Supplementary Information

Kaemtakols A–D, Highly Oxidized Pimarane Diterpenoids with Potent Anti-inflammatory Activity from *Kaempferia takensis*

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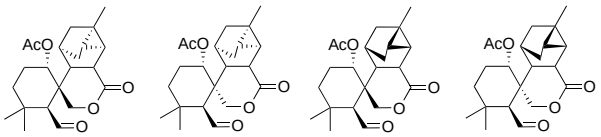
X-ray crystallographic data for compound 1. From a solution of MeOH/EtOH (1:1) and MeOH using the vapor diffusion method, colorless crystals were obtained for kaemtakol A (**1**), respectively. X-ray crystallographic analyses were performed on a Bruker APEX-II CCD diffractometer with Mo Kα radiation at 150 K. Crystallographic data have been deposited in the Cambridge Crystallographic Data Center (Deposition number: CCDC 2247367 for **1**). The data can be obtained free of charge *via* www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 IEZ, UK, fax: +44 1223 336033.

Crystal Data and structure refinement for 1.

Empirical formula	$C_{24}H_{34}O_7$
Formula weight	434.51
Temperature/K	296
Crystal system	hexagonal
Space group	$P6_1$
a/Å	24.4225(6)
b/Å	24.4225(6)
c/Å	7.0814(3)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	3657.9(2)
Z	6
ρ_{calc} g/cm^3	1.184
μ/mm^{-1}	0.086
F(000)	1404.0
Crystal size/mm^3	0.18 × 0.1 × 0.08
Radiation	MoKα (λ = 0.71073 Å)
2θ range for data collection/°	6.068 to 50.77
Index ranges	-29 ≤ h ≤ 29, -29 ≤ k ≤ 29, -8 ≤ l ≤ 8
Reflections collected	101126
Independent reflections	4471 [R_{int} = 0.0996, R_{sigma} = 0.0298]
Data/restraints/parameters	4471/152/350
Goodness-of-fit on F^2	1.241
Final R indexes [$I \geq 2\sigma$ (I)]	R_1 = 0.0695, wR_2 = 0.1416
Final R indexes [all data]	R_1 = 0.0743, wR_2 = 0.1438
Largest diff. peak/hole / e Å^{-3}	0.19/-0.18
Flack parameter	-0.1(4)
CCDC No.	2247367



4 4a 4b 4c

Isomer	Unscaled DP4+ (%)			Scaled DP4+ (%)			DP4+ (%)		
	^{1}H	^{13}C	^{1}H+^{13}C	^{1}H	^{13}C	^{1}H+^{13}C	^{1}H	^{13}C	^{1}H+^{13}C
4	99.77	11.85	100.00	100.00	10.83	100.00	100.00	1.61	100.00
4a	0.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4b	0.00	88.15	0.00	0.00	89.17	0.00	0.00	98.39	0.00
4b	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S1. DP4+ probability Excel sheets of compound **4**

Settings		Type of data (shifts)				TMS 1H	31.560	TMS 13C	196.609
Default		Shielding tensors				Default	μ	σ	ν
						13Cu,sp2	-0.920	1.748	5.364
						13Cu,sp3	2.909	1.600	6.269
Functional	Solvent?	Basis Set				1Hu,sp2	0.347	0.118	4.911
mPW1PW91	PCM	6-31+G(d,p)				1Hu,sp3	-0.018	0.112	3.651
						13Cs	-	1.557	6.227
						1Hs	-	0.104	3.893

Isomer Nº			1	2	3	4	5	6	7	8
DP4+ (%)		H data	100.00%	0.00%	0.00%	0.00%	-	-	-	-
		C data	1.61%	0.00%	98.39%	0.00%	-	-	-	-
		All data	100.00%	0.00%	0.00%	0.00%	-	-	-	-
Type	sp2?	Exp	1	2	3	4	5	6	7	8
C		23.6	170.6247149	166.0710363	170.2803407	166.1648133				
C		34	159.6326916	158.7326665	159.5833846	158.6731829				
C		33.1	162.3857055	165.3667183	162.1938087	165.3556622				
C		34.8	159.4585931	161.4534847	159.2441987	161.5564827				
C		22.9	170.9776921	170.2452721	170.9176461	170.0406355				
C		73.8	121.2870154	125.9502986	121.2986244	125.9837441				
C	x	169.4	30.00567633	29.50233659	29.94643676	29.5232917				
C		21.6	173.1791204	173.3596637	173.0619562	173.2549048				
C		43.5	150.3058609	150.7436402	150.4972178	149.6114323				
C		69.7	127.2923689	125.7732972	127.1125409	126.0997097				
C	x	163.7	37.58403402	36.54194245	37.56537018	36.5265967				
C	x	122.7	73.79334	72.18400054	73.84737816	72.19256535				
C	x	154.6	39.35147054	39.41982371	39.31841577	38.88412405				
C		28.6	158.1969576	159.9276331	159.4091554	159.1315829				
C		17.6	176.634643	176.5119774	176.3068669	176.4159361				
C		20.9	171.9107406	171.2955118	171.5179898	171.1305489				
C		56.2	136.9179855	135.4693969	136.7051155	135.8655984				
C	x	202.9	-6.033386469	-8.52153859	-6.00279668	-8.74188649				
C		23.5	168.2978489	167.9089731	168.7279557	168.5331785				
C		21.6	170.4182378	169.6712606	170.2269731	169.1635508				
C		34.8	164.7061369	164.3018649	163.5504723	164.8702899				
C		35.3	157.0964555	158.016251	156.5687877	157.6556703				
H		5.13	26.3956594	25.12242106	26.43924485	25.03879107				
H		2.17	29.18979415	29.2794193	29.12170571	29.27478807				
H		3.24	28.17063527	28.25612714	28.09744689	28.23263248				
H		1.53	30.2478995	29.61722731	30.24846699	29.61319196				
H		1.63	29.68430051	30.11062334	29.66112114	30.15307149				
H		1.97	29.50667621	29.66704999	29.53082974	29.67073423				
H		1.97	29.51724894	29.77219468	29.4965086	29.77183989				
H		4.83	26.25486691	27.17309897	26.16407482	27.10886389				
H		4.59	26.86488788	26.7618616	26.90755485	26.81057884				
H		0.64	30.97449963	31.048232	30.04327428	29.99615495				
H		1.77	29.91653175	30.03283627	30.81530795	30.89007355				
H	x	9.93	21.20024172	21.25913544	21.15872619	21.30482538				
H		1.3	30.22775554	30.29404829	30.18502727	30.18727246				
H		0.53	30.84150798	30.8786278	29.59963209	29.72533874				
H		1.54	29.74282353	29.65612347	30.90177494	31.08462943				
H		2.84	28.85042375	28.81829948	28.87810566	28.82935975				
H		1.05	30.41044685	30.5082347	30.40293008	30.49165934				
H		1.28	30.12671668	30.09052347	30.06135083	30.09520624				
H		2.05	29.39710183	29.46202128	29.39387589	29.44727568				
H		1.32	30.18183034	30.1908	30.16492085	30.20592977				

Table S2 Conformational analysis of **1**

Conformers of **1**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1460.769971	-916633.156803	2.294767	1.3
II	-1460.773628	-916635.451570	0.000000	61.0
III	-1460.772798	-916634.930745	0.520825	25.6
IV	-1460.771421	-916634.066678	1.384893	6.0
V	-1460.771241	-916633.953728	1.497842	5.0
VI	-1460.769776	-916633.034440	2.417130	1.1

Table S3 Conformational analysis of **2**

Conformers of **2**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1308.178343	-820881.910233	0.080947	18.1
II	-1308.178305	-820881.886388	0.104793	17.4
III	-1308.177672	-820881.489180	0.502000	9.0
IV	-1308.177386	-820881.309715	0.681465	6.6
V	-1308.177650	-820881.475375	0.515805	8.7
VI	-1308.178472	-820881.991180	0.000000	20.7
VII	-1308.178413	-820881.954158	0.037022	19.5

Table S4 Conformational analysis of **3**

Conformers of **3**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1308.189066	-820888.638915	0.919915	9.3
II	-1308.189359	-820888.822773	0.736058	12.6
III	-1308.188057	-820888.005768	1.553062	3.2
IV	-1308.190192	-820889.345480	0.213350	30.2
V	-1308.190532	-820889.558830	0.000000	43.1
VI	-1308.187383	-820887.582833	1.975998	1.6

Table S5 Conformational analysis of **4**

Conformers of **4**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1230.634197	-772222.958618	0.000000	77.8
II	-1230.632999	-772222.206873	0.751745	22.2

Table S6 Conformational analysis of **4a**

Conformers of **4a**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1230.633733	-772222.667458	0.000000	86.3
II	-1230.631981	-772221.568078	1.099380	13.7

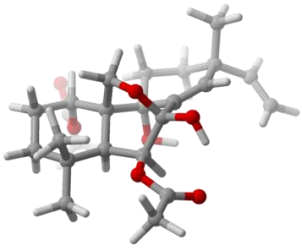
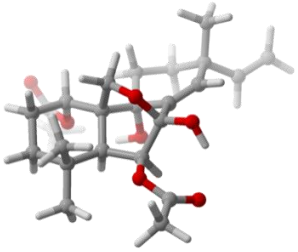
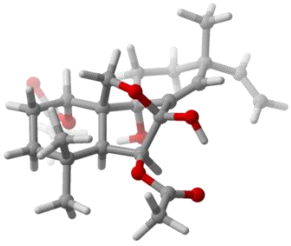
Table S7 Conformational analysis of **4b**

Conformers of **4b**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1230.633964	-772222.812410	0.000000	84.6
II	-1230.632153	-772221.676008	1.136402	12.7
II	-1230.630646	-772220.730365	2.082045	2.6

Table S8 Conformational analysis of **4c**

Conformers of **4c**	Gibbs Free Energy (Hartree)	Gibbs Free Energy (kcal/mol)	Relative Gibbs Free Energy (kcal/mol)	Population (%)
I	-1230.634108	-772222.902770	0.000000	93.9
II	-1230.631497	-772221.264368	1.638402	6.1

Table S9 Coordinates of Compound **1**

	 conformer **1-I**			 conformer **1-II**			 conformer **1-III**		
C	4.166741	-1.665773	1.713068	4.442720	-0.827211	1.539081	4.291352	-1.304017	1.699550
C	3.525316	-1.501101	0.318281	3.747164	-0.819612	0.169477	3.654599	-1.256774	0.293482
C	4.313423	-2.328892	-0.676259	4.561351	-1.532726	-0.893417	4.523669	-2.063040	-0.650294
C	3.822437	-3.224284	-1.532195	5.750301	-2.115370	-0.745443	4.111705	-3.004924	-1.496987
C	2.095437	-1.973887	0.428526	2.435975	-1.564979	0.321267	2.267314	-1.837980	0.412537
C	1.026174	-1.191027	0.294982	1.232164	-1.014621	0.186294	1.142205	-1.147129	0.248880
C	-0.381759	-1.637974	0.647902	-0.050085	-1.735071	0.567049	-0.222933	-1.698611	0.622719
O	-0.503157	-3.002294	0.832076	0.100682	-3.098829	0.730725	-0.240619	-3.067114	0.814117
C	-1.347406	-1.058020	-0.415072	-1.142813	-1.345524	-0.456824	-1.246280	-1.200795	-0.425559
H	-0.969115	-1.321036	-1.412224	-0.749217	-1.513730	-1.468170	-0.862067	-1.436085	-1.427019
O	-2.646827	-1.650259	-0.275580	-2.297421	-2.178543	-0.283396	-2.496359	-1.884162	-0.256708
C	-2.873713	-2.818127	-0.887248	-2.313579	-3.365867	-0.902568	-2.647696	-3.072329	-0.854943
C	-4.317644	-3.212904	-0.776926	-3.640463	-4.045669	-0.724255	-4.053364	-3.576664	-0.699418
O	-2.017308	-3.460645	-1.458548	-1.376512	-3.818685	-1.524155	-1.761299	-3.651208	-1.445892
C	-1.405425	0.494579	-0.265214	-1.499846	0.163382	-0.275542	-1.420591	0.343460	-0.277603
H	-1.196124	0.899925	-1.262396	-1.407726	0.605855	-1.275258	-1.265018	0.751971	-1.283832
C	-2.767276	1.150040	0.144328	-2.951753	0.545671	0.161697	-2.820725	0.905726	0.133085
C	-3.397656	0.640096	1.455377	-3.443484	-0.073407	1.483641	-3.396528	0.377400	1.460869
C	-3.781416	0.951497	-0.998841	-3.934324	0.154933	-0.958765	-3.831303	0.613222	-0.992537
C	-2.538417	2.676363	0.250567	-3.006382	2.088094	0.261165	-2.690748	2.445408	0.201824
C	-1.383719	3.083666	1.158917	-1.942174	2.703415	1.161494	-1.570205	2.947727	1.104015
C	-0.079747	2.444857	0.700556	-0.540125	2.318134	0.711391	-0.219747	2.386131	0.682460
H	0.745387	2.741716	1.362631	0.205763	2.735413	1.402988	0.562529	2.725316	1.376615
O	0.203325	2.941095	-0.621416	-0.284794	2.898613	-0.598680	0.120439	2.903821	-0.634586
C	1.193794	3.835638	-0.777429	0.150018	4.180299	-0.629731	0.709924	4.121454	-0.683259
C	1.413921	4.106919	-2.238702	0.427370	4.610395	-2.043772	1.056185	4.484996	-2.100753
O	1.824387	4.316169	0.133423	0.303549	4.853680	0.355972	0.932402	4.791160	0.291804
C	1.109106	0.280920	-0.062198	1.011045	0.446545	-0.148800	1.104792	0.323169	-0.117364
O	1.030190	0.433804	-1.486959	0.895285	0.548499	-1.568275	1.020893	0.408438	-1.539489
C	2.452418	0.836917	0.429560	2.235504	1.252976	0.309080	2.411021	0.986670	0.344945
C	3.593294	-0.016932	-0.123369	3.493379	0.632402	-0.298840	3.594419	0.201353	-0.220981
H	4.081260	-2.704828	2.065174	4.577401	-1.852484	1.915749	4.300284	-2.332238	2.091955
H	3.672668	-1.015510	2.450936	3.839932	-0.279568	2.278956	3.731207	-0.676849	2.409812
H	5.235518	-1.401405	1.680991	5.431745	-0.347253	1.479900	5.331299	-0.942008	1.665625
H	5.391825	-2.125351	-0.680258	4.079330	-1.555766	-1.878461	5.589133	-1.801326	-0.621396
H	2.755800	-3.461229	-1.572971	6.281022	-2.133392	0.209166	3.059296	-3.290011	-1.574116
H	4.476415	-3.755448	-2.226834	6.240787	-2.603762	-1.590174	4.817399	-3.518277	-2.153459
H	1.935375	-3.017071	0.718736	2.496966	-2.615964	0.619917	2.188310	-2.880454	0.736315
H	-0.693003	-3.394349	-0.035454	-0.000502	-3.505366	-0.144729	-0.386003	-3.476065	-0.054012
H	-4.632382	-3.173348	0.274709	-3.874374	-4.117981	0.346830	-4.746497	-2.907999	-1.230779
H	-4.455289	-4.220666	-1.181874	-3.605677	-5.042480	-1.175557	-4.332423	-3.569268	0.363063
H	-4.937752	-2.497715	-1.337250	-4.431621	-3.446565	-1.198261	-4.127385	-4.589577	-1.108173
H	-3.330132	-0.448278	1.552598	-3.186014	-1.134998	1.558775	-3.247406	-0.701703	1.571917
H	-4.460436	0.929228	1.482055	-4.538662	0.028251	1.546642	-4.476954	0.589110	1.498529
H	-2.931644	1.081704	2.346714	-3.030063	0.430992	2.367265	-2.950978	0.865024	2.338448
H	-4.135314	-0.083896	-1.059756	-4.083653	-0.929132	-1.013380	-3.421645	0.892528	-1.976901
H	-3.340602	1.225020	-1.971030	-3.576150	0.504058	-1.940922	-4.747465	1.204393	-0.833452
H	-4.657508	1.599812	-0.836352	-4.914239	0.624411	-0.775782	-4.113439	-0.444903	-1.025634
H	-3.472342	3.146345	0.599298	-4.007323	2.383426	0.615114	-3.652777	2.865823	0.536719
H	-2.341197	3.075428	-0.757681	-2.896388	2.511324	-0.751722	-2.519880	2.830946	-0.817678
H	-1.580242	2.803999	2.205071	-2.074373	2.381796	2.205788	-1.752357	2.668074	2.152859
H	-1.254334	4.176471	1.153419	-2.019133	3.799956	1.172025	-1.514228	4.045492	1.090566
H	1.677340	3.157561	-2.727090	-0.439698	4.397197	-2.683790	0.176841	4.369661	-2.749087
H	2.213122	4.844446	-2.365635	1.281830	4.039014	-2.437271	1.836360	3.802940	-2.471605
H	0.483610	4.467004	-2.699635	0.663690	5.679325	-2.062118	1.425181	5.515266	-2.135260
H	1.477302	-0.330088	-1.868789	0.580156	1.448049	-1.733007	0.819518	1.335721	-1.726908
H	2.482170	0.842926	1.529996	2.300312	1.272862	1.407982	2.459402	1.029434	1.444045
H	2.583805	1.875256	0.101192	2.148965	2.297998	-0.024222	2.457747	2.024837	-0.016540
H	4.563866	0.407733	0.175686	4.378494	1.244148	-0.067357	4.541438	0.711882	0.014229
H	3.563938	0.035665	-1.223313	3.367979	0.641966	-1.391720	3.490445	0.183908	-1.315387
C	-0.170266	0.918487	0.590856	-0.348826	0.808169	0.562111	-0.210792	0.861303	0.565269
C	-0.268128	0.276415	1.991963	-0.277548	0.138529	1.950967	-0.241252	0.217201	1.967556
H	0.715344	0.306415	2.495619	0.700102	0.351830	2.421573	0.747650	0.321611	2.451197
H	-0.978213	0.802006	2.638270	-1.051571	0.508895	2.631810	-0.975868	0.691629	2.627232
O	-0.726367	-1.062031	1.896611	-0.473492	-1.257939	1.836670	-0.601929	-1.148005	1.876648

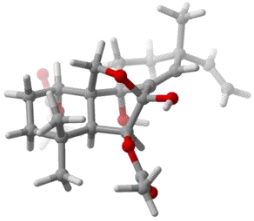
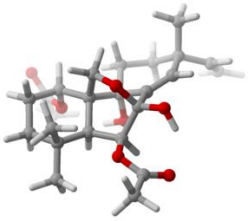
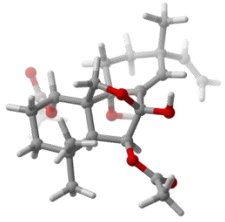
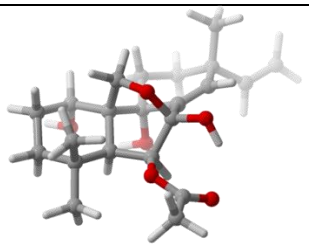
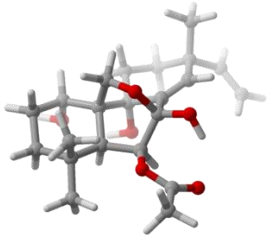
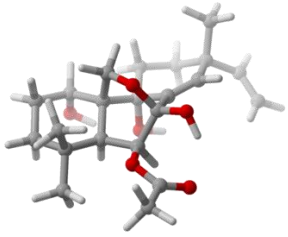
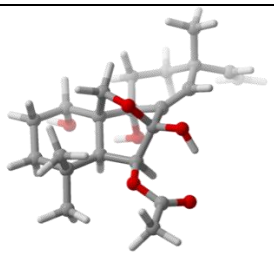
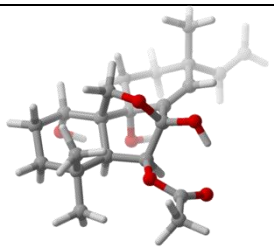
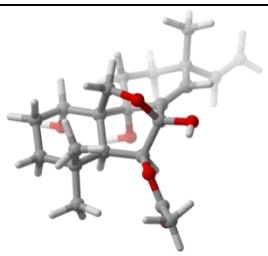
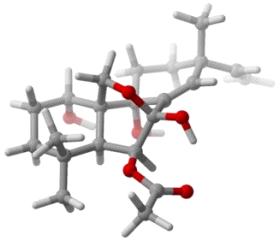
	 conformer **1-IV**			 conformer **1-V**			 conformer **1-VI**		
C	-4.332524	-1.533869	-1.628234	4.090731	-1.651015	1.763502	-4.143766	-1.809487	-1.690775
C	-3.633455	-1.402137	-0.257834	3.505098	-1.569940	0.333704	-3.491030	-1.580613	-0.310397
C	-4.418813	-2.199010	0.763808	4.291912	-2.539322	-0.527468	-4.245140	-2.393312	0.722349
C	-3.934824	-3.119664	1.596688	5.087837	-2.249008	-1.555139	-3.718751	-3.243163	1.603494
C	-2.231221	-1.938135	-0.421684	2.071286	-2.049630	0.415686	-2.051183	-2.023359	-0.422114
C	-1.125731	-1.201851	-0.325241	1.005755	-1.273611	0.236562	-0.999419	-1.212066	-0.328490
C	0.246053	-1.687500	-0.716868	-0.403835	-1.722000	0.581283	0.418429	-1.618372	-0.671528
O	0.276132	-3.057337	-0.846283	-0.532244	-3.088086	0.746405	0.608196	-2.982062	-0.809224
C	1.270282	-1.164009	0.308990	-1.373422	-1.125027	-0.465963	1.366278	-1.041304	0.396505
H	0.926643	-1.417877	1.317766	-0.999272	-1.371495	-1.468560	0.992957	-1.325395	1.387502
O	2.480069	-1.899262	0.076386	-2.675601	-1.708640	-0.318859	2.643635	-1.641909	0.223612
C	3.038573	-2.535220	1.136413	-2.917180	-2.870710	-0.938700	2.936836	-2.699752	1.015825
C	4.259531	-3.295453	0.697379	-4.359604	-3.263720	-0.798515	4.217028	-3.340290	0.558863
O	2.612838	-2.478230	2.259434	-2.076168	-3.508446	-1.534975	2.265238	-3.056974	1.948229
C	1.402099	0.383081	0.173482	-1.425784	0.425317	-0.290011	1.392180	0.514105	0.256776
H	1.246170	0.787208	1.180982	-1.228084	0.838164	-1.286971	1.161420	0.908803	1.253504
C	2.776690	0.980010	-0.275045	-2.780740	1.090798	0.118604	2.747887	1.194211	-0.127515
C	3.344860	0.457956	-1.608260	-3.411636	0.586497	1.430599	3.405171	0.707306	-1.433647
C	3.822642	0.716881	0.825412	-3.799448	0.900364	-1.021507	3.748811	0.989119	1.025365
C	2.612686	2.516088	-0.352412	-2.528761	2.613578	0.217476	2.498532	2.717759	-0.218850
C	1.445156	2.987707	-1.212654	-1.380490	3.008449	1.138058	1.348821	3.117450	-1.137635
C	0.129052	2.400380	-0.719219	-0.075361	2.347948	0.717240	0.047372	2.454960	-0.704447
H	-0.703441	2.745488	-1.347947	0.725284	2.611197	1.423276	-0.773507	2.747614	-1.373919
O	-0.085065	2.887048	0.618723	0.316637	2.858442	-0.588195	-0.258539	2.934117	0.618063
C	-1.042694	3.806168	0.827970	0.999368	4.027040	-0.612606	-1.288575	3.781783	0.778927
C	-1.199368	4.056865	2.300806	1.384425	4.384800	-2.021599	-1.520768	4.034738	2.241236
O	-1.693753	4.320087	-0.049861	1.265018	4.662137	0.374718	-1.941339	4.237510	-0.129435
C	-1.128677	0.271888	0.045228	1.088238	0.199728	-0.107516	-1.117019	0.261370	0.018688
O	-1.004782	0.408346	1.467567	1.022853	0.311646	-1.529202	-1.070897	0.420271	1.442948
C	-2.462108	0.887127	-0.401501	2.439694	0.751321	0.371001	-2.467824	0.779273	-0.495390
C	-3.619445	0.081836	0.188795	3.559671	-0.126187	-0.190175	-3.592067	-0.082906	0.079193
H	-4.306026	-2.574456	-1.985415	4.017067	-2.674233	2.163382	-4.035946	-2.857489	-2.009665
H	-3.838468	-0.902678	-2.382552	3.545955	-0.986926	2.451965	-3.677303	-1.169479	-2.455417
H	-5.386803	-1.223418	-1.555723	5.152819	-1.361841	1.756776	-5.218891	-1.573389	-1.654047
H	-5.486049	-1.947510	0.810418	4.193249	-3.589131	-0.222822	-5.328480	-2.218477	0.732803
H	-2.878899	-3.403692	1.595216	5.239026	-1.227699	-1.911393	-2.645453	-3.449277	1.641105
H	-4.584514	-3.624321	2.314765	5.623038	-3.039496	-2.085231	-4.350032	-3.765305	2.325459
H	-2.131708	-2.988224	-0.711947	1.905625	-3.088598	0.718962	-1.876516	-3.077494	-0.661070
H	1.192069	-3.282055	-1.056391	-0.697611	-3.468110	-0.131337	0.424969	-3.176263	-1.737151
H	4.991893	-2.598818	0.264085	-4.512755	-4.257959	-1.230443	4.040484	-3.813554	-0.418058
H	3.991721	-4.017966	-0.086546	-4.994892	-2.529640	-1.315577	4.533209	-4.095425	1.286069
H	4.696632	-3.815380	1.555991	-4.641381	-3.258383	0.263304	4.999782	-2.581179	0.423342
H	3.268537	-0.631907	-1.686009	-3.353141	-0.503220	1.520592	3.384179	-0.383926	-1.520279
H	4.407529	0.740417	-1.681912	-4.471265	0.886067	1.462956	4.455614	1.039318	-1.453980
H	2.844993	0.890664	-2.484998	-2.936689	1.018399	2.321859	2.928909	1.126046	-2.330763
H	3.412695	0.911368	1.828488	-4.164201	-0.131251	-1.077331	4.112031	-0.043975	1.074382
H	4.689888	1.380979	0.680525	-3.358592	1.164122	-1.996652	3.292772	1.240867	1.996146
H	4.200096	-0.312432	0.805375	-4.667426	1.559538	-0.859485	4.620568	1.648385	0.884557
H	3.552904	2.951448	-0.728411	-3.457351	3.103491	0.552303	3.428919	3.206874	-0.550415
H	2.469456	2.906598	0.668260	-2.317779	3.002727	-0.793085	2.282277	3.101895	0.791218
H	1.593598	2.716496	-2.269028	-1.594487	2.726107	2.180126	1.563963	2.852652	-2.184185
H	1.365367	4.084958	-1.186493	-1.236746	4.098274	1.145010	1.202729	4.208098	-1.122152
H	-0.239232	4.367514	2.735579	0.503581	4.350497	-2.677245	-1.763510	3.073959	2.718087
H	-1.485667	3.108883	2.779053	2.110525	3.648860	-2.399118	-2.339169	4.750287	2.371531
H	-1.962326	4.823586	2.470477	1.834419	5.382831	-2.036534	-0.601694	4.412018	2.710540
H	-1.423513	-0.366881	1.858404	0.895557	1.254455	-1.703691	-1.422856	-0.391357	1.825806
H	-2.527770	0.898629	-1.500365	2.480197	0.786794	1.470641	-2.492395	0.755423	-1.595886
H	-2.538146	1.928673	-0.066371	2.573878	1.783472	0.014808	-2.623424	1.822904	-0.195872
H	-4.580149	0.549983	-0.075237	4.542603	0.314146	0.037423	-4.570324	0.309259	-0.238405
H	-3.547215	0.128996	1.286626	3.443604	-0.135727	-1.283569	-3.565844	0.007812	1.175930
C	0.157776	0.869768	-0.637049	-0.187218	0.829627	0.572928	0.160011	0.928051	-0.610966
C	0.185948	0.250551	-2.050389	-0.283985	0.164424	1.962453	0.282416	0.310162	-2.018883
H	-0.808736	0.335292	-2.524972	0.705079	0.180093	2.456835	-0.692831	0.336778	-2.537438
H	0.900715	0.753852	-2.709139	-0.985134	0.683883	2.624561	0.999538	0.847377	-2.647193
O	0.577415	-1.110675	-1.983971	-0.752243	-1.165517	1.841970	0.747268	-1.029495	-1.928140

Table S10 Coordinates of Compound **2**

	 conformer **2-I**			 conformer **2-II**			 conformer **2-III**		
C	-4.496983	-0.107572	1.431198	-4.481440	-0.187234	1.563594	-4.499818	-0.107093	1.570559
C	-3.795006	0.134034	0.086405	-3.833784	0.107068	0.192993	-3.835316	0.126632	0.196426
C	-4.639358	0.963895	-0.861800	-4.819250	0.904277	-0.637200	-4.799664	0.898150	-0.681651
C	-5.856438	1.458322	-0.639253	-4.566380	2.029911	-1.302603	-4.532844	2.009496	-1.366396
C	-2.524257	0.910704	0.370451	-2.566185	0.882576	0.456215	-2.563204	0.901719	0.445888
C	-1.293529	0.449223	0.163480	-1.339219	0.425923	0.219351	-1.334916	0.432457	0.235360
C	-0.051590	1.160760	0.671828	-0.089916	1.123590	0.728579	-0.079370	1.123907	0.740813
O	-0.271257	2.471305	1.053043	-0.304733	2.423328	1.147924	-0.296934	2.422363	1.160257
C	1.062683	0.996983	-0.388591	1.008042	0.989289	-0.352730	1.016668	0.987170	-0.343067
H	0.665570	1.309413	-1.363647	0.595229	1.326324	-1.313007	0.609526	1.343267	-1.299585
O	2.173782	1.846243	-0.066882	2.124273	1.831091	-0.027384	2.139862	1.817128	-0.012432
C	2.133197	3.118157	-0.482563	2.076884	3.112923	-0.409211	2.107509	3.099664	-0.389865
C	3.422788	3.823708	-0.174855	3.376044	3.807837	-0.118204	3.423249	3.772662	-0.128030
O	1.179072	3.621506	-1.035519	1.110540	3.632255	-0.925506	1.137646	3.635036	-0.885774
C	1.492936	-0.502010	-0.452062	1.438443	-0.507009	-0.462212	1.433820	-0.511960	-0.468582
H	1.418122	-0.781994	-1.509455	1.349570	-0.758617	-1.525605	1.342316	-0.755557	-1.533269
C	2.962131	-0.877904	-0.071966	2.912838	-0.892076	-0.112207	2.908238	-0.911617	-0.129408
C	3.421685	-0.462534	1.338611	3.391786	-0.514775	1.302604	3.401439	-0.543541	1.283776
C	3.924264	-0.260240	-1.104677	3.861106	-0.247037	-1.141035	3.851072	-0.266544	-1.163567
C	3.094788	-2.410600	-0.229479	3.043475	-2.420086	-0.312280	3.024223	-2.439794	-0.337297
C	2.059436	-3.214611	0.548103	2.018611	-3.244984	0.457194	2.002402	-3.265082	0.434792
C	0.639313	-2.833834	0.141737	0.593322	-2.854426	0.079516	0.579291	-2.870113	0.054397
H	-0.084443	-3.371006	0.783481	-0.121807	-3.409304	0.715861	-0.126092	-3.414180	0.713648
O	0.401232	-3.182406	-1.227491	0.337470	-3.165654	-1.295365	0.363136	-3.285532	-1.285198
C	-0.997854	-0.928038	-0.395476	-1.051473	-0.935100	-0.382688	-1.056861	-0.937715	-0.341794
O	-0.871732	-0.811146	-1.810190	-0.944542	-0.777091	-1.794269	-0.892822	-0.860481	-1.772959
C	-2.180132	-1.857490	-0.081727	-2.227733	-1.875731	-0.078933	-2.229671	-1.875493	-0.028893
C	-3.465393	-1.212438	-0.600064	-3.523347	-1.214774	-0.549863	-3.541334	-1.234735	-0.484660
H	-4.687132	0.838046	1.961293	-4.666973	0.744825	2.118830	-4.671440	0.847386	2.090289
H	-3.869547	-0.732522	2.084325	-3.829144	-0.823520	2.181118	-3.862602	-0.732984	2.213700
H	-5.459271	-0.622296	1.285328	-5.445239	-0.704925	1.433083	-5.471630	-0.611398	1.450162
H	-4.154953	1.163156	-1.825524	-5.824825	0.467722	-0.691384	-5.800453	0.454010	-0.756094
H	-6.391178	1.301607	0.300354	-3.576868	2.494183	-1.293245	-3.550706	2.488613	-1.330183
H	-6.367071	2.048086	-1.403564	-5.343189	2.521063	-1.892436	-5.294274	2.481404	-1.990765
H	-2.640578	1.895774	0.832766	-2.667948	1.853216	0.951731	-2.663422	1.886294	0.913332
H	-0.193978	3.018144	0.255153	-0.227191	2.992601	0.365742	-0.163204	3.000813	0.391764
H	3.641841	3.734971	0.898178	3.639988	3.667666	0.938950	3.736962	3.584414	0.907535
H	3.342433	4.877114	-0.461963	3.282797	4.873411	-0.351602	3.330176	4.847555	-0.313851
H	4.247915	3.346803	-0.723704	4.178098	3.361221	-0.724063	4.190133	3.345705	-0.791254
H	4.521478	-0.503832	1.390426	4.492267	-0.555260	1.337709	4.502770	-0.563634	1.300512
H	3.045109	-1.134811	2.121495	3.027435	-1.209267	2.071773	3.065487	-1.259899	2.045728
H	3.097418	0.552430	1.591232	3.069461	0.491951	1.588334	3.067127	0.452366	1.593576
H	4.018999	0.823985	-0.978838	3.959459	0.833135	-0.986553	3.960205	0.812763	-1.007097
H	3.583067	-0.460300	-2.133292	3.505136	-0.418200	-2.169862	3.487121	-0.433754	-2.190254
H	4.926778	-0.704118	-0.993494	4.864425	-0.694949	-1.056332	4.851360	-0.722343	-1.088491
H	4.109708	-2.711585	0.077171	4.062426	-2.728583	-0.027221	4.045776	-2.752705	-0.065815
H	2.998003	-2.663172	-1.298436	2.932529	-2.644124	-1.386195	2.895810	-2.662281	-1.408995
H	2.177854	-3.072064	1.633352	2.150817	-3.130863	1.544231	2.142944	-3.164006	1.522571
H	2.204948	-4.294909	0.374409	2.162318	-4.320233	0.253284	2.128828	-4.333079	0.202255
H	-0.545787	-1.677479	-2.099777	-0.624741	-1.634870	-2.114038	-1.670757	-0.421460	-2.135853
H	-2.249747	-2.052114	1.000148	-2.276605	-2.108311	0.996621	-2.267948	-2.084144	1.050573
H	-2.024539	-2.824835	-0.581491	-2.080167	-2.825025	-0.614531	-2.080344	-2.833830	-0.545737
H	-4.320300	-1.895206	-0.479000	-4.372783	-1.906572	-0.435040	-4.381257	-1.922903	-0.303485
H	-3.333792	-1.044347	-1.679084	-3.415343	-0.998471	-1.622276	-3.511278	-1.091224	-1.578148
C	0.377033	-1.330094	0.262529	0.332557	-1.354706	0.244960	0.332645	-1.363388	0.242506
C	0.272666	-0.899314	1.738817	0.249143	-0.964605	1.733836	0.269801	-0.976469	1.732896
H	-0.690768	-1.237644	2.163845	-0.708574	-1.314026	2.162866	-0.672538	-1.339394	2.183235
H	1.068087	-1.330678	2.356902	1.052745	-1.413379	2.328531	1.091881	-1.418124	2.304787
O	0.390928	0.506709	1.853387	0.370178	0.437698	1.885266	0.372403	0.430230	1.892406
H	0.555257	-4.126948	-1.333254	0.490075	-4.106943	-1.428656	-0.110955	-2.587507	-1.760406

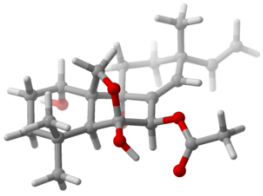
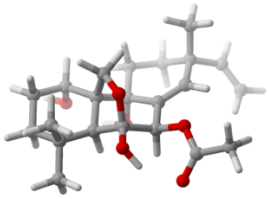
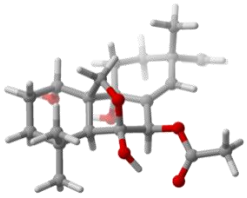
	 conformer **2-IV**			 conformer **2-V**			 conformer **2-VI**		
C	-4.395080	0.100971	1.667863	-4.460860	-0.078920	1.454982	-4.601049	-0.022283	1.353706
C	-3.785351	0.357604	0.269247	-3.796626	0.150417	0.088316	-3.852444	0.271113	0.044785
C	-4.730768	1.288419	-0.465756	-4.672951	0.963659	-0.845512	-4.649899	1.165011	-0.885625
C	-5.441852	1.023545	-1.560374	-5.887558	1.450852	-0.597643	-5.865707	1.668728	-0.677518
C	-2.470170	1.076529	0.486580	-2.521563	0.934496	0.336286	-2.576273	1.006068	0.406508
C	-1.274433	0.552169	0.231462	-1.290034	0.463909	0.144803	-1.350777	0.523803	0.218870
C	0.019998	1.191525	0.702902	-0.044123	1.168350	0.658143	-0.107595	1.162959	0.784342
O	-0.115302	2.511018	1.092783	-0.266000	2.479755	1.032032	-0.333326	2.466670	1.159963
C	1.093312	0.969141	-0.388150	1.081613	0.993919	-0.388874	1.032104	1.029204	-0.242548
H	0.687257	1.306747	-1.351078	0.703660	1.320574	-1.367539	0.680704	1.397478	-1.212530
O	2.260466	1.752083	-0.096499	2.197509	1.830321	-0.051188	2.076270	1.905739	0.208233
C	2.282755	3.025396	-0.508498	2.180875	3.100871	-0.469111	2.598209	2.772941	-0.694175
C	3.624701	3.648772	-0.251143	3.487999	3.780100	-0.181037	3.603981	3.669862	-0.025492
O	1.341546	3.588523	-1.024872	1.230338	3.621517	-1.015010	2.298339	2.799452	-1.857832
C	1.436758	-0.551393	-0.466163	1.496240	-0.509671	-0.454747	1.442756	-0.468603	-0.373948
H	1.320504	-0.822922	-1.521893	1.434598	-0.785994	-1.513642	1.400825	-0.689104	-1.447243
C	2.891770	-1.010813	-0.124973	2.958109	-0.903566	-0.059886	2.888874	-0.897236	0.033338
C	3.410889	-0.627941	1.274129	3.410822	-0.493329	1.355114	3.312954	-0.572564	1.477412
C	3.860689	-0.445161	-1.181005	3.933724	-0.293672	-1.084929	3.905391	-0.239728	-0.920061
C	2.933365	-2.548139	-0.289309	3.073630	-2.437773	-0.217076	2.992743	-2.420144	-0.213516
C	1.874333	-3.295258	0.512839	2.025973	-3.235514	0.549404	1.913293	-3.244930	0.478292
C	0.468287	-2.833690	0.142958	0.616325	-2.847485	0.114932	0.514402	-2.807418	0.054004
H	-0.268618	-3.332279	0.800714	-0.110855	-3.369079	0.768505	-0.239313	-3.365180	0.641698
O	0.177204	-3.161449	-1.221073	0.437844	-3.303008	-1.217356	0.309460	-3.067007	-1.339458
C	-1.072234	-0.835338	-0.343341	-0.998965	-0.921719	-0.388789	-1.063800	-0.829732	-0.405670
O	-0.975724	-0.714631	-1.759844	-0.785504	-0.883524	-1.815761	-0.898047	-0.634111	-1.806578
C	-2.296548	-1.700235	-0.006406	-2.183582	-1.849080	-0.092397	-2.274953	-1.746602	-0.176221
C	-3.557557	-0.970171	-0.471133	-3.482530	-1.207926	-0.583727	-3.529286	-1.046277	-0.698803
H	-4.522636	1.043376	2.222949	-4.640158	0.872971	1.976780	-4.787848	0.899295	1.925788
H	-3.742785	-0.551123	2.268819	-3.812554	-0.691657	2.098592	-4.007727	-0.694003	1.992167
H	-5.382761	-0.375530	1.571178	-5.424061	-0.599566	1.341302	-5.569140	-0.506655	1.152601
H	-4.838635	2.275899	0.001270	-4.219614	1.161319	-1.825527	-4.129426	1.405618	-1.820565
H	-5.389331	0.062717	-2.076947	-6.396964	1.300020	0.356601	-6.434482	1.472531	0.234311
H	-6.110167	1.775320	-1.985402	-6.421353	2.028926	-1.354701	-6.340571	2.306677	-1.426031
H	-2.509918	2.063983	0.958137	-2.633393	1.930978	0.774624	-2.690570	1.974401	0.902303
H	-0.019919	3.055530	0.295004	-0.120210	3.032586	0.247178	0.524522	2.810427	1.442000
H	3.897968	3.513397	0.804237	3.757557	3.632780	0.873487	3.112426	4.260953	0.760604
H	3.589698	4.713309	-0.504455	3.407087	4.847026	-0.412765	4.051740	4.337131	-0.769116
H	4.389130	3.144847	-0.860739	4.280001	3.324830	-0.793902	4.381670	3.061930	0.458760
H	3.019856	-1.283295	2.064264	3.046373	-1.182309	2.129109	4.407108	-0.670857	1.565134
H	3.148704	0.401486	1.539788	3.074875	0.514395	1.621875	2.875907	-1.256075	2.217433
H	4.507859	-0.728585	1.295937	4.510952	-0.520271	1.406108	3.029800	0.447520	1.759911
H	3.481446	-0.620081	-2.200850	4.041547	0.789762	-0.958998	4.116285	0.801467	-0.649302
H	4.838185	-0.947250	-1.097947	3.600057	-0.492012	-2.116349	3.555455	-0.255806	-1.963612
H	4.021900	0.631073	-1.054128	4.929745	-0.749392	-0.965716	4.863075	-0.782913	-0.874457
H	3.937139	-2.907011	-0.009454	4.085383	-2.745710	0.093928	3.988923	-2.765265	0.108036
H	2.795157	-2.790925	-1.355949	2.975884	-2.692807	-1.284782	2.928406	-2.602990	-1.299038
H	2.027673	-3.162018	1.594956	2.135099	-3.101763	1.637230	1.999823	-3.171825	1.573575
H	1.954654	-4.381524	0.334111	2.154426	-4.310540	0.353229	2.041159	-4.315686	0.242652
H	-0.706575	-1.595452	-2.063353	-1.564993	-0.485919	-2.219484	-0.576492	-1.486408	-2.139113
H	-2.341348	-1.913898	1.073199	-2.247496	-2.044964	0.988197	-2.382229	-1.996532	0.891115
H	-2.212964	-2.664463	-0.528448	-2.025698	-2.814707	-0.592701	-2.124376	-2.689166	-0.722682
H	-4.441894	-1.615665	-0.354622	-4.330094	-1.891762	-0.427036	-4.401962	-1.714519	-0.638763
H	-3.432286	-0.766979	-1.544317	-3.423280	-1.070161	-1.678214	-3.359896	-0.826741	-1.763120
C	0.294924	-1.318167	0.275522	0.370797	-1.334841	0.249670	0.284995	-1.307666	0.259399
C	0.255361	-0.888524	1.755292	0.265415	-0.901509	1.724722	0.151598	-0.967033	1.755838
H	-0.714243	-1.173092	2.205163	-0.692753	-1.245229	2.156689	-0.829060	-1.310481	2.135350
H	1.041212	-1.367639	2.350074	1.066850	-1.329163	2.335184	0.921309	-1.452813	2.366119
O	0.457184	0.508131	1.870520	0.372371	0.508803	1.843064	0.288782	0.427705	1.952832
H	0.273844	-4.112793	-1.333593	-0.009462	-2.613470	-1.729367	0.445014	-4.006836	-1.498780



conformer **2-VII**

C	-4.385029	0.179564	1.679243
C	-3.784666	0.381708	0.267257
C	-4.728391	1.288836	-0.499177
C	-5.477354	0.974829	-1.555402
C	-2.465077	1.103620	0.456028
C	-1.268241	0.565443	0.229501
C	0.031639	1.198769	0.697725
O	-0.105851	2.519675	1.079069
C	1.109333	0.965338	-0.387490
H	0.719228	1.319782	-1.351655
O	2.283428	1.733308	-0.084146
C	2.329083	3.004595	-0.496496
C	3.686653	3.599832	-0.260986
O	1.391380	3.586499	-1.001581
C	1.434794	-0.559247	-0.472316
H	1.319545	-0.827487	-1.528680
C	2.885521	-1.035805	-0.131021
C	3.409344	-0.658946	1.269290
C	3.856915	-0.477087	-1.188788
C	2.909833	-2.573467	-0.296399
C	1.847619	-3.315107	0.505661
C	0.447363	-2.846362	0.124382
H	-0.283741	-3.329388	0.802849
O	0.196453	-3.284412	-1.202047
C	-1.075894	-0.832684	-0.312632
O	-0.919928	-0.801275	-1.746880
C	-2.298467	-1.693213	0.030228
C	-3.575522	-0.980224	-0.418183
H	-4.500586	1.142451	2.199959
H	-3.730735	-0.454988	2.296288
H	-5.376474	-0.292776	1.607314
H	-4.800751	2.304981	-0.091307
H	-5.471735	-0.019190	-2.008763
H	-6.140672	1.715341	-2.006839
H	-2.502180	2.107021	0.892849
H	0.061262	3.066048	0.293582
H	4.000223	3.412420	0.774724
H	3.658185	4.674552	-0.467746
H	4.417895	3.113527	-0.923685
H	4.509149	-0.720913	1.275291
H	3.054866	-1.347745	2.048265
H	3.116407	0.354502	1.563802
H	4.032699	0.597360	-1.062753
H	3.474959	-0.649460	-2.208062
H	4.828370	-0.990668	-1.108001
H	3.913423	-2.938199	-0.022579
H	2.759896	-2.817929	-1.360463
H	2.003405	-3.192256	1.589165
H	1.908490	-4.394746	0.302378
H	-1.661592	-0.307127	-2.114285
H	-2.332402	-1.886908	1.112599
H	-2.213329	-2.665246	-0.475020
H	-4.450619	-1.623331	-0.240257
H	-3.530471	-0.838172	-1.511056
C	0.292262	-1.322974	0.271874
C	0.267585	-0.889378	1.750532
H	-0.689427	-1.183872	2.219670
H	1.069285	-1.360135	2.328143
O	0.452510	0.513538	1.866846
H	-0.242327	-2.574341	-1.692804

Table S11 Coordinates of Compound **3**

	 conformer **3-I**			 conformer **3-II**			 conformer **3-III**		
O	1.613090	2.480084	0.368250	1.405491	2.561241	0.362683	1.720187	2.430916	0.304233
C	0.995366	1.240805	0.317107	0.881101	1.279037	0.326774	1.043167	1.221890	0.294782
C	-0.384281	1.334564	-0.384727	-0.524213	1.269492	-0.328562	-0.353965	1.369844	-0.363014
H	-0.215393	1.542453	-1.453419	-0.406617	1.488144	-1.401916	-0.213172	1.546258	-1.441261
O	-1.171839	2.399414	0.168489	-1.371305	2.273012	0.251086	-1.070016	2.483842	0.191712
C	-1.039834	3.624776	-0.347738	-1.347321	3.504682	-0.266432	-0.893291	3.690452	-0.354272
C	-2.085122	4.556139	0.191908	-2.440964	4.355901	0.308842	-1.874368	4.684009	0.195334
O	-0.180749	3.932550	-1.148554	-0.539522	3.875507	-1.093390	-0.045111	3.939169	-1.186499
C	1.810418	0.104785	-0.337852	1.755996	0.208272	-0.360278	1.781172	0.037708	-0.366238
H	1.656128	0.109555	-1.424970	1.565463	0.203504	-1.441536	1.591189	0.032534	-1.447569
C	3.353219	0.166074	-0.098792	3.297235	0.384280	-0.173168	3.332346	0.028969	-0.178583
C	3.785590	0.677901	1.289018	3.737235	0.924223	1.201536	3.833835	0.541371	1.185656
C	3.964800	1.096260	-1.157968	3.801085	1.359799	-1.248151	3.951398	0.912698	-1.272681
C	3.930546	-1.245133	-0.316408	3.970539	-0.979304	-0.416908	3.835171	-1.411224	-0.391252
C	3.276431	-2.288341	0.580124	3.427261	-2.070728	0.496008	3.162160	-2.409409	0.541815
C	1.798231	-2.435605	0.235197	1.953048	-2.326877	0.201460	1.667818	-2.489786	0.248360
H	1.315459	-3.125724	0.952288	1.548307	-3.052452	0.931655	1.177425	-3.146433	0.991218
O	1.677751	-2.984187	-1.084515	1.827952	-2.880407	-1.115664	1.476003	-3.048744	-1.058464
C	1.038329	-1.098142	0.257775	1.096466	-1.050047	0.255767	0.973962	-1.117235	0.275983
C	0.787333	-0.599207	1.700428	0.858929	-0.573865	1.708175	0.798648	-0.584217	1.717336
O	0.810431	0.817647	1.658093	0.774045	0.840838	1.671337	0.883972	0.829424	1.648493
C	-0.350286	-1.216162	-0.494321	-0.304819	-1.271044	-0.449078	-0.445007	-1.178695	-0.424381
O	-0.165656	-1.252511	-1.904168	-0.167126	-1.290762	-1.863991	-0.313218	-1.241438	-1.839113
C	-1.157790	0.047634	-0.232650	-1.194513	-0.071266	-0.153671	-1.180900	0.125658	-0.152779
C	-2.451837	0.034992	0.092576	-2.471308	-0.179159	0.217490	-2.458569	0.178925	0.226632
C	-3.325396	-1.200804	0.182529	-3.237099	-1.471625	0.351577	-3.374590	-1.016146	0.387739
C	-4.575361	-0.916850	-0.629741	-4.597090	-1.374080	-0.312794	-4.718492	-0.650096	-0.215328
C	-5.836307	-0.902119	-0.199364	-5.007809	-0.436719	-1.165585	-5.398040	-1.317876	-1.146014
C	-3.649102	-1.481316	1.656326	-3.457951	-1.768196	1.849158	-3.608674	-1.266041	1.894418
C	-2.588543	-2.386939	-0.467443	-2.448906	-2.604662	-0.335436	-2.737875	-2.233078	-0.290806
C	-1.131841	-2.459092	-0.034255	-0.973372	-2.570418	0.034347	-1.268513	-2.377165	0.079365
H	1.247616	3.036566	-0.339706	0.978334	3.088937	-0.332661	1.361598	2.990997	-0.404511
H	-2.078892	4.517748	1.289696	-2.386524	4.329436	1.405720	-1.844700	4.661088	1.293126
H	-3.078157	4.226892	-0.146670	-3.418016	3.946026	0.014843	-2.891006	4.404150	-0.116714
H	-1.888250	5.574246	-0.158805	-2.339488	5.382883	-0.056250	-1.632126	5.684983	-0.175731
H	3.456450	1.709785	1.449665	3.337441	1.928197	1.377865	3.551711	1.587792	1.342204
H	4.885705	0.646172	1.352537	4.838161	0.974881	1.227729	4.933306	0.465553	1.211601
H	3.391214	0.076771	2.118954	3.417269	0.293752	2.041672	3.444896	-0.032140	2.037525
H	3.579925	2.118303	-1.048782	3.345296	2.350056	-1.120814	3.621011	1.953961	-1.166710
H	3.733193	0.742703	-2.175693	3.561355	0.992351	-2.259047	3.667463	0.556596	-2.276164
H	5.061427	1.128483	-1.054323	4.895202	1.473343	-1.181973	5.051233	0.892117	-1.207017
H	5.018390	-1.219449	-0.143376	5.058729	-0.872742	-0.280812	4.928055	-1.434798	-0.252982
H	3.779723	-1.543247	-1.367329	3.806560	-1.285463	-1.463549	3.636808	-1.716964	-1.432039
H	3.390850	-2.026278	1.642534	3.558924	-1.804257	1.555291	3.324580	-2.138934	1.595843
H	3.763156	-3.272013	0.460185	3.981301	-3.015058	0.353861	3.597180	-3.416872	0.420753
H	2.193637	-3.795985	-1.125381	2.400419	-3.651938	-1.177626	1.949620	-3.885638	-1.104499
H	1.566951	-0.948843	2.397427	1.686023	-0.865277	2.376574	1.586280	-0.957854	2.392484
H	-0.185622	-0.935639	2.091999	-0.071880	-0.982924	2.131626	-0.173645	-0.869008	2.149278
H	0.474109	-1.965376	-2.058196	0.518133	-1.953516	-2.043657	0.285902	-1.986003	-2.005610
H	-2.949148	0.984494	0.302822	-3.020970	0.733960	0.456251	-2.897484	1.157486	0.436289
H	-4.377324	-0.701962	-1.687197	-5.278549	-2.197962	-0.065257	-5.164759	0.261412	0.203697
H	-6.105148	-1.104378	0.839907	-4.365001	0.395356	-1.464072	-5.019840	-2.233367	-1.605961
H	-6.657295	-0.685413	-0.886267	-6.004958	-0.479443	-1.608699	-6.372952	-0.962510	-1.486231
H	-2.731220	-1.693553	2.223591	-2.502275	-1.894150	2.379334	-2.666680	-1.499428	2.412916
H	-4.321649	-2.347695	1.755501	-4.049444	-2.688654	1.981354	-4.310230	-2.102106	2.040572
H	-4.132288	-0.612855	2.129415	-4.001014	-0.941777	2.332696	-4.035960	-0.373450	2.377536
H	-2.609027	-2.267068	-1.562264	-2.534660	-2.480242	-1.425606	-2.796120	-2.107319	-1.382943
H	-3.115148	-3.324180	-0.229542	-2.890794	-3.580149	-0.076391	-3.292931	-3.147467	-0.028640
H	-0.654383	-3.344162	-0.475270	-0.450614	-3.415533	-0.433100	-0.855822	-3.287219	-0.375627
H	-1.066593	-2.569654	1.059565	-0.853560	-2.680906	1.123576	-1.159724	-2.486111	1.169834

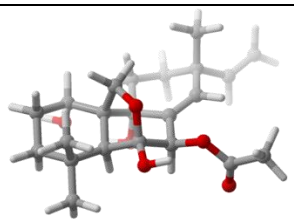
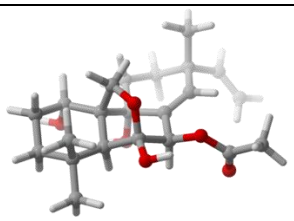
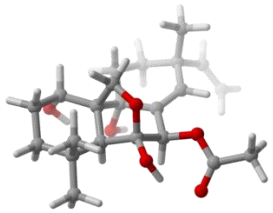
	 conformer **3-IV**			 conformer **3-V**			 conformer **3-VI**		
O	1.47155	2.63433	0.42722	1.28298	2.72360	0.34416	1.42934	2.55059	0.37606
C	0.96887	1.34705	0.38277	0.87454	1.40273	0.35330	0.89845	1.27044	0.33158
C	-0.40968	1.35083	-0.31051	-0.52840	1.28709	-0.27714	-0.50797	1.28079	-0.32603
H	-0.27071	1.58360	-1.37549	-0.45663	1.49767	-1.35394	-0.38179	1.50291	-1.39791
O	-1.17854	2.39938	0.28774	-1.33632	2.30136	0.33162	-1.34412	2.29106	0.25069
C	-1.92833	3.17130	-0.54221	-2.30742	2.85898	-0.43324	-1.29718	3.52398	-0.26923
C	-2.72736	4.16491	0.25520	-3.08685	3.86850	0.36334	-2.33734	4.41111	0.34857
O	-1.94974	3.04940	-1.73730	-2.51525	2.55526	-1.57850	-0.50815	3.86513	-1.12515
C	1.88119	0.33573	-0.32173	1.82876	0.44034	-0.36495	1.75971	0.19352	-0.36322
H	1.71811	0.37772	-1.40608	1.62033	0.44221	-1.44226	1.57089	0.20010	-1.44453
C	3.41362	0.52073	-0.08453	3.35204	0.74098	-0.19577	3.30466	0.34566	-0.18577
C	3.80896	0.99192	1.32816	3.76762	1.27677	1.18771	3.76092	0.87940	1.18583
C	3.92425	1.56248	-1.09280	3.74616	1.78877	-1.24908	3.81230	1.31832	-1.26183
C	4.11013	-0.81964	-0.38357	4.13202	-0.55366	-0.49110	3.95075	-1.02923	-0.43837
C	3.55711	-1.96623	0.45330	3.69767	-1.71403	0.39530	3.41160	-2.11455	0.48245
C	2.09251	-2.22191	0.11125	2.24326	-2.08324	0.11984	1.93343	-2.36531	0.19288
H	1.68165	-2.99148	0.79109	1.91585	-2.86151	0.83428	1.53463	-3.05415	0.96275
O	2.00194	-2.70119	-1.23691	2.13556	-2.60406	-1.21147	1.85350	-3.03108	-1.05730
C	1.21787	-0.96126	0.21849	1.28396	-0.88642	0.23256	1.09616	-1.06543	0.25506
C	0.94515	-0.56634	1.68793	1.04221	-0.47268	1.70248	0.87296	-0.58460	1.70749
O	0.83023	0.84664	1.71267	0.82681	0.92905	1.69921	0.78340	0.83127	1.67164
C	-0.17278	-1.16432	-0.52000	-0.11579	-1.20856	-0.44479	-0.31085	-1.26456	-0.41463
O	-0.01295	-1.10962	-1.93034	-0.01360	-1.17750	-1.86067	-0.06762	-1.32928	-1.83855
C	-1.07855	0.01023	-0.17414	-1.08917	-0.09505	-0.08377	-1.19301	-0.05371	-0.15294
C	-2.34536	-0.12553	0.21737	-2.32523	-0.31397	0.36083	-2.47946	-0.15150	0.19241
C	-3.11021	-1.43311	0.27560	-2.99455	-1.66083	0.46004	-3.25187	-1.43739	0.35253
C	-4.41740	-1.20863	-0.46184	-4.37184	-1.61275	-0.17673	-4.60878	-1.35312	-0.31950
C	-5.65251	-1.33567	0.02174	-4.83062	-0.67356	-1.00366	-5.02397	-0.42190	-1.17709
C	-3.33653	-1.82701	1.74132	-3.15784	-2.04275	1.94423	-3.47517	-1.69458	1.85740
C	-2.31021	-2.51130	-0.48145	-2.14691	-2.70256	-0.29958	-2.46907	-2.59681	-0.29734
C	-0.83354	-2.49305	-0.11236	-0.66403	-2.57007	0.01967	-0.98879	-2.55875	0.05783
H	0.75657	3.18322	0.77745	0.53631	3.23118	0.69086	1.04873	3.06765	-0.35181
H	-2.10379	4.64005	1.02396	-2.41217	4.52891	0.92396	-2.19463	4.43056	1.43796
H	-3.54097	3.63364	0.77153	-3.71288	3.33643	1.09527	-3.33916	4.00346	0.15229
H	-3.15454	4.91574	-0.41779	-3.72741	4.44882	-0.30890	-2.25193	5.42103	-0.06482
H	3.37687	1.97310	1.55180	3.27364	2.22936	1.40688	3.38768	1.89395	1.36188
H	4.90699	1.07062	1.38306	4.85816	1.43676	1.19461	4.86269	0.90263	1.20705
H	3.48849	0.30602	2.12349	3.53118	0.58981	2.01101	3.43155	0.25746	2.02817
H	3.42772	2.52963	-0.94028	3.18890	2.72256	-1.09878	3.36985	2.31506	-1.13269
H	3.73266	1.23500	-2.12732	3.53688	1.42113	-2.26656	3.56680	0.95363	-2.27245
H	5.01105	1.70578	-0.98069	4.82367	2.01075	-1.18624	4.90765	1.41950	-1.19994
H	5.19304	-0.70864	-0.21346	5.20986	-0.36047	-0.36900	5.04331	-0.93518	-0.32878
H	3.97672	-1.06934	-1.44927	3.97469	-0.84109	-1.54395	3.76063	-1.34082	-1.47929
H	3.66130	-1.75950	1.52895	3.82900	-1.47136	1.46040	3.56480	-1.85149	1.54046
H	4.12527	-2.89502	0.27101	4.32446	-2.60410	0.21191	3.93864	-3.06443	0.31079
H	2.57266	-3.47138	-1.32593	2.75436	-3.33577	-1.30374	1.28300	-2.51677	-1.64767
H	1.76688	-0.87259	2.35642	1.91026	-0.70152	2.34279	1.71002	-0.87703	2.36033
H	0.01632	-1.01561	2.07280	0.16436	-0.97633	2.13637	-0.05098	-0.99258	2.14723
H	0.68129	-1.75567	-2.13379	0.71524	-1.77954	-2.07746	-0.91926	-1.45253	-2.27460
H	-2.90946	0.76651	0.50358	-2.93595	0.54027	0.66480	-3.02689	0.76932	0.40628
H	-4.28894	-0.90396	-1.50773	-5.01302	-2.47043	0.06350	-5.28404	-2.18187	-0.07216
H	-5.85247	-1.63137	1.05420	-4.22731	0.19084	-1.29542	-4.39175	0.41991	-1.47136
H	-6.52123	-1.14648	-0.61253	-5.83194	-0.75019	-1.43316	-6.01916	-0.47438	-1.62324
H	-2.37778	-1.99191	2.25421	-2.18253	-2.13591	2.44524	-2.52025	-1.81315	2.39014
H	-3.92821	-2.75284	1.81586	-3.68881	-3.00328	2.04381	-4.07338	-2.60674	2.01209
H	-3.86779	-1.03317	2.28835	-3.73761	-1.27669	2.48196	-4.01223	-0.85183	2.31807
H	-2.39031	-2.32363	-1.56397	-2.28166	-2.54245	-1.37993	-2.59526	-2.53202	-1.39246
H	-2.75006	-3.50160	-0.28598	-2.50434	-3.71834	-0.06677	-2.90676	-3.56228	0.00074
H	-0.30744	-3.30760	-0.62827	-0.09771	-3.35916	-0.49331	-0.45782	-3.40517	-0.39683
H	-0.71293	-2.66726	0.96838	-0.49628	-2.70439	1.10002	-0.87124	-2.65698	1.14682

Table S12 Coordinates of Compound **4**

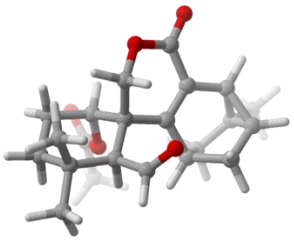
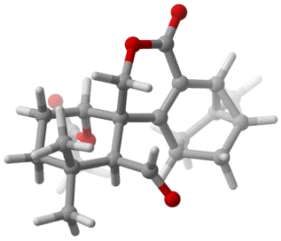
	 conformer **4-I**			 conformer **4-II**		
C	-3.900444	-1.544238	0.369116	-3.910974	-1.465707	0.645211
C	-3.248782	-0.466278	-0.514101	-3.243980	-0.525432	-0.374977
C	-4.012805	-0.438831	-1.852013	-3.984432	-0.695369	-1.712059
C	-3.402495	0.928608	0.125766	-3.389648	0.940418	0.078310
C	-2.470828	1.190168	1.303809	-2.464043	1.328916	1.227934
C	-1.012235	0.982724	0.915770	-1.000955	1.075483	0.880201
H	-0.356640	1.193230	1.770392	-0.353437	1.363155	1.719139
O	-0.669103	1.888761	-0.155240	-0.641366	1.870613	-0.267365
C	-0.335235	3.150717	0.191908	-0.290826	3.155208	-0.038120
C	-0.039820	3.976132	-1.030767	0.014255	3.858906	-1.331861
O	-0.298594	3.542032	1.330212	-0.248612	3.648690	1.059684
C	-0.730307	-0.439452	0.376195	-0.721274	-0.393644	0.484942
C	-0.834310	-1.455527	1.526820	-0.820842	-1.289470	1.730499
O	0.117686	-1.214216	2.563137	0.163608	-0.996386	2.715794
C	1.423161	-1.130944	2.208108	1.463015	-0.991780	2.323008
C	1.694413	-0.867513	0.778672	1.703857	-0.854898	0.870366
C	0.723577	-0.507055	-0.084682	0.722229	-0.524898	0.004057
C	2.340237	0.938195	-1.278531	2.342459	0.811299	-1.300039
C	4.858620	0.832773	-0.593361	4.871379	0.694810	-0.652192
C	3.091708	-0.889042	0.300707	3.089648	-0.937356	0.369152
H	3.839922	-1.191252	1.032556	3.846252	-1.210451	1.103745
O	2.275756	-1.215540	3.054922	2.332394	-1.038252	3.154202
C	-1.722668	-0.724889	-0.787665	-1.725054	-0.801285	-0.639441
H	-1.477206	0.018827	-1.567010	-1.473754	-0.163034	-1.497655
C	-1.510649	-2.051899	-1.483791	-1.488221	-2.214778	-1.130508
O	-0.772089	-2.938030	-1.125443	-1.129710	-2.478115	-2.252999
H	-3.617803	-1.465977	1.426403	-3.587607	-1.291301	1.679214
H	-3.645445	-2.561096	0.030836	-3.738449	-2.527371	0.413179
H	-4.995999	-1.444909	0.323733	-5.000047	-1.305122	0.623075
H	-3.515297	0.209094	-2.591203	-3.529858	-0.079307	-2.503076
H	-5.025414	-0.038928	-1.687014	-5.036426	-0.388886	-1.603835
H	-4.131789	-1.438707	-2.294687	-3.974119	-1.740882	-2.057043
H	-4.451527	1.061655	0.436277	-4.438958	1.127663	0.358202
H	-3.206597	1.687693	-0.649471	-3.172163	1.593899	-0.782347
H	-2.706392	0.534498	2.155769	-2.712115	0.775359	2.146613
H	-2.592120	2.218714	1.671925	-2.580363	2.392867	1.478444
H	-0.963072	4.101713	-1.615448	0.411144	4.857186	-1.120023
H	0.691021	3.463708	-1.671132	-0.909130	3.945530	-1.923305
H	0.339149	4.957220	-0.726033	0.732802	3.276139	-1.924047
H	-0.691285	-2.466348	1.122941	-0.725591	-2.348014	1.439118
H	-1.797385	-1.411602	2.040679	-1.769501	-1.169077	2.258714
H	2.019051	1.755693	-0.616243	2.051715	1.673144	-0.681089
H	2.606931	1.365189	-2.259526	2.598405	1.174664	-2.308952
H	4.806726	1.686132	0.101089	4.847536	1.586956	-0.006782
H	5.209251	1.207953	-1.568531	5.211272	1.007202	-1.652826
H	5.616125	0.134222	-0.208242	5.622382	0.004187	-0.240924
H	-2.097054	-2.173127	-2.426270	-1.675076	-3.040458	-0.400452
C	3.518029	0.161405	-0.723009	3.516161	0.044340	-0.722383
C	3.331628	-1.267922	-1.159353	3.294730	-1.402603	-1.072191
H	4.180413	-1.913673	-1.387707	4.127387	-2.077113	-1.275680
C	2.068103	-1.347197	-1.987989	2.015726	-1.501834	-1.872718
H	1.526773	-2.297343	-1.881958	1.459474	-2.436553	-1.719674
H	2.306253	-1.192119	-3.052417	2.233333	-1.409236	-2.948096
C	1.244863	-0.143139	-1.452660	1.222956	-0.255218	-1.393803
H	0.457610	0.174703	-2.144093	0.427398	0.025804	-2.088486

Table S13 Coordinates of Compound **4a**

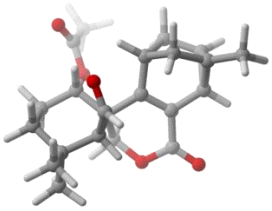
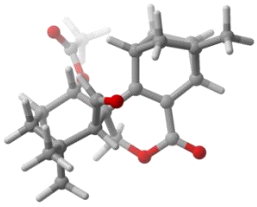
	 conformer **4a-I**			 conformer **4a-II**		
C	3.492657	-2.307392	-1.494308	3.508871	-2.272325	-1.434789
C	2.984699	-1.338382	-0.410082	3.018827	-1.268286	-0.376701
C	3.538439	-1.851396	0.932726	3.603504	-1.723160	0.973639
C	3.515726	0.075571	-0.710606	3.541596	0.136552	-0.735582
C	2.902391	1.158314	0.176748	2.916402	1.253434	0.097724
C	1.388744	1.168444	0.016815	1.404038	1.229251	-0.067248
H	1.165511	1.404120	-1.029596	1.188176	1.397792	-1.131154
O	0.798075	2.184534	0.848890	0.795244	2.302221	0.670352
C	0.629433	3.402705	0.289555	0.606330	3.463682	0.004606
C	-0.030703	4.348782	1.254218	-0.047676	4.489637	0.886513
O	0.954001	3.671060	-0.839761	0.911768	3.626824	-1.150507
C	0.723903	-0.167347	0.379408	0.753912	-0.086105	0.387307
C	0.794081	-0.422879	1.894242	0.844665	-0.237855	1.914194
O	0.172027	-1.654614	2.260708	0.215485	-1.430534	2.375917
C	-1.112340	-1.840909	1.861537	-1.080231	-1.624524	2.017694
C	-1.609922	-0.911843	0.822173	-1.579800	-0.782180	0.907364
C	-0.776162	-0.142146	0.091837	-0.746813	-0.086276	0.107763
C	-2.383617	-0.178091	-1.802359	-2.369733	-0.291905	-1.775038
C	-4.723229	-1.276702	-1.422876	-4.707713	-1.339760	-1.275255
C	-3.059169	-0.832477	0.552419	-3.029098	-0.720438	0.638006
H	-3.695097	-1.477168	1.158403	-3.664402	-1.302765	1.304584
O	-1.756838	-2.741689	2.335192	-1.732988	-2.464847	2.580606
C	1.412078	-1.323210	-0.422909	1.449361	-1.283649	-0.352884
H	1.073524	-2.271715	0.022414	1.120950	-2.212203	0.136515
C	0.937101	-1.343306	-1.868548	0.907741	-1.379158	-1.766418
O	0.860732	-0.373837	-2.586626	0.337325	-2.348099	-2.202249
H	3.203175	-1.996135	-2.509256	3.194908	-1.998339	-2.453414
H	3.118585	-3.330020	-1.324396	3.125261	-3.283625	-1.229707
H	4.592313	-2.347660	-1.471014	4.608762	-2.315143	-1.431323
H	3.524173	-1.094639	1.726695	3.575614	-0.943742	1.745643
H	4.590467	-2.149245	0.804480	4.661775	-1.997015	0.842621
H	2.979149	-2.727535	1.293895	3.070864	-2.602467	1.365280
H	3.300682	0.323256	-1.763061	3.340194	0.340562	-1.801847
H	4.612672	0.076015	-0.604109	4.637895	0.151050	-0.626087
H	3.284750	2.144260	-0.124459	3.286275	2.229576	-0.247986
H	3.176844	1.018463	1.234492	3.188605	1.165430	1.161034
H	-1.112315	4.145748	1.265162	-1.128808	4.287230	0.922512
H	0.131789	5.379842	0.921972	0.110297	5.487340	0.462938
H	0.351000	4.199424	2.272073	0.341454	4.430659	1.910619
H	0.297315	0.410240	2.413163	0.368211	0.636889	2.382265
H	1.814398	-0.504141	2.273470	1.871328	-0.307230	2.279049
H	-1.847648	-1.048844	-2.207583	-1.847978	-1.199854	-2.106615
H	-2.772585	0.404447	-2.652648	-2.768406	0.223116	-2.664099
H	-4.438281	-2.260917	-1.826804	-4.425396	-2.356620	-1.589220
H	-5.194554	-0.700084	-2.234906	-5.184351	-0.838689	-2.133055
H	-5.480010	-1.441647	-0.641584	-5.458327	-1.430454	-0.476089
H	0.668973	-2.352227	-2.267204	1.061720	-0.479680	-2.416790
C	-3.523418	-0.551507	-0.874854	-3.502290	-0.570444	-0.805690
C	-3.610136	0.540505	0.158354	-3.575975	0.613507	0.121291
H	-4.563180	0.852826	0.587253	-4.522931	0.971920	0.526808
C	-2.535737	1.561300	-0.149034	-2.499124	1.595043	-0.287667
H	-2.104163	2.030774	0.747983	-2.057862	2.142826	0.558560
H	-2.937069	2.351800	-0.802246	-2.900308	2.322545	-1.010420
C	-1.482247	0.722022	-0.923341	-1.455384	0.677229	-0.985462
H	-0.799809	1.336783	-1.516515	-0.776647	1.242760	-1.633780

Table S14 Coordinates of Compound **4b**

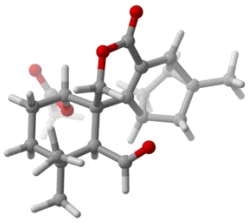
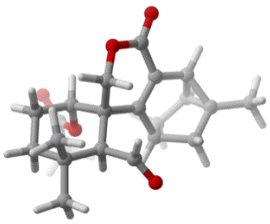
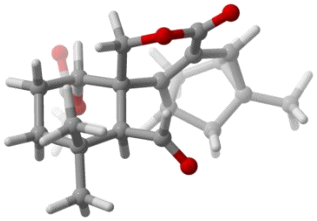
	 conformer **4b-I**			 conformer **4b-II**			 conformer **4b-III**		
C	-3.476208	-2.224127	0.460861	-3.522085	-2.080558	0.811734	3.432203	-2.280159	-0.079672
C	-3.040429	-1.122850	-0.520981	-3.036566	-1.160946	-0.323394	2.902432	-1.091688	0.743943
C	-3.717902	-1.413881	-1.874099	-3.659614	-1.675148	-1.631965	3.310025	-1.328463	2.207431
C	-3.541133	0.257654	-0.049731	-3.526132	0.280877	-0.085148	3.560795	0.215787	0.262978
C	-2.757941	0.850827	1.116015	-2.762562	1.021860	1.009030	3.004377	0.738983	-1.058278
C	-1.271610	0.948202	0.794963	-1.265909	1.063489	0.718570	1.507314	1.009130	-0.946201
H	-0.727708	1.393967	1.637649	-0.736670	1.602672	1.515583	1.111744	1.411817	-1.887475
O	-1.086420	1.790587	-0.363379	-1.042977	1.755487	-0.526388	1.338919	2.026900	0.055274
C	-1.081585	3.125474	-0.156621	-1.010425	3.105531	-0.479820	1.005500	3.267233	-0.371645
C	-0.915656	3.862741	-1.457519	-0.818989	3.678272	-1.857236	0.812820	4.191933	0.796872
O	-1.208141	3.632832	0.928165	-1.135181	3.740224	0.536077	0.865232	3.565141	-1.530534
C	-0.645396	-0.418440	0.430520	-0.647448	-0.342841	0.539727	0.713421	-0.269359	-0.563222
C	-0.579001	-1.304519	1.686548	-0.599735	-1.061502	1.898142	0.739203	-1.123624	-1.850977
O	0.241392	-0.746809	2.713214	0.250725	-0.423741	2.844378	-0.182112	-2.202584	-1.889477
C	1.512391	-0.408433	2.385477	1.532656	-0.178664	2.470875	-1.488774	-1.891780	-1.680804
C	1.790317	-0.239034	0.943163	1.800439	-0.187996	1.016523	-1.740981	-0.673245	-0.881793
C	0.808598	-0.198957	0.019923	0.809005	-0.208215	0.100103	-0.751742	0.017640	-0.273401
C	2.409525	-0.896715	-1.732389	2.377388	-1.105070	-1.593849	-2.212767	0.255301	1.723180
C	4.937142	-1.086689	-1.102029	4.906148	-1.299722	-0.966748	-4.714452	-0.478139	1.537071
C	3.179642	0.008670	0.507273	3.190730	-0.021053	0.549338	-3.139084	-0.332517	-0.553615
H	3.936914	-0.028012	1.289594	3.954824	-0.003084	1.325590	-3.903162	-0.890846	-1.093028
O	2.318648	-0.211529	3.258552	2.353469	0.084121	3.311126	-2.345086	-2.650606	-2.052978
C	-1.483144	-1.047491	-0.720220	-1.484459	-1.117236	-0.527310	1.344161	-0.919457	0.711620
H	-1.371773	-0.353226	-1.572442	-1.343997	-0.561073	-1.464334	1.105093	-0.233500	1.539826
C	-0.937835	-2.354679	-1.253557	-0.915244	-2.492845	-0.808525	0.640230	-2.218037	1.063892
O	-0.036547	-3.002278	-0.776582	-0.441607	-2.813111	-1.872027	0.069284	-2.398775	2.113243
H	-3.273129	-1.974319	1.509776	-3.291870	-1.698904	1.814445	3.306974	-2.157491	-1.163530
H	-2.981102	-3.184411	0.245845	-3.107884	-3.097036	0.735254	2.958370	-3.230861	0.205467
H	-4.562074	-2.384905	0.375793	-4.617524	-2.175141	0.753246	4.512299	-2.390389	0.104313
H	-3.342019	-0.749303	-2.668313	-3.320351	-1.084318	-2.496685	2.961787	-0.509410	2.855309
H	-4.802255	-1.244756	-1.784171	-4.757357	-1.606039	-1.581828	4.406540	-1.386289	2.292057
H	-3.582435	-2.454825	-2.202678	-3.399054	-2.727454	-1.824800	2.890433	-2.266519	2.601220
H	-4.608080	0.175969	0.213992	-4.602120	0.260873	0.152100	4.648634	0.060310	0.181490
H	-3.481483	0.955550	-0.901230	-3.422042	0.843892	-1.027103	3.408458	0.991037	1.030704
H	-2.883336	0.251689	2.030592	-2.921036	0.556329	1.993942	3.192936	0.032442	-1.881365
H	-3.129440	1.855982	1.360157	-3.124644	2.055300	1.104433	3.502648	1.678211	-1.341322
H	-0.795574	4.932671	-1.257943	0.021236	3.186074	-2.365133	1.607398	4.050365	1.540764
H	-1.806635	3.700972	-2.082067	-0.646268	4.757054	-1.783418	-0.146700	3.952150	1.280410
H	-0.048821	3.474978	-2.009729	-1.723636	3.490208	-2.454322	0.787266	5.228360	0.444218
H	-0.194838	-2.293597	1.404630	-0.259063	-2.100492	1.760052	1.712496	-1.588754	-2.022804
H	-1.552776	-1.425367	2.166752	-1.573621	-1.088879	2.392367	0.529131	-0.457690	-2.705680
H	2.666960	-0.804901	-2.800460	2.621974	-1.115403	-2.668140	-2.446865	0.909126	2.579440
H	2.098822	-1.932143	-1.533255	2.046411	-2.115186	-1.314219	-1.775159	-0.676965	2.109554
H	4.901470	-2.165303	-0.882476	4.848895	-2.352296	-0.647677	-4.548719	-1.485091	1.950505
H	5.697932	-0.635775	-0.447624	5.684179	-0.807778	-0.364238	-5.539611	-0.543419	0.812376
H	5.271487	-0.963379	-2.144873	5.231126	-1.282322	-2.019429	-5.037541	0.178703	2.360715
H	-1.431030	-2.707314	-2.191165	-0.959641	-3.236857	0.024596	0.676666	-3.024770	0.295561
C	3.590052	-0.450050	-0.888990	3.575960	-0.614268	-0.804022	-3.461563	0.047495	0.890271
C	3.393695	1.018795	-0.620365	3.416843	0.876205	-0.669230	-3.449174	1.114569	-0.174112
H	4.233934	1.709104	-0.536928	4.273832	1.550474	-0.652221	-4.371203	1.554355	-0.556331
C	2.111222	1.452276	-1.291952	2.138061	1.277635	-1.367377	-2.223303	1.977709	0.037676
H	2.319539	1.821369	-2.309061	2.345489	1.545407	-2.415761	-2.472819	2.820491	0.702630
H	1.573175	2.234264	-0.737196	1.626135	2.122082	-0.883793	-1.794551	2.384952	-0.891011
C	1.305075	0.127432	-1.366550	1.299137	-0.027925	-1.315931	-1.258146	0.998926	0.759113
H	0.503905	0.175353	-2.111376	0.494055	-0.041218	-2.054778	-0.447392	1.499643	1.289807

Table S15 Coordinates of Compound **4c**

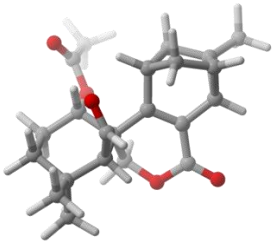
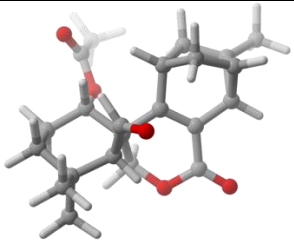
	 conformer **4c-I**			 conformer **4c-II**		
C	-4.048775	-1.571769	1.310189	4.089298	-1.429699	-1.259464
C	-3.252361	-0.808907	0.234833	3.290217	-0.640005	-0.207982
C	-3.751251	-1.322772	-1.129071	3.837409	-1.054177	1.170875
C	-3.528953	0.699239	0.379713	3.512226	0.868169	-0.436076
C	-2.628075	1.571360	-0.494474	2.578108	1.755269	0.384400
C	-1.166250	1.313853	-0.157342	1.131840	1.412118	0.059507
H	-1.011777	1.591358	0.891210	0.981493	1.609081	-1.010712
O	-0.306163	2.128487	-0.976171	0.231582	2.266446	0.784666
C	0.043263	3.333707	-0.475802	-0.160261	3.401300	0.163283
C	0.975429	4.052707	-1.411500	-1.109476	4.186144	1.024261
O	-0.335818	3.751535	0.589301	0.200221	3.713346	-0.944351
C	-0.738415	-0.147827	-0.353066	0.756544	-0.044396	0.372366
C	-0.699243	-0.513885	-1.846271	0.738719	-0.285099	1.890513
O	-0.292202	-1.865959	-2.057623	0.350193	-1.615685	2.221797
C	0.883419	-2.252009	-1.498455	-0.833203	-2.056389	1.721804
C	1.440975	-1.345416	-0.469853	-1.402603	-1.263955	0.608352
C	0.700938	-0.374851	0.105882	-0.674257	-0.350131	-0.064133
C	2.728347	0.975316	0.436999	-2.716981	0.923375	-0.559977
C	5.048876	-0.090287	-0.124029	-5.024005	-0.104080	0.111921
C	2.842640	-1.512711	-0.037336	-2.798273	-1.498050	0.190306
H	3.397148	-2.321337	-0.512694	-3.343874	-2.257165	0.749860
O	1.387530	-3.293071	-1.834853	-1.333817	-3.054397	2.171740
C	-1.716699	-1.083675	0.433978	1.769129	-1.002127	-0.350097
H	-1.522960	-2.112990	0.093907	1.616711	-2.013220	0.055018
C	-1.408726	-1.066689	1.924153	1.394318	-1.112417	-1.815633
O	-1.221607	-0.069682	2.581671	1.111486	-2.150941	-2.359217
H	-3.812202	-1.234848	2.330631	3.816453	-1.155281	-2.289714
H	-3.864032	-2.656608	1.250756	3.926608	-2.512981	-1.150292
H	-5.126842	-1.409432	1.159145	5.165332	-1.230301	-1.141189
H	-3.510386	-0.650397	-1.961659	3.562449	-0.360538	1.975616
H	-4.848324	-1.411475	-1.107251	4.937668	-1.076315	1.138353
H	-3.335183	-2.313446	-1.366347	3.485747	-2.056543	1.457024
H	-3.382238	0.991169	1.432550	3.367000	1.101618	-1.505441
H	-4.587717	0.893169	0.143024	4.562397	1.114914	-0.211774
H	-2.841471	2.632832	-0.302567	2.747831	2.811885	0.131441
H	-2.812549	1.397183	-1.566538	2.765316	1.649949	1.464352
H	1.990503	3.648646	-1.278464	-2.114643	3.747655	0.931498
H	0.985565	5.120326	-1.166619	-1.144326	5.223822	0.675198
H	0.682291	3.892124	-2.456605	-0.814372	4.135523	2.079708
H	-0.000100	0.165991	-2.355374	0.039843	0.429646	2.350825
H	-1.671178	-0.437440	-2.336987	1.717785	-0.158442	2.356746
H	3.212159	1.731663	1.075880	-3.207195	1.595768	-1.282345
H	2.500467	1.433656	-0.538050	-2.499294	1.490515	0.358235
H	5.097888	0.310106	-1.149147	-5.082381	0.407454	1.085870
H	5.576963	-1.055351	-0.116343	-5.538925	-1.071127	0.210841
H	5.597369	0.600446	0.536526	-5.579326	0.500686	-0.623086
H	-1.384381	-2.069502	2.416516	1.387879	-0.155076	-2.398171
C	3.621512	-0.247836	0.326626	-3.593174	-0.292541	-0.315397
C	3.186094	-1.190777	1.416696	-3.139569	-1.345024	-1.290954
H	3.896116	-1.843222	1.926574	-3.835856	-2.062743	-1.726158
C	2.060565	-0.535812	2.183661	-2.021435	-0.765268	-2.126449
H	2.462539	0.042531	3.029794	-2.436568	-0.282013	-3.024879
H	1.320673	-1.245259	2.580063	-1.275874	-1.505838	-2.444047
C	1.454585	0.432368	1.133902	-1.431768	0.320109	-1.185675
H	0.850378	1.219662	1.592844	-0.842009	1.070162	-1.724382

Table S16 Summary of binding energies, amino acid residue involved in the hydrogen bond and hydrophobic interactions of **2** observed in molecular docking studies.

compound	Binding energy (kcal/mol)	Residue involved in the interaction	
		Hydrogen bond	Hydrophobic interaction
2	–8.0	GLN257, ARG260	MET114, TRP84, TYR341, TYR367
AR-C118901	–9.2	GLU371, TRP366, TYR367	HEM901, VAL346, TYR367, PRO344

Datablock 1 - ellipsoid plot

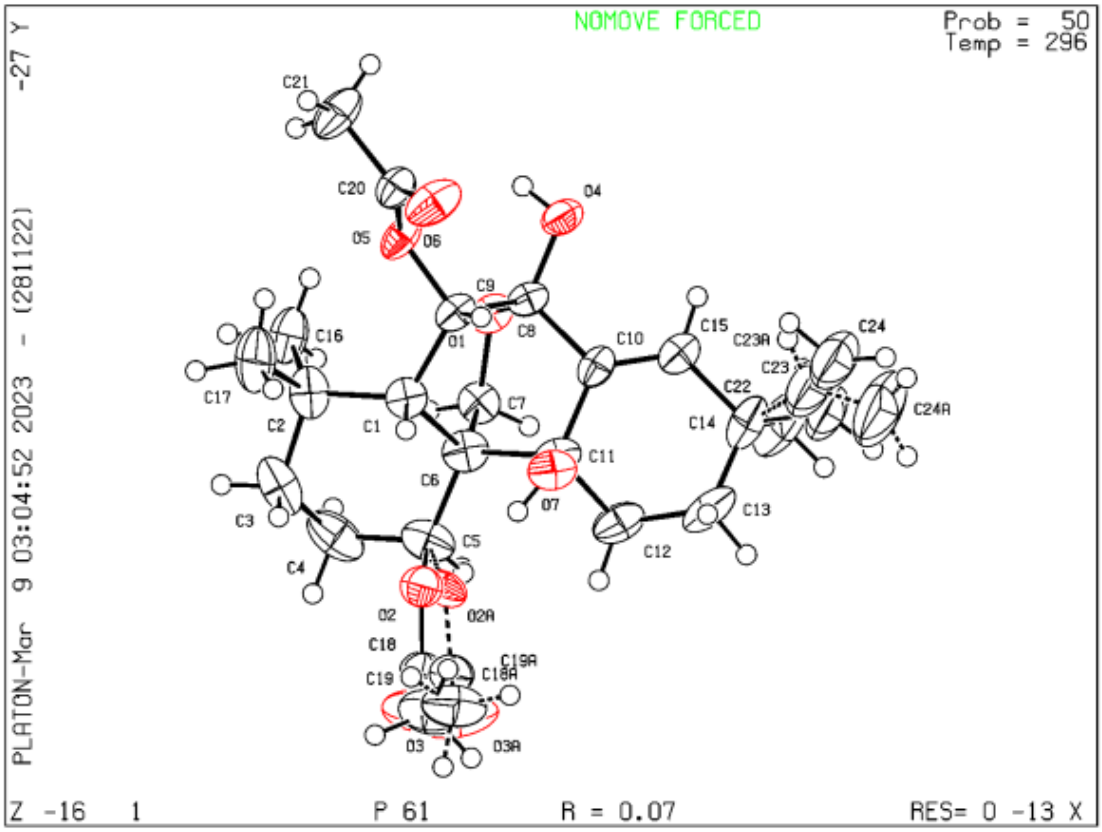


Figure S1 ORTEP drawing of crystal structure of **1**

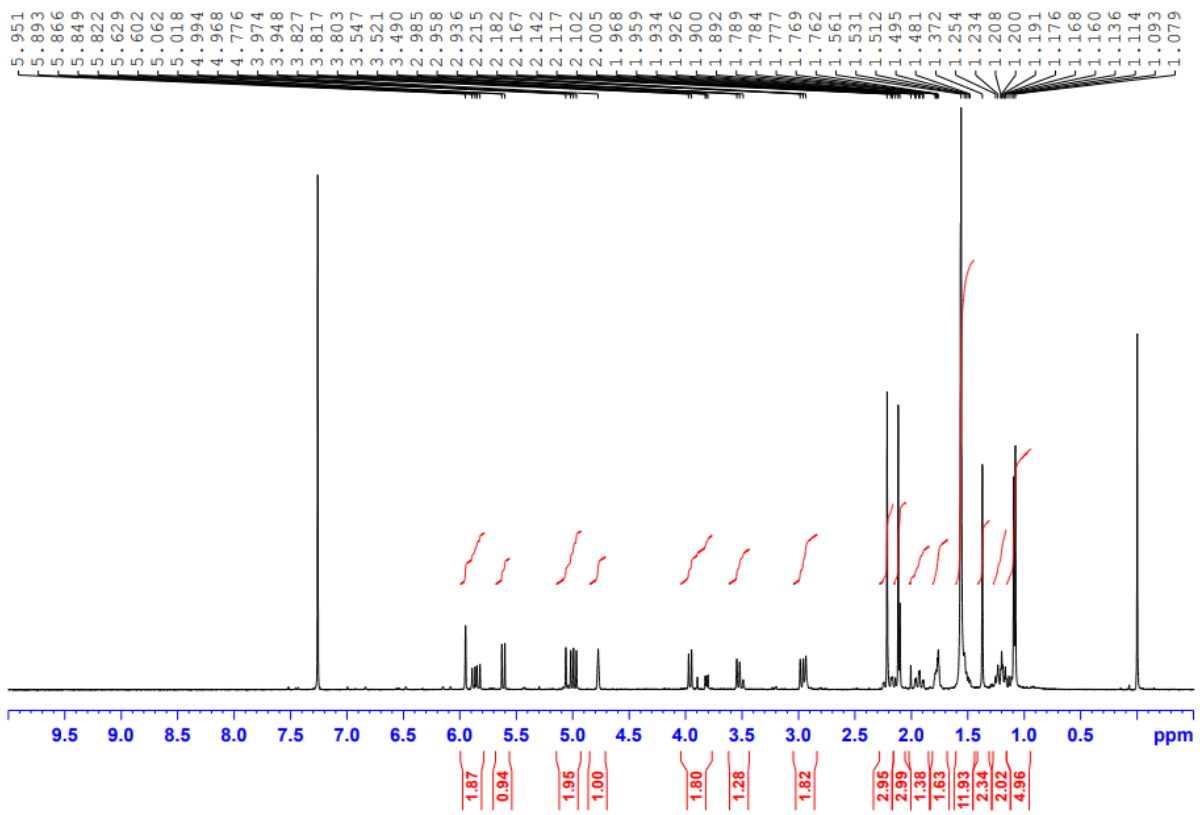


Figure S2 ^{1}H NMR spectrum (400 MHz) of compound **1** in $CDCl_3$

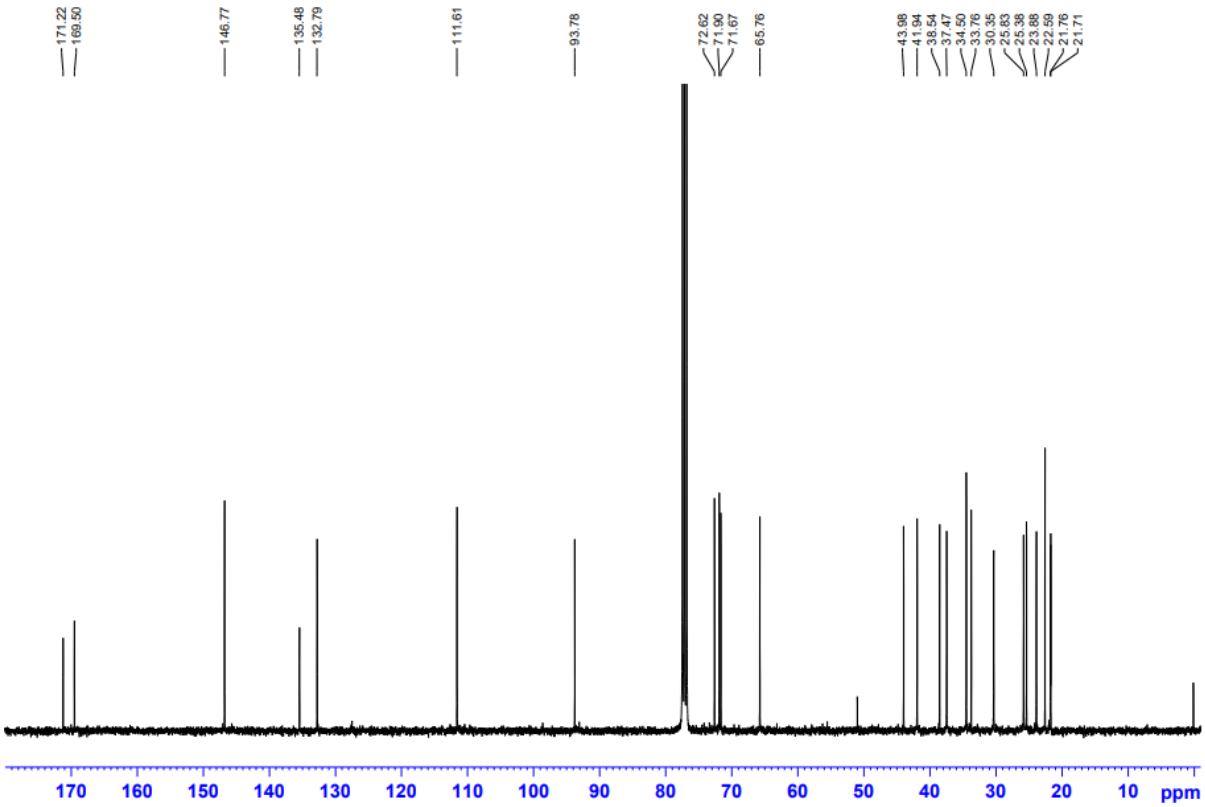


Figure S3 ^{13}C NMR spectrum (100 MHz) of compound **1** in $CDCl_3$

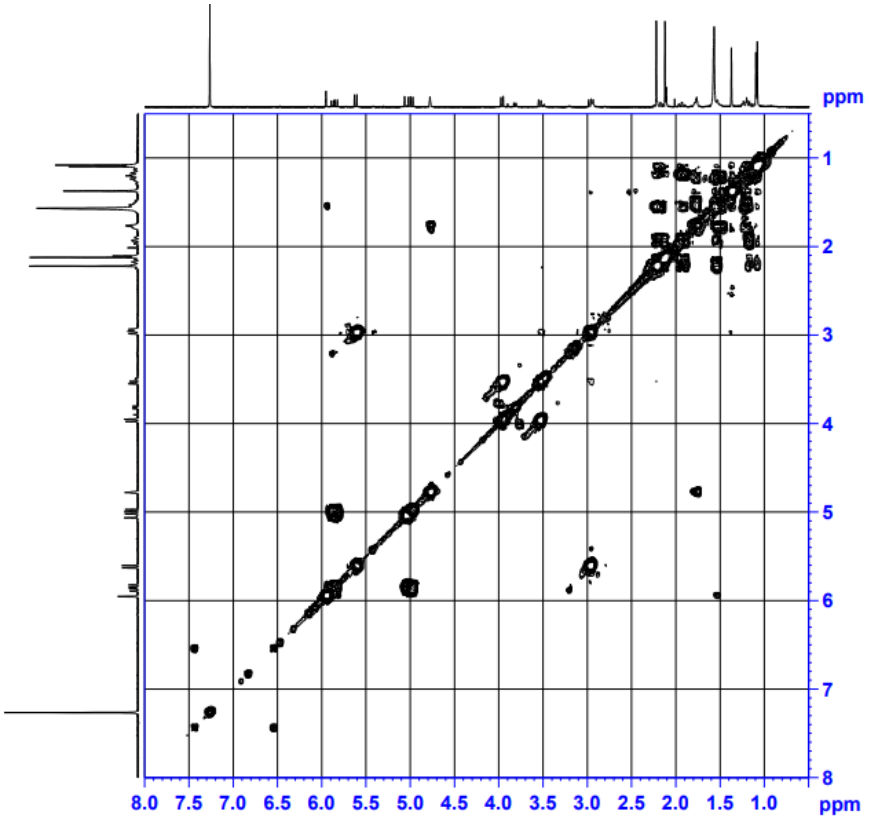


Figure S4 ^{1}H– ^{1}H COSY spectrum of compound **1** in $CDCl_3$

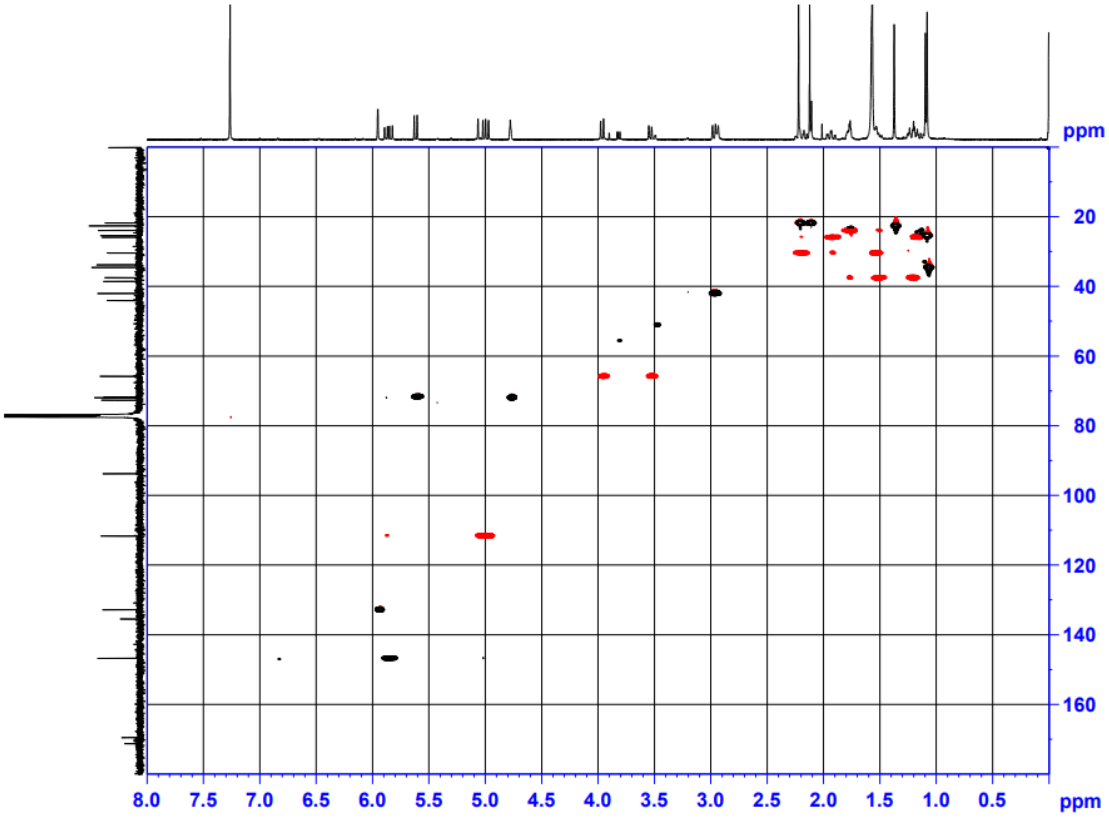


Figure S5 HSQC spectrum of compound **1** in $CDCl_3$

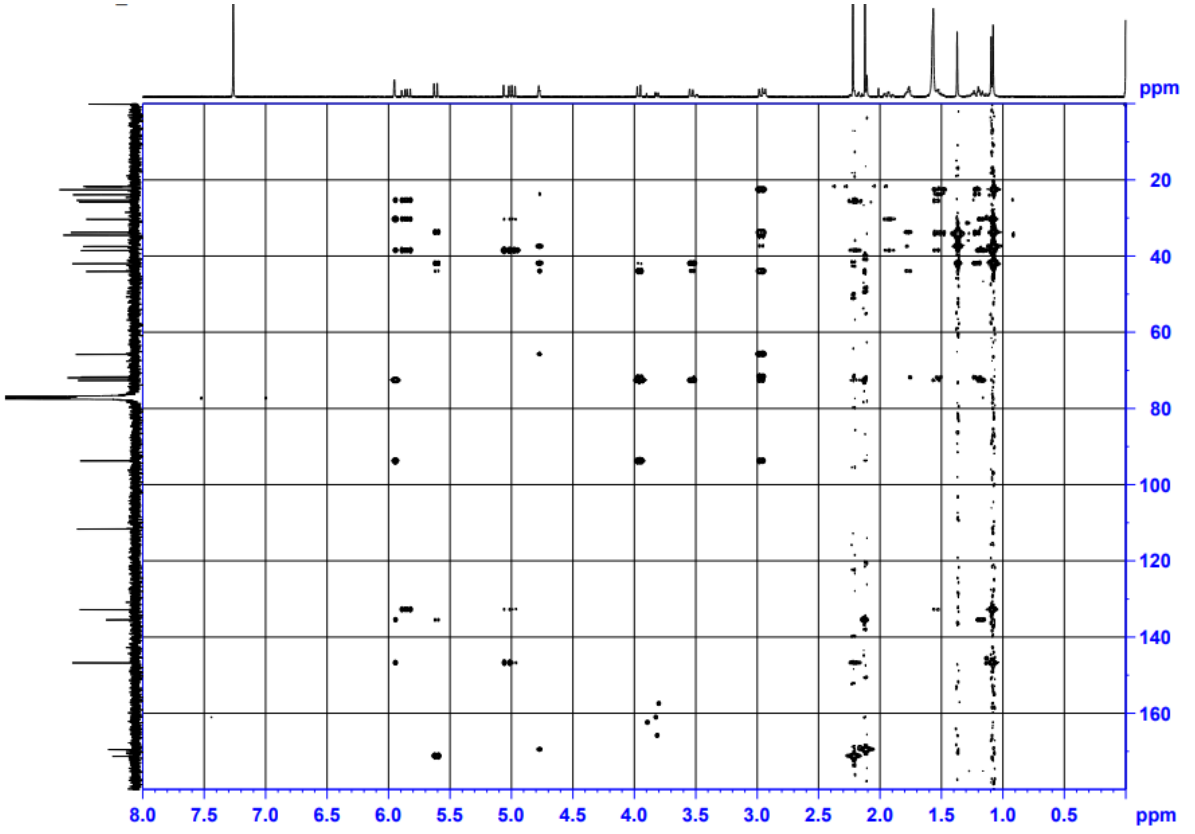


Figure S6 HMBC spectrum of compound **1** in $CDCl_3$

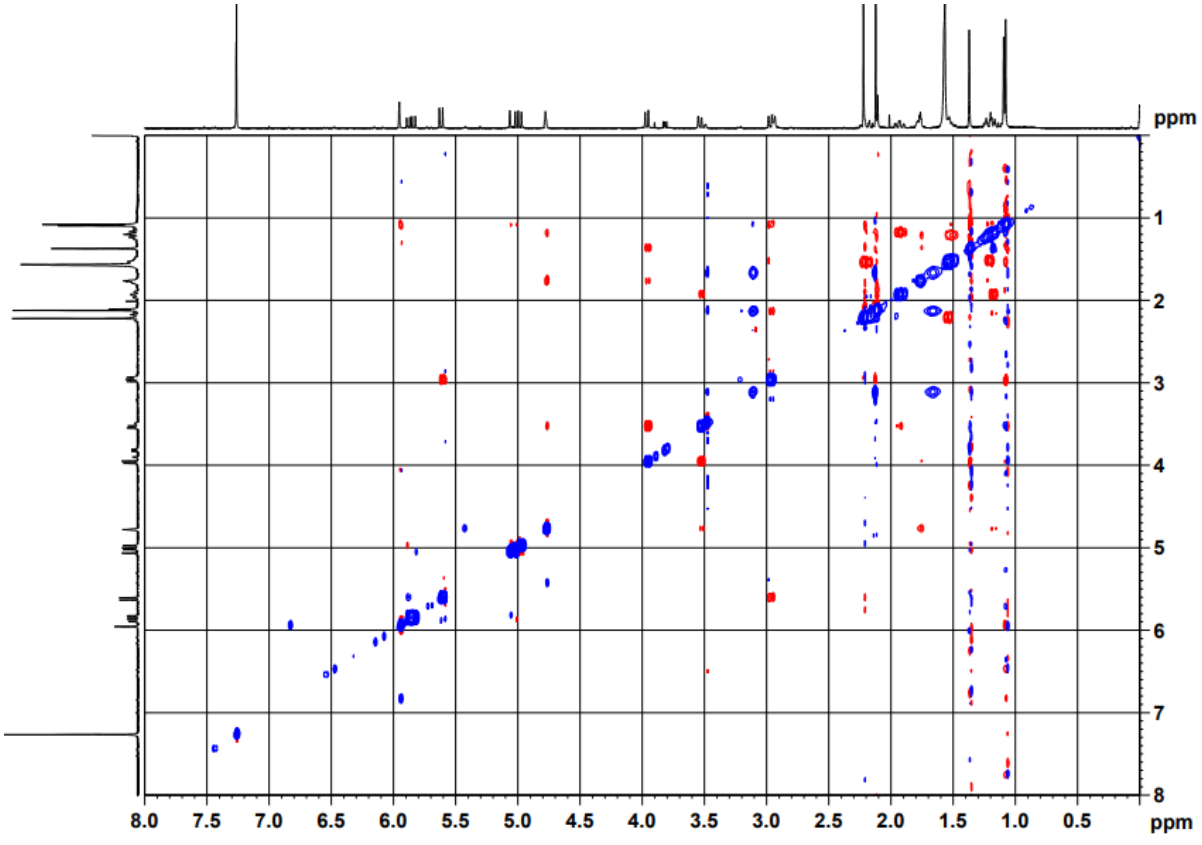
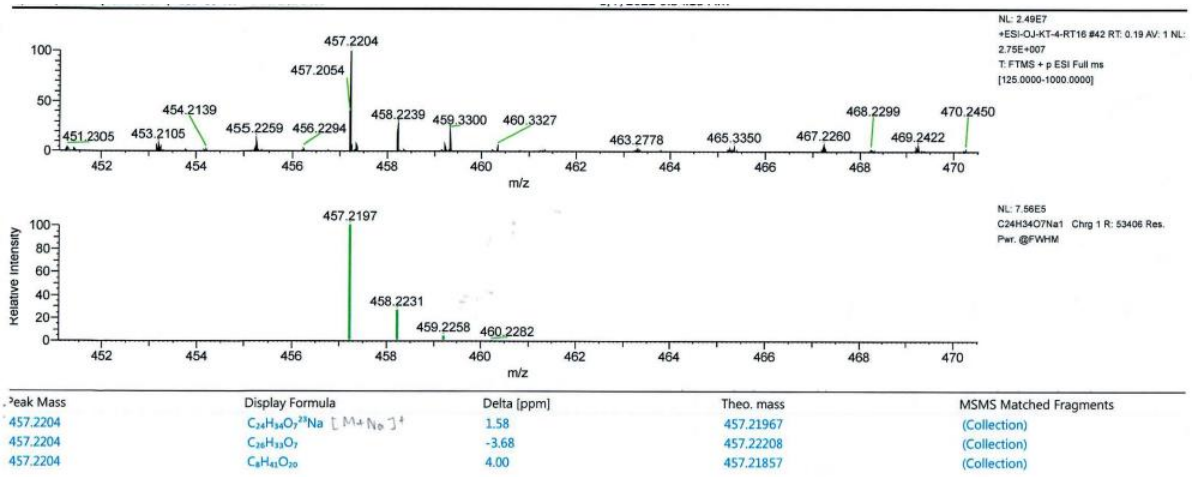


Figure S7 NOESY spectrum of compound **1** in $CDCl_3$



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	MSMS Matched Fragments
457.2204	$C_{24}H_{34}O_7{}^{23}Na$ [M+Na]+	1.58	457.21967	(Collection)
457.2204	$C_{26}H_{33}O_7$	-3.68	457.22208	(Collection)
457.2204	$C_8H_{41}O_{20}$	4.00	457.21857	(Collection)

Figure S8 HREI (+) MS spectrum of compound **1**

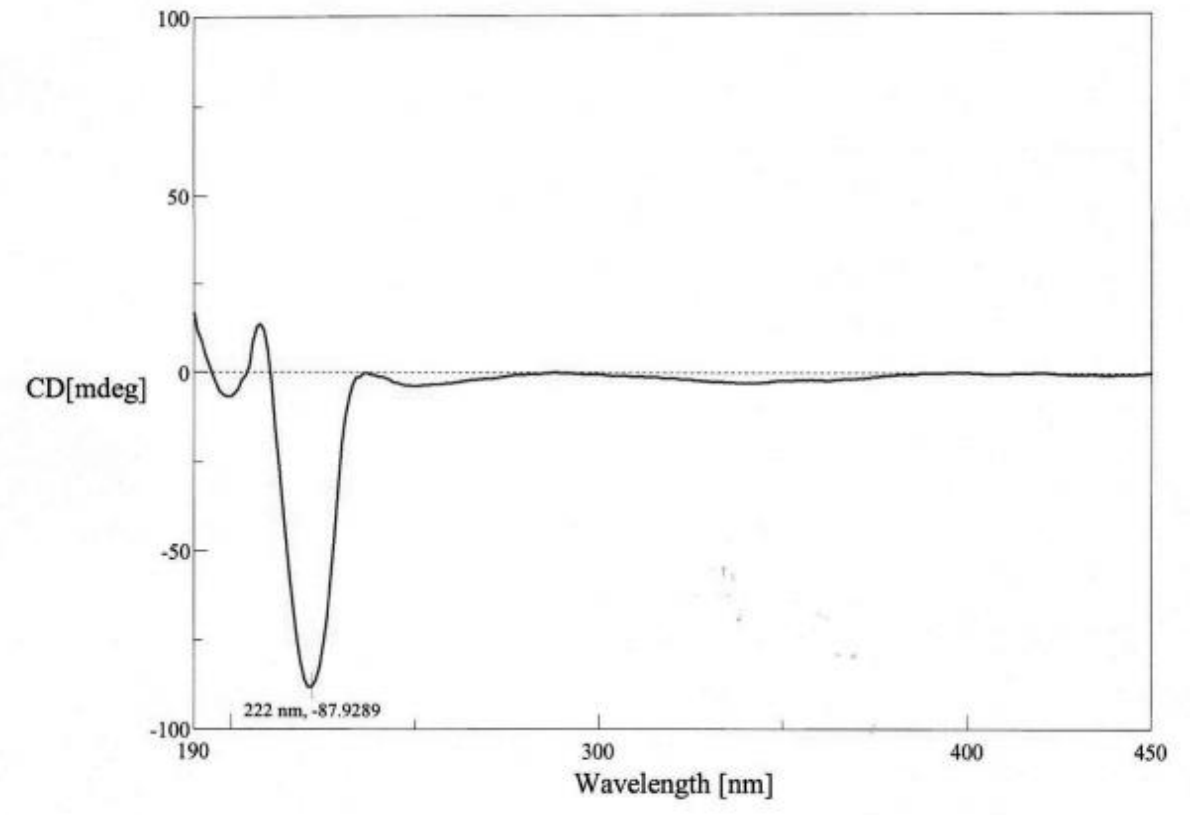


Figure S9 CD spectrum of compound **1**

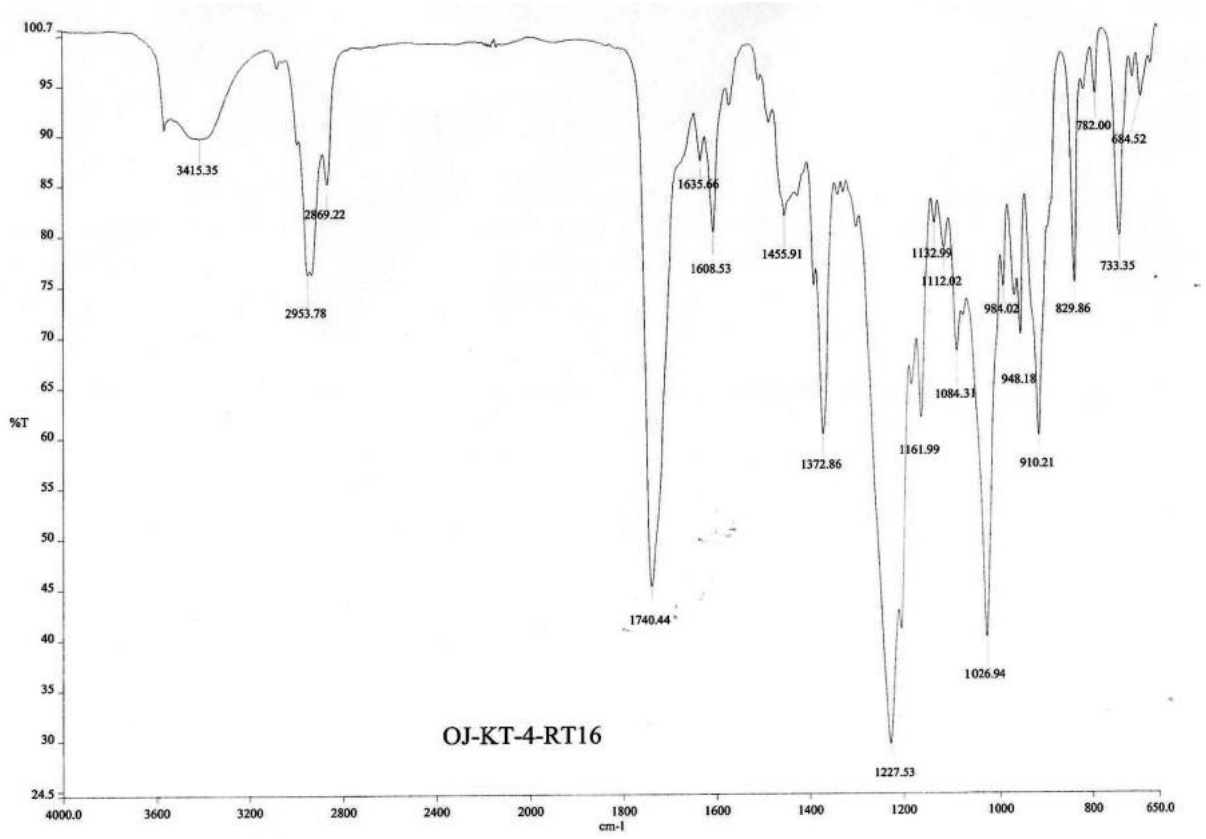


Figure S10 IR spectrum of compound **1**

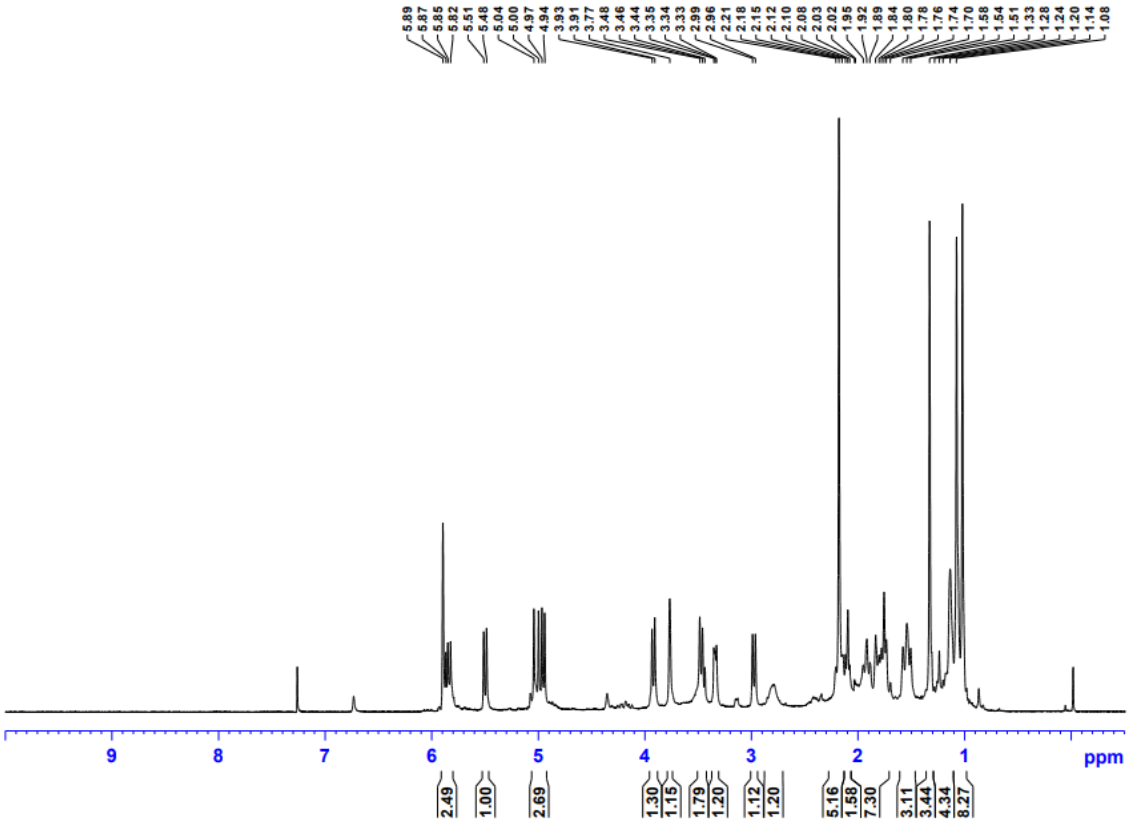


Figure S11 ^{1}H NMR spectrum (400 MHz) of compound **2** in $CDCl_3$

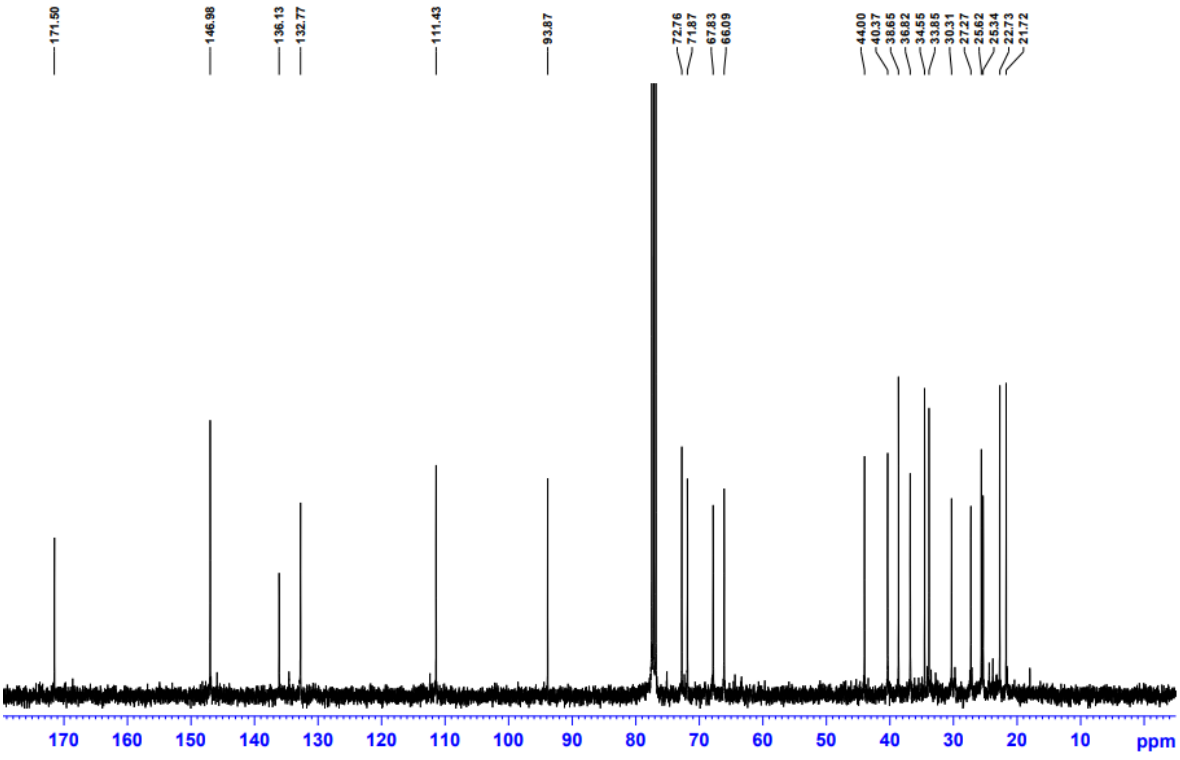


Figure S12 ^{13}C NMR spectrum (100 MHz) of compound **2** in $CDCl_3$

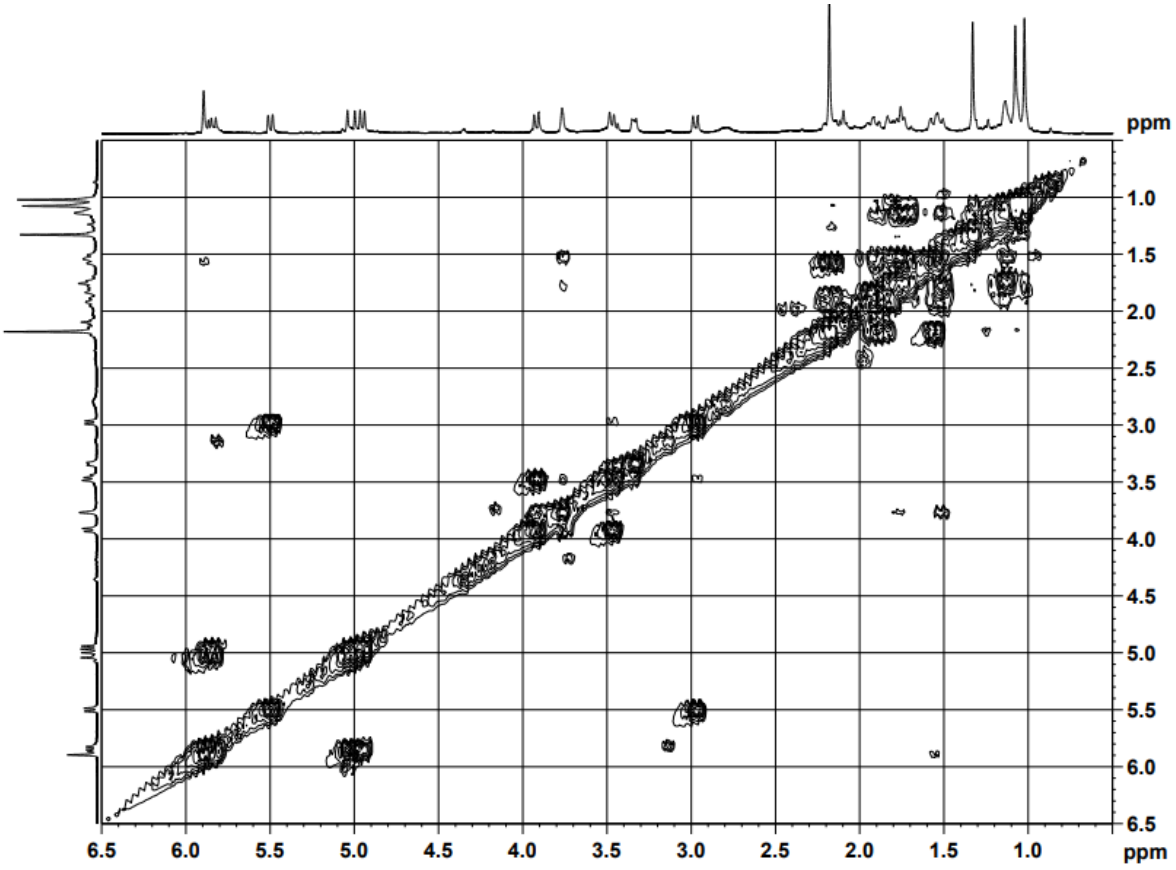


Figure S13 ^{1}H– ^{1}H COSY spectrum of compound **2** in $CDCl_3$

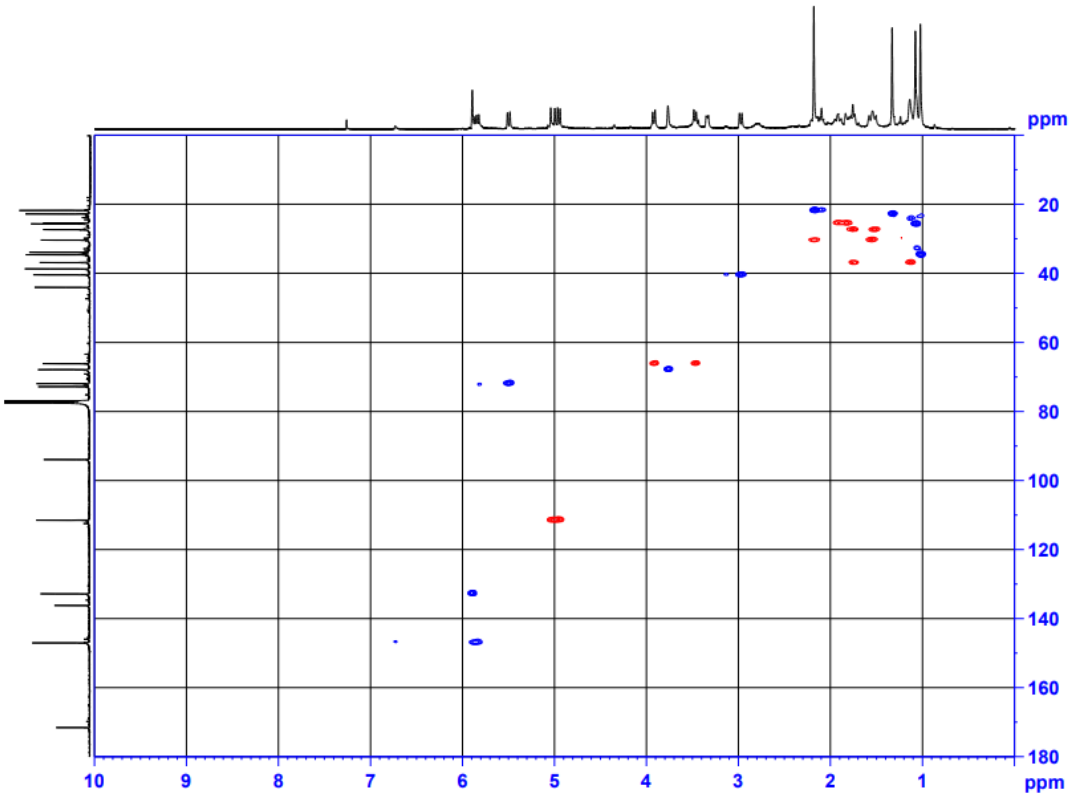


Figure S14 HSQC spectrum of compound **2** in $CDCl_3$

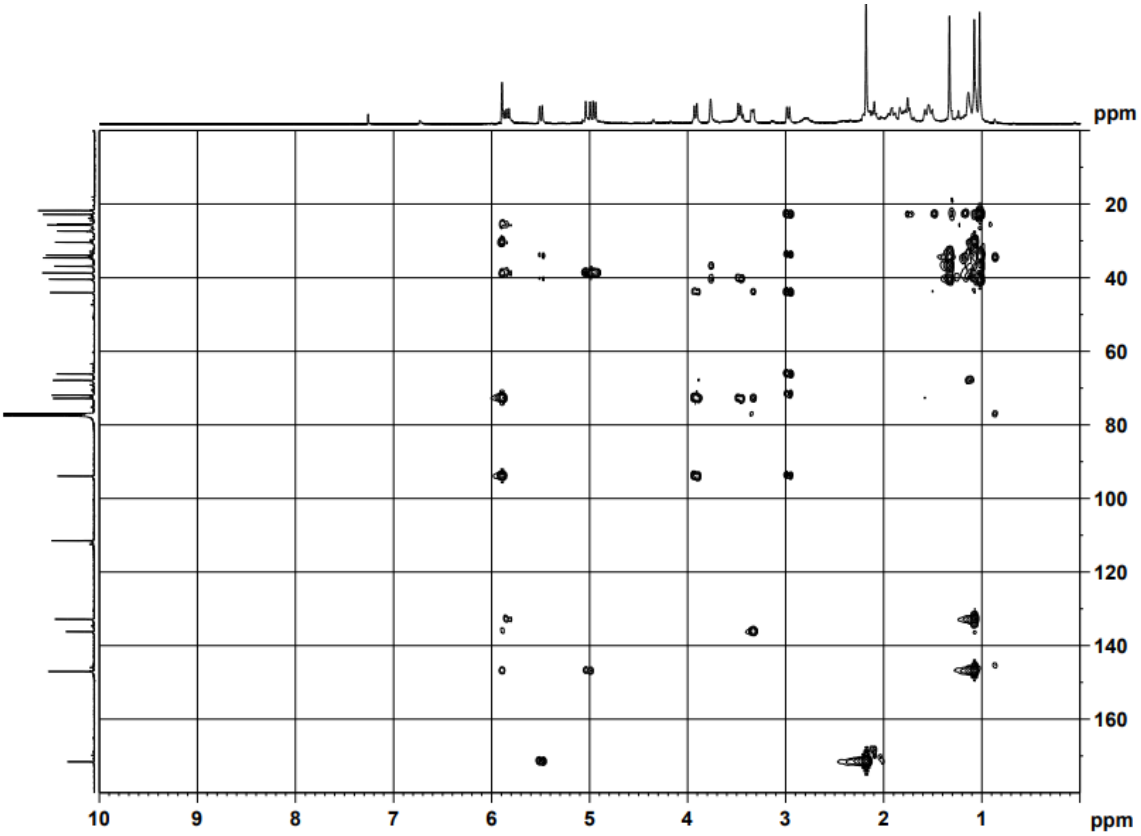


Figure S15 HMBC spectrum of compound **2** in $CDCl_3$

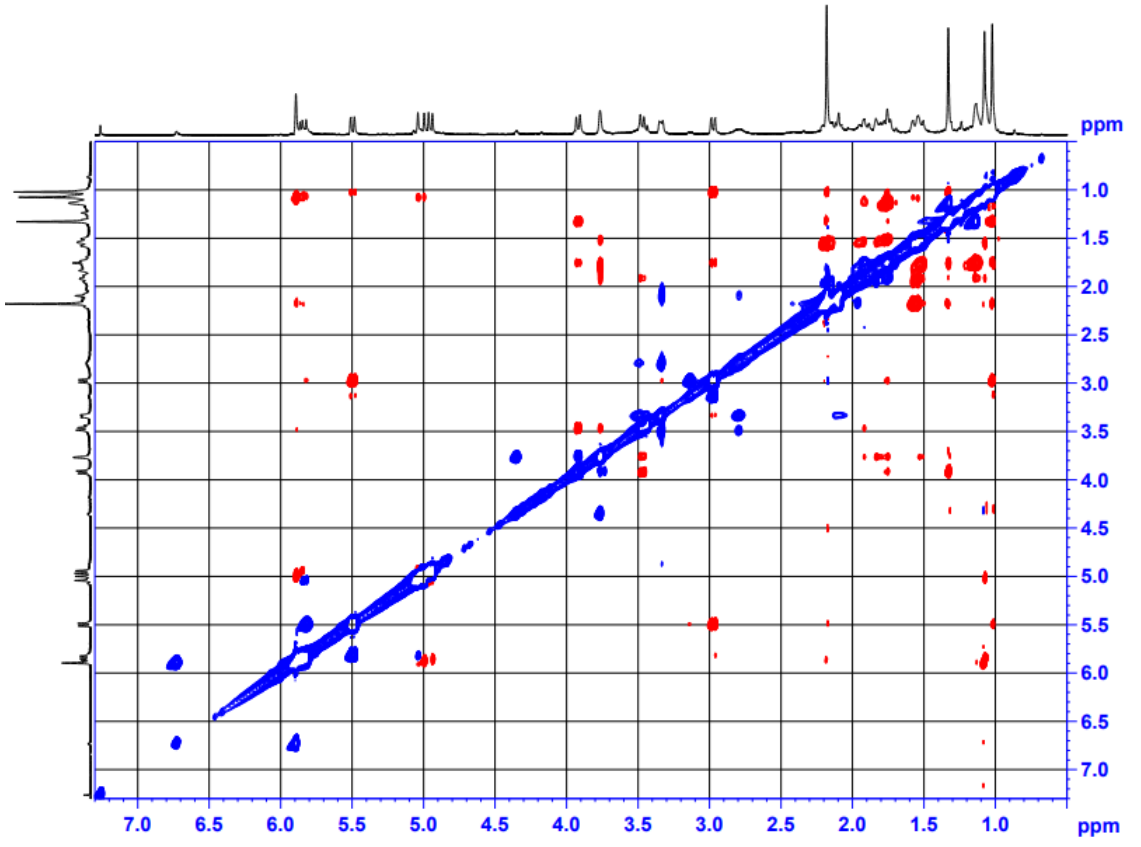
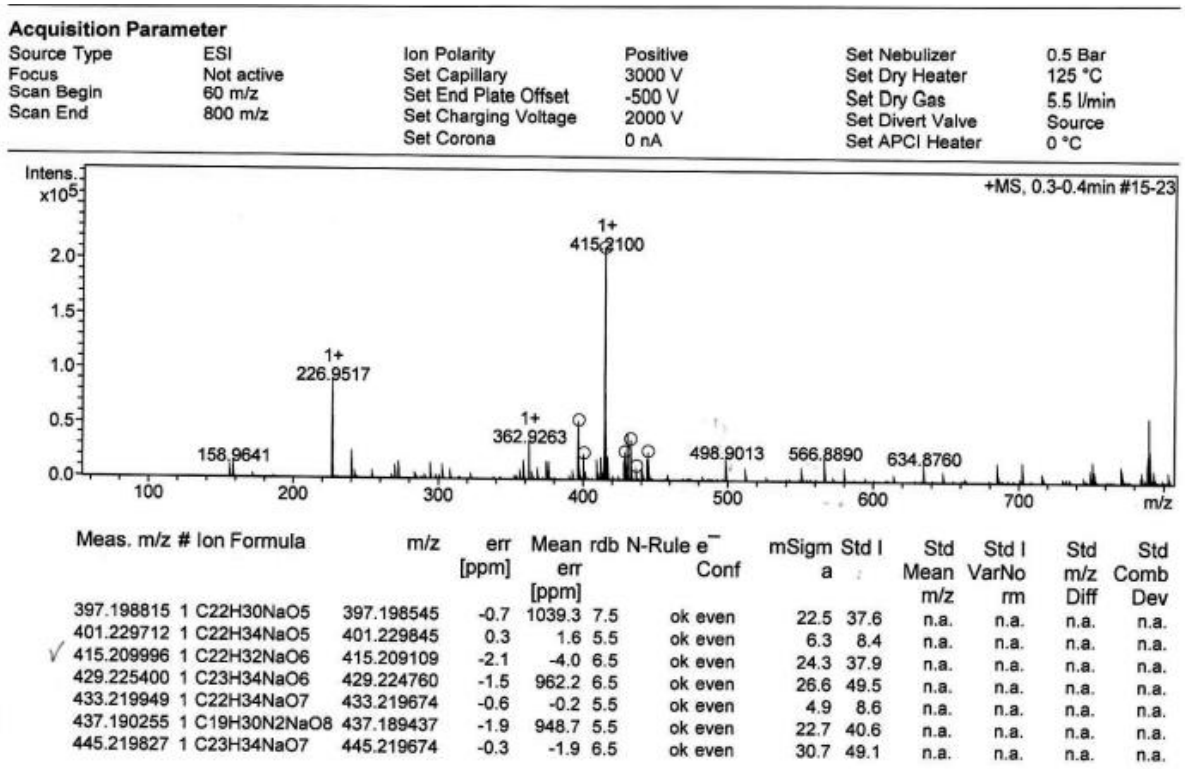


Figure S16 NOESY spectrum of compound **2** in $CDCl_3$



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
397.198815	1	C22H30NaO5	397.198545	-0.7	1039.3	7.5		ok even	22.5	37.6	n.a.	n.a.	n.a.	n.a.
401.229712	1	C22H34NaO5	401.229845	0.3	1.6	5.5		ok even	6.3	8.4	n.a.	n.a.	n.a.	n.a.
√ 415.209996	1	C22H32NaO6	415.209109	-2.1	-4.0	6.5		ok even	24.3	37.9	n.a.	n.a.	n.a.	n.a.
429.225400	1	C23H34NaO6	429.224760	-1.5	962.2	6.5		ok even	26.6	49.5	n.a.	n.a.	n.a.	n.a.
433.219949	1	C22H34NaO7	433.219674	-0.6	-0.2	5.5		ok even	4.9	8.6	n.a.	n.a.	n.a.	n.a.
437.190255	1	C19H30N2NaO8	437.189437	-1.9	948.7	5.5		ok even	22.7	40.6	n.a.	n.a.	n.a.	n.a.
445.219827	1	C23H34NaO7	445.219674	-0.3	-1.9	6.5		ok even	30.7	49.1	n.a.	n.a.	n.a.	n.a.

Figure S17 HREI (+) MS spectrum of compound **2**

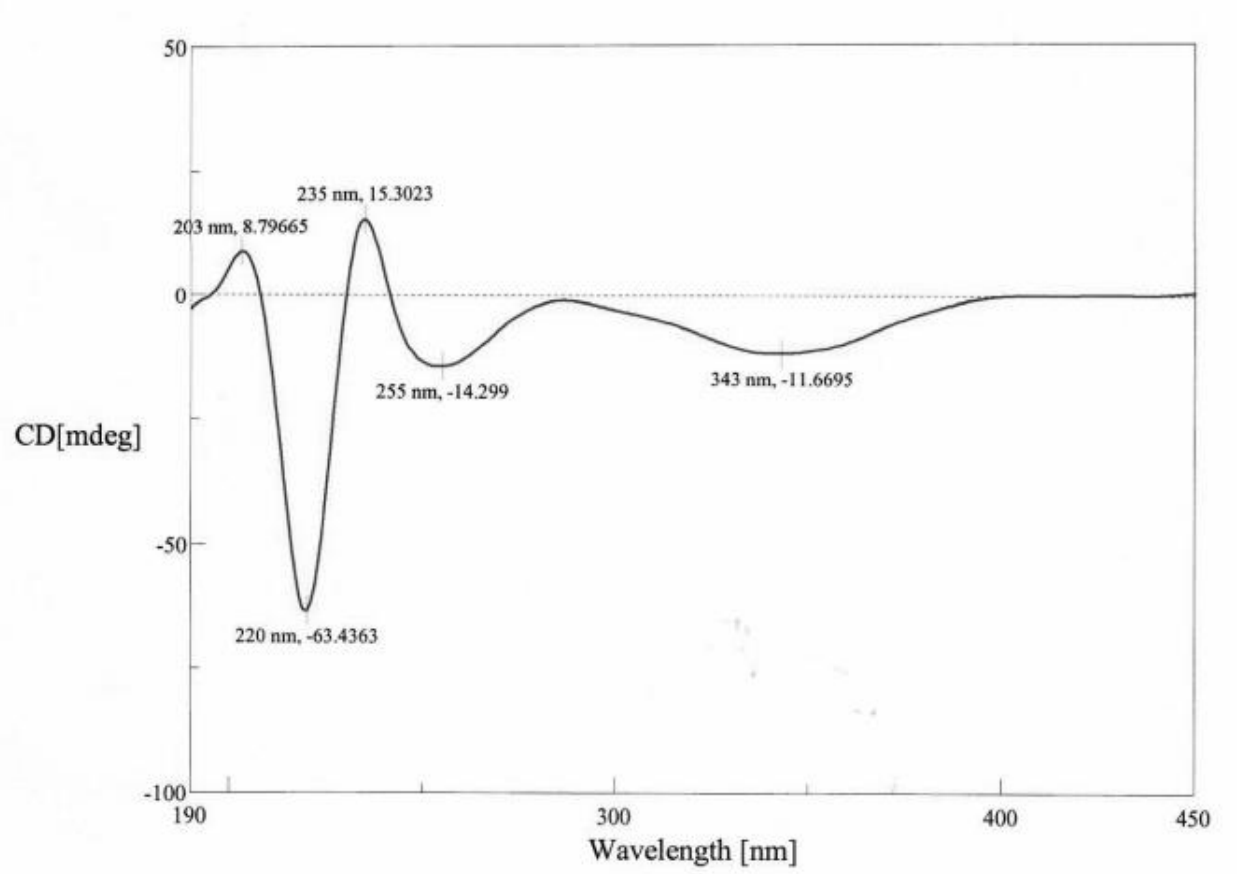


Figure S18 CD spectrum of compound **2**

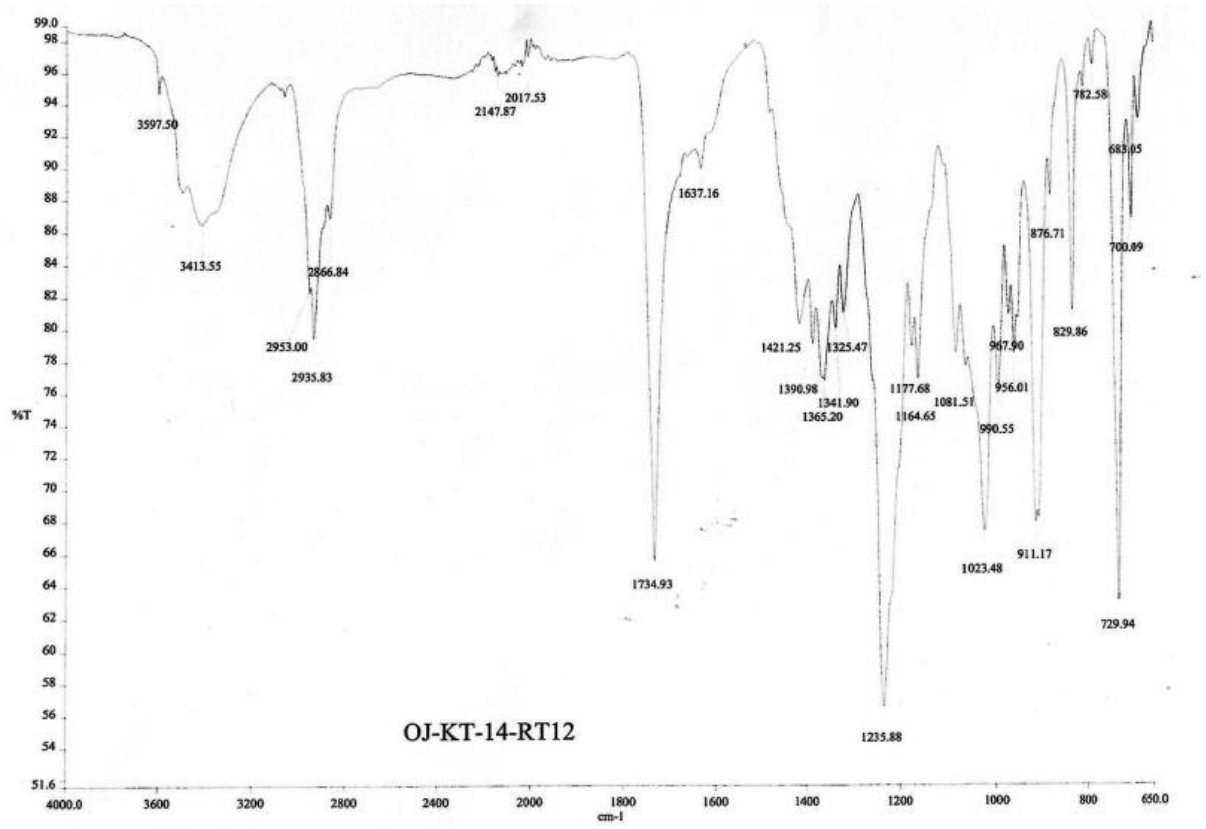


Figure S19 IR spectrum of compound **2**

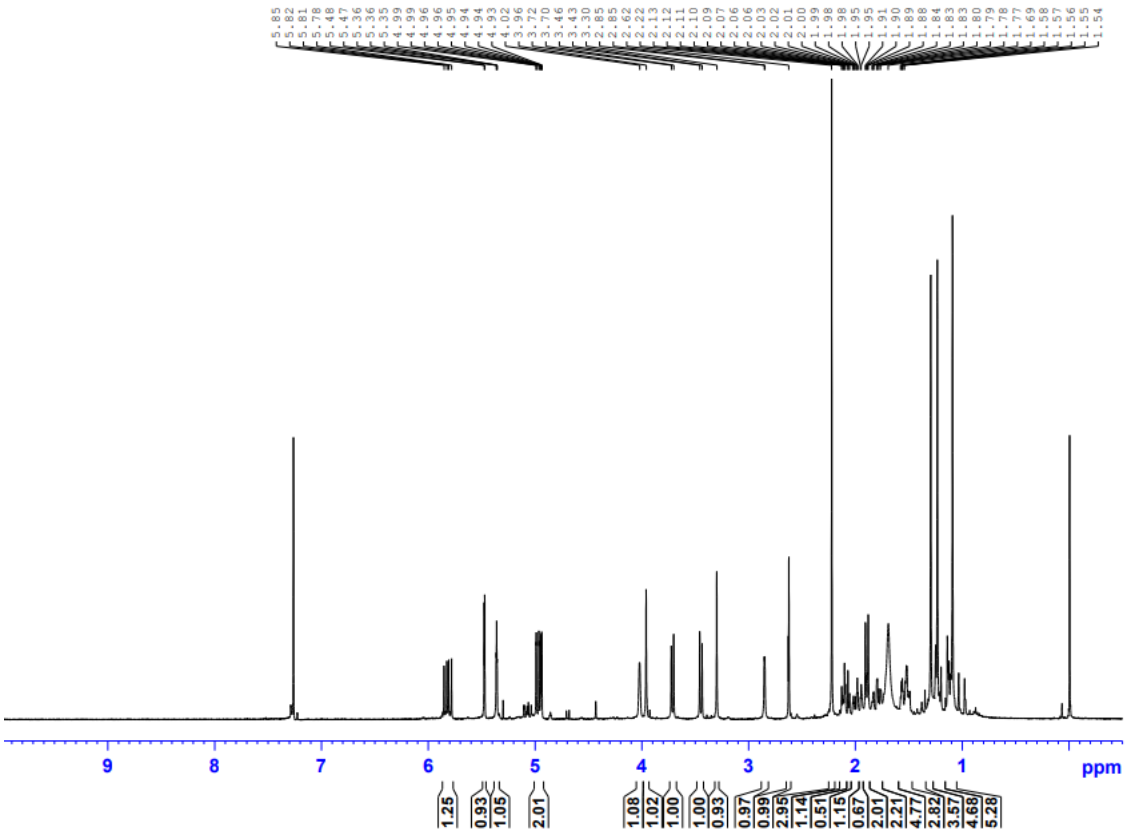


Figure S20 ^{1}H NMR spectrum (400 MHz) of compound **3** in $CDCl_3$

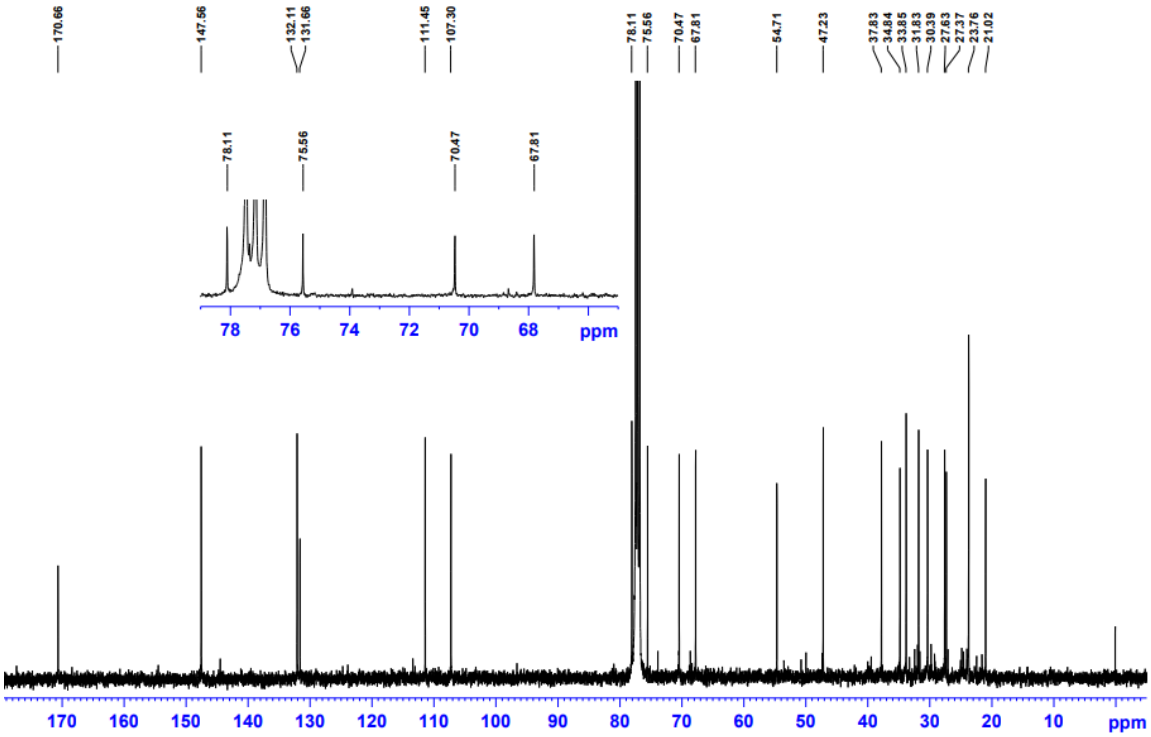


Figure S21 ^{13}C NMR spectrum (100 MHz) of compound **3** in $CDCl_3$

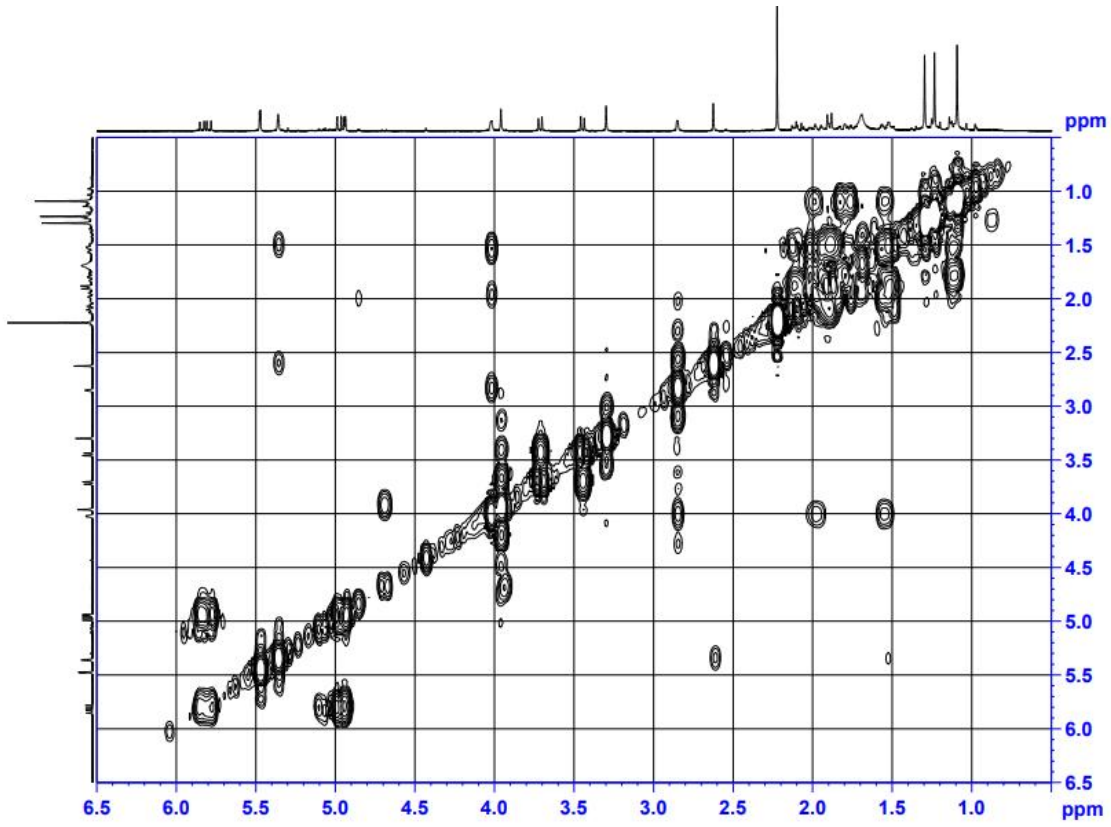


Figure S22 ^{1}H– ^{1}H COSY spectrum of compound **3** in $CDCl_3$

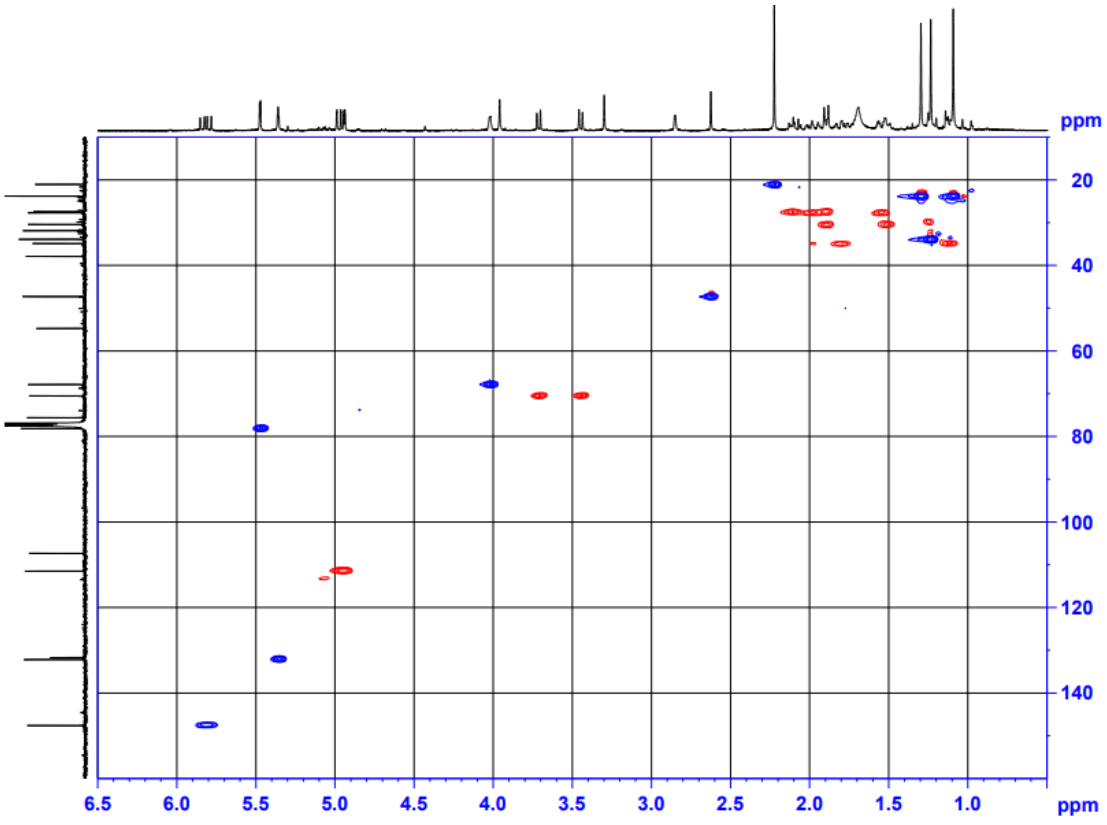


Figure S23 HSQC spectrum of compound **3** in $CDCl_3$

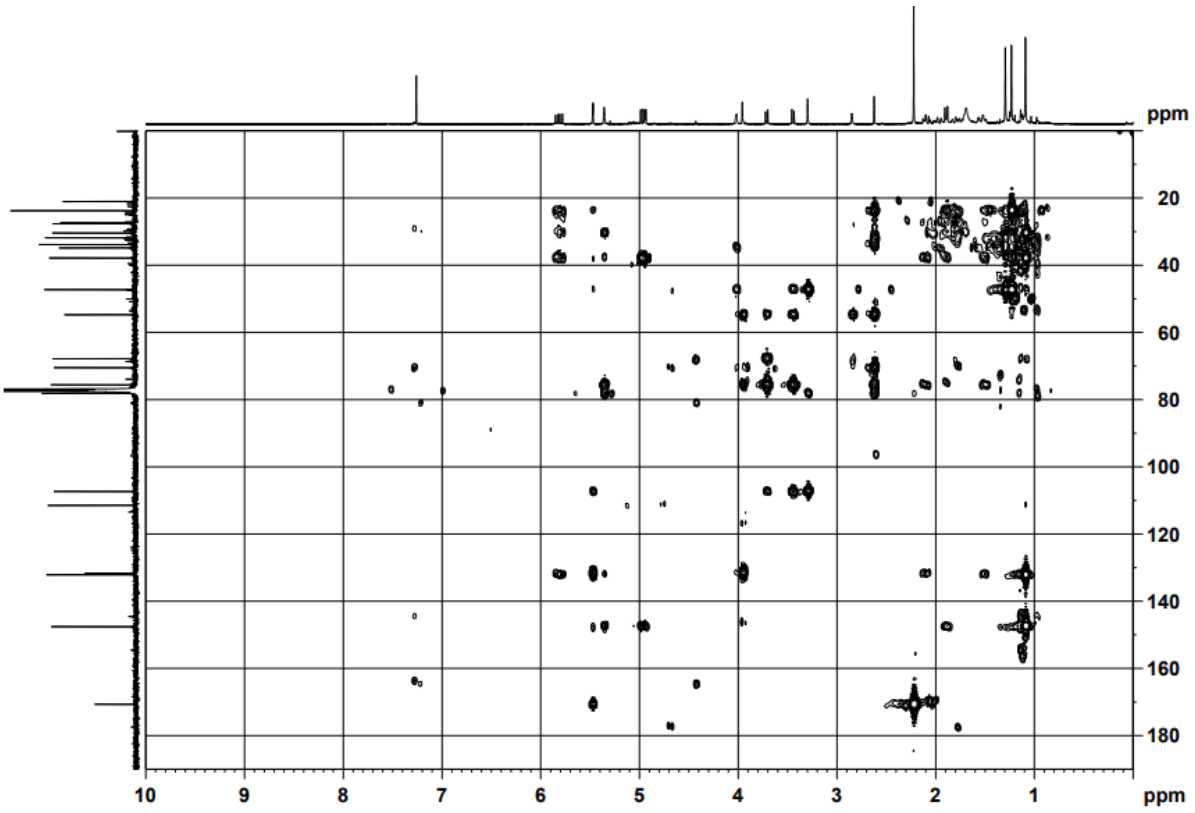


Figure S24 HMBC spectrum of compound **3** in $CDCl_3$

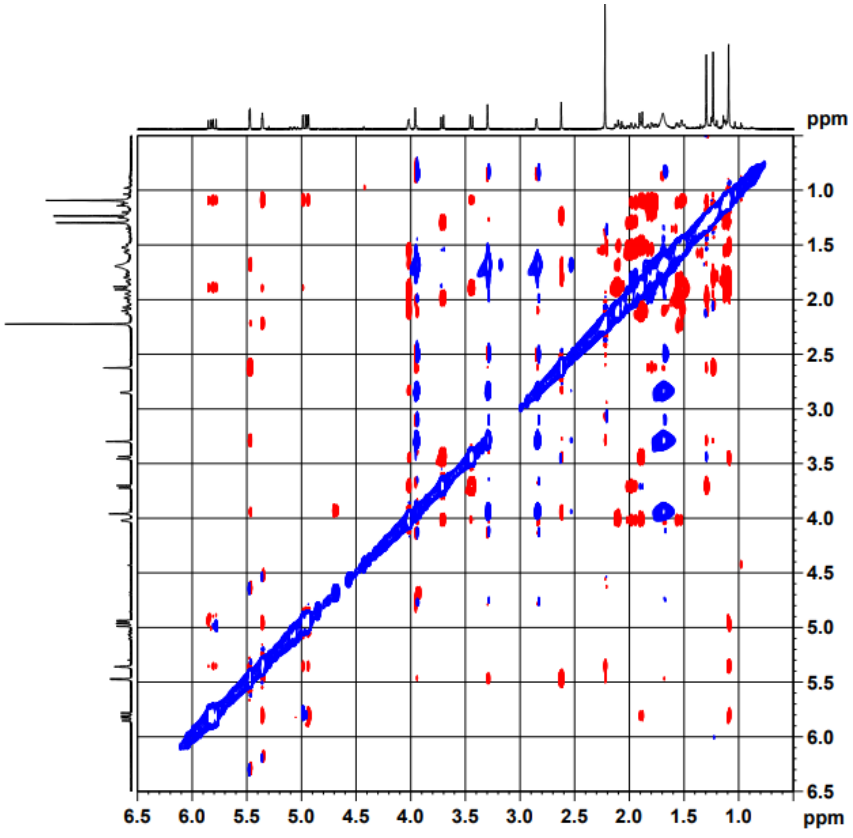


Figure S25 NOESY spectrum of compound **3** in $CDCl_3$

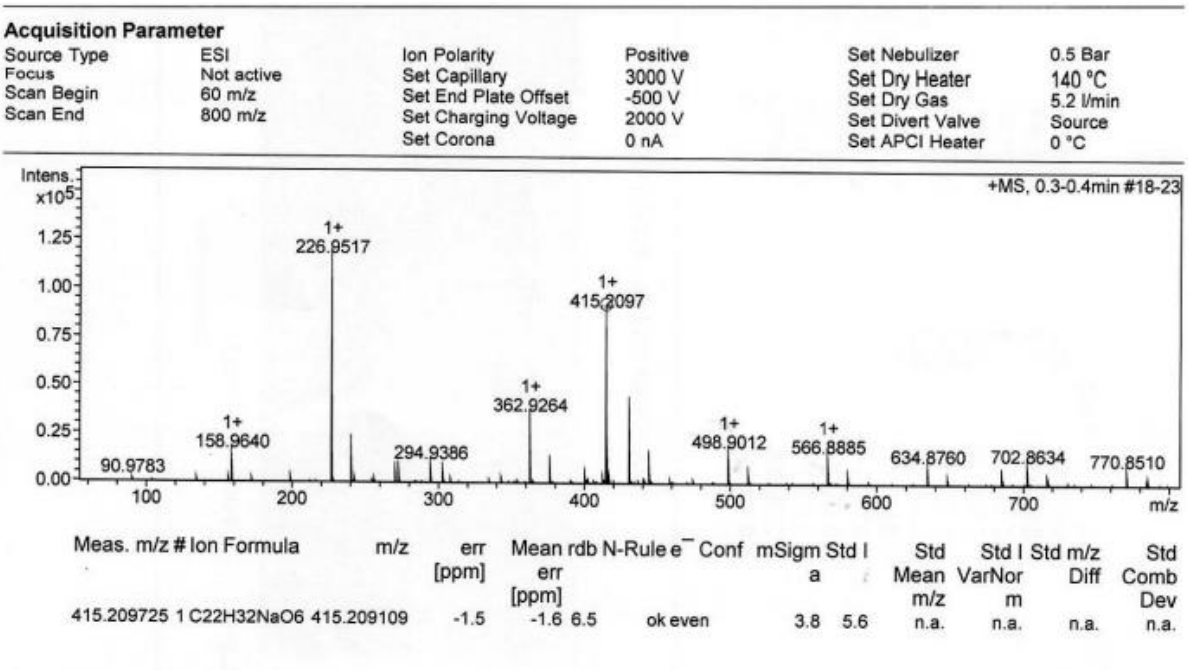


Figure S26 HREI (+) MS spectrum of compound **3**

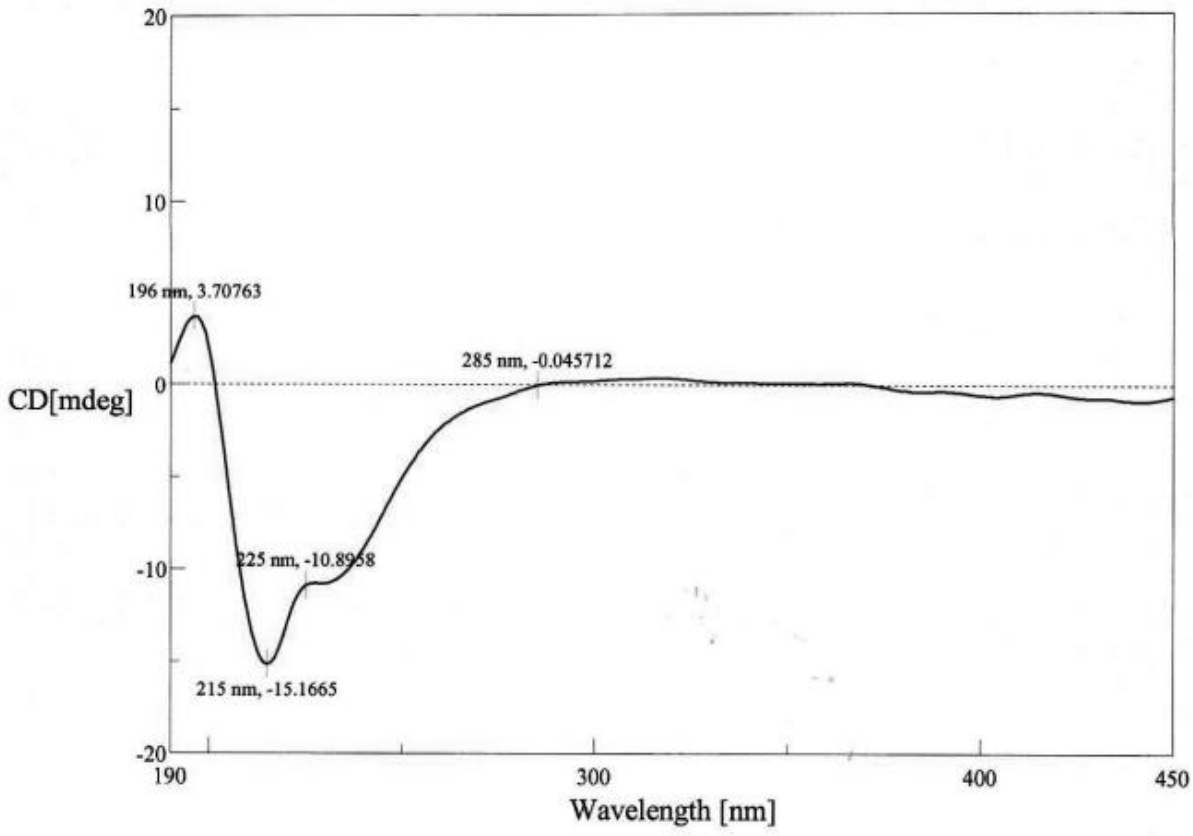


Figure S27 CD spectrum of compound **3**

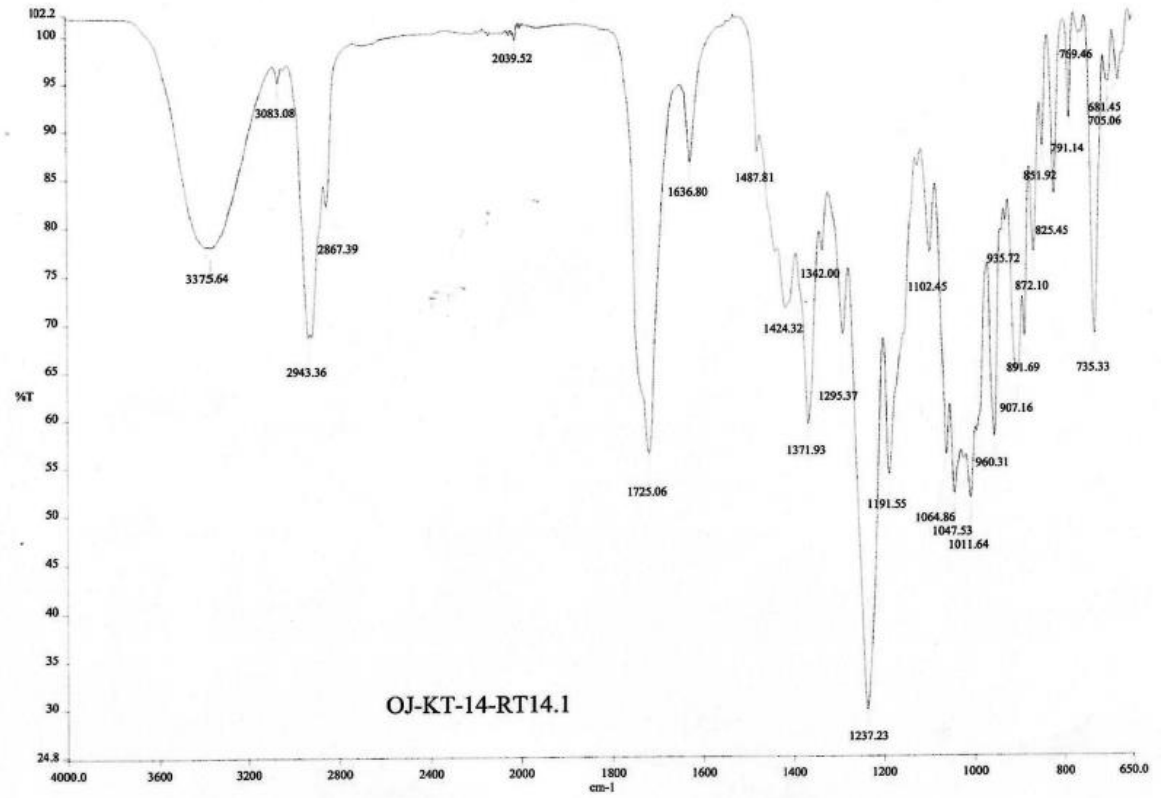


Figure S28 IR spectrum of compound **3**

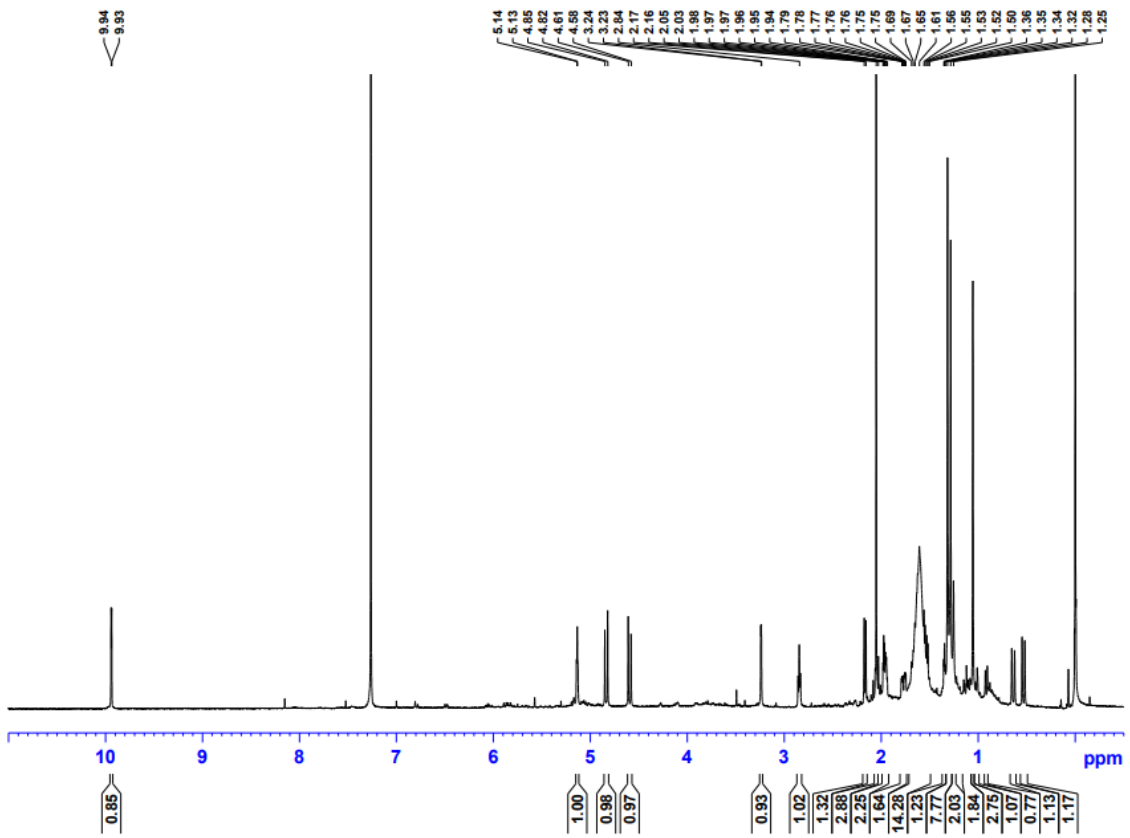


Figure S29 ^{1}H NMR spectrum (400 MHz) of compound **4** in $CDCl_3$

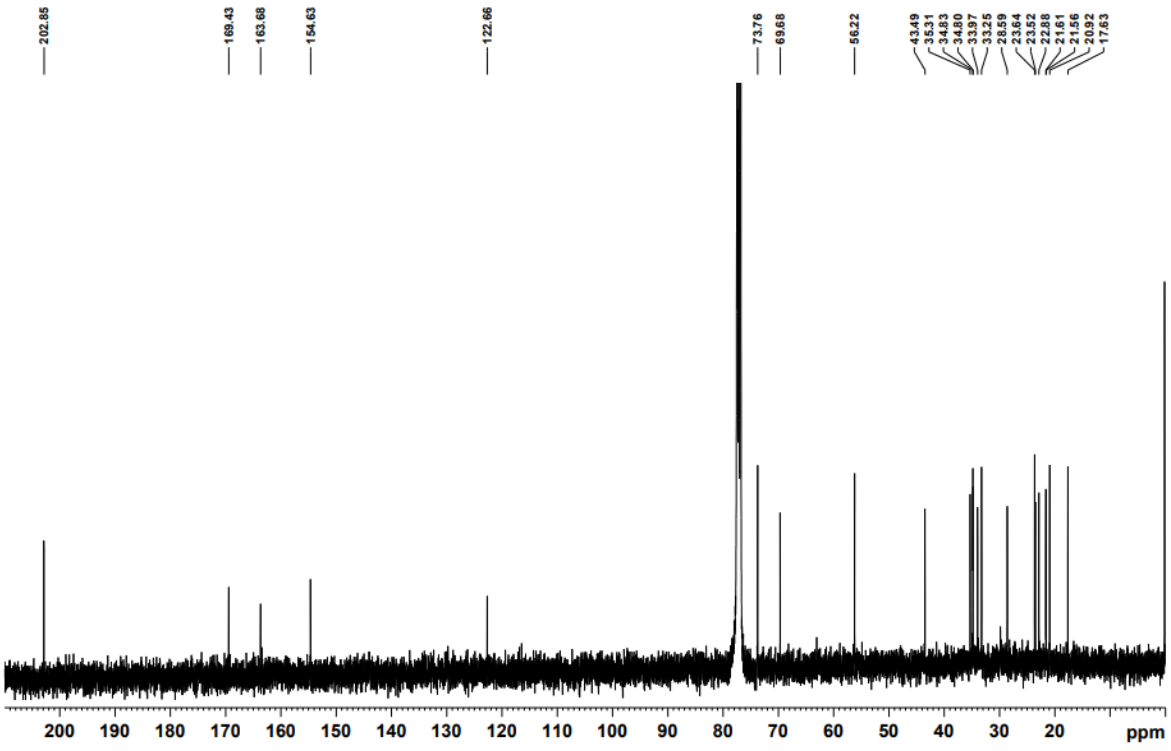


Figure S30 ^{13}C NMR spectrum (100 MHz) of compound **4** in $CDCl_3$

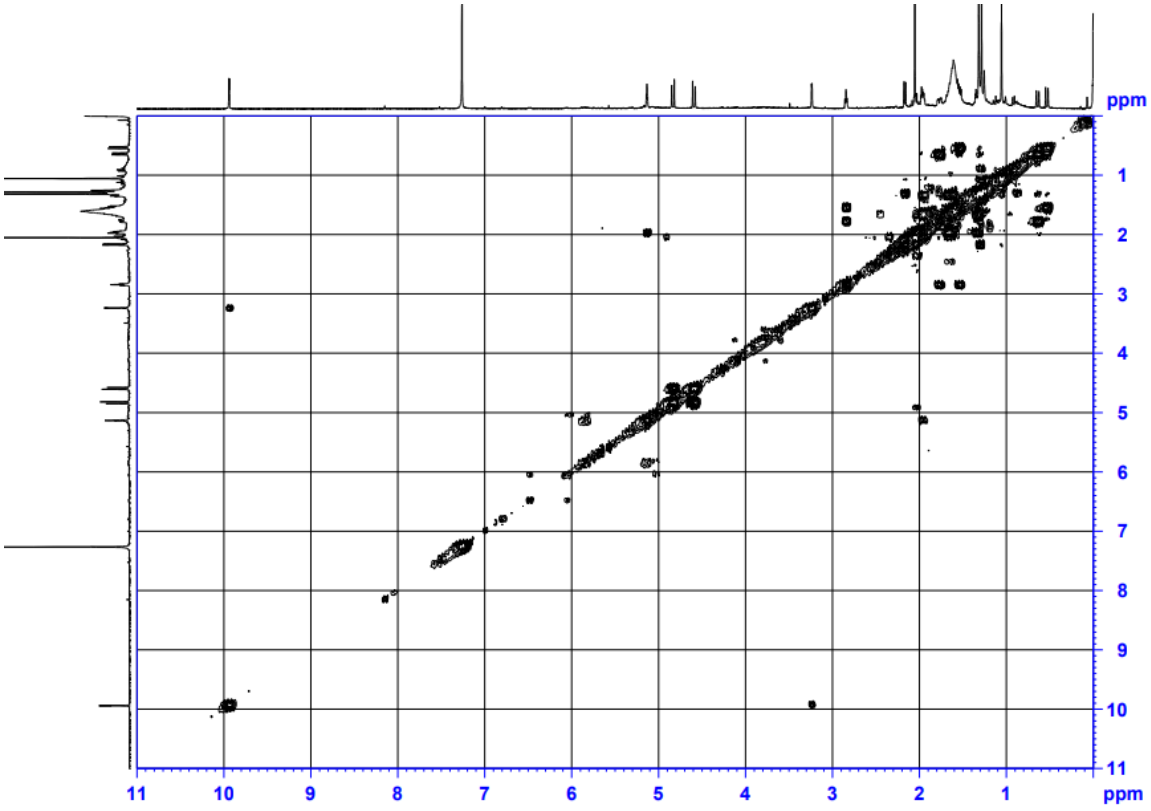


Figure S31 ^{1}H– ^{1}H COSY spectrum of compound **4** in $CDCl_3$

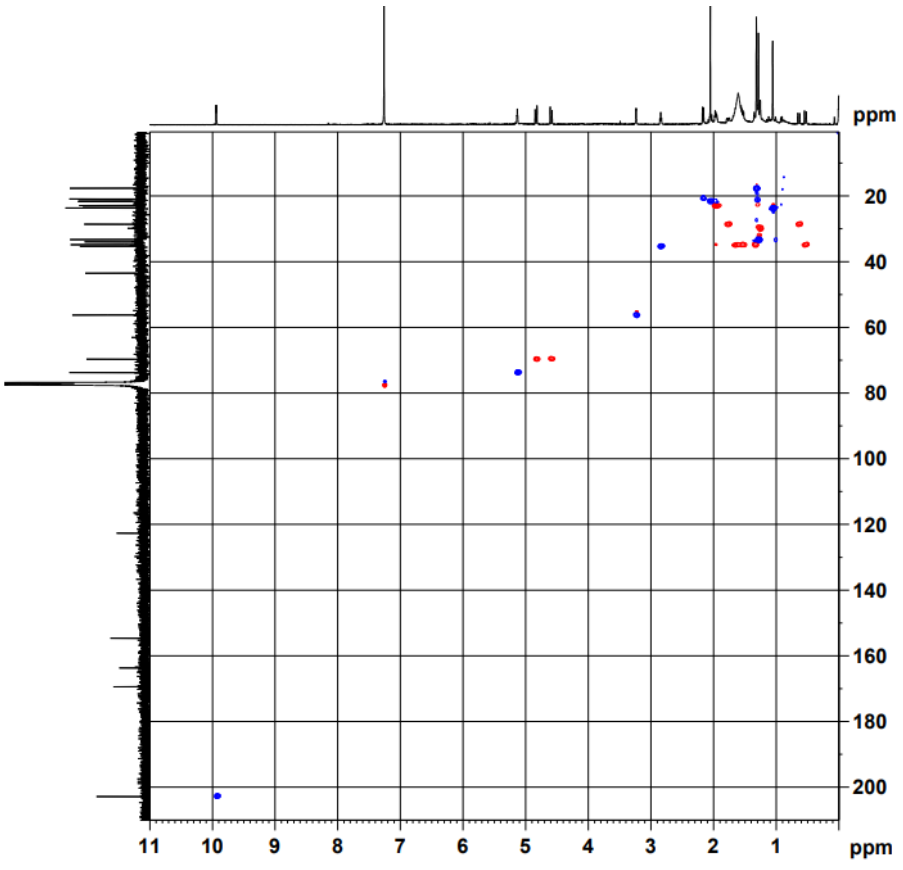


Figure S32 HSQC spectrum of compound **4** in $CDCl_3$

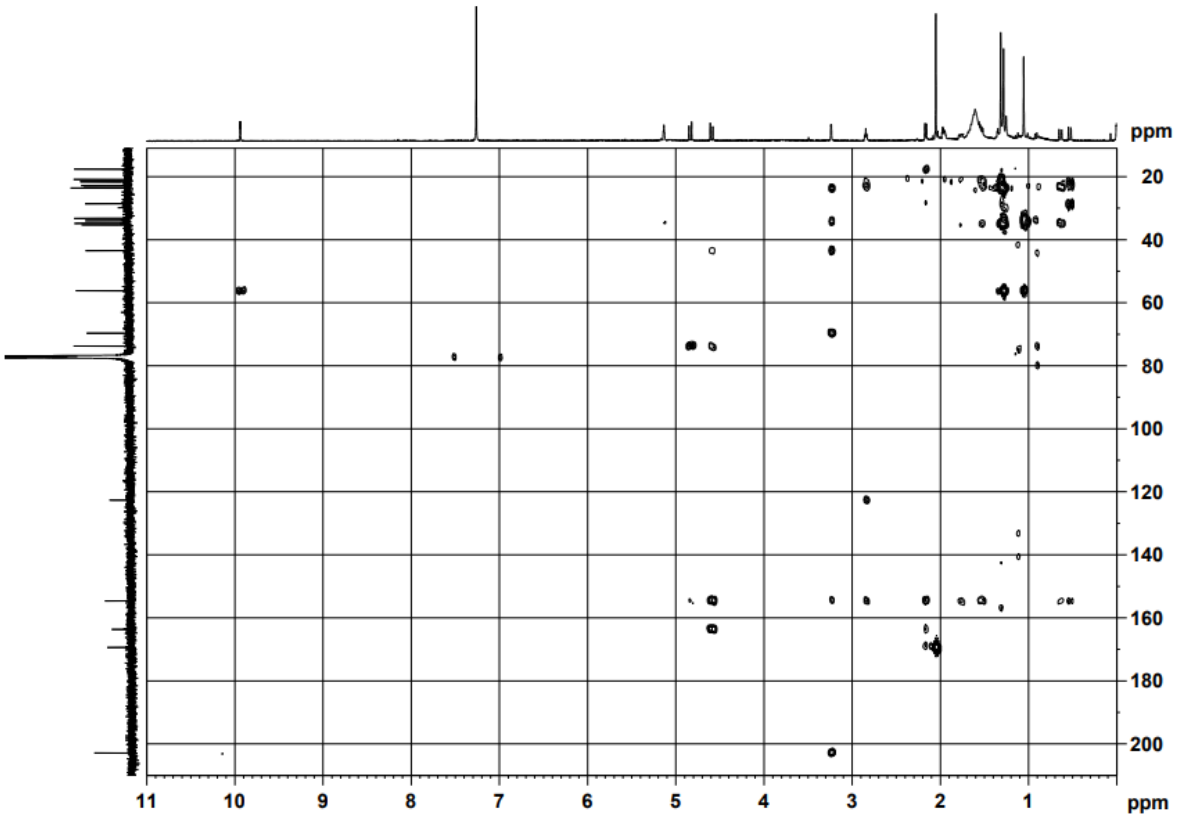


Figure S33 HMBC spectrum of compound **4** in $CDCl_3$

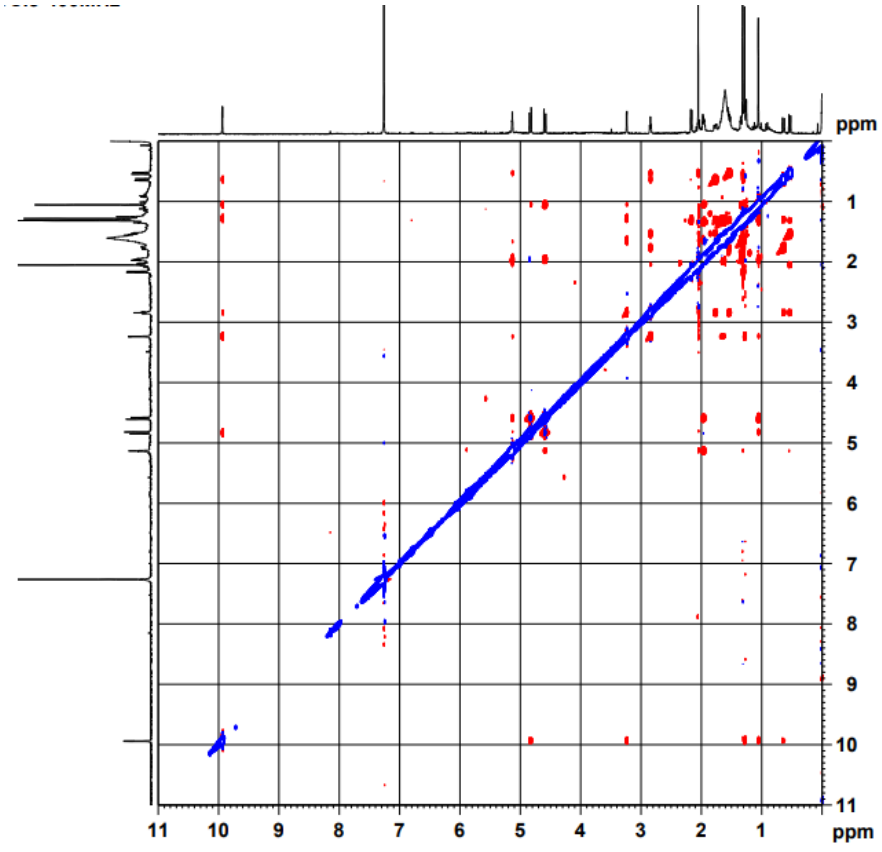


Figure S34 NOESY spectrum of compound **4** in $CDCl_3$

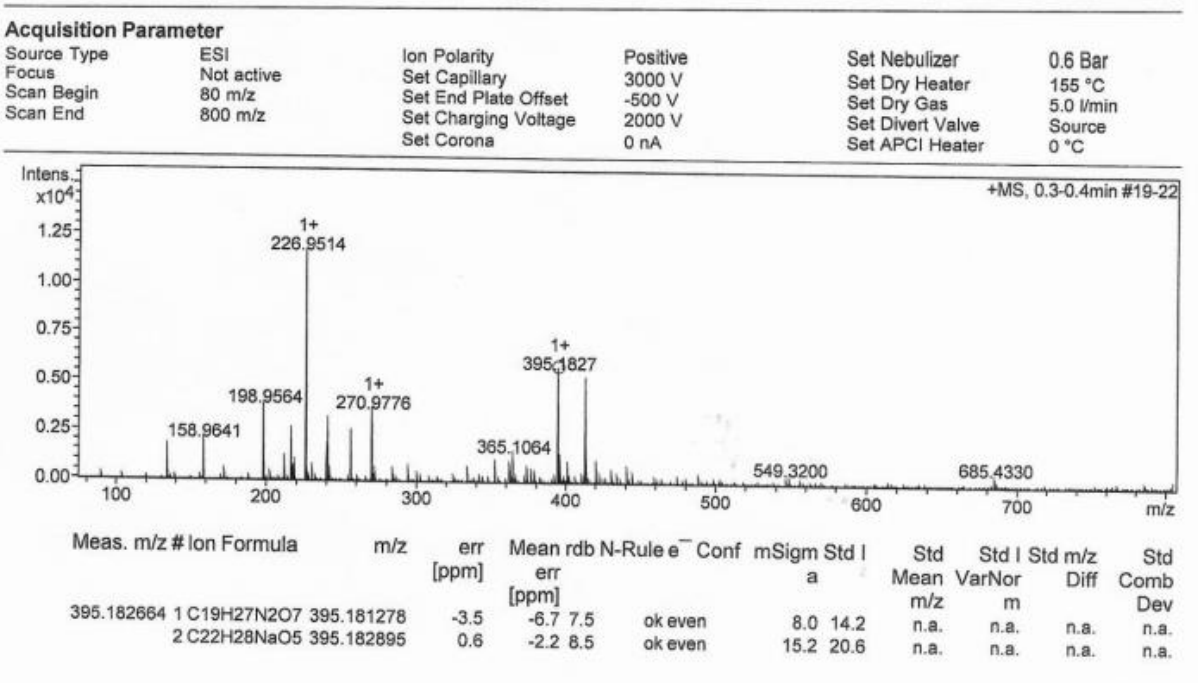


Figure S35 HREI (+) MS spectrum of compound **4**

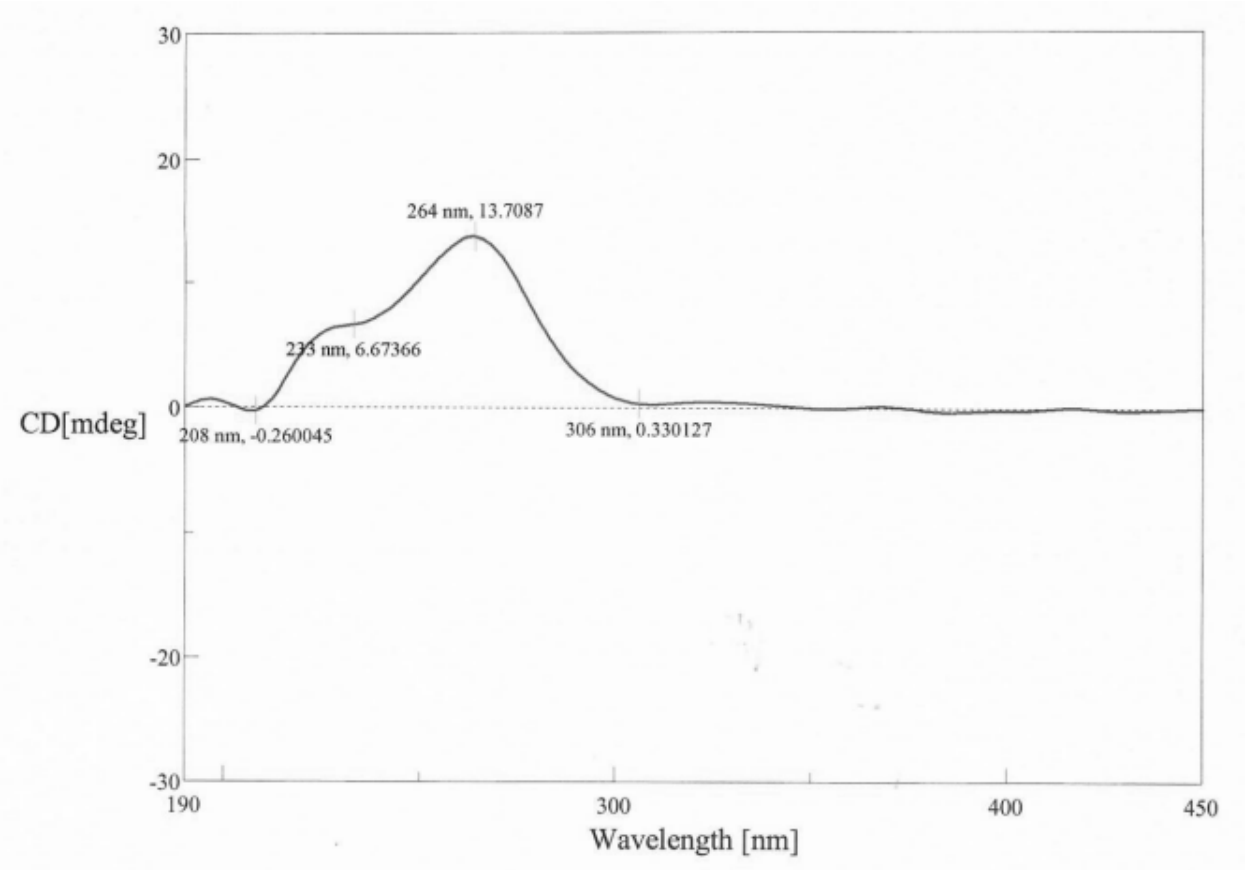


Figure S36 CD spectrum of compound **4**

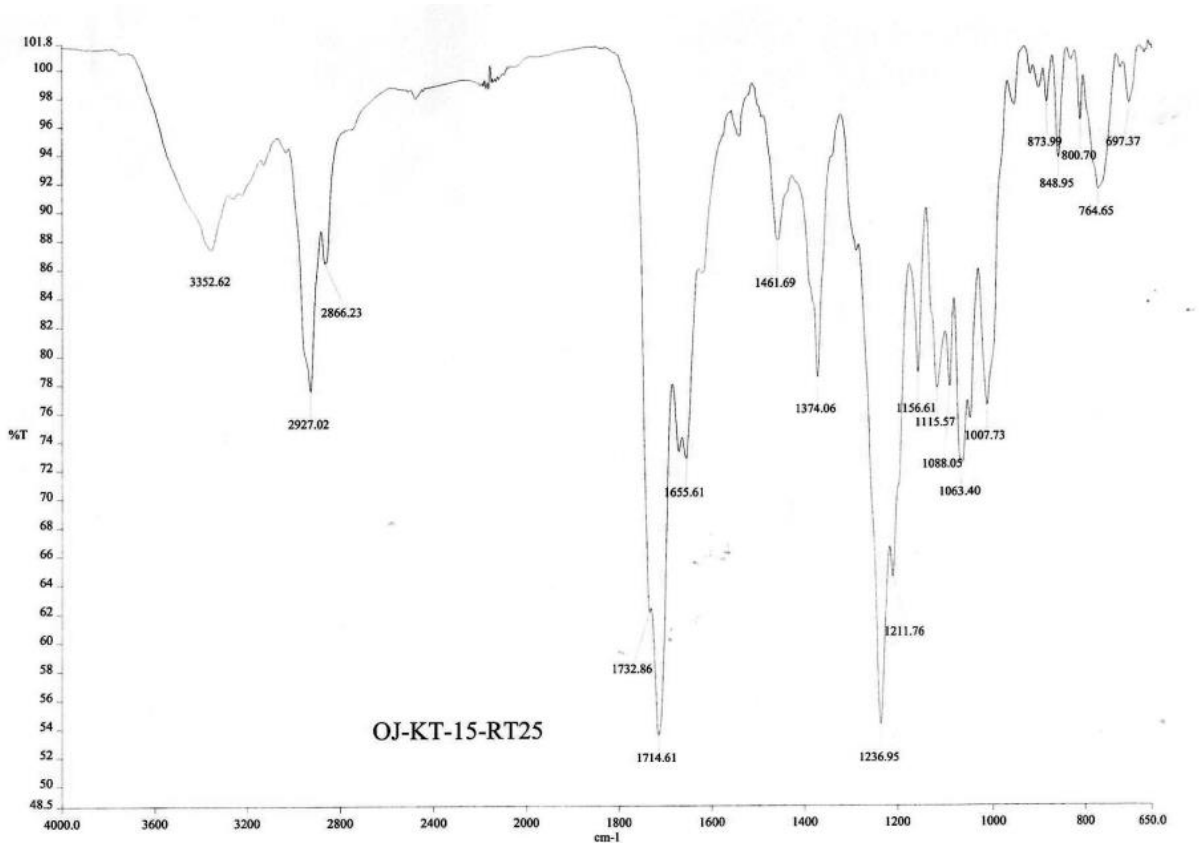


Figure S37 IR spectrum of compound **4**