

Supporting Information

Spiromyrrhenes A–D: Unprecedented Diterpene-Sesquiterpene Heterodimers as intermolecular [4+2] cycloaddition products from *Resina Commiphora* That Inhibit Tumor Stemness in Esophageal Cancer

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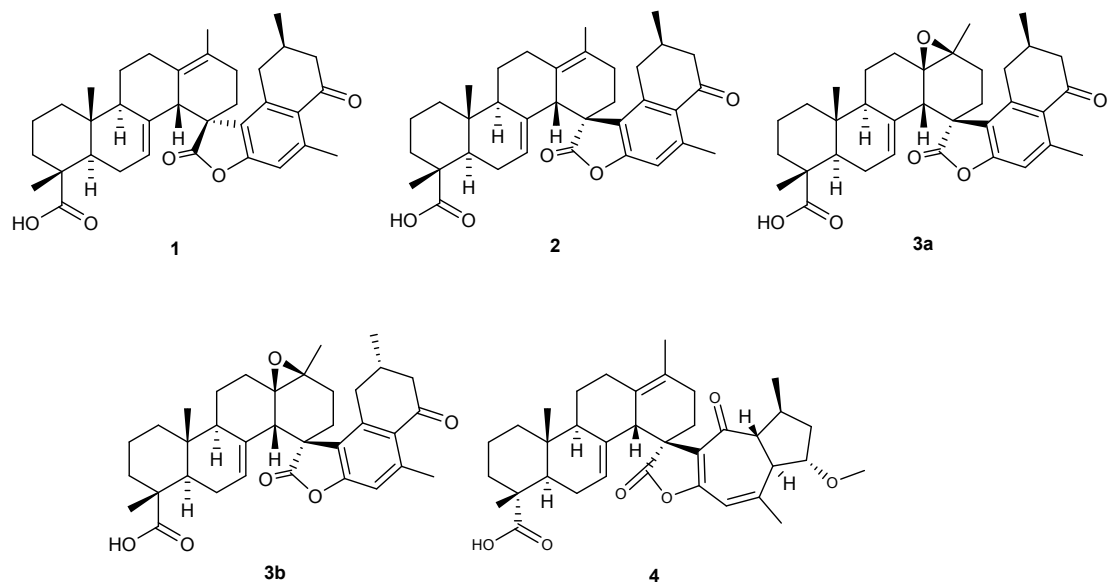


Figure S1. Five model compounds designed for the quantum chemical NMR calculation of compounds **1**, **2**, **3a**, **3b** and **4**.

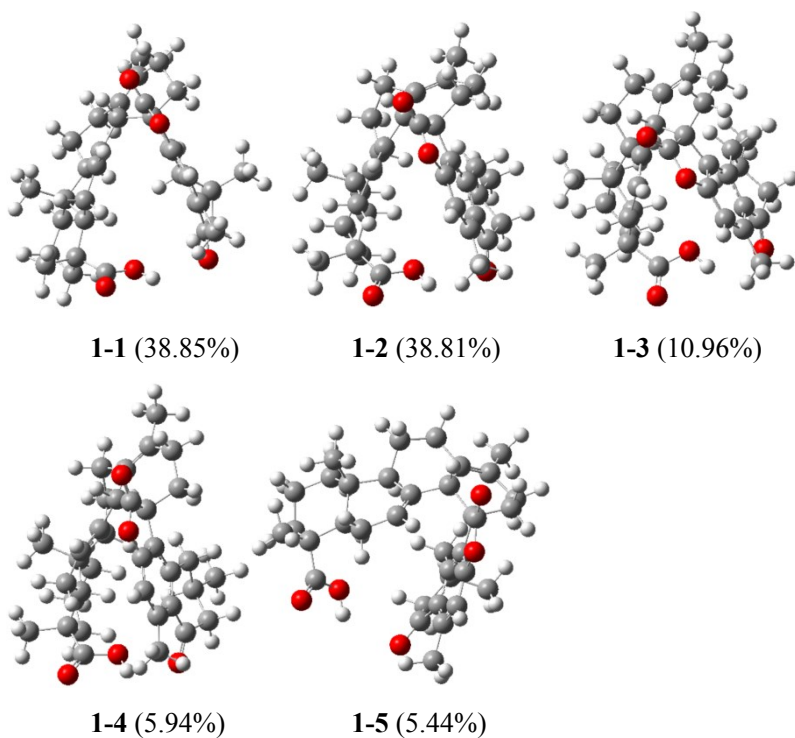
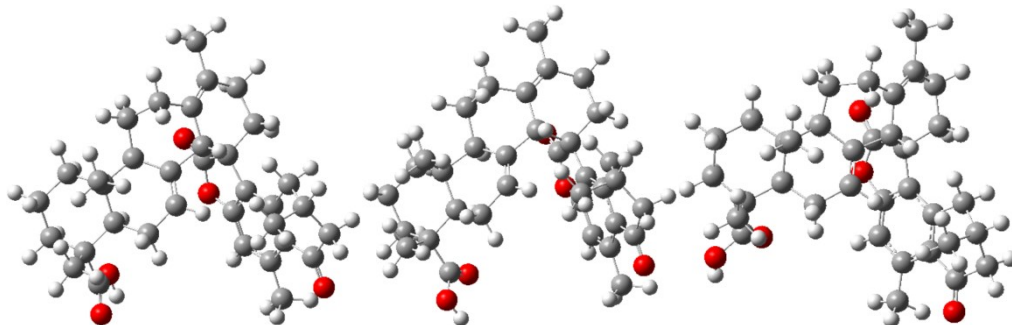


Figure S2. The lowest energy conformers of **1** (the relative populations are in parentheses).



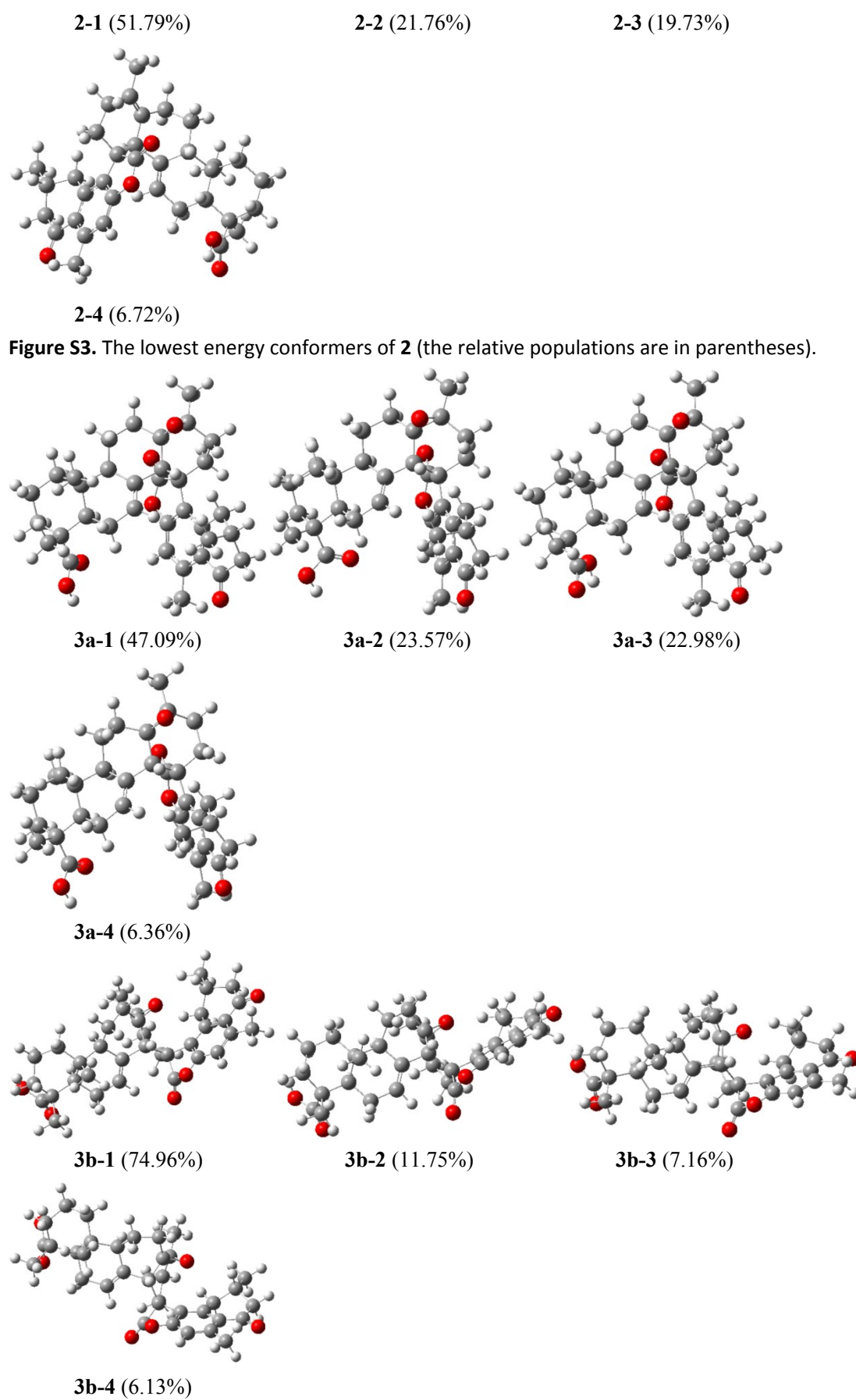


Figure S4. The lowest energy conformers of **3a** and **3b** (the relative populations are in parentheses).

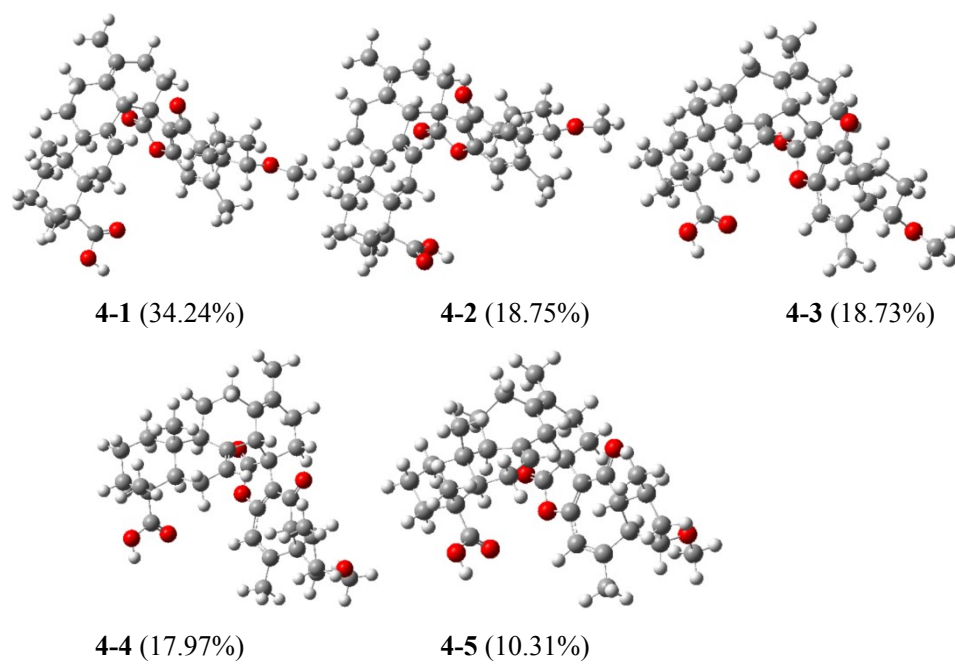


Figure S5. The lowest energy conformers of **4** (the relative populations are in parentheses).

Table S1. Extracted heats and weighting factors of the optimized conformers and the cartesian coordinates for **1**, **2**, **3a**, **3b** and **4**

		B3LYP/6-311+G(d)					
		Conformer	Extracted heats	Boltzmann-calculated contribution (%)			
1		1	-1735.11831655	38.85%			
		2	-1735.11830459	38.81%			
		3	-1735.11707354	10.96%			
		4	-1735.116531716	5.94%			
		5	-1735.116483908	5.44%			
2		1	-1735.12395432	51.79%			
		2	-1735.12312442	21.76%			
		3	-1735.12302682	19.73%			
		4	-1735.12200134	6.72%			
3a		1	-1809.41442350	47.09%			
		2	-1809.41375388	23.57%			
		3	-1809.41370514	22.98%			
		4	-1809.41250073	6.36%			
3b		1	-1809.41489078	74.96%			
		2	-1809.41314070	11.75%			
		3	-1809.41267444	7.16%			
		4	-1809.41252898	6.13%			
4		1	-1849.89166872	34.24%			
		2	-1849.89110932	18.75%			
		3	-1849.89110810	18.73%			
		4	-1849.89103819	17.97%			
		5	-1849.89054895	10.31%			
I-1	X axis(Å)	Y axis(Å)	Z axis(Å)	I-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.7552813427	2.5532594242	2.9549851992	C	-0.8630833324	2.0848169514	3.1826439222
C	0.6287688255	1.9109359709	3.1227282111	C	-0.2919614847	0.6870658457	2.9112026928
C	0.8491845793	0.9612523324	1.9309328747	C	0.9723532802	0.8401259641	2.0593498986
C	0.7785285766	1.6834151812	0.601891705	C	0.8082473949	1.6945024425	0.8168298663
C	-0.1399077073	2.7624238011	0.4384877325	C	-0.1778356473	2.7290534415	0.7835819826
C	-1.0850186471	3.0469225064	1.5500824995	C	-1.1798957432	2.7999812483	1.8852857541
C	1.5606871937	1.2982571575	-0.4880641229	C	1.6296630912	1.505753749	-0.3045301627
C	1.4656616063	2.0459153693	-1.6606153587	C	1.4846210429	2.4050033383	-1.3626585373
C	0.6398900923	3.1417373382	-1.8293649588	C	0.602482341	3.4679120775	-1.389730989
C	-0.2042219894	3.5056105001	-0.7745580052	C	-0.2707292837	3.6337413024	-0.3130885165
C	1.7545949206	2.9449286389	3.2854976562	C	-0.0126384965	-0.0810396402	4.207260495
O	-2.1552741815	3.6284674558	1.3673993811	O	-2.259392845	3.3762812776	1.7501098651
C	-1.1268323462	4.6831129728	-0.9912067305	C	-1.249107243	4.7842312785	-0.3851785522
C	-4.0270985422	0.4130599061	-0.5855458293	C	-3.885336499	0.4072579657	-0.6777302314
O	-4.6126805705	1.0204762185	-1.4590203726	O	-4.4523247556	1.0969106129	-1.5010925373
C	-3.9149336671	-3.0883104524	1.0799216861	C	-3.6215318075	-3.2508601697	0.5904790844

C	-4.3901834531	-1.6670079122	0.7631430632	C	-4.1648351126	-1.8284288592	0.4242219965
C	-3.7802538259	-1.1091301078	-0.5568971291	C	-3.5778734671	-1.0969960825	-0.8198664752
C	-2.2161769801	-1.3038349719	-0.5496999904	C	-2.0031430715	-1.2205732028	-0.8297052858
C	-1.6352216865	-2.6666347453	-0.0475501993	C	-1.3659759744	-2.6008919595	-0.4632646485
C	-2.3895169259	-3.1214561362	1.2282961549	C	-2.0980933507	-3.2214303158	0.7525794968
C	-1.54453834	-0.9199935024	-1.8756454015	C	-1.3500988957	-0.6876422621	-2.1150866035
C	-0.0465847423	-0.9771963834	-1.7494441138	C	0.1506285869	-0.691741354	-1.9888815251
C	0.6000052908	-1.5204841114	-0.7071133792	C	0.8251371024	-1.3303495432	-1.0207756512
C	-0.1454597883	-2.3502059248	0.3325347248	C	0.11500679	-2.2725310307	-0.0459467319
C	-1.695387452	-3.7917110193	-1.1062525896	C	-1.4012330944	-3.5962226728	-1.6499105398
C	-4.50254649	-1.7203927541	-1.772163089	C	-4.2813604226	-1.5924522926	-2.0980093579
C	2.123634634	-1.34090315	-0.5569659777	C	2.3297980034	-1.0497927878	-0.7958496684
C	2.7798498598	-2.0585085379	0.6352414974	C	2.8930592229	-1.9102700677	0.3306886542
C	1.991943592	-3.1282615831	1.3803725127	C	2.4714617922	-3.3454231601	0.1295033084
C	0.7180677633	-3.5783407392	0.6639907806	C	0.9478406231	-3.5429410954	0.2880693528
C	4.0750789685	-1.8102249827	0.920096537	C	3.7020976232	-1.4674068416	1.3118879321
C	4.8772947129	-2.5014190184	1.9944228605	C	4.2406349246	-2.3186148154	2.4378474759
C	2.5812757585	0.1919309448	-0.7245950628	C	2.6999822365	0.4877542786	-0.7242752133
C	3.9106443841	0.501263726	0.0359920443	C	4.0789499709	0.6582189306	-0.0116632558
C	2.9070177055	0.4223736201	-2.21651983	C	2.9881962475	0.9628462785	-2.1693016241
O	2.2763535575	1.5674013377	-2.6718065847	O	2.2985202918	2.1231759386	-2.4412413271
O	3.6182951134	-0.2234591584	-2.9393686813	O	3.7256001469	0.469276913	-2.9801671488
C	4.8081747359	-0.7323318943	0.1535431586	C	4.1830814574	-0.0337442409	1.3442951624
O	-3.4987557916	1.0416163227	0.495140821	O	-3.4323493379	0.9159499055	0.4953906482
H	-0.1960411904	-1.7662709233	1.2656998402	H	0.0357924933	-1.7176048983	0.90131147
H	-1.8643017894	-0.5770700388	0.1913162031	H	-1.6801825316	-0.5517872952	-0.024126484
H	2.574608155	-1.8170964919	-1.4385140801	H	2.8529316999	-1.4014009806	-1.698227712
H	-1.5413244001	1.8264270202	3.2017966565	H	-1.7789832709	2.0527610627	3.7789747902
H	-0.906137089	3.4002673208	3.6347331466	H	-0.118729684	2.6768793284	3.7383622818
H	0.6096707492	1.2991439997	4.0338873317	H	-1.0387708814	0.1273946903	2.3308814664
H	1.8006666672	0.4308877815	2.0247832297	H	1.7379117263	1.3181098187	2.6904067242
H	0.0691542847	0.1892977413	1.9597938229	H	1.371646836	-0.1402516229	1.7908685796
H	0.6335387258	3.6858305093	-2.7677160534	H	0.5740394675	4.1320061316	-2.2468189936
H	1.5813341822	3.5651985016	4.1716828855	H	-0.9274236816	-0.2025141609	4.7971459154
H	1.8285431753	3.6131655724	2.4210946108	H	0.7188349082	0.449498056	4.8295495744
H	2.7249917968	2.4510221643	3.4099066834	H	0.387006099	-1.0797121217	3.9980333253
H	-0.8079959661	5.245222759	-1.8736702006	H	-0.9418863735	5.4773660077	-1.1736716164
H	-2.1588849787	4.3547436512	-1.1452539872	H	-2.2607697483	4.4337568699	-0.6088617612
H	-1.1484343444	5.3550898724	-0.1303227658	H	-1.3186835174	5.3283855292	0.5591307535
H	-4.2452453286	-3.7929951022	0.3071548297	H	-3.9080300841	-3.8832531889	-0.2587591141
H	-4.3809968562	-3.4233628435	2.0145745422	H	-4.0775207962	-3.7080961185	1.4770718533
H	-4.1057978091	-1.0147368741	1.5957688356	H	-3.9194665652	-1.2597704061	1.3270436745
H	-5.484174675	-1.6305399134	0.6907075669	H	-5.2588853212	-1.837586356	0.3436352942

H	-2.0631500329	-4.1283500933	1.5147222485	H	-1.7169115215	-4.2331086368	0.9357598569
H	-2.1167563787	-2.4568497138	2.0612389685	H	-1.8631842171	-2.6322148515	1.6513675296
H	-1.8884898528	-1.5579216097	-2.7006951595	H	-1.6687594223	-1.2602897732	-2.9960073009
H	-1.8284874815	0.1017117687	-2.1624903677	H	-1.6762887911	0.3434062851	-2.3062831955
H	0.5090187633	-0.4750027957	-2.5388172865	H	0.68291451	-0.058450913	-2.6961308863
H	-2.7133455757	-3.9676813152	-1.4598757588	H	-2.3916150535	-3.6488850183	-2.1047468259
H	-1.0747266829	-3.5700297164	-1.9783754426	H	-0.6924304326	-3.3201999459	-2.4353898196
H	-1.3366508984	-4.7342567371	-0.6807096305	H	-1.1518453059	-4.6096844469	-1.3222829701
H	-4.1260513716	-1.3215327556	-2.7157948015	H	-3.9017739309	-1.0999493869	-2.9948767272
H	-5.5692377326	-1.4829939043	-1.729402006	H	-5.3505024463	-1.3694759846	-2.041230128
H	-4.3986397856	-2.8067829732	-1.7904762944	H	-4.1703689265	-2.671320823	-2.2211028704
H	1.7071854038	-2.7497569004	2.3745593666	H	3.0091150637	-4.0327876832	0.7853664942
H	2.629867736	-3.999361693	1.5616671797	H	2.7555104033	-3.6214472544	-0.8965379708
H	0.174492014	-4.2756466276	1.3102764581	H	0.7272891523	-3.8344646542	1.3206764949
H	0.9718559826	-4.1225491341	-0.2540966017	H	0.6436652282	-4.3830125349	-0.3412220559
H	4.3333335479	-3.2909100731	2.5147159338	H	3.7772122845	-3.3039905592	2.5047444728
H	5.7878107484	-2.9428767458	1.5669356159	H	5.3255183767	-2.4604229355	2.3375828127
H	5.2127573549	-1.7770054323	2.7496915333	H	4.0829109543	-1.8131831849	3.4000025044
H	4.4319806391	1.3255456485	-0.4644529766	H	4.8309882966	0.2212342417	-0.6778938683
H	3.6622299908	0.8531363478	1.0414244411	H	4.3087361542	1.7257965698	0.0795177689
H	5.7339394668	-0.4584473635	0.6723598942	H	3.6597624269	0.5308444772	2.1263305639
H	5.1001524851	-1.0803800594	-0.846544728	H	5.2395812858	-0.0264189185	1.6465691867
H	-3.6195390498	2.0050635326	0.4091126225	H	-3.5881171688	1.8777382391	0.5228639065
1-3	X axis(Å)	Y axis(Å)	Z axis(Å)	1-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.645659785	2.2818535866	3.104919452	C	-1.4106900973	2.2115619204	2.9945564667
C	-0.2146844618	0.8327775855	2.8447131233	C	-0.7258124785	0.8427611926	2.8844332132
C	1.0628923608	0.8532250488	1.9994297467	C	0.6055977585	1.0213518859	2.1475242653
C	1.0001081193	1.7204313494	0.7568813635	C	0.5235646326	1.8123579521	0.8541224778
C	0.1239899321	2.8478349574	0.7124300571	C	-0.5183679124	2.7663052691	0.6462858648
C	-0.8889978968	3.0062352105	1.7971676916	C	-1.6406669545	2.8199283106	1.6249919229
C	1.7951161816	1.4386841014	-0.3649304038	C	1.4992705506	1.6582614988	-0.1377781437
C	1.7338507117	2.3299340286	-1.4370341493	C	1.4792561048	2.5387938929	-1.2168489615
C	0.9735884193	3.4840411816	-1.468385887	C	0.5207975407	3.5142628656	-1.4188979475
C	0.1273438668	3.7499381507	-0.3895754006	C	-0.5250858053	3.6182208795	-0.4969859211
C	-0.0193626857	0.0489567157	4.146731043	C	-0.5312628628	0.1848302097	4.254500413
O	-1.9234231154	3.6526082525	1.6348526934	O	-2.7362291135	3.3057792457	1.3441200885
C	-0.7325781848	4.9910353629	-0.4666890936	C	-1.5832067548	4.6647029993	-0.7623981756
C	-3.9908336629	0.4870857673	-0.4430559985	C	-4.0412255052	0.0362820019	-0.8134517608
O	-4.6621590339	1.1980938662	-1.1625408734	O	-4.6516511717	0.6031391222	-1.6970493265
C	-3.8006691327	-3.2549380968	0.5758180608	C	-3.4172351826	-3.507149894	0.6426633638
C	-4.2844743412	-1.8003512079	0.5400836603	C	-4.1092759055	-2.1643439963	0.3890970536
C	-3.7081721893	-1.0116400683	-0.6728453174	C	-3.5412700299	-1.421389835	-0.855893154
C	-2.1436276663	-1.1799799033	-0.7107324349	C	-1.9674462557	-1.3472325755	-0.7627534966

C	-1.5476799989	-2.6117203614	-0.5099910514	C	-1.1907325784	-2.6338245425	-0.3247149249
C	-2.271073108	-3.3146829102	0.6680721547	C	-1.9156316856	-3.3012888212	0.8716807324
C	-1.4880008828	-0.51104693	-1.9256870493	C	-1.3119563582	-0.740401399	-2.0124171168
C	0.0111902045	-0.5576153038	-1.8130506475	C	0.1763957306	-0.622077115	-1.8420393281
C	0.6702985203	-1.3152062967	-0.925413489	C	0.8776512682	-1.1704923598	-0.8378112929
C	-0.0463647975	-2.383980083	-0.1096280108	C	0.2139951052	-2.1168962822	0.1683069903
C	-1.6367832592	-3.4948690435	-1.7759110769	C	-1.0278573053	-3.6578796198	-1.4715265839
C	-4.4435700636	-1.4189436214	-1.9643665367	C	-4.0901396392	-2.0597900327	-2.1461203658
C	2.197838851	-1.1955705499	-0.7161334971	C	2.3692841999	-0.8190462709	-0.7048043803
C	2.6921091307	-1.9833620988	0.5068054124	C	3.1677151416	-1.8578781507	0.0783724422
C	2.1364074609	-3.4003343881	0.6284965386	C	2.5453360727	-3.2260154417	-0.0537356299
C	0.8409750643	-3.6435919521	-0.1607978367	C	1.1731971943	-3.2575317342	0.6370586903
C	3.6090682745	-1.5204902959	1.3809566995	C	4.332500298	-1.5872365439	0.6985480004
C	4.1293881783	-2.3026375518	2.5649230539	C	5.2353913039	-2.60709403	1.349753117
C	2.7204211028	0.2896482559	-0.7944999237	C	2.6904022025	0.7225306478	-0.3236869384
C	4.1565401692	0.3771685092	-0.1895043959	C	3.7158496579	0.8459368699	0.8355145504
C	2.9657847642	0.6605598723	-2.2743987636	C	3.3251096898	1.3260042184	-1.5962226896
O	2.4619305963	1.9176535297	-2.5372999979	O	2.5368788236	2.3544434545	-2.0844108756
O	3.5577716313	0.0339305095	-3.1118104836	O	4.3358423575	1.0039926902	-2.1619795994
C	4.2502032658	-0.1605452137	1.2307204133	C	4.8544098087	-0.1687937044	0.7567038762
O	-3.3977899991	0.9689328792	0.6808100043	O	-3.7080168117	0.660951228	0.343776733
H	-0.0585964058	-2.0559760406	0.9435871779	H	-0.0102128687	-1.5205471952	1.0626014062
H	-1.7962038616	-0.6215464101	0.1660537717	H	-1.7858577268	-0.6367458644	0.0511484172
H	2.6728922992	-1.6870911009	-1.5807046273	H	2.7614762918	-0.9198246164	-1.7256179225
H	-1.5612125694	2.3448790133	3.6994464257	H	-2.378136983	2.1504631143	3.5002622286
H	0.1534025578	2.8029331158	3.6555765176	H	-0.7685660636	2.8920000682	3.5759050797
H	-1.0105584437	0.3466749733	2.2637922338	H	-1.3749404654	0.1951960847	2.2790832772
H	1.8729768672	1.2434753439	2.6355163356	H	1.2935356208	1.5582130006	2.8203500208
H	1.3554316892	-0.1632592557	1.7326470152	H	1.068180054	0.0482077141	1.9643424862
H	1.0030866874	4.1350732703	-2.3355158459	H	0.5786310541	4.1704047125	-2.280575112
H	-0.9454804717	0.0202302957	4.7307921367	H	-1.4916865801	0.0374054372	4.7597012413
H	0.7564866451	0.5091905744	4.7713113692	H	0.0973916216	0.8062377492	4.9042765831
H	0.2828557885	-0.9850027489	3.9454472232	H	-0.048887002	-0.7947011235	4.1594000223
H	-0.357548315	5.6499399678	-1.2552554753	H	-1.2444749029	5.3380618286	-1.5549342099
H	-1.7733919221	4.7389978378	-0.688548681	H	-2.5254443497	4.206250407	-1.0759239823
H	-0.7489056531	5.5416121811	0.4766055583	H	-1.8157431132	5.2529195368	0.1282644703
H	-4.1584390356	-3.8053874791	-0.3025988112	H	-3.5916719473	-4.2004634121	-0.1889770815
H	-4.2386850627	-3.7577399295	1.446670218	H	-3.8609235502	-3.9788852499	1.5279188707
H	-3.9759301282	-1.3078484635	1.4692261199	H	-3.9778464923	-1.5351826422	1.2757975075
H	-5.3800231155	-1.7577235386	0.505619646	H	-5.1893309353	-2.3033874669	0.2565765137
H	-1.9395833961	-4.3579344405	0.7392167866	H	-1.4373960441	-4.2590077968	1.1090300089
H	-1.9721390571	-2.8287284162	1.6080999918	H	-1.7927771542	-2.665405207	1.7607975393
H	-1.8222954323	-0.9675161231	-2.8668909404	H	-1.5423605273	-1.3256494478	-2.9128128888

H	-1.7953859605	0.5416588603	-1.9897020209	H	-1.7231321476	0.2594686614	-2.207128403
H	0.5449242568	0.127393672	-2.4652478681	H	0.6912253095	0.002561544	-2.572188982
H	-2.6630843816	-3.6000596109	-2.131453393	H	-1.9920092327	-3.9788312103	-1.8699574075
H	-1.0406540842	-3.0925697508	-2.5995208904	H	-0.4432563259	-3.2548434641	-2.30216448
H	-1.2663894299	-4.5029660616	-1.5661279278	H	-0.5172181429	-4.559716544	-1.1202548876
H	-4.0662464578	-0.8827853835	-2.8373423694	H	-3.7383952235	-1.5446459155	-3.0415774567
H	-5.5061545426	-1.1771052644	-1.8774881504	H	-5.1820771529	-1.998692158	-2.1534671194
H	-4.3551190339	-2.4896341317	-2.1532525609	H	-3.8113824356	-3.1122052041	-2.2204166546
H	1.9339514946	-3.6134492775	1.6837581065	H	3.181047388	-4.010095294	0.3616642783
H	2.9013958946	-4.1258464484	0.317634449	H	2.4154654748	-3.4606977132	-1.1211401209
H	0.3253646262	-4.5121771337	0.2621356839	H	1.3317190883	-3.1767366636	1.7185711672
H	1.0648961477	-3.8882258074	-1.2053776618	H	0.7175510033	-4.2378895179	0.4722825582
H	3.5129872105	-3.1604729857	2.8377343831	H	4.8969430579	-3.6379731557	1.2384267658
H	5.1430857911	-2.6774360544	2.3645938481	H	6.2450159318	-2.5409178981	0.9222405016
H	4.2086583195	-1.6514109451	3.4450475376	H	5.3408720853	-2.4015398659	2.4237046875
H	4.811302678	-0.2188583236	-0.8351689571	H	4.1083635024	1.8695296581	0.853703806
H	4.5075535703	1.4140907372	-0.2382358027	H	3.1866484753	0.6937855903	1.7788849866
H	3.8193400032	0.5458696352	1.9534244556	H	5.492252393	-0.0468270622	1.6413950655
H	5.3123044818	-0.2364298901	1.5009741855	H	5.4911916537	0.0364675966	-0.1138436626
H	-3.5642827889	1.9275386931	0.7375919577	H	-3.9657676718	1.5999029789	0.2984672323
1-5	X axis(Å)	Y axis(Å)	Z axis(Å)	2-1	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.2947009522	2.6421530052	2.8277049934	C	5.2047167233	-1.4716699707	1.803437339
C	0.9161232789	1.7187100572	3.006639111	C	4.2529397079	-0.4299026837	2.39854594
C	0.9808310668	0.7958580325	1.7753345171	C	3.7163854483	0.4266896197	1.2425155735
C	1.1430163707	1.5627726554	0.4802112702	C	3.0951266486	-0.3717880702	0.1081500623
C	0.4642722254	2.8110950166	0.3419871349	C	3.5323830127	-1.7051031461	-0.1663598126
C	-0.464132947	3.2261914031	1.4301932366	C	4.576308765	-2.3214299731	0.7071287906
C	1.8616948603	1.058951601	-0.6117571443	C	2.1107216097	0.197166738	-0.7088383041
C	1.8976544299	1.8377919408	-1.7708179567	C	1.6271962736	-0.5488235495	-1.7807516932
C	1.3270760548	3.0899160769	-1.9048951816	C	2.0249180587	-1.838878925	-2.0747202732
C	0.5779568318	3.5961034067	-0.8390392595	C	2.9852674337	-2.445674059	-1.2579614723
C	2.2216311389	2.4890604573	3.2618535429	C	3.1390230032	-1.0686976543	3.2432331421
O	-1.4060256303	3.9922742192	1.2256066871	O	4.9647736981	-3.4769568405	0.560709841
C	-0.0737803544	4.9480990703	-1.0170637268	C	3.3894085552	-3.8584897742	-1.6104412243
C	-3.9930634916	0.8812100823	-0.3119033959	C	-3.4917822292	-3.1699907927	-0.5596082928
O	-4.6324442716	1.5807424094	-1.0705432249	O	-3.4228759975	-4.3224647799	-0.1822176771
C	-4.216911779	-2.7035116103	1.1617287029	C	-5.6984820897	-0.0569928771	0.1176002304
C	-4.5104397169	-1.2112121259	0.9659430119	C	-5.2537639468	-1.4034230149	-0.4640756502
C	-3.9145563358	-0.6585175871	-0.3625226325	C	-4.0038628933	-1.9791764112	0.2668914752
C	-2.390387513	-1.0384286839	-0.4486356897	C	-2.8651112934	-0.8876017567	0.2823534815
C	-1.9698287044	-2.5035255727	-0.0970418714	C	-3.2626783449	0.5573181663	0.7328161036
C	-2.7051261571	-2.9593284979	1.1904336931	C	-4.5721948732	0.9782253978	0.0159462386
C	-1.729366757	-0.609728007	-1.7649420905	C	-1.6008742755	-1.3461806323	1.0238084545

C	-0.2436858015	-0.83845889	-1.7108741183	C	-0.5304314528	-0.290566207	1.0023609875
C	0.36436954	-1.5683885057	-0.765577264	C	-0.7144910226	0.9778174706	0.6016626578
C	-0.4316720258	-2.4291595855	0.2072946071	C	-2.1063873793	1.5031612106	0.2315352307
C	-2.2424603322	-3.5115688607	-1.2368914319	C	-3.4329470714	0.6763872627	2.2658380143
C	-4.7732366755	-1.1173319878	-1.5570077407	C	-4.4140863961	-2.5414668107	1.6433192522
C	1.9038758519	-1.6257410013	-0.6356391187	C	0.5102023098	1.9105567755	0.4760516846
C	2.3629300741	-2.304004632	0.6635421316	C	0.1227035017	3.386819964	0.5463920804
C	1.6419696917	-3.6077251445	0.9994245926	C	-1.0977314542	3.5732933364	1.4117119583
C	0.292148835	-3.7874067072	0.2875838055	C	-2.3078819869	2.9950348592	0.6572259742
C	3.3786661512	-1.8561066682	1.4301220165	C	0.7276075575	4.3680121456	-0.1492760792
C	3.8598051046	-2.5401719462	2.6894169591	C	0.3349729223	5.8261212098	-0.1100000057
C	2.6002010082	-0.2476992269	-0.9321850529	C	1.4332037479	1.5636787232	-0.756399096
C	4.07191825	-0.2740942676	-0.4070320163	C	2.470412007	2.7005588826	-0.9644526008
C	2.8122089595	-0.0877088945	-2.4536693732	C	0.55660144	1.4097560394	-2.0164983856
O	2.5065828253	1.2032879095	-2.837347765	O	0.7104749811	0.1380008378	-2.5467564535
O	3.2484251155	-0.8884324186	-3.2361896279	O	-0.1757012176	2.2055537371	-2.5410589339
C	4.1812636415	-0.627423344	1.0680707767	C	1.8401253587	4.0808542597	-1.1298484966
O	-3.2554138221	1.4156745858	0.6971935079	O	-3.1149305644	-2.8238681847	-1.8208480792
H	-0.3419564782	-1.9777140359	1.20908977	H	-2.1635678273	1.4857306907	-0.8651687888
H	-1.923798667	-0.4318223049	0.3360110234	H	-2.5822738106	-0.7774184957	-0.771625781
H	2.2639241258	-2.2835265368	-1.4436318621	H	1.126100638	1.7100822321	1.3628524373
H	-1.2233511053	2.0923302293	3.0312230465	H	6.0690669829	-0.9620406399	1.3508467256
H	-0.2845168928	3.4863682006	3.5277574524	H	5.601279252	-2.1588694897	2.5565838298
H	0.7324764474	1.0838075217	3.8830995204	H	4.8320527521	0.2299638012	3.0575397568
H	1.770325368	0.054622771	1.8839300936	H	2.9992712933	1.1574266712	1.6249338661
H	0.0419512703	0.2270952835	1.7268116665	H	4.5523820761	1.0116515048	0.8309820006
H	1.4246721117	3.6386166607	-2.8355752568	H	1.6021556645	-2.3622979409	-2.9253610537
H	2.1363306146	3.0970167225	4.1692846512	H	3.5654303952	-1.6469666813	4.0698751841
H	2.4720774659	3.1608006137	2.433981927	H	2.5145898903	-1.7487216995	2.6535373013
H	3.0639708544	1.8023900636	3.4014325715	H	2.4849534769	-0.3021879326	3.6734722987
H	0.3750721682	5.4657727099	-1.869774735	H	2.8426590968	-4.1863215264	-2.4994108354
H	-1.1481925115	4.8478920346	-1.1951942495	H	4.4625237921	-3.9369544615	-1.8027276172
H	0.028208069	5.5752197871	-0.1283589188	H	3.1858399488	-4.5526958602	-0.791013341
H	-4.6969857296	-3.3000914429	0.3767374788	H	-6.0277931173	-0.172911264	1.1572427708
H	-4.6610871274	-3.0357417342	2.1079785711	H	-6.5736820844	0.3013320827	-0.437967651
H	-4.0826042044	-0.6581452062	1.8100650517	H	-5.0166666179	-1.2642394582	-1.5247428093
H	-5.5912683308	-1.0246098916	0.9775634362	H	-6.0684472553	-2.1363484719	-0.4110231794
H	-2.5076352372	-4.0224701049	1.3752827775	H	-4.9171665789	1.942797636	0.4069033978
H	-2.2884810383	-2.4122776641	2.048640876	H	-4.3516404237	1.1373547122	-1.0492570137
H	-2.1724833106	-1.1268179026	-2.6264578998	H	-1.8238300815	-1.6279338667	2.0619194098
H	-1.9063510473	0.4592232871	-1.946229547	H	-1.2015188201	-2.2582697145	0.5585593774
H	0.3341151365	-0.3079550797	-2.462369004	H	0.4633354349	-0.6152652317	1.3023364326
H	-3.2939983382	-3.528236074	-1.5285024176	H	-4.2013481881	0.0035807392	2.6473849545

H	-1.654194576	-3.2886521651	-2.1312603909	H	-2.5043695613	0.4536896138	2.798283561
H	-1.9826397791	-4.526169481	-0.9195657899	H	-3.7362862364	1.6880149182	2.549671008
H	-4.3872072671	-0.7424263635	-2.5070081069	H	-3.5615013511	-2.9375597815	2.19849256
H	-5.7904675048	-0.7309296117	-1.4524534744	H	-5.1153264217	-3.3687981723	1.5071123954
H	-4.8287361206	-2.2052226972	-1.6136858243	H	-4.902906738	-1.7848936654	2.2568151302
H	1.4611234711	-3.6463035494	2.07933378	H	-1.27884154	4.6200068621	1.6632014207
H	2.2973588274	-4.4608631068	0.7741866671	H	-0.9686332289	3.0378225084	2.3635992304
H	-0.3029948911	-4.5252895862	0.8357785327	H	-2.4730505311	3.6047197096	-0.2370750299
H	0.436050508	-4.1864239374	-0.7230882951	H	-3.203252022	3.1071461424	1.2742715468
H	3.1473435486	-3.2524937536	3.1083570175	H	-0.5095563786	6.0419201624	0.5451117274
H	4.7957581056	-3.0847060624	2.5003864577	H	1.1807760921	6.4450230091	0.2186741723
H	4.0860877064	-1.7960538324	3.4640485659	H	0.070108717	6.1722409051	-1.1182906866
H	4.6050211786	-1.0323360921	-0.9914954922	H	3.1056084115	2.4608265146	-1.8251119482
H	4.5478249898	0.6910747322	-0.6133820337	H	3.122616659	2.7080956452	-0.0860750005
H	3.8923469086	0.2241430325	1.7014384457	H	1.4402951509	4.2000038446	-2.1463978892
H	5.2388130024	-0.8113633657	1.3018789683	H	2.6283288271	4.8396168384	-1.0269045123
H	-3.3036897595	2.3874501684	0.6386263343	H	-2.8252740124	-3.6419129128	-2.25837134
2-2	X axis(Å)	Y axis(Å)	Z axis(Å)	2-3	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.1322274883	-1.6214766013	1.7341960031	C	5.1383226374	-1.6830785608	1.7332964014
C	4.2285373669	-0.5629609237	2.3734075936	C	4.2673574057	-0.5842803572	2.3491287393
C	3.703822086	0.3442189743	1.2510994102	C	3.7483827048	0.2975428052	1.2042022891
C	3.0524557992	-0.3965068272	0.0941190092	C	3.0597655076	-0.4665634508	0.0847195363
C	3.4283537705	-1.7409763351	-0.2151105707	C	3.4018306328	-1.8282382241	-0.1863197638
C	4.4439241577	-2.4256306284	0.6397859964	C	4.4213832388	-2.504521528	0.6700228823
C	2.0983486561	0.2387932147	-0.7098876937	C	2.103213597	0.1614883861	-0.7217161705
C	1.5827459776	-0.4567065664	-1.8007631766	C	1.5508486141	-0.5591513117	-1.777697292
C	1.9169005099	-1.7573037439	-2.1256822912	C	1.8496140973	-1.8771128497	-2.0635750368
C	2.8464913346	-2.4280392237	-1.3239942404	C	2.7816228705	-2.5400442685	-1.2583591612
C	3.1072954627	-1.1860677793	3.2201868414	C	3.1434585723	-1.1537799945	3.2295156006
O	4.7617504989	-3.6011671148	0.480751698	O	4.7222620308	-3.6877449001	0.5362679781
C	3.1840783111	-3.8493907182	-1.7110081511	C	3.0781297155	-3.9817773841	-1.6006335125
C	-3.3603828641	-3.1333516139	-0.5976595204	C	-3.4886890268	-3.0436609691	-0.5792866042
O	-2.9847204325	-3.0220692914	-1.7480188046	O	-2.5692695798	-3.0298983615	-1.3729827437
C	-5.6379190528	-0.0791784271	-0.0224427134	C	-5.6314784108	0.0762663222	0.0820495075
C	-5.1610012034	-1.4386469654	-0.5431231503	C	-5.2056193656	-1.2935816357	-0.4540309126
C	-3.9358220957	-1.9836971713	0.2489185429	C	-3.9608448667	-1.8689756586	0.2947915569
C	-2.8084826162	-0.8793815878	0.2730638243	C	-2.8147762857	-0.7992076918	0.3168571031
C	-3.232471464	0.575527307	0.6624112068	C	-3.1997105087	0.6694935749	0.7050760227
C	-4.5171334614	0.962508407	-0.1154635616	C	-4.4878188752	1.0874994891	-0.0487495738
C	-1.5675116252	-1.3049201868	1.0714329692	C	-1.5824405326	-1.2462642285	1.1181817164
C	-0.5059680299	-0.240776043	1.0589102589	C	-0.4935980027	-0.2103696683	1.0796714346
C	-0.6847006364	1.0131089571	0.6139215363	C	-0.6442209465	1.0412376957	0.6178534319
C	-2.0645611343	1.5145809573	0.1746724932	C	-2.0167039571	1.5761709969	0.1951156933

C	-3.460941933	0.7431568948	2.1832770617	C	-3.4021172749	0.8530750491	2.2285086967
C	-4.391547702	-2.5064027163	1.627248235	C	-4.3842825318	-2.4154720166	1.6793278773
C	0.5343219667	1.9518439163	0.5139766558	C	0.59842485	1.9431005721	0.4757923467
C	0.1435568626	3.4276026033	0.5997006296	C	0.2480973212	3.4300072684	0.5310636856
C	-1.1315029389	3.6010262742	1.3860566305	C	-0.9978803859	3.6558410299	1.3500139274
C	-2.2847557507	3.0169374087	0.5497597574	C	-2.1921306919	3.0867719203	0.5622888773
C	0.7959041129	4.4209135173	-0.033338058	C	0.905480959	4.3893398731	-0.1475168931
C	0.4134912329	5.8813311661	0.02109293	C	0.5591172602	5.8595346714	-0.123416886
C	1.4736517441	1.6307135812	-0.7156710569	C	1.50636895	1.564925008	-0.761096887
C	2.5438602609	2.746931643	-0.8426022856	C	2.5956294705	2.653937367	-0.9476241924
C	0.6172176145	1.5592038276	-1.996975506	C	0.6223673345	1.4685975125	-2.0219474378
O	0.7043173702	0.292843217	-2.5523202286	O	0.6733458429	0.1843040061	-2.5369957571
O	-0.0565311032	2.4089386068	-2.5156995239	O	-0.0453312601	2.3149422773	-2.5546897376
C	1.9545923954	4.150699934	-0.9643337554	C	2.0319443338	4.0650808168	-1.1005662229
O	-3.299505449	-4.329580241	0.0437035394	O	-4.2661513043	-4.1511717714	-0.4346282944
H	-2.0851005479	1.4628428444	-0.9222081658	H	-2.0542585113	1.5185959369	-0.9010125203
H	-2.4941939269	-0.8084544092	-0.776171569	H	-2.4877993075	-0.7392646645	-0.7284343882
H	1.1456874058	1.7378471395	1.4008419953	H	1.2184813374	1.7346367461	1.3579903761
H	6.0004345745	-1.1295894106	1.2695703865	H	6.0131533689	-1.2267421203	1.2453879065
H	5.5238397505	-2.3366429929	2.4634117862	H	5.5211249306	-2.3849869173	2.4799523298
H	4.8415051296	0.0574149348	3.0401281438	H	4.9028879239	0.043176187	2.9875803159
H	3.0080033259	1.0787764424	1.6651206565	H	3.0781455082	1.0636882242	1.6027991231
H	4.5506484806	0.9224082104	0.8526015742	H	4.6033384096	0.8394588411	0.7732836002
H	1.4655773047	-2.2399021469	-2.9856190225	H	1.3659425847	-2.3806177691	-2.893223615
H	3.5269137198	-1.8031371162	4.0219313045	H	3.559622532	-1.7528715453	4.046599466
H	2.4486889838	-1.8259922796	2.6228041684	H	2.4637704121	-1.7983730805	2.6615626649
H	2.4890912328	-0.4095018789	3.6841257966	H	2.5480248864	-0.3486657966	3.674216926
H	2.6284146438	-4.1267082	-2.6114290718	H	2.4906107032	-4.2800592719	-2.473629529
H	4.2535506414	-3.975380638	-1.8987193186	H	4.1389603137	-4.1379968656	-1.8131526491
H	2.9412228971	-4.5536907111	-0.9110750009	H	2.8430627842	-4.650136418	-0.7682369573
H	-6.0065293935	-0.163694012	1.007295686	H	-5.9644597371	-0.0044251835	1.1240744869
H	-6.4940138271	0.2528345121	-0.6222907214	H	-6.5006820002	0.4280065622	-0.4870332706
H	-4.8758304382	-1.335625876	-1.5960873283	H	-4.9598119223	-1.185074065	-1.519240344
H	-5.9729948257	-2.1756954248	-0.5006637873	H	-6.0276752481	-2.0145307753	-0.3882352363
H	-4.884044811	1.9357597608	0.2315418526	H	-4.8200834219	2.0733644105	0.2974342361
H	-4.2583446395	1.0891912643	-1.1761842621	H	-4.2505448406	1.198098518	-1.1165144922
H	-1.8238859608	-1.560476939	2.1089279519	H	-1.8401705588	-1.4739448244	2.1621625192
H	-1.1432475431	-2.2238121824	0.643099369	H	-1.1888205166	-2.1794635261	0.6966756753
H	0.4784545308	-0.5467992895	1.4059596366	H	0.4880140731	-0.538393164	1.4146387783
H	-4.2550205103	0.0940110817	2.5539023734	H	-4.2080496027	0.2278794622	2.6154665204
H	-2.5579855341	0.5239290497	2.7593812148	H	-2.4975098189	0.6153274946	2.7940860908
H	-3.7593382301	1.7674703009	2.4236130561	H	-3.6718025037	1.8860447583	2.4656959704
H	-3.5615139598	-2.8834452833	2.2280208558	H	-3.5520398435	-2.8971519726	2.2001190466

H	-5.0985551964	-3.3306652266	1.4994811923	H	-5.1757659402	-3.1589686969	1.5659285684
H	-4.8966583507	-1.727328033	2.1983546752	H	-4.7616088388	-1.6198261166	2.3216658911
H	-1.3366274791	4.6458642718	1.625972745	H	-1.1671245359	4.7106885466	1.5740455841
H	-1.0625972347	3.0640399087	2.3432465072	H	-0.9141929672	3.1366744027	2.3158341854
H	-2.3710268948	3.6082585181	-0.3675181697	H	-2.2998405634	3.6703930577	-0.3577499149
H	-3.2261761219	3.1492346099	1.0897131813	H	-3.1098336192	3.24507981	1.1351676692
H	-0.4477158368	6.0925488068	0.6555961577	H	-0.2826200292	6.1077448505	0.5237727724
H	1.2542386452	6.4861139757	0.3866782145	H	1.421826668	6.4533063538	0.207534739
H	0.1816224839	6.2488813424	-0.9878279549	H	0.3134090547	6.2062088757	-1.136450531
H	3.1986352355	2.5300199603	-1.6945726179	H	3.2257266024	2.396632648	-1.8069593178
H	3.1695017428	2.6983465175	0.0533514925	H	3.2411880813	2.6206959662	-0.0651685936
H	1.6112874752	4.3322843623	-1.9922187192	H	1.6642634656	4.2200230831	-2.1243694712
H	2.7542893736	4.8822566973	-0.7823946539	H	2.8508733228	4.7852368246	-0.9642781903
H	-2.9303918021	-4.9636421637	-0.5951901454	H	-3.9271367753	-4.8094305972	-1.0646986464
2-4	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-1	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.9377573219	-1.6839349655	-1.9603010427	C	4.72092	-2.64626	1.32504
C	-4.8978957256	-0.1735897144	-1.7324033798	C	4.20028	-1.36423	1.98355
C	-3.4692582599	0.2013785972	-1.3258197633	C	3.72669	-0.4197	0.86904
C	-2.9780140175	-0.5544245333	-0.1050438189	C	2.7764	-1.04978	-0.13431
C	-3.4306854284	-1.8867112575	0.1461891649	C	2.76132	-2.46133	-0.35453
C	-4.4139934593	-2.5082674	-0.7911548212	C	3.68894	-3.32527	0.4357
C	-2.046676112	0.0188532143	0.7674506419	C	1.9198	-0.24219	-0.88932
C	-1.6016114846	-0.7352930438	1.8503621035	C	1.10694	-0.84684	-1.844
C	-2.0212173025	-2.0222061812	2.1280285272	C	1.05088	-2.20742	-2.07282
C	-2.9520480495	-2.6223157246	1.2727788723	C	1.88031	-3.04337	-1.31624
C	-5.3700147469	0.6093047536	-2.9620111754	C	3.11332	-1.64844	3.0327
O	-4.8066579316	-3.6650506347	-0.6684360674	O	3.66681	-4.55149	0.37707
C	-3.3883644234	-4.0283444211	1.6130936865	C	1.79497	-4.52626	-1.59447
C	3.7467956626	-3.0547815679	0.3864859579	C	-3.62098	-2.74217	-0.38668
O	3.714255727	-4.2049913446	-0.0025521752	O	-3.11941	-2.76672	-1.49376
C	5.7711787775	0.16827879	-0.345546333	C	-5.51769	0.60557	-0.21205
C	5.4177885592	-1.2048808461	0.2365752712	C	-5.19243	-0.84435	-0.58577
C	4.1655720092	-1.8321580278	-0.4463889165	C	-4.09538	-1.46458	0.33067
C	2.9762527868	-0.7967975086	-0.3980306722	C	-2.84184	-0.50815	0.35259
C	3.2841580049	0.6711161849	-0.8444254225	C	-3.09681	1.0164	0.58992
C	4.6023548435	1.1464257795	-0.1797726315	C	-4.26667	1.4858	-0.31424
C	1.7044733158	-1.3059386107	-1.0918803872	C	-1.71972	-1.00473	1.27531
C	0.5854979786	-0.3053144158	-1.0013532564	C	-0.50332	-0.12955	1.1618
C	0.7266048452	0.9653153351	-0.5901797879	C	-0.49708	1.07858	0.57616
C	2.10749979	1.5538008267	-0.2797435377	C	-1.78702	1.76313	0.13116
C	3.3800395445	0.8147612594	-2.3819852027	C	-3.4096	1.35189	2.0677
C	4.5416120546	-2.3598099221	-1.8461137235	C	-4.69675	-1.81275	1.70823
C	-0.5345092851	1.8352358642	-0.3817534438	C	0.84127	1.78663	0.34677

C	-0.2128909	3.3281597344	-0.4023977771	C	0.77498	3.32567	0.35321
C	0.9354414966	3.6054713028	-1.338459279	C	-0.53984	3.96999	-0.04104
C	2.2208247981	3.0588942967	-0.6928457831	C	-1.74005	3.2441	0.56973
C	-0.8074538066	4.2493937857	0.3785316155	C	2.0697	4.02571	0.20401
C	-0.4735230606	5.722551403	0.3868217831	C	2.19574	5.43304	-0.33875
C	-1.3880881331	1.3915670547	0.8616156991	C	1.65177	1.25646	-0.93767
C	-2.446912674	2.4837635079	1.1981092288	C	2.92156	2.13831	-1.20066
C	-0.4820668593	1.1953818992	2.0945185712	C	0.71898	1.33335	-2.16118
O	-0.6916033547	-0.0634913213	2.6378023684	O	0.36603	0.06475	-2.57184
O	0.2943857663	1.9591128736	2.6025773096	O	0.30929	2.30903	-2.73466
C	-1.8444803564	3.8699855492	1.4094830294	C	3.26481	3.11511	-0.06111
O	3.4108990497	-2.7401568702	1.6672482605	O	1.45222	3.90562	1.50655
H	2.212347738	1.5270913101	0.813254789	O	-3.81522	-3.88803	0.31599
H	2.7339705938	-0.713475276	0.6684129342	H	-1.8067	1.76949	-0.96958
H	-1.1744759851	1.6473122569	-1.2540724081	H	-2.45066	-0.57154	-0.67095
H	-5.9448650942	-2.0497766387	-2.1831917799	H	1.48259	1.5249	1.19071
H	-4.3138261799	-1.9354841569	-2.8330161662	H	5.05702	-3.38682	2.05639
H	-5.5647536554	0.0678864918	-0.8912769258	H	5.58591	-2.40599	0.68812
H	-2.8002240436	-0.0158882887	-2.1745250144	H	5.03767	-0.87575	2.49821
H	-3.4005617057	1.2781045851	-1.1587573821	H	3.26392	0.467	1.30996
H	-1.6348434223	-2.5499805728	2.9931771887	H	4.61028	-0.0564	0.32301
H	-6.3941038568	0.3324659537	-3.2348182509	H	0.37827	-2.6112	-2.82139
H	-4.7277906908	0.4069935542	-3.8281606464	H	2.77638	-0.72083	3.5083
H	-5.3534253734	1.6893844177	-2.776946924	H	3.49829	-2.30708	3.81854
H	-2.900908984	-4.3512103427	2.5376227461	H	2.23698	-2.13807	2.59371
H	-4.4720374767	-4.0967310483	1.7388342221	H	1.07401	-4.70879	-2.39635
H	-3.1398351061	-4.7319754588	0.8143926965	H	2.76414	-4.94086	-1.8841
H	6.0586185604	0.0808647345	-1.4003339889	H	1.49002	-5.08554	-0.70612
H	6.6523614978	0.5618178707	0.1756851428	H	-6.28754	0.98572	-0.89443
H	5.2221654412	-1.0897043066	1.3085066003	H	-5.95181	0.66168	0.79377
H	6.2634572911	-1.8967852621	0.1374462386	H	-6.09427	-1.46782	-0.53894
H	4.8821701743	2.131418515	-0.571943168	H	-4.83634	-0.87101	-1.62188
H	4.4219695462	1.2817238261	0.8962143857	H	-4.52354	2.52584	-0.08073
H	1.8941298018	-1.5579644628	-2.1441390683	H	-3.92967	1.47466	-1.36026
H	1.3720337575	-2.2447682068	-0.6273485921	H	-2.0524	-1.06115	2.32094
H	-0.4046207461	-0.6780299152	-1.2542509691	H	-1.43294	-2.03013	1.00419
H	4.1480025794	0.1687760053	-2.808035403	H	0.42987	-0.54766	1.53284
H	2.4339947342	0.5720813189	-2.8735462672	H	-4.24444	0.76803	2.45568
H	3.6415231905	1.8379168988	-2.665988211	H	-2.5495	1.17122	2.71904
H	3.6839687644	-2.7834717238	-2.3724101968	H	-3.68411	2.40526	2.17343
H	5.2808068788	-3.1592057965	-1.7498936713	H	-3.9548	-2.22351	2.39631
H	4.9744208885	-1.5761833871	-2.467626637	H	-5.48418	-2.56245	1.59512
H	1.0509177359	4.6679796189	-1.5612739919	H	-5.14481	-0.93638	2.17678

H	0.7640434715	3.0987973297	-2.2994549263	H	-0.53312	5.01255	0.28615
H	2.4360888879	3.6592216946	0.1971986121	H	-0.61774	3.96245	-1.13462
H	3.0587021772	3.2141995636	-1.3774820902	H	-1.67844	3.31162	1.66164
H	0.3272600187	6.0003564167	-0.2992403196	H	-2.65989	3.75529	0.2661
H	-1.3579730418	6.3213153644	0.1302885528	H	1.29787	6.02652	-0.16389
H	-0.1694458652	6.0340832393	1.3953076008	H	3.03806	5.93895	0.14746
H	-3.0208340733	2.1725368253	2.078477351	H	2.39306	5.41081	-1.41682
H	-3.1547792574	2.5244734311	0.3647922089	H	2.7428	2.73037	-2.10444
H	-1.3835419403	3.9400364706	2.4046393267	H	3.77385	1.4875	-1.41698
H	-2.6581105648	4.6085193599	1.4042395384	H	4.14132	3.70445	-0.35245
H	3.1773910169	-3.5749159101	2.1067691704	H	3.53194	2.5878	0.85885
				H	-3.49157	-4.61267	-0.24666
3a-2	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-3	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.73822	-2.66893	1.336	C	4.87735	-2.35197	1.44246
C	4.23153	-1.37333	1.97809	C	4.22248	-1.12247	2.08035
C	3.75163	-0.44513	0.85271	C	3.71808	-0.21507	0.94858
C	2.786	-1.08658	-0.12846	C	2.86096	-0.91626	-0.09056
C	2.75936	-2.5017	-0.32333	C	2.97771	-2.32205	-0.31633
C	3.69501	-3.35696	0.46647	C	3.94868	-3.10862	0.50369
C	1.9248	-0.28708	-0.88688	C	1.96391	-0.18001	-0.87241
C	1.09458	-0.90377	-1.81854	C	1.24085	-0.84707	-1.85688
C	1.02455	-2.26767	-2.01971	C	1.31852	-2.20508	-2.09609
C	1.8592	-3.09523	-1.26011	C	2.19072	-2.97184	-1.31488
C	3.15355	-1.63326	3.04277	C	3.11962	-1.50289	3.08132
O	3.67264	-4.58384	0.42231	O	4.04148	-4.33027	0.42941
C	1.75601	-4.58249	-1.50612	C	2.25075	-4.45319	-1.60722
C	-3.72793	-2.67789	-0.40787	C	-3.6479	-2.9454	-0.29
O	-2.77448	-2.82531	-1.14651	O	-3.70734	-4.04844	0.21475
C	-5.51557	0.70862	-0.10728	C	-5.60218	0.39694	-0.13229
C	-5.23396	-0.74208	-0.50914	C	-5.2477	-1.04236	-0.52155
C	-4.10594	-1.39485	0.35339	C	-4.10485	-1.62928	0.36039
C	-2.84438	-0.46455	0.37209	C	-2.87589	-0.64037	0.34271
C	-3.06971	1.06485	0.62276	C	-3.17011	0.87418	0.60105
C	-4.25146	1.56303	-0.24823	C	-4.38028	1.31339	-0.26484
C	-1.72086	-0.97894	1.28452	C	-1.70965	-1.10933	1.22401
C	-0.49266	-0.12167	1.15917	C	-0.52955	-0.18689	1.10141
C	-0.47221	1.08556	0.57171	C	-0.57594	1.03031	0.53614
C	-1.75701	1.78925	0.14031	C	-1.89872	1.66577	0.11136
C	-3.34535	1.40194	2.1081	C	-3.44832	1.1878	2.09038
C	-4.66417	-1.78286	1.7435	C	-4.65426	-1.99476	1.75472
C	0.87527	1.77143	0.32488	C	0.73369	1.79915	0.31971
C	0.83256	3.31155	0.31407	C	0.59804	3.3346	0.31465

C	-0.47746	3.97186	-0.06899	C	-0.74104	3.91572	-0.09199
C	-1.67928	3.27178	0.56769	C	-1.90533	3.15034	0.53755
C	2.13453	3.99218	0.13955	C	1.85935	4.09552	0.17587
C	2.27225	5.39212	-0.41965	C	1.92472	5.5058	-0.37043
C	1.66627	1.21233	-0.95967	C	1.58875	1.29573	-0.9433
C	2.93827	2.07926	-1.25675	C	2.8069	2.24797	-1.21368
C	0.71621	1.27289	-2.17064	C	0.67066	1.29244	-2.18074
O	0.34998	0.00009	-2.55346	O	0.44667	-0.00142	-2.6068
O	0.30295	2.24136	-2.7544	O	0.18028	2.22837	-2.75642
C	3.31332	3.06326	-0.13372	C	3.09866	3.24286	-0.07623
O	1.53405	3.89453	1.45169	O	1.23585	3.95064	1.47232
O	-4.63273	-3.67852	-0.23327	O	-3.15944	-2.78056	-1.55035
H	-1.79351	1.78909	-0.96015	H	-1.93828	1.66302	-0.98918
H	-2.45233	-0.52869	-0.65045	H	-2.51345	-0.67675	-0.69222
H	1.51935	1.51008	1.16687	H	1.3705	1.5762	1.17787
H	5.07671	-3.39962	2.07617	H	5.24054	-3.06736	2.1858
H	5.599	-2.44453	0.68765	H	5.74766	-2.03676	0.84673
H	5.07679	-0.88096	2.47601	H	4.99282	-0.56748	2.63096
H	3.2986	0.45124	1.28395	H	3.16867	0.6291	1.37249
H	4.63129	-0.09609	0.2912	H	4.5894	0.22049	0.43673
H	0.33357	-2.6814	-2.74539	H	0.72379	-2.65878	-2.88133
H	2.82738	-0.69567	3.5062	H	2.68522	-0.60949	3.54311
H	3.54247	-2.28126	3.83553	H	3.52528	-2.13018	3.88218
H	2.26967	-2.12418	2.62078	H	2.30745	-2.06311	2.60495
H	1.01519	-4.77479	-2.28719	H	1.58522	-4.69083	-2.44232
H	2.71522	-5.01105	-1.80845	H	3.26444	-4.77697	-1.85675
H	1.46533	-5.12041	-0.60008	H	1.95746	-5.04742	-0.73788
H	-6.30577	1.11057	-0.75303	H	-6.40175	0.75867	-0.79013
H	-5.90682	0.75714	0.91628	H	-6.00803	0.43617	0.88576
H	-6.13965	-1.35376	-0.43522	H	-6.12824	-1.6923	-0.44472
H	-4.9262	-0.75269	-1.56365	H	-4.93284	-1.0524	-1.571
H	-4.47944	2.60769	-0.00622	H	-4.66161	2.34335	-0.01627
H	-3.94561	1.54683	-1.30399	H	-4.07379	1.3201	-1.32054
H	-2.0433	-1.02761	2.33405	H	-2.01183	-1.1965	2.27653
H	-1.45434	-2.00519	1.00357	H	-1.39392	-2.11973	0.9298
H	0.43755	-0.55428	1.52119	H	0.42197	-0.573	1.46021
H	-4.18614	0.83676	2.5116	H	-4.24566	0.56841	2.50065
H	-2.47721	1.20039	2.74198	H	-2.56067	1.03717	2.7117
H	-3.59426	2.4609	2.22176	H	-3.76043	2.22886	2.21277
H	-3.91335	-2.28628	2.35884	H	-3.87364	-2.3634	2.42339
H	-5.51127	-2.46279	1.63416	H	-5.39368	-2.79385	1.6592
H	-5.00919	-0.90575	2.29119	H	-5.14109	-1.14336	2.23002
H	-0.44972	5.01809	0.24499	H	-0.7788	4.96395	0.21388

H	-0.57145	3.95185	-1.16128	H	-0.81948	3.88172	-1.18509
H	-1.59788	3.34652	1.65791	H	-1.83457	3.23116	1.62798
H	-2.59515	3.79665	0.27562	H	-2.84774	3.62186	0.23975
H	1.3853	6.00003	-0.2388	H	0.99817	6.05711	-0.20802
H	3.12816	5.89105	0.0498	H	2.73652	6.05194	0.12407
H	2.45463	5.35617	-1.5	H	2.13603	5.49031	-1.44599
H	2.74643	2.66494	-2.1621	H	2.59167	2.82909	-2.11675
H	3.7797	1.4182	-1.4844	H	3.69276	1.64483	-1.43377
H	4.19256	3.63791	-0.44552	H	3.94753	3.87221	-0.36568
H	3.58818	2.54263	0.78762	H	3.38534	2.73247	0.84708
H	-4.34085	-4.41573	-0.79588	H	-2.92109	-3.66658	-1.87085
3a-4	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-1	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.98402	-2.15825	-1.58074	C	5.05055	-2.01271	1.63142
C	-4.17479	-1.04803	-2.25854	C	4.19268	-0.92708	2.28861
C	-3.71559	-0.0691	-1.16825	C	3.71646	0.02739	1.18396
C	-3.0038	-0.72097	0.00647	C	3.03738	-0.65829	0.00941
C	-3.26817	-2.0811	0.35896	C	3.3588	-2.00858	-0.33288
C	-4.21903	-2.87477	-0.47721	C	4.33438	-2.75948	0.51527
C	-2.10859	0.01457	0.79244	C	2.11824	0.03627	-0.78648
C	-1.54583	-0.59974	1.90762	C	1.58795	-0.60637	-1.90136
C	-1.77402	-1.91074	2.27608	C	1.8742	-1.90841	-2.26172
C	-2.63891	-2.68176	1.49155	C	2.76454	-2.63977	-1.46748
C	-3.01411	-1.6027	-3.09963	C	3.03929	-1.51553	3.11662
O	-4.42245	-4.0718	-0.29435	O	4.59599	-3.94468	0.33086
C	-2.86019	-4.11307	1.92302	C	3.04945	-4.0621	-1.89139
C	3.51065	-3.1781	0.40274	C	-3.53683	-3.29595	-0.28881
O	3.01477	-3.21838	1.51171	O	-3.58591	-4.38148	0.2533
C	5.57831	0.06853	0.3254	C	-5.61036	-0.0247	-0.27659
C	5.17497	-1.37179	0.65521	C	-5.19436	-1.46076	-0.61207
C	4.03921	-1.89921	-0.27175	C	-4.03991	-1.96928	0.30253
C	2.83876	-0.87816	-0.24131	C	-2.84975	-0.93723	0.24999
C	3.1754	0.63755	-0.44414	C	-3.2034	0.57369	0.46418
C	4.37994	1.01575	0.4577	C	-4.42531	0.93781	-0.42057
C	1.6723	-1.30231	-1.14644	C	-1.66173	-1.34988	1.13183
C	0.54038	-0.31552	-1.10507	C	-0.54585	-0.34542	1.08187
C	0.60669	0.89837	-0.53704	C	-0.6375	0.87187	0.52431
C	1.91142	1.42811	0.06561	C	-1.95801	1.38404	-0.06025
C	3.48209	1.00535	-1.9139	C	-3.49404	0.93174	1.93927
C	4.60538	-2.21933	-1.67062	C	-4.58426	-2.29011	1.70934
C	-0.65983	1.76177	-0.49036	C	0.61524	1.75699	0.47508
C	-0.37612	3.26765	-0.68818	C	0.30689	3.25851	0.66792
C	1.04021	3.52234	-1.16082	C	-1.10643	3.48876	1.16063

C	2.01799	2.97416	-0.11149	C	-2.08738	2.9275	0.12172
C	-1.17359	4.32238	-0.00963	C	1.07233	4.32524	-0.02844
C	-0.65084	5.72855	0.21175	C	0.51868	5.71954	-0.24938
C	-1.59372	1.44965	0.7498	C	1.55518	1.45371	-0.76179
C	-2.74377	2.4901	0.82357	C	2.67594	2.52466	-0.85969
C	-0.74777	1.49189	2.03754	C	0.70678	1.45092	-2.04841
O	-0.73508	0.24787	2.63736	O	0.74782	0.20294	-2.64109
O	-0.14209	2.41373	2.5206	O	0.06246	2.34243	-2.53779
C	-2.26392	3.93374	0.97066	C	2.15554	3.95201	-1.02225
O	-1.43568	3.96293	-1.39113	O	1.36315	3.97832	1.35057
O	3.65097	-4.30588	-0.3407	O	-3.02106	-3.16339	-1.54204
H	1.87403	1.23986	1.14661	H	-1.93104	1.19966	-1.14224
H	2.46979	-0.94532	0.79006	H	-2.4949	-0.98725	-0.78675
H	-1.25594	1.48539	-1.36515	H	1.21338	1.49469	1.35274
H	-5.32544	-2.92108	-2.28643	H	5.40359	-2.76106	2.34685
H	-5.88277	-1.72432	-1.1164	H	5.9438	-1.55164	1.1828
H	-4.84152	-0.49855	-2.93544	H	4.82961	-0.34966	2.97086
H	-3.08527	0.70696	-1.60952	H	3.05914	0.78898	1.61042
H	-4.60274	0.45228	-0.77912	H	4.59195	0.57071	0.79834
H	-1.29102	-2.32666	3.15336	H	1.42111	-2.34609	-3.14452
H	-2.46717	-0.79213	-3.5938	H	2.45671	-0.72088	3.59566
H	-3.38876	-2.27625	-3.87785	H	3.4253	-2.16911	3.90616
H	-2.30004	-2.16846	-2.49095	H	2.35478	-2.11118	2.50256
H	-2.2984	-4.31144	2.84025	H	2.5031	-4.28788	-2.81189
H	-3.91799	-4.32506	2.09895	H	4.11629	-4.22934	-2.06017
H	-2.54286	-4.81947	1.15155	H	2.7581	-4.7787	-1.11905
H	6.36921	0.38519	1.01613	H	-6.41287	0.284	-0.9575
H	6.01424	0.12995	-0.67926	H	-6.0349	0.02959	0.73301
H	6.04037	-2.04242	0.5813	H	-6.04943	-2.14218	-0.52254
H	4.82379	-1.41313	1.69255	H	-4.86531	-1.49494	-1.65681
H	4.69799	2.04326	0.24599	H	-4.75449	1.96026	-0.20175
H	4.05002	1.00345	1.50613	H	-4.1085	0.93389	-1.47332
H	1.99835	-1.43745	-2.18718	H	-1.96926	-1.49844	2.17607
H	1.29348	-2.28456	-0.83107	H	-1.27416	-2.32525	0.80588
H	-0.39399	-0.63932	-1.55964	H	0.39806	-0.65731	1.52492
H	4.38409	0.51448	-2.28199	H	-4.38405	0.42791	2.31808
H	2.66191	0.73852	-2.58563	H	-2.66106	0.67222	2.59798
H	3.64987	2.08177	-2.01464	H	-3.67354	2.00563	2.04678
H	3.84251	-2.59894	-2.35351	H	-3.80204	-2.64557	2.38312
H	5.38142	-2.98567	-1.59515	H	-5.32965	-3.08666	1.64188
H	5.05665	-1.33746	-2.12528	H	-5.05973	-1.42127	2.16348
H	1.18794	3.0223	-2.12703	H	-1.23369	2.98359	2.12704
H	1.20754	4.58756	-1.32799	H	-1.28869	4.55061	1.33332

H	3.03815	3.26344	-0.37617	H	-3.10889	3.19973	0.3987
H	1.80396	3.45854	0.84698	H	-1.89228	3.41758	-0.83799
H	0.00409	6.0582	-0.5951	H	-0.13486	6.03906	0.5626
H	-1.49313	6.42821	0.26266	H	1.34596	6.43598	-0.31138
H	-0.10595	5.78983	1.16026	H	-0.03685	5.76624	-1.19257
H	-3.41025	2.23327	1.65463	H	3.34223	2.27399	-1.69278
H	-3.32931	2.39919	-0.09437	H	3.27111	2.46266	0.05441
H	-1.88416	4.10955	1.98197	H	1.75453	4.10193	-2.02962
H	-3.11777	4.60906	0.82677	H	2.99336	4.65175	-0.9032
H	3.299	-5.03514	0.19858	H	-2.75393	-4.05361	-1.82645
3b-2	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-3	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.21713	-2.90125	-1.60021	C	4.97885	-2.21293	1.59248
C	-4.71063	-1.49676	-1.2553	C	4.19086	-1.07886	2.25522
C	-3.48464	-0.62234	-0.97312	C	3.7409	-0.11232	1.15015
C	-2.58041	-1.18795	0.10418	C	3.00729	-0.77445	-0.00516
C	-2.48527	-2.59858	0.30937	C	3.24864	-2.14432	-0.33589
C	-3.2925	-3.51118	-0.55448	C	4.2006	-2.93506	0.50148
C	-1.80729	-0.33625	0.89838	C	2.11347	-0.04064	-0.79409
C	-0.98647	-0.90153	1.87028	C	1.52781	-0.66731	-1.89037
C	-0.86802	-2.25787	2.10054	C	1.7314	-1.98829	-2.23611
C	-1.62233	-3.13525	1.31313	C	2.59537	-2.75696	-1.44838
C	-5.59608	-0.9074	-2.35824	C	3.02618	-1.60043	3.11185
O	-3.22683	-4.73452	-0.47121	O	4.39666	-4.13495	0.32917
C	-1.46782	-4.61186	1.59367	C	2.78775	-4.19992	-1.85367
C	3.75281	-2.65797	0.24965	C	-3.61752	-3.10655	-0.41176
O	3.28387	-2.72324	1.36928	O	-2.70481	-3.21592	-1.20619
C	5.54863	0.74829	0.13504	C	-5.57645	0.19012	-0.24603
C	5.2706	-0.71879	0.4783	C	-5.21351	-1.25592	-0.59501
C	4.18503	-1.35185	-0.44242	C	-4.05684	-1.8131	0.29549
C	2.90262	-0.43337	-0.43331	C	-2.84488	-0.81949	0.26566
C	3.1097	1.10285	-0.63806	C	-3.15116	0.70427	0.47362
C	4.2724	1.58741	0.26726	C	-4.36119	1.10981	-0.4073
C	1.788	-0.94253	-1.35837	C	-1.6838	-1.26099	1.17027
C	0.54677	-0.10768	-1.21361	C	-0.53311	-0.29671	1.11484
C	0.5087	1.08549	-0.5993	C	-0.57882	0.91502	0.54002
C	1.78193	1.80004	-0.15319	C	-1.87864	1.46951	-0.05157
C	3.40028	1.47932	-2.11048	C	-3.43208	1.08086	1.94694
C	4.7846	-1.65215	-1.83208	C	-4.59189	-2.15748	1.70506
C	-0.84756	1.74595	-0.33639	C	0.7058	1.75028	0.47274
C	-0.8278	3.2864	-0.3203	C	0.45632	3.2637	0.65578
C	0.47068	3.96525	0.07044	C	-0.94591	3.55213	1.1504
C	1.68594	3.28664	-0.56417	C	-1.95242	3.01815	0.12122

C	-2.14159	3.94251	-0.14454	C	1.2614	4.29399	-0.05069
C	-2.30719	5.33429	0.42638	C	0.762	5.7071	-0.28149
C	-1.61708	1.17413	0.9532	C	1.62061	1.40251	-0.77215
C	-2.92821	1.99571	1.2256	C	2.78574	2.423	-0.88069
C	-0.69465	1.29497	2.18177	C	0.75964	1.43341	-2.05017
O	-0.30439	0.0439	2.6118	O	0.72089	0.17919	-2.62627
O	-0.32626	2.28942	2.75105	O	0.1621	2.35555	-2.54326
C	-3.30463	2.98835	0.10906	C	2.32668	3.87148	-1.04441
O	-1.53458	3.86556	-1.45555	O	1.54153	3.94738	1.33058
O	3.9416	-3.7787	-0.49372	O	-4.4157	-4.16772	-0.11772
H	1.81204	1.7867	0.94741	H	-1.85643	1.27774	-1.1323
H	2.52234	-0.53124	0.59172	H	-2.46897	-0.89169	-0.76225
H	-1.49952	1.47331	-1.16937	H	1.30344	1.47099	1.34559
H	-3.65291	-2.86561	-2.5461	H	5.31012	-2.97025	2.30894
H	-5.03735	-3.60927	-1.75382	H	5.88354	-1.80172	1.11904
H	-5.30407	-1.55719	-0.33073	H	4.86979	-0.52807	2.91887
H	-2.91213	-0.51586	-1.90903	H	3.12838	0.68338	1.58132
H	-3.80221	0.38532	-0.69926	H	4.63428	0.38511	0.74419
H	-0.19989	-2.62762	2.87034	H	1.22827	-2.41475	-3.09675
H	-5.95669	0.09169	-2.08849	H	2.49415	-0.77279	3.59391
H	-6.4711	-1.54076	-2.5399	H	3.39463	-2.26549	3.9003
H	-5.04434	-0.82118	-3.30248	H	2.3005	-2.16594	2.51688
H	-0.76661	-4.75751	2.42018	H	2.20376	-4.40942	-2.75438
H	-2.42354	-5.07706	1.84926	H	3.83862	-4.43059	-2.04682
H	-1.10363	-5.15286	0.71641	H	2.47629	-4.88502	-1.06095
H	6.31238	1.13633	0.81983	H	-6.38142	0.52675	-0.91064
H	5.97227	0.84053	-0.8726	H	-5.98006	0.25078	0.77202
H	6.19045	-1.31332	0.4099	H	-6.08551	-1.91275	-0.50225
H	4.92495	-0.77988	1.51639	H	-4.89752	-1.28836	-1.64641
H	4.49527	2.63989	0.05555	H	-4.65143	2.14487	-0.19268
H	3.94497	1.54223	1.3154	H	-4.05265	1.0873	-1.46226
H	2.11331	-0.96447	-2.40756	H	-2.00771	-1.37827	2.2142
H	1.53465	-1.98219	-1.10935	H	-1.32886	-2.25037	0.85539
H	-0.37657	-0.54739	-1.58505	H	0.39908	-0.63727	1.56177
H	4.24772	0.92764	-2.51762	H	-4.34376	0.61585	2.32566
H	2.54009	1.2887	-2.75886	H	-2.61256	0.79348	2.61056
H	3.64412	2.54207	-2.19505	H	-3.57041	2.16148	2.04793
H	4.04835	-2.06479	-2.52505	H	-3.83165	-2.64272	2.32324
H	5.59105	-2.38467	-1.74191	H	-5.43964	-2.84174	1.63194
H	5.20808	-0.75416	-2.28239	H	-4.92614	-1.26354	2.23135
H	0.56068	3.94464	1.16271	H	-1.08822	3.06143	2.12224
H	0.42778	5.01167	-0.24136	H	-1.08745	4.6218	1.31319
H	1.6115	3.37111	-1.65405	H	-2.96183	3.32864	0.40278

H	2.593	3.81996	-0.26016	H	-1.74619	3.49457	-0.84303
H	-1.42949	5.95859	0.25641	H	0.12464	6.05863	0.53017
H	-3.16875	5.82309	-0.04335	H	1.61649	6.39005	-0.35244
H	-2.49449	5.28483	1.50532	H	0.20513	5.76759	-1.22308
H	-2.78262	2.57173	2.14535	H	3.43494	2.14162	-1.71747
H	-3.75325	1.30362	1.41963	H	3.38411	2.33791	0.02946
H	-4.19859	3.54224	0.41662	H	1.93092	4.03621	-2.05147
H	-3.55572	2.47651	-0.82449	H	3.19378	4.53511	-0.92781
H	3.6429	-4.52491	0.05437	H	-4.09641	-4.91048	-0.65794
3b-4	X axis(Å)	Y axis(Å)	Z axis(Å)	4-1	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.2333	-2.90902	-1.62998	C	-5.58501	-1.87276	-0.64727
C	-4.73328	-1.51367	-1.25847	C	-4.59246	-3.01106	-0.90104
C	-3.5113	-0.63714	-0.96637	C	-3.42741	-3.03139	0.13994
C	-2.59447	-1.21738	0.09242	C	-2.77092	-1.61074	0.22936
C	-2.49144	-2.6308	0.2734	C	-3.72739	-0.37321	0.33235
C	-3.30647	-3.53255	-0.5943	C	-4.87611	-0.51539	-0.69878
C	-1.81591	-0.37561	0.89207	C	-1.67376	-1.51595	1.30112
C	-0.98159	-0.95367	1.84463	C	-1.04082	-0.1521	1.32245
C	-0.85363	-2.31276	2.04972	C	-1.5167	0.92091	0.67076
C	-1.61317	-3.18022	1.25685	C	-2.85744	0.87733	-0.0682
C	-5.62709	-0.91004	-2.34687	C	-0.68504	2.21102	0.65085
O	-3.24656	-4.75691	-0.52201	C	-1.55017	3.47011	0.57795
C	-1.44449	-4.66051	1.50714	C	-2.95512	3.20351	1.05856
C	3.85554	-2.5987	0.27723	C	-3.62014	2.23635	0.06038
O	2.92135	-2.78205	1.03224	C	-4.31867	-0.1851	1.74998
C	5.54501	0.84179	0.03472	C	-2.38823	-3.99343	-0.45988
C	5.30797	-0.62479	0.40666	O	-1.38171	-3.6858	-1.06762
C	4.191	-1.29033	-0.46066	O	-2.73276	-5.30116	-0.30612
C	2.90376	-0.39556	-0.44805	C	5.60554	-0.40943	1.47605
C	3.08373	1.14429	-0.66711	C	4.20824	-0.36305	2.13765
C	4.2586	1.65675	0.20492	C	3.20219	-0.3819	0.9453
C	1.7869	-0.92169	-1.36193	C	4.03963	-0.5653	-0.35153
C	0.5363	-0.10239	-1.20699	C	5.3825	-1.13006	0.13763
C	0.48652	1.09056	-0.59279	C	2.27888	0.84397	0.89883
C	1.75541	1.82162	-0.15928	C	1.46634	1.07226	-0.29193
C	3.33724	1.52042	-2.14705	C	1.41566	0.29436	-1.41528
C	4.74745	-1.63226	-1.86331	C	2.10724	-0.88457	-1.88309
C	-0.87684	1.73227	-0.31629	C	3.3083	-1.32317	-1.44132
C	-0.87606	3.27289	-0.28247	C	0.46435	2.20694	-0.43673
C	0.41795	3.96399	0.10086	O	0.4741	0.7546	-2.31792
C	1.63278	3.3091	-0.55832	C	3.96937	-1.52003	3.11932
C	-2.19481	3.91296	-0.08554	C	3.93857	-2.54151	-2.05711

C	-2.3693	5.29671	0.50227	C	1.17146	3.58984	-0.38761
C	-1.63163	1.13462	0.97064	O	6.37593	-0.89139	-0.85254
C	-2.94352	1.94405	1.27188	C	7.62819	-1.50297	-0.58394
C	-0.69486	1.2386	2.18973	O	2.18476	1.58958	1.87773
O	-0.29492	-0.01713	2.59441	C	-0.10554	1.92233	-1.82517
O	-0.32209	2.22568	2.7696	O	-0.9086	2.52244	-2.48814
C	-3.34468	2.94423	0.17102	C	0.22503	4.76895	-0.6102
O	-1.60168	3.85677	-1.40376	C	-1.12625	4.63539	0.0534
O	4.7762	-3.57626	0.06076	C	-1.94925	5.89923	-0.03494
H	1.80202	1.80184	0.94081	H	4.27271	0.43413	-0.75617
H	2.52325	-0.49305	0.57618	C	-3.9303	-3.61236	1.48324
H	-1.52998	1.46187	-1.14916	H	-2.26096	-1.49262	-0.73467
H	-3.6689	-2.85249	-2.57477	H	-2.63433	0.74582	-1.13608
H	-5.05015	-3.61796	-1.79655	H	-0.13397	2.23972	1.59855
H	-5.32231	-1.59397	-0.33256	H	2.5264	-1.24506	1.04913
H	-2.94614	-0.50715	-1.90382	H	-6.37061	-1.90728	-1.41203
H	-3.83438	0.36216	-0.66961	H	-6.09302	-2.01247	0.31483
H	-0.17042	-2.693	2.8006	H	-5.09767	-3.98304	-0.89223
H	-5.99163	0.08233	-2.05817	H	-4.16812	-2.87989	-1.90591
H	-6.49963	-1.54483	-2.53543	H	-5.60521	0.29132	-0.5591
H	-5.08026	-0.80448	-3.29202	H	-4.46122	-0.38526	-1.7086
H	-0.72571	-4.81631	2.31641	H	-2.06398	-1.75941	2.29952
H	-2.39217	-5.13663	1.77232	H	-0.89544	-2.26178	1.09519
H	-1.09244	-5.18208	0.61338	H	-0.11892	-0.05693	1.89325
H	6.32916	1.25175	0.6828	H	-3.54784	4.11639	1.1396
H	5.92584	0.92389	-0.99063	H	-2.93629	2.74632	2.05831
H	6.22994	-1.20867	0.31149	H	-3.6486	2.72769	-0.91751
H	5.01013	-0.66728	1.46317	H	-4.66141	2.0714	0.35149
H	4.45487	2.71249	-0.01581	H	-3.54009	-0.04631	2.50427
H	3.96271	1.60888	1.26256	H	-4.96706	0.69478	1.78684
H	2.10117	-0.93867	-2.41491	H	-4.93168	-1.03373	2.05782
H	1.55179	-1.96096	-1.10121	H	-2.05359	-5.82058	-0.76867
H	-0.38429	-0.55497	-1.56981	H	5.96718	0.60354	1.25917
H	4.18915	0.98674	-2.56948	H	6.3495	-0.89904	2.1126
H	2.46928	1.30916	-2.77801	H	4.0763	0.574	2.68435
H	3.55668	2.58783	-2.23982	H	5.30501	-2.21691	0.30965
H	4.00544	-2.14258	-2.48363	H	1.60917	-1.40204	-2.69803
H	5.61356	-2.29106	-1.77588	H	2.95708	-1.47401	3.53593
H	5.06405	-0.73437	-2.3942	H	4.67537	-1.47362	3.95604
H	0.35723	5.01373	-0.19639	H	4.08775	-2.49858	2.63679
H	0.52246	3.92984	1.19161	H	3.32292	-2.93796	-2.86784
H	1.5395	3.4011	-1.64623	H	4.93593	-2.3044	-2.44244
H	2.53649	3.85374	-0.26454	H	4.06894	-3.33672	-1.3116

H	-1.50043	5.93262	0.33009	H	1.98365	3.61215	-1.12379
H	-3.24111	5.78097	0.04694	H	1.63331	3.65428	0.60152
H	-2.5448	5.23351	1.58249	H	8.26709	-1.3088	-1.44817
H	-2.78707	2.51279	2.19445	H	8.10595	-1.08452	0.31218
H	-3.76026	1.24407	1.47272	H	7.52168	-2.59105	-0.45338
H	-4.24059	3.48532	0.49534	H	0.72163	5.68498	-0.25973
H	-3.6014	2.44017	-0.76512	H	0.05142	4.91962	-1.68579
H	4.51121	-4.33176	0.61235	H	-2.93419	5.82165	0.42672
				H	-1.42202	6.73401	0.44621
				H	-2.09454	6.18684	-1.0855
				H	-4.69067	-2.97264	1.93095
				H	-4.37014	-4.59964	1.32791
				H	-3.11964	-3.72257	2.20879
4-2	X axis(Å)	Y axis(Å)	Z axis(Å)	4-3	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-5.67877	-1.82436	-0.62458	C	-5.58521	-1.87248	-0.64689
C	-4.7105	-2.9778	-0.90867	C	-4.59268	-3.01079	-0.90076
C	-3.54341	-3.03655	0.12197	C	-3.42756	-3.03115	0.14014
C	-2.84418	-1.62415	0.19417	C	-2.77103	-1.61054	0.22955
C	-3.77112	-0.37184	0.34729	C	-3.72747	-0.373	0.33262
C	-4.94687	-0.4776	-0.65906	C	-4.87628	-0.51512	-0.69842
C	-1.70092	-1.57101	1.21811	C	-1.67382	-1.51579	1.30126
C	-1.04773	-0.21736	1.25308	C	-1.04083	-0.15195	1.32253
C	-1.52866	0.88035	0.64758	C	-1.51672	0.92105	0.67082
C	-2.88998	0.87116	-0.05575	C	-2.85753	0.87752	-0.06799
C	-0.68216	2.16343	0.6522	C	-0.68495	2.21109	0.65068
C	-1.53424	3.43249	0.60478	C	-1.54996	3.47023	0.57754
C	-2.93028	3.17603	1.11487	C	-2.95485	3.20387	1.05845
C	-3.63156	2.23677	0.11589	C	-3.6202	2.23658	0.06063
C	-4.31619	-0.20204	1.78467	C	-4.31862	-0.18491	1.75031
C	-2.50686	-4.039	-0.40865	C	-2.38848	-3.99324	-0.4598
O	-2.15596	-5.06337	0.1423	O	-1.38186	-3.68565	-1.06739
O	-1.98861	-3.6871	-1.61838	O	-2.73324	-5.30094	-0.30633
C	5.60262	-0.43436	1.53863	C	5.60628	-0.40857	1.47518
C	4.18628	-0.43368	2.1597	C	4.20929	-0.36173	2.13742
C	3.21608	-0.4195	0.93829	C	3.20264	-0.38159	0.94556
C	4.09342	-0.54718	-0.33907	C	4.03948	-0.56565	-0.35152
C	5.4303	-1.11003	0.16973	C	5.3826	-1.13006	0.13733
C	2.28432	0.8005	0.90401	C	2.27894	0.84398	0.8989
C	1.48188	1.04012	-0.29232	C	1.46632	1.07197	-0.29186
C	1.46943	0.29346	-1.43709	C	1.41546	0.29371	-1.41495
C	2.20556	-0.84805	-1.93094	C	2.10662	-0.88565	-1.88228
C	3.4075	-1.27431	-1.47804	C	3.3077	-1.32421	-1.44054
C	0.46815	2.16555	-0.43074	C	0.46442	2.20668	-0.43693

O	0.52976	0.75295	-2.34213	O	0.47389	0.75382	-2.31768
C	3.93612	-1.63211	3.08743	C	3.97097	-1.51792	3.12014
C	4.08908	-2.44237	-2.13545	C	3.93749	-2.5432	-2.05552
C	1.17652	3.5495	-0.37824	C	1.17161	3.58956	-0.38817
O	6.44768	-0.82192	-0.78193	O	6.37553	-0.89201	-0.85349
C	7.70268	-1.42103	-0.49618	C	7.62794	-1.50337	-0.58511
O	2.17355	1.53024	1.8923	O	2.18468	1.58968	1.87772
C	-0.09314	1.88847	-1.82432	C	-0.10552	1.92174	-1.82528
O	-0.91712	2.47248	-2.4751	O	-0.90852	2.5218	-2.48839
C	0.23057	4.72776	-0.60102	C	0.22522	4.76864	-0.61108
C	-1.11141	4.59865	0.08145	C	-1.12602	4.63534	0.05264
C	-1.92592	5.86943	0.01795	C	-1.949	5.89917	-0.03601
H	4.32428	0.46856	-0.70284	H	4.2723	0.43358	-0.75679
C	-4.05518	-3.59903	1.46375	C	-3.93038	-3.61214	1.48347
H	-2.38157	-1.50075	-0.79287	H	-2.26112	-1.4924	-0.7345
H	-2.69575	0.75613	-1.13116	H	-2.63452	0.74603	-1.1359
H	-0.13523	2.16954	1.60282	H	-0.13385	2.23992	1.59837
H	2.54684	-1.2922	0.9911	H	2.52711	-1.24485	1.05035
H	-6.47119	-1.82774	-1.383	H	-6.37086	-1.90699	-1.4116
H	-6.18276	-1.96915	0.3386	H	-6.09315	-2.01221	0.31523
H	-5.24044	-3.93857	-0.90477	H	-5.0979	-3.98277	-0.89192
H	-4.29521	-2.84513	-1.91393	H	-4.16844	-2.87963	-1.90567
H	-5.66001	0.3367	-0.48536	H	-5.60534	0.29161	-0.55868
H	-4.55214	-0.33068	-1.67461	H	-4.46147	-0.38499	-1.70827
H	-2.05111	-1.83941	2.22425	H	-2.06399	-1.75923	2.29968
H	-0.94056	-2.32539	0.96957	H	-0.89552	-2.26163	1.09529
H	-0.11151	-0.15014	1.80377	H	-0.11885	-0.05681	1.89321
H	-3.50812	4.09494	1.22811	H	-3.54746	4.11683	1.13946
H	-2.89279	2.70003	2.10527	H	-2.93586	2.74687	2.05829
H	-3.67743	2.74648	-0.85189	H	-3.649	2.72776	-0.91733
H	-4.66739	2.07884	0.42901	H	-4.66136	2.07167	0.35215
H	-3.51206	-0.08683	2.51611	H	-3.53998	-0.04622	2.50454
H	-4.95129	0.68527	1.85748	H	-4.96696	0.695	1.78729
H	-4.92822	-1.04935	2.09599	H	-4.93166	-1.03352	2.05815
H	-1.36814	-4.39253	-1.86684	H	-2.05411	-5.82038	-0.76893
H	5.95349	0.59125	1.36855	H	5.96787	0.60425	1.25748
H	6.33572	-0.93502	2.17901	H	6.35053	-0.89779	2.1117
H	4.02491	0.47947	2.73793	H	4.07754	0.57574	2.68344
H	5.36428	-2.20332	0.30129	H	5.30523	-2.2168	0.31009
H	1.7489	-1.33672	-2.78723	H	1.60813	-1.40358	-2.69667
H	2.9116	-1.61738	3.47538	H	2.95887	-1.47162	3.53719
H	4.61639	-1.60884	3.94602	H	4.67737	-1.4708	3.95647
H	4.08345	-2.58923	2.57118	H	4.08918	-2.49685	2.63833

H	3.50734	-2.81608	-2.98154	H	3.32145	-2.94019	-2.8657
H	5.08778	-2.15686	-2.48222	H	4.93476	-2.30665	-2.44141
H	4.22712	-3.26883	-1.42628	H	4.06793	-3.33781	-1.30938
H	1.99055	3.57185	-1.11236	H	1.9838	3.61162	-1.12435
H	1.6354	3.61266	0.61247	H	1.63344	3.65424	0.60095
H	8.36258	-1.18791	-1.33454	H	8.26642	-1.30972	-1.44977
H	8.14645	-1.0238	0.42651	H	8.10611	-1.08434	0.31052
H	7.61155	-2.5143	-0.4038	H	7.52154	-2.59137	-0.45382
H	0.73219	5.64534	-0.2622	H	0.72189	5.68476	-0.26091
H	0.04583	4.87115	-1.67581	H	0.05159	4.91898	-1.68671
H	-2.90986	5.79103	0.48148	H	-2.9338	5.82182	0.42598
H	-1.39115	6.69268	0.51054	H	-1.42159	6.73415	0.4446
H	-2.0731	6.17512	-1.02717	H	-2.0946	6.18633	-1.08666
H	-4.87536	-3.00212	1.86165	H	-4.69077	-2.97245	1.93119
H	-4.41986	-4.61944	1.3193	H	-4.37016	-4.59945	1.32818
H	-3.2674	-3.64757	2.218	H	-3.11968	-3.72229	2.20899
4-4	X axis(Å)	Y axis(Å)	Z axis(Å)	4-5	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-5.67937	-1.42367	-0.70547	C	-5.6792	-1.42391	-0.70561
C	-4.79042	-2.64417	-0.96077	C	-4.79024	-2.64443	-0.96077
C	-3.6406	-2.77708	0.08948	C	-3.64043	-2.77722	0.08954
C	-2.86161	-1.42116	0.19894	C	-2.86148	-1.42127	0.19889
C	-3.70587	-0.10439	0.30417	C	-3.70577	-0.10451	0.30403
C	-4.85104	-0.13517	-0.73942	C	-4.85089	-0.1354	-0.73962
C	-1.77203	-1.43327	1.28222	C	-1.7719	-1.4333	1.28217
C	-1.01936	-0.13218	1.32018	C	-1.01929	-0.13217	1.32012
C	-1.3916	0.98398	0.67369	C	-1.39154	0.98395	0.67358
C	-2.72417	1.06752	-0.07588	C	-2.72408	1.0674	-0.07606
C	-0.44804	2.1943	0.67104	C	-0.44808	2.19433	0.67101
C	-1.19647	3.52701	0.61455	C	-1.19658	3.52701	0.61464
C	-2.62413	3.37976	1.07959	C	-2.62432	3.37964	1.07945
C	-3.36255	2.48853	0.06217	C	-3.36249	2.4884	0.06186
C	-4.2935	0.12323	1.71754	C	-4.29344	0.12316	1.71737
C	-2.68528	-3.82164	-0.51175	C	-2.685	-3.82176	-0.51155
O	-1.65193	-3.59833	-1.11156	O	-1.6516	-3.59843	-1.11124
O	-3.14305	-5.09533	-0.37002	O	-3.1428	-5.09545	-0.36987
C	5.07933	-2.02756	1.56823	C	5.07895	-2.0278	1.56816
C	4.10264	-0.96684	2.10276	C	4.10236	-0.96699	2.10271
C	3.14987	-0.77304	0.90556	C	3.14973	-0.77295	0.90545
C	4.01404	-0.97321	-0.38038	C	4.01398	-0.97315	-0.38045
C	5.34163	-1.63935	0.11152	C	5.34146	-1.63946	0.11154
C	2.3762	0.54483	0.89551	C	2.37623	0.54501	0.89542
C	1.58581	0.87664	-0.28951	C	1.58586	0.87686	-0.2896
C	1.47487	0.13099	-1.42865	C	1.47484	0.13119	-1.42873

C	2.0636	-1.09672	-1.91715	C	2.06357	-1.0965	-1.91728
C	3.22295	-1.64759	-1.48808	C	3.22291	-1.64742	-1.48824
C	0.69656	2.10211	-0.41672	C	0.6966	2.10231	-0.41675
O	0.587	0.69361	-2.32909	O	0.58693	0.69381	-2.32912
C	3.41348	-1.35832	3.41136	C	3.41303	-1.35847	3.41122
C	3.72823	-2.90871	-2.13622	C	3.72824	-2.90845	-2.1365
C	1.53007	3.41192	-0.34106	C	1.53	3.41217	-0.3409
O	6.42235	-0.70223	0.10346	O	6.42224	-0.70239	0.10374
C	6.98323	-0.46662	-1.17536	C	6.98336	-0.46673	-1.17497
O	2.3871	1.28736	1.88003	O	2.38714	1.28748	1.87996
C	0.10961	1.8974	-1.81276	C	0.10963	1.89767	-1.8128
O	-0.63277	2.58054	-2.46594	O	-0.63275	2.58081	-2.46596
C	0.69775	4.67782	-0.5426	C	0.69763	4.67805	-0.54227
C	-0.6646	4.65714	0.11187	C	-0.66473	4.65724	0.11219
C	-1.3692	5.9915	0.03888	C	-1.36941	5.99156	0.03937
H	4.29045	0.02413	-0.75492	H	4.29054	0.02416	-0.75497
C	-4.20471	-3.32336	1.42296	C	-4.20458	-3.32338	1.42305
H	-2.33316	-1.3404	-0.75896	H	-2.33303	-1.34059	-0.75902
H	-2.50485	0.92764	-1.14352	H	-2.50472	0.92743	-1.14369
H	0.10293	2.16037	1.61889	H	0.10289	2.16036	1.61885
H	2.39008	-1.572	0.93213	H	2.38985	-1.57184	0.93187
H	-6.45788	-1.38173	-1.47707	H	-6.45766	-1.38203	-1.47726
H	-6.20656	-1.52471	0.25109	H	-6.20644	-1.52489	0.25093
H	-5.38044	-3.56717	-0.9642	H	-5.38023	-3.56744	-0.9641
H	-4.34744	-2.54371	-1.96113	H	-4.34723	-2.54406	-1.96112
H	-5.50593	0.733	-0.6007	H	-5.5058	0.73277	-0.601
H	-4.41529	-0.03605	-1.74395	H	-4.41509	-0.03635	-1.74413
H	-2.19287	-1.64742	2.27481	H	-2.19273	-1.64744	2.27476
H	-1.06178	-2.24475	1.07851	H	-1.06162	-2.24476	1.07849
H	-0.0977	-0.12492	1.89921	H	-0.09766	-0.12486	1.89921
H	-3.13441	4.34048	1.16819	H	-3.13469	4.34032	1.16795
H	-2.65582	2.90943	2.07286	H	-2.65614	2.90929	2.0727
H	-3.3355	2.99182	-0.90967	H	-3.33522	2.9917	-0.90997
H	-4.41767	2.41474	0.34034	H	-4.41767	2.4146	0.33977
H	-3.51413	0.18652	2.48104	H	-3.51409	0.18654	2.48087
H	-4.86212	1.05659	1.75598	H	-4.86212	1.05648	1.75573
H	-4.98242	-0.67038	2.01135	H	-4.98231	-0.67048	2.01121
H	-2.50874	-5.66887	-0.83233	H	-2.50838	-5.66902	-0.83198
H	6.01321	-2.09193	2.13408	H	6.01275	-2.0924	2.13412
H	4.59919	-3.01622	1.59748	H	4.59862	-3.01639	1.59723
H	4.64851	-0.02883	2.25933	H	4.64836	-0.02907	2.25939
H	5.63284	-2.50479	-0.49731	H	5.63271	-2.50483	-0.49735
H	1.51893	-1.55614	-2.73724	H	1.51894	-1.55585	-2.73744

H	2.73717	-0.56858	3.74802	H	2.73677	-0.56867	3.74785
H	4.15226	-1.53128	4.20229	H	4.1517	-1.53154	4.20222
H	2.83494	-2.2838	3.2895	H	2.8344	-2.28387	3.28925
H	3.02867	-3.26473	-2.89617	H	3.02872	-3.26439	-2.89654
H	4.70233	-2.74981	-2.61526	H	4.70236	-2.74947	-2.61548
H	3.86731	-3.70997	-1.39943	H	3.86729	-3.7098	-1.39981
H	2.34273	3.37226	-1.07604	H	1.9939	3.41377	0.64926
H	1.99398	3.41363	0.6491	H	2.34268	3.37265	-1.07587
H	7.80952	0.23372	-1.03581	H	7.80969	0.23352	-1.03523
H	7.37226	-1.39695	-1.61777	H	7.37236	-1.39705	-1.6174
H	6.26014	-0.0206	-1.87496	H	6.26042	-0.02057	-1.87466
H	1.27502	5.53649	-0.17123	H	1.27486	5.53671	-0.17081
H	0.54503	4.86585	-1.61552	H	0.54488	4.86621	-1.61517
H	-2.35769	5.99778	0.49939	H	-2.35774	5.99779	0.50022
H	-0.76907	6.76877	0.53071	H	-0.76914	6.76885	0.53102
H	-1.48623	6.30421	-1.00805	H	-1.48679	6.30429	-1.00751
H	-4.90863	-2.62241	1.87125	H	-4.90869	-2.62249	1.87114
H	-4.7295	-4.26599	1.25465	H	-4.72917	-4.26614	1.25485
H	-3.41323	-3.51206	2.15347	H	-3.41315	-3.5118	2.1537

Table S2. DP4+ analysis results of **3a** (isomer1) and **3b** (Isomer 2)

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d, p)		Type of Data Unscaled Shifts		
		DP4+	100.00%	0.00%	-	-	-	
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	
C	x	198.9	207.7	207.6				
C	x	181.3	188.5	188.8				
C	x	177	187.4	188.0				
C	x	155.5	163.6	163.8				
C	x	144.8	155.8	155.8				
C	x	141.6	152.2	150.7				
C	x	132.4	143.8	142.6				
C	x	128.3	138.5	139.5				
C	x	127.9	133.1	134.0				
C	x	125.9	132.9	133.2				
C	x	112.6	118.4	118.4				
C		64.4	69.80	68.90				
C		63.5	68.50	68.00				
C		50.7	58.40	58.40				
C		49.7	55.04	55.90				
C		48.7	52.29	51.72				
C		46.2	52.15	51.35				
C		45.7	50.57	51.28				
C		43.9	47.63	45.71				
C		37.5	42.07	41.67				
C		37	40.52	41.38				
C		36	39.79	39.99				
C		35	38.22	34.14				
C		29.5	34.51	31.39				
C		28.1	30.88	37.32				
C		26.4	29.6	31.2				
C		25.6	29.5	31				
C		25.1	29	28.9				
C		24.2	28.5	28.7				
C		21.1	23.5	23.9				
C		19.8	22.3	21.7				
C		19.2	21.6	20.4				
C		17.7	20.9	20.2				
C		16.7	18.3	18.8				
C		12.4	13.3	14.2				
H	x	6.83	6.04	6.04				
H	x	4.79	5.38	5.2				
H		3.24	3.36	3.18				
H		3.15	3.16	3.09				
H		2.74	3.1	3.06				
H		2.63	2.94	2.99				
H		2.63	2.73	2.96				
H		2.63	2.54	2.51				
H		2.58	2.54	2.8				
H		2.53	2.43	1.65				
H		2.51	2.32	1.57				
H		2.34	2.19	2.43				
H		2.3	2.17	2.4				
H		2.13	2.15	2.4				
H		2.01	1.94	2.26				
H		1.8	1.88	2.09				
H		1.77	1.86	2				
H		1.74	1.75	1.89				
H		1.73	1.73	1.75				
H		1.69	1.71	1.71				
H		1.62	1.65	1.53				
H		1.62	1.63	1.65				
H		1.59	1.59	1.64				
H		1.55	1.53	1.5				
H		1.55	1.5	1.7				
H		1.54	1.47	1.63				
H		1.51	1.47	1.6				
H		1.47	1.46	1.51				
H		1.47	1.37	1.46				
H		1.47	1.26	1.3				
H		1.2	1.22	1.17				
H		1.15	1.18	1.11				
H		1.15	1.17	1.11				
H		1.15	1.09	1.07				
H		1.13	1.01	1.06				
H		1.13	1.03	1.05				
H		1.13	0.97	1.03				
H		1.01	0.96	0.98				
H		0.73	0.87	0.91				
H		0.73	0.85	0.82				
H		0.73	0.5	0.46				

Functional	Solvent?		Basis Set				Type of Data
mPW1PW91	PCM		6-311+G(d,p)				Unscaled Shifts
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	
sDP4+ (H data)	100.00%	0.00%	-	-	-	-	
sDP4+ (C data)	99.99%	0.01%	-	-	-	-	
sDP4+ (all data)	100.00%	0.00%	-	-	-	-	
uDP4+ (H data)	100.00%	0.00%	-	-	-	-	
uDP4+ (C data)	99.97%	0.03%	-	-	-	-	
uDP4+ (all data)	100.00%	0.00%	-	-	-	-	
DP4+ (H data)	100.00%	0.00%	-	-	-	-	
DP4+ (C data)	100.00%	0.00%	-	-	-	-	
DP4+ (all data)	100.00%	0.00%	-	-	-	-	

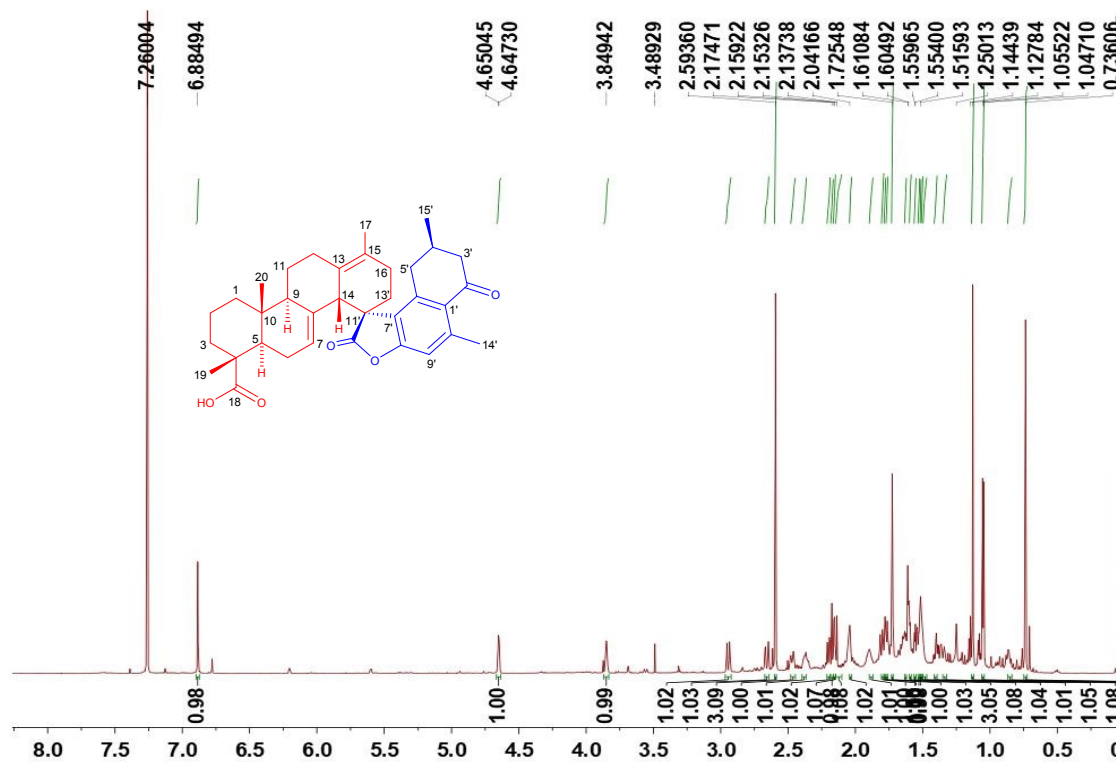


Figure S10. ¹H NMR (800 MHz) spectrum of compound 1 in CDCl₃.

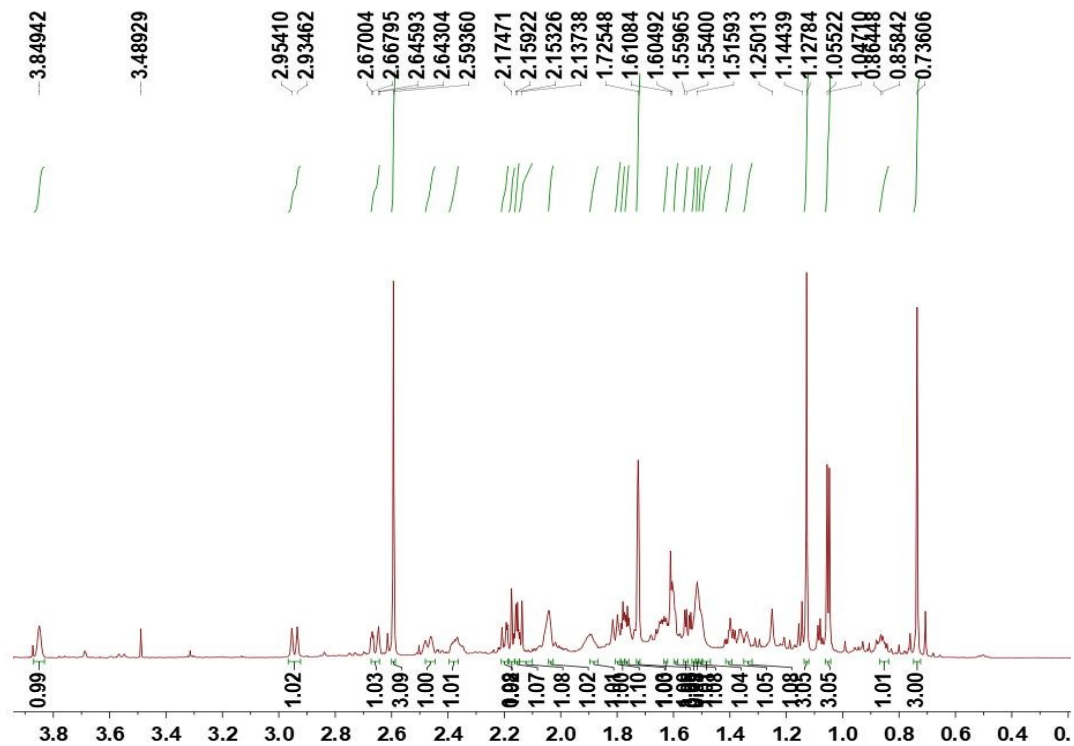


Figure S11. The part of ^1H NMR (800 MHz) spectrum of compound **1** in CDCl_3

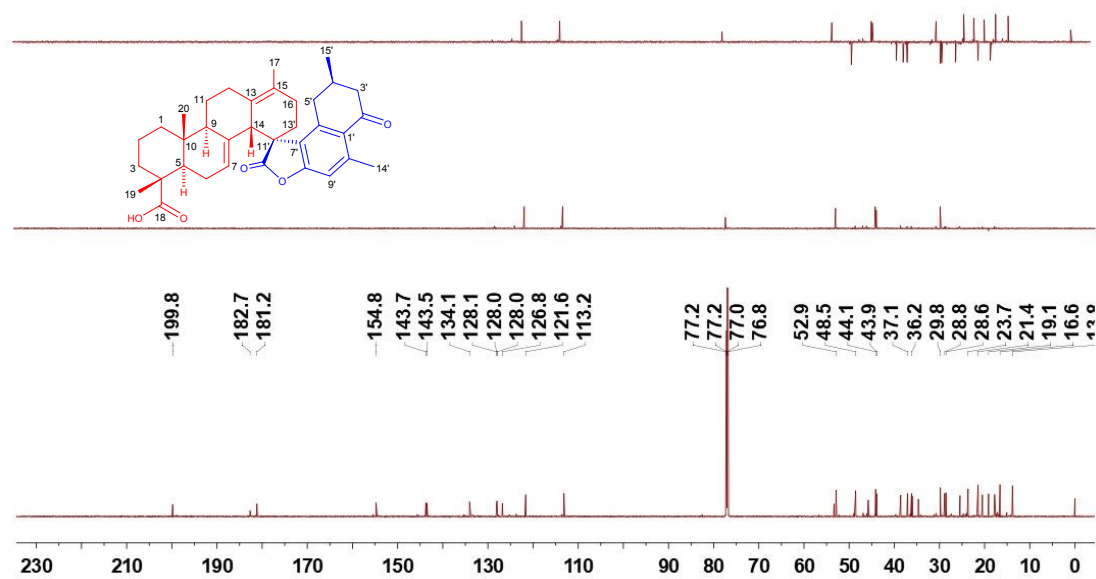


Figure S12. ^{13}C NMR (200 MHz) and DEPT spectra of compound **1** in CDCl_3 .

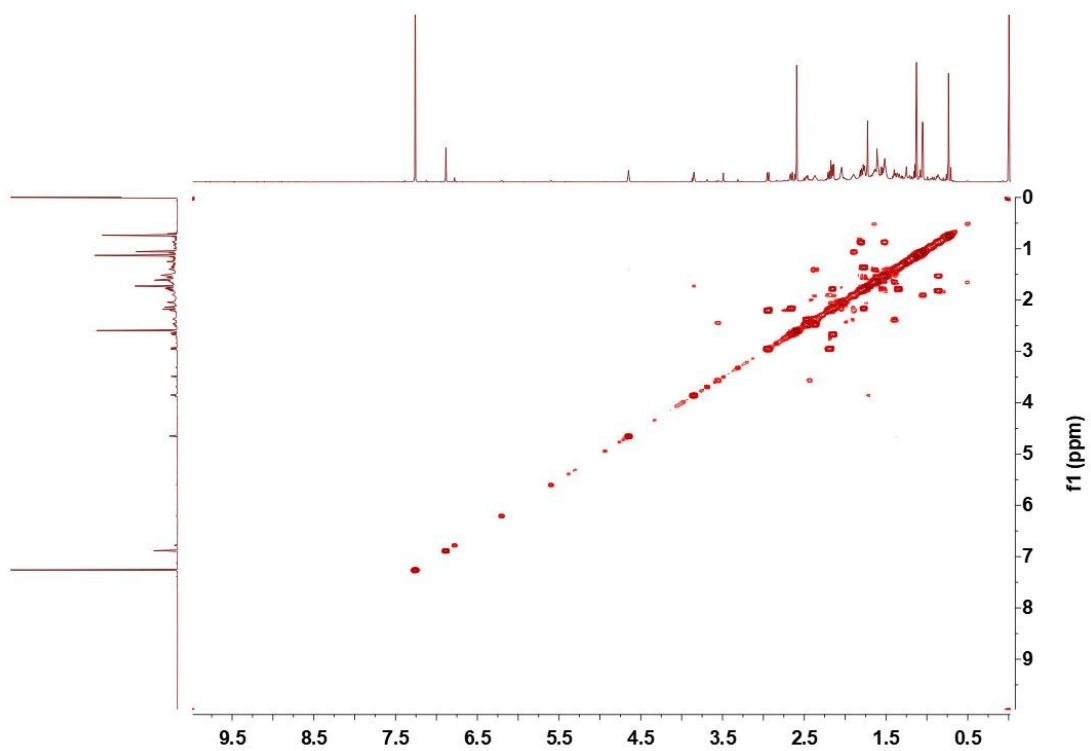


Figure S13. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3 .

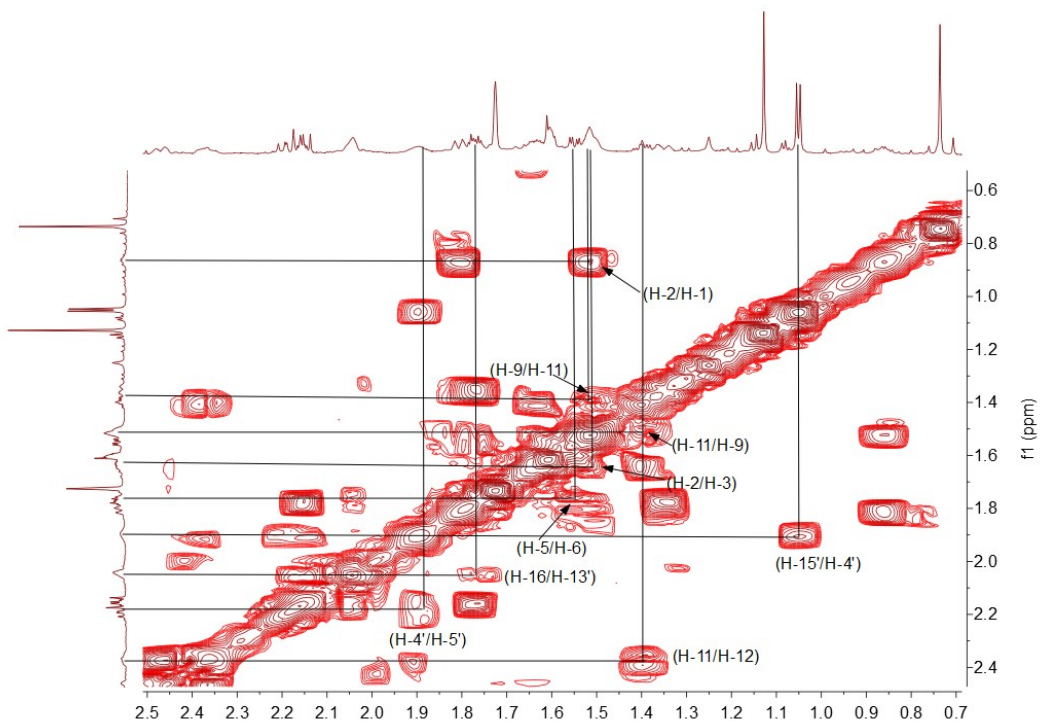


Figure S14. The part of ^1H - ^1H COSY spectrum of compound **1** in CDCl_3 (**1**).

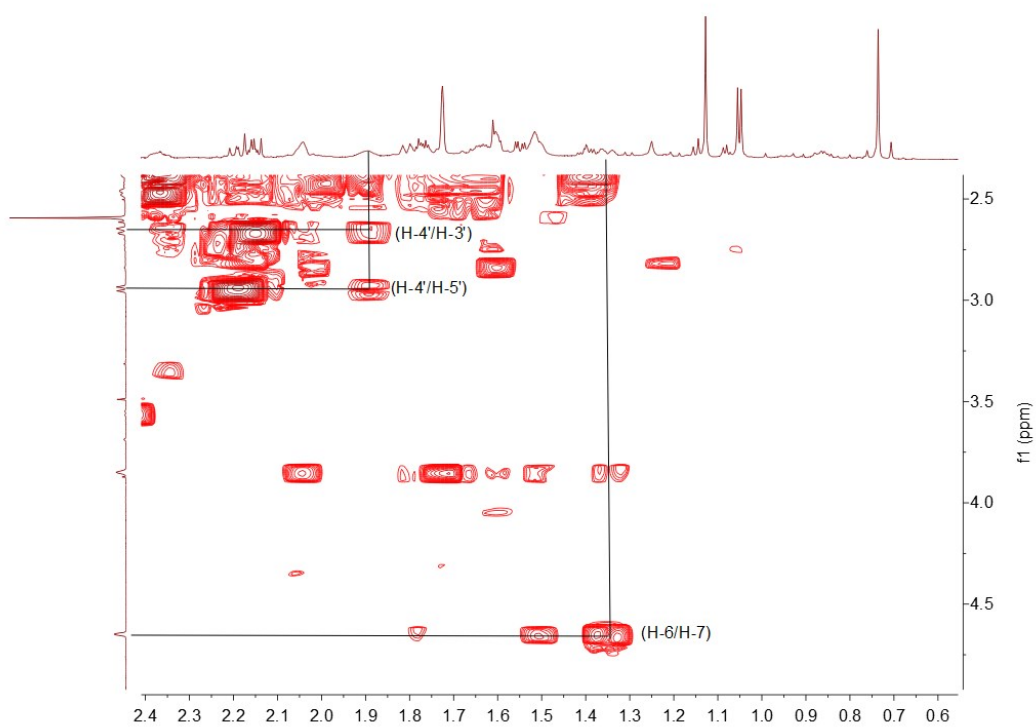


Figure S15. The part of ^1H - ^1H COSY spectrum of compound **1** in CDCl_3 (2).

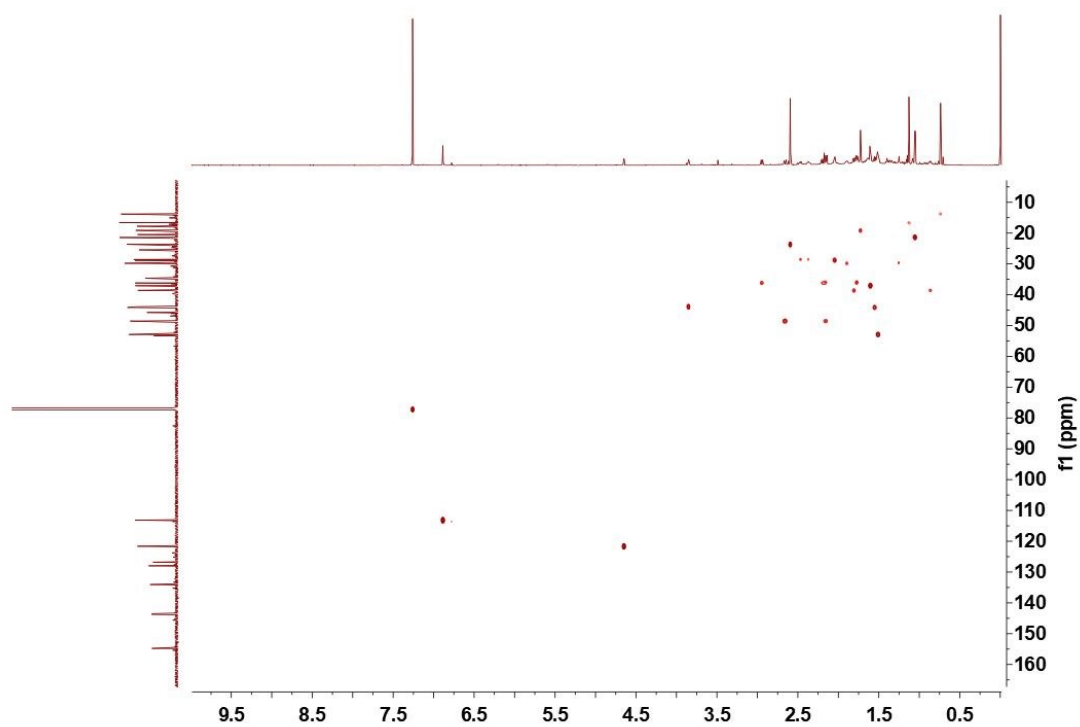


Figure S16. HSQC spectrum of compound **1** in CDCl_3 .

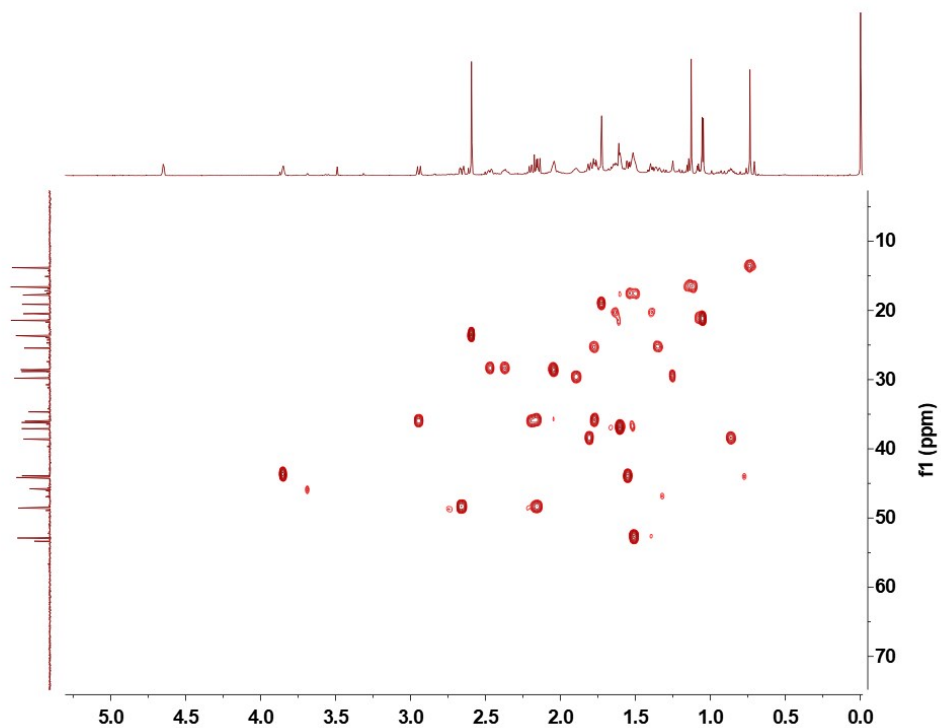


Figure S17. The part of HSQC spectrum of compound **1** in CDCl_3 .

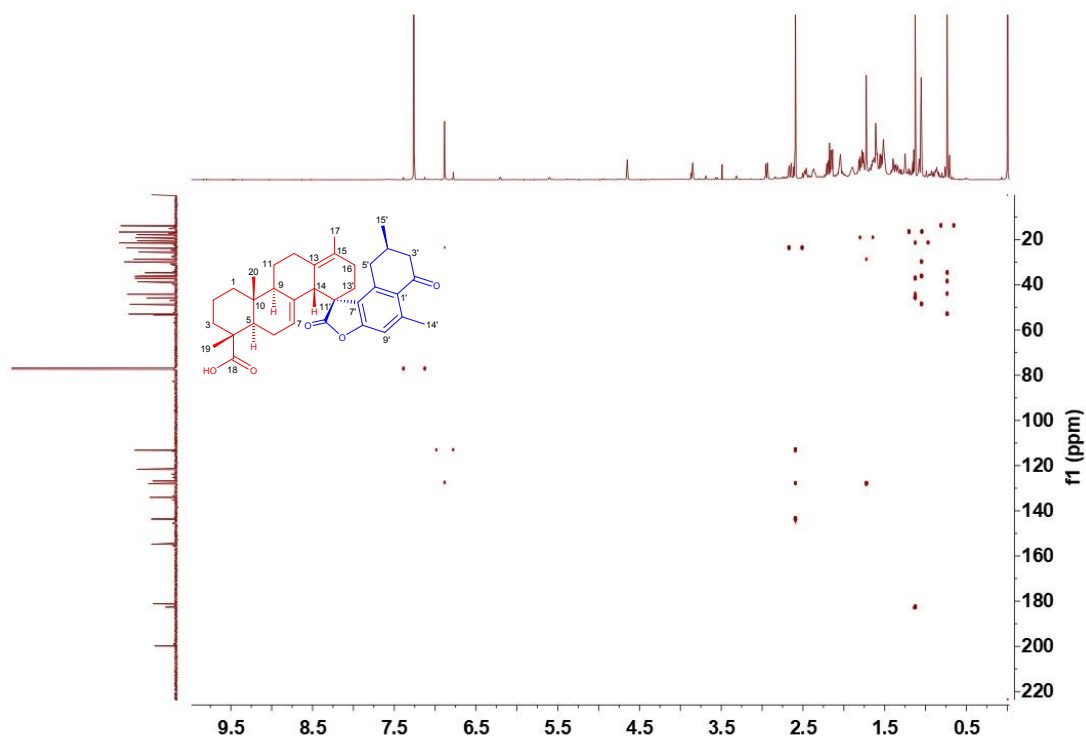


Figure S18. HMBC spectrum of compound **1** in CDCl_3 .

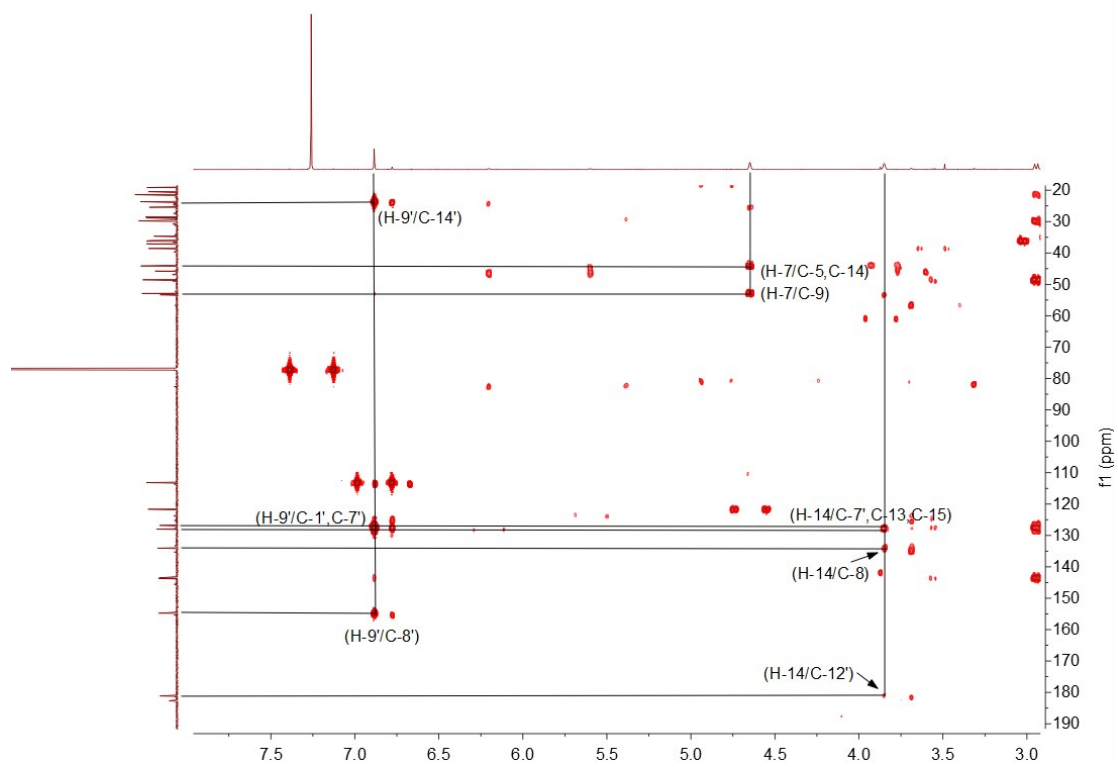


Figure S19. The part of HMBC spectrum of compound **1** in CDCl₃ (1).

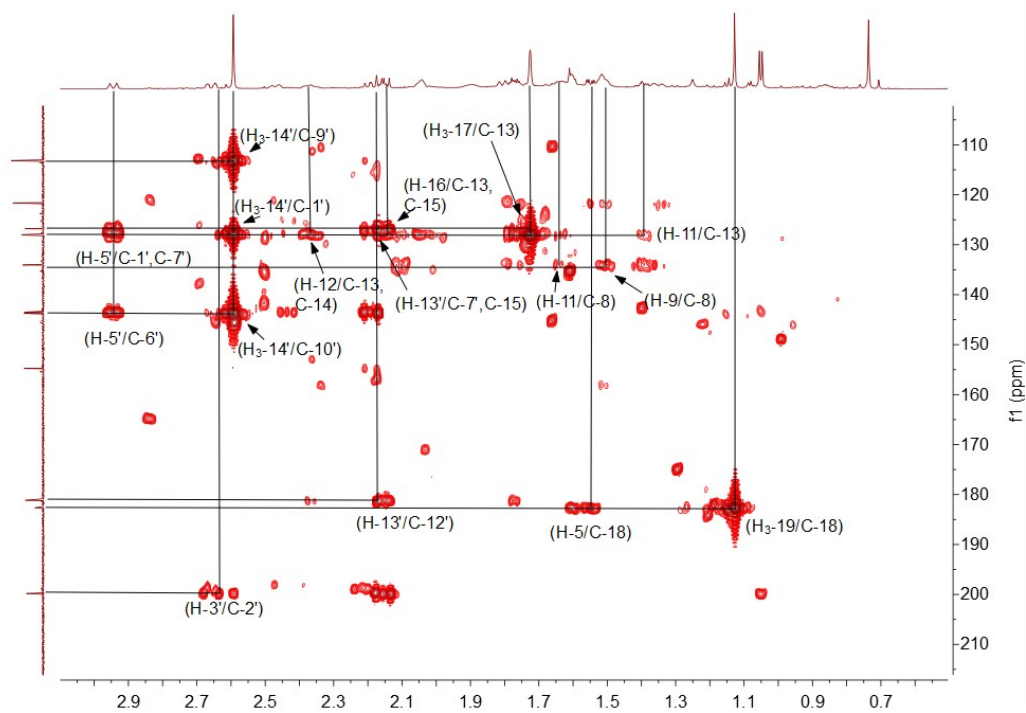


Figure S20. The part of HMBC spectrum of compound **1** in CDCl₃ (2).

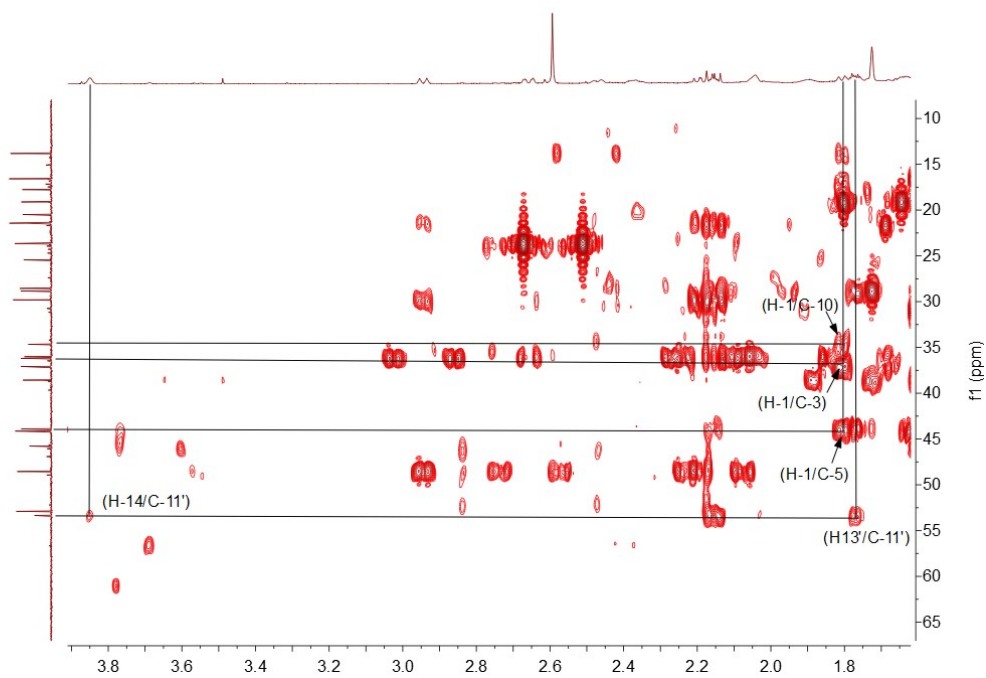


Figure S21. The part of HMBC spectrum of compound **1** in CDCl_3 (2).

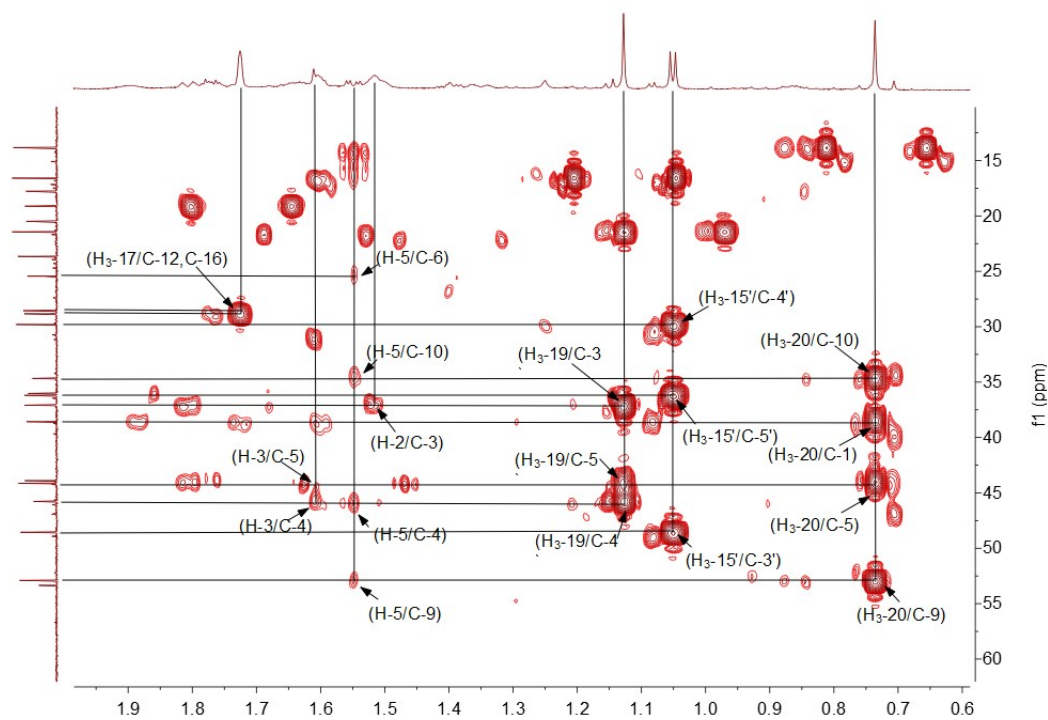


Figure S22. The part of HMBC spectrum of compound **1** in CDCl_3 (3).

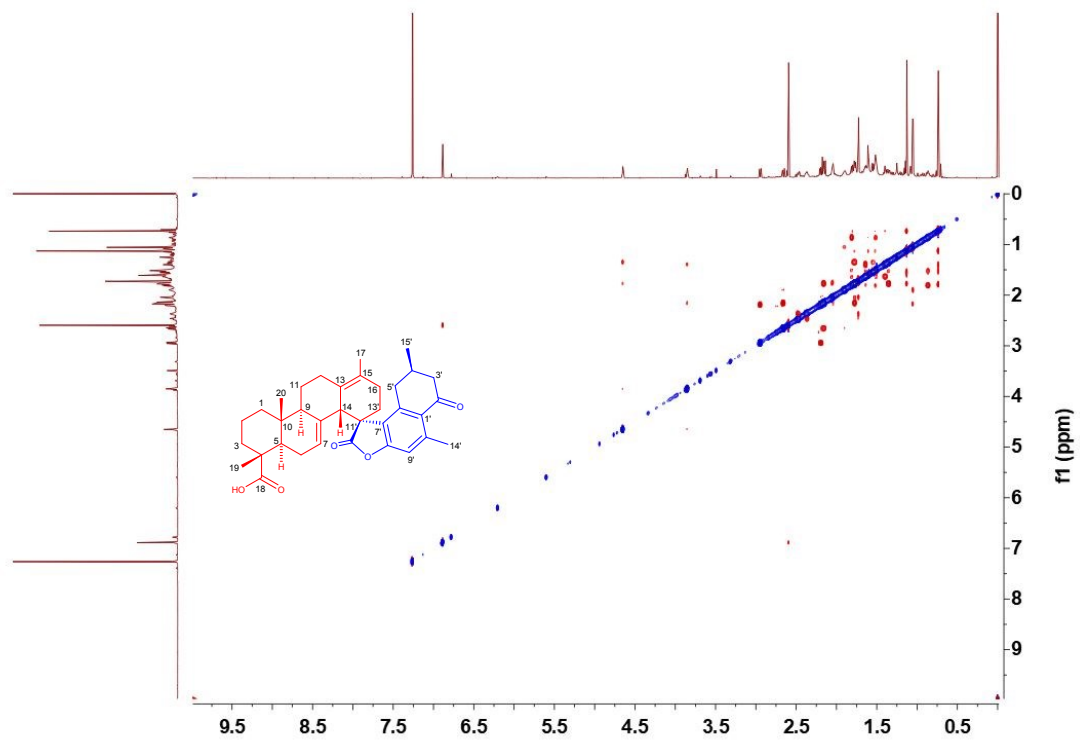


Figure S23. ROESY spectrum of compound **1** in CDCl_3 .

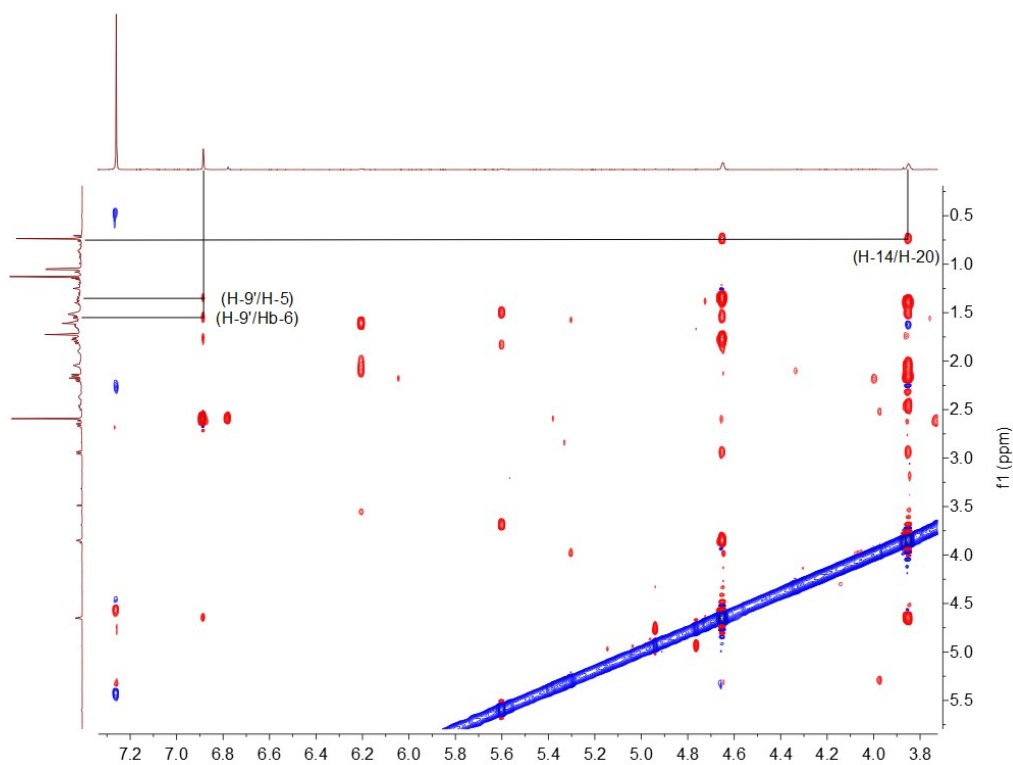


Figure S24. The part of ROESY spectrum of compound **1** in CDCl_3 (1).

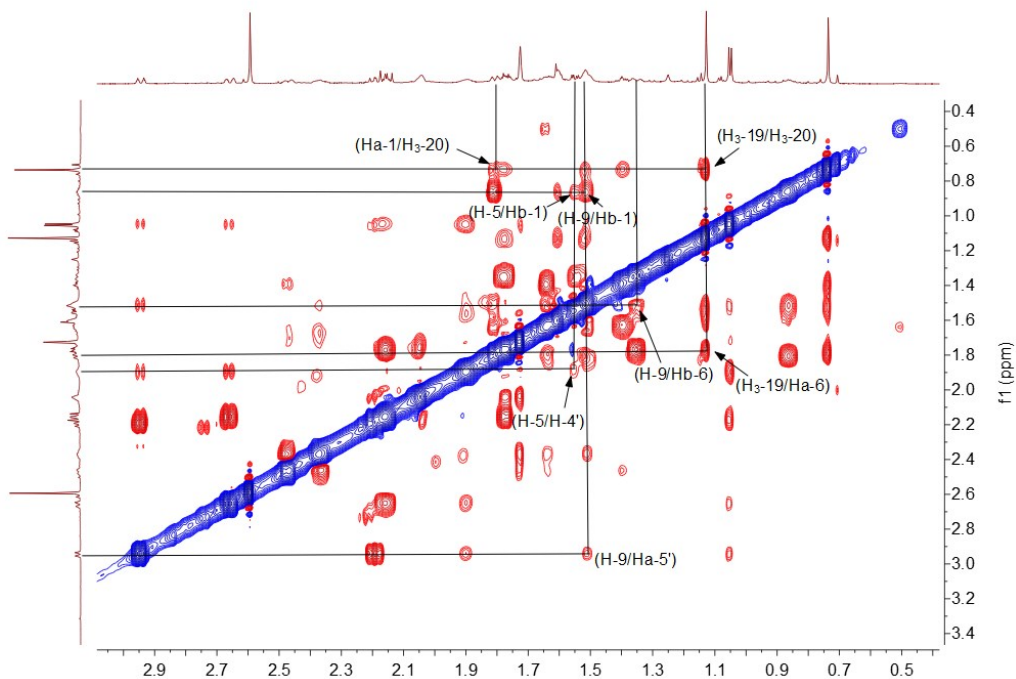


Figure S25. The part of ROESY spectrum of compound **1** in CDCl_3 (2).

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

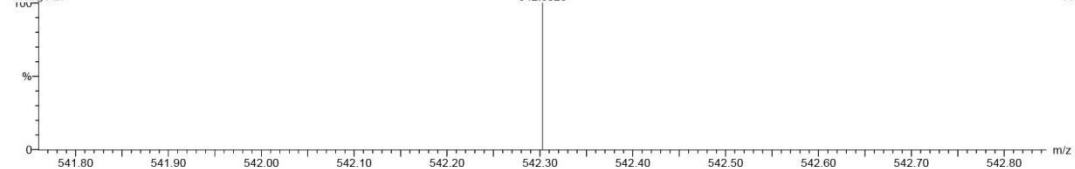
Monoisotopic Mass, Odd and Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:
C: 0-200 H: 0-400 O: 4-6

qjw-62b
03:26:29 20-Sep-2017
Voltage EI+

KIB
M170919EA-02AFAMM 29 (2.662)
542.3028

Autospec Premier
F776
10



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
542.3028	542.3032	-0.4	-0.7	15.0	5546027.0	C35 H42 O5

Figure S26. HRESIMS of compound **1**.

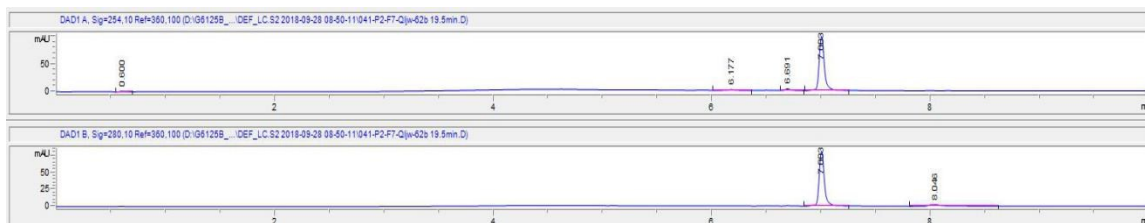


Figure S27. HPLC chromatogram of compound **1**.

(Mobile phase: aqueous MeCN, 10%-100% within 10 min, flow rate 0.25 mL/min)

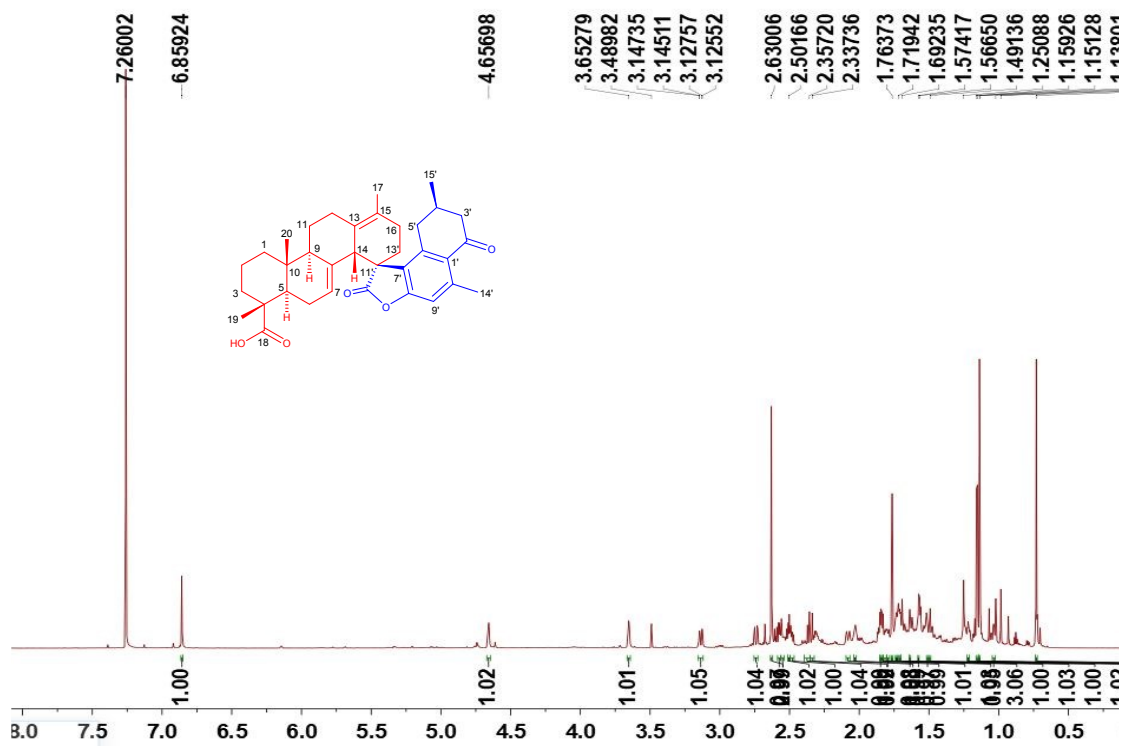


Figure S28. ¹H NMR (800 MHz) spectrum of compound 2 in CDCl₃.

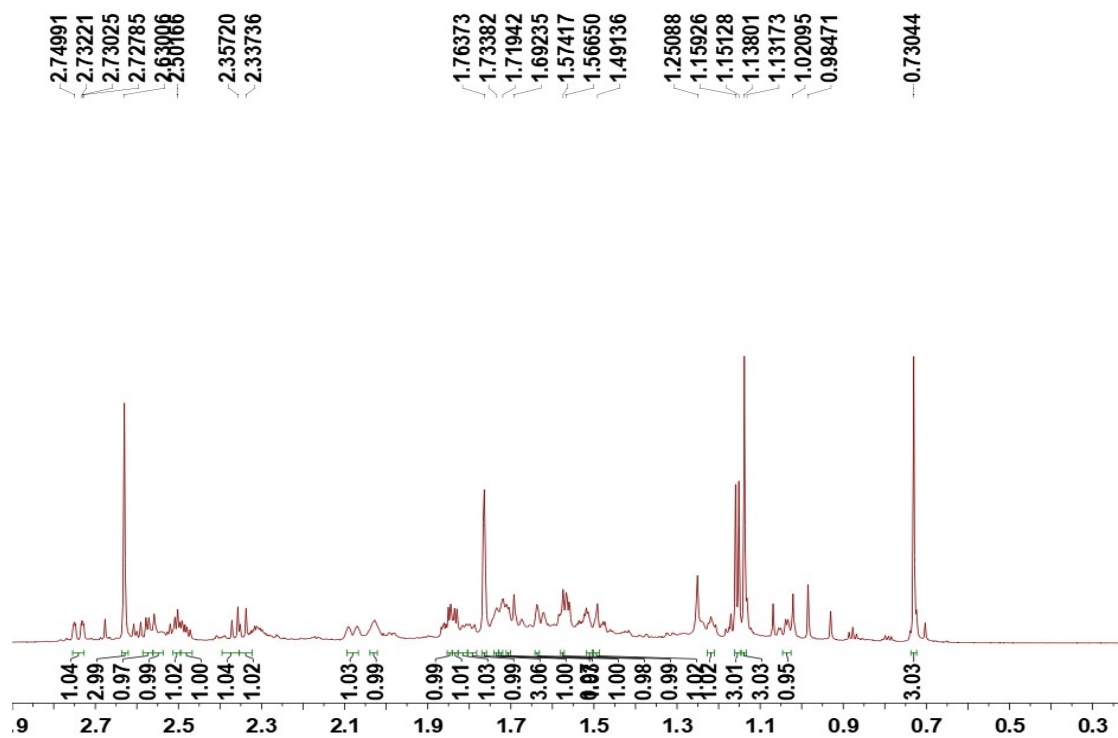


Figure S29. The part of ¹H NMR (800 MHz) spectrum of compound 2 in CDCl₃.

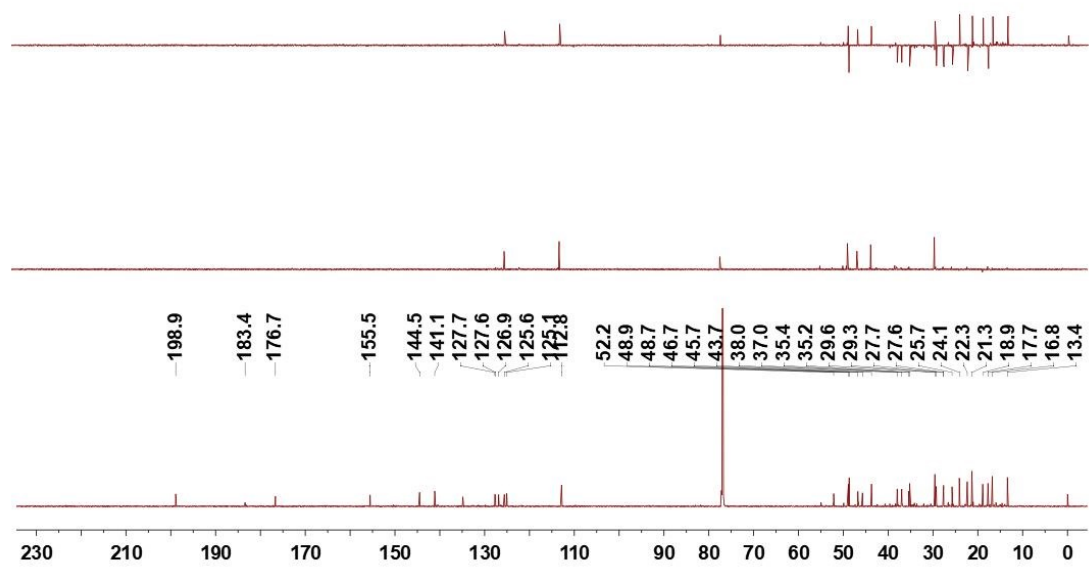


Figure S30. ^{13}C NMR (200 MHz) and DEPT spectra of compound **2** in CDCl_3 .

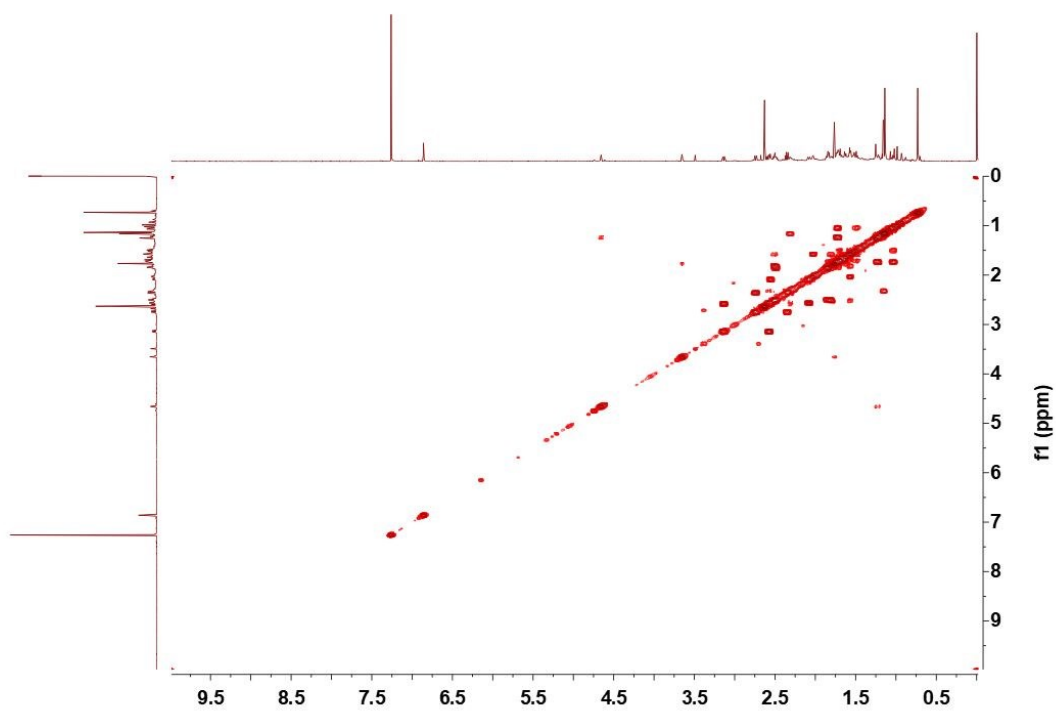


Figure S31. ^1H - ^1H COSY spectrum of compound **2** in CDCl_3 .

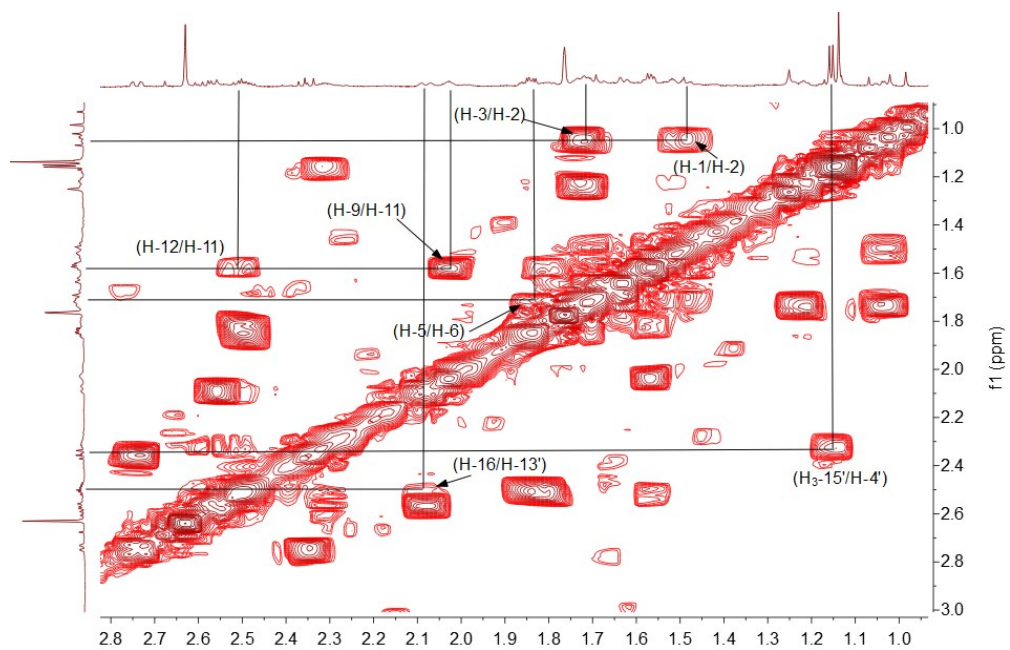


Figure S32. The part of ^1H - ^1H COSY spectrum of compound **2** in CDCl_3 (1).

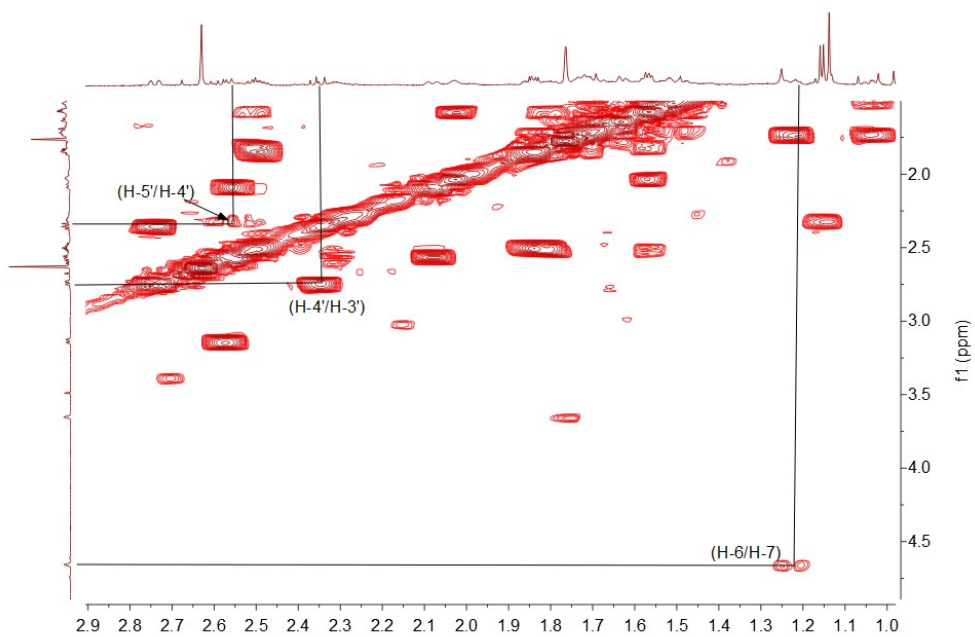


Figure S33. The part of ^1H - ^1H COSY spectrum of compound **2** in CDCl_3 (2).

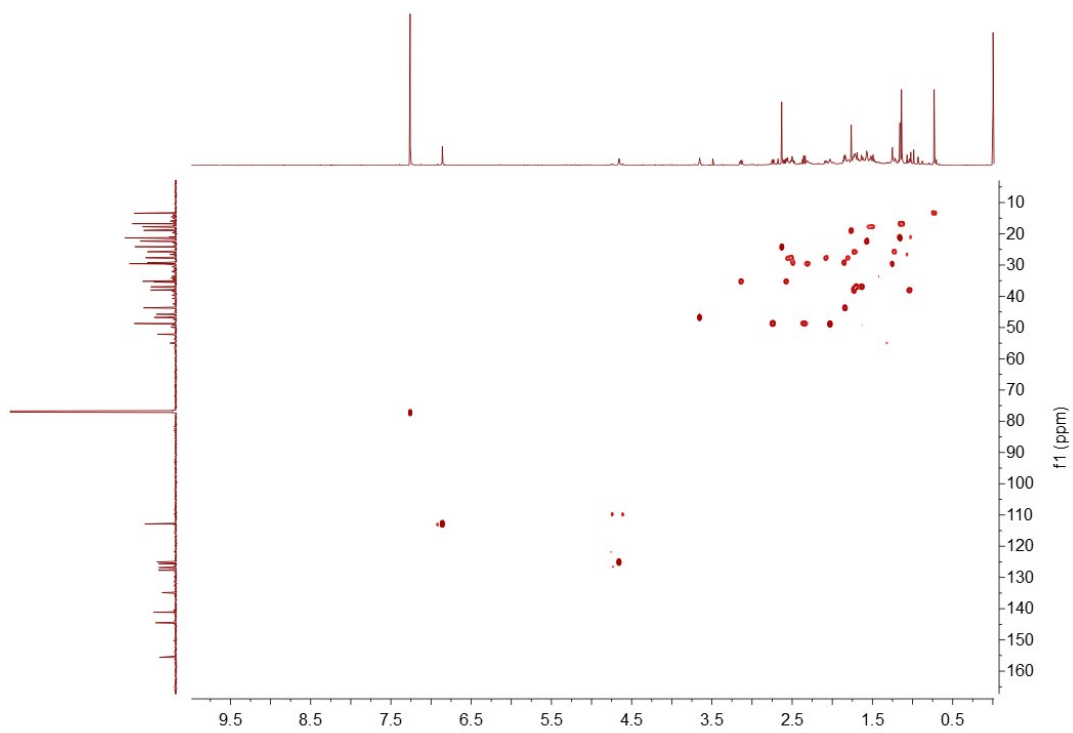


Figure S34. HSQC spectrum of compound **2** in CDCl₃.

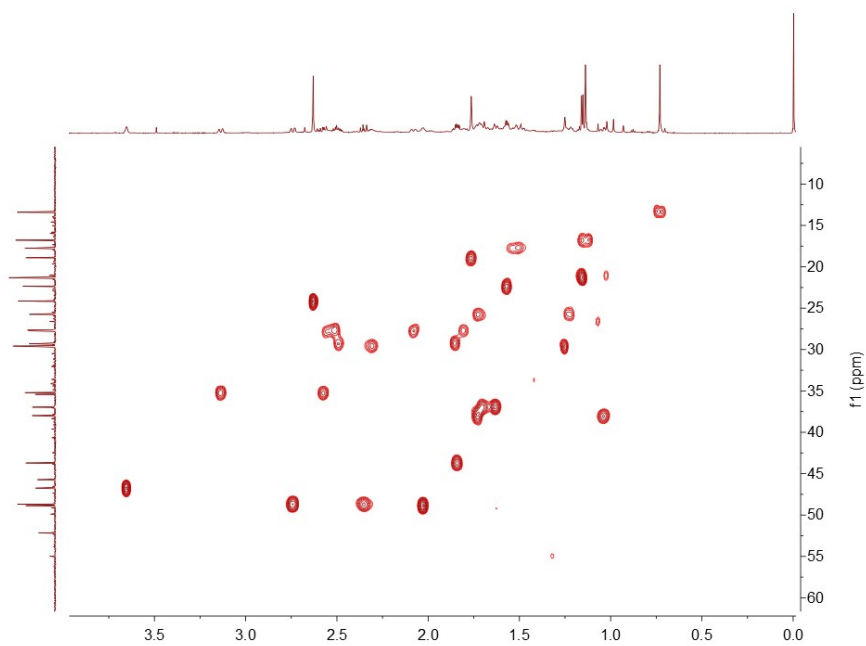


Figure S35. The part of HSQC spectrum of compound **2** in CDCl₃.

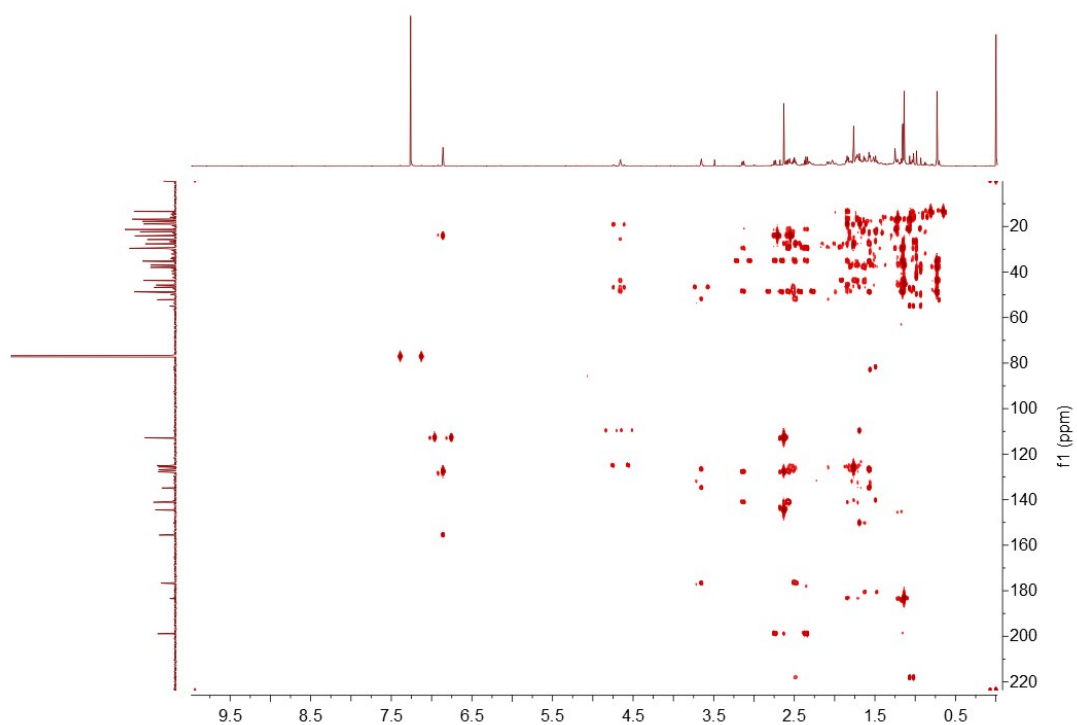


Figure S36. HMBC spectrum of compound **2** in CDCl_3 .

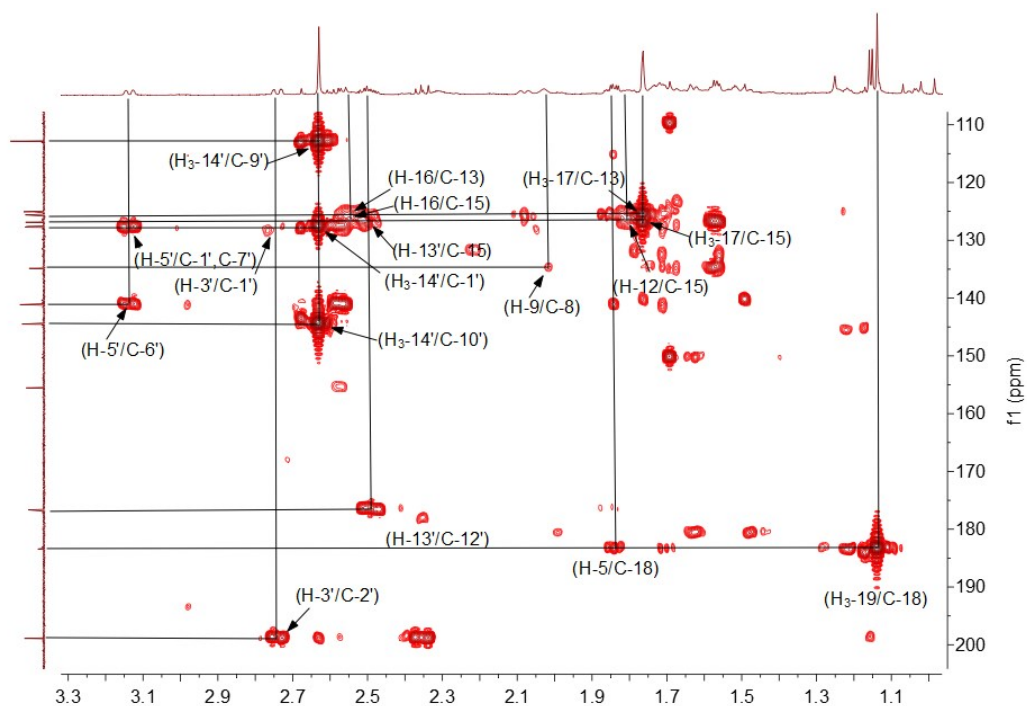


Figure S37. The part of HMBC spectrum of compound **2** in CDCl_3 (1).

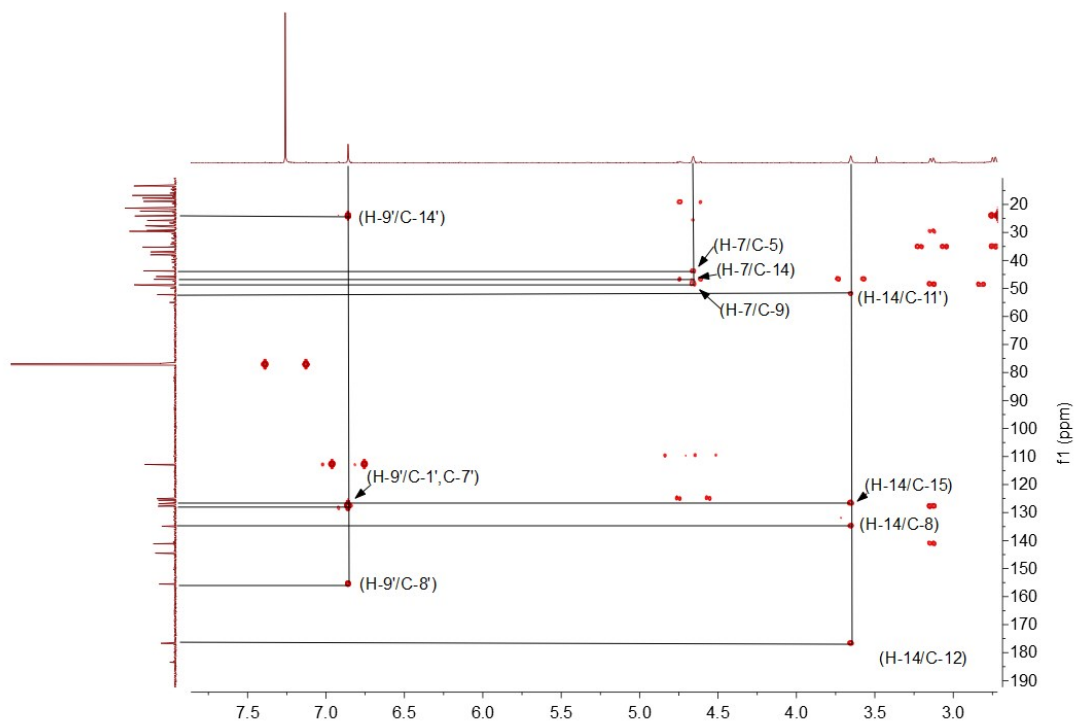


Figure S38. The part of HMBC spectrum of compound 2 in CDCl₃ (2).

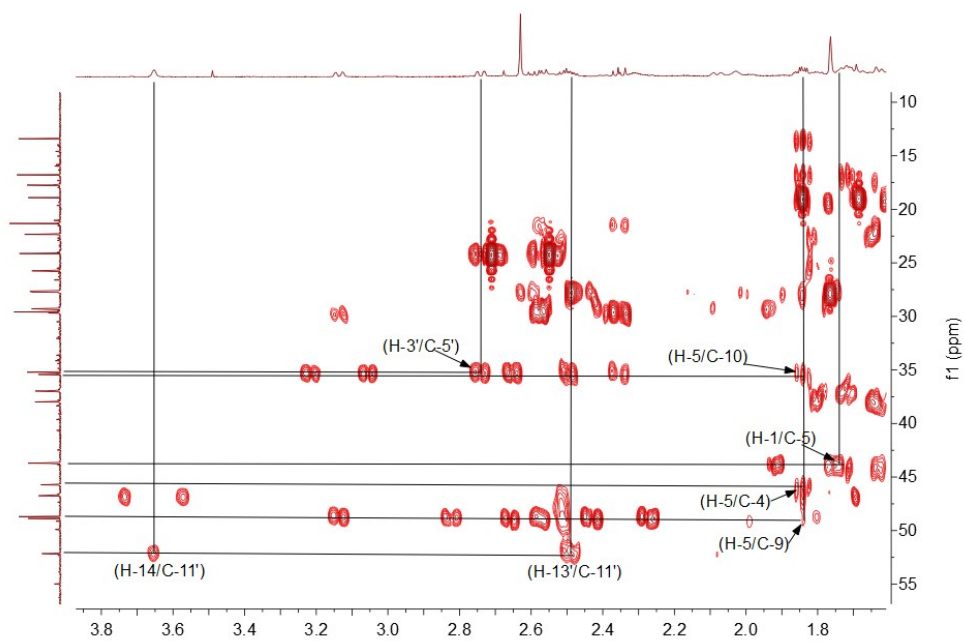


Figure S39. The part of HMBC spectrum of compound 2 in CDCl₃ (3).

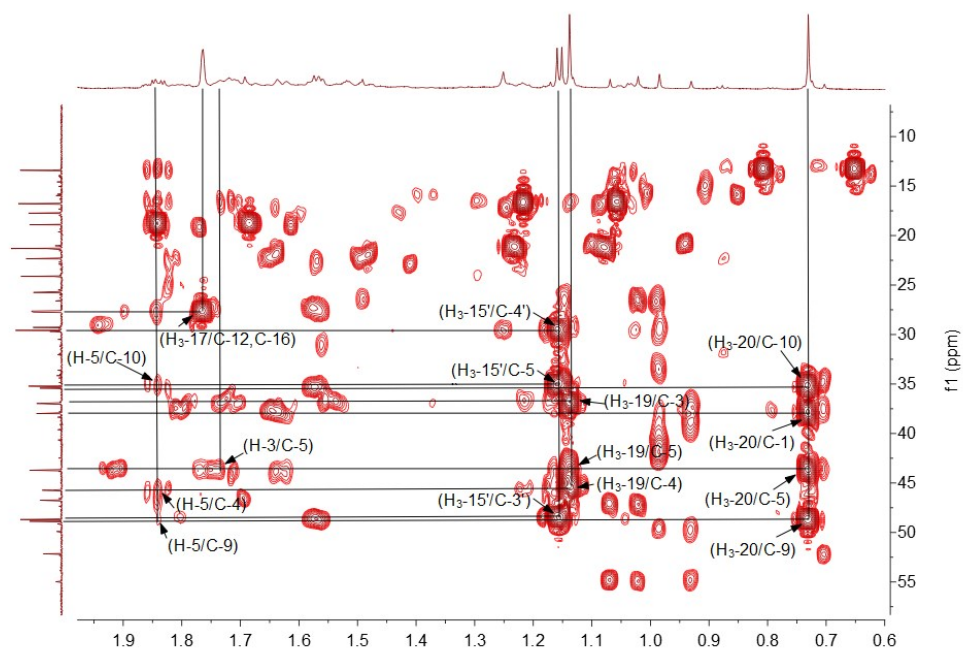


Figure S40. The part of HMBC spectrum of compound **2** in CDCl_3 (4).

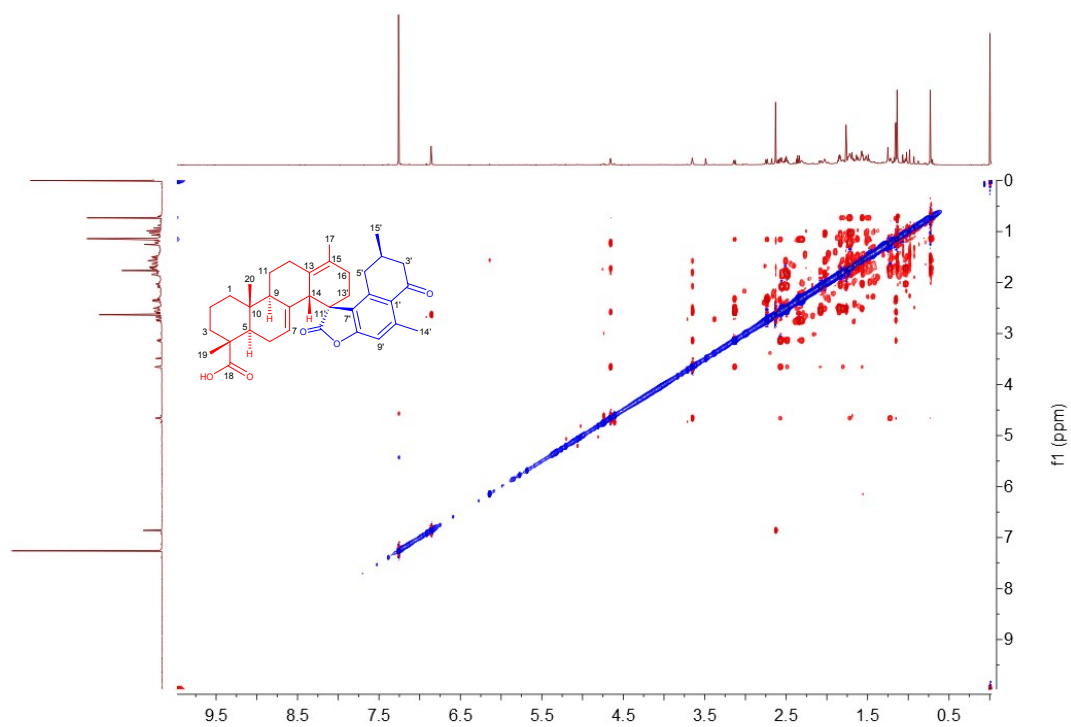


Figure S41. ROESY spectrum of compound **2** in CDCl_3 .

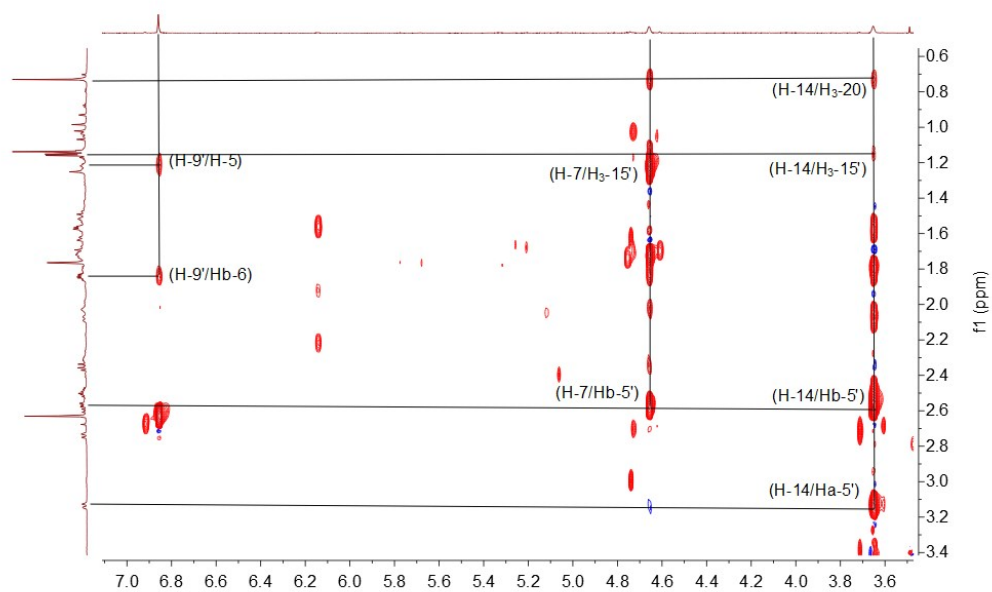


Figure S42. The part of ROESY spectrum of compound **2** in CDCl₃ (1).

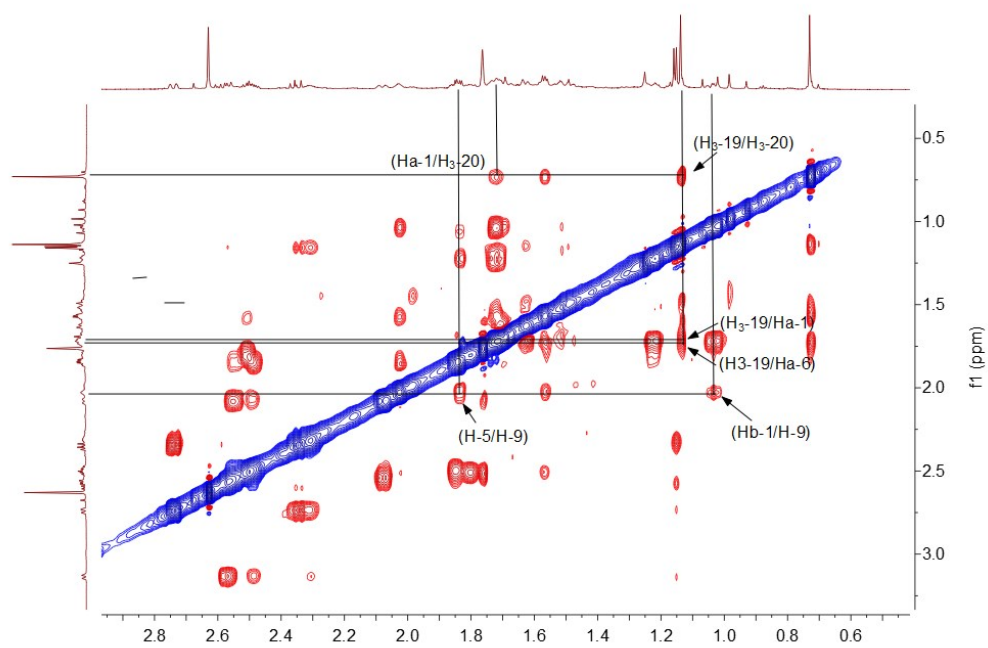
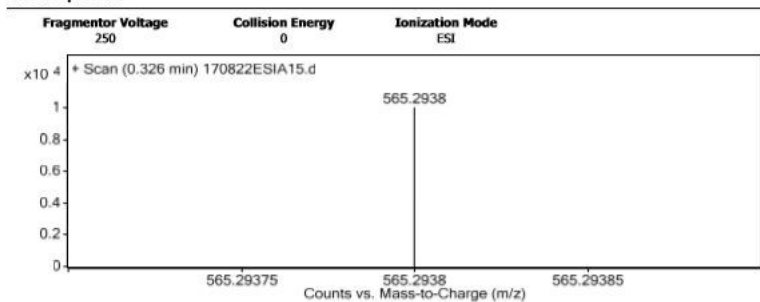


Figure S43. The part of ROESY spectrum of compound **2** in CDCl₃ (2).

Qualitative Analysis Report

Data Filename	170822ESIA15.d	Sample Name	Qljw-62a
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESI.m	Acquired Time	8/22/2017 2:56:29 PM
IRM Calibration Status	Success	DA Method	ESI.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
252.1577	1	17356		
256.2637	1	7563.25		
266.1729	1	19038.55		
274.2748	1	18567.64		
318.3015	1	17317.53		
340.2822	1	9012.65		
362.3273	1	7766.96		
384.3097	1	16316.96		
428.3361	1	13562.52		
565.2938	1	9991.42	C35 H42 Na O5	M+

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	9
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C35 H42 Na O5	565.2930	565.2938	-0.8	1.4	14.5

--- End Of Report ---

Figure S44. HRESIMS of compound 2.

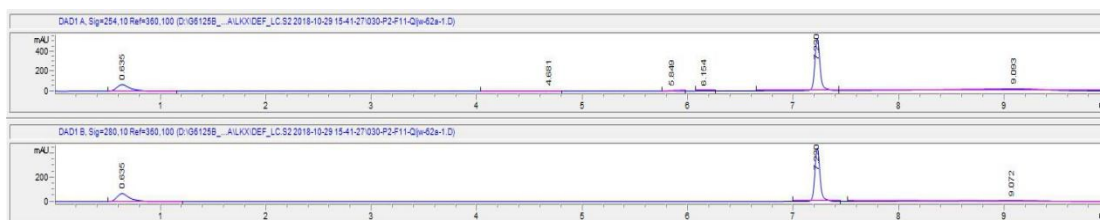


Figure S45. HPLC chromatogram of compound 2.

(Mobile phase: aqueous AcCN, 10%-100% within 10 min, flow rate 0.25 mL/min)

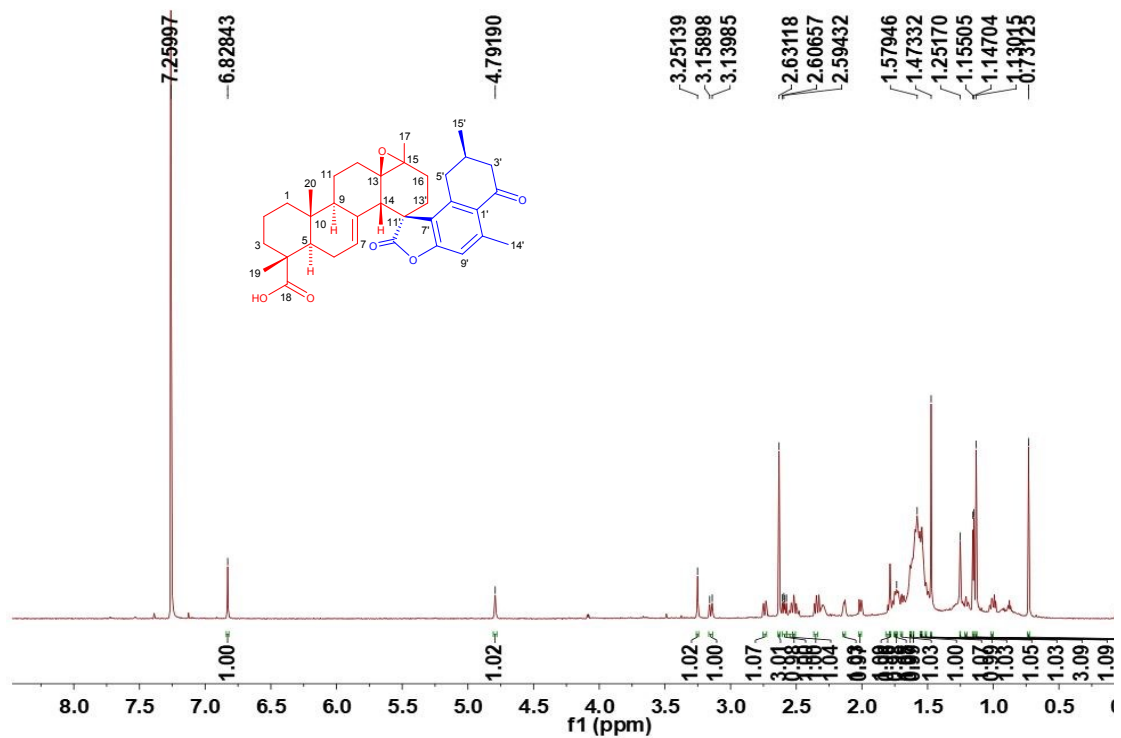


Figure S46. ^1H NMR (800 MHz) spectrum of compound **3** in CDCl_3 .

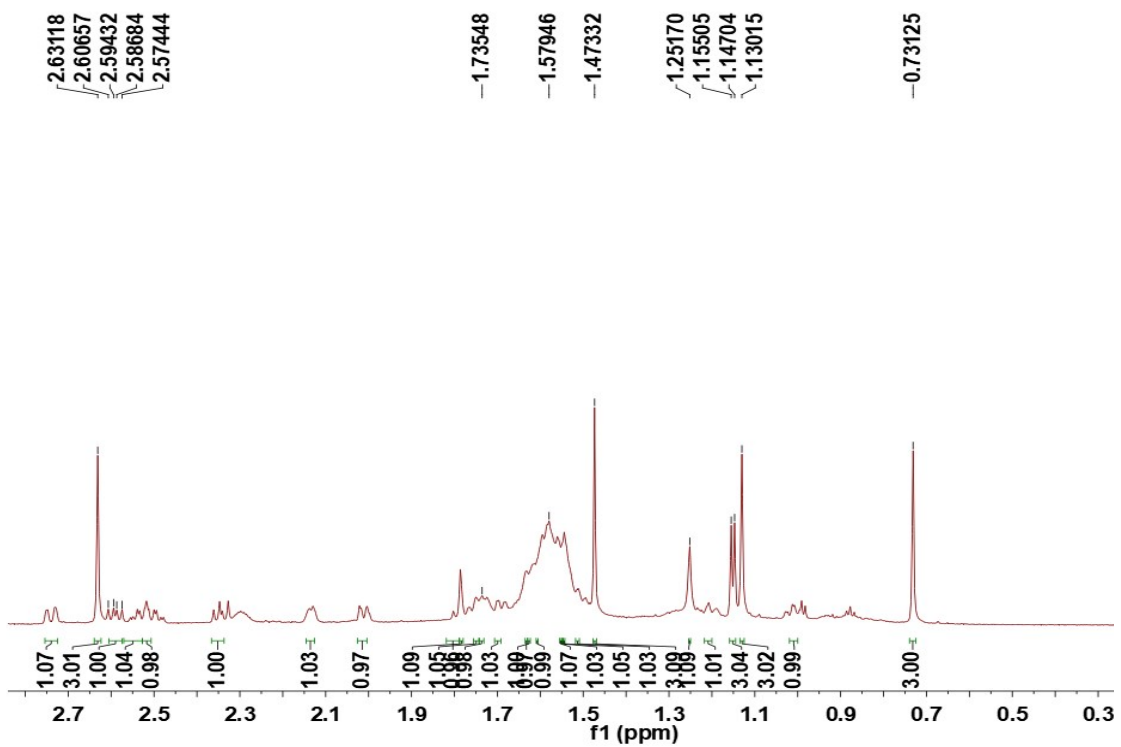


Figure S47. The part of ^1H NMR (800 MHz) spectrum of compound **3** in CDCl_3 .

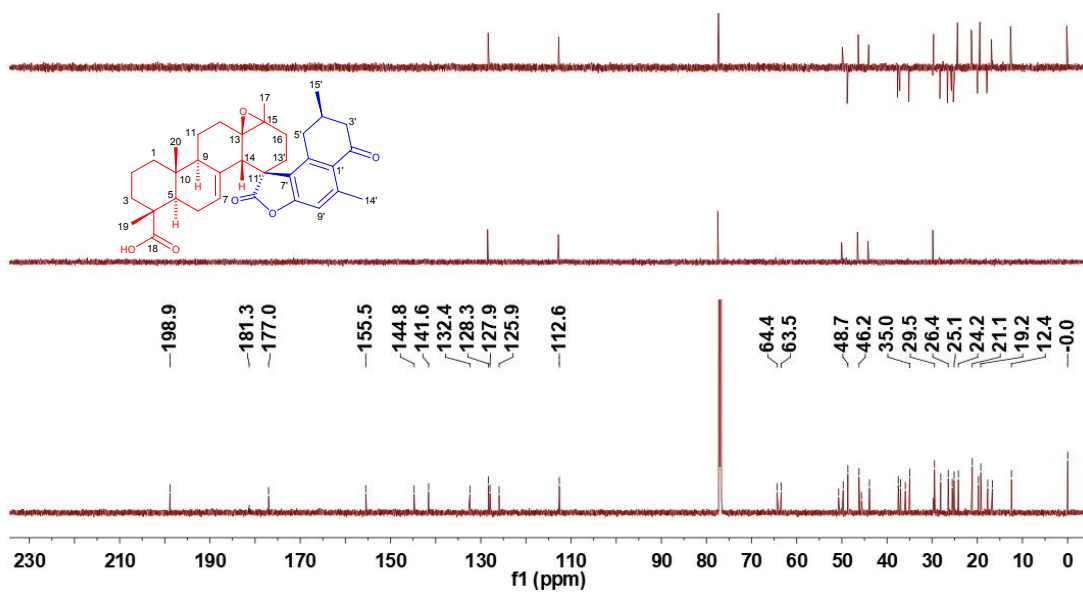


Figure S48. ^{13}C NMR (200 MHz) and DEPT spectra of compound **3** in CDCl_3 .

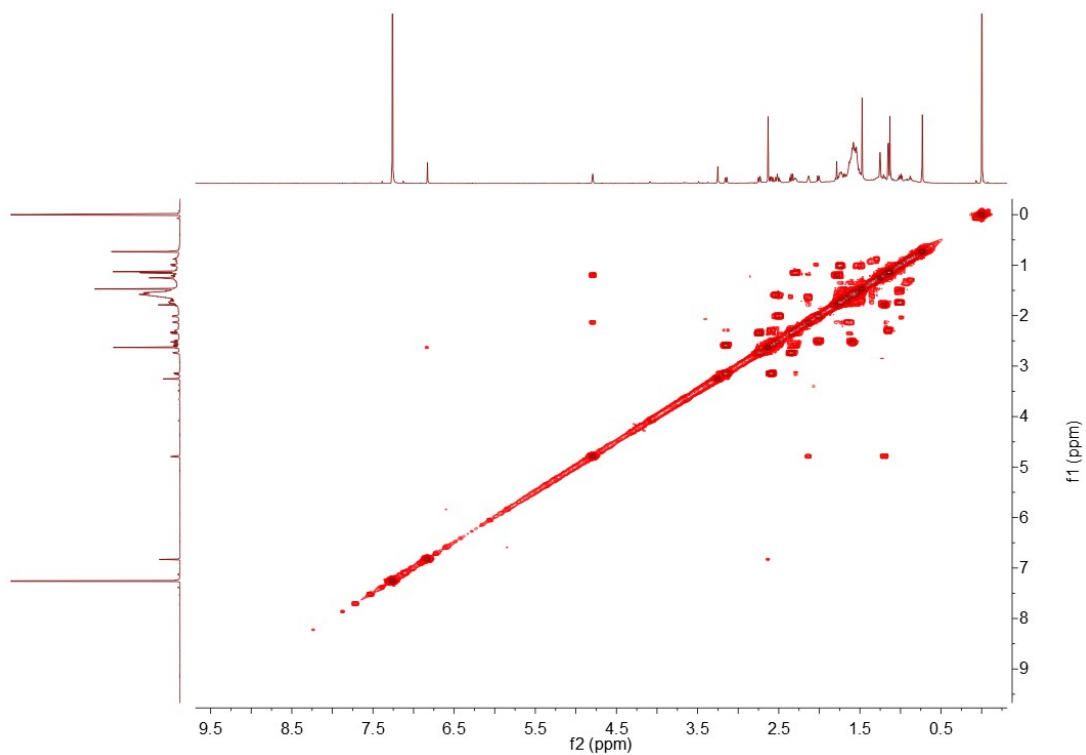


Figure S49. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3 .

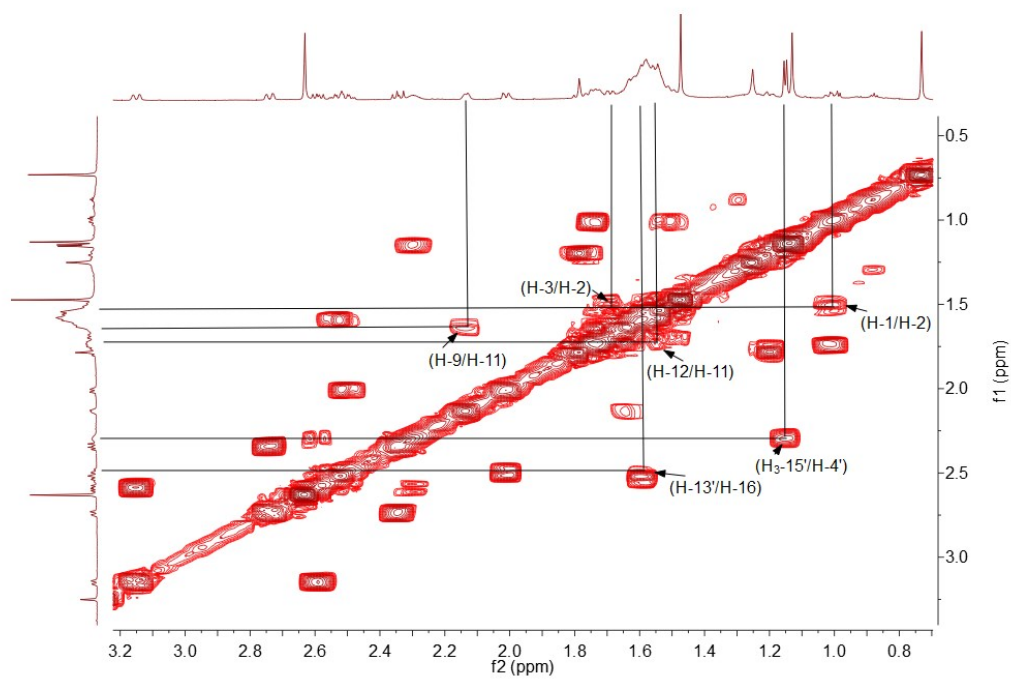


Figure S50. The part of ^1H - ^1H COSY spectrum of compound **3** in CDCl_3 (1).

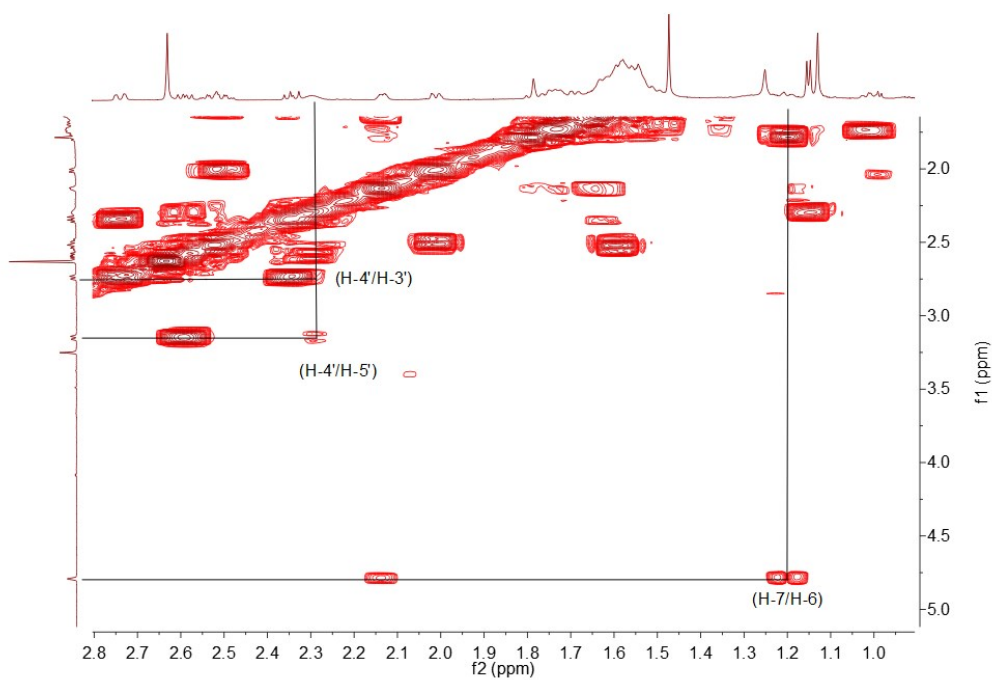


Figure S51. The part of ^1H - ^1H COSY spectrum of compound **3** in CDCl_3 (2).

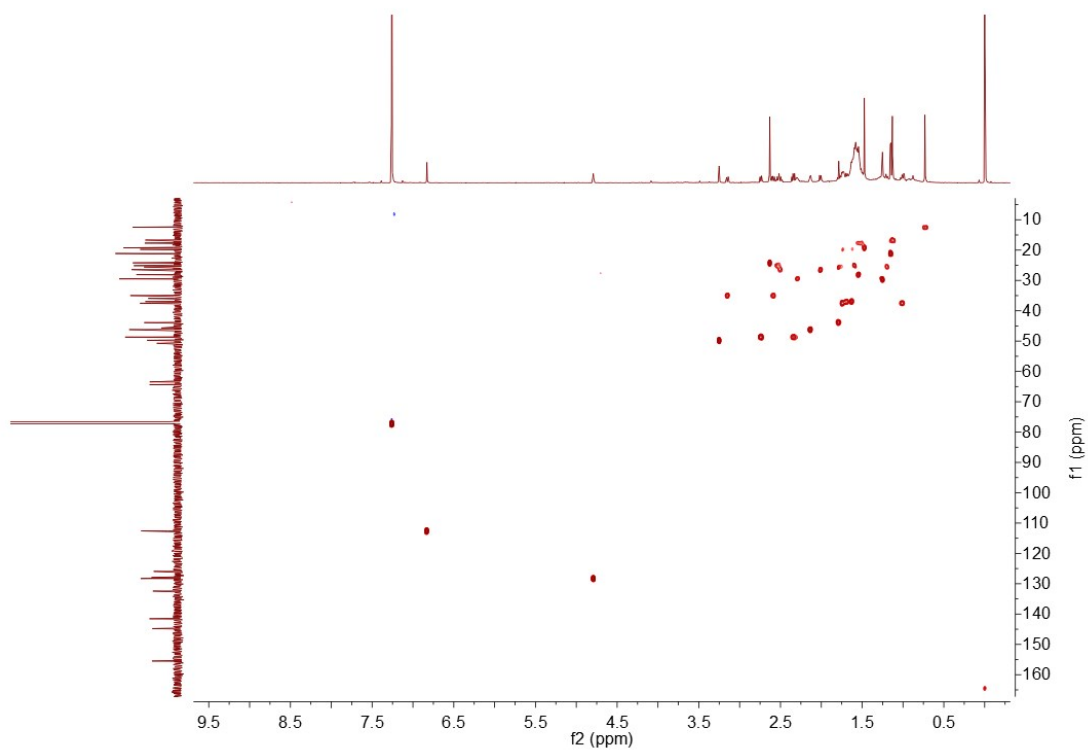


Figure S52. HSQC spectrum of compound **3** in CDCl_3 .

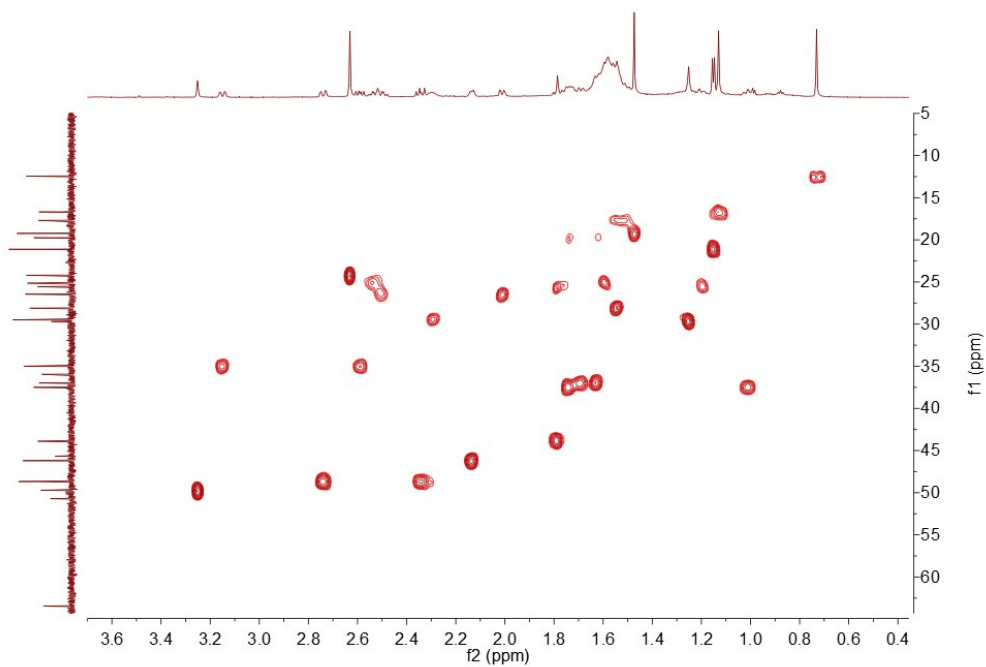


Figure S53. The part of HSQC spectrum of compound **3** in CDCl_3 .

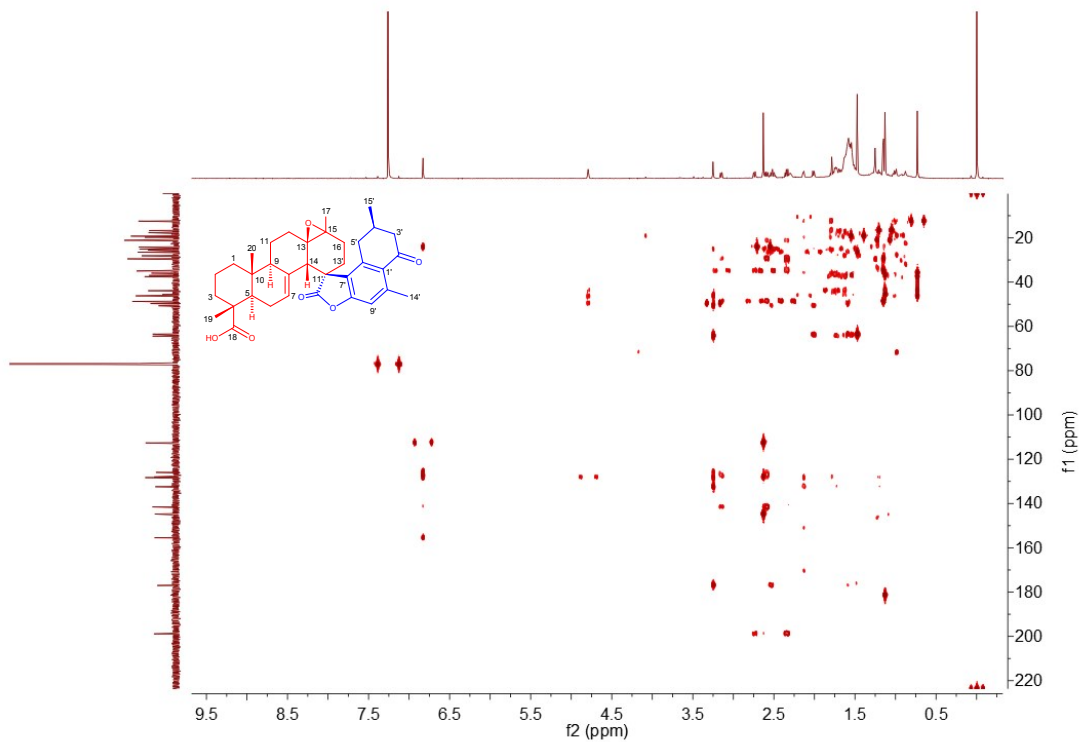


Figure S54. HMBC spectrum of compound **3** in CDCl_3 .

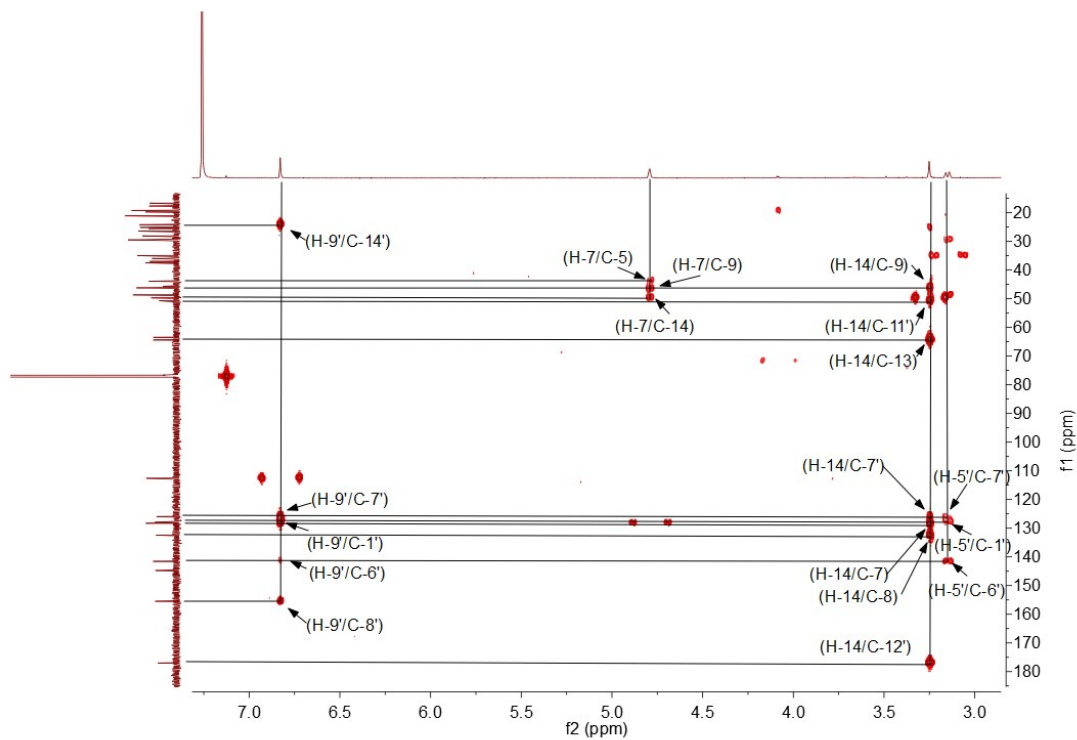


Figure S55. The part of HMBC spectrum of compound **3** in CDCl_3 (1).

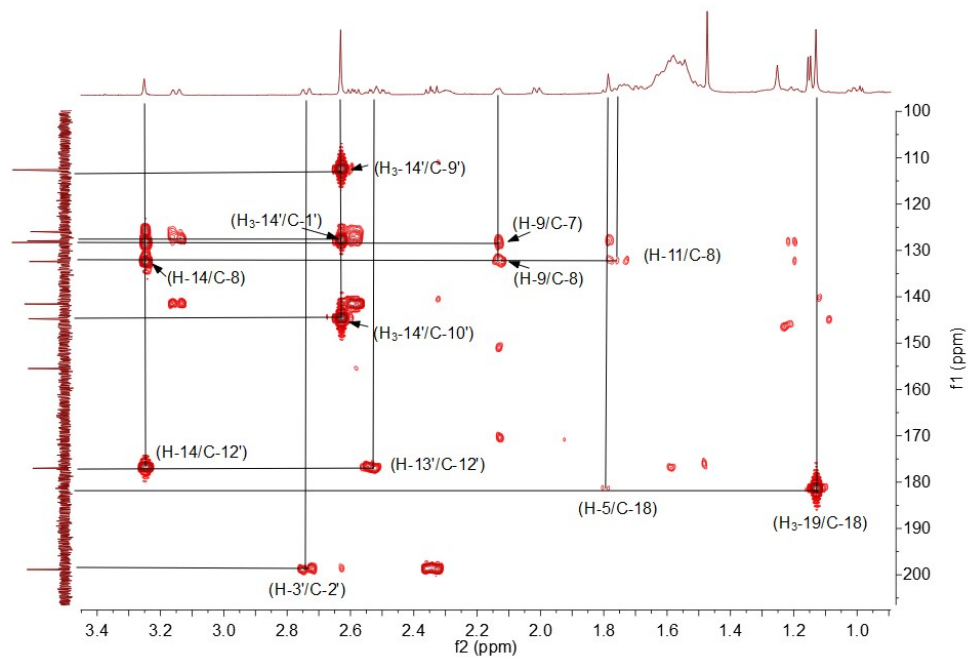


Figure S56. The part of HMBC spectrum of compound **3** in CDCl_3 (2).

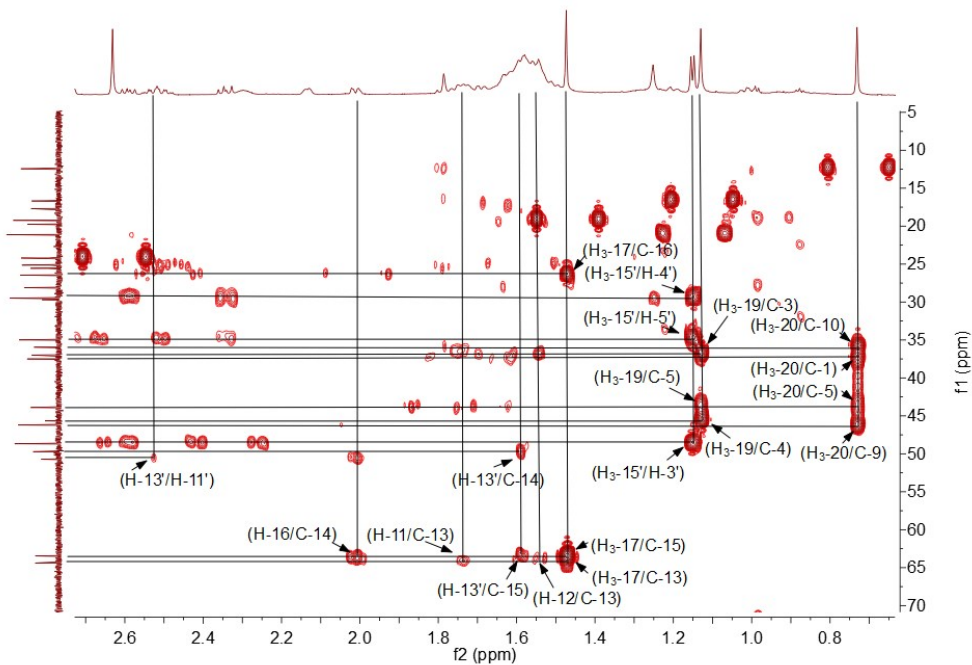


Figure S57. The part of HMBC spectrum of compound **3** in CDCl_3 (3).

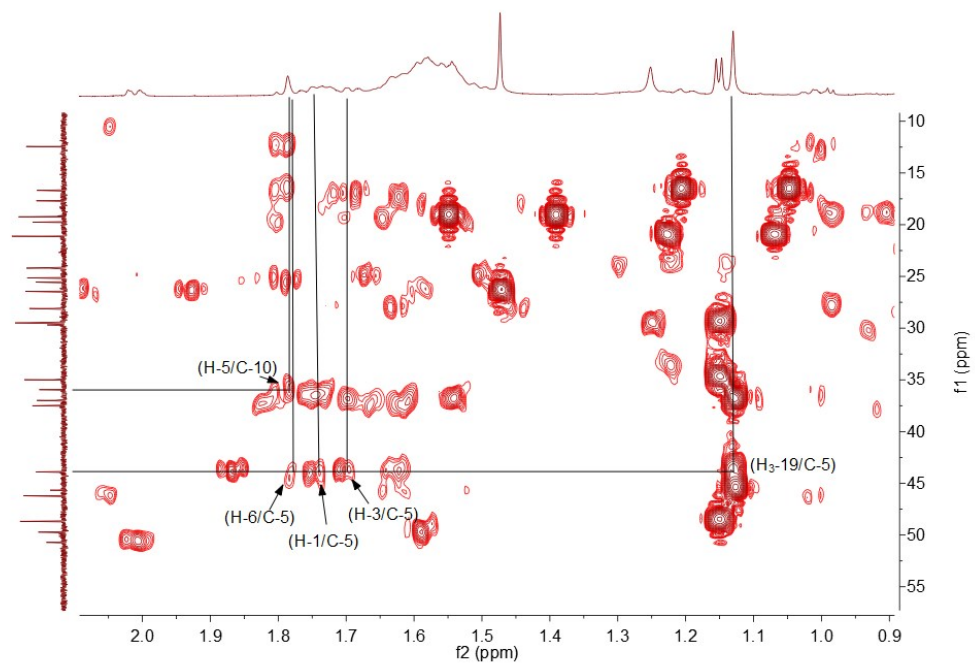


Figure S58. The part of HMBC spectrum of compound **3** in CDCl_3 (**3**).

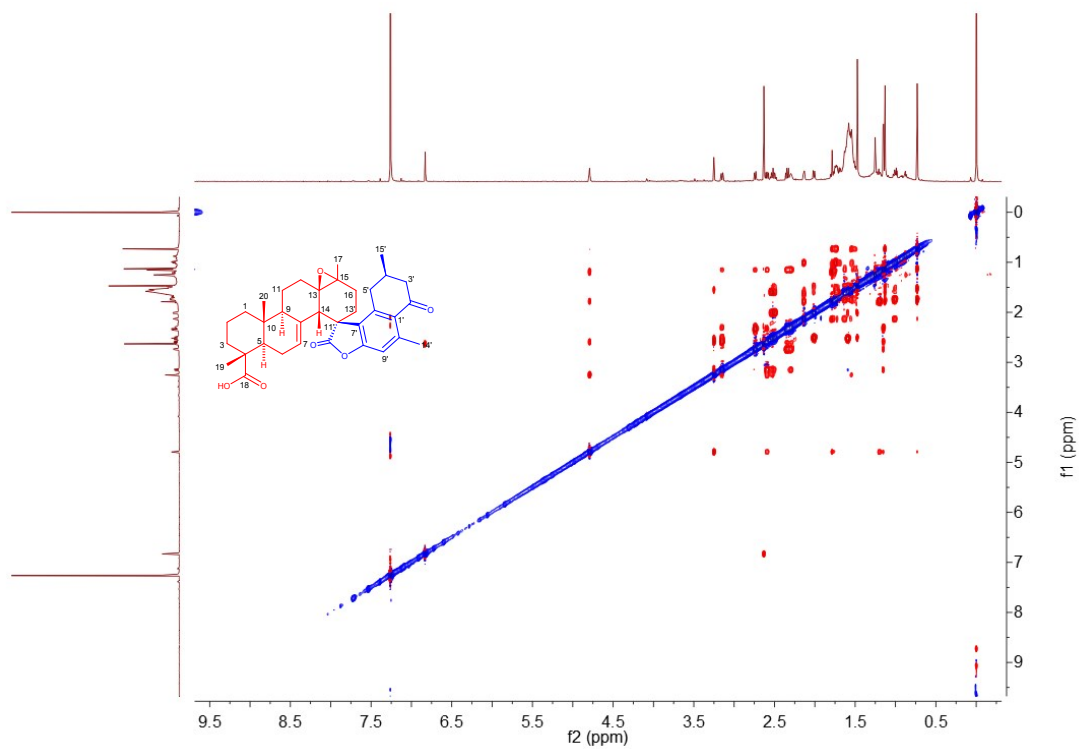


Figure S59. ROESY spectrum of compound **3** in CDCl_3 .

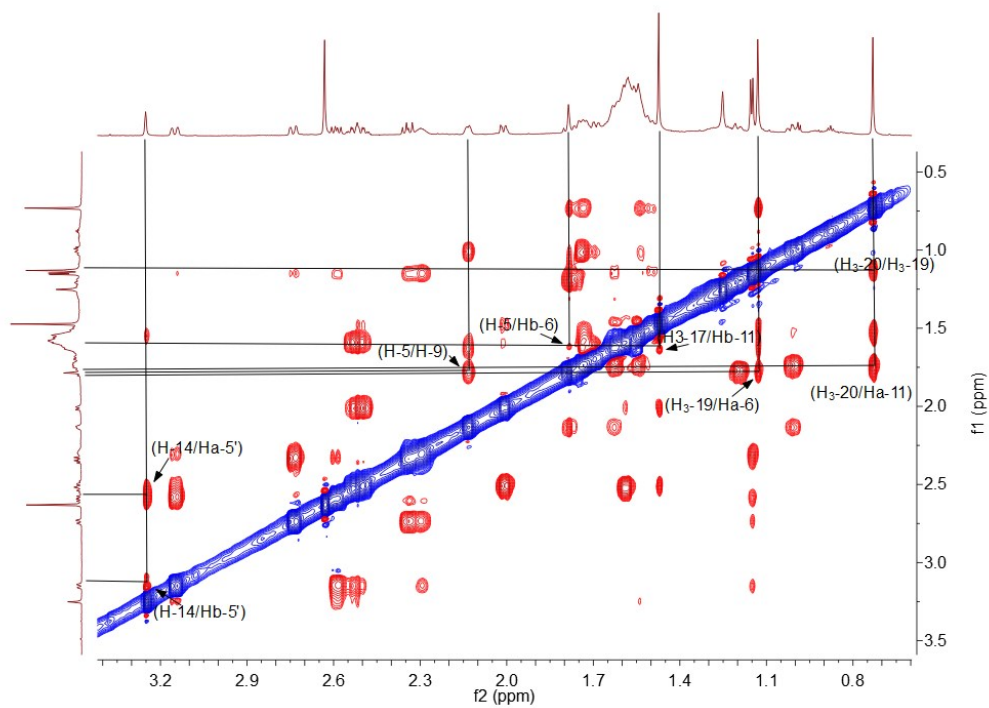


Figure S60. The part of ROESY spectrum of compound **3** in CDCl_3 (1).

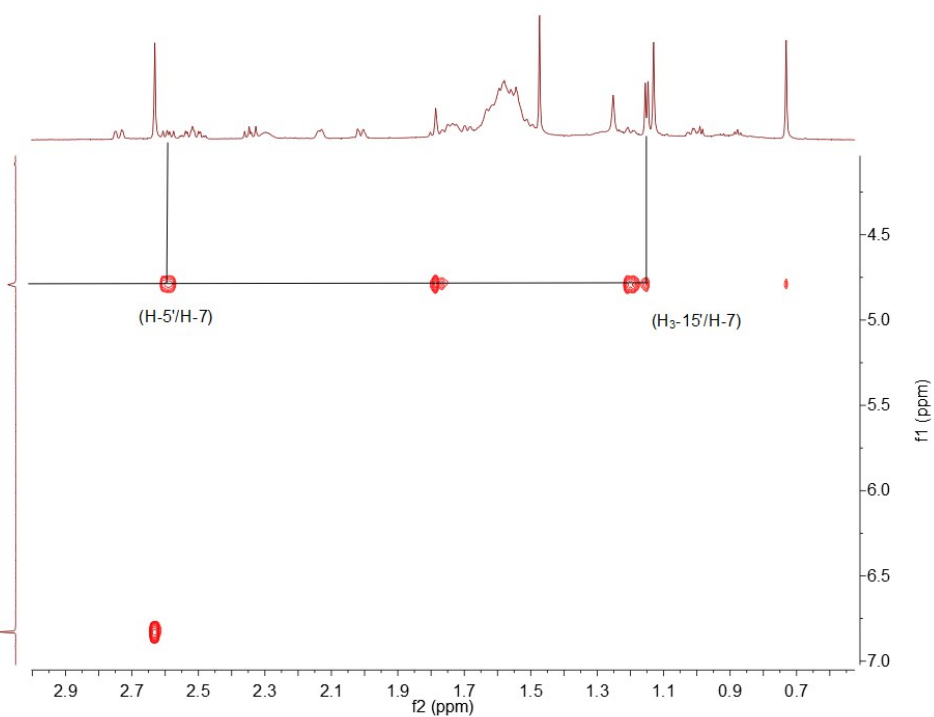


Figure S61. The part of ROESY spectrum of compound **3** in CDCl_3 (2).

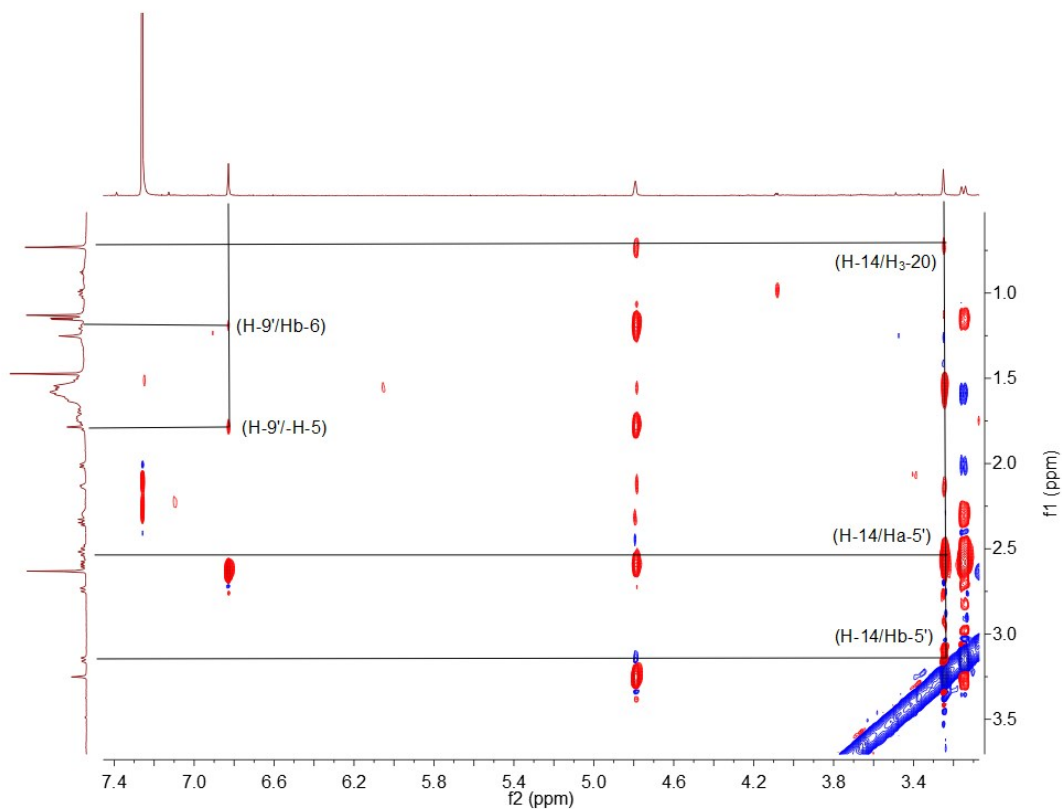
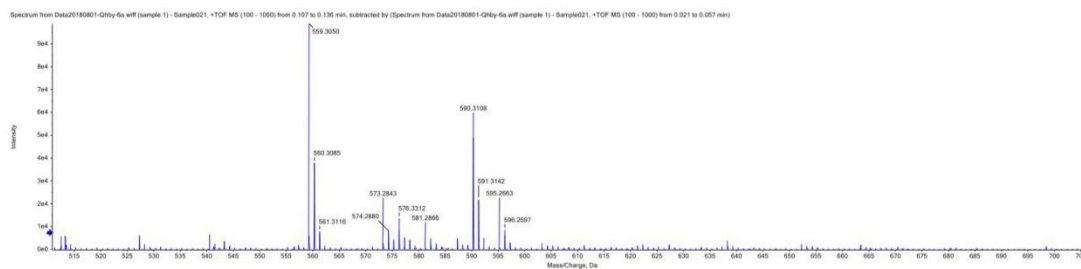


Figure S62. The part of ROESY spectrum of compound **3** in CDCl_3 (3).



$[\text{M}+\text{H}]^+$ m/z 559.3050

Hit	Formula	m/z	RDB	ppm
1	$\text{C}_{35}\text{H}_{43}\text{O}_6$	559.3054	15.0	-0.7

Elements from ~ to $\text{C}_{60}\text{H}_{120}\text{O}_6$

Mass tolerance 5ppm

Figure S63. HRESIMS of compound **3**.

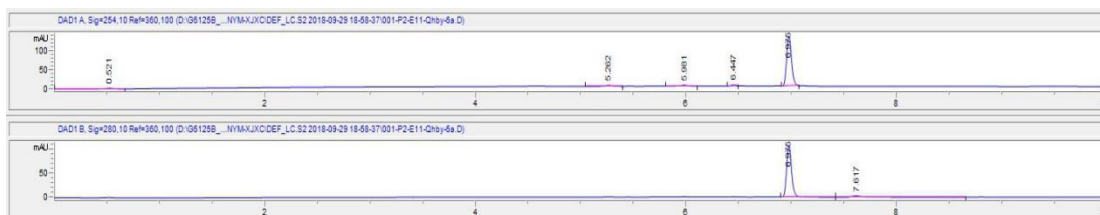


Figure S64. HPLC chromatogram of compound **3**.

(Mobile phase: aqueous AcCN , 10%-100% within 10 min, flow rate 0.25 mL/min)

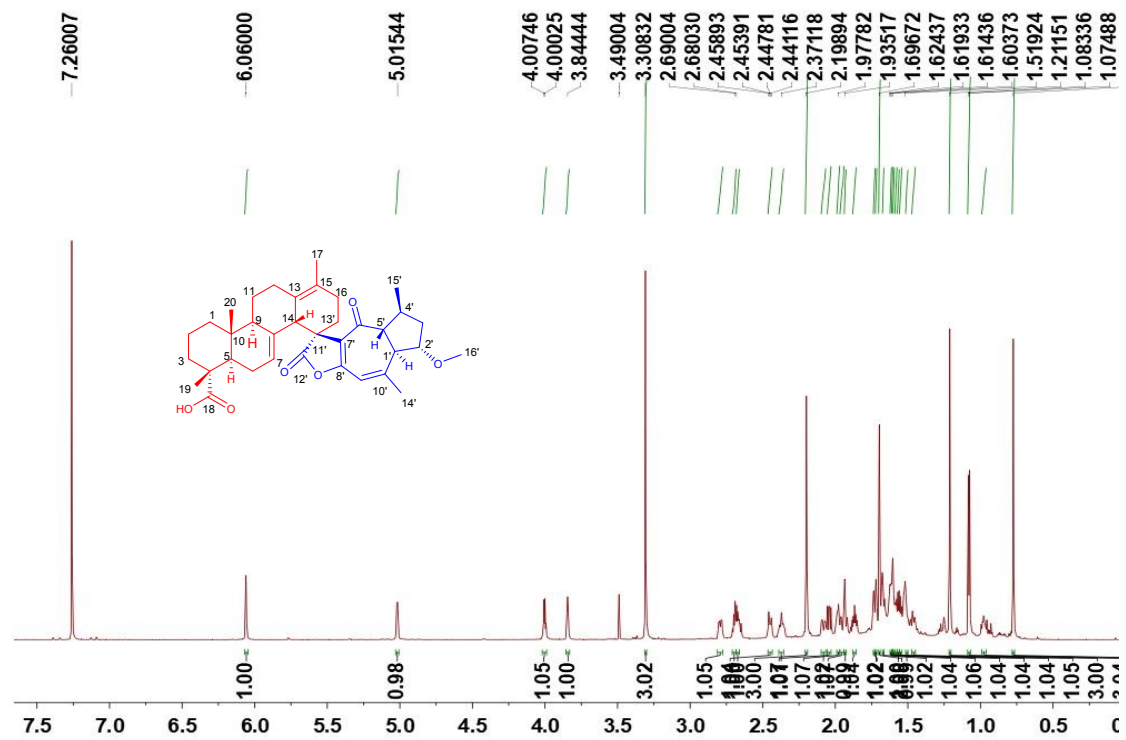


Figure S65. ¹H NMR (800 MHz) spectrum of compound 4 in CDCl₃.

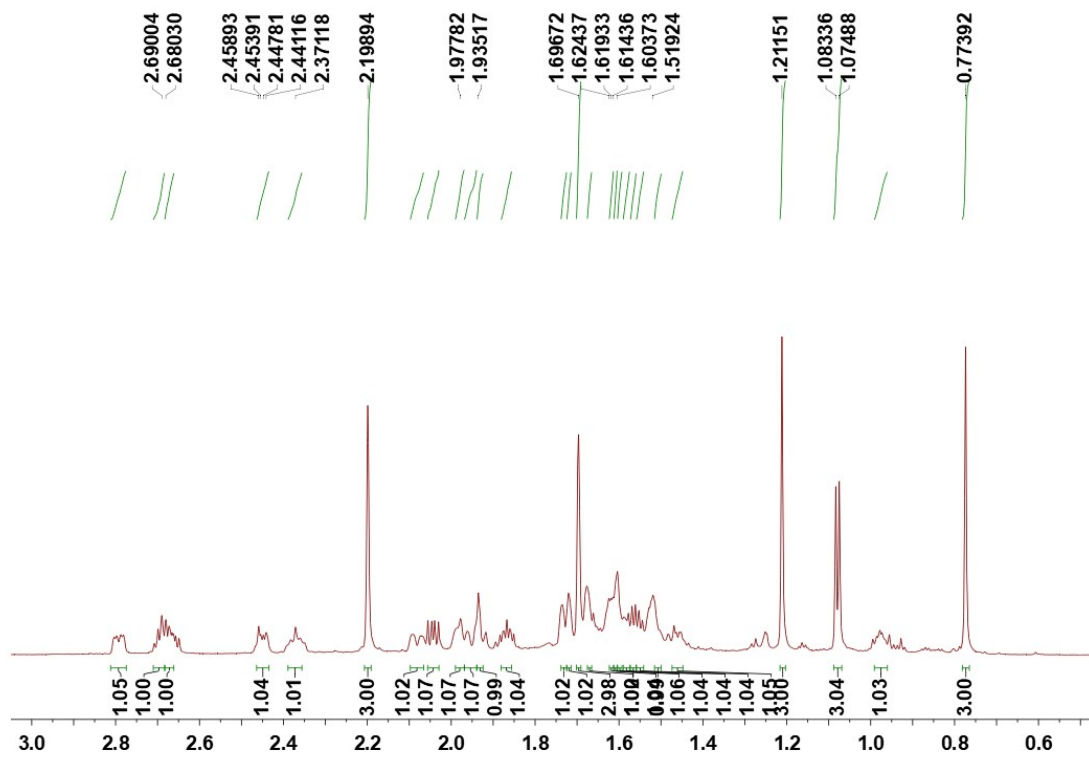


Figure S66. ¹H NMR (800 MHz) spectrum of compound 4 in CDCl₃.

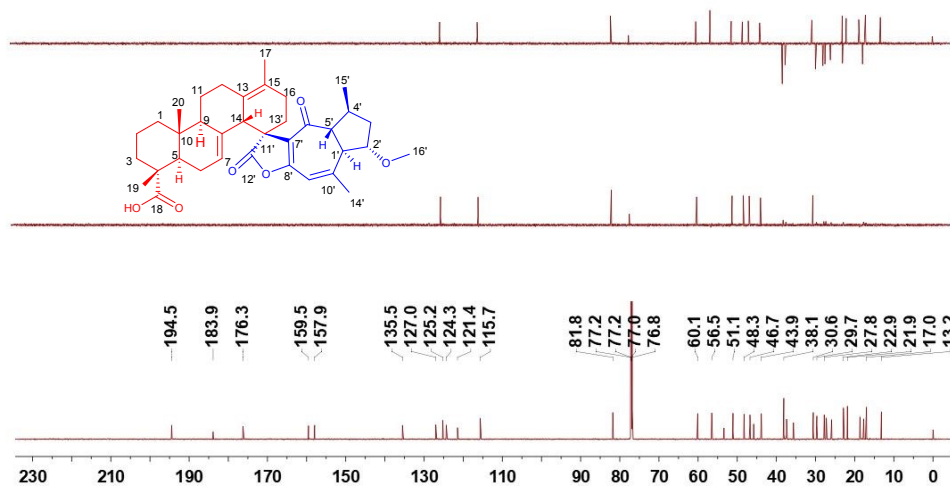


Figure S67. ^{13}C NMR (200 MHz) and DEPT spectra of compound **4** in CDCl_3 .

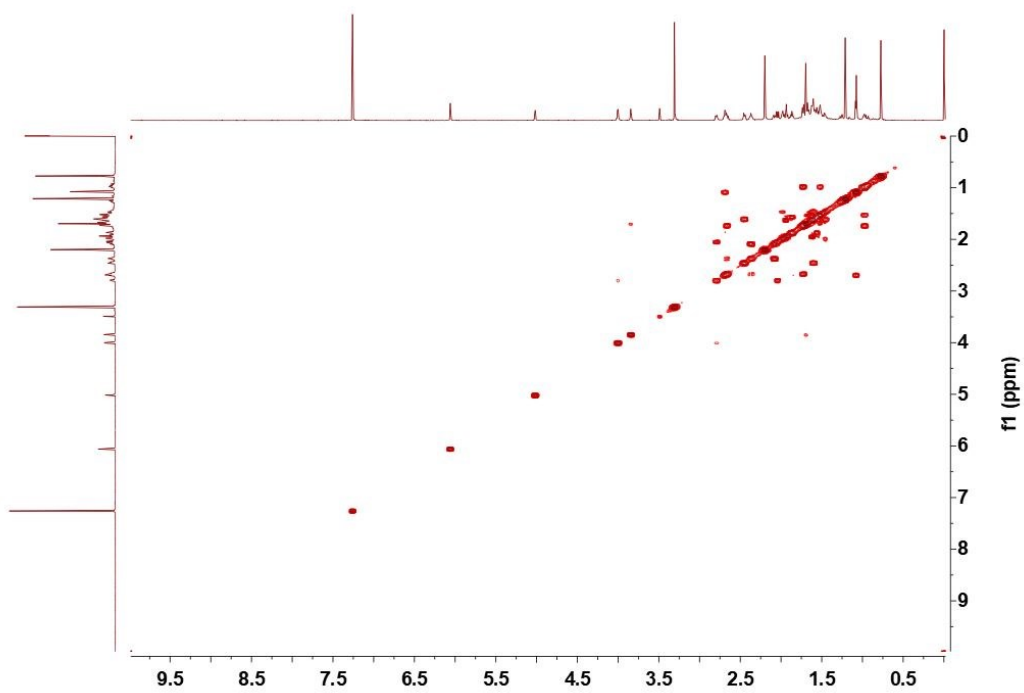


Figure S68. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 .

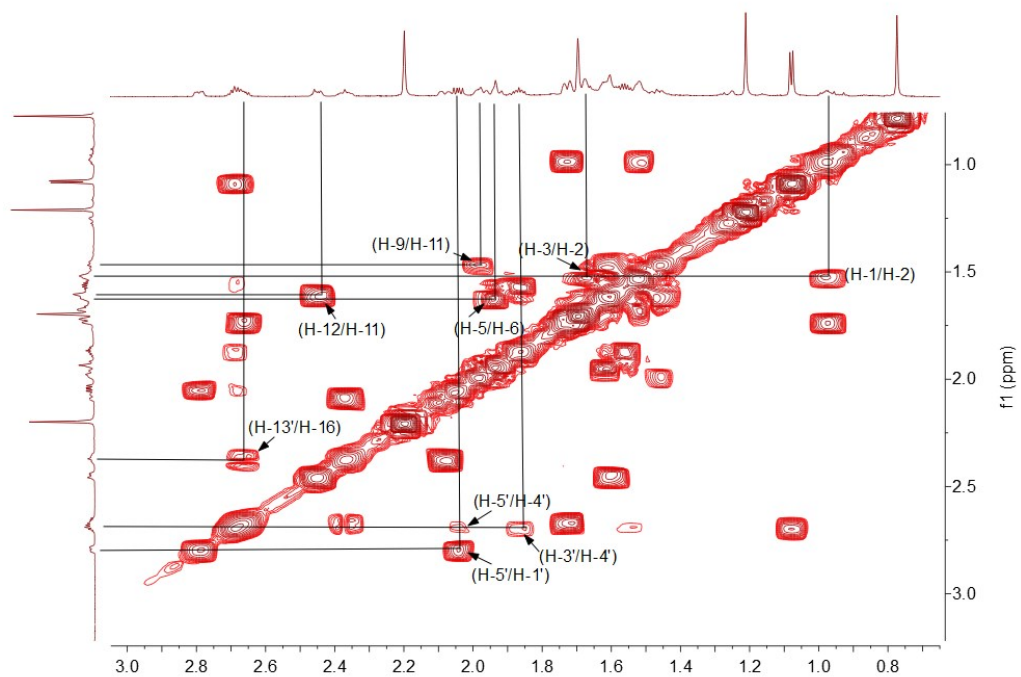


Figure S69. The part of ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 (1).

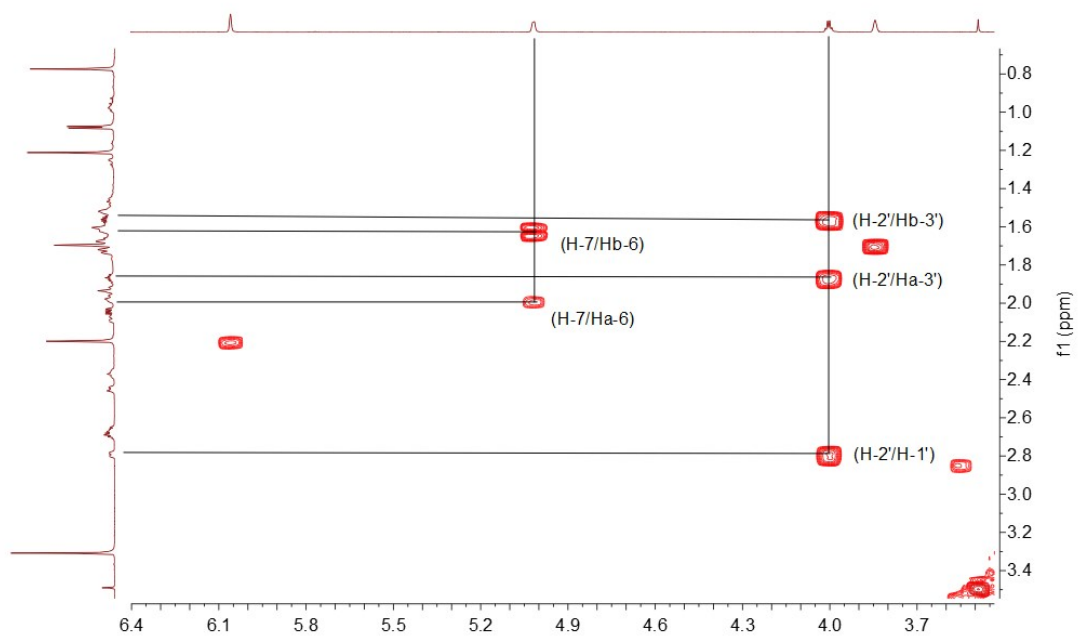


Figure S70. The part of ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 (2).

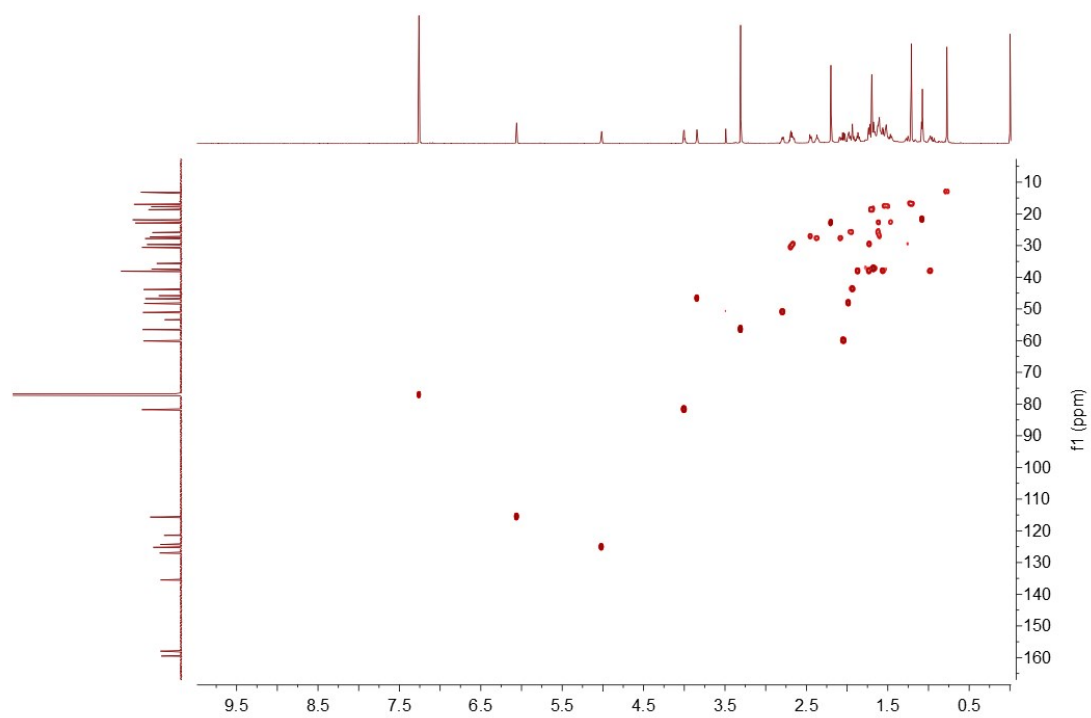


Figure S71. HSQC spectrum of compound 4 in CDCl₃.

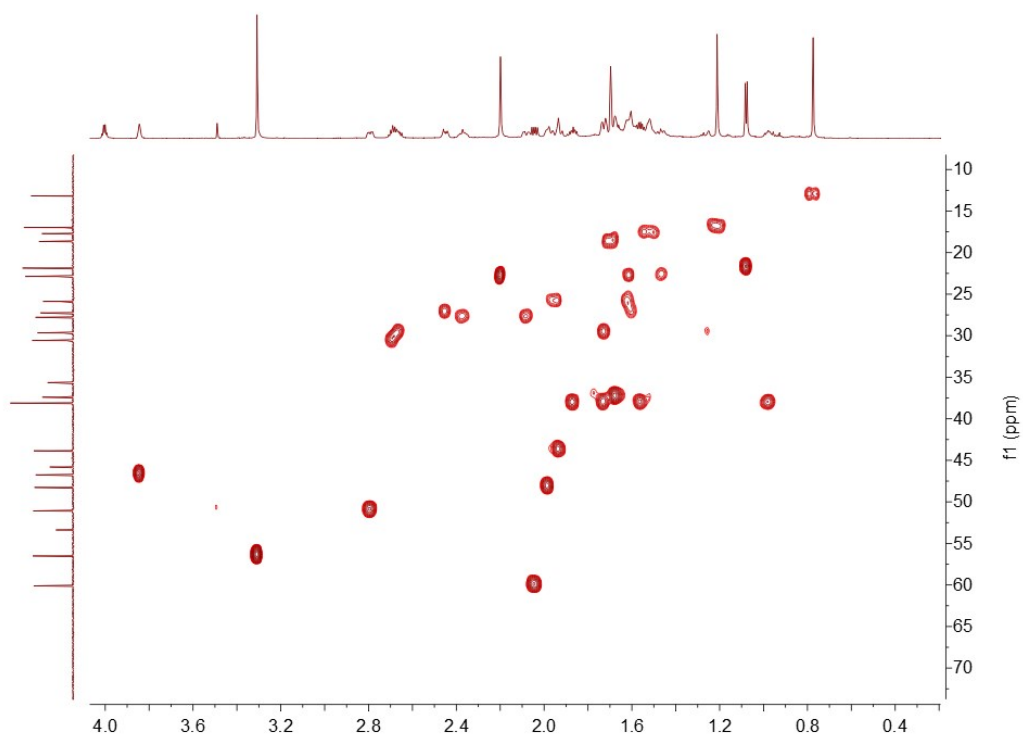


Figure S72. The part of HSQC spectrum of compound 4 in CDCl₃.

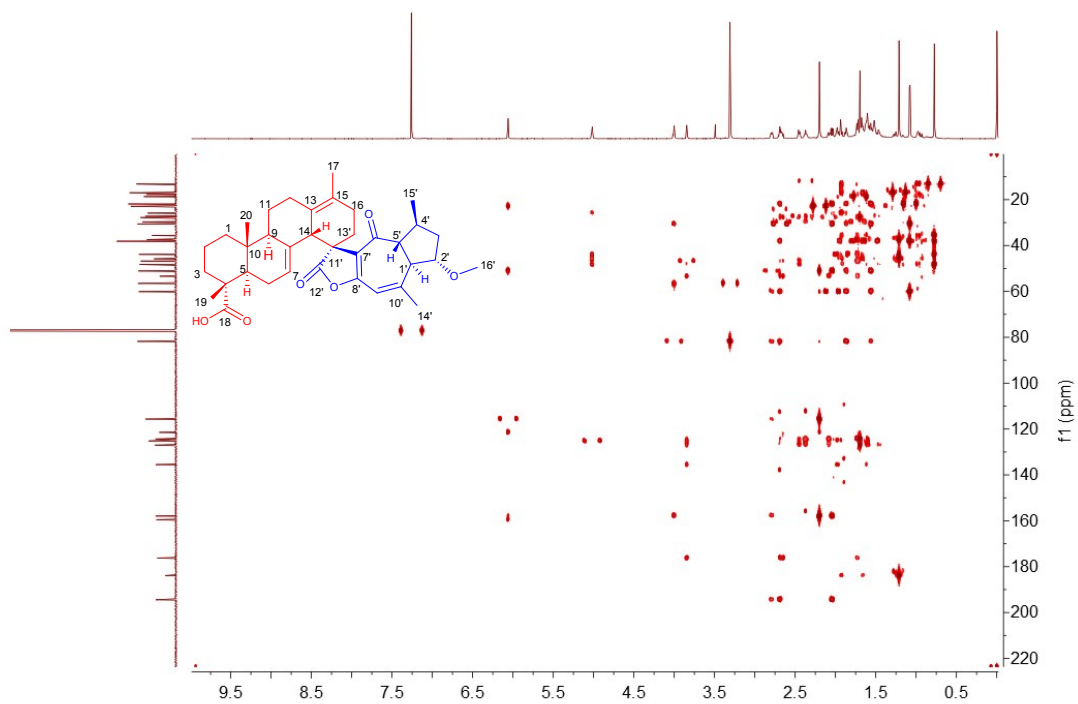


Figure S73. HMBC spectrum of compound **4** in CDCl_3 .

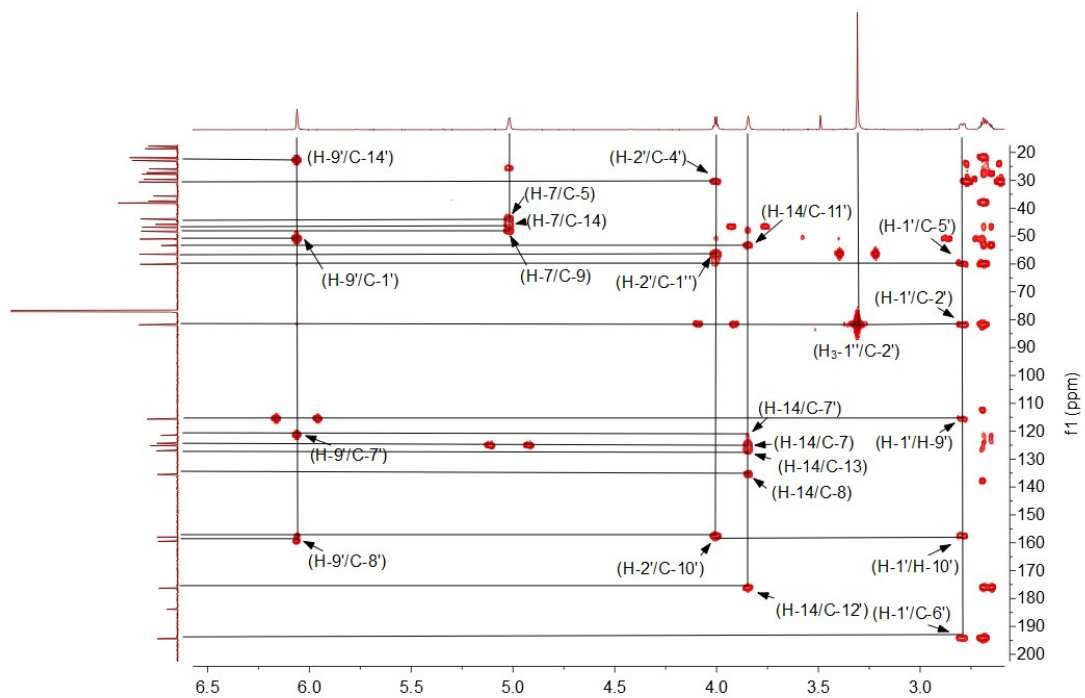


Figure S74. The part of HMBC spectrum of compound **4** in CDCl_3 (1).

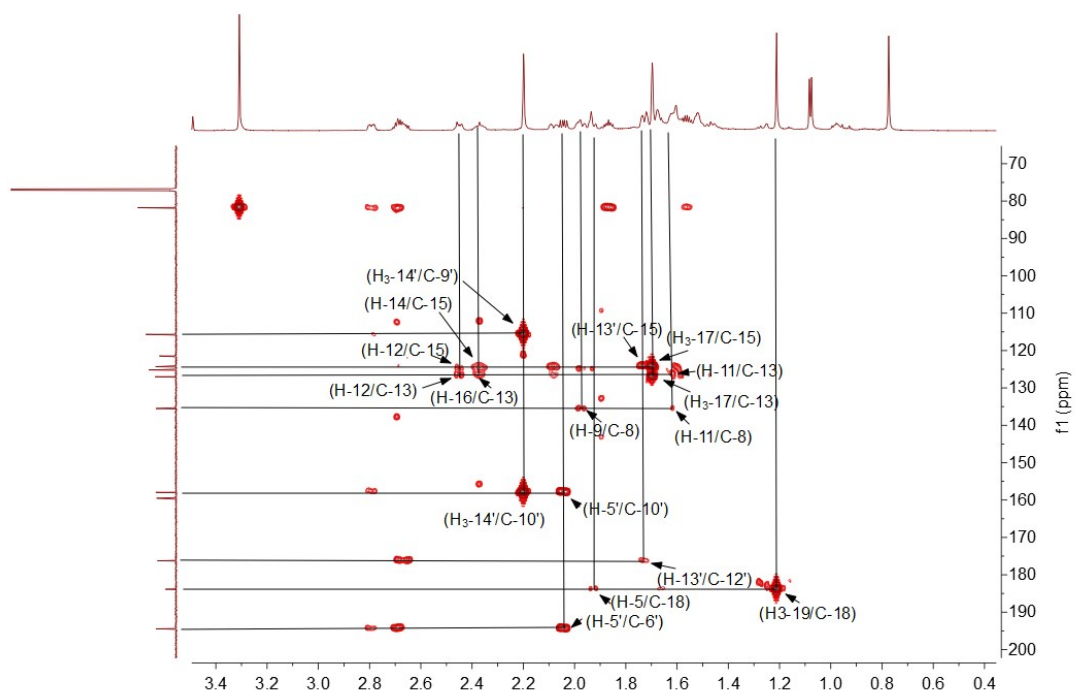


Figure S75. The part of HMBC spectrum of compound **4** in CDCl_3 (2).

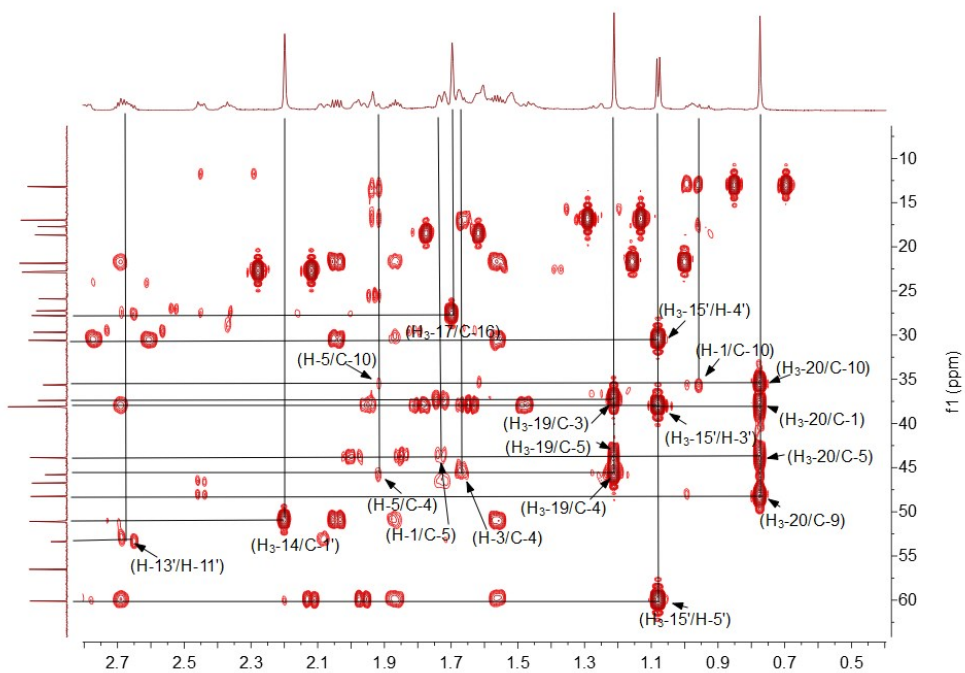


Figure S76. The part of HMBC spectrum of compound **4** in CDCl_3 (3).

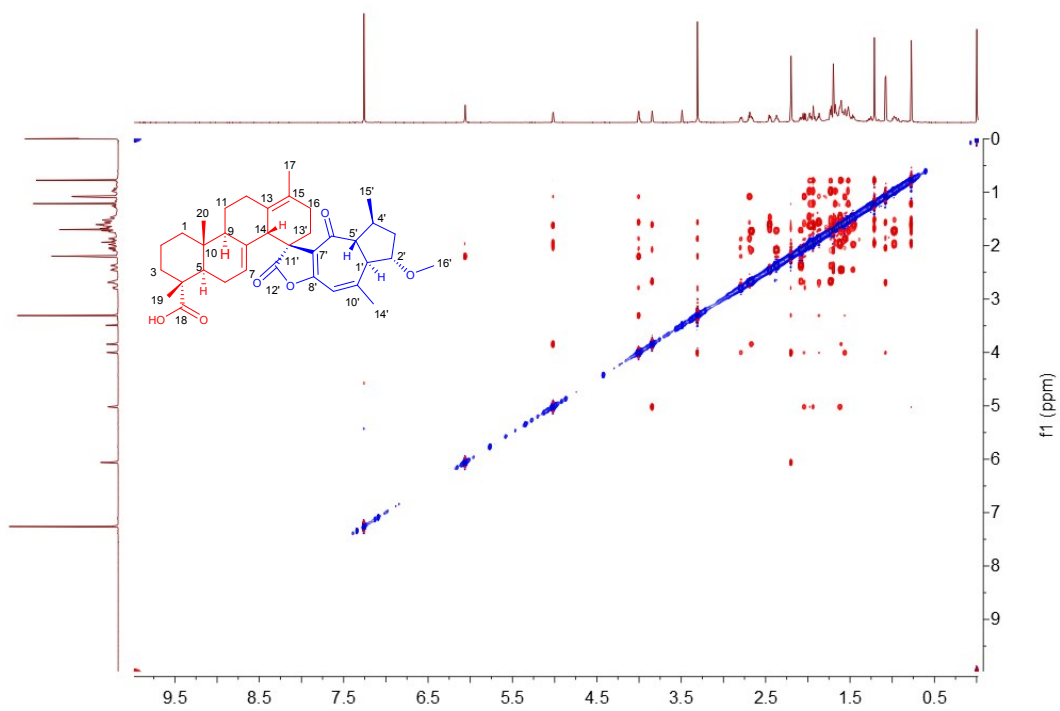


Figure S77. ROESY spectrum of compound **4** in CDCl_3 .

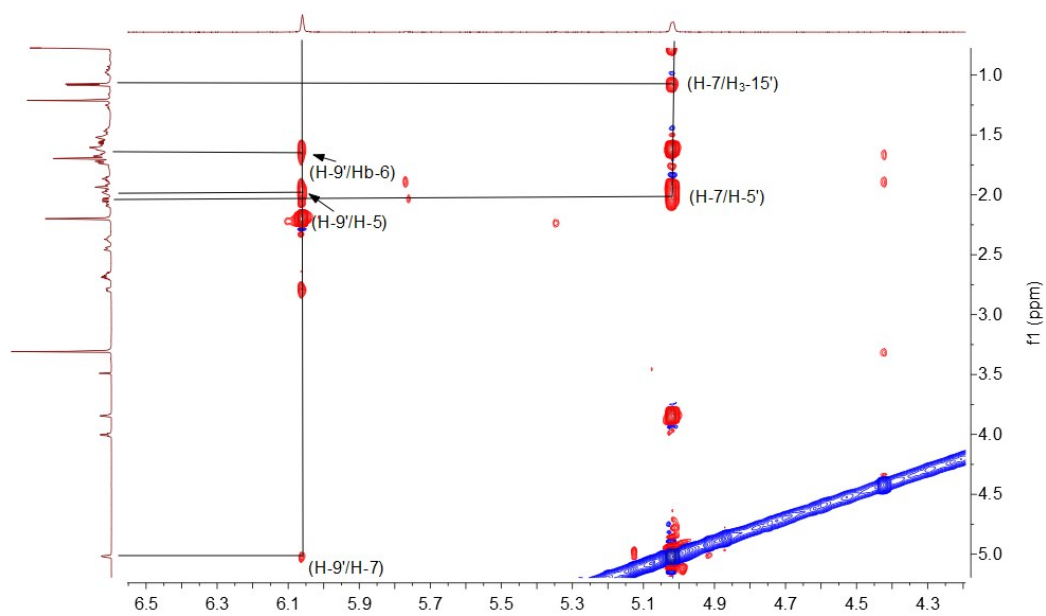


Figure S78. The part of ROESY spectrum of compound **4** in CDCl_3 (1).

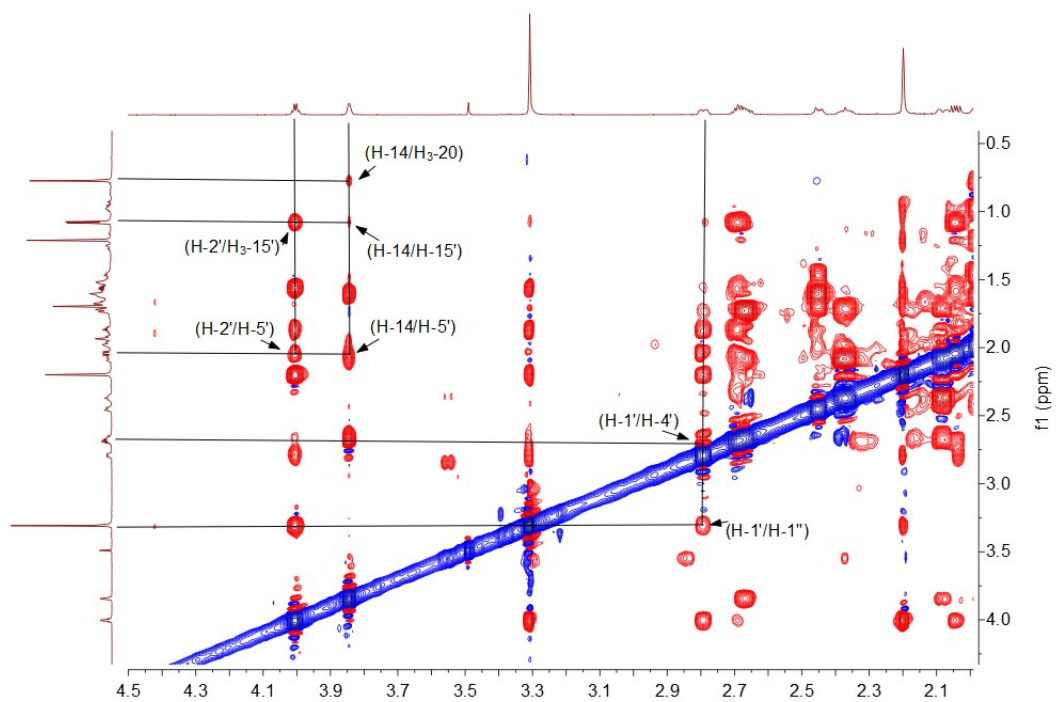


Figure S79. The part of ROESY spectrum of compound **4** in CDCl_3 (2).

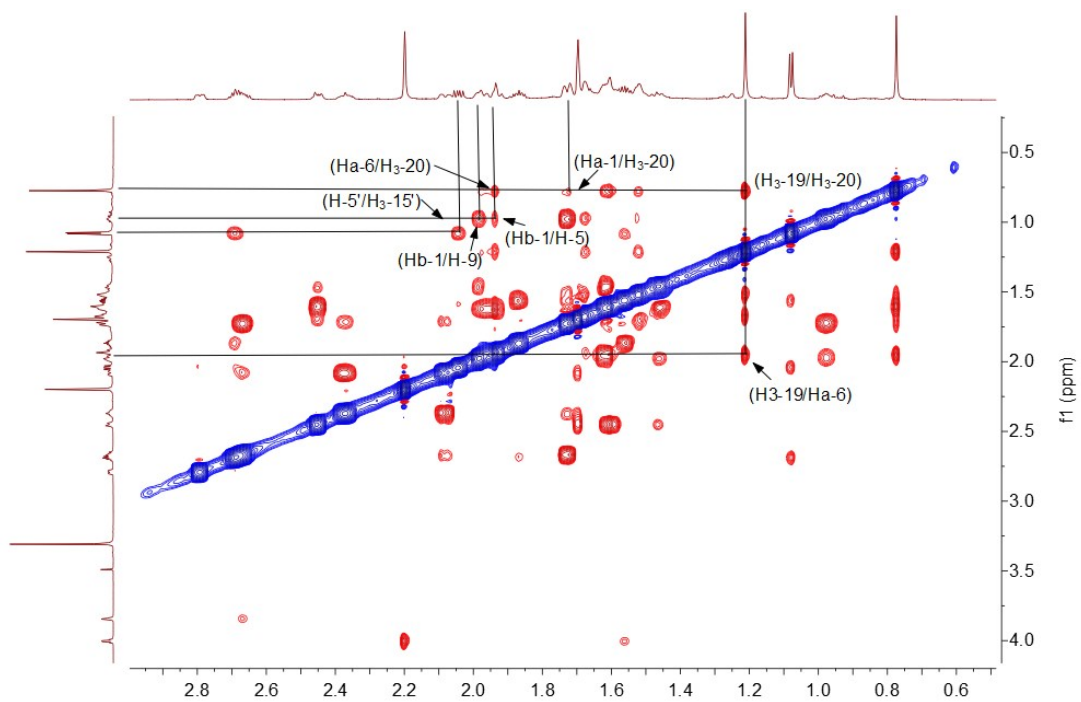


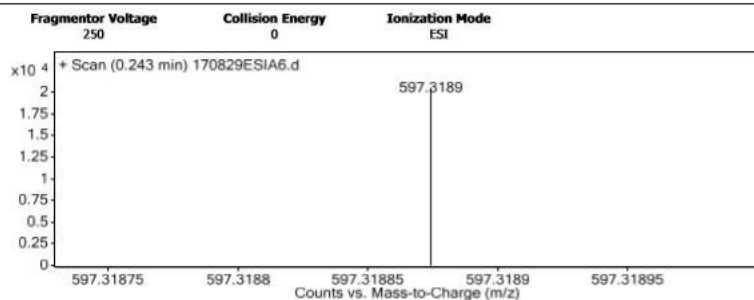
Figure S80. The part of ROESY spectrum of compound **4** in CDCl_3 (3).

Qualitative Analysis Report

Data Filename	170829ESIA6.d	Sample Name	qjw-63c
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESI.m	Acquired Time	8/29/2017 11:22:26 AM
IRM Calibration Status	Success	DA Method	ESI.m
Comment			

Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
122.5479	2	7905.75		
166.0623	1	5976.23		
252.1567		4302.95		
274.274	1	16218.55		
318.3004	1	8840.74		
575.3364	1	5245.28		
597.3189	1	20423.11	C36 H46 Na O6	M+
598.3215	1	6824.93	C36 H46 Na O6	M+
613.308	1	6282.66		
629.3081	1	8627.95		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	2	9
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C36 H46 Na O6	597.3192	597.3189	0.3	0.5	13.5

--- End Of Report ---

Figure S81. HRESIMS of compound 4.