

Supplementary Information

Enhanced Conformational and Configurational Analysis of Furofuran Lignans by VCD Spectroscopy

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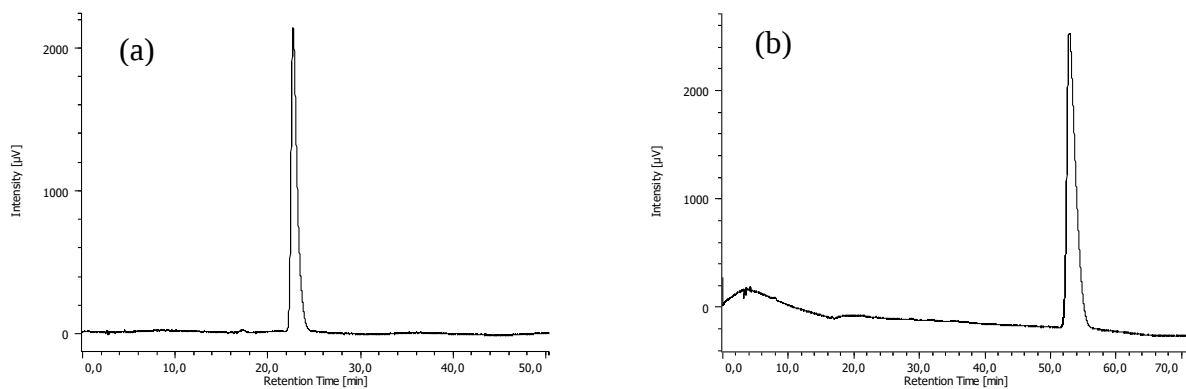


Figure S1. Chiral HPLC analysis of (+)-kobusin (**5**). (a) Lux Cellulose-1 column (Phenomenex®, 4.6 × 250 mm, 5 μm), Hex/EtOH 80:20, 1.0 mL min⁻¹, λ = 280 nm, t_R 22.7 min; (b) CHIRALPAK® IC column (Daicel, 4.6 × 150 mm, 5 μm), Hex/EtOH 80:20, 1 mL min⁻¹, λ = 280 nm, t_R 52.8 min.

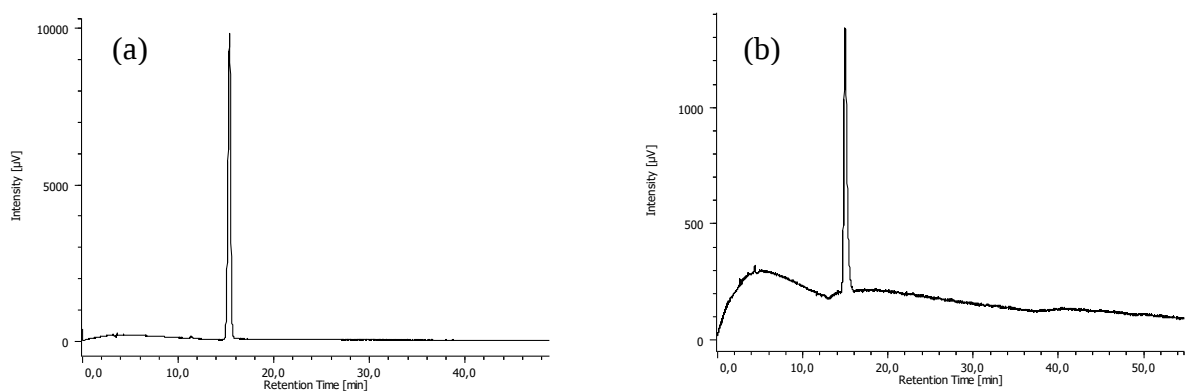


Figure S2. Chiral HPLC analysis of (+)-sesamin (**6**). (a) Lux Cellulose-1 column (Phenomenex®, 4.6 × 250 mm, 5 μm), Hex/EtOH 80:20, 1.0 mL min⁻¹, λ = 280 nm, t_R 14.9 min; (b) CHIRALPAK® IC column (Daicel, 4.6 × 150 mm, 5 μm), Hex/EtOH 80:20, 1 mL min⁻¹, λ = 280 nm, t_R 15.4 min.

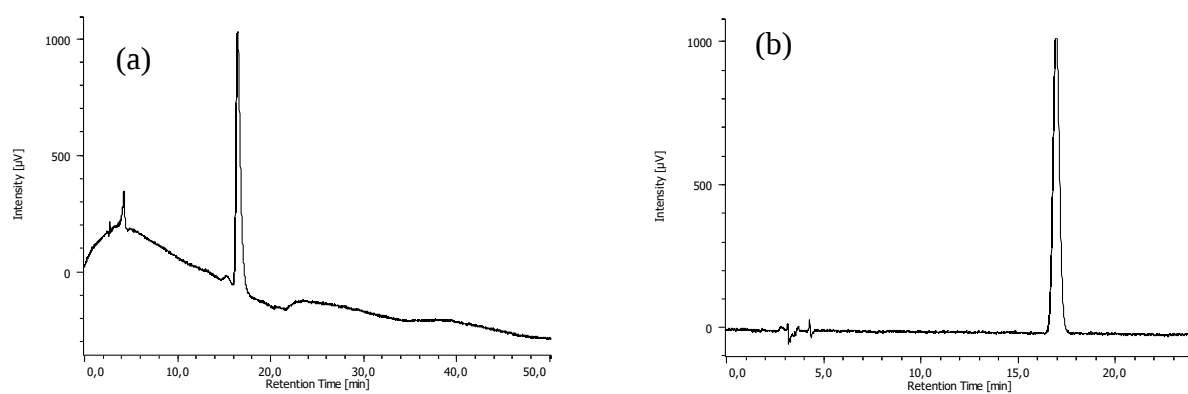


Figure S3. Chiral HPLC analysis of (+)-episesamin (**7**). (a) Lux Cellulose-1 column (Phenomenex®, 4.6 × 250 mm, 5 μm), Hex/EtOH 80:20, 1.0 mL min⁻¹, λ = 280 nm, t_R 16.4 min; (b) CHIRALPAK® IC column (Daicel, 4.6 × 150 mm, 5 μm), Hex/EtOH 80:20, 1 mL min⁻¹, λ = 280 nm, t_R 16.9 min.

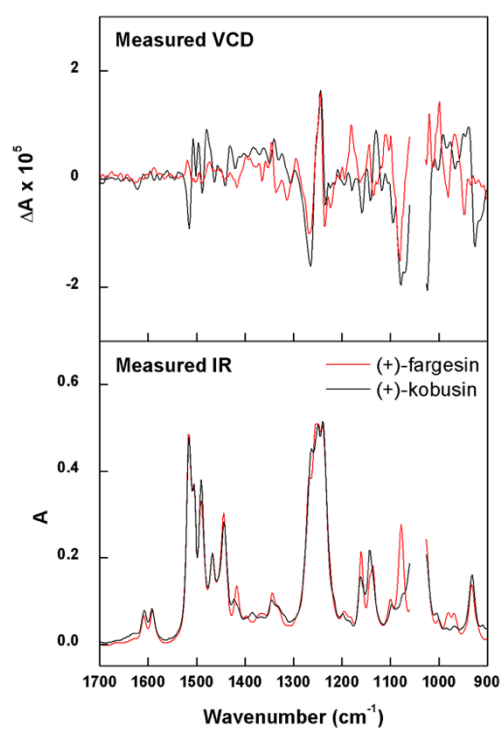


Figure S4. Comparison between experimental IR and VCD spectra of (+)-fargesin (**4**) and (+)-kobusin (**5**) in MeCN- d_3 . Gaps represent intense solvent absorption.

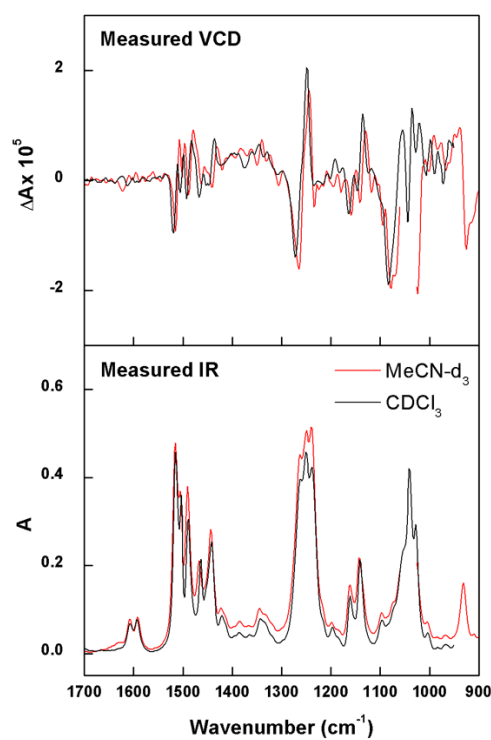


Figure S5. Comparison between experimental IR and VCD spectra of (+)-kobusin (**5**) in different solvents. Gaps represent intense solvent absorption.

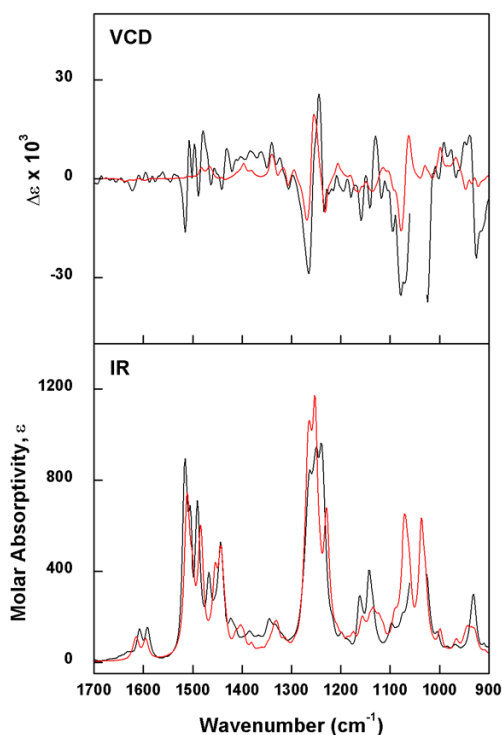


Figure S6. Comparison between experimental IR and VCD spectra of (+)-**5** recorded in MeCN- d_3 (black solid trace) with calculated [B3PW91/PCM(MeCN)/6-311G(d,p)] data for (7*S*,8*R*,7'*S*,8'*R*)-**5** (red trace). Gaps represent intense solvent absorption.

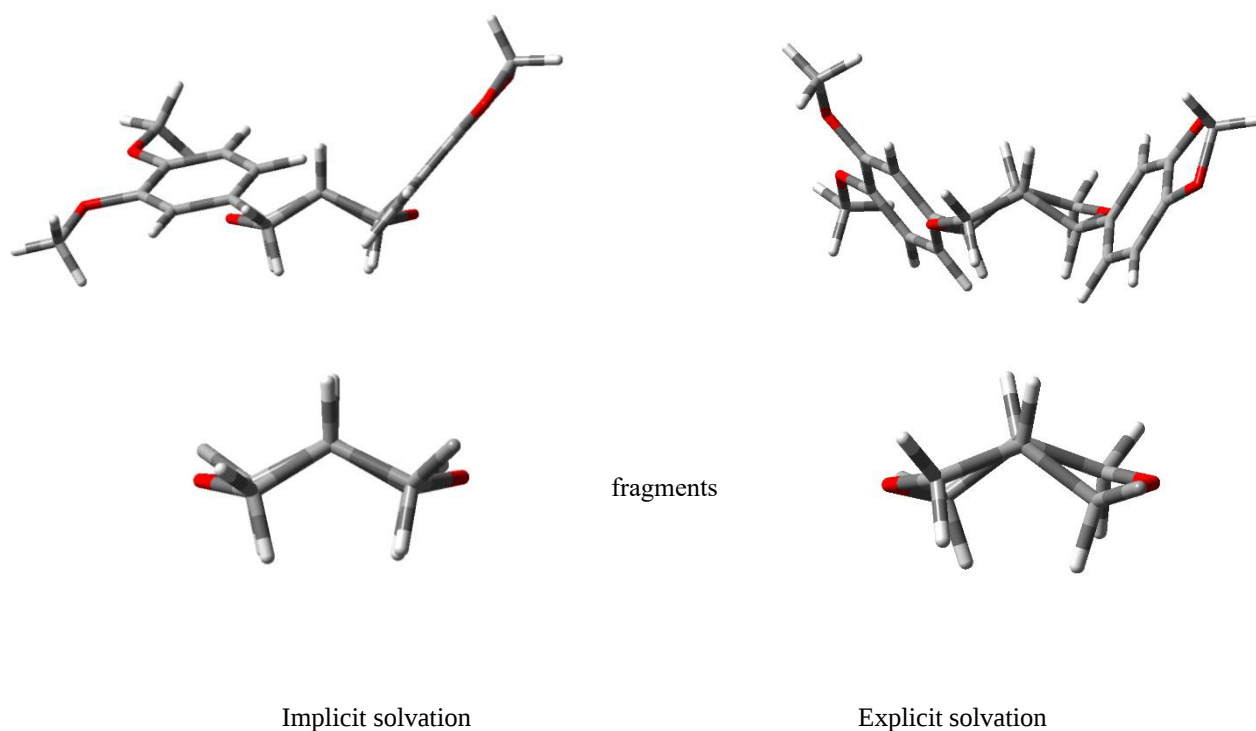


Figure S7. Main structural differences between the lowest-energy conformers generated using implicit and explicit solvation (MD-QM/MM ONIOM) for **5**. Aromatic rings omitted for clarity in fragments.

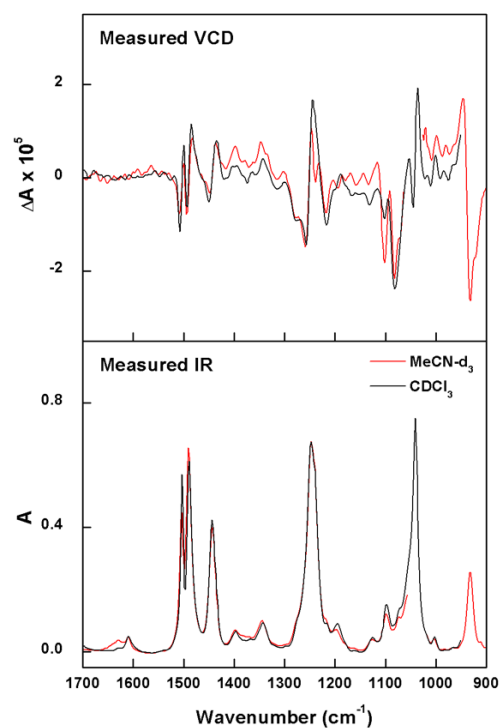


Figure S8. Comparison between experimental IR and VCD spectra of (+)-sesamin (**6**) in different solvents. Gaps represent intense solvent absorption.

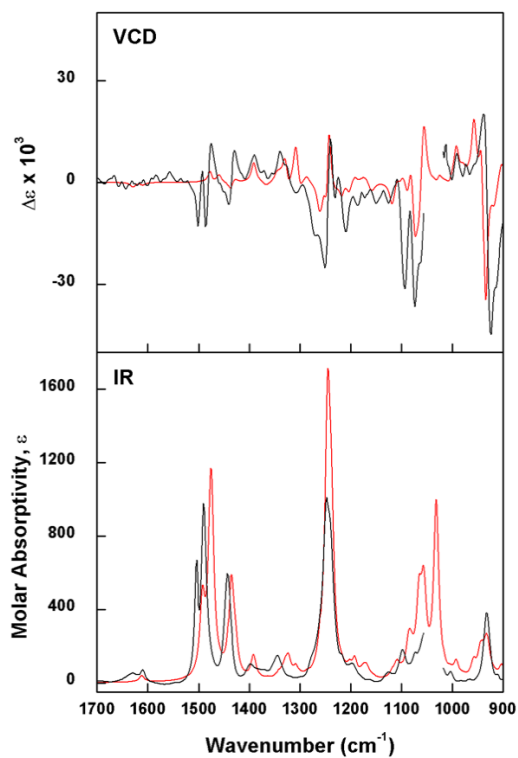


Figure S9. Comparison between experimental IR and VCD spectra of (+)-**6** recorded in MeCN- d_3 (black solid trace) with calculated [B3PW91/PCM(MeCN)/6-311G(d,p)] data for (7S,8R,7'S,8'R)-**6** (red trace). Gaps represent intense solvent absorption.

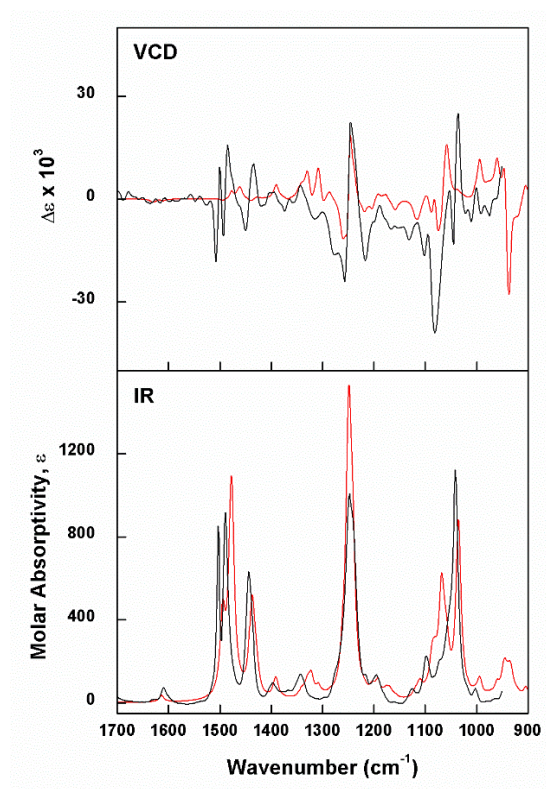


Figure S10. Comparison between experimental IR and VCD spectra of (+)-**6** recorded in CDCl_3 (black solid trace) with calculated [B3PW91/PCM(CHCl_3)/6-311G(d,p)] data for (7*S*,8*R*,7'*S*,8'*R*)-**6** (red trace). Gaps represent intense solvent absorption.

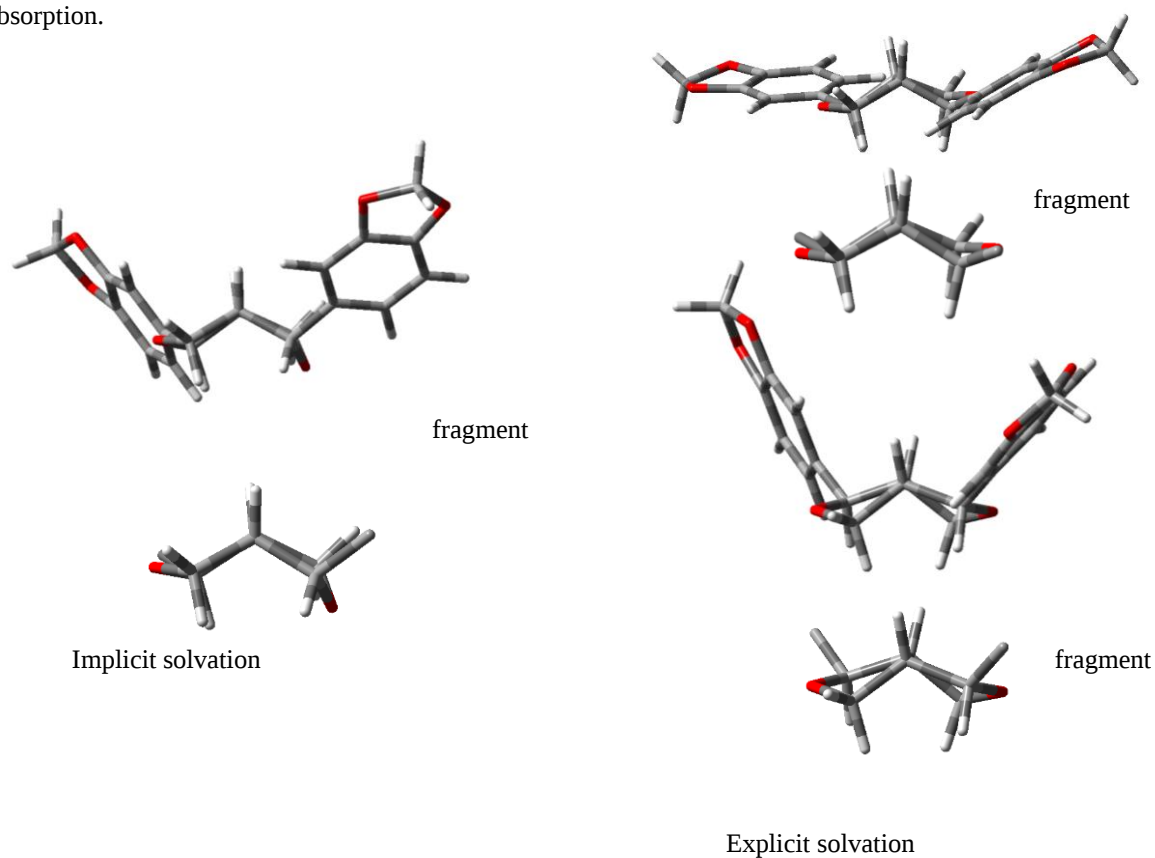


Figure S11. Main structural differences between the lowest-energy conformers generated using implicit and explicit solvation (MD-QM/MM ONIOM) for **6**. Aromatic rings omitted for clarity in the fragments.

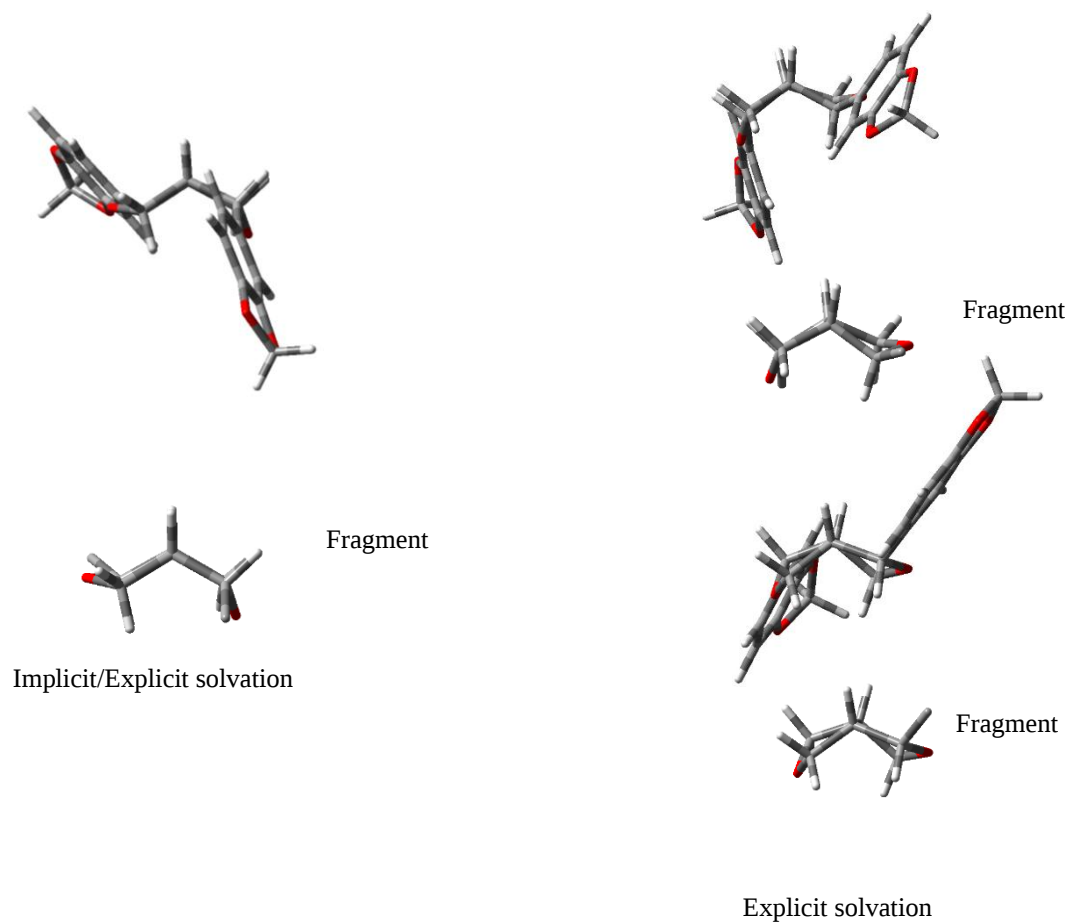


Figure S12. Main structural differences between the lowest-energy conformers generated using implicit and explicit solvation (MD-QM/MM ONIOM) for 7. Aromatic rings omitted for clarity in the fragments.

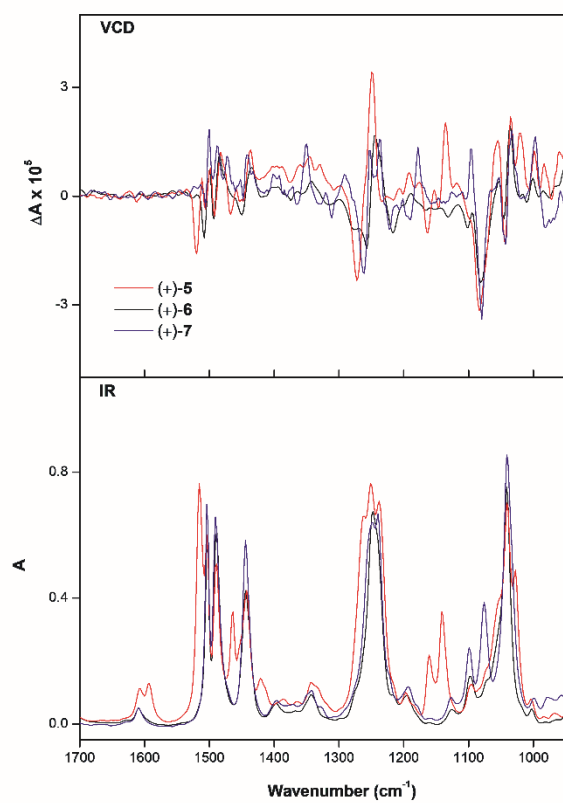


Figure S13. Comparison between experimental IR and VCD spectra of (+)-kobusin (**5**), (+)-sesamin (**6**), and (+)-episesamin (**7**) recorded in CDCl₃.

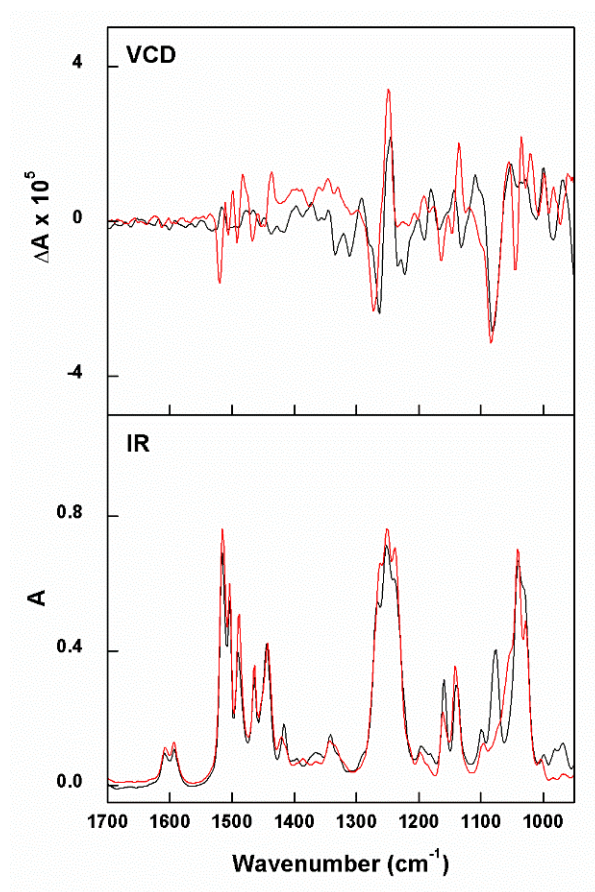


Figure S14. Comparison between experimental IR and VCD spectra of (+)-fargesin (**4**) and (+)-kobusin (**5**) recorded in CDCl_3 .

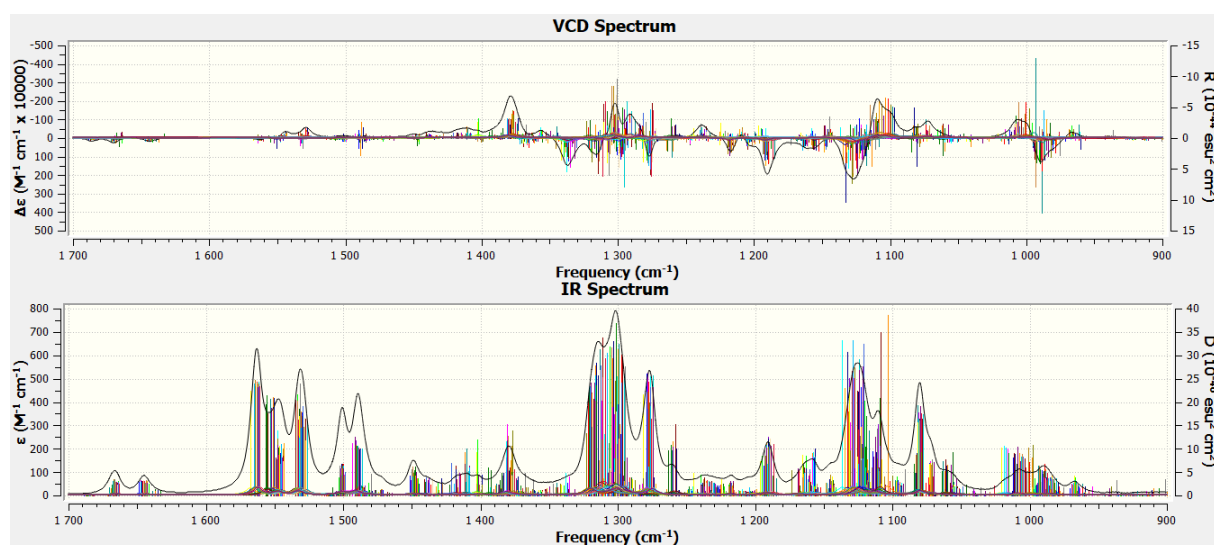


Figure S15. IR (bottom) and VCD (top) spectra of individual MD snapshots for (7S,8R,7'S,8'R)-**5** at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Explicit MeCN solvation. Unscaled frequencies.

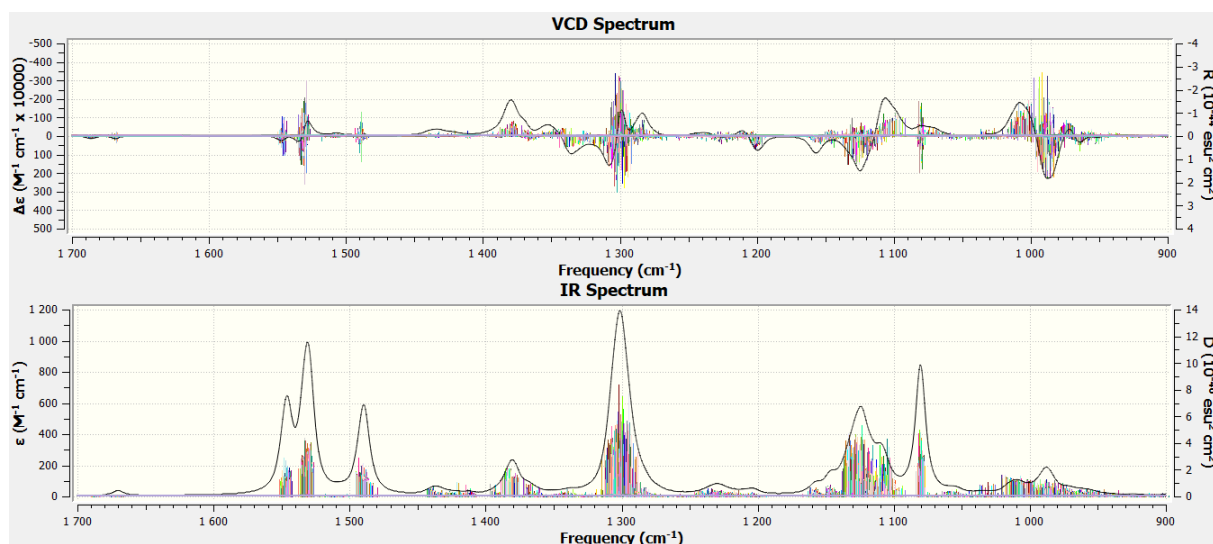


Figure S16. IR (bottom) and VCD (top) spectra of individual MD snapshots for (7S,8R,7'S,8'R)-6 at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Explicit MeCN solvation. Unscaled frequencies.

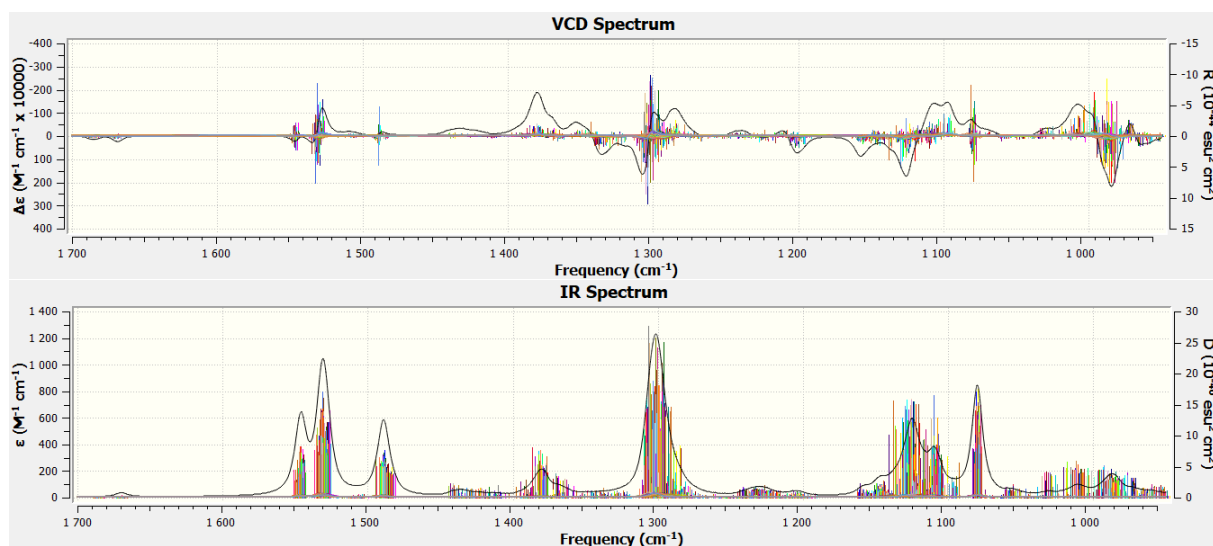


Figure S17. IR (bottom) and VCD (top) spectra of individual MD snapshots for (7S,8R,7'S,8'R)-6 at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Explicit CHCl_3 solvation. Unscaled frequencies.

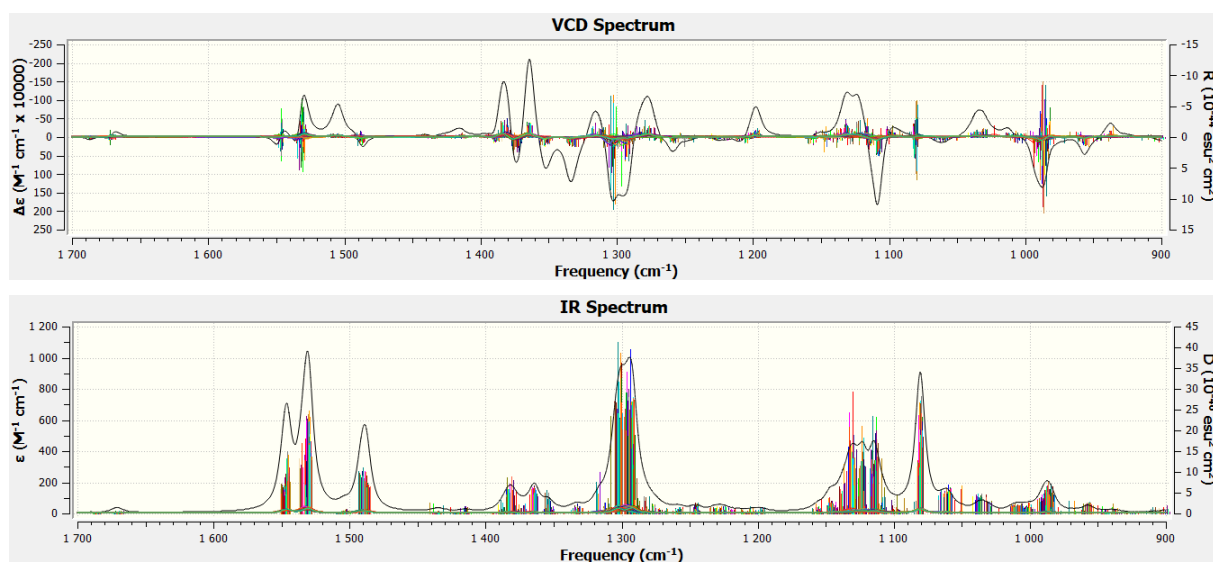
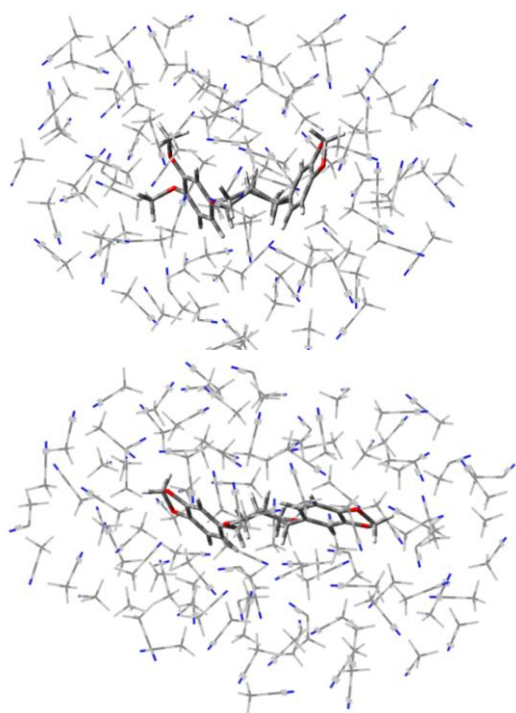
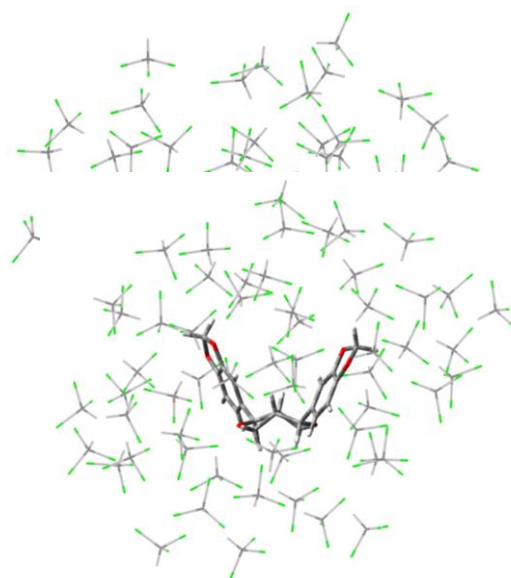


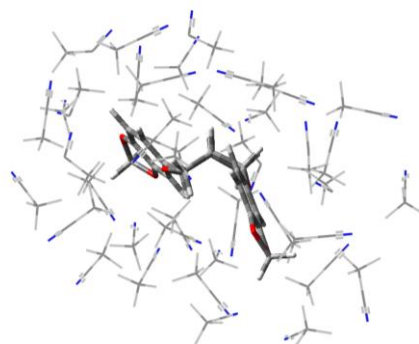
Figure S18. IR (bottom) and VCD (top) spectra of individual MD snapshots for (7S,8R,7'R,8'R)-7 at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Explicit MeCN solvation. Unscaled frequencies.



6 (MeCN)



6 (CHCl_3)



7 (MeCN)

Figure S19. Representative snapshots for 5, 6, and 7.

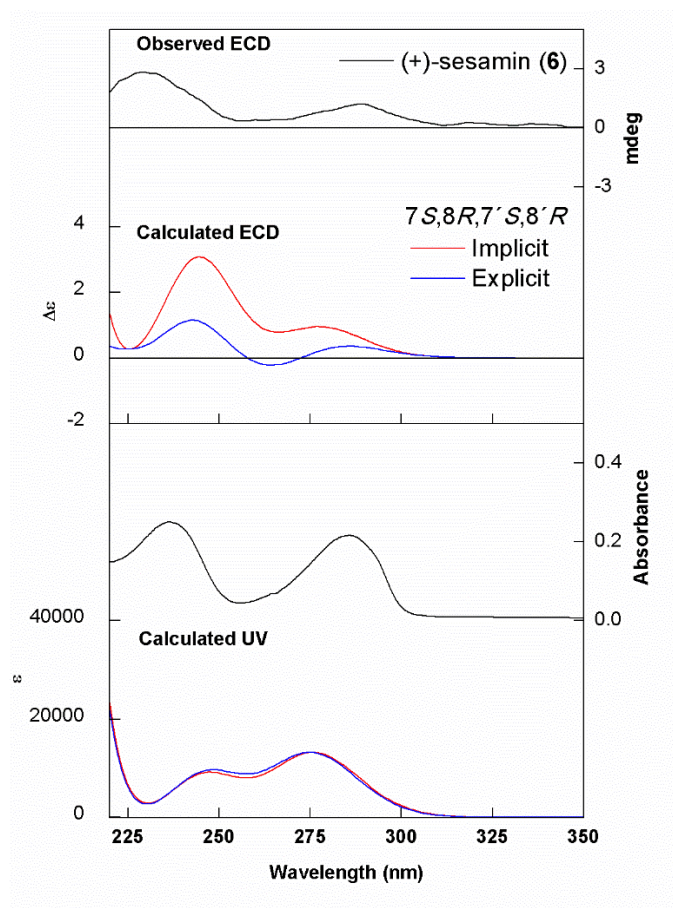


Figure S20. Comparison between experimental UV and ECD spectra of (+)-**6** (black solid trace) with calculated [CAM-B3LYP/PCM(MeCN)/TZVP] data for (7*S*,8*R*,7'*S*,8'*R*)-**6** (red and blue traces). Red trace represents spectra calculated on geometries from the static approach. Blue trace represents spectra calculate on geometries from QM/MM method after removal of explicit solvent molecules.

Cartesian coordinates

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-5

Conf 1 – E = -1264.252428 Hartree

Symbol	X	Y	Z
O	-2.05713	0.253285	-1.726
C	-2.42234	1.323553	-0.86872
C	-1.18977	1.615019	0.005854
C	-1.49484	1.770323	1.510284
O	-1.30998	0.466895	2.059139
C	-0.20558	-0.12065	1.370861
C	-0.37149	0.302819	-0.08375
C	-1.27433	-0.62965	-0.92764
C	-0.65562	2.82265	2.223966
C	-0.04476	2.505761	3.449819
C	-0.5543	4.114993	1.709219
C	0.157508	5.12562	2.37218
C	0.762778	4.785329	3.560775
C	0.661012	3.502907	4.083917
O	1.316725	3.446826	5.283363
O	1.485187	5.573555	4.41404
C	2.052457	4.669898	5.365596
C	-0.54488	-1.61232	-1.80187
C	0.079321	-1.20242	-2.97158
C	-0.4605	-2.95846	-1.42286
C	0.244695	-3.8782	-2.18973
C	0.783284	-2.11705	-3.75663
C	0.87932	-3.45129	-3.3795
O	0.375989	-5.19549	-1.89451
O	1.540726	-4.41162	-4.07209
C	-0.24313	-5.67632	-0.71113
C	2.195937	-4.02941	-5.27201
H	-3.27433	1.026473	-0.2388
H	-2.72624	2.16556	-1.49259
H	-0.63012	2.464874	-0.38293
H	-2.55173	2.011828	1.670023
H	-0.25797	-1.20035	1.527356
H	0.744228	0.246216	1.780103
H	0.58847	0.445959	-0.58206
H	-1.93958	-1.17758	-0.24109
H	-0.13448	1.513089	3.872273

H	-1.04211	4.360962	0.771776
H	0.227022	6.128499	1.968325
H	1.95216	5.086986	6.366949
H	3.101819	4.481334	5.108296
H	0.009615	-0.16772	-3.28676
H	-0.9621	-3.28489	-0.51942
H	1.258079	-1.77788	-4.66877
H	-1.32971	-5.5424	-0.74446
H	-0.01328	-6.73972	-0.66656
H	0.158221	-5.18171	0.179931
H	2.659489	-4.9354	-5.65926
H	1.485599	-3.64218	-6.0104
H	2.970655	-3.2785	-5.08291

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-5

Conf 2 – E = -1264.252325 Hartree

Symbol	X	Y	Z
O	-1.77799	-0.60993	-0.34622
C	-1.8349	0.74015	0.113685
C	-0.38633	1.191079	0.353297
C	-0.022	1.591251	1.797747
O	1.339536	1.195664	1.937583
C	1.497955	-0.04968	1.256608
C	0.452901	-0.08019	0.131647
C	-0.60312	-1.20248	0.20254
C	-0.16797	3.053883	2.119932
C	0.777973	3.97094	1.620802
C	-1.25002	3.501457	2.872558
C	-1.45022	4.864312	3.146294
C	-0.51857	5.741907	2.643052
C	0.572629	5.300445	1.899924
O	1.358803	6.368449	1.568491
O	-0.44824	7.097803	2.796674
C	0.591282	7.524297	1.912248
C	-0.26342	-2.46123	-0.54714
C	0.166934	-3.59638	0.120545
C	-0.3455	-2.48444	-1.94743
C	0.001149	-3.61886	-2.66511
C	0.530434	-4.74481	-0.59075
C	0.45389	-4.77176	-1.97606
O	-0.05748	-3.73016	-4.01523

O	0.775124	-5.83379	-2.75511
C	-0.49406	-2.59904	-4.7538
C	1.227544	-7.01382	-2.10859
H	-2.42308	0.795369	1.040523
H	-2.34645	1.325984	-0.6516
H	-0.09164	1.991036	-0.32839
H	-0.64777	1.011698	2.494822
H	1.346217	-0.88115	1.959101
H	2.524735	-0.09361	0.890303
H	0.919204	-0.08623	-0.85519
H	-0.779	-1.45787	1.259874
H	1.638042	3.635304	1.054821
H	-1.96122	2.780257	3.261738
H	-2.29058	5.207888	3.737179
H	1.228962	8.244912	2.422993
H	0.145769	7.948924	1.004818
H	0.222334	-3.60492	1.204433
H	-0.70503	-1.60222	-2.46144
H	0.865558	-5.61983	-0.04812
H	-0.45905	-2.89607	-5.80076
H	-1.52001	-2.3206	-4.49024
H	0.167752	-1.74043	-4.59779
H	1.426867	-7.73094	-2.90333
H	2.148799	-6.83253	-1.54456
H	0.463265	-7.42002	-1.43736

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-5

Conf 3 – E = -1264.252194 Hartree

Symbol	X	Y	Z
O	-1.96553	-0.41267	0.340853
C	-1.20628	0.564678	-0.36968
C	-0.05669	0.924766	0.562733
C	-0.39402	2.024641	1.597566
O	0.229806	1.5887	2.801609
C	-0.00616	0.190146	2.871291
C	0.122505	-0.34373	1.432964
C	-1.02711	-1.27282	0.987645
C	0.073381	3.408358	1.24111
C	1.442534	3.725603	1.341214
C	-0.83534	4.359129	0.785153
C	-0.4308	5.647707	0.399709

C	0.909625	5.935413	0.507755
C	1.823032	4.99333	0.972359
O	3.079368	5.531284	0.956192
O	1.566896	7.08905	0.185592
C	2.89244	6.92462	0.69602
C	-0.59794	-2.43201	0.099126
C	0.4673	-3.25155	0.446213
C	-1.33471	-2.73869	-1.05146
C	-1.00602	-3.82617	-1.85013
C	0.805034	-4.35411	-0.34316
C	0.084617	-4.65238	-1.49247
O	-1.66502	-4.17999	-2.98228
O	0.338124	-5.69316	-2.32576
C	-2.77337	-3.38681	-3.37867
C	1.41711	-6.55409	-1.99584
H	-1.87241	1.400302	-0.5958
H	-0.8303	0.15055	-1.31381
H	0.851115	1.18656	0.01676
H	-1.48596	2.039804	1.74117
H	-1.01804	5.47E-05	3.258899
H	0.719528	-0.23832	3.56425
H	1.096312	-0.80565	1.275132
H	-1.55393	-1.68296	1.856651
H	2.160277	3.001335	1.706008
H	-1.88882	4.10483	0.732551
H	-1.14086	6.383161	0.041496
H	2.994804	7.487238	1.631458
H	3.612669	7.253612	-0.0523
H	1.048433	-3.05512	1.341327
H	-2.17387	-2.10521	-1.30772
H	1.640795	-4.97715	-0.04987
H	-3.14862	-3.83773	-4.29607
H	-3.56368	-3.39632	-2.62039
H	-2.47413	-2.35249	-3.57917
H	1.444005	-7.31145	-2.77778
H	2.370318	-6.01449	-1.98173
H	1.259584	-7.03978	-1.02673

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-5

Conf 4 – E = -1264.252188 Hartree

Symbol	X	Y	Z
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O	-1.69545	-0.41312	-1.54455
C	-1.03218	0.813127	-1.23981
C	-0.8131	0.781483	0.267545
C	-2.00904	1.301558	1.100398
O	-2.09261	0.409175	2.207088
C	-1.86438	-0.88731	1.675137
C	-0.77191	-0.72994	0.601753
C	-1.08824	-1.42388	-0.74175
C	-1.88359	2.719066	1.586071
C	-1.01781	3.008946	2.659347
C	-2.58621	3.742078	0.955484
C	-2.45153	5.084518	1.345589
C	-1.59624	5.344488	2.390669
C	-0.899	4.325524	3.033673
O	-0.16425	4.854117	4.058134
O	-1.31735	6.539136	2.992685
C	-0.22307	6.270296	3.872748
C	0.112518	-2.05936	-1.42555
C	0.380522	-1.83144	-2.76517
C	0.92911	-2.95473	-0.71734
C	1.996361	-3.59558	-1.33077
C	1.456488	-2.46508	-3.3956
C	2.270675	-3.34476	-2.6973
O	2.830442	-4.47196	-0.71722
O	3.333882	-4.00845	-3.21692
C	2.598446	-4.76173	0.652586
C	3.639278	-3.79432	-4.58632
H	-1.67593	1.628774	-1.57681
H	-0.07574	0.878426	-1.77336
H	0.102359	1.296866	0.562395
H	-2.92121	1.207631	0.490295
H	-2.78948	-1.2748	1.223008
H	-1.57789	-1.54219	2.499501
H	0.201044	-1.02875	0.990511
H	-1.85415	-2.19609	-0.60554
H	-0.48251	2.22111	3.174568
H	-3.25999	3.499934	0.140219
H	-3.00457	5.876913	0.856062
H	-0.40129	6.754944	4.831883
H	0.709215	6.615893	3.410444
H	-0.25324	-1.15908	-3.33093
H	0.719298	-3.15715	0.326313

H	1.648043	-2.2633	-4.44221
H	1.612962	-5.21519	0.804142
H	3.370264	-5.4736	0.940917
H	2.685456	-3.86261	1.272059
H	4.510417	-4.41257	-4.79754
H	2.811148	-4.10219	-5.23383
H	3.884033	-2.74483	-4.7827

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-5

Conf 5 – E = -1264.252021 Hartree

Symbol	X	Y	Z
O	-1.84417	-0.27212	0.284241
C	-0.92872	0.630088	-0.33588
C	0.171106	0.848762	0.696028
C	-0.12572	1.965539	1.726057
O	0.334855	1.443477	2.96714
C	-0.06252	0.080455	2.982019
C	0.136727	-0.4443	1.548693
C	-1.06003	-1.23838	0.984401
C	0.527779	3.29143	1.442258
C	-0.22681	4.318999	0.847746
C	1.877407	3.489037	1.731165
C	2.525176	4.69815	1.443232
C	1.770809	5.684476	0.846923
C	0.425713	5.495545	0.555783
O	-0.09054	6.640795	0.01636
O	2.139738	6.954267	0.497647
C	1.043569	7.464927	-0.26492
C	-0.67962	-2.4212	0.105171
C	0.257707	-3.35707	0.520149
C	-1.34052	-2.62594	-1.11227
C	-1.05998	-3.72829	-1.90908
C	0.54486	-4.47548	-0.26689
C	-0.09889	-4.67369	-1.48153
O	-1.65021	-3.98859	-3.10285
O	0.115813	-5.72124	-2.31723
C	-2.62226	-3.06891	-3.57616
C	1.072192	-6.6932	-1.92425
H	-1.48247	1.535409	-0.59417
H	-0.52062	0.194204	-1.25655
H	1.14483	1.015194	0.232646

H	-1.21756	2.104301	1.776745
H	-1.1206	0.001983	3.273176
H	0.543834	-0.43737	3.726745
H	1.067241	-1.00443	1.465631
H	-1.69969	-1.605	1.795254
H	-1.28291	4.196815	0.635184
H	2.435176	2.687865	2.201514
H	3.570664	4.853405	1.681179
H	1.282683	7.402429	-1.3334
H	0.83327	8.488618	0.042047
H	0.775387	-3.24058	1.466754
H	-2.08202	-1.90086	-1.42166
H	1.280929	-5.18985	0.080181
H	-2.95786	-3.459	-4.53584
H	-3.47658	-3.00192	-2.89403
H	-2.19265	-2.07185	-3.72042
H	1.087351	-7.43536	-2.72097
H	2.070219	-6.25377	-1.82012
H	0.787942	-7.17774	-0.98386

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*R*,8'*S*)-5

Conf 6 – E = -1264.251767 Hartree

Symbol	X	Y	Z
O	-1.02207	-0.91864	-1.27702
C	0.237358	-0.26808	-1.11219
C	-0.07764	1.017106	-0.3562
C	-0.49715	2.206403	-1.25413
O	-1.56508	2.830887	-0.55058
C	-2.35741	1.771766	-0.03453
C	-1.37476	0.677581	0.419804
C	-1.73748	-0.74568	-0.05346
C	0.591238	3.204617	-1.54526
C	1.26363	3.152799	-2.77981
C	0.954319	4.1509	-0.58787
C	1.986123	5.072117	-0.81383
C	2.635276	4.998313	-2.02654
C	2.280903	4.057575	-2.98496
O	3.095362	4.185444	-4.07518
O	3.684764	5.745317	-2.48492
C	3.813323	5.404798	-3.86769
C	-1.43531	-1.84686	0.953094

C	-1.84466	-1.74912	2.275762
C	-0.80533	-3.02367	0.52969
C	-0.57012	-4.07292	1.408662
C	-1.62202	-2.79954	3.170091
C	-0.98497	-3.96222	2.75625
O	0.041918	-5.23725	1.075435
O	-0.71832	-5.03086	3.5491
C	0.474419	-5.39787	-0.2669
C	-1.11681	-4.95885	4.909227
H	0.658137	-0.10745	-2.10721
H	0.926137	-0.90065	-0.5381
H	0.736447	1.316149	0.305903
H	-0.88011	1.801186	-2.20434
H	-3.02262	1.3841	-0.82041
H	-2.96968	2.174293	0.773898
H	-1.21964	0.717407	1.497232
H	-2.79833	-0.80703	-0.32148
H	0.991154	2.434168	-3.54446
H	0.41091	4.183405	0.349083
H	2.263791	5.808281	-0.06903
H	4.864931	5.251959	-4.10774
H	3.368816	6.197609	-4.48106
H	-2.35287	-0.85989	2.634283
H	-0.50337	-3.09938	-0.50684
H	-1.95085	-2.69699	4.196694
H	0.934311	-6.38375	-0.31496
H	-0.36707	-5.35643	-0.96679
H	1.214479	-4.63892	-0.54223
H	-0.81436	-5.90346	5.358671
H	-0.61755	-4.1342	5.429497
H	-2.20216	-4.84449	5.003359

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-5

Conf 7 – E = -1264.251609 Hartree

Symbol	X	Y	Z
O	-1.05634	0.389349	-1.60019
C	-0.81936	1.68699	-1.05632
C	0.253387	1.522055	0.030756
C	-0.13063	1.976391	1.454357
O	0.547128	1.058953	2.309338
C	0.460928	-0.22993	1.702675

C	0.409752	-0.00304	0.18448
C	-0.82617	-0.55378	-0.55759
C	0.252242	3.38757	1.810316
C	1.604905	3.698917	2.051454
C	-0.71858	4.383132	1.87017
C	-0.39437	5.719688	2.154742
C	0.931543	6.000146	2.387991
C	1.90688	5.008058	2.339354
O	3.13193	5.562391	2.584731
O	1.517162	7.203387	2.663895
C	2.862913	6.892576	3.034079
C	-0.67156	-1.93384	-1.13663
C	0.045118	-2.14668	-2.3105
C	-1.22402	-3.03995	-0.48713
C	-1.05145	-4.32755	-0.97445
C	0.221475	-3.43132	-2.81919
C	-0.31346	-4.53614	-2.15629
O	-1.56529	-5.38296	-0.26739
O	-0.1756	-5.82337	-2.5588
C	-2.69133	-6.02343	-0.8727
C	0.557925	-6.07656	-3.7495
H	-1.74994	2.089727	-0.63158
H	-0.50776	2.334527	-1.87703
H	1.195432	1.991887	-0.25761
H	-1.21896	1.86343	1.582407
H	-0.44283	-0.7482	2.053594
H	1.331707	-0.80256	2.024982
H	1.314724	-0.36225	-0.30861
H	-1.68429	-0.55237	0.133943
H	2.369651	2.932749	2.022059
H	-1.758	4.122498	1.699716
H	-1.1525	6.49226	2.196355
H	2.959191	6.935262	4.125431
H	3.543872	7.586272	2.542235
H	0.464733	-1.30075	-2.8431
H	-1.80388	-2.91922	0.422942
H	0.786108	-3.56486	-3.73361
H	-2.99062	-6.82258	-0.19446
H	-3.52069	-5.31714	-0.98825
H	-2.42949	-6.44869	-1.8444
H	0.542912	-7.15683	-3.88356
H	0.090674	-5.5968	-4.61561

H	1.594811	-5.73743	-3.65751
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B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-5

Conf 8 – E = -1264.251037 Hartree

Symbol	X	Y	Z
O	-1.82716	-1.6737	-0.76253
C	-2.62136	-0.79763	0.020756
C	-1.70638	0.379848	0.39723
C	-1.83804	0.816493	1.86311
O	-0.88743	-0.00968	2.560892
C	0.262075	-0.0893	1.722672
C	-0.28715	-0.23687	0.303839
C	-0.5535	-1.70355	-0.12373
C	-1.59597	2.284873	2.15937
C	-2.08639	2.781503	3.385012
C	-0.86938	3.124573	1.316985
C	-0.60496	4.464161	1.646072
C	-1.09206	4.919121	2.848877
C	-1.81859	4.09181	3.69926
O	-2.21789	4.803258	4.795437
O	-1.01346	6.171796	3.386254
C	-1.50977	6.043241	4.721677
C	0.476912	-2.3045	-1.03749
C	1.427118	-3.18876	-0.55323
C	0.511086	-1.94276	-2.39265
C	1.478673	-2.45354	-3.24449
C	2.416173	-3.70346	-1.39777
C	2.455358	-3.34761	-2.73838
O	1.577628	-2.1668	-4.56642
O	3.364734	-3.79592	-3.63836
C	0.619199	-1.2807	-5.12446
C	4.356619	-4.70233	-3.18028
H	-2.96716	-1.3147	0.928664
H	-3.49044	-0.5074	-0.5714
H	-1.85014	1.204913	-0.29978
H	-2.81438	0.541253	2.272994
H	0.855437	-0.94362	2.056547
H	0.873944	0.8172	1.816443
H	0.340987	0.263707	-0.43506
H	-0.6261	-2.31769	0.78793
H	-2.65847	2.15097	4.056367

H	-0.49156	2.749734	0.372915
H	-0.04693	5.111471	0.980493
H	-2.19303	6.864527	4.935071
H	-0.66714	6.024336	5.422625
H	1.40927	-3.49321	0.488285
H	-0.24756	-1.26874	-2.76973
H	3.148973	-4.3924	-0.9971
H	0.876946	-1.18915	-6.1784
H	-0.39607	-1.68123	-5.03319
H	0.664958	-0.2932	-4.65293
H	4.972578	-4.93274	-4.04809
H	4.981587	-4.25175	-2.40175
H	3.908225	-5.62585	-2.79856

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-5

Conf 9 – E = -1264.251005 Hartree

Symbol	X	Y	Z
O	-1.45089	-1.21962	-1.5237
C	-0.04921	-1.11975	-1.29382
C	0.210784	0.360618	-1.01855
C	0.494112	1.203855	-2.28791
O	-0.25812	2.399725	-2.10812
C	-1.49768	1.9853	-1.55572
C	-1.16077	0.891537	-0.52809
C	-2.09334	-0.32928	-0.59007
C	1.941345	1.531198	-2.53107
C	2.577005	2.501721	-1.73142
C	2.656549	0.855962	-3.51583
C	4.021228	1.09979	-3.74107
C	4.620289	2.051875	-2.94988
C	3.909486	2.737959	-1.96914
O	4.747089	3.601531	-1.3205
O	5.92276	2.464565	-2.94309
C	5.951734	3.611941	-2.09022
C	-2.38359	-1.01683	0.727427
C	-3.60064	-1.66233	0.897567
C	-1.44773	-1.07169	1.773141
C	-1.71884	-1.75827	2.94935
C	-3.89175	-2.35396	2.075428
C	-2.96376	-2.41339	3.10659
O	-0.86983	-1.85704	4.00211

O	-3.14801	-3.05263	4.286913
C	0.396777	-1.22479	3.898123
C	-4.38675	-3.71523	4.494069
H	0.459002	-1.49527	-2.18534
H	0.250956	-1.74094	-0.44013
H	1.004667	0.510063	-0.28449
H	0.097598	0.65867	-3.1589
H	-2.1426	1.575627	-2.34769
H	-1.98446	2.860497	-1.12316
H	-1.10632	1.316724	0.474272
H	-3.05102	-0.073	-1.05244
H	2.031659	3.045094	-0.96971
H	2.147322	0.124385	-4.1345
H	4.574908	0.569097	-4.50603
H	5.984953	4.520409	-2.70314
H	6.80963	3.545587	-1.42199
H	-4.34353	-1.63199	0.106613
H	-0.49829	-0.56122	1.673363
H	-4.85274	-2.84178	2.180314
H	0.912359	-1.43745	4.833264
H	0.978816	-1.63028	3.063604
H	0.295195	-0.14058	3.780151
H	-4.32729	-4.1521	5.489604
H	-5.22654	-3.01325	4.455831
H	-4.54251	-4.51108	3.757974

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-5

Conf 10 – E = -1264.250658 Hartree

Symbol	X	Y	Z
O	-2.23328	-2.08856	0.357295
C	-2.94054	-0.85618	0.465363
C	-1.87868	0.234975	0.602848
C	-2.26435	1.408604	1.519504
O	-1.82462	1.049567	2.831401
C	-1.20674	-0.23598	2.824977
C	-0.78581	-0.50705	1.380115
C	-0.92523	-1.97159	0.925509
C	-1.65944	2.731015	1.090104
C	-2.25094	3.417827	0.011065
C	-0.53967	3.256624	1.724856
C	0.043922	4.466645	1.313808

C	-0.5401	5.112388	0.24957
C	-1.66493	4.596029	-0.38617
O	-2.06538	5.454424	-1.372
O	-0.20391	6.310087	-0.31978
C	-0.99963	6.398837	-1.50329
C	0.130381	-2.39813	-0.07287
C	-0.12051	-2.45253	-1.43275
C	1.409764	-2.73232	0.397285
C	2.422536	-3.09869	-0.47702
C	0.890498	-2.82459	-2.32603
C	2.16032	-3.14526	-1.86854
O	3.683164	-3.43633	-0.10764
O	3.203951	-3.51832	-2.65138
C	3.997887	-3.41306	1.276045
C	2.985982	-3.58836	-4.05189
H	-3.60083	-0.87479	1.343848
H	-3.5616	-0.74169	-0.42605
H	-1.54139	0.575765	-0.37677
H	-3.3565	1.523158	1.543359
H	-1.91939	-0.99502	3.176057
H	-0.36372	-0.2124	3.519542
H	0.212051	-0.11375	1.183342
H	-0.86686	-2.63925	1.796112
H	-3.13658	3.037912	-0.48693
H	-0.11747	2.720038	2.565294
H	0.911255	4.877328	1.816842
H	-0.3878	6.137633	-2.37513
H	-1.41348	7.402915	-1.5882
H	-1.11007	-2.21853	-1.80561
H	1.604091	-2.70675	1.463752
H	0.670719	-2.86322	-3.38576
H	5.043301	-3.70888	1.348424
H	3.875617	-2.40954	1.697721
H	3.381372	-4.12249	1.838575
H	3.933676	-3.904	-4.48548
H	2.211811	-4.32244	-4.30028
H	2.707139	-2.61209	-4.46306

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 1 – E = -1223.788403 Hartree

Symbol	X	Y	Z
C	-2.85624	-1.52738	1.858877
C	-3.37867	-2.75969	2.173407
C	-3.7526	-3.67651	1.196745
C	-3.62498	-3.38976	-0.14193
C	-3.10221	-2.1299	-0.47691
C	-2.7121	-1.21182	0.492907
C	2.370031	2.369122	-2.35536
C	3.69064	2.467509	-2.82307
C	4.691624	2.247871	-1.90614
C	4.410362	1.944315	-0.57694
C	3.123281	1.840318	-0.10738
C	2.080617	2.055405	-1.03041
C	0.653774	1.905199	-0.58155
O	0.4685	2.527872	0.686076
C	-0.78214	2.056985	1.164802
C	0.174879	0.448626	-0.3738
C	-0.86982	0.573289	0.76192
C	-0.62088	-0.12778	-1.53768
O	-1.96971	0.27897	-1.30485
C	-2.20403	0.167261	0.09679
H	3.911516	2.718317	-3.85345
O	6.044436	2.324928	-2.08092
O	5.580851	1.823402	0.118784
C	6.610751	1.811676	-0.87256
O	-4.19495	-4.82491	1.793644
H	-3.91519	-4.10346	-0.90369
H	-3.00579	-1.85551	-1.52029
H	1.555082	2.546448	-3.04946
H	2.914116	1.618987	0.931837
H	-0.00893	2.383804	-1.31971
H	-1.59954	2.626841	0.698479
H	-0.81246	2.22096	2.243014
H	1.016267	-0.18809	-0.09566
H	-0.62685	-0.07292	1.604896
H	-0.54516	-1.22205	-1.56002
H	-0.32362	0.262135	-2.51385
H	-2.98729	0.898553	0.327486
H	6.94665	0.780915	-1.03674
H	7.429238	2.455874	-0.55343
O	-3.57998	-3.30388	3.411023
C	-4.32755	-4.50095	3.179366

H	-2.57382	-0.83137	2.640787
H	-5.38381	-4.32094	3.412558
H	-3.91427	-5.30867	3.782384

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-6

Conf 2 – E = -1223.788392 Hartree

Symbol	X	Y	Z
C	-3.66884	-0.64007	0.588032
C	-4.82547	-0.88256	-0.11477
C	-5.3249	0.016478	-1.05102
C	-4.6858	1.204826	-1.31554
C	-3.50847	1.469409	-0.59686
C	-2.99351	0.570021	0.331426
C	3.77724	1.534635	0.208501
C	5.024448	1.424355	-0.42782
C	5.450953	0.155055	-0.74061
C	4.68165	-0.96702	-0.44544
C	3.454814	-0.87244	0.165878
C	2.997768	0.41836	0.498221
C	1.646622	0.583471	1.136337
O	1.464015	-0.38769	2.162157
C	0.077183	-0.36882	2.465576
C	0.439188	0.382365	0.190237
C	-0.65799	-0.18335	1.125126
C	-0.16718	1.673988	-0.34207
O	-1.09726	2.087617	0.658788
C	-1.74753	0.912137	1.136099
H	5.626	2.296124	-0.65478
O	6.599102	-0.2314	-1.37238
O	5.328067	-2.08911	-0.88308
C	6.64222	-1.6544	-1.24015
O	-6.45525	-0.49998	-1.62249
H	-5.07363	1.905502	-2.04529
H	-2.98626	2.404304	-0.75969
H	3.418498	2.519679	0.488243
H	2.866233	-1.75193	0.395843
H	1.576482	1.591069	1.575717
H	-0.14677	0.469389	3.142123
H	-0.16775	-1.30269	2.973788
H	0.700054	-0.31118	-0.61085

H	-1.04653	-1.13372	0.76036
H	-0.67737	1.502603	-1.29814
H	0.556364	2.481786	-0.4732
H	-2.05692	1.138678	2.162954
H	6.924774	-2.09893	-2.19373
H	7.34464	-1.92468	-0.44285
O	-5.63008	-1.98667	-0.06829
C	-6.79221	-1.63715	-0.82502
H	-3.30279	-1.35811	1.313321
H	-7.60677	-1.3737	-0.13968
H	-7.06535	-2.46814	-1.47434

B3PW91/PCM(MeCN)6-311G(d,p)
(7R,8S,7'R,8'S)-6

Conf 3 – E = -1223.788176 Hartree

Symbol	X	Y	Z
C	-0.87588	3.482621	1.205653
C	-1.14547	4.488473	2.101854
C	-0.31175	4.761048	3.182952
C	0.836054	4.038007	3.408525
C	1.125807	3.008951	2.497744
C	0.290816	2.722627	1.421429
C	1.721389	-2.82328	-2.37182
C	1.648673	-3.87596	-3.29864
C	0.588912	-4.74296	-3.17073
C	-0.3649	-4.58694	-2.16871
C	-0.3078	-3.5598	-1.25804
C	0.76496	-2.65377	-1.37474
C	0.848095	-1.47816	-0.43874
O	0.573011	-1.89692	0.894898
C	0.236812	-0.73905	1.663358
C	-0.17081	-0.35021	-0.69883
C	-0.27542	0.321094	0.679233
C	0.284094	0.772969	-1.64027
O	0.398738	1.960223	-0.85191
C	0.607559	1.57307	0.503125
H	2.398325	-4.00772	-4.06937
O	0.306329	-5.86298	-3.90017
O	-1.27168	-5.60707	-2.24193
C	-0.99929	-6.26742	-3.48023
O	-0.80015	5.830799	3.878295
H	1.491609	4.2614	4.241411

H	2.028253	2.42364	2.640056
H	2.549348	-2.12513	-2.43758
H	-1.04557	-3.45662	-0.47207
H	1.865042	-1.05847	-0.49416
H	1.121342	-0.38142	2.207693
H	-0.51627	-1.03849	2.394375
H	-1.12135	-0.78663	-1.01135
H	-1.29823	0.628849	0.904643
H	-0.43439	0.976489	-2.43622
H	1.251809	0.536044	-2.10285
H	1.661494	1.288443	0.650082
H	-1.73601	-5.95459	-4.22963
H	-1.01323	-7.34591	-3.32734
O	-2.1797	5.382035	2.089204
C	-2.10515	6.065014	3.34285
H	-1.52205	3.289177	0.358455
H	-2.85813	5.655069	4.026347
H	-2.24523	7.133467	3.18313

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 4 – E = -1223.787986 Hartree

Symbol	X	Y	Z
C	3.56559	0.24783	0.74351
C	4.75383	-0.43907	0.80674
C	5.36577	-0.96761	-0.32639
C	4.81333	-0.8234	-1.57752
C	3.60493	-0.11231	-1.65828
C	2.98222	0.4111	-0.52864
C	-3.49699	1.06238	1.17265
C	-4.68178	0.52358	1.69583
C	-5.3279	-0.42167	0.93164
C	-4.83009	-0.8178	-0.30292
C	-3.67186	-0.29347	-0.82988
C	-2.98719	0.666	-0.0636
C	-1.7409	1.3308	-0.63368
O	-1.24965	0.65469	-1.78998
C	-0.34652	-0.35067	-1.33038
C	-0.54042	1.38956	0.33548
C	0.42984	0.30542	-0.19604
C	0.28945	2.684	0.24947
O	1.64929	2.28293	0.17118

C	1.66259	1.12106	-0.65212
H	-5.06881	0.83376	2.65899
O	-6.4634	-1.12913	1.21702
O	-5.63989	-1.78497	-0.83204
C	-6.80412	-1.7936	-0.00211
O	6.50954	-1.62201	0.03563
H	5.29249	-1.23217	-2.45881
H	3.1515	0.03851	-2.63246
H	-2.97812	1.81945	1.75133
H	-3.29511	-0.60085	-1.79708
H	-2.01513	2.33593	-0.97285
H	0.27387	-0.64898	-2.17845
H	-0.89608	-1.23041	-0.97218
H	-0.84186	1.18896	1.36281
H	0.7159	-0.41011	0.57656
H	0.18059	3.33201	1.12043
H	0.01555	3.25501	-0.65021
H	1.50917	1.41877	-1.70132
H	-7.08917	-2.82281	0.21274
H	-7.61168	-1.24542	-0.50237
O	5.49847	-0.74697	1.91091
C	6.72898	-1.26811	1.40343
H	3.0993	0.65863	1.63038
H	7.0069	-2.15713	1.96831
H	7.50325	-0.49371	1.45916

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 5 – E = -1223.786994 Hartree

Symbol	X	Y	Z
C	-3.58813	-0.61928	-0.76997
C	-4.77626	-0.99749	-0.18716
C	-5.4175	-0.21252	0.76211
C	-4.89262	0.9927	1.17028
C	-3.67531	1.38406	0.59333
C	-3.02104	0.59835	-0.35533
C	3.43643	0.94359	1.17293
C	4.63008	0.43674	1.70479
C	5.31948	-0.47495	0.93624
C	4.85715	-0.87157	-0.31212
C	3.69093	-0.3754	-0.85016
C	2.96611	0.55186	-0.07975
C	1.66126	1.08713	-0.60552

O	1.52607	2.46687	-0.28345
C	0.16096	2.78222	-0.51094
C	0.39215	0.42129	-0.01967
C	-0.64956	1.56726	-0.02522
C	-0.23731	-0.64361	-0.90972
O	-1.10553	0.07142	-1.78891
C	-1.73589	1.08783	-1.0114
H	4.99494	0.74552	2.67708
O	6.47886	-1.13893	1.22696
O	5.71273	-1.79541	-0.84431
C	6.86312	-1.77421	0.00521
O	-6.58938	-0.81018	1.1369
H	-5.3979	1.61118	1.90228
H	-3.24334	2.33174	0.89753
H	2.87086	1.67289	1.74077
H	3.35174	-0.68479	-1.83227
H	1.6373	0.96911	-1.70074
H	-0.01102	2.95044	-1.58458
H	-0.06515	3.70374	0.02758
H	0.59478	0.04906	0.98574
H	-1.05723	1.74443	0.96925
H	-0.80456	-1.36733	-0.31084
H	0.47943	-1.18908	-1.52749
H	-1.9963	1.88282	-1.7191
H	7.65842	-1.19087	-0.47407
H	7.18086	-2.79564	0.21112
O	-5.52719	-2.11301	-0.43853
C	-6.53425	-2.12416	0.57619
H	-3.10267	-1.22733	-1.5225
H	-6.25612	-2.84213	1.35716
H	-7.49705	-2.36875	0.12901

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-6

Conf 6 – E = -1223.786195 Hartree

Symbol	X	Y	Z
C	-4.19504	-0.85561	0.057829
C	-5.22327	0.052493	0.133575
C	-5.02569	1.409781	-0.09935
C	-3.78605	1.911005	-0.42047
C	-2.72702	0.991792	-0.49627
C	-2.91041	-0.3704	-0.26377

C	3.689636	-0.95783	1.407002
C	4.911459	-0.32939	1.698184
C	5.423636	0.508056	0.735069
C	4.76464	0.720528	-0.47271
C	3.567229	0.11534	-0.7686
C	3.01913	-0.74147	0.206608
C	1.685902	-1.38969	-0.04455
O	1.63478	-1.90887	-1.37026
C	0.262542	-2.16341	-1.62413
C	0.459346	-0.44634	0.064975
C	-0.50429	-0.97016	-1.03145
C	-0.34332	-0.60925	1.356133
O	-1.30516	-1.62184	1.073853
C	-1.77181	-1.37331	-0.26504
H	5.432985	-0.50526	2.63118
O	6.601158	1.201209	0.740856
O	5.512909	1.552006	-1.25834
C	6.538678	2.058863	-0.4015
O	-6.21742	2.068897	0.000745
H	-3.63458	2.966572	-0.61086
H	-1.74357	1.371441	-0.74769
H	3.26057	-1.63179	2.141135
H	3.069505	0.27529	-1.71705
H	1.548854	-2.21675	0.669323
H	-0.04464	-3.09644	-1.12812
H	0.133311	-2.27804	-2.70128
H	0.76227	0.588739	-0.1017
H	-0.70119	-0.22782	-1.80448
H	-0.83899	0.330165	1.632743
H	0.253106	-0.94896	2.205894
H	-2.16115	-2.33317	-0.61743
H	6.276641	3.074059	-0.08049
H	7.493647	2.035733	-0.92507
O	-6.5466	-0.17814	0.385392
C	-7.12905	1.116411	0.555225
H	-4.36703	-1.91093	0.237599
H	-7.26076	1.319285	1.624553
H	-8.07448	1.162907	0.016244

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 7 – E = -1223.7861 Hartree

Symbol	X	Y	Z
C	3.087854	0.458483	0.303286
C	4.282199	1.141297	0.286195
C	5.453167	0.573295	-0.20164
C	5.478158	-0.71112	-0.69565
C	4.26438	-1.41293	-0.69137
C	3.08076	-0.85562	-0.20736
C	-3.25213	-0.03395	1.510398
C	-4.40983	0.739483	1.673326
C	-5.15789	0.99031	0.544478
C	-4.78635	0.495622	-0.69927
C	-3.65705	-0.2724	-0.87211
C	-2.87341	-0.5358	0.26612
C	-1.60505	-1.33306	0.119
O	-1.42822	-2.19294	1.238358
C	-0.07747	-2.62172	1.176659
C	-0.30222	-0.49379	0.048946
C	0.741939	-1.38567	0.768437
C	0.26871	-0.33098	-1.35925
O	1.126875	-1.45131	-1.55003
C	1.80803	-1.67346	-0.30111
H	-4.70353	1.1249	2.642338
O	-6.29959	1.732449	0.419083
O	-5.68435	0.910314	-1.64299
C	-6.77351	1.469104	-0.90371
O	6.48591	1.454158	-0.05355
H	6.393902	-1.15915	-1.06197
H	4.248068	-2.42645	-1.0791
H	-2.6423	-0.26443	2.375907
H	-3.38964	-0.66262	-1.84752
H	-1.66776	-1.94464	-0.79539
H	0.029722	-3.41525	0.421759
H	0.193932	-3.02614	2.152738
H	-0.44856	0.465702	0.547923
H	1.162587	-0.90246	1.650343
H	0.827973	0.608758	-1.4537
H	-0.48782	-0.35845	-2.14697
H	2.086694	-2.73092	-0.30972
H	-7.59343	0.742255	-0.85891
H	-7.0873	2.402351	-1.36972
O	4.545958	2.397725	0.755379
C	5.875582	2.692702	0.319854

H	2.199382	0.92439	0.712001
H	6.435447	3.139848	1.140449
H	5.834978	3.355829	-0.55221

B3PW91/PCM(CHCl₃)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-**6**

Conf 1 – E = -1223.784313 Hartree

Symbol	X	Y	Z
C	-2.10247	2.867745	0.689711
C	-3.36353	3.390506	0.843941
C	-4.17851	3.054768	1.920893
C	-3.75944	2.1826	2.897711
C	-2.46779	1.649922	2.758875
C	-1.65101	1.972824	1.679052
C	1.717958	-3.3838	-0.47818
C	1.952894	-4.3643	-1.45517
C	2.614061	-3.96621	-2.59298
C	3.029325	-2.65082	-2.76726
C	2.796591	-1.6792	-1.82281
C	2.116662	-2.06186	-0.64964
C	1.897933	-1.03829	0.455691
O	1.044372	-1.52682	1.48696
C	-0.2927	-1.20859	1.105419
C	1.245906	0.281813	-0.01268
C	-0.21059	0.188735	0.505168
C	1.788341	1.545927	0.680573
O	0.655923	2.294703	1.090531
C	-0.29592	1.337174	1.539481
H	1.629058	-5.38923	-1.31949
O	2.939204	-4.69856	-3.70191
O	3.630831	-2.52013	-3.98817
C	3.802458	-3.85602	-4.46595
O	-5.38041	3.694882	1.801524
H	-4.39355	1.926972	3.737835
H	-2.09537	0.975527	3.523108
H	1.220059	-3.65964	0.443434
H	3.133157	-0.66149	-1.9856
H	2.86377	-0.84413	0.936562
H	-0.91462	-1.26965	2.001425
H	-0.66818	-1.93042	0.369026
H	1.281008	0.386428	-1.09679
H	-0.9449	0.342101	-0.28748

H	2.390866	2.180235	0.028307
H	2.392617	1.268538	1.557502
H	0.020522	0.943078	2.518399
H	4.843919	-4.16588	-4.31338
H	3.519448	-3.90386	-5.51726
O	-4.03237	4.252599	0.019637
C	-5.1978	4.64164	0.74748
H	-1.47118	3.142027	-0.14609
H	-6.06325	4.618858	0.085619
H	-5.04331	5.639286	1.176975

B3PW91/PCM(CHCl₃)6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 2 – E = -1223.784064 Hartree

Symbol	X	Y	Z
C	-2.84019	-1.55002	1.848801
C	-3.36299	-2.78417	2.15487
C	-3.75043	-3.68799	1.171935
C	-3.63714	-3.38567	-0.16446
C	-3.11441	-2.12404	-0.49049
C	-2.71018	-1.21876	0.485542
C	2.362448	2.335562	-2.35444
C	3.682047	2.430151	-2.82458
C	4.684016	2.248405	-1.90076
C	4.404379	1.986086	-0.56293
C	3.118169	1.886491	-0.09047
C	2.075011	2.062089	-1.02029
C	0.649255	1.908617	-0.56953
O	0.462164	2.527246	0.698174
C	-0.78668	2.053615	1.174445
C	0.176419	0.449329	-0.36365
C	-0.87254	0.569964	0.768645
C	-0.61434	-0.12996	-1.52929
O	-1.96246	0.27863	-1.30322
C	-2.20314	0.162833	0.096535
H	3.902343	2.651007	-3.86187
O	6.036667	2.331984	-2.07739
O	5.575778	1.89854	0.137155
C	6.605263	1.867121	-0.85215
O	-4.18963	-4.84229	1.760493
H	-3.9389	-4.08987	-0.93049
H	-3.02966	-1.83571	-1.53112

H	1.546193	2.485801	-3.05351
H	2.908799	1.701813	0.955644
H	-0.01631	2.384922	-1.30698
H	-1.60552	2.622646	0.70903
H	-0.81753	2.216493	2.25304
H	1.020773	-0.18265	-0.08319
H	-0.63153	-0.07854	1.610605
H	-0.53911	-1.22461	-1.54832
H	-0.31228	0.257147	-2.50515
H	-2.98969	0.891825	0.324024
H	6.955477	0.835409	-0.98124
H	7.415998	2.531452	-0.55364
O	-3.55205	-3.34262	3.388479
C	-4.30626	-4.53273	3.149554
H	-2.54724	-0.86496	2.636422
H	-5.35993	-4.35125	3.395994
H	-3.89104	-5.34935	3.739783

B3PW91/PCM(CHCl₃)6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 3 – E = -1223.784064 Hartree

Symbol	X	Y	Z
C	-2.19505	2.687738	1.492547
C	-3.27656	2.821066	2.332909
C	-3.25594	2.365907	3.644615
C	-2.14286	1.753305	4.173886
C	-1.03843	1.598463	3.323584
C	-1.05331	2.046646	2.003083
C	1.779625	-1.03546	-3.36471
C	1.798335	-2.057	-4.32763
C	1.940315	-3.34361	-3.8637
C	2.055072	-3.6204	-2.50469
C	2.026186	-2.63179	-1.55122
C	1.883808	-1.30552	-2.00318
C	1.80173	-0.18663	-1.00244
O	2.740977	-0.39067	0.046423
C	2.365267	0.506799	1.078547
C	0.438913	-0.04747	-0.28297
C	0.824939	0.51735	1.106604
C	-0.47622	1.0212	-0.86612
O	-0.07561	2.235675	-0.23443
C	0.190098	1.924928	1.131719

H	1.714227	-1.84334	-5.38619
O	1.970079	-4.51261	-4.57202
O	2.161159	-4.97171	-2.32368
C	2.36668	-5.51064	-3.63004
O	-4.44413	2.665112	4.25324
H	-2.12208	1.408927	5.200785
H	-0.14841	1.120674	3.719953
H	1.691904	-0.00597	-3.69635
H	2.124335	-2.85583	-0.49647
H	2.022543	0.767449	-1.50691
H	2.74995	1.513918	0.857773
H	2.818271	0.156864	2.007619
H	-0.05111	-1.02021	-0.21516
H	0.445601	-0.10903	1.913278
H	-1.52862	0.798884	-0.64734
H	-0.36643	1.15877	-1.94426
H	0.91653	2.673149	1.468339
H	1.746562	-6.39749	-3.75833
H	3.431174	-5.73819	-3.76728
O	-4.47925	3.421175	2.077628
C	-5.30442	3.095657	3.197058
H	-2.21062	3.063667	0.477585
H	-5.98287	2.277577	2.923821
H	-5.85235	3.982651	3.514107

B3PW91/PCM(CHCl₃)/6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-6

Conf 4 – E = -1223.783631 Hartree

Symbol	X	Y	Z
C	-0.90649	3.470565	1.27389
C	-1.16921	4.457214	2.193059
C	-0.35351	4.676129	3.299265
C	0.768858	3.915911	3.529218
C	1.054983	2.910498	2.591925
C	0.238112	2.67883	1.489026
C	1.650273	-2.73629	-2.46717
C	1.581874	-3.7641	-3.42124
C	0.549628	-4.66295	-3.29076
C	-0.38494	-4.55708	-2.26492
C	-0.33563	-3.55078	-1.33098
C	0.713205	-2.61788	-1.44484
C	0.791976	-1.4686	-0.47639

O	0.516044	-1.92163	0.844007
C	0.175346	-0.78637	1.641266
C	-0.22973	-0.33655	-0.70961
C	-0.33457	0.299946	0.684578
C	0.223253	0.811186	-1.6221
O	0.342046	1.976022	-0.80389
C	0.551382	1.554378	0.539057
H	2.311148	-3.85175	-4.21729
O	0.240224	-5.73332	-4.08235
O	-1.30633	-5.56024	-2.38472
C	-0.77432	-6.44496	-3.37147
O	-0.86816	5.693925	4.052446
H	1.405089	4.091829	4.387988
H	1.944966	2.305231	2.729866
H	2.464462	-2.02142	-2.52652
H	-1.06029	-3.48339	-0.52932
H	1.80797	-1.0438	-0.51983
H	1.056807	-0.44199	2.199435
H	-0.57955	-1.10653	2.361678
H	-1.17842	-0.76884	-1.03373
H	-1.35622	0.605823	0.918272
H	-0.49682	1.036719	-2.41077
H	1.188883	0.584733	-2.09476
H	1.605021	1.262655	0.677865
H	-1.56536	-6.73561	-4.06244
H	-0.32889	-7.31725	-2.87722
O	-2.21825	5.333747	2.22179
C	-1.89577	6.274053	3.247142
H	-1.54012	3.315483	0.409722
H	-2.77724	6.458007	3.86097
H	-1.5217	7.198462	2.789841

B3PW91/PCM(CHCl₃)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-6

Conf 5 – E = -1223.783134 Hartree

Symbol	X	Y	Z
C	-1.49317	1.215668	3.298964
C	-2.64278	1.126231	4.050852
C	-3.89132	1.434319	3.526471
C	-4.04417	1.844761	2.220948
C	-2.88299	1.931914	1.441335
C	-1.6262	1.624832	1.959982

C	1.728377	-0.45143	-3.47934
C	1.939369	-1.41141	-4.47996
C	2.502395	-2.60496	-4.08988
C	2.856953	-2.84083	-2.76818
C	2.667073	-1.90289	-1.77943
C	2.074684	-0.6828	-2.14851
C	1.897223	0.407716	-1.09924
O	2.086279	-0.08356	0.226006
C	0.8176	-0.55586	0.675745
C	0.502667	1.069407	-1.08357
C	-0.19152	0.463841	0.161361
C	0.515522	2.579101	-0.78208
O	-0.48535	2.798032	0.19805
C	-0.40376	1.689182	1.084633
H	1.67371	-1.22276	-5.51309
O	2.83836	-3.68712	-4.85611
O	3.428363	-4.07959	-2.6641
C	3.187554	-4.71061	-3.92257
O	-4.85006	1.237082	4.482065
H	-5.01963	2.088483	1.817457
H	-2.95686	2.266301	0.413426
H	1.288413	0.498787	-3.76362
H	2.963528	-2.0849	-0.75446
H	2.682166	1.157384	-1.25052
H	0.861683	-0.62968	1.764621
H	0.608671	-1.55259	0.266289
H	-0.05445	0.85887	-1.99581
H	-1.15265	0.006619	-0.07912
H	0.280259	3.202151	-1.64653
H	1.498471	2.879545	-0.38885
H	0.490404	1.799957	1.719167
H	2.351231	-5.41403	-3.82339
H	4.09574	-5.21192	-4.25664
O	-2.77891	0.727864	5.351944
C	-4.12831	1.044625	5.699424
H	-0.5247	0.987388	3.729445
H	-4.14512	1.973206	6.283744
H	-4.56476	0.213685	6.253083

B3PW91/PCM(CHCl₃)/6-311G(d,p)

(7R,8S,7'R,8'S)-6

Conf 6 – E = -1223.782823 Hartree

Symbol	X	Y	Z
C	-2.01906	2.273755	2.506606
C	-3.15192	2.890581	2.986578
C	-4.14663	3.364848	2.141149
C	-4.05053	3.240266	0.773331
C	-2.90567	2.606824	0.27075
C	-1.904	2.127243	1.112432
C	1.544059	-3.31099	-1.4038
C	2.281332	-4.15463	-2.24599
C	3.506579	-3.69521	-2.6742
C	3.994901	-2.45452	-2.28513
C	3.285376	-1.61938	-1.45249
C	2.026549	-2.06444	-1.01005
C	1.190395	-1.1605	-0.14223
O	0.451394	-1.92773	0.798921
C	-0.58979	-1.09691	1.309547
C	0.116412	-0.34034	-0.88794
C	-0.9315	-0.08083	0.209715
C	0.522913	1.061847	-1.3648
O	-0.32699	1.991352	-0.69491
C	-0.70764	1.409076	0.544707
H	1.906748	-5.12556	-2.54709
O	4.403425	-4.29685	-3.51372
O	5.213432	-2.23962	-2.86709
C	5.584873	-3.49852	-3.43224
O	-5.15835	3.907622	2.884743
H	-4.82595	3.616883	0.117156
H	-2.78078	2.503519	-0.80039
H	0.582538	-3.64038	-1.02887
H	3.688953	-0.66057	-1.14751
H	1.858448	-0.46524	0.392657
H	-0.24769	-0.59151	2.22411
H	-1.42737	-1.74522	1.571333
H	-0.29259	-0.94445	-1.69986
H	-1.94806	-0.21249	-0.16538
H	0.386468	1.207597	-2.43742
H	1.573408	1.275047	-1.12008
H	0.126766	1.489181	1.261038
H	6.313113	-3.99107	-2.77581
H	5.987404	-3.3421	-4.43276
O	-3.50767	3.122045	4.286399
C	-4.64372	3.986036	4.214703

H	-1.24616	1.922931	3.180952
H	-4.3306	5.016513	4.424255
H	-5.40284	3.645904	4.918688

B3PW91/PCM(CHCl₃)6-311G(d,p)

(7*R*,8*S*,7'*R*,8'*S*)-**6**

Conf 7 – E = -1223.782377 Hartree

Symbol	X	Y	Z
C	-0.70695	2.340547	2.504593
C	-0.78487	2.534864	3.862276
C	0.347332	2.585242	4.670016
C	1.6119	2.448868	4.147627
C	1.706515	2.259591	2.75955
C	0.578525	2.197824	1.946854
C	0.610178	-1.93732	-4.00067
C	0.256527	-3.21202	-4.46366
C	-0.55052	-3.96718	-3.64358
C	-0.99964	-3.48285	-2.42117
C	-0.66575	-2.22988	-1.96146
C	0.16976	-1.43843	-2.77491
C	0.663885	-0.07517	-2.33326
O	1.906559	-0.17382	-1.61525
C	1.574606	-0.39357	-0.24906
C	-0.26084	0.704393	-1.38453
C	0.363163	0.498659	0.019915
C	-0.20041	2.230361	-1.56943
O	-0.15705	2.781522	-0.26438
C	0.720456	1.938213	0.472967
H	0.595358	-3.58475	-5.42265
O	-1.07082	-5.21141	-3.86194
O	-1.81621	-4.41021	-1.83555
C	-1.65715	-5.59573	-2.61675
O	-0.02821	2.756248	5.973054
H	2.491904	2.493543	4.777587
H	2.690121	2.168852	2.310457
H	1.253928	-1.31908	-4.61798
H	-1.05103	-1.87761	-1.01227
H	0.895478	0.506802	-3.22999
H	2.451372	-0.13404	0.349082
H	1.338035	-1.45061	-0.07045
H	-1.29293	0.356956	-1.43642
H	-0.33401	0.045965	0.727653

H	-1.06836	2.646393	-2.08314
H	0.707964	2.50791	-2.12544
H	1.758507	2.146159	0.168678
H	-2.63337	-6.04427	-2.79869
H	-0.98409	-6.28798	-2.09591
O	-1.90277	2.674314	4.637088
C	-1.42333	3.060577	5.925729
H	-1.59309	2.312908	1.882913
H	-1.94525	2.489102	6.693069
H	-1.56541	4.140123	6.059447

B3PW91/PCM(MeCN)6-311G(d,p)
(7R,8S,7'S,8'S)-7

Conf 1 – E = -1223.789981 Hartree

Symbol	X	Y	Z
C	-2.9509	5.502211	1.126853
C	-2.61436	4.308582	1.759363
C	-2.38911	5.864643	-0.07483
C	-1.45731	4.974191	-0.63292
C	-1.10762	3.784101	-0.00149
C	-1.70188	3.430627	1.226415
C	-0.0655	2.882831	-0.60429
O	-0.49077	1.52581	-0.53343
C	0.671058	0.746684	-0.78815
C	1.817187	1.445113	-0.04093
C	1.313656	2.903262	0.100447
C	2.380933	3.725184	-0.62488
O	2.996769	2.822985	-1.53726
C	3.147482	1.605018	-0.81708
C	3.532792	0.480539	-1.74437
C	3.319495	0.591322	-3.13003
C	3.67133	-0.48783	-3.90873
C	4.218573	-1.64499	-3.36877
C	4.445053	-1.77109	-2.01655
C	4.093232	-0.6792	-1.21041
O	3.600742	-0.60926	-5.26927
C	3.878093	-1.98601	-5.53682
O	4.508284	-2.52694	-4.37321
O	-3.90521	6.152758	1.856923
C	-3.97411	5.448999	3.099603
O	-3.34993	4.177908	2.904121
H	-2.66296	6.78688	-0.57268

H	-1.00105	5.224252	-1.58509
H	-1.45789	2.497177	1.718395
H	0.080375	3.159582	-1.66026
H	0.870513	0.715576	-1.86782
H	0.476204	-0.26855	-0.44037
H	1.99192	0.973585	0.926927
H	1.20094	3.209259	1.141553
H	3.126758	4.108294	0.085363
H	1.981745	4.564092	-1.19861
H	3.951062	1.730742	-0.07453
H	2.907906	1.495189	-3.55943
H	4.885947	-2.66752	-1.59759
H	4.265704	-0.74387	-0.14073
H	4.556689	-2.06148	-6.38554
H	2.936767	-2.51757	-5.72171
H	-5.01754	5.302565	3.376288
H	-3.42616	6.009544	3.866245

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'S,8'S)-7

Conf 2 – E = -1223.789884 Hartree

Symbol	X	Y	Z
C	0.529308	2.59893	6.032084
C	0.292372	1.250768	5.77947
C	1.157292	3.405246	5.111834
C	1.549534	2.803333	3.905206
C	1.325236	1.453482	3.649496
C	0.674937	0.648166	4.60538
C	1.81178	0.83543	2.367776
O	0.830367	-0.05333	1.845643
C	1.502091	-0.83162	0.863594
C	2.88607	-1.14772	1.450977
C	3.096319	-0.02128	2.493774
C	4.368965	0.679156	2.014488
O	4.448407	0.401132	0.62121
C	4.087745	-0.96791	0.490581
C	3.855592	-1.32705	-0.95492
C	3.745759	-2.69051	-1.29372
C	3.513263	-2.99712	-2.61346
C	3.402797	-2.01428	-3.59174
C	3.520268	-0.67893	-3.28559
C	3.746589	-0.34935	-1.93908

O	3.403348	-4.23052	-3.19136
C	2.969333	-3.98187	-4.53152
O	3.221863	-2.60335	-4.8124
O	0.009456	2.934012	7.250477
C	-0.34508	1.692545	7.864571
O	-0.38374	0.70278	6.833511
H	1.327795	4.457597	5.303927
H	2.038548	3.412526	3.152149
H	0.472847	-0.39785	4.411171
H	2.000911	1.634673	1.63402
H	1.599368	-0.25733	-0.06799
H	0.896765	-1.71717	0.666252
H	2.898444	-2.13851	1.906659
H	3.198523	-0.40313	3.510708
H	5.252231	0.27654	2.529507
H	4.35457	1.76359	2.141081
H	4.914517	-1.58848	0.872888
H	3.846005	-3.4717	-0.54835
H	3.446422	0.084815	-4.05047
H	3.844341	0.690729	-1.65516
H	1.893372	-4.17896	-4.60763
H	3.542039	-4.60338	-5.21893
H	-1.33093	1.781438	8.319627
H	0.418568	1.419868	8.602586

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*S*,8'*S*)-7

Conf 3 – E = -1223.789513 Hartree

Symbol	X	Y	Z
C	-1.91519	5.743514	1.91193
C	-0.93079	5.064966	1.199129
C	-2.80038	5.079916	2.728876
C	-2.66509	3.684343	2.808718
C	-1.68983	2.997749	2.091073
C	-0.79014	3.69978	1.264674
C	-1.61388	1.497249	2.160074
O	-0.25676	1.078003	2.255343
C	-0.2618	-0.31052	1.951575
C	-1.24664	-0.48072	0.785472
C	-2.17607	0.751155	0.923365
C	-3.56061	0.133931	1.133254
O	-3.31768	-1.16822	1.653699

C	-2.22421	-1.67454	0.899741
C	-1.67766	-2.93481	1.52097
C	-0.70758	-3.66397	0.804143
C	-0.21163	-4.80326	1.391844
C	-0.64775	-5.24193	2.63798
C	-1.60233	-4.55317	3.348458
C	-2.11176	-3.38103	2.765217
O	0.700263	-5.68861	0.889919
C	1.009399	-6.56744	1.975344
O	-0.02243	-6.41663	2.952818
O	-1.79588	7.086597	1.690796
C	-0.8579	7.21138	0.619015
O	-0.16594	5.964912	0.511014
H	-3.55646	5.611034	3.294274
H	-3.34071	3.129852	3.451677
H	-0.01165	3.181742	0.718516
H	-2.16087	1.151328	3.051111
H	-0.59724	-0.88546	2.825964
H	0.76039	-0.6047	1.710638
H	-0.72093	-0.49574	-0.16994
H	-2.14828	1.398602	0.045694
H	-4.10292	0.062647	0.180237
H	-4.18357	0.671983	1.850582
H	-2.57788	-1.91444	-0.11648
H	-0.36537	-3.34663	-0.17466
H	-1.94976	-4.90198	4.313567
H	-2.86454	-2.80878	3.292163
H	1.97236	-6.27919	2.413508
H	1.022121	-7.59594	1.61646
H	-0.14601	8.002966	0.850274
H	-1.39631	7.411048	-0.31503

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'S,8'S)-7

Conf 4 – E = -1223.789426 Hartree

Symbol	X	Y	Z
C	5.589241	-0.28574	-0.14082
C	4.808142	-0.2945	-1.29305
C	5.024384	-0.2673	1.112826
C	3.621234	-0.26311	1.175564
C	2.833502	-0.26248	0.028068
C	3.435147	-0.27934	-1.24601

C	1.334234	-0.21114	0.136015
O	0.745625	-1.13118	-0.77752
C	-0.62573	-0.76495	-0.86031
C	-0.64985	0.770838	-0.87856
C	0.693279	1.156024	-0.20983
C	0.266842	1.978954	1.007574
O	-1.06488	1.566657	1.294518
C	-1.70366	1.452879	0.028056
C	-3.03565	0.759803	0.161795
C	-3.32222	-0.0271	1.291714
C	-4.54779	-0.6526	1.32801
C	-5.47767	-0.52215	0.304039
C	-5.2222	0.251167	-0.80606
C	-3.97821	0.896122	-0.85657
O	-5.07249	-1.43022	2.323354
C	-6.26128	-1.99758	1.767617
O	-6.61337	-1.21307	0.625516
O	6.911477	-0.2727	-0.4854
C	6.937156	-0.52934	-1.89189
O	5.620154	-0.28878	-2.3927
H	5.633551	-0.26402	2.008521
H	3.141817	-0.26912	2.148945
H	2.836206	-0.29248	-2.14822
H	1.038868	-0.48332	1.16152
H	-1.16939	-1.15396	0.011171
H	-1.03998	-1.21997	-1.76087
H	-0.7237	1.144335	-1.90066
H	1.346751	1.72154	-0.87574
H	0.285784	3.053249	0.77733
H	0.873431	1.801839	1.898042
H	-1.87929	2.464068	-0.37137
H	-2.60915	-0.12127	2.100096
H	-5.95351	0.365297	-1.59703
H	-3.74839	1.519125	-1.71516
H	-7.06413	-1.95007	2.502253
H	-6.05977	-3.02876	1.453186
H	7.207266	-1.57775	-2.06559
H	7.63823	0.152114	-2.37235

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'S,8'S)-7

Conf 5 – E = -1223.788938 Hartree

Symbol	X	Y	Z
C	5.657085	-0.13707	0.132786
C	4.890075	-0.23574	-1.02458
C	5.07806	-0.08407	1.379085
C	3.67571	-0.13962	1.428853
C	2.901587	-0.22835	0.275318
C	3.517051	-0.27861	-0.99094
C	1.40055	-0.23297	0.369947
O	0.85248	-1.18176	-0.53841
C	-0.53042	-0.86623	-0.63453
C	-0.61083	0.667446	-0.66619
C	0.713451	1.107482	0.006904
C	0.248832	1.924545	1.213793
O	-1.06434	1.45745	1.501194
C	-1.69471	1.308497	0.235324
C	-2.99408	0.555913	0.366865
C	-3.87776	0.553423	-0.73078
C	-5.04712	-0.15717	-0.59898
C	-5.36912	-0.84002	0.569449
C	-4.52796	-0.83943	1.657239
C	-3.32364	-0.12733	1.533442
O	-6.06878	-0.28319	-1.49764
C	-6.93633	-1.27756	-0.94576
O	-6.60354	-1.41325	0.437749
O	6.981409	-0.08171	-0.20015
C	7.033597	-0.40702	-1.59135
O	5.713451	-0.24678	-2.11582
H	5.676487	-0.01121	2.279077
H	3.186119	-0.12136	2.396992
H	2.928466	-0.36062	-1.89621
H	1.106975	-0.50491	1.396049
H	-1.06736	-1.26373	0.23768
H	-0.92169	-1.34456	-1.53322
H	-0.69301	1.031776	-1.69088
H	1.3503	1.69086	-0.65986
H	0.222068	2.99593	0.971071
H	0.85934	1.783891	2.108039
H	-1.91408	2.309856	-0.16949
H	-3.65265	1.094017	-1.64348
H	-4.78562	-1.36123	2.571097
H	-2.63239	-0.10202	2.366148
H	-6.76682	-2.23242	-1.45744

H	-7.97061	-0.94854	-1.03984
H	7.348336	-1.45072	-1.70949
H	7.711442	0.278107	-2.09908

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*S*,8'*S*)-7

Conf 6 – E = -1223.788837 Hartree

Symbol	X	Y	Z
C	5.568919	-0.10725	-0.46389
C	4.959552	0.082051	0.769809
C	4.832331	-0.33886	-1.60457
C	3.438081	-0.36972	-1.46554
C	2.8184	-0.18138	-0.23078
C	3.591537	0.046198	0.921961
C	1.316446	-0.18223	-0.12605
O	0.764953	-1.2085	-0.94261
C	-0.62029	-0.90746	-1.05121
C	-0.70696	0.617053	-1.21782
C	0.622946	1.119105	-0.6014
C	0.168229	2.045667	0.527782
O	-1.14325	1.610546	0.868626
C	-1.78461	1.338732	-0.37241
C	-3.08061	0.600216	-0.15155
C	-3.33537	-0.04484	1.071683
C	-4.52835	-0.72134	1.189667
C	-5.45583	-0.77463	0.156797
C	-5.23127	-0.14211	-1.04543
C	-4.02107	0.552965	-1.18
O	-5.02045	-1.38654	2.278677
C	-6.17427	-2.08292	1.801343
O	-6.55769	-1.47413	0.565922
O	6.924818	0.004358	-0.32645
C	7.158889	0.015773	1.083918
O	5.913958	0.316736	1.72008
H	5.310951	-0.48779	-2.56506
H	2.822458	-0.56084	-2.3366
H	3.133182	0.18313	1.894834
H	1.027787	-0.36365	0.921661
H	-1.1452	-1.23103	-0.14225
H	-1.01909	-1.46399	-1.90018
H	-0.79976	0.886284	-2.27064
H	1.252575	1.637362	-1.32597

H	0.140855	3.089751	0.186332
H	0.785222	1.988892	1.426896
H	-2.01194	2.294812	-0.8695
H	-2.6238	0.004332	1.88523
H	-5.96141	-0.17081	-1.84516
H	-3.81637	1.067645	-2.11342
H	-6.98401	-1.98154	2.522792
H	-5.91742	-3.13449	1.62494
H	7.886159	0.790118	1.32521
H	7.500766	-0.97565	1.404339

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*S*,8'*S*)-7

Conf 7 – E = -1223.788432 Hartree

Symbol	X	Y	Z
C	0.158744	2.178872	6.021575
C	1.167873	2.786331	5.285
C	-0.41377	0.992603	5.619245
C	0.07701	0.417246	4.438852
C	1.089396	1.020306	3.694116
C	1.648116	2.240447	4.116009
C	1.627575	0.354055	2.455944
O	0.575834	-0.27047	1.731038
C	1.215325	-1.13816	0.803887
C	2.382208	-1.78223	1.567944
C	2.659381	-0.77376	2.710984
C	4.115152	-0.36288	2.4835
O	4.363075	-0.60319	1.103116
C	3.735737	-1.84789	0.818479
C	3.676943	-2.08669	-0.66957
C	3.900612	-1.03144	-1.57136
C	3.811883	-1.32193	-2.91412
C	3.515911	-2.59694	-3.37889
C	3.301153	-3.6465	-2.5138
C	3.390894	-3.36691	-1.14293
O	4.024287	-0.48748	-3.97693
C	3.593829	-1.22462	-5.12374
O	3.533657	-2.60227	-4.74653
O	-0.15441	2.960159	7.099252
C	0.872477	3.953472	7.152886

O	1.51835	3.96754	5.877038
H	-1.21043	0.528779	6.188467
H	-0.34732	-0.51565	4.087121
H	2.419653	2.739968	3.541059
H	2.100992	1.114824	1.814546
H	1.584702	-0.56066	-0.05461
H	0.474054	-1.85515	0.449158
H	2.102113	-2.7662	1.945877
H	2.506652	-1.20653	3.700676
H	4.791969	-0.97147	3.099065
H	4.316586	0.69166	2.682013
H	4.329574	-2.65538	1.275071
H	4.144134	-0.03869	-1.21687
H	3.084071	-4.64383	-2.87673
H	3.233164	-4.17436	-0.43499
H	4.317591	-1.0998	-5.92826
H	2.594578	-0.88419	-5.42112
H	1.601105	3.683071	7.926597
H	0.425268	4.928246	7.343739

B3PW91/PCM(MeCN)6-311G(d,p)

(7*R*,8*S*,7'*S*,8'*S*)-7

Conf 8 – E = -1223.788216 Hartree

Symbol	X	Y	Z
C	4.419877	-2.72793	-3.1245
C	3.373234	-1.83082	-3.29615
C	4.992034	-2.94097	-1.89015
C	4.466967	-2.21552	-0.81141
C	3.417542	-1.31288	-0.97548
C	2.853899	-1.10547	-2.24773
C	2.845425	-0.58263	0.210813
O	3.876909	-0.24232	1.128165
C	3.216628	0.097681	2.340243
C	2.078883	-0.92157	2.497628
C	1.818681	-1.392	1.044402
C	0.357469	-1.00794	0.800405
O	0.086418	0.046696	1.716225
C	0.709762	-0.34514	2.932305
C	0.740435	0.797303	3.915293
C	1.101303	0.518615	5.248818
C	1.140603	1.575693	6.126623
C	0.825577	2.872999	5.735218

C	0.457954	3.16504	4.442867
C	0.423965	2.096822	3.531314
O	1.426236	1.55943	7.463024
C	1.529727	2.934622	7.842254
O	0.903829	3.707373	6.816067
O	4.716479	-3.31946	-4.32128
C	3.986993	-2.57409	-5.29916
O	2.980975	-1.83088	-4.60567
H	5.810154	-3.63928	-1.76022
H	4.896649	-2.34456	0.174796
H	2.046392	-0.399	-2.40282
H	2.355415	0.341356	-0.13605
H	2.815355	1.118509	2.276061
H	3.952359	0.061778	3.144539
H	2.38045	-1.74336	3.148244
H	1.986504	-2.46177	0.912648
H	-0.3065	-1.86012	1.001679
H	0.154843	-0.63804	-0.20665
H	0.127996	-1.16919	3.37652
H	1.33391	-0.48854	5.576519
H	0.20149	4.173869	4.142371
H	0.139391	2.28301	2.503569
H	2.587915	3.212885	7.914969
H	1.006439	3.0908	8.784808
H	3.512649	-3.26052	-5.99955
H	4.665685	-1.87969	-5.80875

B3PW91/PCM(MeCN)6-311G(d,p)

(7R,8S,7'S,8'S)-7

Conf 9 – E = - 1223.788191 Hartree

Symbol	X	Y	Z
C	4.993521	1.170503	-2.41737
C	4.676979	1.78197	-1.21078
C	4.178221	0.211328	-2.97541
C	3.009586	-0.11755	-2.27389
C	2.685483	0.4906	-1.06242
C	3.537846	1.462618	-0.50711
C	1.399987	0.15075	-0.35526
O	1.087446	-1.22522	-0.52656
C	-0.27875	-1.3591	-0.15692
C	-0.99096	-0.12527	-0.73005
C	0.150957	0.912625	-0.86904

C	-0.30336	2.066374	0.027977
O	-1.19623	1.483002	0.969758
C	-1.99337	0.578146	0.216705
C	-2.80263	-0.31283	1.124116
C	-3.82987	-1.08937	0.551478
C	-4.55418	-1.89864	1.394068
C	-4.30166	-1.95682	2.760821
C	-3.30799	-1.2041	3.341127
C	-2.55633	-0.3748	2.492283
O	-5.56716	-2.76061	1.080298
C	-6.11174	-3.17537	2.336102
O	-5.1487	-2.85875	3.34349
O	6.161114	1.692135	-2.90214
C	6.697697	2.470614	-1.8298
O	5.63606	2.705416	-0.90072
H	4.429491	-0.26576	-3.91514
H	2.346439	-0.87615	-2.67204
H	3.313906	1.940258	0.440003
H	1.513472	0.361363	0.720396
H	-0.37125	-1.38597	0.937549
H	-0.64426	-2.30385	-0.5611
H	-1.45636	-0.35583	-1.68913
H	0.303606	1.23367	-1.90034
H	-0.82657	2.832619	-0.56081
H	0.504999	2.545274	0.584066
H	-2.68934	1.159893	-0.40926
H	-4.04704	-1.05164	-0.51024
H	-3.11274	-1.24996	4.405821
H	-1.77184	0.243349	2.909881
H	-6.28038	-4.2515	2.320105
H	-7.03854	-2.62258	2.530677
H	7.057867	3.422957	-2.21711
H	7.496585	1.906187	-1.33409

QM/MM B3PW91/6-311G(d,p):UFF - MeCN

(7R,8S,7'R,8'S)-5

Symbol	X	Y	Z
H	25.0951739	23.5850855	21.6527813
C	25.2816473	24.6460517	21.7505085
C	24.640955	25.5355718	20.8992
C	26.1798655	25.096708	22.7155395
O	23.768032	25.1813351	19.9269837

C	24.909539	26.9165404	21.0195348
H	26.6960939	24.3844769	23.3473252
C	26.4479431	26.4499497	22.8432119
C	23.3102541	23.8468698	19.9111313
O	24.2549734	27.725006	20.1502726
C	25.8042558	27.3510072	21.9889162
C	27.4052888	26.9469277	23.8929993
H	22.5644584	23.7988221	19.1196397
H	22.84507	23.5748944	20.8661655
H	24.1133201	23.1355464	19.6860243
C	24.5237468	29.1086741	20.209769
H	26.0176376	28.4086029	22.0828706
H	27.6979082	27.9806992	23.6483453
O	28.5723259	26.1242572	23.8928349
C	26.8675431	26.9048612	25.3470514
H	24.2259986	29.5422074	21.1710528
H	25.5843436	29.3206598	20.038204
H	23.9330982	29.5645346	19.4171627
C	29.1479318	26.2040825	25.1794705
H	25.9213619	26.3661594	25.3886347
C	26.7516405	28.2390231	26.0851809
C	27.9680681	26.1841548	26.1519309
H	29.7240218	27.1362588	25.2890291
H	29.835033	25.3628566	25.2884098
H	25.7581784	28.6856476	26.0554034
H	27.4675262	28.9693614	25.6781726
O	27.0494174	27.9529715	27.4392742
H	27.6915448	25.1568955	26.3815244
C	28.1132601	27.0106093	27.452287
H	29.0679883	27.5593236	27.4221056
C	28.0767442	26.1892176	28.7176403
C	29.1294056	25.3171007	28.9838217
C	26.9936656	26.2834674	29.6030714
H	29.9573131	25.2584074	28.2857489
C	29.1510905	24.5056015	30.1237463
H	26.1777011	26.9646152	29.4074304
C	27.0308689	25.4836496	30.7224279
H	29.9713315	23.8285065	30.3239645
C	28.0805031	24.6141044	30.9812579
O	26.1207514	25.4126123	31.7399175
O	27.8650744	23.9724748	32.1694201
C	26.5352821	24.3164879	32.5471649

H	26.524304	24.6163743	33.596046
H	25.8705197	23.460747	32.3693948
C	29.279662	33.6340093	26.5588131
C	29.1203796	34.036326	27.988641
H	29.1775537	33.1348234	28.6315892
H	29.9150027	34.7505676	28.2929821
H	28.1291655	34.5141427	28.1269576
N	30.2318235	34.1089808	25.8446604
C	30.0655853	24.479105	19.9764659
C	29.1721553	24.9240634	20.9341546
H	28.1548877	24.9740292	20.498578
H	29.1705398	24.2279398	21.7954061
H	29.4723007	25.9320506	21.2797986
N	30.8130232	24.1064284	19.1757499
C	17.6663036	21.044415	22.5559551
C	17.5799336	22.389047	23.1951848
H	17.7641377	22.3007268	24.2850651
H	18.332577	23.068661	22.7469809
H	16.5670418	22.8098733	23.0303574
N	18.7483069	20.361673	22.623989
C	28.8154294	22.3886098	25.9241898
C	28.8559203	22.1214632	24.5684833
H	29.7935711	21.5810551	24.3263792
H	27.988537	21.4907897	24.2901735
H	28.8188855	23.0746888	24.0039612
N	28.7828919	22.6113613	27.0586644
C	35.2372563	24.4793231	25.4562006
C	34.4537227	25.3687012	24.7424262
H	34.4963945	25.1180965	23.6627777
H	33.404796	25.3008997	25.0957891
H	34.8317995	26.3999769	24.8944183
N	35.8912907	23.7346535	26.0535451
C	25.0697053	27.5709534	14.8110866
C	25.7678143	27.2899012	15.9720486
H	26.7480808	27.8075285	15.9480091
H	25.1849016	27.6342012	16.8508237
H	25.9313301	26.1973057	16.0473582
N	24.4866704	27.8047314	13.8392881
C	31.7604736	29.8873026	20.0529449
C	31.3432841	30.9474846	20.9704329
H	32.2089105	31.6016098	21.2005532
H	30.5403442	31.5484808	20.49895

H	30.9617641	30.4958427	21.9083214
N	32.0900589	29.0474153	19.3285594
C	28.4243132	28.3144246	20.0237552
C	28.0460642	27.6912558	18.8491645
H	28.6752529	26.7943553	18.6878408
H	26.9813759	27.389635	18.9140791
H	28.1823628	28.3889046	18.0008925
N	28.7391165	28.8338383	21.0079841
C	22.6649695	20.8044545	34.4871308
C	23.8228755	21.4831653	34.8230535
H	24.2020252	22.0314224	33.9368384
H	23.6066185	22.2021952	35.6393255
H	24.5905921	20.7596558	35.1651091
N	21.6964062	20.2365124	34.2076059
C	19.4124118	22.4127267	35.9678322
C	20.6099039	22.9583559	36.6057876
H	21.2440905	22.1276204	36.9770988
H	21.1824843	23.5608156	35.8713246
H	20.3096924	23.6016296	37.4573874
N	18.4639489	21.9819546	35.4642007
C	19.7761603	25.6028905	23.7242731
C	19.658343	25.7887994	25.1688021
H	19.244651	24.8680231	25.627221
H	20.6606886	25.9931423	25.5964266
H	18.9846195	26.6443027	25.3773317
N	19.8771013	25.4534624	22.5818654
C	34.071368	25.3852115	29.6099389
C	32.8031262	25.3115799	30.3336705
H	31.9993438	25.7597554	29.7185026
H	32.5585592	24.2527641	30.5470784
H	32.8871094	25.8693284	31.2863655
N	35.0745446	25.4434201	29.0364326
C	19.3031997	20.3573578	26.3088189
C	18.7010074	21.4547819	27.0653307
H	18.9467326	22.4184711	26.5759208
H	17.5995719	21.3267737	27.092329
H	19.1004225	21.4531183	28.1001847
N	19.7806431	19.4893931	25.7109611
C	32.4782002	27.8017501	26.4347043
C	33.6499562	28.5133229	26.7681606
H	33.4245043	29.2706375	27.5460966
H	34.4265188	27.813459	27.1428588

H	34.033537	29.0298057	25.8653104
N	31.8630077	27.1103262	27.3200547
C	32.9694174	22.4293898	23.3473677
C	31.9019545	23.3433475	22.9436649
H	31.123062	22.7759094	22.3959314
H	31.4554181	23.8140487	23.8431849
H	32.3185815	24.1302035	22.2825241
N	33.8148265	21.7065479	23.6661567
C	23.9504976	25.5788311	39.1916867
C	23.0747866	24.8379203	38.2845306
H	23.6676548	24.0881975	37.7222088
H	22.2897231	24.3217217	38.8734493
H	22.6000861	25.5412888	37.5710603
N	24.6433532	26.1655358	39.9091108
C	23.1708074	33.2778643	27.2677491
C	22.6688805	32.0513654	26.6495139
H	23.1249517	31.1718671	27.1469076
H	21.5658723	32.0081364	26.7551833
H	22.9369901	32.0448055	25.574125
N	23.5693484	34.2482986	27.7558346
C	28.7781707	21.0444301	30.1049192
C	29.4184039	19.992186	29.2643511
H	29.3249702	19.0037719	29.7605424
H	28.9307383	19.9534749	28.2686331
H	30.4925134	20.2338096	29.1321904
N	27.5333437	20.973267	30.3981477
C	27.801307	31.8063667	22.7144006
C	28.6720034	32.975194	22.5970583
H	28.800249	33.2337675	21.5264638
H	28.2148558	33.8323862	23.131881
H	29.6612428	32.7463905	23.0429632
N	27.1108288	30.8828067	22.8080369
C	19.3777532	25.7237548	29.4184275
C	18.5090686	24.5300668	29.1987667
H	19.0074678	23.632756	29.6174286
H	17.5408088	24.682136	29.7182224
H	18.3212128	24.3694405	28.1164372
N	19.791245	26.427033	28.4309165
C	25.9805655	19.5170755	27.4826229
C	25.3085479	18.8770986	28.6122413
H	25.0778285	19.6388673	29.3840547
H	24.3665088	18.4062238	28.2641855

H	25.9727334	18.1016475	29.0453511
N	26.512787	20.0240599	26.5896649
C	34.8974866	28.9138277	30.1759959
C	33.5509915	28.8950495	30.7459357
H	33.5525448	28.2938131	31.6777291
H	33.2314802	29.9313968	30.9779568
H	32.847152	28.4458457	30.0159593
N	35.9624353	28.9279558	29.7237339
C	22.3772777	25.6649379	16.1190508
C	21.2776992	26.3697686	15.4615788
H	20.5970785	26.7930139	16.2287595
H	21.6871938	27.1896245	14.8370573
H	20.7157822	25.6620156	14.8186611
N	23.2472055	25.1081025	16.6397962
C	21.5453249	35.5011182	21.0562541
C	22.7714215	36.1398375	20.578535
H	22.5147372	36.9453083	19.8605401
H	23.3224979	36.5723889	21.4384259
H	23.4082783	35.3853934	20.0751835
N	20.5762071	34.9957454	21.4358898
C	25.5103608	23.3859246	27.0969965
C	25.5915355	23.1198024	28.5304283
H	26.6518045	23.1449097	28.8483599
H	25.0206973	23.8921845	29.0829697
H	25.1640806	22.1205447	28.7445829
N	25.446065	23.5979535	25.9623085
C	27.4448003	36.5216421	25.7243202
C	26.3594176	35.6785509	25.5641312
H	26.1794743	35.1209248	26.5058529
H	25.4606752	36.2770827	25.3111119
H	26.5686437	34.9613895	24.7453781
N	28.3532492	37.2258163	25.858247
C	26.5778518	24.7155408	36.8538347
C	26.581735	23.2799876	36.5778798
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H	31.9749723	18.7265943	32.0778958
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QM/MM B3PW91/6-311G(d,p):UFF - MeCN

(7R,8S,7'R,8'S)-5

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C	24.6126189	22.1582423	28.2996692
H	26.902785	25.141972	29.2232815
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C	23.7497581	22.5034932	31.8031349
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H	25.2696392	22.4994808	26.2897958
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H	24.5553778	20.4066775	26.2545825
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H	25.2657778	24.3884671	24.4577909
O	25.6477679	26.2416366	23.6186293
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H	28.2462079	19.4641214	26.7084769
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C	28.703767	22.8889526	21.5467203
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QM/MM B3PW91/6-311G(d,p):UFF - MeCN

(7R,8S,7'R,8'S)-6

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C	25.0697222	26.8348909	26.4577064
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H	32.3576225	31.3084035	21.5630621
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H	29.9725124	22.9515367	27.1701272
H	29.9526963	24.3884428	26.0715
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H	19.9372793	20.0842103	30.2772924
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H	21.7176922	19.7533839	30.2283098
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H	32.5265455	28.364948	23.1759919
H	32.2585015	28.0602184	24.9338368
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H	35.5568382	30.2384119	31.3637612

H	36.3301367	29.2595257	30.0499517
H	34.8911068	30.2942062	29.6812061
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QM/MM B3PW91/6-311G(d,p):UFF - MeCN

(7R,8S,7'R,8'S)-7

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O	32.6021647	24.8350975	26.942363
C	30.4726167	24.8223815	26.2149219
H	28.920683	24.6951811	29.7049007
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C	32.5566918	25.1393851	25.5532266
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C	29.1033035	24.7878373	26.312404
C	27.052402	24.6952177	27.7569451
H	32.7559059	26.2090603	25.4057136
H	33.2816634	24.5223553	25.0240066
H	28.4847086	24.7991432	25.4231511
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C	25.2729184	25.2079565	29.0796996
H	26.1121387	25.4054274	25.9008318
C	26.773563	27.1426271	27.0273486
C	24.9206401	25.8077916	27.7021916
H	24.7442164	24.2583224	29.2296647
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H	27.4391644	27.4301008	26.2140913
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H	24.1281743	25.2254254	27.2354729
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H	24.527556	27.7154795	28.6840147
C	23.259411	27.6184622	26.9670358
C	22.0735518	27.6527847	27.6923073
C	23.2461366	27.8089784	25.5750763
H	22.1061663	27.5283336	28.7684874
C	20.8317093	27.8507933	27.0733591

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H	19.9097067	27.8840933	27.6395607
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H	19.957602	27.4925554	22.9470719
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H	28.838398	22.6384928	24.0894502
H	29.7003019	23.7420666	22.9463986
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C	31.3195811	27.1249379	31.3269331
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C	16.6055289	29.1036386	23.6690257
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