880
C	-0.6559130	-0.0918840	0.0041320
C	0.5324510	2.1083470	-0.0521630
H	0.6499470	-1.5377340	-0.8834110
H	0.6596050	-1.5536480	0.8469580
H	0.4829430	2.7451280	-0.9496680

H	0.5050080	2.8145730	0.7934430
C	-1.9190740	-0.9033260	0.0066940
C	-3.0882070	1.2722220	0.3335250
C	-3.1286320	-0.0629370	-0.4097370
H	-2.1018060	-1.3405300	1.0007190
H	-1.8126980	-1.7567390	-0.6791250
H	-3.1437130	1.0688070	1.4172750
H	-3.9553750	1.8879560	0.0675360
H	-3.0793970	0.1406530	-1.4847250
C	-0.6931990	1.2535070	-0.0080400
C	1.8667560	-0.0276540	-0.0115260
C	1.8357230	1.3633450	-0.0330010
C	3.1132080	-0.6846700	0.0040190
C	3.0353270	2.0883640	-0.0366940
H	3.0011920	3.1766360	-0.0525510
C	4.2519370	1.4295770	-0.0203500
H	5.1807170	1.9972420	-0.0234620
C	4.3035570	0.0357760	0.0001040
H	5.2635450	-0.4714810	0.0120760
C	-4.4224430	-0.7902790	-0.1775180
O	-5.1955730	-1.1322110	-1.0357580
O	-4.6384400	-1.0311690	1.1193050
H	-5.4815000	-1.5022540	1.1979350
O	3.0509980	-2.0347500	0.0210140
C	4.2492880	-2.7668680	0.0375970
H	4.8579160	-2.5654020	-0.8552350
H	4.8483840	-2.5406150	0.9309370
H	3.9728700	-3.8239990	0.0507410
N	-1.8842260	1.9654340	-0.0397440
H	-1.8197180	2.9150250	0.2989500

Electronic Energy (RPW6B95D3/def2-SVP)= -862.756679750 (Hartree/Particle)

Dipole Moment= 3.2046 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301547 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.455133
Sum of electronic and thermal Energies= -862.438420
Sum of electronic and thermal Enthalpies= -862.437476
Sum of electronic and thermal Free Energies= -862.500671

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762499236 (Hartree/Particle)
Corrected Free Energy= -863.506490486 (Hartree/Particle)

CONFORMER 10

CARTESIAN COORDINATES

C	0.6270800	0.8596600	-0.0951730
C	-0.6545970	0.0926780	-0.1028870
C	0.5307110	-2.1097230	-0.0023520
H	0.6303400	1.5746230	0.7446460
H	0.6894340	1.5119380	-0.9835580
H	0.4473860	-2.7522220	0.8899920
H	0.5332630	-2.8106540	-0.8508270
C	-1.9187330	0.9005490	-0.0884910
C	-3.1082560	-1.2526540	-0.3880280
C	-3.1005540	0.0649270	0.4015010
H	-2.1515270	1.3050870	-1.0853800
H	-1.7841190	1.7741300	0.5656400
H	-3.2723630	-1.0075860	-1.4485860
H	-3.9370380	-1.8946540	-0.0726580
H	-2.9774340	-0.1641510	1.4658500

C	-0.6916460	-1.2530110	-0.0949410
C	1.8675730	0.0249840	-0.0175630
C	1.8337400	-1.3651170	0.0378690
C	3.1143170	0.6812200	0.0078830
C	3.0310370	-2.0895090	0.1188640
H	2.9948230	-3.1770200	0.1610480
C	4.2478880	-1.4315060	0.1437470
H	5.1746890	-1.9989340	0.2068230
C	4.3022150	-0.0387470	0.0883070
H	5.2622850	0.4680750	0.1086100
C	-4.4109650	0.7828300	0.2725770
O	-5.1831180	0.9983160	1.1727530
O	-4.6582390	1.1578540	-0.9870320
H	-5.5201710	1.6000980	-1.0009030
O	3.0548150	2.0304260	-0.0491760
C	4.2536920	2.7615040	-0.0290390
H	4.8941990	2.5104000	-0.8862820
H	3.9798890	3.8179390	-0.0845740
H	4.8189280	2.5847330	0.8969250
N	-1.8724450	-1.9704150	-0.2242070
H	-1.9241400	-2.8101730	0.3366910

Electronic Energy (RPW6B95D3/def2-SVP)= -862.756482340 (Hartree/Particle)

Dipole Moment= 1.8950 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301594 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454888
Sum of electronic and thermal Energies= -862.438198
Sum of electronic and thermal Enthalpies= -862.437254
Sum of electronic and thermal Free Energies= -862.500028

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.762327183 (Hartree/Particle)
Corrected Free Energy= -863.505872843 (Hartree/Particle)

CONFORMER 11

CARTESIAN COORDINATES

C	0.5508070	-0.9262550	-0.5428630
C	-0.8221700	-0.3532720	-0.6759780
C	-0.0415270	1.9536000	-0.1097220
H	0.8521920	-1.4238660	-1.4810110
H	0.5410400	-1.7497140	0.1907750
H	-0.0222340	2.7672950	-0.8501710
H	-0.3670880	2.4357500	0.8270150
C	-1.9336410	-1.3180790	-0.9715640
C	-3.4077400	0.6540600	-1.1721710
C	-3.2779490	-0.7285550	-0.5462280
H	-1.7279490	-2.2749540	-0.4674420
H	-1.9820910	-1.5768830	-2.0397320
H	-4.3544880	1.1193050	-0.8862480
H	-3.4127510	0.5360760	-2.2649750
H	-4.0966110	-1.3734850	-0.8957660
C	-1.0806170	0.9601250	-0.5211990
C	1.6120810	0.0534500	-0.1485180
C	1.3428400	1.4011920	0.0682270
C	2.9300860	-0.4169440	0.0168170
C	2.3774450	2.2675120	0.4472710
H	2.1570920	3.3206800	0.6145360
C	3.6665780	1.7916280	0.6069700
H	4.4664540	2.4685280	0.9017300
C	3.9565680	0.4441080	0.3928500

H	4.9717250	0.0807390	0.5207940
C	-3.4171170	-0.6205890	0.9620110
O	-3.7832380	0.3725600	1.5334150
O	-3.1330120	-1.7191310	1.6686530
H	-2.8654790	-2.4416020	1.0876520
O	3.1021970	-1.7377490	-0.2131480
C	4.3862380	-2.2878900	-0.0686840
H	5.1031810	-1.8277030	-0.7632190
H	4.7632840	-2.1693450	0.9569430
H	4.3004910	-3.3530290	-0.2972540
N	-2.3246500	1.5247550	-0.7718060
H	-2.5930770	2.2189470	-0.0856520

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754663893 (Hartree/Particle)

Dipole Moment= 4.5494 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301536 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.453128
Sum of electronic and thermal Energies= -862.436639
Sum of electronic and thermal Enthalpies= -862.435694
Sum of electronic and thermal Free Energies= -862.498169

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759752889 (Hartree/Particle)
Corrected Free Energy= -863.503257996 (Hartree/Particle)

CONFORMERS of IMINE TRANS-2

CONFORMER 1

CARTESIAN COORDINATES

C	0.6624085239	0.7286708891	0.7221728626
C	-0.5436342673	0.1754250845	-0.0353911300
C	0.5842930697	-2.0782478583	0.4813371395
H	0.4991895039	0.6067982758	1.8047428313
H	0.7586578686	1.8025802898	0.5385319145
H	0.5971606163	-2.2639986448	1.5682689885
H	0.5209454134	-3.0661354877	0.0136844785
H	-0.3181067690	0.2910897412	-1.1088680238
C	-1.8458063140	0.8940954837	0.2616222809
C	-3.0493197556	-1.2846619604	0.0520289809
C	-2.9740031589	0.1662052648	-0.4403596145
H	-1.7959430710	1.9397225650	-0.0612035227
H	-2.0317360876	0.9039163249	1.3451108232
H	-3.6622817084	-1.8784566561	-0.6375440297
H	-3.5785944116	-1.3228193397	1.0174741492
C	-0.6896232952	-1.3111601685	0.2034293978
N	-1.7848493472	-1.9514495921	0.2342688659
C	1.9079013678	0.0151741888	0.2901068578
C	1.8532121483	-1.3677147924	0.1106371805
C	3.1012726223	0.7012696658	0.0108029474
C	2.9734042334	-2.0632204102	-0.3503272257
H	2.9200968185	-3.1413362812	-0.4910558534
C	4.1466204162	-1.3753796248	-0.6224184009
H	5.0226344941	-1.9123825070	-0.9817417774
C	4.2216434750	0.0040132725	-0.4437531404
H	5.1483805514	0.5254798722	-0.6633354374
C	-4.2971480945	0.8617109482	-0.2812643555
O	-4.4732088747	1.9002855832	0.3030345057
O	-5.2889345171	0.1859785193	-0.8658360843

H	-6.1115050098	0.6767019608	-0.7194526261
H	-2.7685374841	0.1428899400	-1.5217263695
O	3.0816559894	2.0378297145	0.2082745239
C	4.2370915475	2.7835900802	-0.0772121845
H	5.0845838230	2.4716741762	0.5492405789
H	4.5264555806	2.6923956539	-1.1336925466
H	3.9988164798	3.8278225539	0.1392192006

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755447425 (Hartree/Particle)

Dipole Moment= 2.5720 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301307 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454140
Sum of electronic and thermal Energies= -862.437733
Sum of electronic and thermal Enthalpies= -862.436789
Sum of electronic and thermal Free Energies= -862.499205

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761827821 (Hartree/Particle)
Corrected Free Energy= -863.505585396 (Hartree/Particle)

CONFORMER 2

CARTESIAN COORDINATES

C	0.6444535054	0.7070888228	0.7109000375
C	-0.5557192142	0.1425715223	-0.0481836120
C	0.5949266222	-2.1012860043	0.4620204217
H	0.4821618932	0.5814162959	1.7930834338
H	0.7303526478	1.7821901360	0.5291114459
H	0.6114002351	-2.2952074349	1.5474009110
H	0.5402199019	-3.0862129719	-0.0130041511
H	-0.3326981438	0.2631775677	-1.1214396987
C	-1.8634672597	0.8482338907	0.2540523765
C	-3.0464010141	-1.3331715443	0.0532299226
C	-2.9900570818	0.1118734567	-0.4615717318
H	-1.8121892691	1.8962518644	-0.0639664390
H	-2.0520003265	0.8445825151	1.3363410932
H	-3.6591392820	-1.9441286574	-0.6231312446
H	-3.5658322876	-1.3520660194	1.0233661435
C	-0.6865435419	-1.3445950256	0.1911573273
N	-1.7769844866	-1.9920543582	0.2302513895
C	1.8966899521	0.0067913167	0.2768936047
C	1.8561689635	-1.3761609708	0.0936721356
C	3.0828360575	0.7059997557	-0.0007393388
C	2.9835136094	-2.0585707247	-0.3695083195
H	2.9413556446	-3.1367500599	-0.5134408606
C	4.1495207980	-1.3578668316	-0.6396957826
H	5.0309636453	-1.8848479732	-1.0005599739
C	4.2103227479	0.0216919323	-0.4571860199
H	5.1315748485	0.5534915055	-0.6750876005
C	-4.3258639446	0.7812595687	-0.3017793159
O	-5.0655769197	1.0843837086	-1.2029869374
O	-4.6297749421	1.0000417010	0.9810394438
H	-5.5039440875	1.4166594261	1.0128093651
H	-2.7873158959	0.1029101881	-1.5386864314
O	3.0494473231	2.0416856624	0.2003926766
C	4.1954929260	2.8006536843	-0.0885262125
H	4.4838571372	2.7109653970	-1.1453771412
H	3.9452369911	3.8423317664	0.1266368313
H	5.0477746922	2.4999296504	0.5368797359

Electronic Energy (RPW6B95D3/def2-SVP)= -862.753984482 (Hartree/Particle)

Dipole Moment= 4.1018 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301621 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452364
Sum of electronic and thermal Energies= -862.435953
Sum of electronic and thermal Enthalpies= -862.435009
Sum of electronic and thermal Free Energies= -862.497638

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760960586 (Hartree/Particle)
Corrected Free Energy= -863.504614104 (Hartree/Particle)

CONFORMER 3

CARTESIAN COORDINATES

C	0.7949470813	0.3787992308	-1.5518237320
C	-0.6310648074	-0.1551012903	-1.3246175220
C	0.6646147574	-2.2851373911	-0.8380539602
H	0.7819742115	1.4718274911	-1.5856399854
H	1.1437266710	0.0445432655	-2.5397321751
H	0.5755582248	-3.2740713684	-0.3818029048
H	0.8782801830	-2.4073082517	-1.9115570647
H	-1.0908306286	-0.2979250468	-2.3148977587
C	-1.5213451090	0.7845884671	-0.5296639600
C	-2.6978449311	-1.2157008096	0.4185433035
C	-2.8659793125	0.1138581709	-0.3313662877
H	-1.6408109542	1.7413543627	-1.0496632018
H	-1.0627664132	1.0040575560	0.4453609787
H	-3.5838818761	-1.8443451792	0.2645976591
H	-2.6622805230	-1.0285002723	1.5033759819
C	-0.6166229084	-1.5166069785	-0.6598710823
N	-1.5222534760	-1.9851468255	0.0953006839
C	1.7716913178	-0.1065727652	-0.5225858844
C	1.7442987437	-1.4617157990	-0.1866651969
C	2.7184367721	0.7342751632	0.0824718153
C	2.6387637338	-1.9814693905	0.7488218523
H	2.5990069088	-3.0369282983	1.0110670381
C	3.5720246372	-1.1399311664	1.3385392643
H	4.2771283498	-1.5347091162	2.0678331356
C	3.6186370469	0.2140599592	1.0149786252
H	4.3553708882	0.8544485777	1.4905338330
C	-3.8593553044	1.0018914534	0.3648565638
O	-3.6582612583	2.1380338187	0.7106199011
O	-5.0220042737	0.3796670673	0.5730057727
H	-5.6127769684	0.9958422922	1.0314514482
H	-3.2983594794	-0.1085648397	-1.3191127310
O	2.6954666591	2.0312450295	-0.2943792020
C	3.5976931857	2.9281919303	0.3010449514
H	4.6405515020	2.6526674749	0.0900753925
H	3.3943795073	3.9112802515	-0.1304828872
H	3.4586628496	2.9778222728	1.3902133401

Electronic Energy (RPW6B95D3/def2-SVP)= -862.753817507 (Hartree/Particle)

Dipole Moment= 1.7761 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301831 (Hartree/Particle)

Sum of electronic and zero-point Energies= -862.451986
Sum of electronic and thermal Energies= -862.435770
Sum of electronic and thermal Enthalpies= -862.434826
Sum of electronic and thermal Free Energies= -862.496851

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760302357 (Hartree/Particle)
Corrected Free Energy= -863.503335850 (Hartree/Particle)

CONFORMER 4

CARTESIAN COORDINATES

C	0.7252413943	0.2709116889	-1.5642695972
C	-0.6784688041	-0.2916009192	-1.2784654099
C	0.6945469565	-2.3563055265	-0.7224282547
H	0.6793960889	1.3597539262	-1.6559686177
H	1.0629372572	-0.1063641772	-2.5404650076
H	0.6450749765	-3.3251215300	-0.2194587481
H	0.8968341331	-2.5222778921	-1.7923371433
H	-1.1630392490	-0.4824572247	-2.2485960838
C	-1.5699447698	0.6559120090	-0.4945454397
C	-2.6912615030	-1.3452239865	0.5254172718
C	-2.9037959144	-0.0426197753	-0.2386523882
H	-1.7273970709	1.5868294435	-1.0491676459
H	-1.0888246517	0.9161600245	0.4598676599
H	-3.5537972677	-2.0103413348	0.3836026315
H	-2.6782037464	-1.1287690012	1.6032843926
C	-0.6102390045	-1.6242098287	-0.5603412917
N	-1.4921657034	-2.0893942486	0.2235553706
C	1.7350711334	-0.1315847902	-0.5312284053
C	1.7562089473	-1.4686798304	-0.1287661347
C	2.6637681808	0.7676861577	0.0145594052
C	2.6811544643	-1.9125388685	0.8161365137
H	2.6795616526	-2.9542800792	1.1310020515
C	3.5954027261	-1.0134649722	1.3480326779
H	4.3233988613	-1.3488321854	2.0845553081
C	3.5940693362	0.3233517821	0.9567682857
H	4.3168967415	1.0093943506	1.3879172217
C	-3.8905677616	0.8500563549	0.4669487308
O	-4.4249565235	0.6091470796	1.5197750970
O	-4.1236089486	1.9720298717	-0.2161192872
H	-4.7585152613	2.5016177191	0.2890746256
H	-3.3467959400	-0.2541946365	-1.2234865680
O	2.5939229185	2.0425443331	-0.4266856421
C	3.4822622719	2.9941143113	0.1009900515
H	3.3610941409	3.1011387667	1.1881550611
H	4.5281531669	2.7336153478	-0.1140584352
H	3.2454806262	3.9460334784	-0.3804839389

Electronic Energy (RPW6B95D3/def2-SVP)= -862.753753135 (Hartree/Particle)

Dipole Moment= 5.0151 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302063 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.451690
Sum of electronic and thermal Energies= -862.435552
Sum of electronic and thermal Enthalpies= -862.434607
Sum of electronic and thermal Free Energies= -862.496547

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759893025 (Hartree/Particle)
Corrected Free Energy= -863.502686890 (Hartree/Particle)

CONFORMER 5

CARTESIAN COORDINATES

C	0.7358422269	0.3344894678	-1.5767662616
C	-0.6791281768	-0.2068930222	-1.3035941525
C	0.6478459664	-2.3190730131	-0.8189940603
H	0.7136753607	1.4266911055	-1.6286150424
H	1.0600448808	-0.0139867227	-2.5680738767
H	0.5783033337	-3.3010748662	-0.3446793989
H	0.8353846560	-2.4574523410	-1.8953813594
H	-1.1669162699	-0.3628809504	-2.2781252477
C	-1.5504335972	0.7363872751	-0.4923395997
C	-2.6902085812	-1.2533043992	0.5036009504
C	-2.8990655407	0.0616421758	-0.2640448173
H	-1.6759742338	1.6885939086	-1.0211326923
H	-1.0725648061	0.9560621874	0.4725034687
H	-3.5712069044	-1.8976841015	0.3826711873
H	-2.6271481280	-1.0367124201	1.5805020019
C	-0.6350839988	-1.5583615029	-0.6213470436
N	-1.5172966325	-2.0201926314	0.1645079369
C	1.7431026739	-0.1267081998	-0.5660715133
C	1.7371227464	-1.4768085387	-0.2089949693
C	2.6971442886	0.7320959762	0.0006173430
C	2.6620741473	-1.9740069873	0.7091598558
H	2.6396580250	-3.0256768514	0.9881223971
C	3.6032085173	-1.1150939252	1.2599233838
H	4.3320264732	-1.4925060913	1.9749625397
C	3.6277214662	0.2342765050	0.9155047737
H	4.3710282928	0.8882975001	1.3613582306
C	-3.8797276140	0.9422028785	0.4586220061
O	-4.9878224950	1.2144410719	0.0723008912
O	-3.3903960359	1.3981887715	1.6154925232
H	-4.0733184392	1.9440515868	2.0330398656
H	-3.3549866583	-0.1541437104	-1.2369741720
O	2.6510784333	2.0231943937	-0.3937456920
C	3.5588637255	2.9374978137	0.1658788326
H	4.5987410679	2.6700255034	-0.0687111980
H	3.3337701857	3.9125109590	-0.2730653135
H	3.4477476468	3.0003228779	1.2575734815

Electronic Energy (RPW6B95D3/def2-SVP)= -862.752336192 (Hartree/Particle)

Dipole Moment= 4.2321 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302040 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.450296
Sum of electronic and thermal Energies= -862.434067
Sum of electronic and thermal Enthalpies= -862.433123
Sum of electronic and thermal Free Energies= -862.495325

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759406635 (Hartree/Particle)
Corrected Free Energy= -863.502395443 (Hartree/Particle)

CONFORMER 6

CARTESIAN COORDINATES

C	0.8781762388	0.0470429279	-1.8221410060
C	-0.6197882054	-0.2347403043	-1.7014974125
C	0.2935526791	-2.2599575835	-0.4259518983
H	1.0479699065	1.0572485337	-2.2046908237
H	1.3158641698	-0.6467608538	-2.5550145126

H	-0.0270854666	-3.0504431864	0.2575691327
H	0.7665128801	-2.7370959104	-1.3002221439
H	-1.0316996035	-0.4250181609	-2.7048462205
C	-1.3951250186	0.9540536047	-1.1028908629
C	-3.1032507272	-0.8896473358	-1.0085548414
C	-2.7337957326	0.5213889732	-0.5110845939
H	-1.5480024358	1.7028979386	-1.8866418839
H	-0.7842350572	1.4129383267	-0.3178173566
H	-3.1906931361	-0.8603876278	-2.1064544096
H	-4.0758313595	-1.1919842210	-0.6084890165
C	-0.8977111520	-1.4776753332	-0.8972787419
N	-2.0820600678	-1.8223966775	-0.5816655605
C	1.5568667475	-0.1436124876	-0.4978414012
C	1.2715932734	-1.3111087830	0.2134632399
C	2.4369883151	0.8006469709	0.0509750751
C	1.8527098220	-1.5441473566	1.4599130621
H	1.6164592494	-2.4540362961	2.0082780574
C	2.7287917361	-0.6060615309	1.9884796548
H	3.1899302040	-0.7786334480	2.9592790750
C	3.0249579911	0.5652538029	1.2958353017
H	3.7081677396	1.2873536394	1.7324579297
C	-2.6982445305	0.4969507315	1.0015655913
O	-1.7310590400	0.7079122928	1.6880922888
O	-3.8912222537	0.1970909422	1.5181977403
H	-3.7997412361	0.1738155271	2.4823289137
H	-3.5400845782	1.2093904252	-0.7936727542
O	2.6625391331	1.9110260286	-0.6847891570
C	3.5110366448	2.9047153263	-0.1690311025
H	3.5422094845	3.7074751617	-0.9096404400
H	3.1316481785	3.3063890453	0.7811309524
H	4.5294339386	2.5234333159	-0.0093887077

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755900337 (Hartree/Particle)

Dipole Moment= 3.0349 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302487 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.453414
Sum of electronic and thermal Energies= -862.437557
Sum of electronic and thermal Enthalpies= -862.436613
Sum of electronic and thermal Free Energies= -862.497379

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761541013 (Hartree/Particle)
Corrected Free Energy= -863.503019676 (Hartree/Particle)

CONFORMER 7

CARTESIAN COORDINATES

C	0.5457075350	1.1045935187	0.3174725435
C	-0.6097741417	0.5597101272	-0.5184531877
C	0.0832428634	-1.6118890024	0.6640966144
H	0.2037011021	1.2015104935	1.3603546372
H	0.8198193842	2.1089832314	-0.0166628141
H	-0.1922418176	-1.3442319497	1.6988571510
H	-0.0522773671	-2.6923852011	0.5641071801
H	-0.2977133709	0.5795976082	-1.5759701861
C	-1.8944560586	1.3989550772	-0.4043046675
C	-2.7578707664	-0.6743072077	-1.5307935296
C	-3.1410261249	0.5807627173	-0.7255953561
H	-1.8198566023	2.2541727242	-1.0835415722
H	-1.9740389692	1.7927471433	0.6143003206
H	-2.2711847550	-0.3527463335	-2.4658810411

H	-3.6542253538	-1.2393579565	-1.8053269122
C	-0.8812147615	-0.8947482487	-0.2360304634
N	-1.8737274819	-1.5084772857	-0.7447761608
C	1.7288344150	0.1853536694	0.2603254850
C	1.5018813275	-1.1833654214	0.4163706501
C	3.0362435918	0.6470315966	0.0420363736
C	2.5600808462	-2.0903666200	0.3493895165
H	2.3702800609	-3.1556554413	0.4664608522
C	3.8485139308	-1.6216719209	0.1339107586
H	4.6808484916	-2.3211628481	0.0808465233
C	4.0964058417	-0.2597472900	-0.0198711856
H	5.1119854217	0.0855886928	-0.1885779287
C	-3.8527370055	0.1313584239	0.5306586655
O	-3.4439223490	0.2661633218	1.6562304878
O	-5.0121673667	-0.4672209816	0.2552570313
H	-5.4038140193	-0.7570430104	1.0926573954
H	-3.8642625087	1.1622680184	-1.3099178644
O	3.1846548914	1.9827008628	-0.0948505732
C	4.4670521919	2.5027586346	-0.3355515451
H	4.3559439071	3.5864747610	-0.4205883708
H	5.1565018930	2.2763196167	0.4899015106
H	4.8936111694	2.1108341886	-1.2696795618

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755313528 (Hartree/Particle)

Dipole Moment= 3.4235 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302063 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.453250
Sum of electronic and thermal Energies= -862.437190
Sum of electronic and thermal Enthalpies= -862.436246
Sum of electronic and thermal Free Energies= -862.497927

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761090124 (Hartree/Particle)
Corrected Free Energy= -863.503703596 (Hartree/Particle)

CONFORMER 8

CARTESIAN COORDINATES

C	0.1033920667	0.5206625813	-0.7246463124
C	-0.8567043375	-0.5606413274	-1.2280665299
C	0.4126475599	-2.3449140969	0.0115692250
H	-0.3718187169	1.1255486730	0.0605600547
H	0.3106522131	1.2274622175	-1.5373945271
H	0.3380697333	-2.9814414590	0.8998256910
H	0.6147868728	-3.0181996266	-0.8375334053
H	-0.3922568118	-0.9917850791	-2.1276657618
C	-2.2392280328	-0.0343597879	-1.5972336763
C	-3.2284831670	-1.4948711388	0.1680369444
C	-3.1917193020	-0.0869922620	-0.4024907808
H	-2.6696293366	-0.6585849891	-2.3886923542
H	-2.1702446367	0.9846340849	-1.9939870375
H	-3.8017359973	-2.1453033151	-0.5086681454
H	-3.7707138701	-1.4936156381	1.1207410630
C	-0.9134255034	-1.6858623417	-0.2251162604
N	-1.9384247931	-2.1088644018	0.3924123124
C	1.3994887870	-0.0297932637	-0.2024632474
C	1.5572067139	-1.3716690237	0.1446369176
C	2.4875308997	0.8504977015	-0.0401524079
C	2.7903719683	-1.8278504460	0.6272204768
H	2.9028171932	-2.8766761694	0.8966814479
C	3.8540049225	-0.9534189152	0.7666625563

H	4.8102909319	-1.3124206475	1.1427385181
C	3.7132168090	0.3936939437	0.4359358097
H	4.5527931424	1.0715681946	0.5563362752
C	-2.8399193923	0.9225279120	0.6650972219
O	-2.6352307799	0.6732862738	1.8254642400
O	-2.7921985930	2.1657514611	0.1791372171
H	-2.5742040824	2.7626129087	0.9107041882
H	-4.1962149265	0.1953864752	-0.7473092392
O	2.2430392084	2.1368250636	-0.3734552435
C	3.2800893627	3.0771478144	-0.2557988207
H	4.1349316229	2.8171697110	-0.8957308118
H	2.8714896144	4.0381374606	-0.5775524152
H	3.6295798841	3.1643030680	0.7824840865

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755843730 (Hartree/Particle)

Dipole Moment= 5.0178 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302063 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.453780
Sum of electronic and thermal Energies= -862.437694
Sum of electronic and thermal Enthalpies= -862.436750
Sum of electronic and thermal Free Energies= -862.497931

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760945244 (Hartree/Particle)
Corrected Free Energy= -863.503032514 (Hartree/Particle)

CONFORMER 9

CARTESIAN COORDINATES

C	0.7759806828	0.0806954291	-1.8658694431
C	-0.7195098743	-0.1907761383	-1.6945045652
C	0.2268584157	-2.2623749481	-0.5247553025
H	0.9414109769	1.0992092602	-2.2277259100
H	1.1779713769	-0.5971143558	-2.6332389190
H	-0.0696856389	-3.0761095250	0.1420700637
H	0.6559508531	-2.7080128852	-1.4372513693
H	-1.1671515381	-0.3652669324	-2.6852699072
C	-1.4677452445	0.9992442994	-1.0603200830
C	-3.1782049807	-0.8285046883	-0.8716336323
C	-2.7534039720	0.5617416655	-0.3604983383
H	-1.7059145985	1.7177512196	-1.8515249536
H	-0.8031712747	1.5054921564	-0.3536193460
H	-3.3431818647	-0.7695511157	-1.9594662710
H	-4.1249397695	-1.1229444862	-0.4072754393
C	-0.9765483562	-1.4506064113	-0.9086501329
N	-2.1468396040	-1.7887036717	-0.5391490978
C	1.5022268202	-0.1536851584	-0.5742624178
C	1.2380156303	-1.3435516454	0.1069700646
C	2.4019371086	0.7707624315	-0.0240272971
C	1.8600511762	-1.6194115770	1.3242057051
H	1.6394131634	-2.5463014611	1.8501849710
C	2.7556854586	-0.7006109644	1.8543109399
H	3.2488226957	-0.9061424940	2.8027415481
C	3.0308125482	0.4932134390	1.1920454341
H	3.7297675170	1.2003436899	1.6284056465
C	-2.6711922410	0.4550627335	1.1476428146
O	-3.6312891174	0.2624925231	1.8506945482
O	-1.4361106663	0.5617932033	1.6371708543
H	-1.4874624052	0.4445576522	2.5978957652
H	-3.5695925695	1.2662801840	-0.5571424996
O	2.6039555654	1.9054704723	-0.7291220776

C	3.4739268044	2.8792086488	-0.2113744599
H	3.4804980023	3.7066625022	-0.9249728968
H	3.1310304028	3.2491328589	0.7651946671
H	4.4963474476	2.4908491225	-0.1025161730

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754099765 (Hartree/Particle)

Dipole Moment= 5.4463 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302554 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.451546
Sum of electronic and thermal Energies= -862.435718
Sum of electronic and thermal Enthalpies= -862.434774
Sum of electronic and thermal Free Energies= -862.495365

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759681801 (Hartree/Particle)
Corrected Free Energy= -863.500947036 (Hartree/Particle)

CONFORMER 10

CARTESIAN COORDINATES

C	0.4602969016	1.0325545969	0.2462726663
C	-0.6408650478	0.4922515836	-0.6654437599
C	0.0489366181	-1.7026988149	0.4745825932
H	0.0570347971	1.0866894461	1.2702864468
H	0.7253527941	2.0527098898	-0.0447585153
H	-0.2432006885	-1.5118955634	1.5220229748
H	-0.0640891220	-2.7776410024	0.3074643990
H	-0.2307989744	0.4633630994	-1.6881652083
C	-1.8974541319	1.3865949836	-0.6917574094
C	-2.9764888189	-0.7284012561	-1.4466256021
C	-3.1841062758	0.5763086818	-0.6623556009
H	-1.8871277838	1.9911659852	-1.6045093570
H	-1.8696378964	2.0832025463	0.1524683497
H	-2.6563352942	-0.4788657562	-2.4710021328
H	-3.9207500235	-1.2780986586	-1.5249750988
C	-0.9508907553	-0.9543526906	-0.3647173289
N	-1.9954735494	-1.5536717237	-0.7738570630
C	1.6658280917	0.1435394366	0.2073966957
C	1.4616377653	-1.2348981282	0.2838970751
C	2.9704926348	0.6406717797	0.0621857263
C	2.5402603006	-2.1172593820	0.2107836464
H	2.3684453116	-3.1905538652	0.2669766167
C	3.8256104684	-1.6142716305	0.0682329815
H	4.6737006786	-2.2942153361	0.0106720170
C	4.0508589905	-0.2416104536	-0.0055055861
H	5.0647031007	0.1305405331	-0.1180589909
C	-3.6514943568	0.1909117475	0.7236936658
O	-4.7334096557	-0.2815788644	0.9621199738
O	-2.7330747635	0.3951350587	1.6729025967
H	-3.1029071911	0.0906812512	2.5156764250
H	-4.0114131236	1.1366414404	-1.1124744281
O	3.0955856026	1.9842840305	-0.0029436422
C	4.3745491438	2.5405752231	-0.1690114751
H	4.8439437032	2.2034730829	-1.1039880421
H	4.2434986148	3.6247959328	-0.2056477261
H	5.0375709492	2.2874011131	0.6702273349

Electronic Energy (RPW6B95D3/def2-SVP)= -862.753607597 (Hartree/Particle)

Dipole Moment= 5.6012 (Debye)

Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302034 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.451574
Sum of electronic and thermal Energies= -862.435569
Sum of electronic and thermal Enthalpies= -862.434625
Sum of electronic and thermal Free Energies= -862.495509

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758864937 (Hartree/Particle)
Corrected Free Energy= -863.500766340 (Hartree/Particle)

CONFORMER 11

CARTESIAN COORDINATES

C	0.2168615133	0.6658855751	-0.6370662384
C	-0.7596094454	-0.2982150983	-1.3185195344
C	0.3789942939	-2.2672533025	-0.2225773838
H	-0.2814034119	1.1746597602	0.1981648299
H	0.4784678228	1.4657478889	-1.3403653326
H	0.2239362312	-2.9741165603	0.6000400788
H	0.5983210952	-2.8794847026	-1.1128764604
H	-0.2654553553	-0.6336833905	-2.2433857598
C	-2.0983510520	0.3428410034	-1.6895113255
C	-3.2533175030	-1.3996883493	-0.3226700561
C	-3.1734492600	0.0887791653	-0.6409084621
H	-2.4541080980	-0.0816248146	-2.6348592617
H	-1.9707978716	1.4193641398	-1.8468040265
H	-3.7018273489	-1.9209558165	-1.1814273554
H	-3.9327670350	-1.5710963747	0.5186301809
C	-0.9099849762	-1.5432144861	-0.4815080168
N	-1.9896957485	-2.0358861408	-0.0289604387
C	1.4726443889	0.0049543922	-0.1491169871
C	1.5593697016	-1.3719942121	0.0517602876
C	2.5944573344	0.8080073043	0.1390962729
C	2.7538007672	-1.9387898605	0.5147777996
H	2.8095948163	-3.0152857071	0.6681118667
C	3.8507122705	-1.1379704796	0.7801045404
H	4.7770237448	-1.5818725911	1.1402952065
C	3.7815525877	0.2424564202	0.5959622406
H	4.6466140103	0.8616035659	0.8133594994
C	-3.0164819729	0.9747195270	0.5762487137
O	-2.4609534548	2.0451089737	0.5780680454
O	-3.6183452720	0.4870138600	1.6603719115
H	-3.5144156567	1.1373387894	2.3714329414
H	-4.1486141206	0.3938473596	-1.0506404386
O	2.4227023258	2.1339213986	-0.0572711649
C	3.4992734784	3.0008770123	0.1919214338
H	4.3623073265	2.7670846766	-0.4473074797
H	3.1492679812	4.0108909974	-0.0347593317
H	3.8169841818	2.9578730125	1.2431931628

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754462843 (Hartree/Particle)

Dipole Moment= 1.6303 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301986 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452477
Sum of electronic and thermal Energies= -862.436309
Sum of electronic and thermal Enthalpies= -862.435365

Sum of electronic and thermal Free Energies= -862.497502

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758992334 (Hartree/Particle)
Corrected Free Energy= -863.502031491 (Hartree/Particle)

CONFORMER 12

CARTESIAN COORDINATES

C	0.1093387432	0.6256639837	-0.6354230752
C	-0.8449178107	-0.3631225573	-1.3112107167
C	0.3725840985	-2.3172762571	-0.2983913143
H	-0.3732107635	1.0996985573	0.2309086856
H	0.3311454623	1.4482501521	-1.3258601810
H	0.2741936315	-3.0597190240	0.5009758823
H	0.5773339947	-2.8811444027	-1.2231529163
H	-0.3548689201	-0.6738846481	-2.2461707351
C	-2.2124705663	0.2189975399	-1.6498547148
C	-3.2553467292	-1.4245331345	-0.0869271561
C	-3.1992021584	0.0412914866	-0.4941281187
H	-2.6253668018	-0.3002767379	-2.5223353134
H	-2.1276930859	1.2793027076	-1.9150152825
H	-3.8264608226	-1.9794605134	-0.8460770649
H	-3.8177908941	-1.5361355329	0.8475517053
C	-0.9384261070	-1.6094121202	-0.4672344534
N	-1.9806177213	-2.0866312253	0.0772838873
C	1.3947022097	-0.0095782471	-0.1869628263
C	1.5304359424	-1.3889378445	-0.0275982732
C	2.4934905344	0.8233542230	0.1030433741
C	2.7532109196	-1.9262237977	0.3940770262
H	2.8487099132	-3.0038496068	0.5161306927
C	3.8279187494	-1.0956744562	0.6596927361
H	4.7761193295	-1.5176730458	0.9877707955
C	3.7086938686	0.2862534254	0.5184856095
H	4.5567714019	0.9280789475	0.7369158135
C	-2.8664536720	1.0014746229	0.6250377654
O	-2.9037007569	2.2001964674	0.5053707708
O	-2.5080354806	0.4055758010	1.7626893236
H	-2.3128858180	1.0983652648	2.4120177428
H	-4.1918147891	0.3584796570	-0.8384267491
O	2.2701170452	2.1470904499	-0.0488454455
C	3.3187740000	3.0461847065	0.2070738937
H	2.9261328311	4.0487033245	0.0207008347
H	3.6598982826	2.9815046796	1.2497873420
H	4.1757983270	2.8660624228	-0.4569276245

Electronic Energy (RPW6B95D3/def2-SVP)= -862.754369116 (Hartree/Particle)

Dipole Moment= 2.2187 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302144 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452225
Sum of electronic and thermal Energies= -862.436125
Sum of electronic and thermal Enthalpies= -862.435181
Sum of electronic and thermal Free Energies= -862.496719

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.759683190 (Hartree/Particle)
Corrected Free Energy= -863.502033074 (Hartree/Particle)

CONFORMER 13

CARTESIAN COORDINATES

C	0.8192451751	0.2060127432	-1.8209621627
C	-0.6700664694	-0.1011515589	-1.6625831731
C	0.2981594517	-2.2238568066	-0.6029666683
H	0.9643436638	1.2500426500	-2.1116933858
H	1.2245713711	-0.4091996979	-2.6375973575
H	0.0038629885	-3.0677574729	0.0265000418
H	0.7378053773	-2.6307395974	-1.5286579242
H	-1.1396618287	-0.1580022816	-2.6561177694
C	-1.4077389365	0.9889136198	-0.8596032078
C	-3.1271651675	-0.8454124727	-1.0044203371
C	-2.8034406789	0.5196386057	-0.3883996444
H	-1.5000755734	1.8828875548	-1.4839460760
H	-0.7811771371	1.2687921287	-0.0032410320
H	-3.2046254386	-0.7321146343	-2.0954717785
H	-4.0939234101	-1.2184605892	-0.6494214781
C	-0.9057512551	-1.4191871063	-0.9822712450
N	-2.0825302848	-1.7913951110	-0.6519545403
C	1.5580256588	-0.1014269003	-0.5513777045
C	1.3000480312	-1.3243366289	0.0703498765
C	2.4690992390	0.7907091196	0.0345770391
C	1.9321805066	-1.6635480388	1.2661353178
H	1.7156506217	-2.6162132875	1.7452508881
C	2.8347593720	-0.7746412161	1.8332433702
H	3.3358201740	-1.0287043932	2.7654784237
C	3.1084655205	0.4497035195	1.2287140020
H	3.8145094857	1.1321440025	1.6922408453
C	-2.8773660480	0.4996753985	1.1313814179
O	-3.1296008931	1.4850398901	1.7757232592
O	-2.6265833530	-0.6559562474	1.7449410692
H	-2.3925745731	-1.3566624631	1.0999579242
H	-3.5567258364	1.2497726907	-0.6985566252
O	2.6692214574	1.9551420444	-0.6179077390
C	3.5510183676	2.9006648513	-0.0675351346
H	3.2208944108	3.2287392804	0.9280191229
H	4.5721635250	2.5021687022	0.0111622457
H	3.5536121380	3.7584331838	-0.7443410878

Electronic Energy (RPW6B95D3/def2-SVP)= -862.753967755 (Hartree/Particle)

Dipole Moment= 6.8761 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302648 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.451319
Sum of electronic and thermal Energies= -862.435584
Sum of electronic and thermal Enthalpies= -862.434640
Sum of electronic and thermal Free Energies= -862.495576

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760881555 (Hartree/Particle)
Corrected Free Energy= -863.502489800 (Hartree/Particle)

CONFORMER 14

CARTESIAN COORDINATES

C	0.5822583720	1.0758274318	0.4169665338
C	-0.6091658679	0.5853861486	-0.4026978494
C	0.1243978227	-1.6576324850	0.6046300007
H	0.2873768693	1.1059208058	1.4779807336
H	0.8448553666	2.0990663812	0.1361728750
H	-0.1266654254	-1.4410112964	1.6574928342
H	-0.0156768587	-2.7309511720	0.4511404774
H	-0.3797973318	0.7371180113	-1.4697243053

C	-1.9136198047	1.3442125890	-0.0977686216
C	-2.7203750113	-0.5663584589	-1.5237039218
C	-3.1573367490	0.5943055689	-0.6279257006
H	-1.8555990413	2.3414415755	-0.5448739170
H	-1.9887047656	1.4952856381	0.9858737232
H	-2.1975613004	-0.1588894105	-2.4016459834
H	-3.5859772620	-1.1251943370	-1.8956617875
C	-0.8431142198	-0.8883994884	-0.2408379841
N	-1.8501540851	-1.4612472358	-0.7790208533
C	1.7590480632	0.1606346121	0.2532772086
C	1.5362794276	-1.2146576268	0.3375558759
C	3.0583221509	0.6348974327	0.0143042129
C	2.5877112244	-2.1173084661	0.1786755057
H	2.3997290042	-3.1874258787	0.2396910708
C	3.8680556151	-1.6360861442	-0.0561547086
H	4.6964657883	-2.3310548978	-0.1804067145
C	4.1128651390	-0.2675830362	-0.1394551314
H	5.1224161241	0.0864672814	-0.3250701464
C	-4.0409513598	0.1370479282	0.5247803466
O	-4.8169885233	0.8789773247	1.0695769013
O	-3.9185854889	-1.1238643112	0.9377818027
H	-3.2082979823	-1.5913272512	0.4502778567
H	-3.7812706068	1.2873216647	-1.2002313536
O	3.2036437643	1.9754924690	-0.0489105980
C	4.4776918453	2.5104149965	-0.3036623601
H	4.8698811546	2.1751663318	-1.2740795995
H	4.3645011812	3.5970426724	-0.3197792464
H	5.1952355745	2.2355776428	0.4820503706

Electronic Energy (RPW6B95D3/def2-SVP)= -862.752988678 (Hartree/Particle)

Dipole Moment= 8.1807 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302389 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.450600
Sum of electronic and thermal Energies= -862.434743
Sum of electronic and thermal Enthalpies= -862.433799
Sum of electronic and thermal Free Energies= -862.494620

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760014008 (Hartree/Particle)
Corrected Free Energy= -863.501645330 (Hartree/Particle)

CONFORMER 15

CARTESIAN COORDINATES

C	0.6595135092	0.7320017235	0.7200149052
C	-0.5424729497	0.1811994244	-0.0456626373
C	0.5825785476	-2.0740977571	0.4691190678
H	0.4905318800	0.6067428222	1.8012618899
H	0.7565192144	1.8064289620	0.5401103208
H	0.5873545172	-2.2620617801	1.5557322441
H	0.5218667621	-3.0609031177	-0.0010735553
H	-0.3125862980	0.3024779419	-1.1175457217
C	-1.8461114007	0.8962792395	0.2514794118
C	-3.0468419138	-1.2787980691	0.0196402506
C	-2.9738505225	0.1792063884	-0.4626890473
H	-1.7950078502	1.9449473495	-0.0607738255
H	-2.0400784101	0.8952262062	1.3331417035
H	-3.6450870574	-1.8867195099	-0.6745960646
H	-3.5832398285	-1.3238733148	0.9806012125
C	-0.6885001580	-1.3057874130	0.1849326556
N	-1.7841638740	-1.9460627613	0.2053264469

C	1.9071679869	0.0198871848	0.2920957327
C	1.8538481755	-1.3624541208	0.1086214449
C	3.1017696760	0.7071657625	0.0210554244
C	2.9768852389	-2.0567557631	-0.3470237597
H	2.9247808774	-3.1345440140	-0.4905198759
C	4.1515451571	-1.3678841354	-0.6101779987
H	5.0299851205	-1.9038466463	-0.9650644072
C	4.2250199558	0.0111547966	-0.4282409730
H	5.1529485541	0.5333125868	-0.6410451727
C	-4.3012427447	0.8723659502	-0.2751829494
O	-4.4733618892	1.8349791473	0.4225710304
O	-5.3380860789	0.3337486447	-0.9295570402
H	-5.0590933658	-0.4099255945	-1.4774368875
H	-2.7624947252	0.1711779036	-1.5435655186
O	3.0801613091	2.0431813380	0.2210087646
C	4.2356090237	2.7909492708	-0.0595623592
H	5.0808534942	2.4806726926	0.5706869136
H	4.5296007512	2.6999890784	-1.1147692673
H	3.9944834521	3.8347715549	0.1556238773

Electronic Energy (RPW6B95D3/def2-SVP)= -862.750470178 (Hartree/Particle)

Dipole Moment= 5.1646 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301212 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.449258
Sum of electronic and thermal Energies= -862.432820
Sum of electronic and thermal Enthalpies= -862.431876
Sum of electronic and thermal Free Energies= -862.494143

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758093771 (Hartree/Particle)
Corrected Free Energy= -863.501766593 (Hartree/Particle)

CONFORMER 16

CARTESIAN COORDINATES

C	0.6067055670	0.7380980964	0.6529862119
C	-0.5816678584	0.0872750238	-0.0532767172
C	0.6092514163	-2.0773812081	0.6598762245
H	0.4478780747	0.7010235912	1.7422706755
H	0.6722765529	1.7953205715	0.3804716076
H	0.6252469555	-2.1534549066	1.7599919414
H	0.5754730257	-3.1078149707	0.2918808437
H	-0.3643208446	0.1240847164	-1.1338034322
C	-1.9031912032	0.7892783686	0.1921650459
C	-3.0422375743	-1.4319702496	0.1285461417
C	-3.0200027751	-0.0268776957	-0.4596293083
H	-1.8629746342	1.8123827220	-0.2022753803
H	-2.0899248623	0.8700955765	1.2725424204
H	-3.6211400001	-2.0996487604	-0.5234854715
H	-3.5983462791	-1.4095599407	1.0768038092
C	-0.6847552522	-1.3785379670	0.3067240123
N	-1.7613997217	-2.0452030597	0.3790051153
C	1.8711586140	0.0262217661	0.2766435718
C	1.8565238948	-1.3682427784	0.2198755762
C	3.0421992696	0.7198964177	-0.0694301841
C	2.9946595867	-2.0685103123	-0.1862818655
H	2.9728372675	-3.1558811198	-0.2316647436
C	4.1456820694	-1.3729581610	-0.5258782270
H	5.0355836155	-1.9136636914	-0.8430190037
C	4.1806642127	0.0182881599	-0.4691004954
H	5.0904988460	0.5454977790	-0.7397477974

C	-4.3671166512	0.6454485028	-0.3193794597
O	-5.2873716802	0.2076295068	0.3173911270
O	-4.4986532942	1.8173826111	-0.9514446382
H	-3.7007760733	2.0384538468	-1.4473203358
H	-2.8034573109	-0.0833693930	-1.5378837878
O	2.9842017132	2.0673535841	0.0110467646
C	4.1170928861	2.8177993511	-0.3445668157
H	4.9747343224	2.5858687687	0.3024206013
H	4.4061455042	2.6425215100	-1.3904218040
H	3.8495793398	3.8697801327	-0.2189950679

Electronic Energy (RPW6B95D3/def2-SVP)= -862.750477186 (Hartree/Particle)

Dipole Moment= 7.8982 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301623 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.448855
Sum of electronic and thermal Energies= -862.432521
Sum of electronic and thermal Enthalpies= -862.431577
Sum of electronic and thermal Free Energies= -862.493467

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.757988930 (Hartree/Particle)
Corrected Free Energy= -863.500978744 (Hartree/Particle)

CONFORMER 17

CARTESIAN COORDINATES

C	0.6156294376	0.8217775045	0.1298187802
C	-0.6016163863	0.1437922980	-0.4984475651
C	0.5519807187	-2.1051427907	-0.2259482683
H	0.4050399776	1.0153970411	1.1936446846
H	0.7566189756	1.8093655277	-0.3236836938
H	0.5372959367	-2.9384484688	0.4862201282
H	0.4678837629	-2.5685625391	-1.2223709885
H	-0.4245821616	0.0906719657	-1.5853562383
C	-1.8739310872	0.9315018655	-0.2264825417
C	-2.9621672609	-1.1434998199	0.5805258993
C	-3.0909881052	0.0454854572	-0.3804845088
H	-1.9347093361	1.8039605985	-0.8862355353
H	-1.8593199750	1.3201985080	0.8007679503
H	-3.7686262478	-1.8701660886	0.4091512226
H	-3.0946699755	-0.7956664619	1.6170648457
C	-0.6903569479	-1.2843650404	-0.0219941039
N	-1.7088466777	-1.8498793232	0.4852713352
C	1.8803142846	0.0259640451	0.0065926327
C	1.8570535763	-1.3577632661	-0.1562123447
C	3.1225544285	0.6867874151	0.0814959462
C	3.0583240061	-2.0703920907	-0.2592019924
H	3.0296179396	-3.1511565273	-0.3878668023
C	4.2710558866	-1.4066861653	-0.1947051424
H	5.2030148119	-1.9633177535	-0.2747264006
C	4.3152037720	-0.0235975915	-0.0240052789
H	5.2730406344	0.4849416821	0.0286688450
C	-4.3764274596	0.7968173376	-0.1347905861
O	-4.4375444100	1.9199776651	0.2875035676
O	-5.5037795001	0.1203886793	-0.3881139939
H	-5.3130397824	-0.7515492769	-0.7550038237
H	-3.1311898609	-0.3574062364	-1.4050365743
O	3.0612400096	2.0242088064	0.2624265605
C	4.2590490549	2.7556147552	0.3232127716
H	4.8845953398	2.4356496567	1.1683163670
H	4.8403776594	2.6556246388	-0.6041802327

H	3.9813009568	3.8034448414	0.4604133849

Electronic Energy (RPW6B95D3/def2-SVP)= -862.750664761 (Hartree/Particle)

Dipole Moment= 4.9059 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301435 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.449230
Sum of electronic and thermal Energies= -862.432835
Sum of electronic and thermal Enthalpies= -862.431890
Sum of electronic and thermal Free Energies= -862.493976

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758516807 (Hartree/Particle)
Corrected Free Energy= -863.501828046 (Hartree/Particle)

CONFORMER 18

CARTESIAN COORDINATES

C	0.8019843933	0.3823775200	-1.5618711266
C	-0.6257323456	-0.1527934445	-1.3473891561
C	0.6665428962	-2.2815873270	-0.8492692396
H	0.7883256131	1.4753671736	-1.5956973321
H	1.1599715240	0.0484398222	-2.5465030478
H	0.5741024786	-3.2707333689	-0.3942961886
H	0.8880529803	-2.4024151997	-1.9212105403
H	-1.0763369037	-0.2986499111	-2.3413826452
C	-1.5215385348	0.7880667049	-0.5609368092
C	-2.6970144640	-1.2052446145	0.3936674861
C	-2.8692308197	0.1220304322	-0.3650562871
H	-1.6390016424	1.7431627385	-1.0840827515
H	-1.0702974541	1.0109995999	0.4163379508
H	-3.5721761862	-1.8545262841	0.2453362970
H	-2.6613277887	-1.0108257423	1.4770814711
C	-0.6145330764	-1.5117917478	-0.6794772219
N	-1.5225492000	-1.9770384566	0.0751282759
C	1.7689326026	-0.1022495239	-0.5230088476
C	1.7399591483	-1.4575310736	-0.1879774880
C	2.7074338394	0.7397969001	0.0931736355
C	2.6250238154	-1.9768657302	0.7565213881
H	2.5837575327	-3.0324733481	1.0178049159
C	3.5506239362	-1.1342739281	1.3566664689
H	4.2484684222	-1.5284595683	2.0932002257
C	3.5982680480	0.2200771662	1.0349144883
H	4.3284960479	0.8613117353	1.5192551494
C	-3.8536674467	1.0209809405	0.3434874571
O	-3.6001948432	2.1240789122	0.7456786737
O	-5.0773914887	0.5115672811	0.5351507177
H	-5.1605299501	-0.3654457018	0.1414607413
H	-3.2962318198	-0.1017504431	-1.3557728798
O	2.6858120206	2.0370826099	-0.2820314161
C	3.5767414244	2.9359317085	0.3275996729
H	3.4230741921	2.9819344280	1.4149463879
H	4.6233096004	2.6649642604	0.1296350242
H	3.3752513692	3.9193670431	-0.1039345117

Electronic Energy (RPW6B95D3/def2-SVP)= -862.748808696 (Hartree/Particle)

Dipole Moment= 3.8515 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301948 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.446861
Sum of electronic and thermal Energies= -862.430711
Sum of electronic and thermal Enthalpies= -862.429766
Sum of electronic and thermal Free Energies= -862.491171

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.756463120 (Hartree/Particle)
Corrected Free Energy= -863.498825424 (Hartree/Particle)

CONFORMER 19

CARTESIAN COORDINATES

C	0.7174612126	0.2368953405	-1.5705589437
C	-0.6860534888	-0.3215152943	-1.2766100114
C	0.6872365262	-2.3728868096	-0.6745046203
H	0.6716431281	1.3236043168	-1.6851341277
H	1.0565213335	-0.1603747191	-2.5382134853
H	0.6371047653	-3.3307954901	-0.1512013611
H	0.8923757319	-2.5615685077	-1.7400693257
H	-1.1694985345	-0.5308822805	-2.2433077917
C	-1.5784783457	0.6398943272	-0.5108172795
C	-2.7030808620	-1.3385702321	0.5406494982
C	-2.9182606467	-0.0508104303	-0.2486123236
H	-1.7105842254	1.5668166731	-1.0824629259
H	-1.1041915636	0.9140155586	0.4426097873
H	-3.5649406562	-2.0064191426	0.4084382675
H	-2.6945729256	-1.0954465483	1.6124864862
C	-0.6185663771	-1.6392993491	-0.5315046374
N	-1.5032295686	-2.0876559917	0.2586508459
C	1.7253884622	-0.1435498243	-0.5274085607
C	1.7467202574	-1.4718724155	-0.0971609324
C	2.6526662701	0.7677669003	0.0004606564
C	2.6703926942	-1.8951508073	0.8582833087
H	2.6690849417	-2.9300273492	1.1949469492
C	3.5831360117	-0.9843407561	1.3725437702
H	4.3101435402	-1.3036200008	2.1171263597
C	3.5816900734	0.3439359875	0.9532536477
H	4.3033972619	1.0393675897	1.3710089413
C	-3.8938002062	0.8661418412	0.4559753258
O	-4.3092060268	0.7004835970	1.5712335026
O	-4.2856093686	1.9383642945	-0.2421291155
H	-3.9059180374	1.9356622273	-1.1293773974
H	-3.3592239670	-0.2878100987	-1.2293400707
O	2.5827161890	2.0326767083	-0.4681628927
C	3.4707809303	2.9957191220	0.0390613419
H	3.3482419985	3.1272283933	1.1233465884
H	4.5167667603	2.7299834755	-0.1688799568
H	3.2348302361	3.9365605697	-0.4640767993

Electronic Energy (RPW6B95D3/def2-SVP)= -862.748870289 (Hartree/Particle)

Dipole Moment= 7.0506 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.301962 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.446908
Sum of electronic and thermal Energies= -862.430712
Sum of electronic and thermal Enthalpies= -862.429768
Sum of electronic and thermal Free Energies= -862.492017

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.756449266 (Hartree/Particle)

Corrected Free Energy= -863.499595977 (Hartree/Particle)

CONFORMERS of ENAMINE F

CONFORMER 1

CARTESIAN COORDINATES

C	0.6048660315	-0.7788328456	-0.3737634485
C	-0.5906902397	-0.1090951035	0.2877554321
C	0.5820003424	2.0297453494	-0.1591254570
H	0.4202785386	-0.8099470156	-1.4620295596
H	0.6792075480	-1.8197826421	-0.0442984259
H	0.5841943858	3.1142722102	-0.2701838174
H	-0.4862837461	-0.2053144535	1.3828730485
C	-1.8915821550	-0.7929950169	-0.1090831204
C	-3.0676563336	1.3946794329	-0.1711582087
C	-3.0949441221	-0.0084652759	0.3998239849
H	-1.9063868723	-1.8154011599	0.2823725377
H	-1.9481650754	-0.8649168429	-1.2054965546
H	-3.8669299312	1.9991108493	0.2694935837
H	-3.2740373531	1.3372452131	-1.2539396951
C	-0.5967461104	1.3763384299	0.0120102452
N	-1.7976566646	2.0231881208	0.1084511301
C	1.8909154352	-0.0533549007	-0.1235273028
C	1.8596511604	1.3496871146	-0.0648639918
C	3.1138541064	-0.7275822730	-0.0300046842
C	3.0643036840	2.0580879615	0.0799292509
H	3.0437510544	3.1458732624	0.1215756773
C	4.2656980980	1.3749235191	0.1788968786
H	5.1959097270	1.9285690896	0.2972208859
C	4.3071816668	-0.0174722487	0.1318962107
H	5.2584387374	-0.5345340360	0.2113095377
H	-1.7659506102	3.0167656867	-0.0731979070
C	-4.4058969241	-0.6818784334	0.0928898248
O	-5.3470047579	-0.1492669409	-0.4385685806
O	-4.4245851823	-1.9536103237	0.4895181605
H	-5.2944846999	-2.3214337932	0.2727380937
H	-3.0275767670	0.0467737436	1.4976814380
O	3.0572664731	-2.0780683877	-0.1193531440
C	4.2481668114	-2.8133584048	-0.0173935803
H	4.7438091071	-2.6512123389	0.9504226102
H	3.9763624260	-3.8682656467	-0.1061418989
H	4.9536837264	-2.5564210323	-0.8203881671

Electronic Energy (RPW6B95D3/def2-SVP)= -862.763828747 (Hartree/Particle)

Dipole Moment= 2.1833 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302356 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.461473
Sum of electronic and thermal Energies= -862.445163
Sum of electronic and thermal Enthalpies= -862.444219
Sum of electronic and thermal Free Energies= -862.505903

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.767081470 (Hartree/Particle)
Corrected Free Energy= -863.509155723 (Hartree/Particle)

CONFORMER 2

CARTESIAN COORDINATES

C	0.6110911983	-0.7946309389	-0.3463054143
C	-0.5868951936	-0.1210894140	0.3074774941
C	0.5791049453	2.0165788813	-0.1616061963
H	0.4265734005	-0.8387316353	-1.4340737489
H	0.6895307095	-1.8314151755	-0.0048924995
H	0.5775737411	3.0997380585	-0.2850567730
H	-0.4828875010	-0.2049380140	1.4034483983
C	-1.8851305177	-0.8116329253	-0.0858544020
C	-3.0620288122	1.3627757851	-0.1917821134
C	-3.0956570755	-0.0319198629	0.4208808290
H	-1.8881864226	-1.8344279413	0.3094245613
H	-1.9480110475	-0.8882224045	-1.1805633697
H	-3.8674195054	1.9814116958	0.2198126647
H	-3.2393660805	1.2725402177	-1.2766719238
C	-0.5968116357	1.3608103494	0.0145497331
N	-1.8015598702	2.0031343207	0.1023431110
C	1.8945992083	-0.0618321599	-0.1037022934
C	1.8591072743	1.3415428412	-0.0594915182
C	3.1197809489	-0.7310733301	-0.0028922447
C	3.0610834332	2.0555615925	0.0781227659
H	3.0367789703	3.1436315676	0.1084217299
C	4.2647287658	1.3774198959	0.1842270774
H	5.1931401132	1.9352326731	0.2968296395
C	4.3106152254	-0.0152058379	0.1516338935
H	5.2635482031	-0.5282794690	0.2365604832
H	-1.7753041686	2.9954325842	-0.0879176244
C	-4.3822952765	-0.7473835237	0.1076157240
O	-5.1427851223	-1.1964912013	0.9255923631
O	-4.5939504461	-0.8507976964	-1.2067399759
H	-5.4269370915	-1.3282006631	-1.3388057802
H	-3.0500996014	0.0504501638	1.5126123473
O	3.0676956740	-2.0824767253	-0.0779026408
C	4.2609462696	-2.8128728616	0.0323140042
H	4.9658661334	-2.5623878271	-0.7732300569
H	4.7556825250	-2.6387726141	0.9985000255
H	3.9924367975	-3.8694976622	-0.0451667352

Electronic Energy (RPW6B95D3/def2-SVP)= -862.761768993 (Hartree/Particle)

Dipole Moment= 2.1122 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302553 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.459216
Sum of electronic and thermal Energies= -862.442859
Sum of electronic and thermal Enthalpies= -862.441915
Sum of electronic and thermal Free Energies= -862.503956

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.765917096 (Hartree/Particle)
Corrected Free Energy= -863.508104103 (Hartree/Particle)

CONFORMER 3

CARTESIAN COORDINATES

C	0.6362599819	-0.7753824345	-0.4396558206
C	-0.5717586099	-0.1620508239	0.2538006983
C	0.5835335118	2.0131867453	-0.0438598915
H	0.4594652465	-0.7382897928	-1.5290181664
H	0.7194089675	-1.8346362666	-0.1775387591
H	0.5756130710	3.1026230720	-0.0840880698
H	-0.4750613149	-0.3290717323	1.3411801653

C	-1.8638435416	-0.8256966480	-0.2006607692
C	-3.0579610791	1.3523112844	-0.1284810965
C	-3.0753764588	-0.0940985279	0.3429382428
H	-1.8781559220	-1.8748431832	0.1130219803
H	-1.9120800051	-0.8251112544	-1.2996047988
H	-3.8640754939	1.9162466050	0.3499353828
H	-3.2462214836	1.3758278966	-1.2172299191
C	-0.5888514794	1.3385416031	0.0770348472
N	-1.7964599042	1.9677108671	0.2108013667
C	1.9133699080	-0.0548551553	-0.1340579406
C	1.8673768859	1.3409763197	0.0148881077
C	3.1430472018	-0.7209249969	-0.0756226916
C	3.0630730368	2.0512654352	0.2136392255
H	3.0302330810	3.1338056383	0.3252728705
C	4.2710411510	1.3757745841	0.2767686898
H	5.1945616002	1.9300317159	0.4371120924
C	4.3275779153	-0.0101765632	0.1400660952
H	5.2839862029	-0.5210426805	0.1924976730
H	-1.7718948515	2.9718515432	0.0976796648
C	-4.3620101666	-0.7933716972	-0.0159653194
O	-4.4397857523	-1.9113687357	-0.4552861550
O	-5.4330568758	-0.0367787796	0.2261378976
H	-6.2208494920	-0.5493440381	-0.0100966561
H	-3.0338592716	-0.0867996351	1.4441411393
O	3.1016397941	-2.0633011912	-0.2524345127
C	4.2997506988	-2.7913979365	-0.1916614505
H	4.7884705897	-2.6881243292	0.7876846019
H	4.0396457582	-3.8409293233	-0.3510709190
H	5.0067918102	-2.4751039147	-0.9718185815

Electronic Energy (RPW6B95D3/def2-SVP)= -862.763517129 (Hartree/Particle)

Dipole Moment= 2.9558 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302167 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.461351
Sum of electronic and thermal Energies= -862.444995
Sum of electronic and thermal Enthalpies= -862.444051
Sum of electronic and thermal Free Energies= -862.505998

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.766754242 (Hartree/Particle)
Corrected Free Energy= -863.509235113 (Hartree/Particle)

CONFORMER 4

CARTESIAN COORDINATES

C	0.2374341735	-0.8642952958	0.4064851868
C	-0.7286141728	0.0307245757	1.1737442896
C	0.1143662970	1.8630390123	-0.2688068278
H	-0.2676985596	-1.2278726306	-0.5048432723
H	0.4681427747	-1.7517298753	1.0038728587
H	0.0078077099	2.8440903741	-0.7319074062
H	-0.2363706526	0.3118490455	2.1187976888
C	-2.0408756994	-0.6942324852	1.5221126260
C	-3.3568419948	1.3191911765	0.9182382093
C	-3.2244853044	-0.1756074899	0.7117375235
H	-2.2836302493	-0.5492541111	2.5804959494
H	-1.9224792210	-1.7720938652	1.3697828709
H	-3.6553175656	1.5042356437	1.9612782344
H	-4.1466223895	1.7185081556	0.2736474761
C	-0.9270809382	1.3347503357	0.4301191802
N	-2.1128206597	1.9849891270	0.5958201549

C	1.4967426581	-0.1472058369	0.0273616912
C	1.4038308711	1.2070529738	-0.3362529663
C	2.7301552590	-0.8050081907	-0.0432527491
C	2.5578592116	1.8803352957	-0.7732915646
H	2.4890038656	2.9282430162	-1.0607969472
C	3.7723727824	1.2162808765	-0.8293500862
H	4.6640163129	1.7449179616	-1.1632621931
C	3.8773725464	-0.1244549093	-0.4623854325
H	4.8382213959	-0.6270914880	-0.5132401463
H	-2.1992529257	2.8650787922	0.1094513845
C	-3.1344599299	-0.5083966296	-0.7626189296
O	-3.3352086675	0.2675234238	-1.6610087941
O	-2.8338263093	-1.7911069009	-0.9729797968
H	-2.8148568571	-1.9391997724	-1.9305657434
H	-4.1379741424	-0.6703272995	1.0700408083
O	2.7264560593	-2.1155115189	0.3013379039
C	3.9344479783	-2.8282563510	0.2626986909
H	4.3581745213	-2.8543086370	-0.7514282689
H	4.6820918816	-2.3977748470	0.9441902619
H	3.7089465313	-3.8494057626	0.5806057801

Electronic Energy (RPW6B95D3/def2-SVP)= -862.759723534 (Hartree/Particle)

Dipole Moment= 3.6632 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302392 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457332
Sum of electronic and thermal Energies= -862.441108
Sum of electronic and thermal Enthalpies= -862.440163
Sum of electronic and thermal Free Energies= -862.501688

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761355383 (Hartree/Particle)
Corrected Free Energy= -863.503319849 (Hartree/Particle)

CONFORMER 5

CARTESIAN COORDINATES

C	0.3290601762	-0.9660059802	0.2549641175
C	-0.7181672626	-0.1772661767	1.0319539818
C	0.1526889795	1.8075327097	-0.1862891311
H	-0.1294352708	-1.2548636209	-0.7052514238
H	0.5581221635	-1.8947631302	0.7866684252
H	0.0455958340	2.8345040753	-0.5357867304
H	-0.3149828495	0.0255465031	2.0379747206
C	-2.0133432209	-1.0029936873	1.2053642613
C	-3.2432488619	1.1573092553	1.1937963065
C	-3.2672290634	-0.2919898617	0.7245674244
H	-2.1493002306	-1.2490982487	2.2635565429
H	-1.9106796021	-1.9515640648	0.6671377595
H	-3.2156021476	1.1766367733	2.2956813813
H	-4.1494141840	1.6817441439	0.8784209889
C	-0.9013854114	1.1949513788	0.4189867141
N	-2.1040820457	1.8052089850	0.5980769394
C	1.5806676569	-0.1862681037	-0.0049329293
C	1.4583650978	1.1887489154	-0.2684789304
C	2.8367690097	-0.7996592020	-0.0709973045
C	2.6070519792	1.9269175644	-0.6038363421
H	2.5162882669	2.9916954049	-0.8128347292
C	3.8436576222	1.3051493489	-0.6585561142
H	4.7303136667	1.8836245181	-0.9140831217
C	3.9777944065	-0.0561277235	-0.3889280456
H	4.9559551674	-0.5244730382	-0.4369014127

H	-2.1974777205	2.7652809415	0.3038947375
C	-3.3759197419	-0.3218190841	-0.7836861627
O	-2.5763979022	-0.8272014728	-1.5296958723
O	-4.4758385953	0.2936770359	-1.2176547249
H	-4.4772657301	0.2555143391	-2.1859257517
H	-4.1641551317	-0.7818636144	1.1251061601
O	2.8615814017	-2.1324980818	0.1752720914
C	4.0920599182	-2.8051163589	0.1399280104
H	3.8858620568	-3.8531991839	0.3720365644
H	4.5604196482	-2.7440599777	-0.8529007559
H	4.7956068480	-2.4054531797	0.8843741407

Electronic Energy (RPW6B95D3/def2-SVP)= -862.760650701 (Hartree/Particle)

Dipole Moment= 4.8987 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302137 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.458514
Sum of electronic and thermal Energies= -862.442174
Sum of electronic and thermal Enthalpies= -862.441230
Sum of electronic and thermal Free Energies= -862.502794

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.761871832 (Hartree/Particle)
Corrected Free Energy= -863.504015131 (Hartree/Particle)

CONFORMER 6

CARTESIAN COORDINATES

C	0.6360896382	-0.9583957674	-0.1466016244
C	-0.5787153130	-0.3259651319	0.5211899729
C	0.3970727108	1.8686365365	-0.1568727578
H	0.3804406838	-1.1431746548	-1.2047949987
H	0.8337943655	-1.9413672927	0.2917704403
H	0.2997323673	2.9411588483	-0.3240754303
H	-0.4592843366	-0.3880260917	1.6170640370
C	-1.8478949894	-1.0779048335	0.1208890712
C	-2.8807765009	0.9654535842	1.1771766259
C	-3.1369224116	-0.4577811487	0.6640064263
H	-1.7618941601	-2.1239771800	0.4347926296
H	-1.9048953422	-1.0862839625	-0.9739474611
H	-2.4855691672	0.9063193529	2.2037370140
H	-3.8156774799	1.5289607042	1.2247203730
C	-0.6935361130	1.1391324568	0.1827655701
N	-1.9629066720	1.6438977551	0.2921336272
C	1.8686911415	-0.1064383553	-0.1015544017
C	1.7270101073	1.2890266086	-0.1725708761
C	3.1479723575	-0.6745137346	-0.0854019711
C	2.8763479091	2.0946557535	-0.2307829257
H	2.7681527440	3.1765904423	-0.2871615271
C	4.1352689371	1.5161546046	-0.2061670168
H	5.0225262464	2.1461383390	-0.2470744795
C	4.2883349481	0.1333212525	-0.1278494264
H	5.2825372976	-0.3022664706	-0.1108020630
H	-2.0503836634	2.6493030606	0.2437378500
C	-4.2346505891	-0.4613936594	-0.3782535809
O	-4.1330682477	-0.8450307726	-1.5148365231
O	-5.3786451248	0.0178694836	0.1146766010
H	-6.0399816315	-0.0016892281	-0.5929111159
H	-3.5338586138	-1.0369379478	1.5077654892
O	3.1962950805	-2.0276539480	-0.0413610921
C	4.4485569687	-2.6599261449	-0.0040461883
H	5.0271320257	-2.3628116355	0.8822954090

H	4.2579275864	-3.7352953359	0.0389561681
H	5.0426086709	-2.4372145082	-0.9018446806

Electronic Energy (RPW6B95D3/def2-SVP)= -862.759698676 (Hartree/Particle)

Dipole Moment= 3.9975 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302653 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457045
Sum of electronic and thermal Energies= -862.440777
Sum of electronic and thermal Enthalpies= -862.439833
Sum of electronic and thermal Free Energies= -862.502190

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.763111838 (Hartree/Particle)
Corrected Free Energy= -863.505603162 (Hartree/Particle)

CONFORMER 7

CARTESIAN COORDINATES

C	0.7451995179	-0.4794153523	1.5686349085
C	-0.7241707974	-0.0857448065	1.4725533677
C	-0.0116619291	1.7921168851	-0.0041169968
H	0.8328928461	-1.5594763796	1.7291024492
H	1.1723557499	-0.0090615834	2.4683747112
H	-0.2381182484	2.7107958019	-0.5448912956
H	-1.1091350624	-0.0060265508	2.4971279606
C	-1.6119787209	-1.1022473293	0.7368125968
C	-3.2386771759	0.7567398218	1.2780164448
C	-2.9990217828	-0.4904619416	0.4265181908
H	-1.7223883407	-1.9974746306	1.3584584817
H	-1.1193971328	-1.4162554857	-0.1905470267
H	-3.2610837568	0.4715854137	2.3371436503
H	-4.2065056765	1.2051132658	1.0410663945
C	-0.9408104919	1.2460503472	0.8148711546
N	-2.2029152006	1.7491173818	1.0311935307
C	1.5739890557	-0.0611702382	0.3889314139
C	1.2260997230	1.1005824006	-0.3191560750
C	2.7369703333	-0.7600503156	0.0434852588
C	2.0576838860	1.5462229360	-1.3598157405
H	1.7872734593	2.4460093644	-1.9099995214
C	3.2023952192	0.8395335770	-1.6912524984
H	3.8401392845	1.1888184108	-2.5018050283
C	3.5534622047	-0.3194139191	-1.0024755397
H	4.4548018169	-0.8600947052	-1.2738779296
H	-2.4834737457	2.4532853467	0.3613290014
C	-3.1704410818	-0.1391667396	-1.0341939402
O	-3.5563158220	0.9262186326	-1.4475748684
O	-2.8718214028	-1.1553065145	-1.8420111705
H	-3.0130995377	-0.8618933901	-2.7547066945
H	-3.7763139690	-1.2369686329	0.6389999596
O	3.0107676243	-1.8572147725	0.7893163533
C	4.1468844741	-2.6210557194	0.4805351162
H	4.1673075221	-3.4554480237	1.1862157047
H	4.1025721954	-3.0186649997	-0.5434301967
H	5.0712830661	-2.0363954877	0.5906764993

Electronic Energy (RPW6B95D3/def2-SVP)= -862.757841158 (Hartree/Particle)

Dipole Moment= 3.5447 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302767 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.455074
Sum of electronic and thermal Energies= -862.438952
Sum of electronic and thermal Enthalpies= -862.438008
Sum of electronic and thermal Free Energies= -862.499382

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760857950 (Hartree/Particle)
Corrected Free Energy= -863.502398792 (Hartree/Particle)

CONFORMER 8

CARTESIAN COORDINATES

C	0.7565911792	-0.7192361593	1.4599596434
C	-0.7135018762	-0.3147334491	1.4347648541
C	-0.0047971238	1.7620801133	0.2438202318
H	0.8427420523	-1.8112346186	1.4529203126
H	1.1913469305	-0.3934279843	2.4180902252
H	-0.2321588915	2.7512744190	-0.1529646339
H	-1.0803802822	-0.3628857691	2.4682427539
C	-1.6200018727	-1.2350867563	0.5980650507
C	-3.2297529124	0.5376559296	1.3757728742
C	-2.9838275183	-0.5747076820	0.3480785133
H	-1.7451934172	-2.1859106788	1.1275551265
H	-1.1434830601	-1.4528206253	-0.3642153875
H	-3.2275606179	0.0977572326	2.3813691952
H	-4.2053619539	1.0050222237	1.2297457818
C	-0.9342257720	1.0956624361	0.9667597005
N	-2.1994712143	1.5558869131	1.2539175726
C	1.5823583397	-0.1276175877	0.3545003937
C	1.2333119188	1.1267952933	-0.1710995806
C	2.7465576020	-0.7647210674	-0.0916900277
C	2.0641095767	1.7249878126	-1.1327651676
H	1.7923575809	2.6968343224	-1.5415491810
C	3.2099532425	1.0778528737	-1.5664636558
H	3.8471520795	1.5457289039	-2.3153023406
C	3.5625142716	-0.1708977148	-1.0594403710
H	4.4646138808	-0.6633839884	-1.4088176630
H	-2.4819601402	2.3841206005	0.7468333741
C	-3.0852259339	-0.0309286086	-1.0645758235
O	-2.3878851236	-0.3553951536	-1.9904971673
O	-4.0731209521	0.8574089691	-1.1929656346
H	-4.0977413368	1.1419140179	-2.1189280079
H	-3.7904076525	-1.3171296319	0.4296580303
O	3.0224720045	-1.9605057909	0.4820433287
C	4.1619857034	-2.6659637572	0.0657979180
H	5.0838269015	-2.1001321533	0.2621526341
H	4.1853368902	-3.5950311725	0.6410459803
H	4.1202870459	-2.9088604162	-1.0055555584

Electronic Energy (RPW6B95D3/def2-SVP)= -862.757730192 (Hartree/Particle)

Dipole Moment= 3.6861 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302865 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.454866
Sum of electronic and thermal Energies= -862.438777
Sum of electronic and thermal Enthalpies= -862.437833
Sum of electronic and thermal Free Energies= -862.499917

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.760449483 (Hartree/Particle)
Corrected Free Energy= -863.502636291 (Hartree/Particle)

CONFORMER 9

CARTESIAN COORDINATES

C	0.7536795617	-0.6906495209	1.4297224302
C	-0.7023130963	-0.2418788413	1.3468869335
C	0.1195822236	1.8237179905	0.2097817440
H	0.8076735532	-1.7844882555	1.4061352972
H	1.1488755372	-0.3965095706	2.4148055932
H	-0.0696072113	2.8151373366	-0.2012655491
H	-1.1122286285	-0.2962040774	2.3639040137
C	-1.5967019104	-1.1204074729	0.4595954321
C	-3.1864418616	0.6825161080	1.2749270971
C	-3.0360775873	-0.5621882775	0.3675564062
H	-1.6185736064	-2.1362107416	0.8694383416
H	-1.1457391986	-1.1827853169	-0.5377658666
H	-3.1821092592	0.3355929185	2.3163177698
H	-4.1542257988	1.1662348581	1.1134737537
C	-0.8662878051	1.1712643460	0.8697705058
N	-2.1373049170	1.6511849628	1.0582782381
C	1.6527581751	-0.1046699431	0.3804032709
C	1.3633440983	1.1660081934	-0.1430978380
C	2.8244875875	-0.7646118033	-0.0087283123
C	2.2637535113	1.7565613550	-1.0459811902
H	2.0401286612	2.7408837600	-1.4542202234
C	3.4167783695	1.0874197647	-1.4232309807
H	4.1074285143	1.5508093322	-2.1261497704
C	3.7097797524	-0.1774600112	-0.9178275285
H	4.6186530385	-0.6866404462	-1.2227604315
H	-2.3886271097	2.4557716660	0.5014507437
C	-3.4654445846	-0.2083671916	-1.0323500355
O	-4.5407500267	-0.4737680070	-1.5077129142
O	-2.5401979669	0.4867136410	-1.6979089363
H	-2.9001258548	0.7012228049	-2.5717657385
H	-3.7632753629	-1.3040048886	0.7099766043
O	3.0366718890	-1.9762460523	0.5597140749
C	4.1781861936	-2.7058487286	0.1938970350
H	4.1422311053	-3.6472145470	0.7481349295
H	4.1921863717	-2.9241740382	-0.8834836538
H	5.1025809509	-2.1714705492	0.4556173761

Electronic Energy (RPW6B95D3/def2-SVP)= -862.755022032 (Hartree/Particle)

Dipole Moment= 0.9261 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302974 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.452048
Sum of electronic and thermal Energies= -862.435887
Sum of electronic and thermal Enthalpies= -862.434943
Sum of electronic and thermal Free Energies= -862.496745

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.758782048 (Hartree/Particle)
Corrected Free Energy= -863.500505016 (Hartree/Particle)

CONFORMER 10

CARTESIAN COORDINATES

C	0.5919450138	-0.9976947148	-0.0734712225

C	-0.6199291896	-0.3229290060	0.5556351357
C	0.3646251721	1.8297743468	-0.2219929885
H	0.3448848726	-1.2373486438	-1.1224192991
H	0.7847249398	-1.9556450442	0.4187467153
H	0.2715114584	2.8892094545	-0.4593835529
H	-0.4966317886	-0.3182981297	1.6524752284
C	-1.8983106372	-1.0865314596	0.2172901369
C	-2.8846928325	1.0317160281	1.1716577008
C	-3.1851511088	-0.4090464393	0.7490962062
H	-1.8271889923	-2.1102060744	0.5981048119
H	-1.9474269302	-1.1681086482	-0.8773051622
H	-2.4175939063	1.0390026418	2.1667236515
H	-3.8041838368	1.6210834309	1.2420140021
C	-0.7249408321	1.1173743169	0.1249966824
N	-2.0180493345	1.6335494851	0.1652955228
C	1.8265264124	-0.1462112258	-0.0596216785
C	1.6965000701	1.2443766690	-0.1902875412
C	3.1037280123	-0.7184544014	-0.0060784548
C	2.8454344236	2.0453628834	-0.2666145545
H	2.7406663512	3.1239869920	-0.3692517000
C	4.1019913975	1.4639013025	-0.2025464636
H	4.9926642678	2.0874915928	-0.2576431914
C	4.2458198436	0.0850203866	-0.0679052612
H	5.2378853953	-0.3534892154	-0.0217099192
H	-2.0580374022	2.6453870820	0.1307999755
C	-4.2396901018	-0.4326173553	-0.3375095446
O	-5.1960294225	-1.1622936329	-0.3458808890
O	-4.0179292763	0.4193746297	-1.3395046634
H	-3.2227072077	0.9600772470	-1.1277307288
H	-3.5925524622	-0.9599482960	1.6005741928
O	3.1461170811	-2.0669476457	0.0943408765
C	4.3957726051	-2.7023805680	0.1730132205
H	4.1992309776	-3.7738237162	0.2603024787
H	4.9997627990	-2.5208296354	-0.7272111773
H	4.9649950712	-2.3690747398	1.0523116131

Electronic Energy (RPW6B95D3/def2-SVP)= -862.761008961 (Hartree/Particle)

Dipole Moment= 6.2361 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.303546 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.457463
Sum of electronic and thermal Energies= -862.441677
Sum of electronic and thermal Enthalpies= -862.440733
Sum of electronic and thermal Free Energies= -862.500751

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.765363088 (Hartree/Particle)
Corrected Free Energy= -863.505105127 (Hartree/Particle)

CONFORMER 11

CARTESIAN COORDINATES

C	0.5989621306	-0.7784056458	-0.3601506999
C	-0.5931466407	-0.0995107262	0.2984391175
C	0.5802133180	2.0327869905	-0.1727121454
H	0.4105337827	-0.8214100632	-1.4472203075
H	0.6741778703	-1.8156224067	-0.0191266515
H	0.5830791509	3.1161916576	-0.2934703224
H	-0.4881149030	-0.1867006873	1.3940720215
C	-1.8957960949	-0.7855050900	-0.0913664516
C	-3.0659794730	1.3999244198	-0.1756939378
C	-3.1024080419	0.0031665506	0.4113544008

H	-1.8833813231	-1.8103213962	0.3016032219
H	-1.9555944737	-0.8694366864	-1.1862601359
H	-3.8688911355	2.0087304017	0.2516024791
H	-3.2642696815	1.3278185476	-1.2586370480
C	-0.5983325272	1.3831545634	0.0090957886
N	-1.7987397653	2.0311590467	0.1081331542
C	1.8865611832	-0.0514389050	-0.1222975241
C	1.8575841336	1.3519435595	-0.0780078797
C	3.1089177059	-0.7264478600	-0.0265416975
C	3.0633627606	2.0605116052	0.0540184923
H	3.0441463845	3.1486616477	0.0842515259
C	4.2643076230	1.3768290615	0.1549111454
H	5.1957494576	1.9304122444	0.2631474656
C	4.3036653937	-0.0159952785	0.1226476497
H	5.2546178987	-0.5333637063	0.2035129547
H	-1.7676869854	3.0234408820	-0.0808519147
C	-4.4186156814	-0.6688389845	0.0925236030
O	-5.3116984821	-0.1459109591	-0.5180691407
O	-4.5611556465	-1.9206271127	0.5372509067
H	-3.7815464767	-2.2098518527	1.0270327278
H	-3.0371476523	0.0737585141	1.5090246197
O	3.0500023406	-2.0775653791	-0.1006278735
C	4.2402253755	-2.8136007043	0.0062354141
H	3.9663519690	-3.8690201051	-0.0686069208
H	4.9432047052	-2.5676112147	-0.8023314513
H	4.7393094599	-2.6402428406	0.9702973160

Electronic Energy (RPW6B95D3/def2-SVP)= -862.758885210 (Hartree/Particle)

Dipole Moment= 3.5278 (Debye)
Number of imaginary frequencies 0

THERMOCHEMICAL DATA (Temperature 298.150 Kelvin. Pressure 1.00000 Atm)

Zero-point correction= 0.302320 (Hartree/Particle)
Sum of electronic and zero-point Energies= -862.456565
Sum of electronic and thermal Energies= -862.440228
Sum of electronic and thermal Enthalpies= -862.439284
Sum of electronic and thermal Free Energies= -862.500907

Electronic Energy SP (RPW6B95D3/def2-QZVPP)= -863.763497846 (Hartree/Particle)
Corrected Free Energy= -863.505519636 (Hartree/Particle)
