

Supporting Information

Rec. Nat. Prod. 17:3 (2023) 522-528

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

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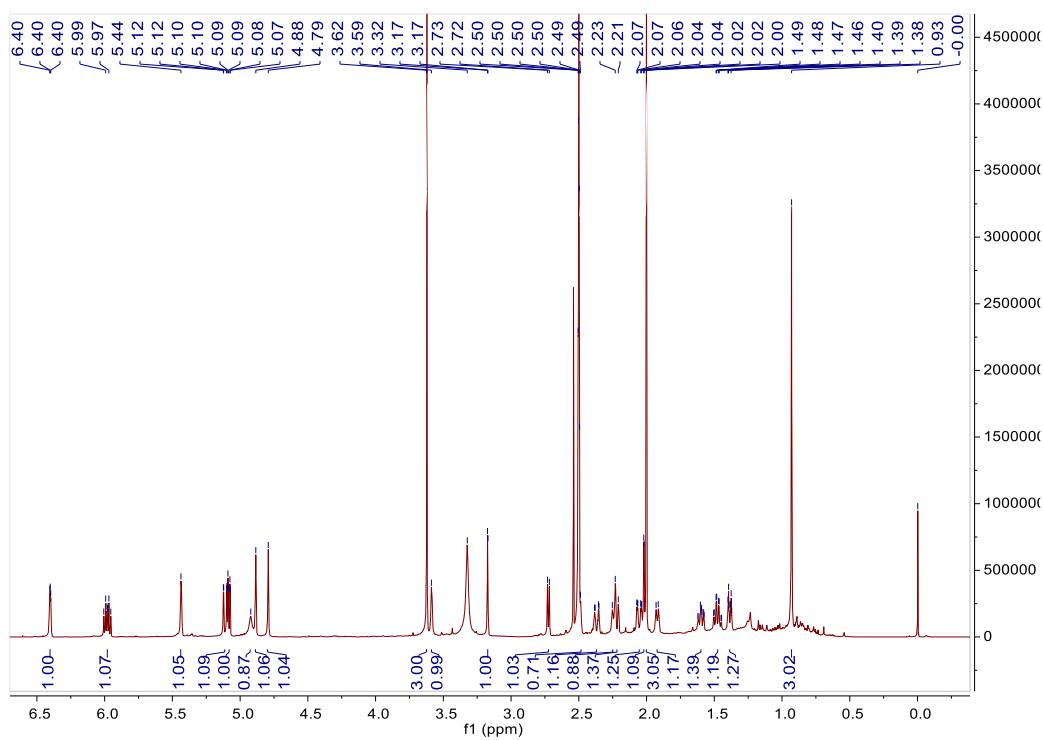


Figure S4: $^1\text{H-NMR}$ (700 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

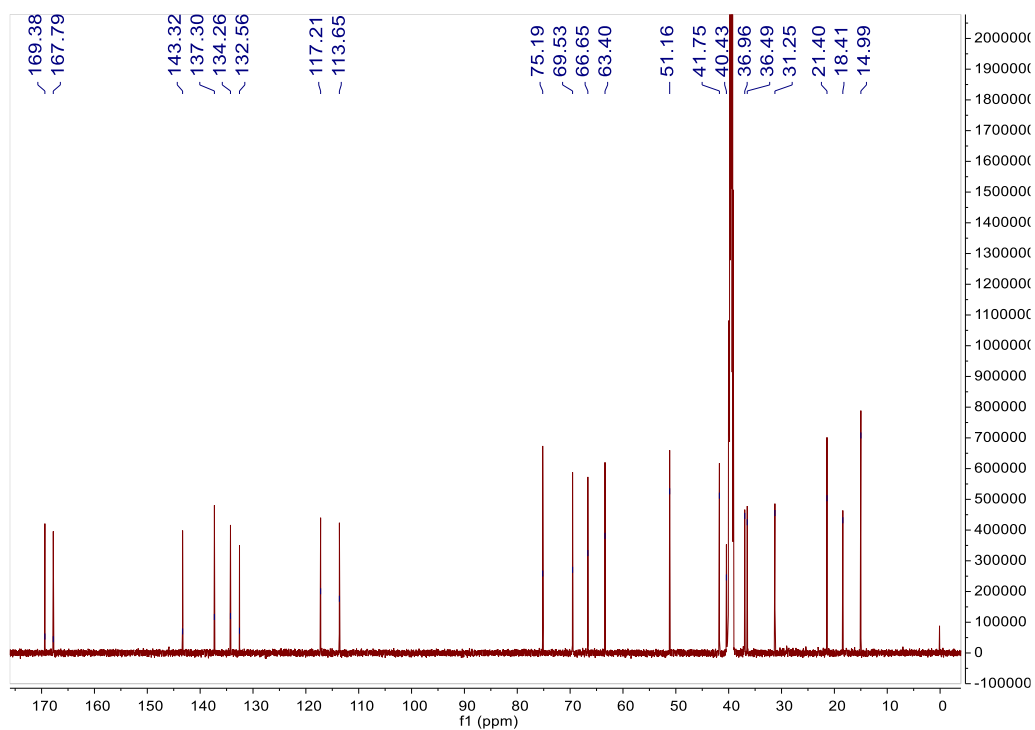


Figure S5: $^{13}\text{C-NMR}$ (700 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

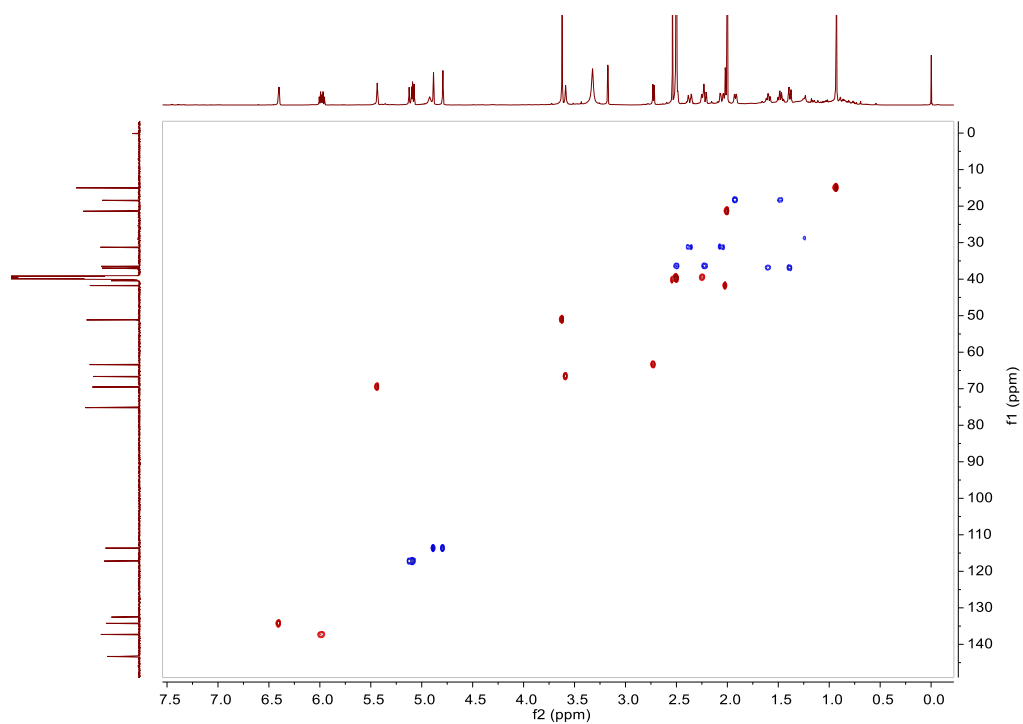


Figure S6: HSQC spectrum of compound **1**

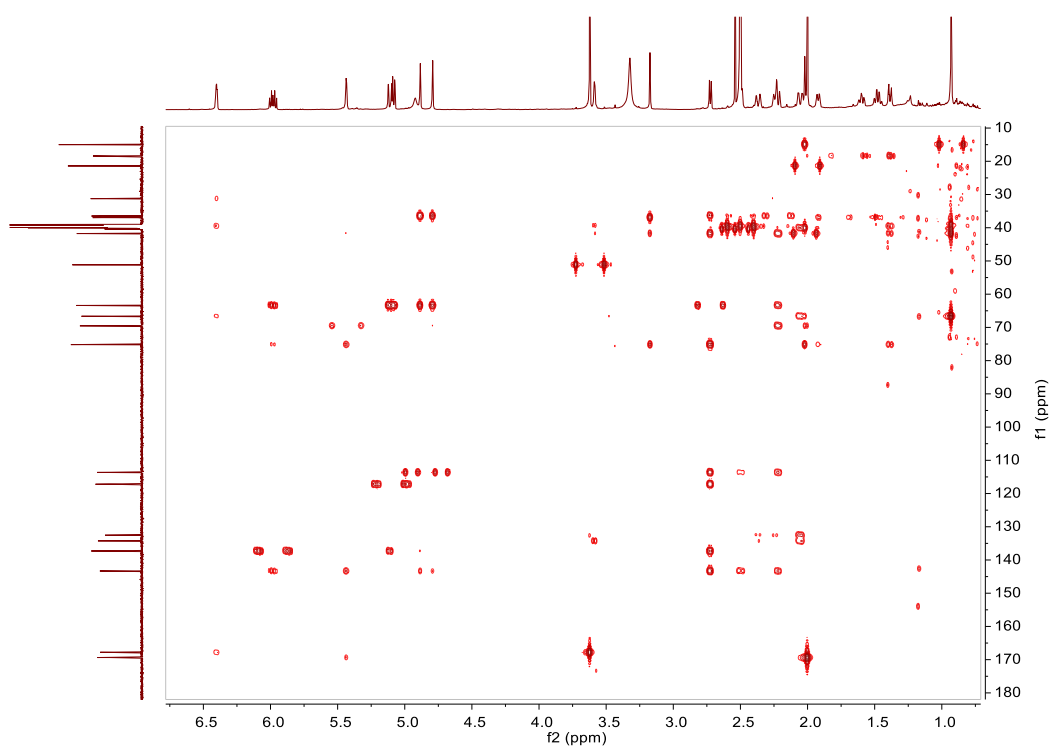


Figure S7: HMBC spectrum of compound **1**

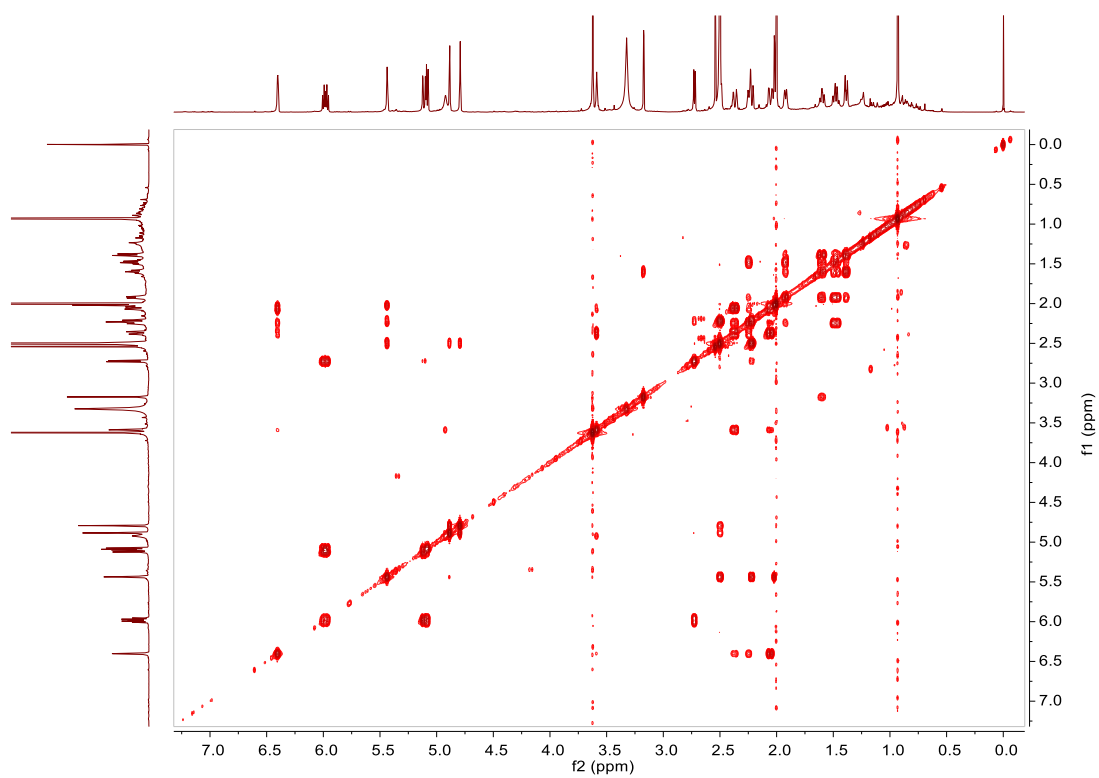


Figure S8: ^1H - ^1H COSY spectrum of compound **1**

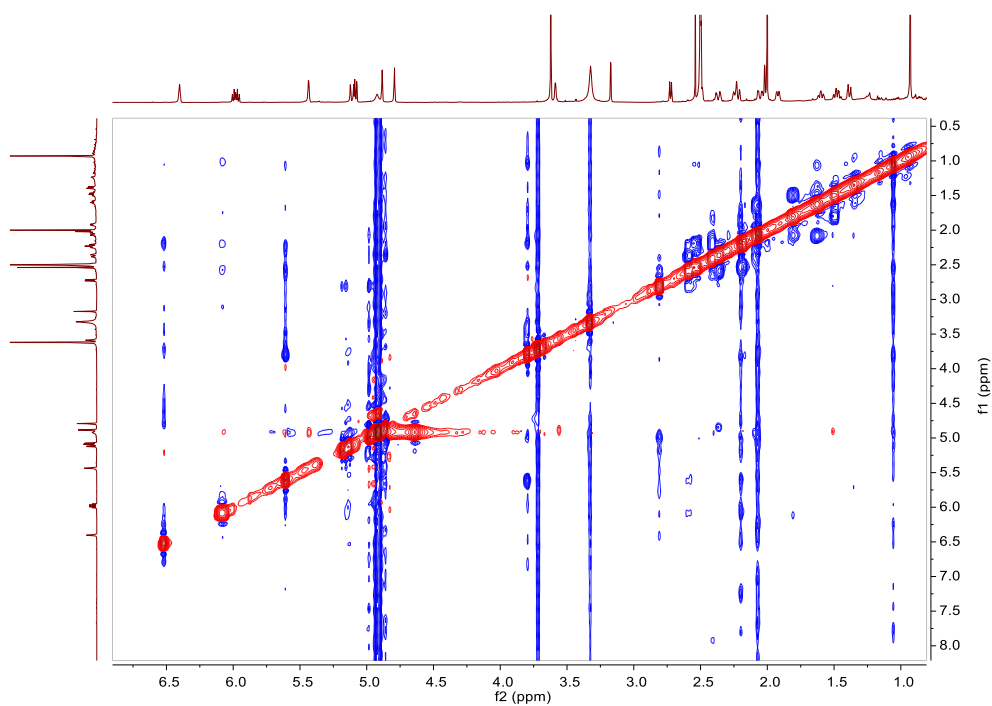


Figure S9: NOESY spectrum of compound **1**

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