

Supporting Information

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A Previously Undescribed Cleistanthane-Type Diterpenoid from *Peniophora incarnate*

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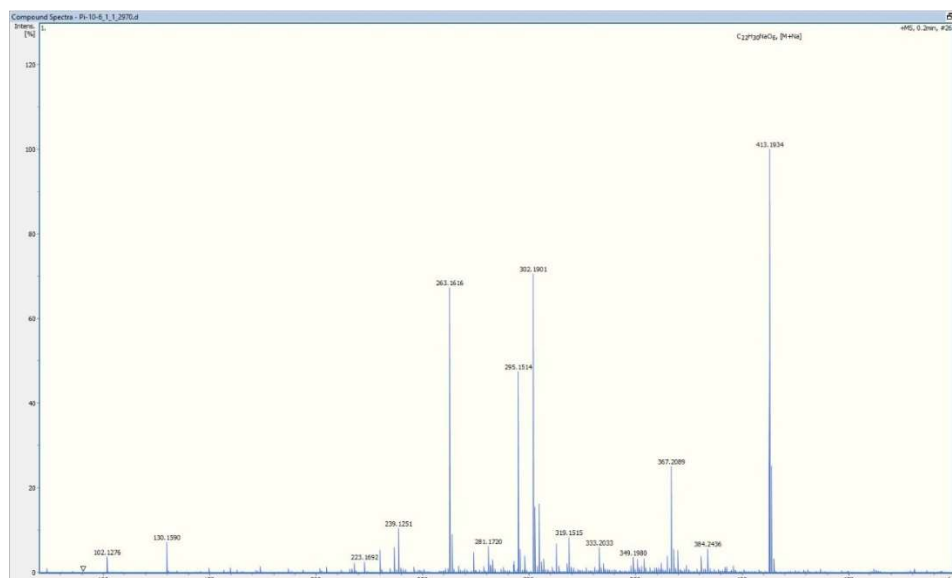


Figure S1: HR-ESI-MS spectrum of compound **1**



Figure S2: The IR spectrum of compound **1**

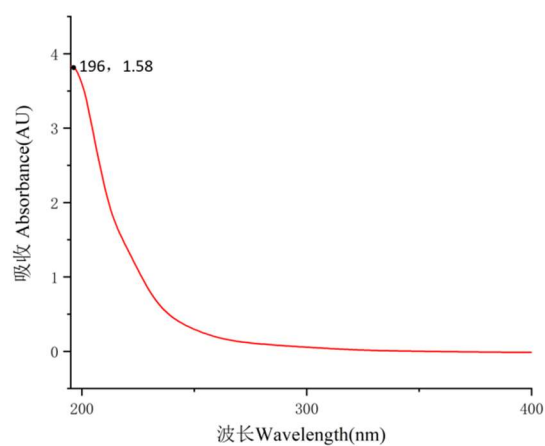


Figure S3: The UV spectrum of compound **1**

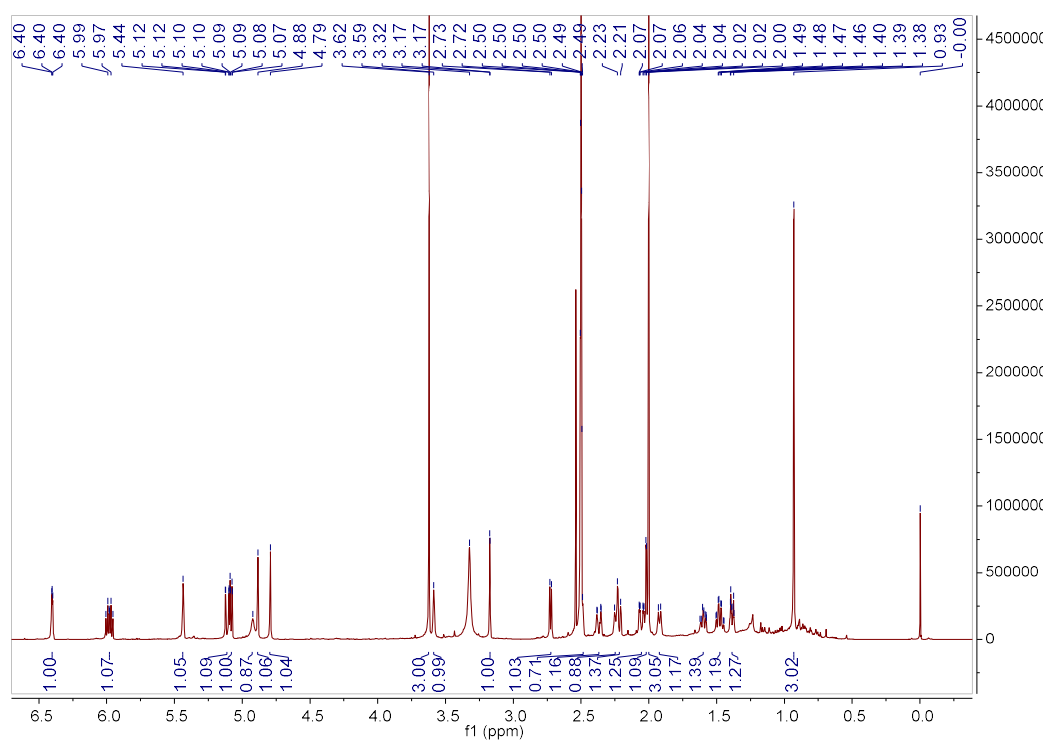


Figure S4: ^1H -NMR (700 MHz, $\text{DMSO}-d_6$) spectrum of compound **1**

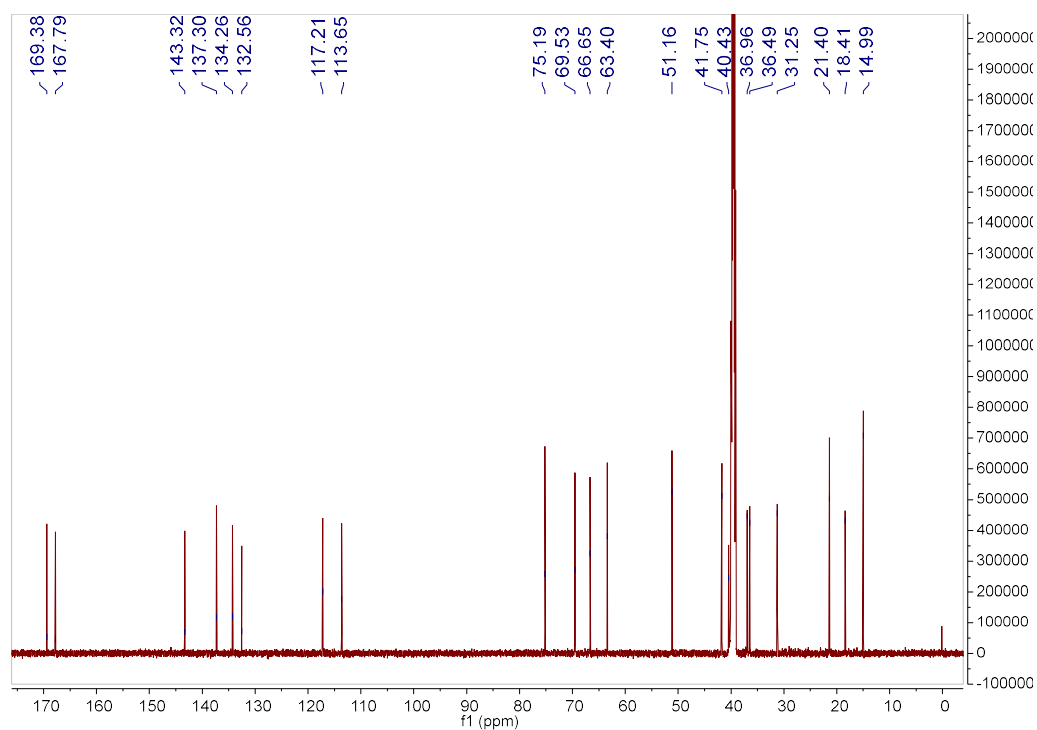


Figure S5: ^{13}C -NMR (700 MHz, $\text{DMSO}-d_6$) spectrum of compound **1**

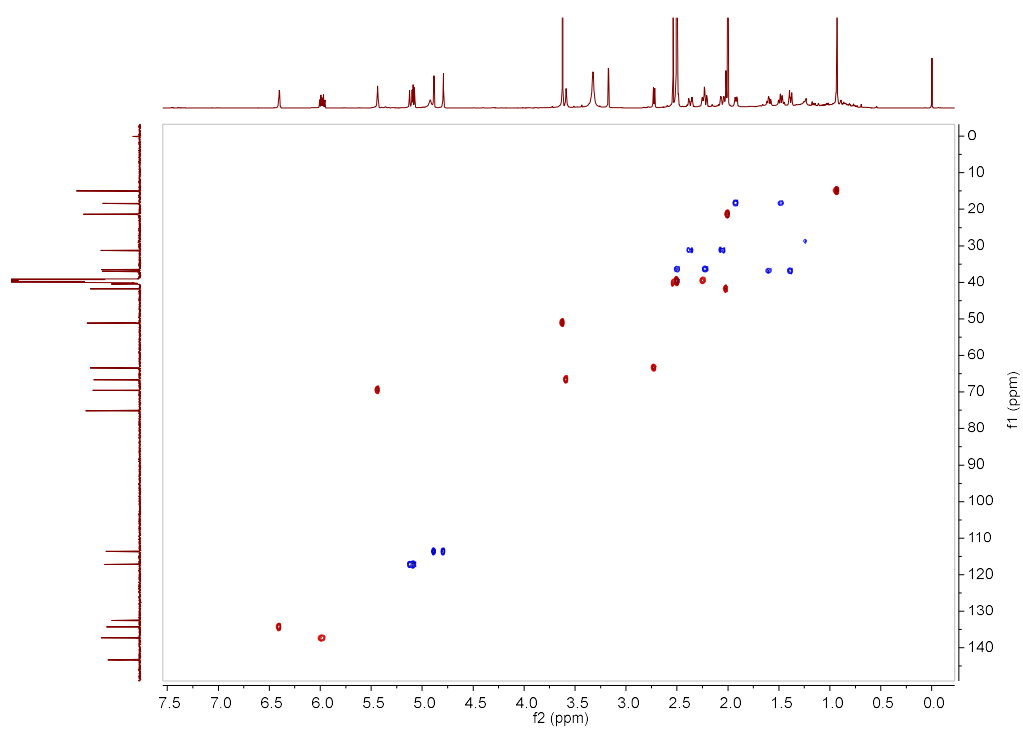


Figure S6: HSQC spectrum of compound **1**

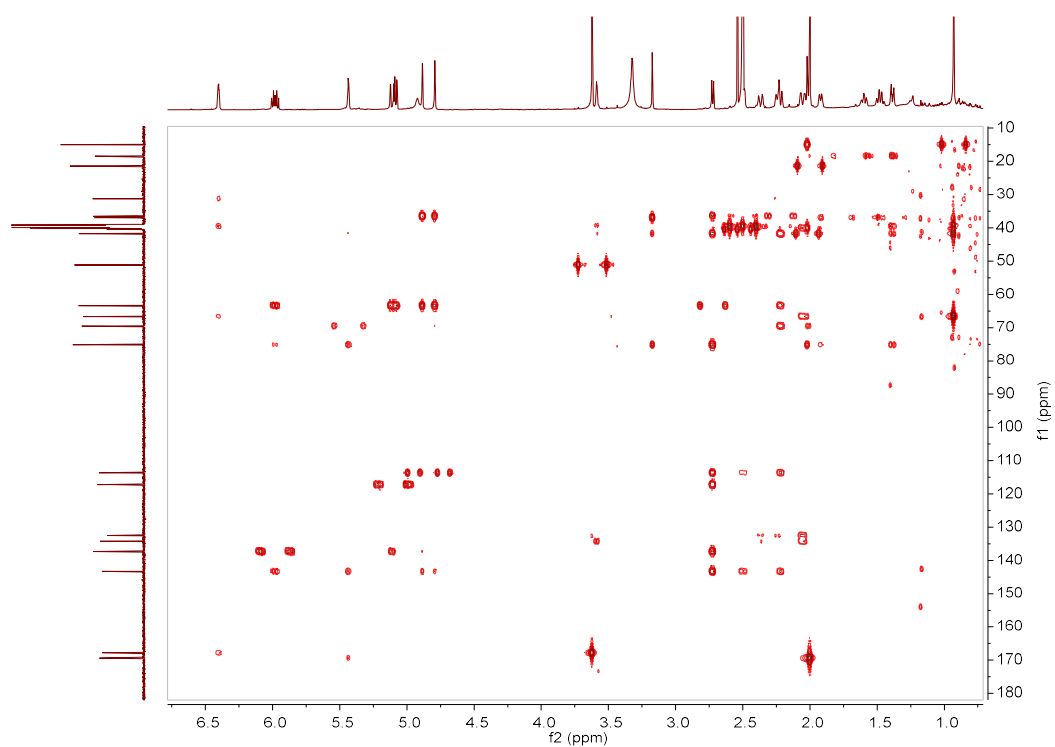


Figure S7: HMBC spectrum of compound **1**

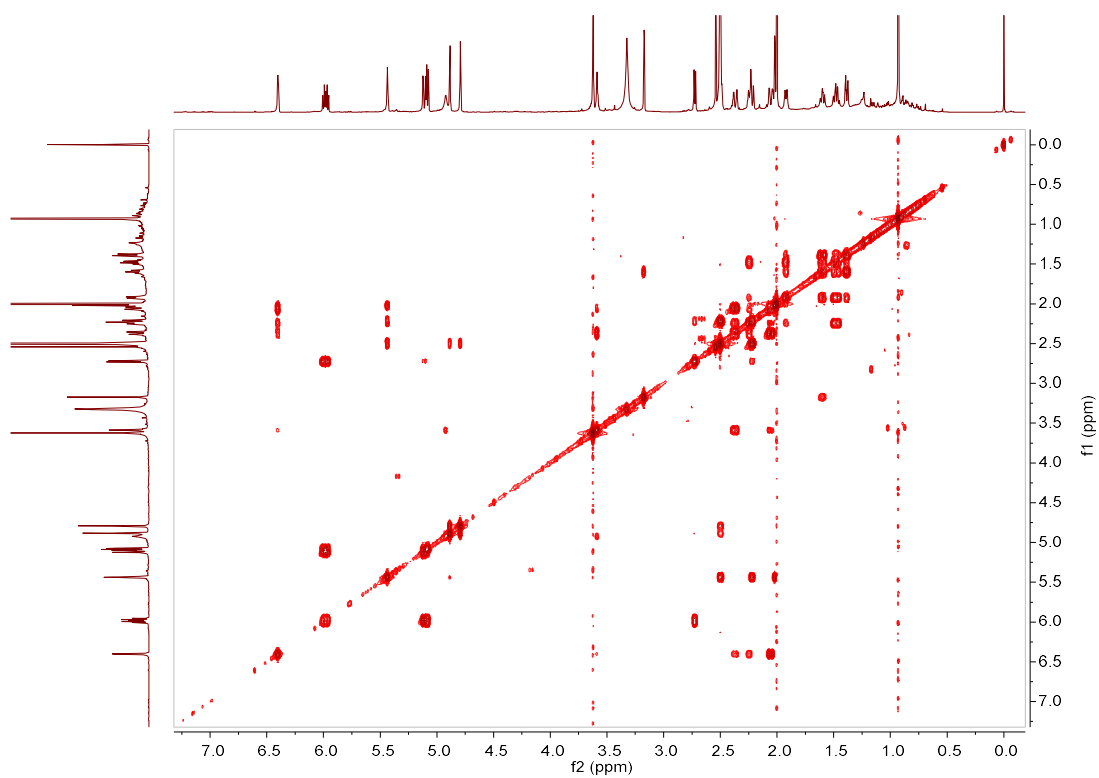


Figure S8: ^1H - ^1H COSY spectrum of compound **1**

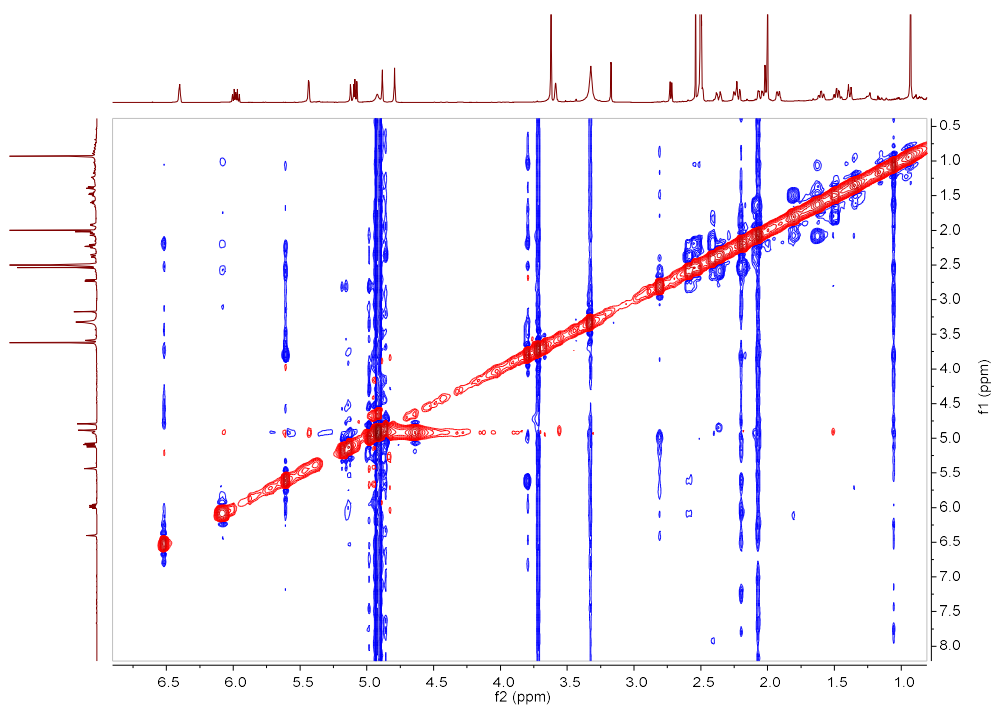


Figure S9: NOESY spectrum of compound **1**

Computational Details

The theoretical calculations of compound **1** was performed using Gaussian 16.¹ Conformational analysis was initially carried out using Conflex 8 to generate conformations by Boltzman Jump, then minimize them by Smart Minimizer using the MMFF molecular mechanics force field. All geometries with relative energy from 0-5.0 kcal/mol were used in optimizations at the B3LYP/6-31G (d, p) in the gas and further at WB97XD/DGDZVP in the methanol. Room-temperature equilibrium populations were calculated according to the Boltzmann distribution law. The theoretical calculation of ECD was performed using TD-DFT at the CAM-B3LYP/DGDZVP level in the methanol. The ECD spectra were obtained by weighing the Boltzmann distribution rate of each geometric conformation. SpecDis 1.71 was used to sum up single CD spectra after a Boltzmann statistical weighting, and for the Gauss curve generation ($\sigma = 0.3$ eV) and for the comparison with experimental data.²

References

- [1] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, G.A. Petersson and H. Nakatsuji *et.al.* (2016). Gaussian 16, Revision B.01, Gaussian, Inc., Wallingford CT, 2016.
- [2] T. Bruhn, A. Schaumlöffel Y. Hemberger and G. Pescitelli (2017). SpecDis version 1.71, Berlin, Germany, 2017.

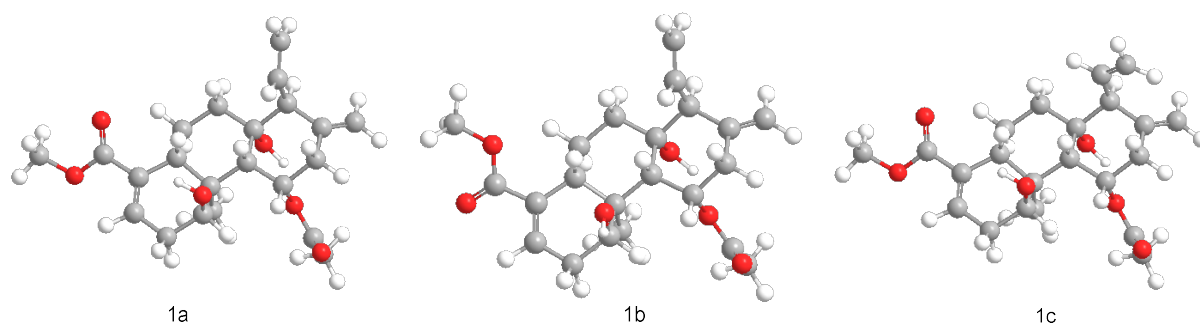


Figure S10 : Most stable conformers of 1S,5R,8R,9S,10S,11S,14S-**1** calculated with DFT at the CAM-B3LYP/DGDZVP level

Table 1 : Optimized Z-Matrixes of 1S,5R,8R,9S,10S,11S,14S-1 with simplified structures in the methanol at WB97XD/DGDZVP level.

	1a			1b			1c		
C	2.202413	2.203632	-0.14974	1.921583	2.325783	-0.11371	2.188559	2.222594	-0.31193
C	3.427682	1.35489	0.12475	3.219894	1.606571	0.19276	3.414043	1.371916	-0.06143
C	1.875369	3.059243	1.051267	1.474161	3.134221	1.081328	1.899486	3.156272	0.848362
C	4.583763	1.538339	-0.51647	4.368714	1.914039	-0.41305	4.547159	1.517046	-0.7511
C	3.216237	0.245568	1.120021	3.096365	0.474611	1.177316	3.230288	0.301963	0.983154
C	1.030426	1.284917	-0.62893	0.864943	1.29455	-0.63093	1.002221	1.290641	-0.73866
C	0.784981	0.139243	0.397554	0.711426	0.122645	0.382512	0.771703	0.200594	0.34994
C	2.060934	-0.65967	0.687135	2.053204	-0.54173	0.708477	2.047799	-0.60214	0.637201
O	2.454073	-1.3642	-0.51885	2.552944	-1.19596	-0.48682	2.393847	-1.37621	-0.54141
C	3.131848	-2.51913	-0.39761	3.341549	-2.27565	-0.34682	3.044221	-2.54131	-0.37962
C	3.476176	-3.0819	-1.74659	3.782577	-2.79445	-1.68537	3.339247	-3.17823	-1.70728
O	3.410671	-3.02209	0.672588	3.638566	-2.75238	0.730623	3.336235	-3.00051	0.706816
C	-0.4994	-0.7053	0.1339	-0.47024	-0.85048	0.077799	-0.52282	-0.64969	0.164839
C	-0.75449	-1.67839	1.311473	-0.64563	-1.85538	1.234147	-0.76908	-1.53354	1.412751
C	-0.23585	2.113762	-0.84059	-0.47509	1.988871	-0.87062	-0.27199	2.094639	-1.01023
O	1.382785	0.79995	-1.92861	1.301228	0.859593	-1.9229	1.343324	0.735986	-2.0145
C	-2.03701	-2.48187	1.090442	-1.83652	-2.78339	0.982686	-2.05593	-2.34668	1.262544
O	-0.77047	-1.01587	2.575614	-0.80778	-1.11652	2.44419	-0.77159	-0.78103	2.625312
C	-3.1769	-1.6423	0.600866	-3.0424	-2.06833	0.460687	-3.19894	-1.53879	0.729128
C	-1.68047	0.303982	0.076527	-1.75046	0.030832	0.00129	-1.70087	0.356038	0.044604
C	-1.48475	1.27389	-1.09599	-1.62305	1.025187	-1.16102	-1.51324	1.227364	-1.20398
C	-3.02627	-0.39485	0.132358	-3.01356	-0.80768	0.009928	-3.04874	-0.32935	0.169777
C	-4.25047	0.409357	-0.14059	-4.33548	-0.20671	-0.33178	-4.27203	0.461341	-0.1437
O	-5.27177	-0.32315	-0.6051	-4.41477	1.079419	0.040962	-5.3049	-0.29563	-0.53764
C	-6.51304	0.373924	-0.78993	-5.65503	1.746016	-0.23667	-6.54416	0.395656	-0.75555
O	-4.3363	1.608869	0.064728	-5.2665	-0.80374	-0.84512	-4.34692	1.673452	-0.02655
C	1.969401	4.389419	1.063087	1.438033	4.467096	1.104568	2.757063	3.499433	1.810964
C	-0.42918	-1.5571	-1.15315	-0.27979	-1.6749	-1.21513	-0.47392	-1.59229	-1.05916
H	2.415749	2.869915	-0.99112	2.088657	3.017185	-0.94519	2.369447	2.854905	-1.18954

H	1.562373	2.554031	1.963918	1.182728	2.592528	1.980122	0.924147	3.634551	0.855504
H	4.70443	2.331256	-1.24999	4.427412	2.720515	-1.13935	4.650498	2.284394	-1.51387
H	5.446208	0.906713	-0.31925	5.286252	1.374195	-0.19315	5.407716	0.878978	-0.56663
H	2.962504	0.652835	2.104897	2.77479	0.847278	2.155999	3.01685	0.75262	1.957386
H	4.120429	-0.35413	1.243763	4.053836	-0.02947	1.324616	4.13154	-0.30502	1.09325
H	0.587109	0.640544	1.352189	0.434324	0.596258	1.330596	0.613527	0.758743	1.281875
H	1.884581	-1.39963	1.466718	1.928909	-1.29979	1.48077	1.886805	-1.29825	1.459174
H	2.568801	-3.19416	-2.34232	2.909907	-2.99816	-2.30816	2.411273	-3.3097	-2.26642
H	4.134234	-2.38697	-2.27147	4.380259	-2.03318	-2.19	3.987325	-2.52092	-2.28971
H	3.970765	-4.04365	-1.63198	4.370582	-3.7002	-1.55657	3.825454	-4.13947	-1.55779
H	0.073452	-2.38704	1.384549	0.252057	-2.48166	1.310354	0.057347	-2.23786	1.53029
H	-0.40964	2.730127	0.046244	-0.73394	2.576451	0.014956	-0.47782	2.76911	-0.17718
H	-0.05139	2.800319	-1.67304	-0.34247	2.697271	-1.69475	-0.08927	2.71774	-1.89098
H	2.072265	0.126408	-1.83111	2.049928	0.255457	-1.80866	2.031078	0.065396	-1.88981
H	-2.3147	-2.9676	2.030709	-2.09444	-3.30078	1.912797	-2.32395	-2.76499	2.237353
H	-1.8599	-3.29477	0.378024	-1.55355	-3.57624	0.280872	-1.8891	-3.20736	0.605873
H	-1.61409	-0.55406	2.674718	-0.83311	-1.74338	3.178402	-1.61022	-0.30497	2.694662
H	-4.17148	-2.07414	0.658671	-3.98774	-2.60434	0.47298	-4.1947	-1.95941	0.831877
H	-1.62527	0.926635	0.98195	-1.78274	0.629082	0.921598	-1.63302	1.047721	0.897545
H	-2.34106	1.944079	-1.17939	-2.5392	1.607357	-1.26895	-2.37318	1.883398	-1.34324
H	-1.40628	0.72822	-2.04009	-1.46387	0.499313	-2.10629	-1.42795	0.608055	-2.10035
H	-7.2141	-0.37312	-1.15346	-5.52162	2.766222	0.114227	-7.25559	-0.37069	-1.05262
H	-6.85981	0.792017	0.155722	-5.85968	1.736363	-1.30778	-6.87366	0.885238	0.161527
H	-6.39479	1.172104	-1.52335	-6.47396	1.264456	0.298606	-6.43137	1.136594	-1.54756
H	1.740562	4.962702	1.956503	1.126295	5.007091	1.993647	2.473735	4.218484	2.573597
H	2.27552	4.946181	0.180338	1.716708	5.05922	0.235843	3.762113	3.088843	1.868808
H	0.159186	-2.46335	-0.98705	0.399996	-2.51383	-1.04633	0.091196	-2.49932	-0.82962
H	-1.4274	-1.86548	-1.4735	-1.23214	-2.08579	-1.55926	-1.47984	-1.89816	-1.35743
H	0.031331	-1.01206	-1.97354	0.135028	-1.07311	-2.01988	-0.00085	-1.11809	-1.91595

Table 2 : Energy analysis for 1S,5R,8R,9S,10S,11S,14S-1

Conf.	Steric Energy (kJ/mol)	Relative Energy (kJ/mol)	Distribution (%)^a
1a	-1307.4948241	0	56.42
1b	-1307.4945027	0.0003214	40.13
1c	-1307.4921907	0.0026334	3.46