

Conformational preferences induced by cyclization in orbitides: a vibrational CD study

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Electronic Supplementary File

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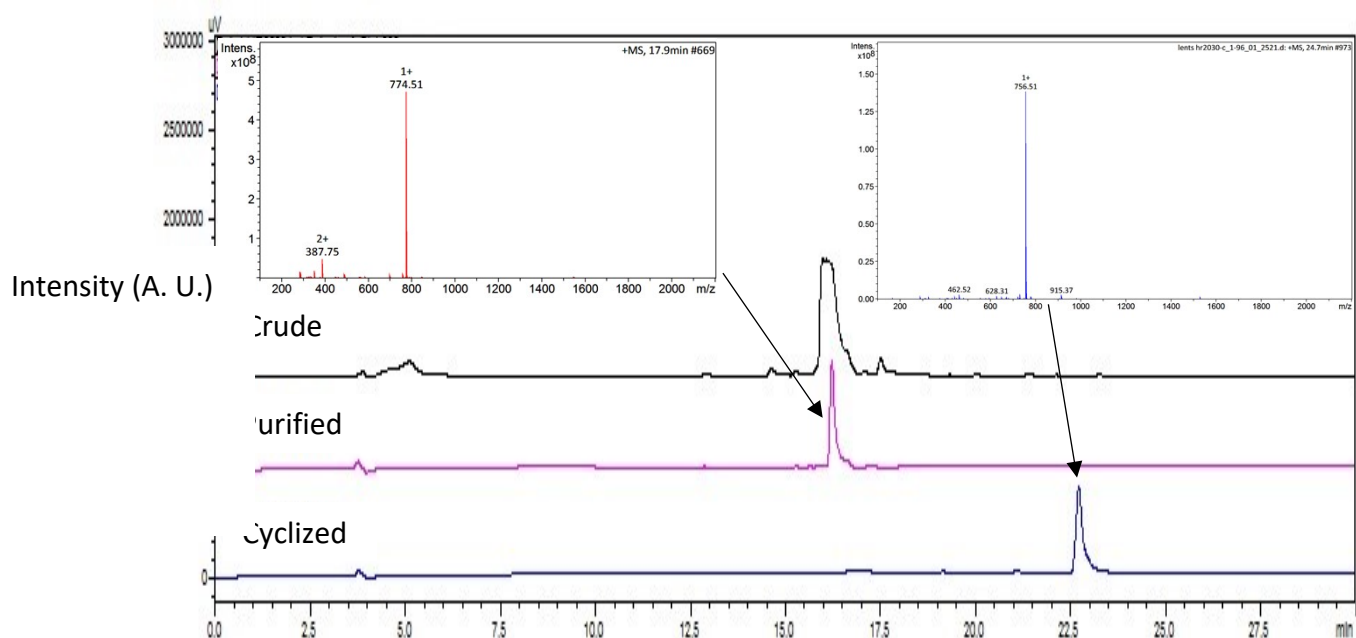


Figure S1. Chromatogram profiles of D-pohlianin A presenting the crude, purified and cyclized peptides. Inset, mass spectra of the purified and cyclized D-pohlianin A, confirming the success of the orbitide synthesis, indicated by the arrows.

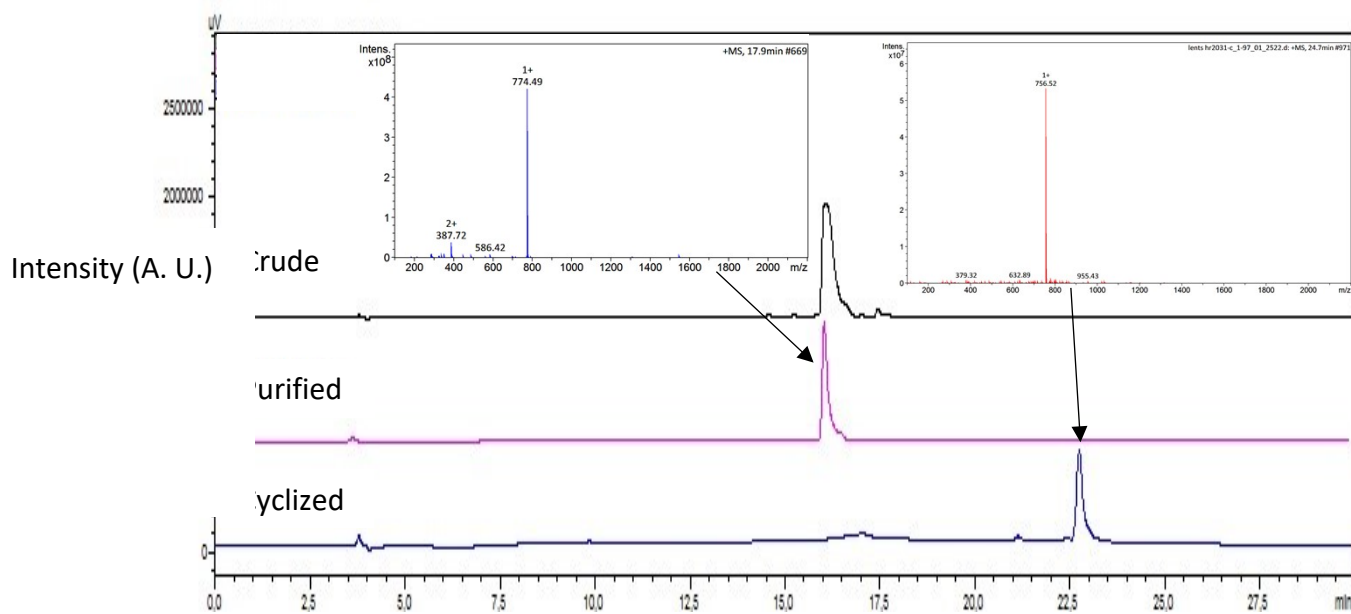


Figure S2. Chromatogram profiles of L-pohlianin A presenting the crude, purified and cyclized peptides. Inset, the mass spectra of the purified and cyclized L-pohlianin A, confirming the success of the orbitide synthesis, indicated by the arrows.

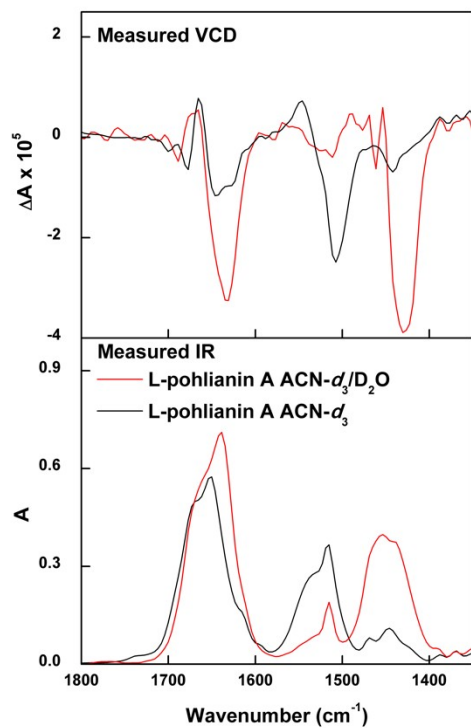


Figure S3. Experimental IR and VCD spectra of all-L **1** (cyclic) in 75:25 ACN- d_3 /D $_2$ O and 100% ACN- d_3 .

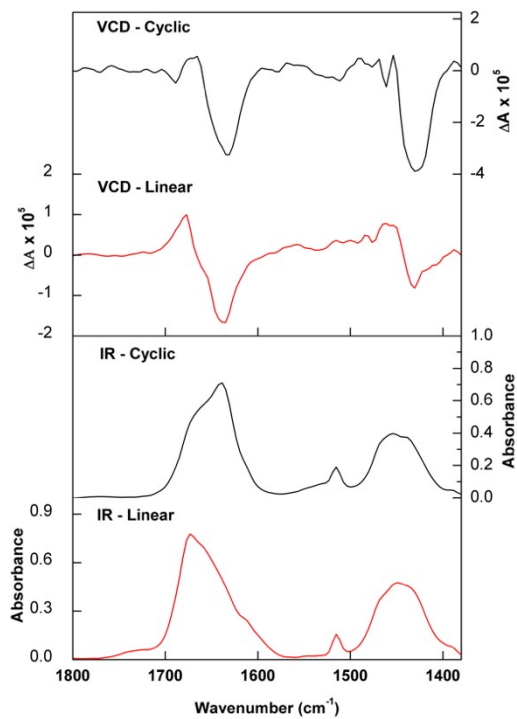


Figure S4. Experimental IR and VCD spectra of all-L **1** (cyclic) and all-L **1a** (linear) in 75:25 ACN- d_3 /D $_2$ O.

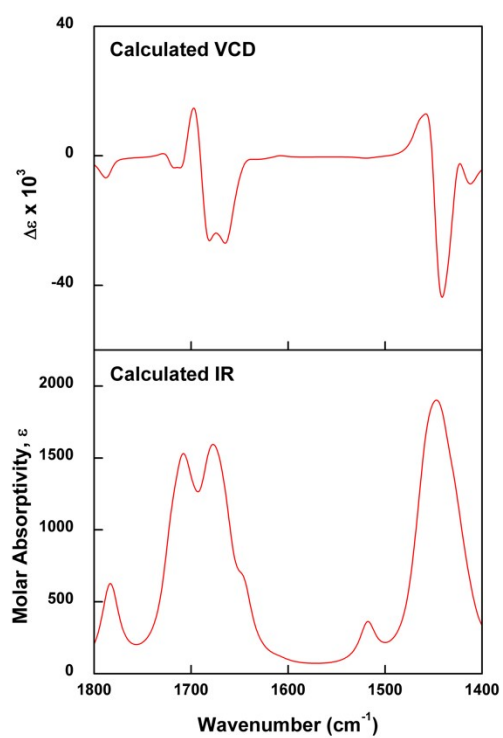


Figure S5. Calculated IR and VCD for the simple average of the four lowest-energy conformers identified for all-L **1a** (linear) at the B3PW91/PCM(DMSO)/cc-pVDZ.

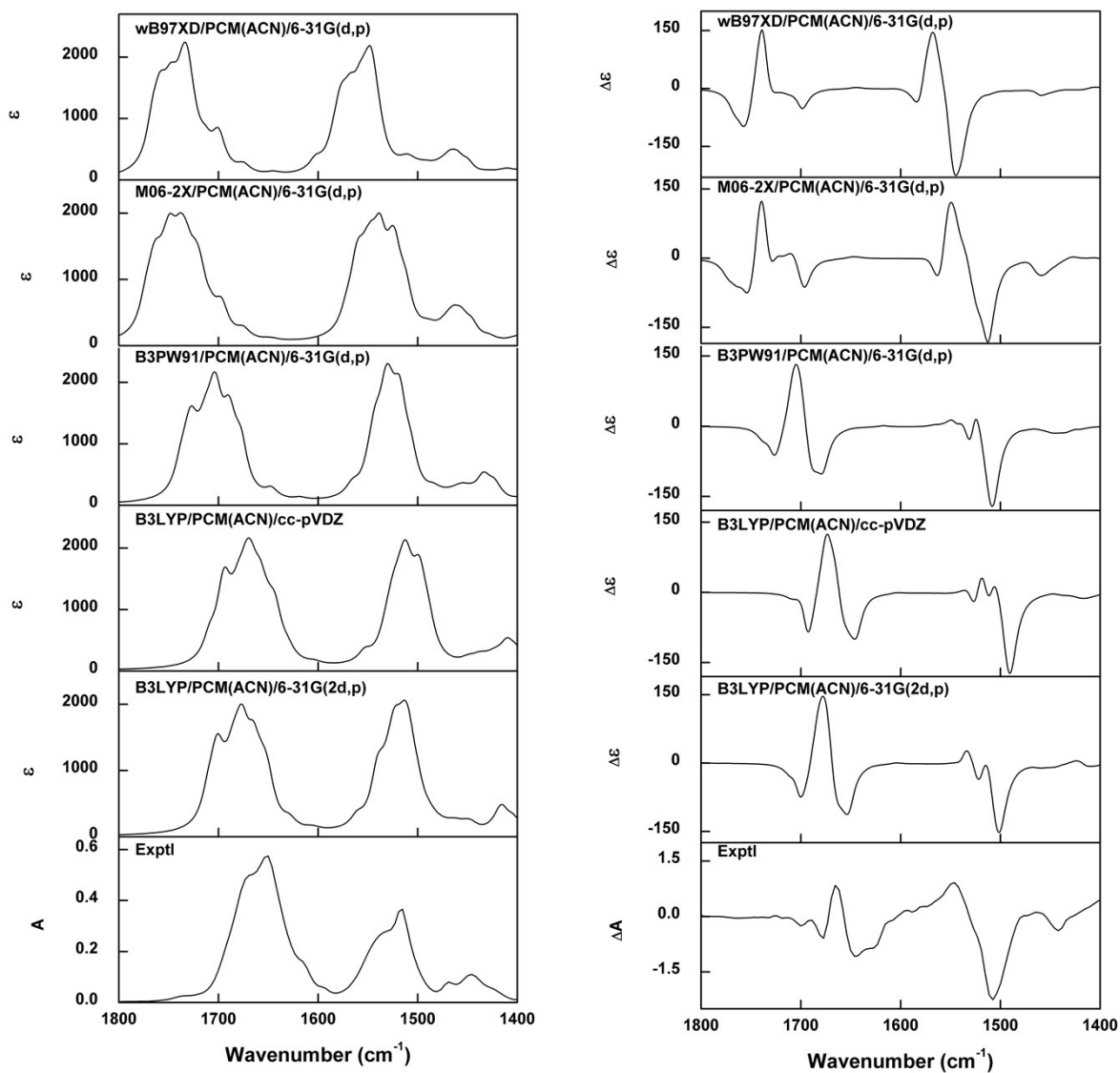


Figure S6. (Left) Comparison of experimental IR spectrum (bottom, measured in 100% ACN-*d*₃) with calculated data at different levels of theory for the simple average of the three lowest-energy conformers identified for all-L **1** (cyclic). (Right) Comparison of experimental VCD spectrum (bottom, measured in 100% ACN-*d*₃) with calculated data at different levels of theory for the simple average of the three lowest-energy conformers identified for all-L **1** (cyclic).

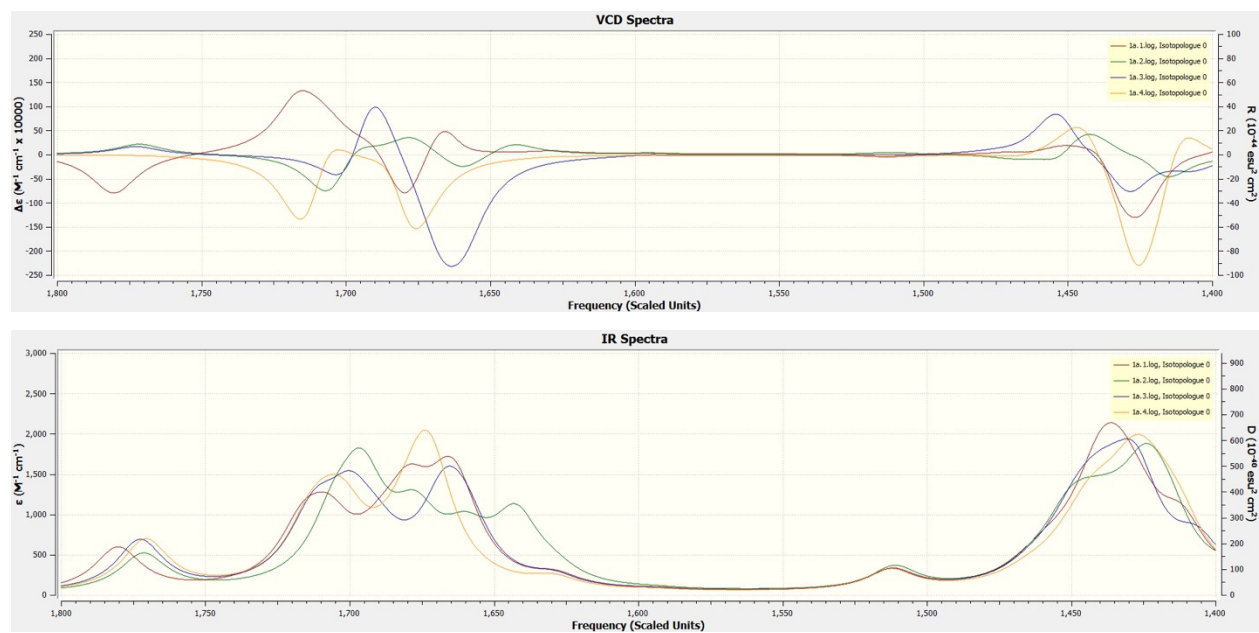


Figure S7. Calculated IR and VCD of the individual conformers identified for all-L **1a** (linear) at the B3PW91/PCM(DMSO)/6-31G(d,p).

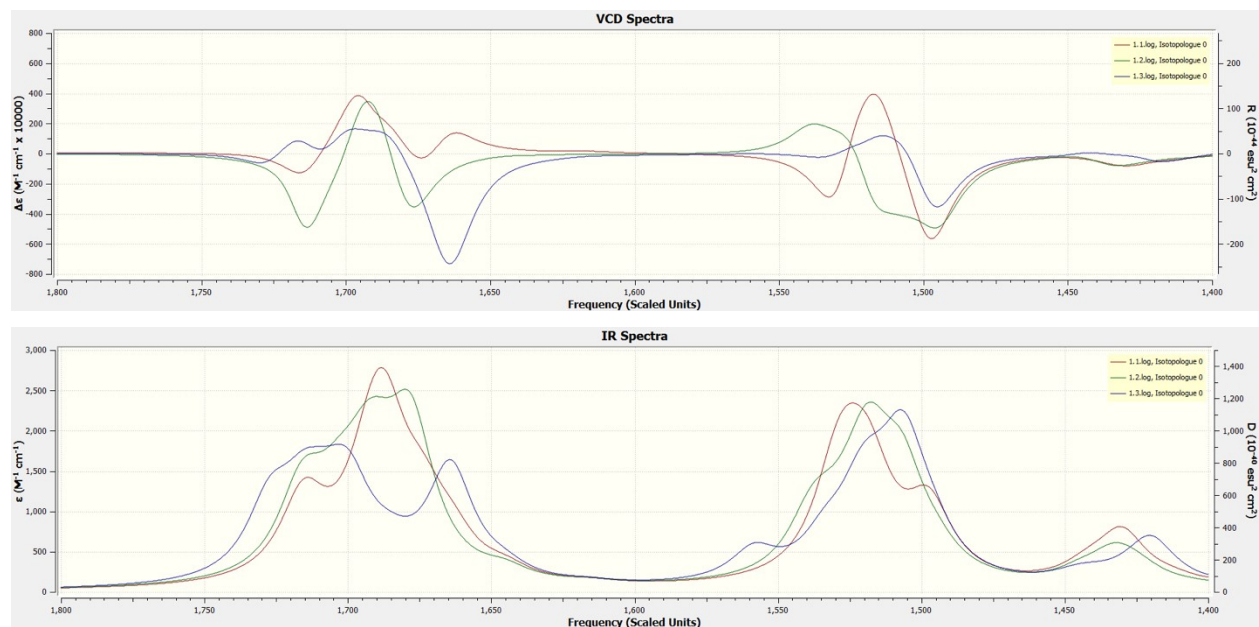


Figure S8. Calculated IR and VCD of the individual conformers identified for all-L **1** (cyclic) at the B3PW91/PCM(ACN)/cc-pVDZ.

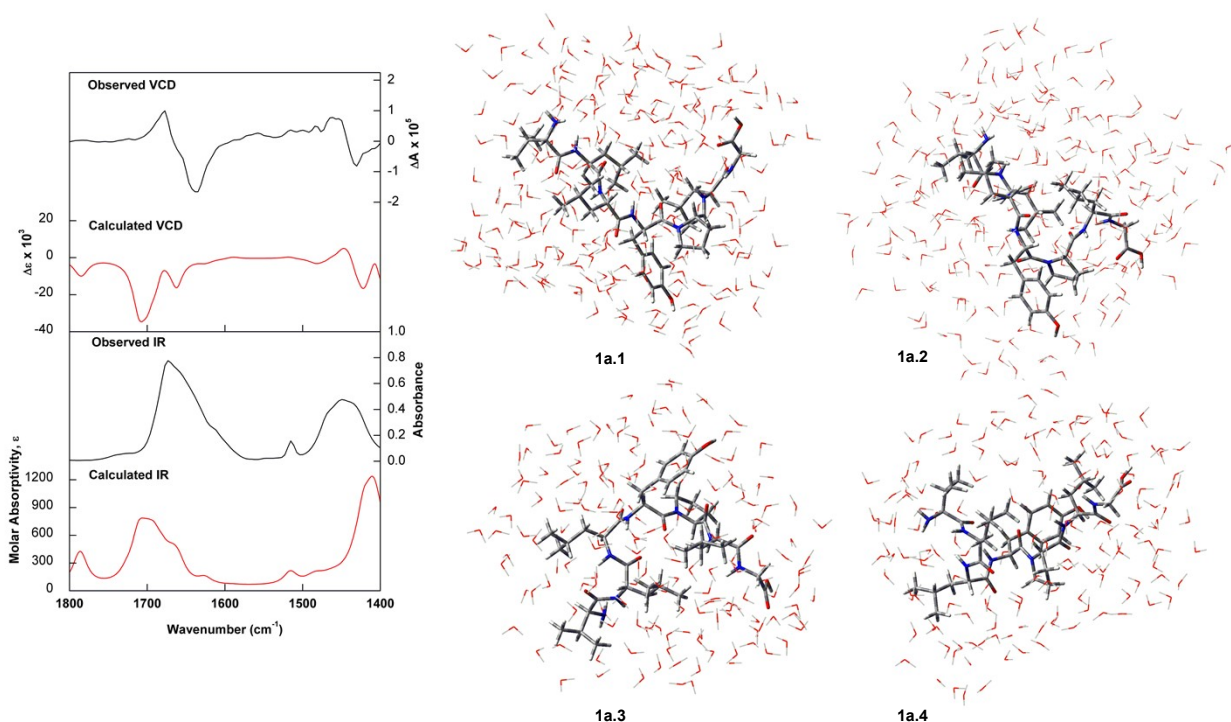


Figure S9. (Left) Comparison of experimental IR and VCD spectra of **1a** (linear) recorded in 75:25 proportion of ACN- d_3 /D $_2$ O (black trace) with QM/MM simulated IR and VCD spectra for the simple average of the four lowest-energy conformers identified for all-L **1a** using the two-layer ONIOM approach (red trace). (Right) Optimized structures with implicit water molecules.

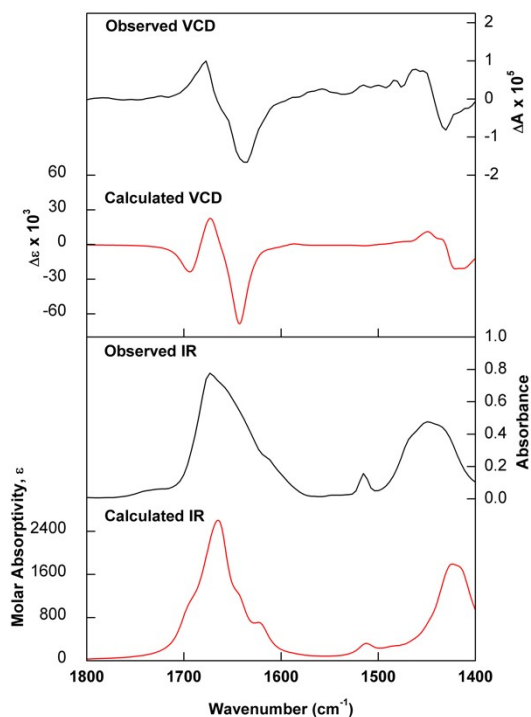


Figure S10. Comparison of experimental IR and VCD spectra of **1a** (linear) recorded in 75:25 proportion of ACN- d_3 /D $_2$ O (black trace) with calculated [B3LYP/PCM(H $_2$ O)]/6-31G(d)] IR and VCD spectra for the Boltzmann average of the four lowest-energy conformers identified for all-L **1a** in zwitterionic form (linear) (red trace).

Table S1. Dihedral angles (in degrees) of lowest-energy conformers identified for all-L **1** (cyclic) at the B3PW91/PCM(ACN)/cc-pVDZ level.

Confs	Pro ₁		Leu ₂		Gly ₃		Val ₄		Leu ₅		Leu ₆		Tyr ₇	
	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
1.1	-102	7	-122	17	83	-58	-69	-21	-116	33	70	-76	-133	131
1.2	-102	13	-79	-42	-145	178	-64	-32	-93	-15	-130	63	-64	133
1.3	-91	-0.3	-79	-24	90	-51	-73	-24	-110	-78	-127	159	-62	143
Lit*	-74	-15	-63	-27	-172	177	-56	-39	-82	-8	-157	71	-64	144

* Auvin-Guette et al., *Tetrahedron* **1999**, 55, 11495-11510

Table S2. Relative energies (E_{rel}) and conformer populations of all-L **1a** (linear).

Conformer	B3PW91/PCM(DMSO)/6-31G(d,p)		B3PW91/PCM(DMSO)/cc-pVDZ	
	E_{rel} (kcal/mol) ¹	Population (%)	E_{rel} (kcal/mol) ²	Population (%)
1a.1	0.0	61.57	0.0	92.6
1a.2	0.436	29.46	1.62	5.95
1a.3	1.545	4.53	2.79	0.82
1a.4	1.560	4.42	2.96	0.63

¹ Referenced to $G = -2582.840897$ Hartree; ² Referenced to $G = -2582.924874$ Hartree;

Table S3. Relative energies (E_{rel}) and conformer populations (Pop.) of all-L **1** (cyclic).

Confs.	B3PW91/ PCM(ACN)/ 6-31G(d,p)		B3LYP/ PCM(ACN)/ 6-31G(2d,p)		B3LYP/ PCM(ACN)/ cc-pVDZ		B3PW91/ PCM(ACN)/ cc-pVDZ		M06-2X/ PCM(ACN)/ 6-31G(d,p)		wB97XD/ PCM(ACN)/ 6-31G(d)	
	E_{rel} (kcal/mol) ¹	Pop. (%)	E_{rel} (kcal/mol) ²	Pop. (%)	E_{rel} (kcal/mol) ³	Pop. (%)	E_{rel} (kcal/mol) ⁴	Pop. (%)	E_{rel} (kcal/mol) ⁵	Pop. (%)	E_{rel} (kcal/mol) ⁶	Pop. (%)
1.1	0.0	65.1	0.04	47.8	0.41	32.9	0.756	21.5	3.71	0.2	0.157	43.4
1.2	0.381	34.2	0.0	51.2	0.0	65.8	0.0	77.1	0.0	99.8	0.0	56.6
1.3	2.76	0.7	2.39	1	2.38	1.3	2.38	1.4	7.31	-	4.02	-

¹Referenced to $G = -2506.416241$ Hartree, ²Referenced to $G = -2507.393486$ Hartree, ³Referenced to $G = -2507.392854$ Hartree, ⁴Referenced to $G = -2506.495521$ Hartree, ⁵Referenced to $G = -2506.287044$ Hartree, ⁶Referenced to $G = -2506.549633$ Hartree

CARTESIAN COORDINATES**Conformer 1.1**

B3PW91/PCM(ACN)/cc-pVDZ opt

Total energy = -2506.494316 Hartree

Imaginary frequencies = 0

N	1.12959	2.120511	0.034059
H	0.758123	2.493982	0.910282
C	2.411615	1.441529	0.043505
H	2.463552	0.871196	-0.89127
C	2.474177	0.546272	1.281834
O	2.177091	1.015689	2.379445
C	3.553046	2.487928	0.084862
H	3.386348	3.169952	-0.76302
H	3.427844	3.076324	1.007003
C	4.946517	1.91386	0.021153
C	5.694001	1.681223	1.185632
H	5.263119	1.928701	2.159457
C	5.541919	1.596849	-1.20817
H	4.9945	1.778545	-2.13736

C	6.981218	1.151093	1.131871
H	7.557753	0.980894	2.043391
C	6.827827	1.062177	-1.27917
H	7.27169	0.82824	-2.25095
C	7.557064	0.835879	-0.10507
O	8.815965	0.325573	-0.1038
H	9.09022	0.160425	-1.01807
N	2.858555	-0.75504	1.148485
C	3.480561	-1.37222	-0.0275
H	3.920648	-0.61549	-0.68973
C	2.541567	-2.21319	-0.90801
O	3.005372	-2.84944	-1.84903
C	4.581956	-2.24948	0.586775
H	5.462472	-1.62002	0.783932
H	4.877148	-3.05837	-0.09304
C	3.955805	-2.72802	1.896792
H	4.702819	-3.03892	2.639778
H	3.296785	-3.5912	1.714671
C	3.144867	-1.52368	2.377781
H	2.21252	-1.80501	2.88864
H	3.714382	-0.87965	3.065688
N	1.215673	-2.18783	-0.60024
H	0.955712	-1.72408	0.265858
C	0.273893	-3.11512	-1.20442
H	0.848254	-3.63302	-1.99133
C	-0.87462	-2.43417	-1.95617
O	-1.88337	-3.08202	-2.27015
C	-0.27405	-4.14023	-0.2037
H	-0.74969	-3.5937	0.630425
H	-1.08059	-4.68778	-0.71498
C	0.747746	-5.13539	0.357823
H	1.566066	-4.55802	0.825789
C	0.094532	-5.97994	1.453659
H	-0.73949	-6.57683	1.046377
H	-0.30974	-5.35084	2.262976
H	0.818426	-6.67968	1.900218
C	1.357483	-6.0262	-0.7259
H	2.05214	-6.75687	-0.28195
H	0.573553	-6.59183	-1.25849
H	1.925279	-5.44606	-1.46901
N	-0.72837	-1.14132	-2.29839
H	0.100837	-0.61936	-2.02432
C	-1.66603	-0.48403	-3.19178
H	-1.16612	0.383981	-3.63153

H	-1.95695	-1.18762	-3.98847
C	-2.93105	0.02487	-2.5012
O	-3.25272	1.217851	-2.52847
N	-3.66122	-0.90523	-1.84579
H	-3.35481	-1.87911	-1.93725
C	-4.91904	-0.54903	-1.21184
H	-5.4865	0.087195	-1.91048
C	-4.7487	0.364551	0.014893
O	-5.68532	1.063062	0.392745
C	-5.78204	-1.78518	-0.88765
H	-6.66562	-1.37233	-0.37233
C	-6.26062	-2.47283	-2.16733
H	-5.42271	-2.90538	-2.73797
H	-6.95193	-3.29449	-1.9252
H	-6.78918	-1.76781	-2.8275
C	-5.09625	-2.77113	0.06011
H	-4.77962	-2.28921	0.99781
H	-5.78812	-3.58606	0.322316
H	-4.20738	-3.23625	-0.39747
N	-3.52881	0.35479	0.609131
H	-2.83378	-0.27906	0.227588
C	-3.10968	1.309188	1.621514
H	-3.96039	2.000275	1.739482
C	-1.92096	2.151698	1.10807
O	-1.04604	2.561336	1.877729
C	-2.7797	0.661491	2.96747
H	-1.95322	-0.0554	2.818912
H	-2.37922	1.451964	3.621855
C	-3.94854	-0.04529	3.664164
H	-4.33795	-0.81829	2.976028
C	-3.44521	-0.75462	4.922693
H	-4.25745	-1.30966	5.418243
H	-2.64056	-1.47051	4.689357
H	-3.04478	-0.02811	5.650569
C	-5.09757	0.908517	3.998016
H	-4.74872	1.739407	4.635553
H	-5.55228	1.336096	3.091533
H	-5.89386	0.380341	4.546797
N	-1.93442	2.406985	-0.21597
H	-2.65719	1.975899	-0.79179
C	-0.88684	3.09058	-0.9723
H	-1.26344	3.122957	-2.0034
C	0.36505	2.198244	-1.07524
O	0.641574	1.613053	-2.12895

C	-0.56606	4.525097	-0.52231
H	-0.44199	4.555834	0.571428
H	0.415899	4.779312	-0.95608
C	-1.56921	5.60098	-0.96813
H	-1.70134	5.496661	-2.06226
C	-2.94493	5.469346	-0.3119
H	-3.43378	4.515025	-0.55381
H	-3.61141	6.281093	-0.6456
H	-2.86373	5.535348	0.786765
C	-0.98288	6.989058	-0.70035
H	-0.01704	7.127839	-1.21218
H	-0.81455	7.14322	0.379349
H	-1.66533	7.781293	-1.04685

Conformer 1.2

B3PW91/PCM(ACN)/cc-pVDZ opt

Total energy = -2506.495521 Hartree

Imaginary frequencies = 0

N	0.232661	-0.54797	-1.83085
C	1.514059	-1.04485	-1.35767
H	1.571441	-0.86667	-0.27348
C	2.642963	-0.3196	-2.1109
O	2.581246	-0.20302	-3.33315
C	1.559328	-2.55811	-1.64505
H	0.661117	-3.00306	-1.1866
H	1.472834	-2.68746	-2.73552
C	2.788928	-3.26718	-1.13649
C	3.892757	-3.4949	-1.96797
H	3.864526	-3.15726	-3.00718
C	2.860555	-3.73169	0.186393
H	2.010186	-3.58248	0.857548
C	5.030145	-4.15603	-1.50336
H	5.875867	-4.32862	-2.17488
C	3.989644	-4.38974	0.666306
H	4.034932	-4.75187	1.695319
C	5.085649	-4.60642	-0.1792
O	6.159276	-5.25954	0.335885
H	6.838323	-5.3408	-0.35022
N	3.695835	0.178387	-1.40639
C	4.074138	-0.10275	-0.01759
H	3.620842	-1.03859	0.33653
C	3.705666	0.985925	1.007312
O	4.201915	0.951362	2.133099

C	5.600501	-0.23501	-0.1076
H	5.851839	-1.23954	-0.47981
H	6.069782	-0.09169	0.873209
C	5.96284	0.832637	-1.13965
H	6.948005	0.674749	-1.59963
H	5.971846	1.828705	-0.6686
C	4.831932	0.734381	-2.16472
H	4.564131	1.703594	-2.61085
H	5.073102	0.0479	-2.99172
N	2.847392	1.949475	0.606859
H	2.35657	1.844187	-0.28296
C	2.470518	3.032939	1.500602
H	3.352406	3.267536	2.111946
C	1.39518	2.632388	2.52407
O	1.447864	3.012436	3.693329
C	2.046818	4.251602	0.667161
H	2.899834	4.50984	0.014487
H	1.225302	3.943577	-0.00161
C	1.61704	5.499273	1.449854
H	0.738367	5.233229	2.065626
C	2.70971	6.009166	2.390745
H	3.641304	6.221905	1.838245
H	2.39485	6.942603	2.884187
H	2.934682	5.276736	3.179729
C	1.182658	6.590437	0.469498
H	0.375723	6.240468	-0.19418
H	0.817134	7.481191	1.004366
H	2.025978	6.906239	-0.16836
N	0.381586	1.880881	2.038324
H	0.435895	1.5139	1.089024
C	-0.62676	1.30624	2.888552
H	-1.52359	1.946739	2.968632
H	-0.227	1.19589	3.90894
C	-1.04449	-0.04065	2.322024
O	-0.60124	-0.44766	1.245522
N	-1.96334	-0.74776	3.020453
H	-2.20258	-0.44168	3.958541
C	-2.25003	-2.1305	2.651258
H	-1.29749	-2.67782	2.564241
C	-2.86694	-2.25183	1.250133
O	-2.65913	-3.25007	0.566871
C	-3.0944	-2.81534	3.751976
H	-2.54509	-2.61614	4.690858
C	-4.50338	-2.2374	3.893388

H	-5.1196	-2.46039	3.008003
H	-5.00487	-2.68032	4.767301
H	-4.50083	-1.14553	4.038616
C	-3.13098	-4.331	3.558946
H	-3.66878	-4.80288	4.395247
H	-3.64313	-4.60646	2.624729
H	-2.11666	-4.75731	3.524085
N	-3.65281	-1.22359	0.83392
H	-3.82798	-0.45949	1.478636
C	-4.31701	-1.22683	-0.45835
H	-4.38753	-2.27915	-0.76865
C	-3.5064	-0.52965	-1.56542
O	-3.81568	-0.66607	-2.74837
C	-5.7234	-0.61787	-0.3099
H	-6.19767	-1.13238	0.544631
H	-5.61389	0.440878	-0.01324
C	-6.66447	-0.70294	-1.51897
H	-6.19147	-0.16813	-2.3587
C	-6.91446	-2.14389	-1.96459
H	-7.64218	-2.17425	-2.79116
H	-5.99186	-2.62438	-2.3228
H	-7.32248	-2.75318	-1.13943
C	-7.98034	0.002375	-1.18452
H	-8.5015	-0.49995	-0.35122
H	-7.81393	1.051159	-0.88983
H	-8.65997	0.000782	-2.05123
C	-1.62223	1.019734	-2.02857
H	-1.80342	0.633782	-3.0443
C	-0.16038	0.723193	-1.65586
O	0.594741	1.593665	-1.20478
C	-1.90848	2.521743	-1.97289
C	-3.30298	2.950669	-2.4442
H	-4.04864	2.385919	-1.8549
C	-3.51096	4.437855	-2.15067
H	-3.38127	4.661411	-1.07949
H	-2.78765	5.0556	-2.71042
H	-4.52195	4.763315	-2.44299
C	-3.54304	2.650727	-3.9251
H	-4.53427	3.014874	-4.23987
H	-2.78905	3.151692	-4.55684
H	-3.50955	1.571049	-4.13342
H	-0.44491	-1.22259	-2.16801
H	-1.75037	2.861436	-0.93613
H	-1.1431	3.033328	-2.58085

N	-2.47905	0.245215	-1.14277
H	-2.21125	0.1801	-0.1646

Conformer 1.3

B3PW91/PCM(ACN)/cc-pVDZ opt

Total energy = -2506.491713 Hartree

Imaginary frequencies = 0

N	2.389501	-1.3948	-0.5966
C	3.3736	-0.33981	-0.42958
H	2.996312	0.367093	0.323267
C	3.586584	0.363482	-1.78542
O	3.589945	-0.30382	-2.81583
C	4.71223	-0.93586	0.046391
H	5.092582	-1.59445	-0.75015
H	5.435016	-0.10952	0.135609
C	4.622226	-1.69251	1.350344
C	4.430764	-1.02328	2.567562
H	4.358092	0.067436	2.586738
C	4.730145	-3.08993	1.384865
H	4.898082	-3.64276	0.456369
C	4.341036	-1.71779	3.77215
H	4.195943	-1.17218	4.708637
C	4.642918	-3.79929	2.581443
H	4.730803	-4.88736	2.597022
C	4.444993	-3.11534	3.785879
O	4.368721	-3.85042	4.924889
H	4.233726	-3.25569	5.677562
N	3.784875	1.713359	-1.7904
C	4.005923	2.581158	-0.62537
H	4.524133	2.034929	0.175915
C	2.757526	3.197814	0.014431
O	2.887896	3.959658	0.970072
C	4.917619	3.720985	-1.16041
H	5.720043	3.956881	-0.45015
H	4.320486	4.635135	-1.29659
C	5.426701	3.213263	-2.50955
H	6.315279	2.575713	-2.37653
H	5.690067	4.029515	-3.19657
C	4.26506	2.368591	-3.01511
H	3.46528	2.99661	-3.44328
H	4.533995	1.600477	-3.74878
N	1.561274	2.903392	-0.54337
H	1.513739	2.174651	-1.2512

C	0.331433	3.49143	-0.04193
H	0.576859	4.513069	0.282398
C	-0.1915	2.816232	1.234789
O	-0.91903	3.428853	2.02429
C	-0.71218	3.532038	-1.16932
H	-0.2123	3.980157	-2.04626
H	-0.96414	2.494896	-1.45139
C	-2.00449	4.309366	-0.88625
H	-2.49578	3.852273	-0.01028
C	-1.74469	5.780285	-0.55827
H	-1.19256	6.278533	-1.3739
H	-2.69452	6.320963	-0.42056
H	-1.16479	5.896123	0.369458
C	-2.94826	4.176061	-2.08283
H	-3.16933	3.120617	-2.30889
H	-3.90483	4.686836	-1.89087
H	-2.50512	4.625489	-2.98805
N	0.197718	1.542033	1.44274
H	0.617605	1.030854	0.665415
C	-0.04261	0.850665	2.690065
H	-0.02643	1.596815	3.500691
H	0.761642	0.126139	2.864359
C	-1.35982	0.084839	2.779065
O	-1.40619	-1.08699	3.137668
N	-2.4724	0.795262	2.441228
H	-2.36701	1.807751	2.358625
C	-3.78697	0.209664	2.657142
H	-3.77734	-0.31959	3.624031
C	-4.1012	-0.90164	1.641236
O	-4.92432	-1.77511	1.907034
C	-4.87268	1.309411	2.719436
H	-4.46452	2.065156	3.415372
C	-5.12566	1.989082	1.373424
H	-4.19831	2.35216	0.904502
H	-5.61418	1.30122	0.664843
H	-5.79028	2.856748	1.504538
C	-6.17197	0.781654	3.326817
H	-6.90379	1.598712	3.421671
H	-6.6142	-0.00673	2.700144
H	-6.0033	0.358956	4.329458
N	-3.43359	-0.83264	0.460951
H	-2.73163	-0.10339	0.38176
C	-3.46059	-1.90303	-0.52657
H	-4.11941	-2.67244	-0.10581

C	-2.07598	-2.57294	-0.59497
O	-1.86102	-3.64956	-0.04395
C	-3.9843	-1.45214	-1.89483
H	-3.35398	-0.63255	-2.28306
H	-3.85953	-2.29496	-2.59821
C	-5.44828	-0.99158	-1.9174
H	-5.54357	-0.15202	-1.20514
C	-5.80442	-0.46571	-3.30896
H	-6.83518	-0.07833	-3.33408
H	-5.13082	0.349291	-3.61944
H	-5.73085	-1.26635	-4.06491
C	-6.41867	-2.09118	-1.48246
H	-6.254	-2.39426	-0.43751
H	-7.46042	-1.74198	-1.56345
H	-6.31706	-2.98547	-2.12164
C	0.25453	-2.30547	-1.38097
H	0.390574	-3.12735	-0.6632
C	1.133167	-1.12073	-0.98204
O	0.707846	0.042707	-1.05247
C	0.645222	-2.76132	-2.80249
C	-0.10183	-3.99273	-3.32943
H	-1.18443	-3.77675	-3.27563
C	0.256204	-4.21869	-4.79964
H	0.024687	-3.33339	-5.41341
H	1.332173	-4.43448	-4.91608
H	-0.30162	-5.07267	-5.2151
C	0.175593	-5.24598	-2.49808
H	-0.33527	-6.12006	-2.93264
H	1.255857	-5.47152	-2.47085
H	-0.18392	-5.13754	-1.46386
H	2.70666	-2.3579	-0.59435
H	0.478288	-1.9107	-3.48572
H	1.731332	-2.95609	-2.81957
N	-1.13018	-1.89456	-1.29337
H	-1.33505	-0.96854	-1.65443

Conformer 1a.1

B3PW91/PCM(DMSO)/6-31G(d,p) opt

Total energy = -2582.840897 Hartree

Imaginary frequencies = 0

N	8.19696	-0.95657	0.40907
H	7.94418	-1.23434	1.35312
C	7.66006	0.37323	0.11543

H	7.68113	1.04669	0.98536
C	6.18314	0.26194	-0.27196
O	5.42217	1.24204	-0.23946
C	8.49306	1.05098	-1.0046
H	9.53033	1.00745	-0.63961
C	8.43187	0.29516	-2.33391
H	9.14917	0.72027	-3.04317
H	8.66818	-0.76534	-2.20851
H	7.43705	0.36919	-2.78726
C	8.1354	2.52655	-1.18303
H	7.10296	2.64565	-1.52261
H	8.2446	3.08058	-0.24476
H	8.79654	2.98658	-1.92461
N	5.78651	-0.96463	-0.65463
H	6.49825	-1.6885	-0.59247
C	4.46047	-1.24691	-1.18873
H	4.14539	-0.34114	-1.71993
C	3.46609	-1.47193	-0.02783
O	3.00427	-2.57513	0.25331
C	4.51965	-2.43753	-2.14139
H	5.36154	-2.27465	-2.82703
H	4.74792	-3.33432	-1.55327
C	3.2469	-2.69137	-2.96469
H	2.41509	-2.82055	-2.26064
C	2.9092	-1.53084	-3.90457
H	2.02973	-1.77181	-4.51115
H	2.68313	-0.60577	-3.36522
H	3.74002	-1.32666	-4.59124
C	3.40032	-3.99412	-3.75399
H	3.60097	-4.84275	-3.09113
H	2.49152	-4.2188	-4.32214
H	4.23003	-3.92445	-4.46826
N	3.15776	-0.32791	0.64072
H	3.72912	0.48998	0.41545
C	2.33636	-0.31948	1.8359
H	2.04586	-1.36209	2.00766
C	1.01205	0.44054	1.65083
O	0.27069	0.65736	2.61223
C	3.08758	0.21805	3.06173
H	3.41421	1.24486	2.8461
H	2.36249	0.28866	3.88005
C	4.29705	-0.61376	3.50936
H	4.99217	-0.6874	2.66109
C	5.02398	0.1067	4.64808

H	4.37311	0.20695	5.52524
H	5.91656	-0.44686	4.95818
H	5.33857	1.11282	4.35
C	3.90978	-2.03502	3.92653
H	3.48931	-2.60787	3.09435
H	4.78574	-2.58252	4.29065
H	3.16933	-2.01646	4.73577
N	0.71177	0.80799	0.39068
H	1.37192	0.64248	-0.3586
C	-0.50327	1.51588	0.04815
H	-1.3005	1.14205	0.69556
C	-0.75821	1.23056	-1.43503
O	0.1978	1.25994	-2.21873
C	-0.33126	3.0401	0.28608
H	0.01543	3.15042	1.31838
H	0.47342	3.38596	-0.37143
C	-1.57979	3.85612	0.06893
C	-1.83851	4.47891	-1.15693
H	-1.11779	4.38972	-1.96624
C	-2.52743	4.00904	1.09159
H	-2.3476	3.54857	2.06049
C	-2.99812	5.22264	-1.36516
H	-3.17285	5.70256	-2.32526
C	-3.69166	4.74547	0.90051
H	-4.41717	4.86288	1.69964
C	-3.93265	5.35764	-0.33414
O	-5.08228	6.07171	-0.4679
H	-5.1259	6.44752	-1.35643
N	-2.01419	0.98672	-1.85714
C	-3.22085	0.88519	-1.0432
H	-3.27289	1.7	-0.3159
C	-3.30557	-0.47344	-0.33522
O	-2.78729	-1.48985	-0.80844
C	-4.34714	1.0084	-2.09166
H	-5.27486	0.53472	-1.76358
H	-4.54238	2.07092	-2.26641
C	-3.74329	0.35302	-3.33603
H	-3.82939	-0.73469	-3.26565
H	-4.23148	0.6745	-4.25881
C	-2.27399	0.76859	-3.28744
H	-2.08935	1.70073	-3.83411
H	-1.59309	0.01003	-3.68107
N	-4.02827	-0.48169	0.80461
H	-4.48385	0.36904	1.10706

C	-4.28711	-1.69701	1.57474
H	-3.39899	-2.32726	1.45594
C	-5.47961	-2.46687	0.96579
O	-6.5684	-2.56798	1.52345
C	-4.52207	-1.36761	3.04523
H	-5.32395	-0.62072	3.10826
H	-4.91915	-2.26624	3.53089
C	-3.28221	-0.87724	3.8084
H	-2.80792	-0.07647	3.22388
C	-3.69962	-0.28926	5.15856
H	-4.39938	0.54413	5.03367
H	-4.19103	-1.04813	5.77975
H	-2.83067	0.08129	5.71232
C	-2.25074	-1.99175	4.00458
H	-1.36808	-1.61373	4.52996
H	-2.67228	-2.80955	4.60155
H	-1.90577	-2.41456	3.05544
N	-5.20005	-3.03613	-0.23308
H	-4.3066	-2.81228	-0.66434
C	-6.21743	-3.70014	-0.99509
H	-5.76764	-4.44409	-1.65861
H	-6.89113	-4.23257	-0.31693
C	-7.06022	-2.75283	-1.83375
O	-6.93758	-1.54924	-1.88478
H	9.21203	-0.93326	0.38062
O	-7.98361	-3.43598	-2.52612
H	-8.49824	-2.79427	-3.04255

Conformer 1a.2

B3PW91/PCM(DMSO)/6-31G(d,p) opt

Total energy = -2582.840201 Hartree

Imaginary frequencies = 0

N	7.357677	-2.78917	0.216929
H	7.147805	-2.79328	1.211001
C	7.566369	-1.4163	-0.24777
H	8.058759	-0.78085	0.503385
C	6.214679	-0.75003	-0.52018
O	6.100031	0.482699	-0.61785
C	8.467441	-1.40865	-1.5108
H	9.360787	-1.97889	-1.21463
C	7.827696	-2.12398	-2.70294
H	7.475928	-3.12417	-2.43452

H	6.975055	-1.55744	-3.09351
H	8.553755	-2.22746	-3.5156
C	8.930223	-0.00079	-1.88636
H	9.444751	0.486861	-1.05159
H	9.626439	-0.04662	-2.73011
H	8.084447	0.630379	-2.17194
N	5.181142	-1.59812	-0.65228
H	5.409908	-2.57949	-0.51274
C	3.846434	-1.18186	-1.05894
H	3.98102	-0.33675	-1.74492
C	3.054049	-0.65318	0.15668
O	2.07747	-1.24681	0.627872
C	3.128312	-2.33378	-1.75768
H	3.83564	-2.79248	-2.46067
H	2.882744	-3.08963	-1.00267
C	1.8497	-1.94899	-2.51884
H	1.191317	-1.41608	-1.82112
C	2.132593	-1.03642	-3.71524
H	2.600707	-0.09108	-3.42185
H	2.798454	-1.52992	-4.43388
H	1.203893	-0.78825	-4.23973
C	1.121984	-3.21705	-2.97278
H	0.193358	-2.97191	-3.49875
H	1.746831	-3.80344	-3.65777
H	0.86702	-3.85793	-2.12197
N	3.51756	0.512001	0.651524
H	4.360613	0.896139	0.221881
C	2.976874	1.119811	1.862903
H	2.617002	0.299617	2.494791
C	1.749872	1.992377	1.515638
O	1.760994	3.221567	1.590641
C	4.034309	1.937918	2.598099
H	4.340773	2.768815	1.951253
H	3.546786	2.400342	3.465076
C	5.273795	1.163609	3.069585
H	5.761439	0.726555	2.187925
C	6.268379	2.133926	3.712785
H	5.837988	2.599708	4.607778
H	7.184165	1.61548	4.015815
H	6.549286	2.936142	3.021718
C	4.926537	0.027797	4.034774
H	4.402937	0.412371	4.91872
H	4.288772	-0.73129	3.570585
H	5.834585	-0.47708	4.381088

N	0.664716	1.283323	1.132842
H	0.741481	0.274435	1.013618
C	-0.55612	1.944978	0.719074
H	-0.65823	2.840617	1.336208
C	-1.69047	0.951966	0.984997
O	-1.50255	-0.25219	0.741688
C	-0.49588	2.384282	-0.77242
H	0.546352	2.663389	-0.95812
H	-0.71386	1.520864	-1.40941
C	-1.38881	3.551337	-1.11265
C	-2.54804	3.406535	-1.88235
H	-2.8188	2.425584	-2.26278
C	-1.0657	4.8356	-0.6541
H	-0.16594	4.977053	-0.05943
C	-3.36323	4.494423	-2.1825
H	-4.25921	4.372605	-2.78338
C	-1.86992	5.933912	-0.94249
H	-1.59674	6.921296	-0.57742
C	-3.02725	5.766178	-1.71105
O	-3.85438	6.797089	-2.03282
H	-3.50893	7.615943	-1.65516
N	-2.85244	1.405966	1.490867
C	-3.85116	0.456656	2.025887
H	-3.31066	-0.36696	2.505015
C	-4.76383	-0.15729	0.938399
O	-5.94745	0.152669	0.824453
C	-4.64046	1.303803	3.024325
H	-5.6606	0.936376	3.139176
H	-4.14117	1.2743	3.997993
C	-4.5729	2.710402	2.427801
H	-5.2855	2.796051	1.602079
H	-4.78623	3.49963	3.152147
C	-3.14294	2.794523	1.901755
H	-2.45318	3.100601	2.697849
H	-3.03368	3.479341	1.05915
N	-4.15789	-1.11023	0.184054
H	-3.14086	-1.1659	0.266178
C	-4.8557	-1.8406	-0.85677
H	-5.84323	-1.37459	-0.94225
C	-5.14254	-3.30593	-0.48657
O	-5.67515	-4.06675	-1.29562
C	-4.1353	-1.78201	-2.20945
H	-3.13013	-2.20897	-2.08922
H	-4.67694	-2.44843	-2.88969

C	-4.0206	-0.38549	-2.83172
H	-3.49257	0.256275	-2.11233
C	-3.17875	-0.4564	-4.10825
H	-2.18649	-0.87601	-3.91089
H	-3.66505	-1.08866	-4.86099
H	-3.04243	0.537415	-4.5475
C	-5.38625	0.244322	-3.11801
H	-5.97715	-0.3941	-3.78623
H	-5.96753	0.407948	-2.2052
H	-5.26884	1.216849	-3.60776
N	-4.80189	-3.68887	0.758231
H	-4.38502	-3.03055	1.403434
C	-5.06522	-5.01621	1.242462
H	-6.12334	-5.28233	1.130821
H	-4.4963	-5.77428	0.689127
C	-4.6882	-5.09939	2.701506
O	-4.22065	-4.18174	3.343223
H	8.212119	-3.32639	0.103289
O	-4.93153	-6.31486	3.198216
H	-4.66956	-6.31203	4.133619

Conformer 1a.3

B3PW91/PCM(DMSO)/6-31G(d,p) opt

Total energy = -2582.838435 Hartree

Imaginary frequencies = 0

N	7.282095	-3.34316	0.744917
H	7.427005	-2.77365	1.573757
C	7.316826	-2.50401	-0.45415
H	8.042035	-1.67996	-0.37919
C	5.958245	-1.82718	-0.65295
O	5.823533	-0.83039	-1.38142
C	7.719982	-3.35071	-1.68978
H	8.672747	-3.82	-1.40174
C	6.721477	-4.46895	-1.9988
H	6.51535	-5.08439	-1.11838
H	5.769336	-4.06301	-2.35815
H	7.117576	-5.1226	-2.78251
C	7.991458	-2.48838	-2.92255
H	7.083444	-1.98014	-3.25832
H	8.746433	-1.72242	-2.71655
H	8.35995	-3.11201	-3.74354
N	4.93709	-2.3982	0.00803
H	5.193388	-3.17599	0.611331

C	3.554673	-1.962	-0.12966
H	3.441603	-1.61898	-1.16447
C	3.302465	-0.7497	0.793797
O	2.676372	-0.8232	1.847467
C	2.596322	-3.11105	0.168488
H	2.975151	-4.01168	-0.33138
H	2.621771	-3.30016	1.247817
C	1.143373	-2.86653	-0.27011
H	0.830819	-1.88625	0.113352
C	0.991198	-2.85589	-1.79375
H	1.60216	-2.08334	-2.27194
H	1.283045	-3.82344	-2.22018
H	-0.0495	-2.66747	-2.07714
C	0.227447	-3.92405	0.350948
H	0.510915	-4.93059	0.01947
H	0.279674	-3.9053	1.444743
H	-0.81568	-3.76073	0.060491
N	3.840707	0.411573	0.331873
H	4.479866	0.329764	-0.46004
C	3.842939	1.610357	1.150489
H	3.981915	1.318326	2.196973
C	2.5004	2.357496	1.141734
O	2.261824	3.200657	2.008603
C	4.952229	2.582904	0.725757
H	4.784807	2.863969	-0.32287
H	4.818788	3.495089	1.319021
C	6.393446	2.076907	0.894408
H	6.514656	1.168601	0.288831
C	7.366137	3.127415	0.351078
H	8.401208	2.777027	0.420735
H	7.159872	3.358919	-0.69953
H	7.291271	4.061835	0.92048
C	6.724544	1.732916	2.348042
H	7.768549	1.415988	2.441759
H	6.581557	2.604912	2.997928
H	6.101983	0.920309	2.735953
N	1.665262	2.067306	0.122382
H	1.923823	1.311663	-0.49835
C	0.359268	2.684204	-0.04002
H	0.338396	3.537366	0.638633
C	-0.69972	1.630845	0.329323
O	-0.89458	0.674189	-0.42936
C	0.170246	3.174976	-1.48514
H	1.074226	3.731763	-1.7554

H	0.112381	2.299563	-2.13994
C	-1.04814	4.047449	-1.66912
C	-2.22731	3.549765	-2.23594
H	-2.26881	2.510885	-2.5515
C	-1.03152	5.390122	-1.27266
H	-0.12754	5.810951	-0.83778
C	-3.3495	4.355157	-2.40462
H	-4.25861	3.961349	-2.84856
C	-2.14541	6.210078	-1.43147
H	-2.10597	7.251505	-1.12031
C	-3.31346	5.692367	-2.00038
O	-4.43611	6.438661	-2.18835
H	-4.2817	7.336317	-1.86776
N	-1.34821	1.747955	1.506599
C	-2.2541	0.680025	1.932955
H	-1.69337	-0.26166	1.984228
C	-3.45554	0.514438	0.998101
O	-4.03179	1.479645	0.501828
C	-2.71764	1.132761	3.331234
H	-3.63074	1.729432	3.231277
H	-2.93246	0.282612	3.981968
C	-1.57036	2.013664	3.825231
H	-1.8709	2.698766	4.621665
H	-0.74637	1.395921	4.198336
C	-1.13463	2.752032	2.561586
H	-0.08959	3.065656	2.597846
H	-1.76652	3.630449	2.379666
N	-3.86208	-0.76737	0.846489
H	-3.40873	-1.50338	1.373332
C	-5.11823	-1.13999	0.231873
H	-5.69781	-0.22157	0.100496
C	-5.83631	-2.09329	1.191215
O	-5.20415	-2.83987	1.93722
C	-4.92638	-1.85175	-1.12291
H	-4.30556	-2.7392	-0.94422
H	-5.90371	-2.21901	-1.46397
C	-4.29276	-0.99493	-2.22706
H	-3.35214	-0.58592	-1.83423
C	-3.96	-1.87506	-3.43501
H	-3.28677	-2.69504	-3.16228
H	-4.86937	-2.31694	-3.86074
H	-3.47513	-1.29059	-4.22412
C	-5.19001	0.17466	-2.63846
H	-4.73412	0.739257	-3.45898

H	-6.16682	-0.18408	-2.98638
H	-5.35123	0.871219	-1.81079
N	-7.18843	-2.07483	1.128606
H	-7.64169	-1.44675	0.481547
C	-8.00114	-3.00634	1.863708
H	-7.39166	-3.41161	2.677241
H	-8.85928	-2.5019	2.315668
C	-8.53735	-4.19057	1.076881
O	-9.36643	-4.95187	1.527087
H	8.046473	-4.01159	0.72082
O	-7.99321	-4.31448	-0.13907
H	-8.38527	-5.10231	-0.55113

Conformer 1a.4

B3PW91/PCM(DMSO)/6-31G(d,p) opt

Total energy = -2582.838412 Hartree

Imaginary frequencies = 0

N	6.094918	1.45382	2.528886
H	6.321031	0.465323	2.591409
C	4.64259	1.640354	2.512284
H	4.109497	0.903126	3.131024
C	4.10865	1.439419	1.091041
O	2.908303	1.255598	0.854206
C	4.276526	3.044769	3.061834
H	4.778871	3.095444	4.039483
C	4.820505	4.182302	2.194597
H	5.890432	4.067358	1.998773
H	4.30078	4.228673	1.231009
H	4.670363	5.144285	2.694816
C	2.777025	3.2024	3.313621
H	2.209703	3.145646	2.380835
H	2.399815	2.422485	3.983413
H	2.575724	4.172373	3.779868
N	5.045587	1.470579	0.118562
H	5.993157	1.641697	0.447316
C	4.708307	1.476645	-1.29115
H	3.887663	2.186139	-1.4502
C	4.138235	0.145247	-1.80273
O	3.578136	0.100455	-2.89679
C	5.918343	1.881544	-2.14297
H	6.740343	1.185955	-1.92615
H	5.642191	1.724137	-3.19166
C	6.407442	3.327229	-1.96067

H	6.613481	3.495528	-0.89394
C	7.721084	3.522971	-2.72245
H	8.108036	4.537837	-2.58394
H	8.489805	2.820398	-2.38309
H	7.57549	3.365899	-3.79806
C	5.36532	4.354602	-2.40789
H	5.749389	5.372459	-2.28432
H	5.11441	4.218567	-3.46683
H	4.437142	4.285823	-1.83195
N	4.293615	-0.92839	-0.99393
H	4.818071	-0.80046	-0.13895
C	3.77674	-2.2403	-1.31563
H	3.476552	-2.19213	-2.36823
C	2.489835	-2.60216	-0.55247
O	2.018476	-3.73668	-0.66134
C	4.833102	-3.33612	-1.12614
H	5.128027	-3.35937	-0.06759
H	4.344823	-4.29445	-1.33243
C	6.087777	-3.18888	-1.99741
H	6.54767	-2.21698	-1.7686
C	7.098054	-4.28066	-1.63493
H	6.693436	-5.27647	-1.85303
H	8.024335	-4.16545	-2.20754
H	7.35495	-4.25131	-0.57035
C	5.769026	-3.21845	-3.49441
H	6.689076	-3.1638	-4.08602
H	5.253484	-4.14766	-3.76675
H	5.135985	-2.37916	-3.79918
N	1.927217	-1.62945	0.197566
H	2.326586	-0.69334	0.212564
C	0.694007	-1.85216	0.936691
H	0.572549	-2.93391	1.00505
C	-0.46433	-1.21564	0.150017
O	-0.51433	0.00932	-0.00031
C	0.799595	-1.24669	2.346437
H	1.708134	-1.65309	2.80449
H	0.941111	-0.16678	2.244209
C	-0.39655	-1.54499	3.217491
C	-1.43519	-0.61851	3.37361
H	-1.378	0.335618	2.856633
C	-0.5057	-2.76653	3.892595
H	0.288945	-3.50366	3.800443
C	-2.54101	-0.89358	4.171869
H	-3.34022	-0.16812	4.289351

C	-1.60623	-3.05977	4.694103
H	-1.66508	-4.01329	5.214036
C	-2.63202	-2.12007	4.836021
O	-3.7326	-2.34035	5.605892
H	-3.67677	-3.22023	5.999613
N	-1.38345	-2.03519	-0.40582
C	-2.38929	-1.47243	-1.30366
H	-1.90473	-0.77943	-1.99806
C	-3.48273	-0.73941	-0.51874
O	-4.02001	-1.22796	0.471103
C	-2.94909	-2.71474	-2.02079
H	-3.97891	-2.57574	-2.35868
H	-2.33131	-2.92035	-2.90088
C	-2.79936	-3.82819	-0.98134
H	-3.62021	-3.77562	-0.2616
H	-2.79065	-4.82613	-1.42618
C	-1.47774	-3.49969	-0.28507
H	-0.62058	-3.97217	-0.77723
H	-1.48369	-3.80198	0.765507
N	-3.86721	0.457811	-1.03716
H	-3.28777	0.88785	-1.74455
C	-4.84369	1.289435	-0.3512
H	-4.65606	1.228924	0.724959
C	-6.28064	0.787975	-0.53587
O	-7.14369	1.016865	0.309478
C	-4.69389	2.740885	-0.84099
H	-3.64365	3.025681	-0.68881
H	-4.87253	2.758302	-1.9245
C	-5.59285	3.789904	-0.1705
H	-6.63796	3.495853	-0.32988
C	-5.35613	3.886288	1.338276
H	-4.30569	4.113324	1.558724
H	-5.96633	4.685203	1.772886
H	-5.62041	2.956335	1.849332
C	-5.37455	5.147596	-0.84361
H	-6.03534	5.907055	-0.41302
H	-4.34148	5.491129	-0.70979
H	-5.57384	5.099861	-1.91973
N	-6.53133	0.133225	-1.69455
H	-5.76521	-0.01715	-2.33488
C	-7.85075	-0.30511	-2.0527
H	-7.82716	-1.30833	-2.48631
H	-8.44728	-0.35514	-1.13586
C	-8.6108	0.585632	-3.02141

O	-9.64458	0.240812	-3.55336
H	6.491108	1.889926	3.356198
O	-8.043	1.783255	-3.20633
H	-8.61273	2.278619	-3.81794