Supporting Information

Conformational Simulations of Aqueous Solvated α-Conotoxin GI and Its

Single-disulfide Analogues Using a Polarizable Force Field Model

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Figure S1. Comparison of CPU time (on a single CPU) made between conventional method and molecular fragmentation scheme at B3LYP/6-31G(*d*) level.

1gcn	HSQGTFTSDYSKYLD-
	SRRAQDFVQWLMNT
Frag1:	His1-Ser2-Gln3
Frag2:	Gly4-Thr5-Phe6
Frag3:	Thr7-Ser8-Asp9-Tyr10
Frag4:	Ser11-Lys12-Tyr13
Frag5:	Leu14-Asp15-Ser16-Arg17
Frag6:	Arg18-Ala19
Frag7:	Gln20-Asp21-Phe22
Frag8:	Val23-Gln24-Trp25
Frag9:	Leu26-Met27-Asn28-Thr29
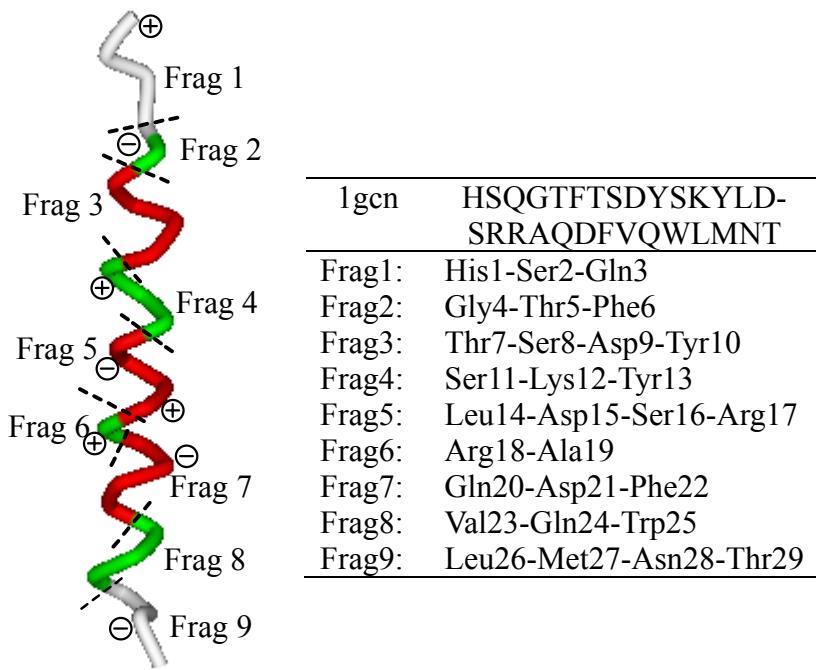
Figure S2. Fragmentation scheme on the basis of secondary structure of glucagon (PDB code: 1gcn).
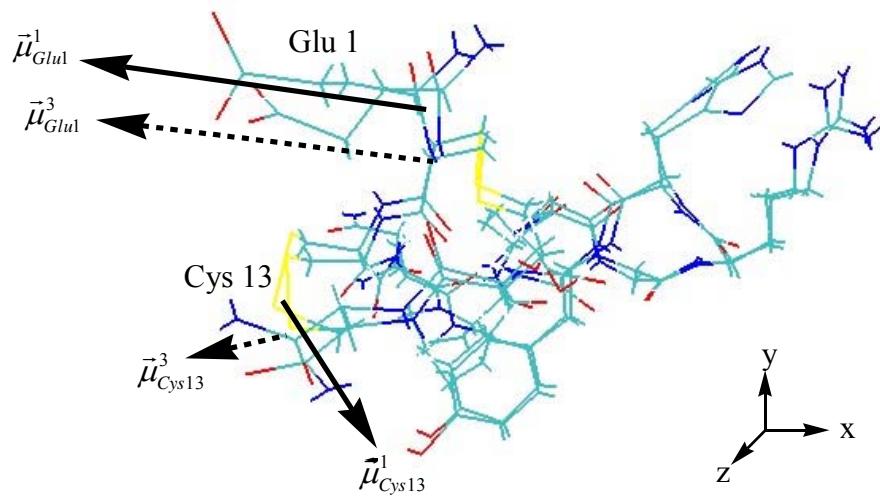
Conformer	$E_{\text{int}}^{Glu1-Cys13}$
1	19.3 kcal/mol
3	19.9 kcal/mol

Figure S3. The dipole moments of two residues, Glu 1 and Cys 13, $\vec{\mu}_{Glu1}$ and $\vec{\mu}_{Cys13}$, respectively, and their interaction energies, E_{int}, in conformers 1 and 3.
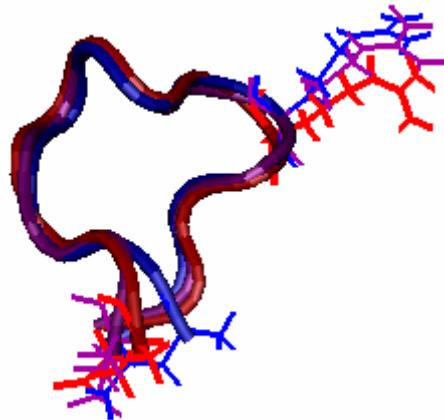
(a)
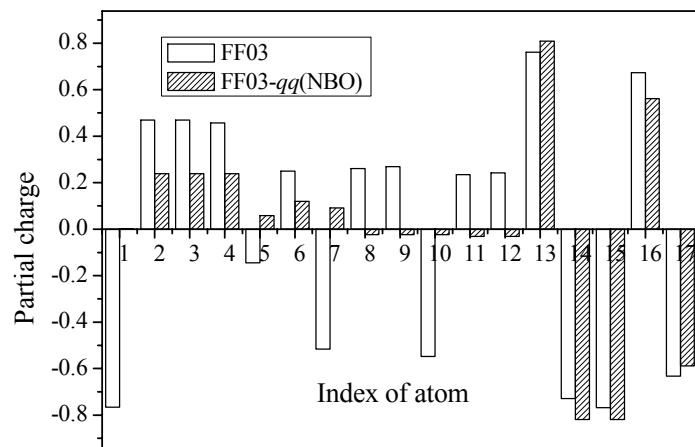
(b)

Figure S4. (a) Structural superposition of conformers 3 (blue), 5 (purple), and 6 (red). The polar residues Glu1 and Arg9 are shown in lines. (b) Comparison of partial charges on Glu 1 of conformer 6 made between FF03 and FF03-*qq*(NBO) force fields.
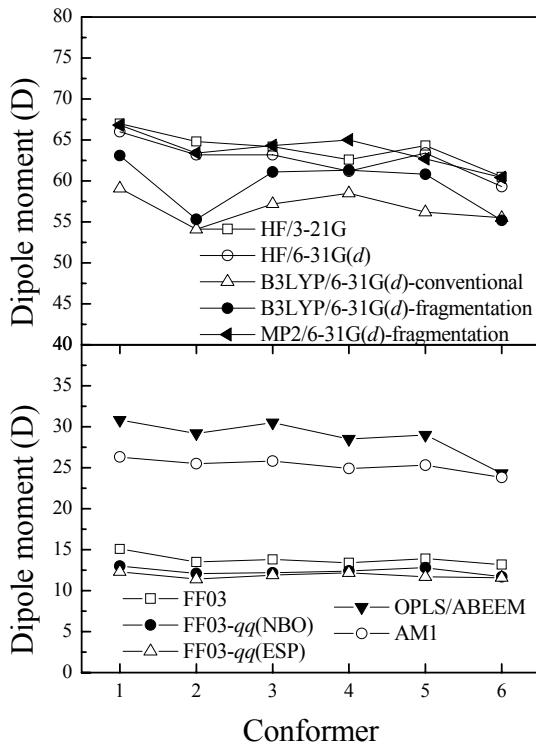
Figure S5. Dipole moments (Debye) for six conformers of α-conotoxin GI, generated from MD simulations. The quantum chemical calculations are carried out at various levels including AM1, HF, conventional B3LYP, and energy-based fragmentation B3LYP and MP2 (labeled as B3LYP-fragmentation and MP2-fragmentation, respectively). The molecular mechanical calculations are implemented in conventional FF03 and OPLS force fields, respectively, with NBO or ESP charges (designated FF03(or OPLS)-qq(NBO) and FF03(or OPLS)-qq(ESP), respectively) and with fragment dipoles (designated FF03(or OPLS)-$\mu\mu$(NBO) and FF03(or OPLS)-$\mu\mu$(ESP), respectively).
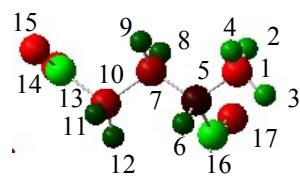
(a) Index of atoms on Glu 1
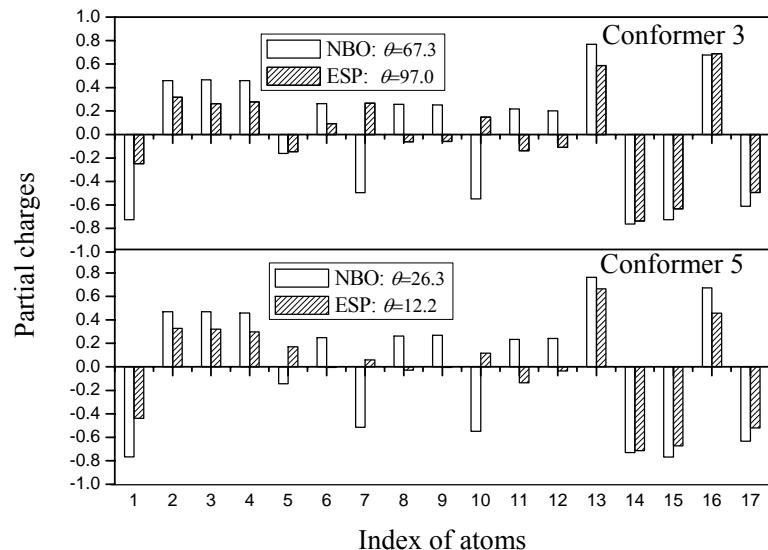
(b) NBO vs. ESP

Figure S6. Comparison of NBO and ESP charges on the terminal residue Glu 1 made between conformers 3 and 5.
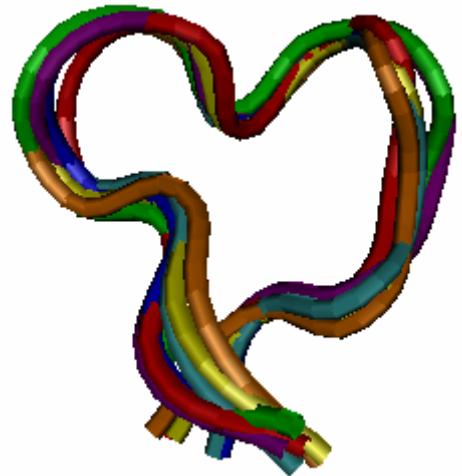
Figure S7. The time-averaged conformations of α-conotoxin GI taken during a molecular dynamics (MD) simulation period of 1ns (orange), 2 ns (yellow), 3 ns (green), 4 ns (purple), and 8 ns (cyan), respectively, in comparison with experimental NMR (red) and x-ray (blue) structures. The MD simulations are carried out in the framework of standard FF03.
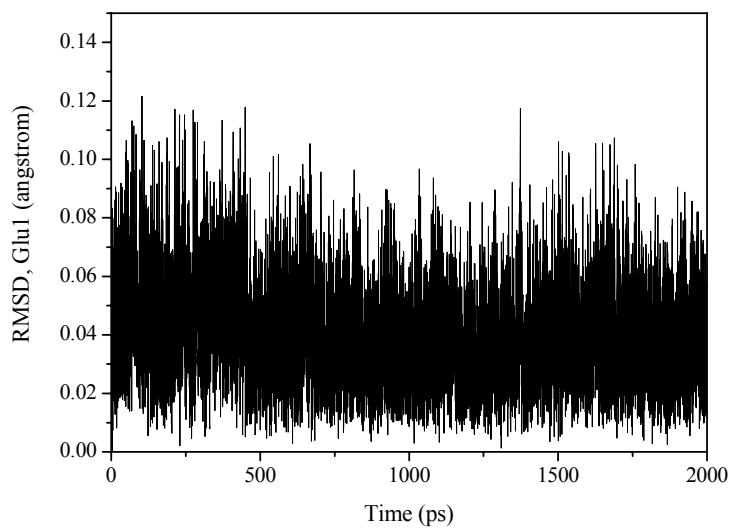
Figure S8. Backbone atom root-mean-square deviations (RMSD) of Glu 1 from the initial structure of α-conotoxin GI varied as a function of time. The molecular dynamics simulations are carried out at 300 K by using FF03 with NBO charges, updated every 2 ps.

(a)
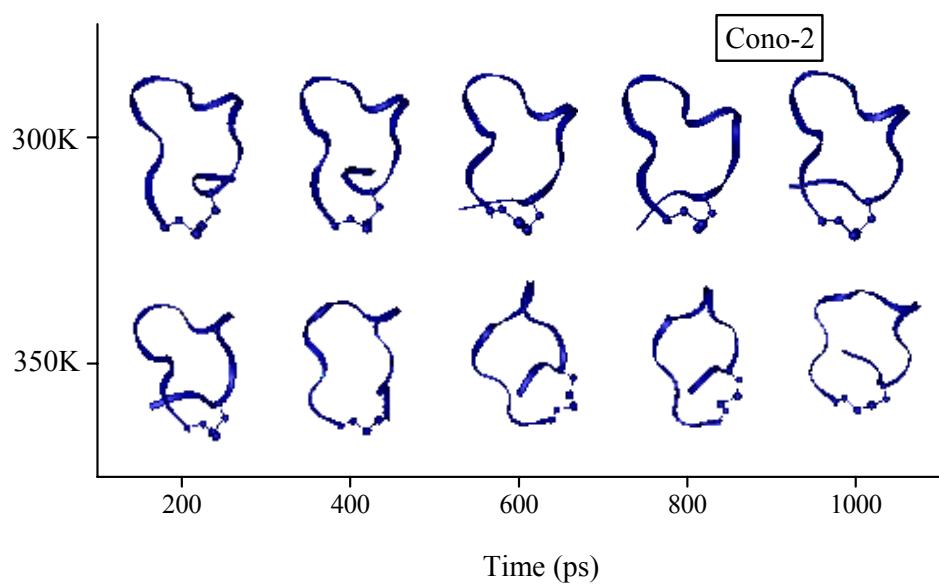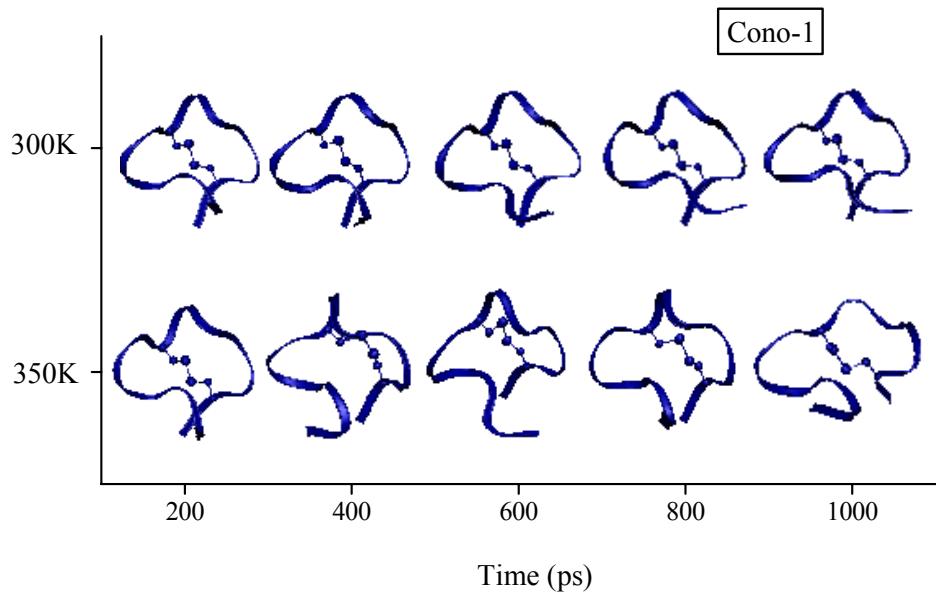
Figure S9. Snapshots of representative unfolding trajectories for (a) Cono-1 and (b) Cono-2 at several MD steps using standard FF03 at 300 K (top) and 350 K (bottom), respectively. The backbones of α-conotoxin GI analogues are shown in ribbon representations and the disulfide bonds are given in CPK forms.

Table S1. Terms of total energies (kcal/mol) for six α-conotoxin GI conformers, obtained by the standard FF03, polarizable model with NBO and ESP charges (designated FF03-qq(NBO) and FF03-qq(ESP), respectively), and the polarizable model with fragment dipoles determined by NBO and ESP charges (designated FF03-$\mu\mu$(NBO) and FF03-$\mu\mu$(ESP), respectively). The charges and dipole moments are obtained from energy-based fragmentation B3LYP/6-31G(d) calculations.

Conformer	Bond stretching + Angle bending + Torsion rotating	Van der Waals	Electrostatic		
			Standard	FF03-qq-NBO (ESP)	FF03-$\mu\mu$-NBO (ESP)
1	280.3	203.0	-267.8	-276.3 (-325.7)	-33.1 (-32.3)
2	288.3	202.1	-265.9	-259.8 (-328.7)	3.9 (0.4)
3	290.9	161.7	-272.0	-278.5 (-370.8)	-13.7 (-13.3)
4	269.2	146.0	-257.8	-255.2 (-323.9)	-10.7 (-11.8)
5	297.2	143.7	-269.2	-268.1 (-298.2)	-24.7 (27.9)
6	282.7	177.2	-259.1	-290.2 (-329.8)	-50.3 (5.9)

Table S2. The dipole-dipole interaction energies (kcal/mol) of six α-conotoxin GI conformers evaluated on the basis of fragment-centered and residue-centered dipoles, respectively. The dipole moments are calculated by NBO charges taken from molecular fragmentation calculation (at B3LYP/6-31G(*d*) level).

	Fragment-centered	Residue-centered
1	-33.1	257.4
2	3.9	10.3
3	-13.7	17.6
4	-10.7	-10.1
5	-24.7	-96.2
6	-50.3	-142.8

Table S3. The dihedral angles of ϕ and φ (deg) of solvated α-conotoxin GI calculated from the FF03-qq(NBO) and FF03-$\mu\mu$(NBO) force fields. The deviations with respect to the x-ray structure[a] are given in parenthesis.

| Residue | FF03-qq(NBO: B3LYP/6-31G(d)) | | | | | | FF03-$\mu\mu$(NBO) B3LYP/6-31G(d) | |
| | Residue-based fragmentation | | Secondary-structure-based Fragmentation | | Conventional | | | |
	ϕ	φ	ϕ	φ	ϕ	φ	ϕ	φ
Glu 1	-- (--)	168.8 (10.6)	-- (--)	152.9 (5.3)	-- (--)	155.9 (2.3)	-- (--)	164.3 (6.1)
Cys 2	-166.0 (19.0)	117.6 (18.1)	-155.4 (8.4)	98.3 (1.2)	-146.0 (1.0)	105.7 (6.2)	-152.6 (5.6)	104.5 (5.0)
Cys 3	-110.9 (6.3)	-6.8 (2.1)	-100.7 (3.9)	-10.8 (6.4)	-106.8 (2.2)	-8.9 (4.2)	-104.4 (0.2)	4.6 (9.3)
Asn 4	-99.0 (16.3)	159.4 (11.5)	-80.8 (1.9)	138.8 (17.9)	-84.7 (2.0)	139.9 (8.0)	-92.2 (9.5)	143.9 (4.0)
Pro 5	-52.2 (2.6)	-32.9 (3.1)	-50.8 (4.0)	-32.2 (3.8)	-47.7 (7.1)	-35.6 (0.4)	-52.0 (2.8)	-28.8 (7.2)
Ala 6	-62.0 (1.1)	-17.0 (3.5)	-65.5 (2.4)	-13.4 (0.1)	-60.1 (3.0)	-16.3 (2.8)	-60.9 (2.2)	-5.2 (6.3)
Cys 7	-68.6 (7.7)	-34.3 (3.7)	-61.4 (0.5)	-35.9 (5.3)	-61.9 (1.0)	-33.0 (2.4)	-62.9 (2.0)	-36.5 (5.9)
Gly 8	57.4 (3.1)	-133.6 (9.2)	56.7 (2.4)	-122.6 (1.8)	54.5 (0.2)	-124.5 (0.1)	54.1 (0.2)	-120.3 (4.1)
Arg 9	-62.1 (1.4)	-17.0 (2.8)	-62.8 (0.7)	-9.7 (4.5)	-61.9 (1.6)	-16.4 (2.2)	-69.5 (6.0)	-6.2 (8.0)
His 10	-78.9 (15.6)	-9.9 (12.5)	-95.9 (1.4)	0.6 (2.0)	-87.1 (7.4)	1.6 (4.2)	-104.6 (10.1)	6.8 (4.2)
Tyr 11	-55.4 (0.4)	131.1 (2.3)	-54.3 (1.4)	138.8 (10.0)	-53.4 (2.4)	137.2 (8.4)	-56.7 (0.9)	136.3 (7.5)
Ser 12	-174.7 (15.5)	114.7 (10.5)	-169.1 (10.2)	116.1 (11.9)	-171.3 (12.1)	95.2 (9.0)	-171.7 (12.5)	112.2 (8.0)
Cys 13	-168.1 (27.4)	-- (--)	-154.3 (13.6)	-- (--)	-147.9 (7.2)	-- (--)	-162.4 (21.7)	-- (--)
Mean deviation	(9.7)	(7.4)	(4.2)	(5.8)	(3.9)	(4.2)	(6.1)	(6.3)

[a]The experimental crystal results come from reference 53.

Table S4. Total energy (kcal/mol) of α-conotoxin GI in different charge iteration steps during molecular dynamics simulation.

MD step	Iteration step	Total energy	RMSD of NBO charges[a]
1	--	-11619.56	--
2	0	-11626.20	0.016
	1	-11620.57	0.015
3	0	-11625.41	0.014
	1	-11619.86	0.009

[a] In the last column, the RMSD deviation of NBO charges from the last iteration step is listed.

Conformer 1 (16.00 ps)

N	-6.53757839	2.11002503	0.92666930
H	-7.17157839	2.52102503	0.19766930
H	-5.73257839	2.69202503	0.88166930
H	-6.91857839	2.19802503	1.83366930
C	-6.19257839	0.69102503	0.74066930
H	-5.71257839	0.36802503	1.63966930
C	-7.41857839	-0.28797497	0.68266930
H	-7.93157839	-0.05597497	-0.24333070
H	-6.96957839	-1.24197497	0.38366930
C	-8.37457839	-0.38997497	1.93166930
H	-7.75957839	-0.66097497	2.79566930
H	-8.81157839	0.60502503	2.03666930
C	-9.44357839	-1.44497497	1.73566930
O	-9.01057839	-2.59297497	1.72366930
O	-10.57457839	-1.09397497	1.32166930
C	-5.28157839	0.42902503	-0.45433070
O	-5.69357839	0.73702503	-1.57833070
N	-4.08157839	-0.13697497	-0.20433070
H	-3.74257839	-0.16797497	0.78166930
C	-3.09257839	-0.54297497	-1.19133070
H	-3.54357839	-0.76197497	-2.13533070
C	-2.22757839	0.75902503	-1.40233070
H	-2.92257839	1.61202503	-1.49833070
H	-1.48757839	0.92802503	-0.65533070
S	-1.27657839	0.63402503	-2.94933070
C	-2.22357839	-1.71397497	-0.57233070
O	-1.56957839	-1.49997497	0.42466930
N	-2.36657839	-2.91397497	-1.19633070
H	-2.82157839	-2.93397497	-2.08233070
C	-1.82157839	-4.09797497	-0.71633070
H	-1.77157839	-3.89697497	0.32966930
C	-2.81357839	-5.22197497	-0.88133070
H	-3.20857839	-5.30797497	-1.92633070
H	-2.32157839	-6.10997497	-0.49333070
S	-4.24757839	-4.95597497	0.29366930
C	-0.43257839	-4.48997497	-1.22333070
O	0.14942161	-5.33697497	-0.54733070
N	0.03242161	-3.94797497	-2.32633070
H	-0.47857839	-3.21997497	-2.76033070
C	1.19342161	-4.51897497	-3.05333070
H	1.13242161	-5.61697497	-2.99933070
C	1.05942161	-4.22897497	-4.57133070
H	0.60642161	-3.21797497	-4.72133070
H	2.03342161	-4.07497497	-4.91333070
C	0.27642161	-5.33297497	-5.32833070
O	-0.62757839	-5.93597497	-4.79233070
N	0.70242161	-5.57697497	-6.54133070
H	0.21742161	-6.35797497	-7.06233070
H	1.40842161	-4.98697497	-7.00233070
C	2.48942161	-3.95597497	-2.57433070
O	2.46342161	-2.88897497	-2.00933070
N	3.66742161	-4.65497497	-2.86833070
C	3.82242161	-5.92297497	-3.59733070
H	3.62342161	-5.74297497	-4.69133070
H	3.12642161	-6.66697497	-3.23133070

C	5.27442161	-6.36397497	-3.26533070
H	5.73942161	-6.90797497	-4.11333070
H	5.31542161	-6.95197497	-2.35233070
C	6.04942161	-5.05897497	-3.14133070
H	6.38342161	-4.65697497	-4.11733070
H	6.90542161	-5.29097497	-2.61033070
C	5.04142161	-4.12997497	-2.51433070
H	5.17042161	-4.29697497	-1.47233070
C	5.23242161	-2.68697497	-2.99433070
O	5.88842161	-1.93797497	-2.28133070
N	4.69542161	-2.42497497	-4.16933070
H	4.38542161	-3.22397497	-4.66633070
C	4.86442161	-1.14097497	-4.85933070
H	5.93742161	-0.93197497	-4.84033070
C	4.36242161	-1.38497497	-6.28533070
H	3.31142161	-1.86297497	-6.34633070
H	4.44142161	-0.47097497	-6.86333070
H	4.88042161	-2.26397497	-6.65933070
C	4.13242161	0.07202503	-4.17333070
O	4.40342161	1.23502503	-4.44233070
N	3.16142161	-0.19397497	-3.28833070
H	2.82242161	-1.18397497	-3.19733070
C	2.49542161	0.92702503	-2.56533070
H	1.98442161	1.59002503	-3.29133070
C	1.36542161	0.43002503	-1.64933070
H	1.81142161	-0.00897497	-0.73833070
H	0.77542161	1.25802503	-1.25933070
S	0.17142161	-0.69097497	-2.43333070
C	3.41042161	1.80902503	-1.68733070
O	3.16742161	2.96902503	-1.53733070
N	4.59542161	1.32502503	-1.24933070
H	4.73242161	0.31302503	-1.29233070
C	5.54242161	1.97302503	-0.44133070
H	6.17442161	1.22702503	-0.03733070
H	6.03542161	2.67002503	-1.03833070
C	4.92842161	2.72502503	0.63566930
O	4.25742161	2.05202503	1.51266930
N	5.10842161	4.04702503	0.63666930
H	5.66442161	4.53602503	-0.07933070
C	4.55642161	4.88202503	1.75466930
H	4.93842161	4.53702503	2.70066930
C	5.14342161	6.29202503	1.62666930
H	4.93742161	6.78102503	2.55866930
H	6.21442161	6.17402503	1.48166930
C	4.51842161	7.17402503	0.61566930
H	4.33942161	6.63402503	-0.29833070
H	3.58142161	7.52502503	1.09766930
C	5.37142161	8.40302503	0.40966930
H	5.73642161	8.92302503	1.33266930
H	6.27242161	8.02302503	-0.02333070
N	4.69942161	9.47402503	-0.37533070
H	4.98342161	9.65202503	-1.31633070
C	3.66642161	10.23802503	0.01566930
N	3.29242161	10.36102503	1.27066930
H	3.62042161	9.84902503	2.05566930
H	2.51442161	11.01002503	1.47366930
N	3.05942161	11.07502503	-0.77533070

H	3.40342161	11.18302503	-1.72033070
H	2.24842161	11.50202503	-0.50133070
C	2.99742161	4.87502503	1.89266930
O	2.47342161	4.86502503	3.00066930
N	2.22942161	4.66902503	0.79966930
H	2.66142161	4.57602503	-0.12033070
C	0.77042161	4.65802503	0.81766930
H	0.46542161	5.36002503	1.63766930
C	0.21742161	5.08702503	-0.55433070
H	0.62542161	4.53602503	-1.35033070
H	-0.83357839	4.99502503	-0.57533070
C	0.43842161	6.52102503	-0.95733070
N	1.36742161	6.87202503	-1.91833070
C	1.34342161	8.23502503	-1.90833070
H	2.09442161	8.84202503	-2.40933070
N	0.32942161	8.65602503	-1.14733070
H	0.12042161	9.55702503	-0.81133070
C	-0.19557839	7.60502503	-0.45333070
H	-1.01057839	7.66902503	0.33166930
C	0.13542161	3.29102503	1.24566930
O	-1.05357839	3.13502503	1.05566930
N	0.94842161	2.30302503	1.62766930
H	1.85942161	2.55602503	1.73666930
C	0.46842161	0.96302503	2.06466930
H	0.09742161	0.34202503	1.21566930
C	1.68042161	0.14802503	2.50566930
H	2.35042161	-0.04597497	1.67866930
H	2.10342161	0.66002503	3.31666930
C	1.19442161	-1.17397497	3.03366930
C	0.87142161	-2.26497497	2.18966930
H	0.80742161	-2.06297497	1.10966930
C	0.61042161	-3.53797497	2.72366930
H	0.55042161	-4.39997497	2.03766930
C	0.60542161	-3.71297497	4.12066930
O	0.44742161	-4.93997497	4.71966930
H	0.11242161	-5.61797497	4.14066930
C	0.82342161	-2.64297497	4.97966930
H	0.74642161	-2.74897497	6.03566930
C	1.07642161	-1.32897497	4.41566930
H	1.21942161	-0.47197497	5.03166930
C	-0.59857839	0.99602503	3.09466930
O	-0.52857839	1.79202503	3.98566930
N	-1.56257839	0.11402503	2.98766930
H	-1.56457839	-0.55197497	2.19666930
C	-2.60257839	-0.07197497	4.03766930
H	-2.08757839	-0.58897497	4.83466930
C	-3.39657839	1.15602503	4.50666930
H	-2.95657839	2.10202503	4.00566930
H	-4.43557839	1.02602503	4.22566930
O	-3.31757839	1.22902503	5.85266930
H	-3.64357839	2.14502503	6.15066930
C	-3.59257839	-1.05197497	3.45466930
O	-4.14857839	-0.83297497	2.39766930
N	-3.75657839	-2.25297497	4.07066930
H	-3.34757839	-2.37197497	4.97166930
C	-4.38157839	-3.46597497	3.46966930
H	-5.08657839	-3.23497497	2.64466930
C	-3.12357839	-4.19797497	2.87466930
H	-2.56857839	-3.51797497	2.25566930

H	-2.40457839	-4.46397497	3.72266930
S	-3.52157839	-5.67697497	1.96866930
C	-5.20857839	-4.20597497	4.48666930
O	-4.92957839	-4.11397497	5.64666930
N	-6.23857839	-4.86397497	4.02266930
H	-6.65157839	-4.78897497	3.05066930
H	-6.77057839	-5.30897497	4.64866930

Conformer 2 (148.50 ps)

N	-5.31094466	4.83651120	-1.11869697
H	-5.26894466	5.04651120	-2.07769697
H	-4.44494466	5.20051120	-0.69969697
H	-6.05194466	5.39851120	-0.73269697
C	-5.36794466	3.38251120	-0.93569697
H	-5.01794466	3.27751120	0.05030303
C	-6.82894466	2.87751120	-1.15169697
H	-7.12194466	3.10451120	-2.12869697
H	-6.86494466	1.84751120	-0.97969697
C	-7.94494466	3.41251120	-0.21169697
H	-7.80894466	3.19151120	0.81430303
H	-7.92594466	4.48851120	-0.18969697
C	-9.29094466	2.91251120	-0.57669697
O	-9.68994466	3.35451120	-1.67169697
O	-9.81894466	1.98351120	0.08530303
C	-4.35994466	2.63651120	-1.84169697
O	-4.28894466	2.84251120	-3.04869697
N	-3.76294466	1.64051120	-1.18469697
H	-4.03994466	1.36851120	-0.23869697
C	-2.75094466	0.77251120	-1.78169697
H	-3.04894466	0.47051120	-2.68269697
C	-1.39894466	1.46851120	-1.76069697
H	-1.53294466	2.58151120	-1.92569697
H	-1.02294466	1.46551120	-0.71069697
S	-0.06694466	0.79551120	-2.82569697
C	-2.64994466	-0.52248880	-0.91469697
O	-2.37794466	-0.37348880	0.27630303
N	-2.82294466	-1.74448880	-1.54769697
H	-2.91494466	-1.72248880	-2.57369697
C	-2.86194466	-3.11448880	-0.93269697
H	-2.76294466	-3.16748880	0.17130303
C	-4.21694466	-3.82048880	-1.28869697
H	-4.31294466	-3.79948880	-2.39769697
H	-4.16494466	-4.90748880	-1.12869697
S	-5.58594466	-2.93548880	-0.46969697
C	-1.75094466	-4.05048880	-1.42269697
O	-1.47694466	-5.07448880	-0.77969697
N	-1.15194466	-3.73648880	-2.56369697
H	-1.35194466	-2.79648880	-2.91169697
C	-0.11394466	-4.52948880	-3.18269697
H	-0.48094466	-5.51048880	-3.40469697
C	0.26205534	-3.82248880	-4.48769697
H	-0.69994466	-3.58848880	-4.98769697
H	0.78805534	-2.92248880	-4.26869697
C	1.11505534	-4.76748880	-5.39469697
O	2.29205534	-4.94148880	-5.13569697
N	0.50605534	-5.55348880	-6.26469697
H	0.86405534	-6.47048880	-6.44269697
H	-0.44094466	-5.47348880	-6.51269697
C	1.18605534	-4.68748880	-2.31169697
O	1.43405534	-3.75948880	-1.51169697

N	1.81805534	-5.88148880	-2.30369697	H	5.69105534	9.33251120	1.08230303
C	1.35505534	-7.11948880	-2.91669697	N	7.48305534	8.62351120	-0.49969697
H	1.19505534	-6.85348880	-3.91969697	H	8.23905534	8.27051120	-1.07769697
H	0.40505534	-7.52948880	-2.55769697	H	6.91605534	9.46451120	-0.63869697
C	2.46705534	-8.14148880	-2.72569697	C	3.95905534	3.72251120	2.68930303
H	2.60005534	-8.77248880	-3.61369697	O	3.48505534	4.52751120	3.49530303
H	2.19205534	-8.74248880	-1.86769697	N	3.32005534	3.39851120	1.59130303
C	3.64505534	-7.25948880	-2.37669697	H	3.89205534	2.77251120	1.01630303
H	4.10305534	-6.94848880	-3.31369697	C	2.01405534	3.89051120	1.20630303
H	4.43205534	-7.74148880	-1.71069697	H	1.76005534	4.81151120	1.85030303
C	3.12105534	-6.09948880	-1.65869697	C	2.04805534	4.35051120	-0.26969697
H	3.06505534	-6.35348880	-0.56969697	H	2.12305534	3.41451120	-0.85569697
C	4.06005534	-4.88348880	-1.76969697	H	1.13305534	4.76051120	-0.58869697
O	4.50605534	-4.31648880	-0.74169697	C	3.21605534	5.23651120	-0.56069697
N	4.15605534	-4.30448880	-2.97969697	N	4.49405534	4.90651120	-1.02869697
H	3.80205534	-4.87848880	-3.71269697	C	5.11505534	6.05251120	-1.21369697
C	5.12905534	-3.21748880	-3.24269697	H	6.07605534	6.24651120	-1.54069697
H	6.08405534	-3.39948880	-2.65169697	N	4.29505534	7.08351120	-0.88169697
C	5.45305534	-3.22148880	-4.70869697	H	4.56205534	8.08151120	-0.92469697
H	4.62905534	-3.25948880	-5.38769697	C	3.14205534	6.61351120	-0.44069697
H	6.18905534	-2.38848880	-4.83469697	H	2.32705534	7.27951120	-0.15269697
H	5.96305534	-4.17848880	-4.95169697	C	0.89505534	2.88951120	1.43430303
C	4.71205534	-1.75748880	-2.86469697	O	-0.21394466	3.04451120	0.91930303
O	5.52105534	-0.81148880	-3.02469697	N	1.14705534	1.67651120	2.00030303
N	3.49105534	-1.49548880	-2.37969697	H	2.10905534	1.52651120	2.33730303
H	2.87205534	-2.25448880	-2.37469697	C	0.09905534	0.66851120	2.31130303
C	2.99405534	-0.33148880	-1.69469697	H	-0.35494466	0.39051120	1.30930303
H	2.87405534	0.38351120	-2.50669697	C	0.75805534	-0.56848880	3.03630303
C	1.66505534	-0.56448880	-1.00769697	H	1.63405534	-0.73048880	2.41030303
H	1.80505534	-1.33248880	-0.26269697	H	1.09205534	-0.33248880	4.07230303
H	1.48705534	0.33451120	-0.37969697	C	-0.17894466	-1.82248880	2.92030303
S	0.30605534	-1.00748880	-1.99369697	C	0.16605534	-2.87948880	1.97130303
C	3.92605534	0.22551120	-0.57569697	H	1.04805534	-2.75748880	1.31630303
O	4.08505534	1.42851120	-0.43169697	C	-0.57994466	-4.08948880	1.94430303
N	4.36705534	-0.69248880	0.32730303	H	-0.17294466	-4.87048880	1.30130303
H	4.06305534	-1.67848880	0.13430303	C	-1.68994466	-4.24448880	2.79930303
C	5.34605534	-0.37348880	1.33730303	O	-2.29294466	-5.40848880	2.74030303
H	5.35205534	-1.22448880	2.02630303	H	-1.98294466	-5.95148880	1.97430303
H	6.26805534	-0.25648880	0.82530303	C	-2.03694466	-3.29148880	3.74430303
C	4.91805534	0.79551120	2.15330303	H	-2.77094466	-3.49448880	4.44630303
O	3.91205534	0.70051120	2.81230303	C	-1.23394466	-2.15948880	3.77130303
N	5.68505534	1.85451120	2.16630303	H	-1.42394466	-1.36448880	4.52230303
H	6.51205534	1.89551120	1.59330303	C	-1.06694466	1.28151120	3.13230303
C	5.31505534	3.04751120	3.03330303	O	-0.90194466	1.68451120	4.33030303
H	5.20105534	2.60251120	4.11030303	N	-2.33194466	1.24251120	2.60230303
C	6.49205534	4.07051120	3.09530303	H	-2.42794466	0.82951120	1.68130303
H	6.30305534	4.70551120	3.92630303	C	-3.56994466	1.66851120	3.33430303
H	7.41805534	3.56651120	3.25630303	H	-3.56894466	1.29551120	4.41230303
C	6.70605534	4.96051120	1.84830303	C	-3.63494466	3.21551120	3.36930303
H	6.99405534	4.28251120	1.01130303	H	-2.73894466	3.60951120	3.80930303
H	5.77705534	5.47051120	1.56230303	H	-3.88694466	3.68851120	2.38430303
C	7.80405534	5.99551120	2.01530303	O	-4.64894466	3.55251120	4.23830303
H	7.64105534	6.58351120	2.97330303	H	-4.38394466	4.35951120	4.77930303
H	8.74005534	5.47951120	2.15730303	C	-4.75594466	0.95651120	2.66630303
N	7.84605534	6.82751120	0.81030303	O	-5.27494466	1.34151120	1.63730303
H	8.36405534	6.48251120	0.07130303	N	-5.15794466	-0.16748880	3.21030303
C	7.21205534	7.95351120	0.57830303	H	-4.75194466	-0.42848880	4.06530303
N	6.30405534	8.54451120	1.34330303	C	-5.90294466	-1.25648880	2.58730303
H	5.87905534	7.97851120	2.05730303	H	-6.15594466	-0.83448880	1.57030303

C	-4.93294466	-2.41548880	2.40430303	H	-3.22225560	-1.68595784	-7.46582477
H	-4.00494466	-1.94748880	2.04730303	C	-0.79425560	-2.33495784	-3.90382477
H	-4.63294466	-2.91048880	3.39330303	O	0.03274440	-1.72195784	-3.17182477
S	-5.54794466	-3.68848880	1.35030303	N	-0.59925560	-3.61895784	-4.23382477
C	-7.09294466	-1.69848880	3.39430303	C	-1.50925560	-4.49195784	-4.93182477
O	-7.91994466	-2.37048880	2.83130303	H	-1.69125560	-4.33195784	-5.97282477
N	-7.26194466	-1.43048880	4.69130303	H	-2.46625560	-4.40295784	-4.47782477
H	-6.51294466	-1.03448880	5.23230303	C	-0.95125560	-5.88495784	-4.67882477
H	-8.02694466	-1.87048880	5.22630303	H	-1.32425560	-6.59995784	-5.38382477

Conformer 3 (279.50 ps)

				H	-1.19925560	-6.31295784	-3.71382477
N	-2.48825560	5.61504216	3.74817523	C	0.57674440	-5.60295784	-4.72282477
H	-2.83925560	6.59204216	3.63317523	H	0.91974440	-5.44895784	-5.73382477
H	-1.46525560	5.53104216	3.66017523	H	1.05074440	-6.44395784	-4.28682477
H	-2.70425560	5.33804216	4.71417523	C	0.65974440	-4.28895784	-3.92182477
C	-3.25625560	4.73504216	2.80417523	H	0.54574440	-4.47295784	-2.89482477
H	-3.22525560	3.71504216	3.19917523	C	1.98474440	-3.51495784	-4.16482477
C	-4.74325560	4.95104216	2.88117523	O	2.90674440	-3.58695784	-3.37782477
H	-5.05825560	5.06804216	3.94617523	N	1.98774440	-2.71295784	-5.22382477
H	-4.91625560	5.89604216	2.35317523	H	1.18274440	-2.77595784	-5.91082477
C	-5.59125560	3.93004216	2.16117523	C	3.13474440	-1.75595784	-5.51982477
H	-5.13425560	3.62704216	1.20217523	H	4.01574440	-2.30395784	-5.64582477
H	-5.80125560	3.09304216	2.82117523	C	2.72374440	-0.92695784	-6.72482477
C	-6.88425560	4.73504216	1.85017523	H	2.56874440	-1.63795784	-7.53882477
O	-7.05025560	5.44104216	0.81917523	H	1.77374440	-0.41695784	-6.47282477
O	-7.73825560	4.67204216	2.69917523	H	3.47874440	-0.14695784	-6.97482477
C	-2.67925560	4.65904216	1.46217523	C	3.57374440	-0.69395784	-4.43582477
O	-2.47525560	5.69004216	0.82717523	O	4.69774440	-0.12395784	-4.46282477
N	-2.60925560	3.43704216	0.89217523	N	2.71074440	-0.45895784	-3.46182477
H	-2.82725560	2.60204216	1.50017523	H	1.88574440	-1.06395784	-3.51282477
C	-2.06825560	3.17404216	-0.46182477	C	2.86574440	0.33904216	-2.29882477
H	-2.52025560	3.94704216	-1.15782477	H	3.38574440	1.28304216	-2.55582477
C	-0.50325560	3.28404216	-0.42382477	C	1.46574440	0.54004216	-1.64082477
H	-0.35625560	4.26404216	0.00817523	H	0.99374440	-0.43995784	-1.45982477
H	0.03274440	2.53104216	0.18417523	H	1.56874440	1.17204216	-0.77282477
S	0.41074440	3.32904216	-1.99382477	S	0.28174440	1.41604216	-2.67282477
C	-2.51825560	1.72004216	-0.84782477	C	3.76574440	-0.43095784	-1.29582477
O	-2.20225560	0.75304216	-0.13182477	O	4.39874440	0.15304216	-0.47182477
N	-3.35225560	1.57904216	-1.89482477	N	3.97374440	-1.78795784	-1.42982477
H	-3.61425560	2.44404216	-2.34882477	H	3.39474440	-2.32895784	-2.05382477
C	-4.26525560	0.35604216	-2.11982477	C	4.98474440	-2.48795784	-0.58682477
H	-4.21125560	-0.36295784	-1.31882477	H	5.12574440	-3.58895784	-0.84282477
C	-5.70825560	0.95304216	-2.18482477	H	5.98674440	-2.03395784	-0.73382477
H	-5.77725560	1.71804216	-2.94582477	C	4.71074440	-2.50395784	0.97517523
H	-6.43725560	0.10704216	-2.42982477	O	3.60774440	-2.77395784	1.45117523
S	-6.44625560	1.60804216	-0.69982477	N	5.78174440	-2.09695784	1.70317523
C	-3.76725560	-0.51795784	-3.29782477	H	6.59974440	-1.85695784	1.18317523
O	-4.61225560	-1.32595784	-3.67582477	C	5.76274440	-1.80795784	3.15117523
N	-2.54025560	-0.52995784	-3.72682477	H	5.63574440	-2.71895784	3.72117523
H	-1.85225560	0.19004216	-3.37682477	C	7.19574440	-1.39895784	3.52717523
C	-1.89825560	-1.50895784	-4.60682477	H	7.28974440	-1.39895784	4.60217523
H	-2.61825560	-2.20795784	-4.93182477	H	7.86474440	-2.16895784	3.22617523
C	-1.46125560	-0.77595784	-5.83482477	C	7.77574440	-0.13995784	2.93617523
H	-2.24425560	-0.02295784	-6.03482477	H	7.53974440	-0.02895784	1.86017523
H	-0.52925560	-0.28895784	-5.64882477	H	7.36674440	0.65904216	3.51817523
C	-1.30325560	-1.70895784	-7.02782477	C	9.27774440	-0.18895784	2.90817523
O	-0.21025560	-2.26395784	-7.18182477	H	9.60174440	-0.56795784	3.84917523
N	-2.32525560	-2.11395784	-7.73882477	H	9.65074440	-0.98695784	2.23317523
H	-2.28325560	-2.87395784	-8.35882477	N	9.87874440	1.10504216	2.53617523
				H	9.56374440	1.50604216	1.65317523

C	10.71574440	1.72504216	3.30617523
N	11.12174440	1.30604216	4.46717523
H	10.61974440	0.50604216	4.93917523
H	11.80874440	1.81204216	4.92117523
N	11.06274440	2.91804216	2.93417523
H	10.67474440	3.29504216	2.08717523
H	11.68774440	3.46404216	3.47317523
C	4.73274440	-0.74995784	3.54017523
O	4.33074440	-0.71695784	4.70317523
N	4.32974440	0.10404216	2.61017523
H	4.51674440	-0.10095784	1.62717523
C	3.34774440	1.11004216	2.84517523
H	3.14974440	1.15204216	3.93317523
C	3.90874440	2.41604216	2.25817523
H	4.30274440	2.37204216	1.31517523
H	3.08374440	3.11904216	2.11517523
C	5.00174440	3.06604216	3.14017523
N	5.05374440	2.94104216	4.50217523
C	6.03174440	3.77504216	4.91617523
H	6.24274440	3.98304216	5.98417523
N	6.74774440	4.25104216	3.87117523
H	7.40874440	5.02304216	3.98517523
C	6.14774440	3.74904216	2.70117523
H	6.27874440	4.07704216	1.67517523
C	1.95174440	0.81504216	2.18117523
O	1.00474440	1.65004216	2.22117523
N	1.74174440	-0.42495784	1.65117523
H	2.49674440	-1.06195784	1.70417523
C	0.43774440	-1.07595784	1.42517523
H	-0.17025560	-0.54995784	0.62017523
C	0.66674440	-2.51695784	0.99617523
H	1.46474440	-2.57395784	0.28517523
H	1.00974440	-2.99695784	1.91117523
C	-0.47325560	-3.36495784	0.42217523
C	-1.52525560	-2.77395784	-0.28982477
H	-1.69325560	-1.72195784	-0.44982477
C	-2.46825560	-3.59295784	-0.97482477
H	-3.17725560	-3.16495784	-1.61282477
C	-2.44025560	-4.99995784	-0.79282477
O	-3.31025560	-5.88495784	-1.45382477
H	-3.93525560	-5.38595784	-2.01182477
C	-1.48025560	-5.58395784	0.07017523
H	-1.35725560	-6.63295784	0.24817523
C	-0.43825560	-4.76495784	0.63717523
H	0.46074440	-5.21295784	1.18117523
C	-0.48525560	-0.94495784	2.63117523
O	-0.24025560	-1.50995784	3.70417523
N	-1.68625560	-0.32395784	2.40117523
H	-1.95225560	-0.01095784	1.47517523
C	-2.73725560	-0.20595784	3.49017523
H	-2.83125560	-1.23795784	3.81917523
C	-2.21625560	0.68304216	4.59517523
H	-1.14425560	0.65104216	4.85617523
H	-2.26125560	1.74504216	4.22317523
O	-3.16025560	0.73804216	5.65617523
H	-3.90525560	1.33904216	5.50017523
C	-4.09925560	0.33604216	2.96817523
O	-4.06725560	1.34004216	2.27417523
N	-5.18925560	-0.31995784	3.29917523

H	-5.07225560	-1.14595784	3.94017523
C	-6.45325560	-0.26495784	2.54917523
H	-6.55525560	0.80804216	2.40817523
C	-6.28225560	-0.82895784	1.11217523
H	-5.23525560	-0.75295784	0.69417523
H	-6.56825560	-1.83095784	1.08117523
S	-7.44325560	-0.02995784	-0.05382477
C	-7.78025560	-0.51095784	3.24717523
O	-8.90025560	-0.57295784	2.62517523
N	-7.76325560	-0.75195784	4.54817523
H	-6.89125560	-0.65195784	5.02517523
H	-8.67925560	-0.74095784	5.05417523

Conformer 4 (358.50 ps)

N	-3.36449275	7.06772991	0.19201318
H	-3.94249275	7.53172991	0.85301318
H	-3.27049275	7.65872991	-0.59698682
H	-2.50649275	6.92972991	0.73001318
C	-3.82149275	5.81872991	-0.26498682
H	-4.00949275	5.18272991	0.58401318
C	-5.12549275	5.85672991	-0.97398682
H	-5.90449275	6.44572991	-0.47198682
H	-4.92949275	6.30172991	-1.99498682
C	-5.68749275	4.46672991	-1.27498682
H	-4.96649275	3.75572991	-1.61798682
H	-6.02449275	4.18872991	-0.24098682
C	-7.01149275	4.58172991	-2.10198682
O	-6.86149275	4.49872991	-3.34198682
O	-8.05249275	4.79372991	-1.50298682
C	-2.74549275	5.14572991	-1.11298682
O	-2.29349275	5.70672991	-2.07398682
N	-2.32049275	3.93472991	-0.61798682
H	-2.87749275	3.59372991	0.12601318
C	-1.49549275	3.02572991	-1.38098682
H	-1.36949275	3.51472991	-2.38098682
C	-0.13049275	3.04872991	-0.70598682
H	0.13650725	4.13572991	-0.69798682
H	-0.26949275	2.66972991	0.30401318
S	1.29150725	2.26672991	-1.38998682
C	-2.09949275	1.64472991	-1.44698682
O	-2.08449275	0.89772991	-0.48398682
N	-2.72749275	1.29072991	-2.57598682
H	-2.74649275	1.98372991	-3.36498682
C	-3.57849275	0.06572991	-2.71898682
H	-3.81349275	-0.29027009	-1.74098682
C	-4.89749275	0.52572991	-3.40098682
H	-4.52949275	1.35472991	-4.01498682
H	-5.42949275	-0.23627009	-3.98998682
S	-6.04349275	1.26572991	-2.29798682
C	-2.93549275	-1.01127009	-3.58398682
O	-3.51949275	-2.05627009	-3.81098682
N	-1.76449275	-0.71527009	-4.16498682
H	-1.24749275	0.13672991	-3.98298682
C	-0.97549275	-1.68827009	-4.83098682
H	-1.59949275	-2.21827009	-5.56098682
C	0.05650725	-0.97627009	-5.74498682
H	-0.41749275	-0.08127009	-6.15098682
H	0.91050725	-0.60927009	-5.20298682
C	0.65750725	-1.86927009	-6.89898682

O	1.61050725	-2.63727009	-6.69398682		H	8.66950725	-2.35027009	5.54501318
N	0.12250725	-1.87627009	-8.10898682		N	9.44650725	-0.94827009	4.18701318
H	0.61950725	-2.37927009	-8.87998682		H	9.90650725	-1.72927009	3.75601318
H	-0.58149275	-1.20527009	-8.30598682		C	10.17250725	0.14072991	3.96101318
C	-0.29349275	-2.69527009	-3.89598682		N	10.06750725	1.18672991	4.81701318
O	0.20850725	-2.34327009	-2.83498682		H	9.41450725	1.17772991	5.59301318
N	-0.22549275	-4.03327009	-4.24498682		H	10.75550725	1.97672991	4.73201318
C	-1.00049275	-4.55427009	-5.40498682		N	11.05450725	0.25572991	2.99801318
H	-0.65249275	-4.17027009	-6.37198682		H	11.31850725	-0.60127009	2.52301318
H	-2.08949275	-4.38827009	-5.33398682		H	11.42750725	1.17272991	2.75101318
C	-0.84849275	-6.06827009	-5.23798682		C	4.09950725	-0.43827009	4.88901318
H	-0.83049275	-6.59327009	-6.19398682		O	3.65550725	0.22072991	5.82701318
H	-1.75549275	-6.46627009	-4.68298682		N	4.11150725	0.06772991	3.64901318
C	0.49650725	-6.30027009	-4.44598682		H	4.55550725	-0.35227009	2.89101318
H	1.35850725	-6.23727009	-5.16898682		C	3.47550725	1.40072991	3.33701318
H	0.58450725	-7.22427009	-3.83098682		H	3.48950725	1.94772991	4.23501318
C	0.51550725	-5.07627009	-3.52998682		C	4.25250725	2.02572991	2.19701318
H	0.09450725	-5.30927009	-2.52798682		H	4.29450725	1.37372991	1.31701318
C	1.99650725	-4.74127009	-3.18398682		H	3.81050725	2.94272991	1.91401318
O	2.42850725	-5.07527009	-2.06498682		C	5.70350725	2.47172991	2.60301318
N	2.64950725	-3.99627009	-4.07598682		N	6.75650725	2.56372991	1.69001318
H	2.24950725	-3.73727009	-4.98198682		C	7.82250725	2.84872991	2.55001318
C	4.00050725	-3.43127009	-3.83598682		H	8.83450725	3.15972991	2.22601318
H	4.63850725	-4.34827009	-3.71098682		N	7.39650725	3.07972991	3.80301318
C	4.49850725	-2.75427009	-5.14298682		H	7.85950725	3.57772991	4.47301318
H	4.44750725	-3.46227009	-5.95698682		C	6.08450725	2.86072991	3.87801318
H	3.76150725	-1.95827009	-5.36498682		H	5.51350725	2.93672991	4.75801318
H	5.49150725	-2.27927009	-4.96398682		C	2.00850725	1.29472991	2.95101318
C	4.13250725	-2.49227009	-2.69598682		O	1.42750725	2.21972991	2.36901318
O	5.27650725	-2.14227009	-2.30498682		N	1.31950725	0.14672991	3.19101318
N	2.99050725	-2.01927009	-2.12198682		H	1.79050725	-0.64027009	3.68101318
H	2.10650725	-2.24627009	-2.59098682		C	0.01150725	-0.17127009	2.55701318
C	3.02050725	-1.16727009	-0.92698682		H	-0.02849275	0.23272991	1.49801318
H	3.61450725	-0.24627009	-1.16198682		C	-0.28449275	-1.67927009	2.46001318
C	1.63750725	-0.82427009	-0.63898682		H	0.42350725	-2.14127009	1.75201318
H	1.03150725	-1.77827009	-0.67798682		H	-0.06749275	-2.12627009	3.41201318
H	1.57550725	-0.27727009	0.34001318		C	-1.63149275	-2.03527009	1.88101318
S	0.87150725	0.33772991	-1.85098682		C	-1.80849275	-2.22627009	0.48501318
C	3.64650725	-1.80227009	0.29101318		H	-0.94449275	-2.00827009	-0.15298682
O	4.54450725	-1.22727009	0.88901318		C	-3.00049275	-2.70027009	-0.02298682
N	3.27550725	-3.07027009	0.60801318		H	-3.23349275	-2.82527009	-1.08398682
H	2.55250725	-3.55327009	0.10001318		C	-4.08749275	-3.03927009	0.85501318
C	3.72550725	-3.75027009	1.83201318		O	-5.22649275	-3.61827009	0.35001318
H	3.13850725	-4.64327009	1.89101318		H	-5.12849275	-3.80027009	-0.60298682
H	4.75650725	-3.95827009	1.79201318		C	-3.87249275	-2.77327009	2.23401318
C	3.61450725	-2.90027009	3.07001318		H	-4.72349275	-2.94227009	2.88801318
O	2.44150725	-2.56027009	3.33801318		C	-2.68149275	-2.24427009	2.74301318
N	4.67150725	-2.65027009	3.84101318		H	-2.66949275	-2.05527009	3.79901318
H	5.56050725	-3.10327009	3.54201318		C	-1.15849275	0.49772991	3.27701318
C	4.63850725	-1.84927009	5.05801318		O	-1.08949275	0.62772991	4.50901318
H	4.02150725	-2.39227009	5.72701318		N	-2.22249275	0.97172991	2.61301318
C	6.03550725	-1.85327009	5.63901318		H	-2.30849275	0.81672991	1.57601318
H	6.00550725	-1.42127009	6.65601318		C	-3.30849275	1.70872991	3.22701318
H	6.35250725	-2.89527009	5.70601318		H	-3.67849275	1.04972991	4.00401318
C	7.03650725	-1.03327009	4.83801318		C	-2.84649275	3.00972991	3.84801318
H	6.96650725	-1.36727009	3.81401318		H	-2.05449275	2.81372991	4.57001318
H	6.80050725	0.05972991	5.05801318		H	-2.42049275	3.70872991	3.10501318
C	8.44250725	-1.38427009	5.28101318		O	-3.98349275	3.76772991	4.36301318
H	8.71650725	-0.86327009	6.20801318		H	-4.48349275	4.04672991	3.57701318

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C   -4.38349275   1.94972991   2.14601318
O   -4.15049275   2.70472991   1.21801318
N   -5.58949275   1.44872991   2.33201318
H   -5.59349275   0.76972991   3.13001318
C   -6.53449275   1.36372991   1.15901318
H   -6.28549275   2.21772991   0.53401318
C   -6.24949275  -0.06927009   0.45601318
H   -5.20149275  -0.28627009   0.41501318
H   -6.68349275  -0.93327009   0.92001318
S   -6.88949275  -0.28427009  -1.22898682
C   -8.01449275   1.59172991   1.52201318
O   -8.89449275   1.31172991   0.70001318
N   -8.27249275   2.14972991   2.70201318
H   -7.50049275   2.39672991   3.27801318
H   -9.23349275   2.42872991   3.04801318
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Conformer 5 (461.00 ps)

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N   -1.93782872   5.98355995  -5.49524111
H   -2.36282872   5.52255995  -6.30824111
H   -0.91482872   5.90955995  -5.66824111
H   -2.06682872   6.99455995  -5.39324111
C   -2.38882872   5.24255995  -4.31324111
H   -1.90782872   5.71755995  -3.47324111
C   -3.80982872   5.37455995  -4.10024111
H   -3.88582872   6.45855995  -4.01424111
H   -4.19782872   4.94055995  -4.96824111
C   -4.52082872   4.73855995  -2.85024111
H   -4.57382872   3.66255995  -2.88324111
H   -4.05182872   4.96955995  -1.89424111
C   -5.98882872   5.25755995  -2.83324111
O   -6.82882872   4.90555995  -3.71224111
O   -6.32182872   6.19755995  -2.01024111
C   -1.88982872   3.81855995  -4.23224111
O   -2.20682872   3.05955995  -5.10924111
N   -1.20782872   3.43855995  -3.18724111
H   -1.20782872   4.00455995  -2.36524111
C   -0.48782872   2.14655995  -3.02424111
H   -0.09182872   1.94055995  -4.03824111
C    0.70017128   2.22455995  -2.06724111
H    1.03417128   3.27155995  -1.89024111
H    0.39417128   1.95955995  -1.04324111
S    2.12317128   1.20855995  -2.60624111
C   -1.54382872   1.07755995  -2.60724111
O   -1.67582872   0.77755995  -1.47124111
N   -2.45082872   0.61955995  -3.50124111
H   -2.36682872   0.96155995  -4.42124111
C   -3.41782872  -0.45544005  -3.26724111
H   -3.77982872  -0.33144005  -2.27324111
C   -4.66482872  -0.25144005  -4.12324111
H   -4.44382872  -0.05944005  -5.18124111
H   -5.33782872  -1.10844005  -4.21424111
S   -5.84182872   1.06655995  -3.61324111
C   -2.90582872  -1.89844005  -3.35324111
O   -3.60782872  -2.80544005  -2.81324111
N   -1.62482872  -2.16644005  -3.72024111
H   -1.11682872  -1.51944005  -4.28424111
C   -1.14782872  -3.58544005  -3.64224111
H   -1.94482872  -4.21344005  -4.04424111
C    0.10617128  -3.78544005  -4.55124111
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H   -0.06982872  -3.28544005  -5.55224111
H    0.91617128  -3.28344005  -4.00724111
C    0.42517128  -5.22644005  -4.84224111
O    1.17317128  -5.92844005  -4.15424111
N   -0.18682872  -5.70744005  -5.93224111
H    0.24617128  -6.49344005  -6.33524111
H   -0.79682872  -5.08544005  -6.46624111
C   -0.80382872  -4.11544005  -2.22724111
O   -0.25782872  -3.29944005  -1.42224111
N   -1.05682872  -5.36644005  -1.85824111
C   -1.93582872  -6.29644005  -2.53724111
H   -1.37182872  -7.10444005  -3.05224111
H   -2.67282872  -5.86644005  -3.16724111
C   -2.52882872  -7.02744005  -1.27324111
H   -2.91682872  -8.00144005  -1.50124111
H   -3.34382872  -6.42944005  -0.77124111
C   -1.32682872  -7.07044005  -0.33124111
H   -0.52082872  -7.72244005  -0.63924111
H   -1.62482872  -7.25044005   0.67875889
C   -0.77582872  -5.70044005  -0.54824111
H   -1.38382872  -5.01444005   0.09275889
C    0.69717128  -5.61044005  -0.16524111
O    1.01817128  -5.27844005   0.98175889
N    1.59217128  -5.81644005  -1.15124111
H    1.24917128  -5.88044005  -2.10324111
C    3.05017128  -5.74844005  -0.91224111
H    3.37717128  -6.29544005   0.00175889
C    3.74717128  -6.54144005  -2.12524111
H    3.37217128  -7.54344005  -2.14124111
H    3.48917128  -5.94744005  -3.00524111
H    4.81117128  -6.61544005  -2.04524111
C    3.51617128  -4.28644005  -0.70024111
O    4.67617128  -4.01044005  -0.31124111
N    2.73317128  -3.21344005  -0.83924111
H    1.84817128  -3.30444005  -1.19324111
C    3.05617128  -1.90044005  -0.25624111
H    3.92517128  -1.50244005  -0.87224111
C    1.89717128  -0.95944005  -0.61424111
H    1.00617128  -1.35744005  -0.20924111
H    1.97717128   0.04855995  -0.20224111
S    1.72217128  -0.78244005  -2.39324111
C    3.41317128  -1.98044005   1.23575889
O    4.10817128  -1.07944005   1.64975889
N    2.87517128  -2.96244005   2.00375889
H    2.16817128  -3.63244005   1.66375889
C    3.20617128  -3.09344005   3.44475889
H    2.51317128  -3.79644005   3.91475889
H    4.23517128  -3.51044005   3.56075889
C    2.94217128  -1.91444005   4.34275889
O    1.87117128  -1.30244005   4.37075889
N    3.99017128  -1.51744005   4.97275889
H    4.81917128  -2.01944005   4.67775889
C    4.11117128  -0.14644005   5.63775889
H    3.52217128  -0.17944005   6.59975889
C    5.54517128  -0.02044005   6.27375889
H    5.48117128   0.57555995   7.20975889
H    5.98917128  -1.02444005   6.53075889
C    6.57317128   0.65155995   5.40175889
H    6.44617128   0.22155995   4.39675889
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H	6.14417128	1.68355995	5.28175889
C	7.97517128	0.76355995	6.05475889
H	7.90017128	1.46955995	6.90275889
H	8.22817128	-0.22544005	6.41575889
N	9.00517128	1.27755995	5.11075889
H	9.23817128	0.70755995	4.28375889
C	9.89317128	2.21555995	5.46975889
N	9.77517128	2.99755995	6.51775889
H	9.07717128	2.83955995	7.24075889
H	10.36317128	3.80555995	6.62475889
N	10.91517128	2.50455995	4.63375889
H	11.24517128	1.71455995	4.04575889
H	11.55917128	3.26855995	4.91275889
C	3.74317128	1.13055995	4.83275889
O	3.40317128	2.12455995	5.48875889
N	3.77017128	1.06755995	3.49375889
H	4.15617128	0.21455995	3.08775889
C	3.22517128	2.16255995	2.63075889
H	3.13517128	3.02155995	3.26575889
C	4.29717128	2.51055995	1.53675889
H	4.33517128	1.76155995	0.75875889
H	3.94217128	3.34255995	0.92775889
C	5.70117128	2.81455995	2.11175889
N	6.81217128	1.97555995	1.82475889
C	7.90317128	2.59055995	2.43175889
H	8.94217128	2.41655995	2.27075889
N	7.51517128	3.80155995	2.93375889
H	8.11517128	4.57955995	3.26475889
C	6.12417128	3.91155995	2.82075889
H	5.45717128	4.74555995	3.11475889
C	1.83317128	1.96555995	1.98275889
O	1.34017128	2.79055995	1.19475889
N	1.13717128	0.91555995	2.43575889
H	1.41717128	0.53355995	3.35875889
C	-0.19182872	0.53355995	1.92875889
H	-0.10982872	0.54455995	0.84375889
C	-0.59682872	-0.86944005	2.37475889
H	0.13217128	-1.55244005	1.90075889
H	-0.52982872	-0.99344005	3.48475889
C	-2.07182872	-1.20244005	2.02375889
C	-2.53982872	-1.51044005	0.70375889
H	-1.88282872	-1.53944005	-0.18524111
C	-3.85982872	-1.84444005	0.50475889
H	-4.18582872	-2.08444005	-0.47724111
C	-4.83682872	-1.75244005	1.59175889
O	-6.14382872	-2.06144005	1.39475889
H	-6.37982872	-2.51044005	0.53375889
C	-4.41982872	-1.13544005	2.81975889
H	-5.09682872	-1.05844005	3.61875889
C	-3.01682872	-0.93944005	3.05775889
H	-2.63082872	-0.61744005	4.01575889
C	-1.20582872	1.50155995	2.36375889
O	-1.42082872	1.71155995	3.50875889
N	-1.81782872	2.10555995	1.36075889
H	-1.70682872	1.78955995	0.42575889
C	-2.55382872	3.34755995	1.54575889
H	-2.88682872	3.45955995	2.60875889
C	-1.69082872	4.48555995	1.08675889
H	-2.11282872	5.47855995	1.12075889

H	-0.73782872	4.39855995	1.62975889
O	-1.31382872	4.28055995	-0.29724111
H	-1.29382872	5.20055995	-0.72624111
C	-3.86682872	3.26555995	0.78075889
O	-4.46082872	4.31455995	0.56475889
N	-4.46682872	2.11055995	0.50275889
H	-4.10882872	1.27055995	0.97575889
C	-5.79482872	2.00355995	-0.17124111
H	-5.66782872	2.57155995	-1.12624111
C	-6.06982872	0.52155995	-0.59124111
H	-5.10982872	0.01955995	-0.73224111
H	-6.57782872	0.02955995	0.26975889
S	-6.98382872	0.24355995	-2.12124111
C	-7.04082872	2.56055995	0.62475889
O	-7.39782872	1.96155995	1.67475889
N	-7.77082872	3.62155995	0.15575889
H	-7.49982872	3.94455995	-0.75324111
H	-8.61882872	3.97355995	0.67575889

Conformer 6 (561.25 ps)

N	4.04408432	5.99883531	-4.31599868
H	4.08408432	7.03183531	-4.13399868
H	4.10208432	5.86683531	-5.30299868
H	4.90308432	5.65583531	-3.90799868
C	2.71508432	5.56483531	-3.76199868
H	2.74108432	5.76483531	-2.68999868
C	1.53508432	6.48183531	-4.18199868
H	1.59108432	7.56283531	-3.86499868
H	1.39708432	6.38083531	-5.28099868
C	0.12808432	6.05283531	-3.55699868
H	-0.03291568	4.93083531	-3.77999868
H	0.04808432	6.13483531	-2.49399868
C	-1.01391568	6.80383531	-4.26799868
O	-1.30791568	6.68083531	-5.49499868
O	-1.71391568	7.47983531	-3.46199868
C	2.55708432	4.03783531	-4.08699868
O	2.85508432	3.59883531	-5.19799868
N	2.05908432	3.22183531	-3.08999868
H	1.84908432	3.70983531	-2.14299868
C	1.56908432	1.83483531	-3.25399868
H	1.86108432	1.43383531	-4.19599868
C	2.39808432	0.96283531	-2.21599868
H	3.32408432	1.43683531	-2.15199868
H	1.86008432	1.10383531	-1.27699868
S	2.68108432	-0.76116469	-2.46699868
C	0.03808432	1.83683531	-3.08499868
O	-0.42891568	2.50983531	-2.14599868
N	-0.73291568	1.16683531	-3.88999868
H	-0.30491568	0.54083531	-4.54999868
C	-2.17591568	1.02583531	-3.66199868
H	-2.36291568	1.48383531	-2.66799868
C	-2.93191568	1.88883531	-4.76899868
H	-2.32091568	1.86283531	-5.68199868
H	-3.92591568	1.49683531	-4.99499868
S	-3.21791568	3.68083531	-4.49099868
C	-2.67391568	-0.36516469	-3.67299868
O	-3.75991568	-0.62416469	-3.08899868
N	-2.00091568	-1.32816469	-4.24999868
H	-1.08991568	-1.10716469	-4.66399868

C	-2.49291568	-2.68316469	-4.37699868	H	1.53208432	-2.60816469	8.07800132
H	-3.50791568	-2.51316469	-4.83599868	C	3.55608432	-2.10116469	7.32200132
C	-1.70291568	-3.44116469	-5.44699868	H	3.68308432	-2.80816469	6.48600132
H	-1.94791568	-2.99816469	-6.36299868	H	4.07408432	-1.12516469	7.03200132
H	-0.64091568	-3.46416469	-5.33099868	C	4.06308432	-2.68416469	8.63200132
C	-2.05791568	-4.90616469	-5.50299868	H	3.83908432	-1.98816469	9.46400132
O	-1.75791568	-5.58016469	-4.52899868	H	3.65408432	-3.64916469	8.84300132
N	-2.52791568	-5.44216469	-6.62999868	N	5.52208432	-2.80016469	8.59300132
H	-2.87091568	-6.37416469	-6.63699868	H	5.82708432	-3.76316469	8.41400132
H	-2.85891568	-4.79916469	-7.36199868	C	6.52908432	-1.95916469	8.94300132
C	-2.54991568	-3.32816469	-2.93799868	N	6.29208432	-0.77516469	9.43100132
O	-1.63491568	-3.12016469	-2.14599868	H	5.33708432	-0.48816469	9.65600132
N	-3.54391568	-4.12016469	-2.61199868	H	7.07108432	-0.14016469	9.72200132
C	-4.73791568	-4.45316469	-3.40899868	N	7.77608432	-2.28916469	8.56700132
H	-4.50391568	-5.11116469	-4.27999868	H	8.03008432	-3.11716469	8.04500132
H	-5.14491568	-3.60916469	-3.82999868	H	8.42308432	-1.52416469	8.63900132
C	-5.68691568	-5.14716469	-2.50899868	C	1.81208432	-0.44316469	5.37200132
H	-6.36791568	-5.86016469	-3.00699868	O	1.39708432	0.66383531	5.62500132
H	-6.38091568	-4.44116469	-2.01799868	N	2.76708432	-0.66116469	4.48000132
C	-4.74191568	-5.80816469	-1.51399868	H	3.23008432	-1.58316469	4.42300132
H	-4.25791568	-6.56516469	-2.03099868	C	3.28808432	0.26083531	3.45000132
H	-5.36391568	-6.16916469	-0.65299868	H	3.61608432	1.09183531	4.07800132
C	-3.67391568	-4.75116469	-1.29099868	C	4.50108432	-0.39716469	2.81900132
H	-4.06691568	-3.96216469	-0.58699868	H	4.19708432	-1.31516469	2.28300132
C	-2.49391568	-5.46616469	-0.64899868	H	5.05008432	0.22183531	2.13000132
O	-2.32491568	-5.52516469	0.54900132	C	5.51408432	-0.82916469	3.86400132
N	-1.55191568	-6.01716469	-1.49299868	N	5.50508432	-2.09116469	4.49000132
H	-1.65991568	-5.94716469	-2.50599868	C	6.52408432	-2.02316469	5.37600132
C	-0.38891568	-6.68016469	-1.03099868	H	6.66608432	-2.75516469	6.15000132
H	-0.62791568	-7.27116469	-0.19399868	N	7.11108432	-0.79216469	5.38500132
C	0.10908432	-7.53316469	-2.19999868	H	7.92008432	-0.54016469	5.98200132
H	-0.69091568	-8.21216469	-2.55199868	C	6.44008432	-0.00816469	4.52300132
H	0.28108432	-6.88816469	-3.02499868	H	6.64508432	0.98183531	4.27200132
H	0.90308432	-8.22816469	-1.92899868	C	2.27808432	0.64383531	2.27200132
C	0.81208432	-5.82716469	-0.53499868	O	2.62908432	1.30383531	1.32200132
O	1.85508432	-6.45316469	-0.24199868	N	1.04608432	0.13383531	2.36100132
N	0.70908432	-4.46516469	-0.60099868	H	0.73308432	-0.52016469	3.08400132
H	0.02308432	-3.96116469	-1.15999868	C	-0.01491568	0.79583531	1.69500132
C	1.68908432	-3.61216469	0.10700132	H	0.14108432	0.83983531	0.61400132
H	2.75308432	-3.81116469	-0.11599868	C	-1.30991568	0.08883531	2.05300132
C	1.35408432	-2.12416469	-0.11199868	H	-1.31291568	-0.96416469	1.75600132
H	0.44108432	-1.87316469	0.53600132	H	-1.45591568	0.18083531	3.12700132
H	2.14108432	-1.54216469	0.20800132	C	-2.52791568	0.58583531	1.34000132
S	0.94508432	-1.62916469	-1.88499868	C	-3.09091568	-0.18816469	0.26300132
C	1.74608432	-3.80816469	1.63800132	H	-2.54491568	-0.99616469	-0.09099868
O	2.70508432	-3.33616469	2.24200132	C	-4.43491568	0.10483531	-0.18699868
N	0.76708432	-4.44916469	2.23000132	H	-4.88891568	-0.48316469	-0.94499868
H	-0.04991568	-4.76716469	1.72600132	C	-5.17591568	1.15683531	0.32500132
C	0.64808432	-4.55116469	3.70400132	O	-6.41691568	1.37583531	-0.15899868
H	-0.18891568	-5.20916469	3.95900132	H	-6.81691568	0.67983531	-0.70099868
H	1.57308432	-4.91816469	4.00200132	C	-4.55691568	2.04983531	1.20300132
C	0.55708432	-3.18016469	4.40600132	H	-5.17391568	2.83383531	1.67100132
O	-0.23491568	-2.38116469	3.97700132	C	-3.24691568	1.73983531	1.78700132
N	1.28008432	-2.91216469	5.49500132	H	-2.88991568	2.22283531	2.70800132
H	1.86108432	-3.64716469	5.81500132	C	-0.12091568	2.22683531	2.11500132
C	1.26608432	-1.63116469	6.25800132	O	0.01508432	2.53383531	3.31600132
H	0.27708432	-1.44316469	6.58900132	N	-0.17691568	3.12983531	1.12500132
C	2.07508432	-1.80716469	7.58500132	H	0.01908432	2.76283531	0.24600132
H	1.99308432	-0.94216469	8.19300132	C	-0.11191568	4.63683531	1.16900132

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H   -0.16091568   5.02383531    2.18600132        H   -2.51191568   5.29083531   -2.02499868
C    1.34208432   5.00083531    0.74900132        C   -3.85591568   3.72583531   -1.57499868
H    1.41108432   6.07483531    0.97800132        H   -3.21491568   2.84183531   -1.61499868
H    2.07808432   4.51883531    1.38600132        H   -4.62991568   3.59183531   -0.81199868
O    1.52208432   4.77283531   -0.64899868        S   -4.68991568   3.80883531   -3.14099868
H    1.63208432   5.65983531   -0.98299868        C   -4.09891568   6.14283531   -0.97999868
C   -1.17391568   5.34983531    0.32500132        O   -4.77091568   6.21583531    0.03000132
O   -1.13591568   6.56383531    0.11200132        N   -4.19091568   7.02283531   -1.93899868
N   -2.18391568   4.59083531   -0.13099868        H   -3.43091568   7.07883531   -2.58999868
H   -2.22591568   3.63383531    0.11100132        H   -4.94891568   7.66183531   -1.91099868
C   -3.11191568   4.99483531   -1.16899868
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