

Unprecedented monoterpenoid polyprenylated acylphloroglucinols with a rare 6/6/5/4 tetracyclic core, enhanced MCF-7 cells sensitivity to camptothecin by inhibiting the DNA damage response

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1. Previously reported MTPAPs

In the past decades, a series of polycyclic polypropenylated acylphloroglucinols (PPAPs) have been reported isolating from the plants of genera *Hypericum* and *Garcinia*. Monoterpeneoid polypropenylated acylphloroglucinols (MTPAPs), a special type of structurally diverse PPAPs, generally decorated with a geranyl or a cyclic monoterpene fragment at C-3 of the phloroglucinol ring. To date, approximately 110 MTPAPs (Table S1) have been identified, which can be divided into six types due to their different ring system, including the uncyclized MTPAPs and cyclized MTPAPs with 6/5, 6/6, 6/5/6, 6/6/6 and 6/7/5 ring system.¹⁻²⁴ Most of them were obtained from the genus *Hypericum*. Our work on *Hypericum elodeoides* have found three pairs of novel scaffolds MTPAPs, (\pm)-Hypersines A – C (**1–3**), which were characterized by an unusual large tensional four-membered carbocycle concurrently merged with five- and six-membered rings in the part of monoterpene fragment.

Table S1. Previously Reported MTPAPs

No.	Names	No.	Names
1-2	chinesin I-II ¹	34-41	tomoeones A–H ⁹
3-4	hypercalin B–C ²	42-45	(±)-japonicols A–D ¹⁰
5-6	isomeric homologues of hypercalin C (5a/5b) ²	46-47	hyperpatulone E–F ¹¹
7	paglucinol ³	48-56	hyperpatulols A–I ¹²
8-9	yojironins C–D ⁴	57-68	hyperbeanols F–Q ¹³
10-11	empetrikarinens A–B ⁵	69-74	faberiones A–F ¹⁴
12-13	empetrikarinols A–B ⁵	75-76	hyphenrone J–K ¹⁵
14-15	empetriferdinan A–B ⁵	77-81	hypascyrin A–E ¹⁶
16	empetriferdinol ⁵	82	ent-hyphenrone J ¹⁶
17-18	empetrifranzinan A/B ⁵	83	hypascyrin K ¹⁶
19	empetrifranzinan C ⁵	84-85	hyperpatulone A–B ¹⁷
20	madeleinol A ⁶	86-87	spirohypatone A–B ¹⁸
21	empetrifranzinan D ⁶	88-89	hypatone A–B ¹⁹
22	madeleinol B ⁶	90-94	hyperhenols A–E ²⁰
23	3-geranyl-2,4,6-trihydroxybenzophenone ⁷	95	longisglucinols B–C ²¹
24	3-geranyl-1-(2'-methylpropanoyl)-phloroglucinol ⁸	96-100	bellumone F–J ²²
25	3-geranyl-1-(2'-methylbutanoyl)-phloroglucinol ⁸	101-103	hyperelodione A–C ²³

26-33 hyperascyrone A–H⁹ 104-111 elodeoidols A–I²⁴

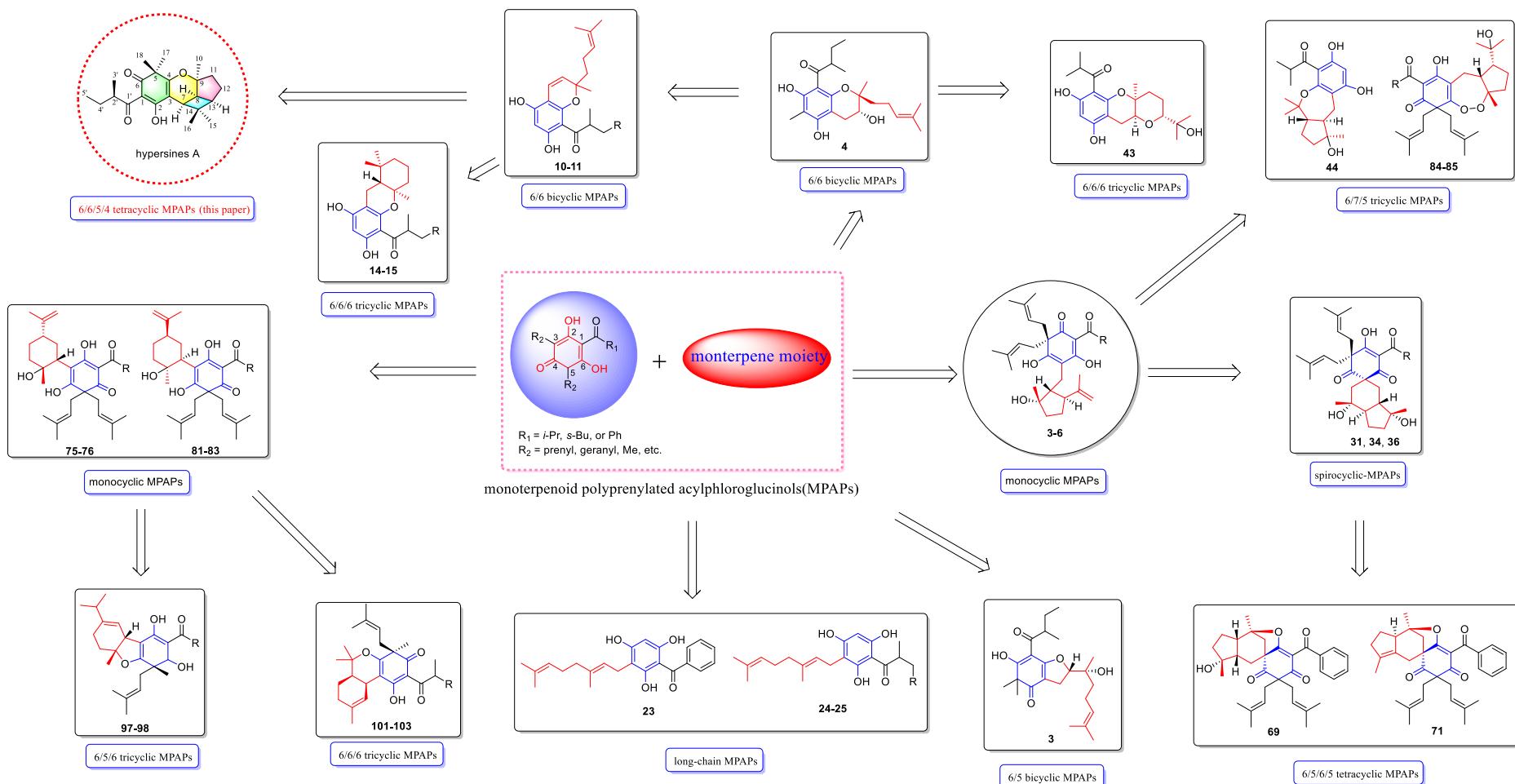


Figure S1. MTPAPs derivatives reported previously

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2. The HPLC chromatogram and ^1H NMR data of 1 – 3

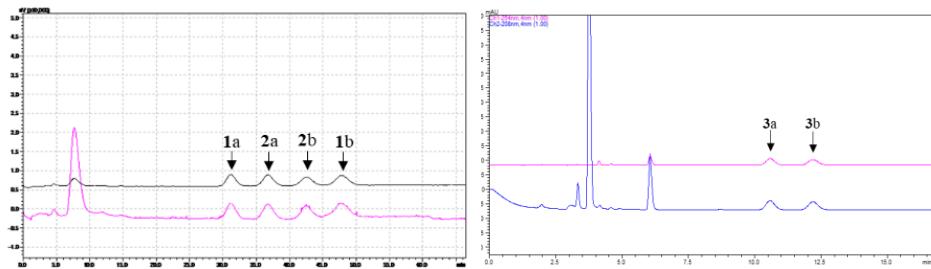


Figure S2. Chiral HPLC chromatogram of 1a/b–3a/b.

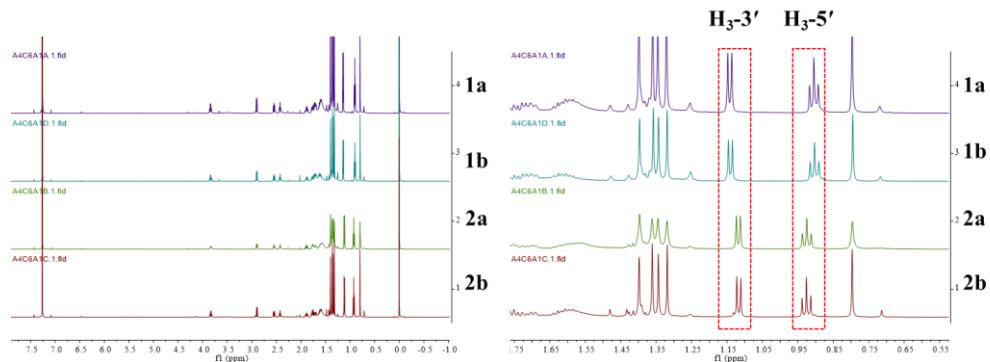


Figure S3. Comparing the ^1H NMR data of 1a/b and 2a/b (left) and partial enlarged detail(right).

3. Computational details

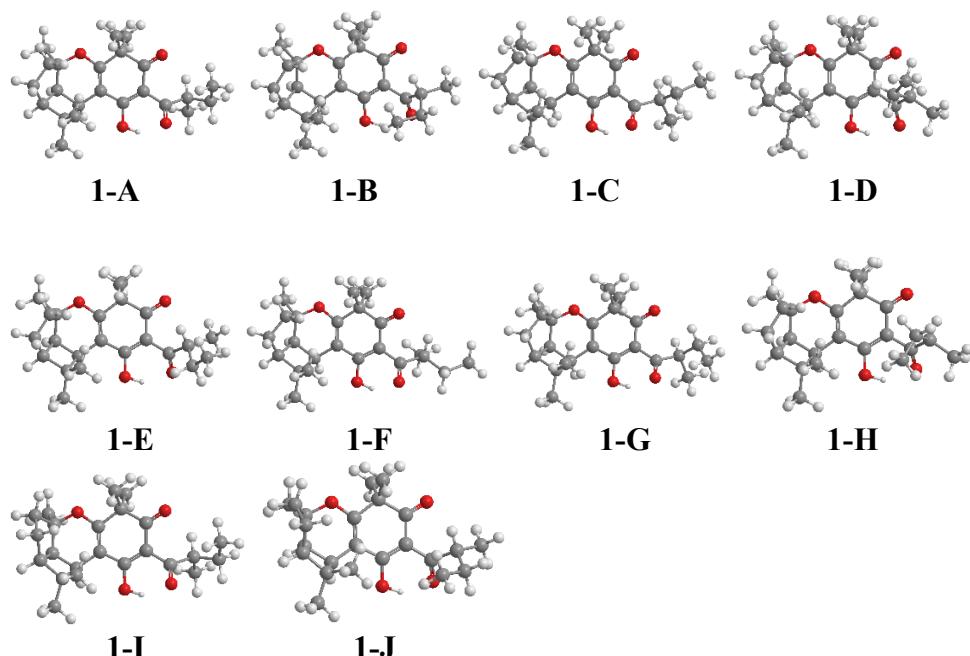


Figure S4. Conformers of isomer 1 for NMR calculation.

Table S3. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer 1 at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
1-A	-1196.706236	0	20.59%	0
1-B	-1196.706235	0.000188253	20.58%	0
1-C	-1196.705827	0.256337631	13.35%	0
1-D	-1196.705827	0.256400382	13.35%	0
1-E	-1196.705129	0.694527515	6.37%	0
1-F	-1196.705126	0.696410043	6.35%	0
1-G	-1196.704621	1.01323959	3.72%	0
1-H	-1196.704616	1.016377137	3.70%	0
1-I	-1196.704316	1.204378983	2.69%	0
1-J	-1196.704313	1.206575267	2.68%	0

Table S4. Optimized Z-matrixes of isomer **1** in the gas phase (\AA) at B3LYP/6-31G* level.

1-A				1-B			
C	-10.3581	1.4893	2.6921	C	-10.0935	1.5916	2.5954
C	-10.2352	0.0081	2.2748	C	-9.8813	0.1163	2.1933
C	-10.1958	-0.2848	0.7671	C	-10.0896	-0.2342	0.7122
C	-10.7189	0.8757	-0.0877	C	-10.8942	0.824	-0.0512
C	-11.1341	2.0266	0.4915	C	-11.3236	1.9466	0.5713
O	-11.0992	2.3378	1.8194	O	-11.073	2.3197	1.8596
C	-10.8249	0.7186	-1.539	C	-11.2275	0.6062	-1.4593
C	-11.3234	1.6816	-2.3662	C	-11.9405	1.4936	-2.2106
C	-11.7199	2.9978	-1.8377	C	-12.4966	2.7169	-1.6069
C	-11.7028	3.2149	-0.2954	C	-12.1653	3.0287	-0.1174
C	-13.1766	3.4346	0.1446	C	-13.5208	3.1423	0.6374
C	-10.801	4.4544	-0.0218	C	-11.3585	4.3581	-0.1082
O	-12.0498	3.9208	-2.587	O	-13.2178	3.4829	-2.2513
C	-11.4599	1.3841	-3.8054	C	-12.1411	1.2144	-3.6465
O	-10.5648	0.7958	-4.4172	O	-12.3938	0.0748	-4.0463
C	-12.7906	1.681	-4.5412	C	-11.8795	2.3206	-4.6966
C	-13.7011	0.4332	-4.528	C	-13.1401	2.587	-5.5495
C	-12.5957	2.2097	-5.9876	C	-10.6524	2.0146	-5.5949
C	-11.8394	3.548	-6.0753	C	-9.3172	1.8921	-4.8354
O	-10.4058	-0.4733	-2.046	O	-10.7852	-0.5589	-2.0068
C	-8.9237	2.033	2.7864	C	-8.7375	2.2907	2.4082
C	-8.0331	0.8112	3.0371	C	-7.6826	1.1837	2.5101
C	-8.7548	-0.3937	2.4023	C	-8.367	-0.117	2.0463
C	-11.1184	1.6403	4.0195	C	-10.6094	1.7144	4.0381
C	-8.6909	-0.6448	0.8714	C	-8.5602	-0.4217	0.536
C	-8.4074	-2.1223	0.5285	C	-8.1767	-1.8718	0.1741
C	-7.7268	0.2512	0.0572	C	-7.8746	0.5412	-0.4633

H	-8.5666	-1.2817	3.0098	H	-7.9695	-0.9542	2.6245
H	-10.9434	-0.6108	2.8269	H	-10.3991	-0.5521	2.8823
H	-10.8094	-1.1521	0.5113	H	-10.6363	-1.1735	0.5965
H	-13.7949	2.5542	-0.0407	H	-14.0736	2.2009	0.6279
H	-13.2436	3.6545	1.211	H	-13.3742	3.4175	1.6827
H	-13.6385	4.2758	-0.3764	H	-14.1698	3.9062	0.2045
H	-10.7864	4.714	1.0375	H	-10.401	4.2587	-0.6233
H	-11.1507	5.3434	-0.5507	H	-11.9054	5.1735	-0.5863
H	-9.7665	4.2807	-0.3242	H	-11.1425	4.686	0.9095
H	-13.3136	2.4607	-3.9907	H	-11.6573	3.2409	-4.1576
H	-14.6662	0.6455	-4.9893	H	-12.9788	3.4084	-6.2481
H	-13.902	0.0919	-3.511	H	-13.9919	2.8628	-4.9248
H	-13.2537	-0.399	-5.0747	H	-13.4289	1.7103	-6.132
H	-12.0817	1.4619	-6.5956	H	-10.8296	1.1033	-6.1707
H	-13.5738	2.3447	-6.4521	H	-10.5491	2.8111	-6.334
H	-11.7854	3.9016	-7.1052	H	-8.4876	1.7478	-5.5283
H	-12.3335	4.3208	-5.4846	H	-9.1084	2.7911	-4.2543
H	-10.8164	3.4574	-5.7081	H	-9.3158	1.0445	-4.1491
H	-10.4242	-0.3842	-3.009	H	-11.1766	-0.6123	-2.8906
H	-8.6481	2.5109	1.8478	H	-8.6964	2.7583	1.426
H	-8.8067	2.7927	3.5594	H	-8.5673	3.0885	3.1314
H	-7.9508	0.6477	4.1133	H	-7.3847	1.0735	3.5545
H	-7.0164	0.9435	2.6649	H	-6.774	1.4102	1.9509
H	-10.6429	1.0682	4.8159	H	-9.9341	1.2302	4.7432
H	-11.1581	2.6828	4.3356	H	-10.7091	2.7585	4.3349
H	-12.146	1.2901	3.9221	H	-11.5908	1.2514	4.1415
H	-8.5657	-2.3152	-0.5335	H	-8.5071	-2.1243	-0.8345
H	-7.3783	-2.394	0.7651	H	-7.0972	-2.0192	0.2165
H	-9.0594	-2.8002	1.0806	H	-8.632	-2.594	0.8527
H	-6.6892	0.0804	0.3437	H	-6.7893	0.4987	-0.3732
H	-7.8088	0.0421	-1.0099	H	-8.1269	0.2795	-1.4913
H	-7.9326	1.3118	0.1782	H	-8.1774	1.5763	-0.3268

Continued table S4.

1-C				1-D			
C	-10.354	1.496	2.7167	C	-10.0282	1.6417	2.579
C	-10.2348	0.0102	2.3156	C	-9.914	0.1372	2.2522
C	-10.1773	-0.2976	0.8114	C	-10.1636	-0.2756	0.7937
C	-10.682	0.8577	-0.0618	C	-10.9158	0.7884	-0.0142
C	-11.0985	2.0159	0.5011	C	-11.2662	1.9659	0.5538
O	-11.079	2.34	1.8263	O	-10.9677	2.3926	1.8149
C	-10.7676	0.6877	-1.5132	C	-11.2867	0.5181	-1.404
C	-11.2471	1.6454	-2.3591	C	-11.977	1.3978	-2.1861

C	-11.6549	2.9652	-1.8439	C	-12.4687	2.6708	-1.6297
C	-11.6511	3.1987	-0.3041	C	-12.0597	3.0561	-0.1772
C	-13.1276	3.4331	0.1199	C	-13.3743	3.3123	0.6156
C	-10.7439	4.4353	-0.0354	C	-11.1661	4.3234	-0.287
O	-11.9866	3.8789	-2.6032	O	-13.1969	3.4222	-2.2819
C	-11.3578	1.339	-3.8021	C	-12.2101	1.0595	-3.6082
O	-10.4959	0.6703	-4.379	O	-12.528	-0.0884	-3.9307
C	-12.6268	1.7345	-4.5941	C	-11.925	2.1073	-4.7211
C	-13.3435	0.484	-5.159	C	-12.3668	1.6299	-6.1293
C	-12.2924	2.772	-5.6976	C	-10.438	2.5574	-4.7041
C	-13.5316	3.4228	-6.3342	C	-10.1543	3.8032	-5.56
O	-10.3491	-0.5127	-1.9992	O	-10.9017	-0.6888	-1.9017
C	-8.9176	2.0323	2.8239	C	-8.6333	2.2433	2.3453
C	-8.0379	0.8078	3.0988	C	-7.6488	1.0782	2.4934
C	-8.7587	-0.3992	2.4667	C	-8.4192	-0.198	2.1023
C	-11.13	1.6646	4.0328	C	-10.5193	1.8707	4.0175
C	-8.6763	-0.6663	0.9394	C	-8.6507	-0.5641	0.6112
C	-8.3982	-2.149	0.6154	C	-8.3595	-2.0509	0.3183
C	-7.6955	0.2151	0.1292	C	-7.9217	0.3051	-0.4416
H	-8.5839	-1.2821	3.0857	H	-8.0675	-1.029	2.7178
H	-10.954	-0.599	2.8642	H	-10.4629	-0.4608	2.9806
H	-10.7931	-1.1635	0.5561	H	-10.7666	-1.1851	0.733
H	-13.5795	4.2712	-0.4148	H	-13.9879	4.0894	0.1554
H	-13.75	2.5546	-0.0611	H	-13.9886	2.4128	0.689
H	-13.2032	3.6657	1.183	H	-13.1695	3.6448	1.6341
H	-11.0825	5.3205	-0.5778	H	-11.6764	5.1417	-0.7993
H	-10.7384	4.7065	1.021	H	-10.8881	4.7003	0.6983
H	-9.7075	4.2514	-0.3251	H	-10.2388	4.1247	-0.8279
H	-13.3095	2.205	-3.8874	H	-12.5396	2.9742	-4.4861
H	-12.7437	-0.0137	-5.9231	H	-11.765	0.7893	-6.4781
H	-14.3011	0.7421	-5.6107	H	-12.2862	2.4254	-6.8695
H	-13.5521	-0.2473	-4.3764	H	-13.4097	1.3082	-6.1302
H	-11.6774	3.5719	-5.2776	H	-10.124	2.7888	-3.6841
H	-11.6823	2.3087	-6.476	H	-9.7962	1.7373	-5.033
H	-13.2405	4.1908	-7.0514	H	-9.1171	4.1219	-5.4515
H	-14.1434	2.6961	-6.8684	H	-10.324	3.6157	-6.6202
H	-14.1572	3.9002	-5.5789	H	-10.7879	4.6397	-5.262
H	-10.3603	-0.4371	-2.9643	H	-11.3151	-0.7709	-2.7732
H	-8.6272	2.4987	1.8841	H	-8.5746	2.6587	1.3408
H	-8.806	2.7992	3.5905	H	-8.4046	3.0633	3.0264
H	-7.9709	0.6548	4.1775	H	-7.3456	1.0017	3.5393
H	-7.0156	0.9302	2.7387	H	-6.7347	1.2185	1.9151
H	-10.6679	1.0978	4.8408	H	-9.8682	1.3811	4.7413

H	-11.1678	2.7104	4.338	H	-10.5495	2.9329	4.2607
H	-12.1583	1.3192	3.9259	H	-11.5268	1.4771	4.1523
H	-8.5439	-2.3519	-0.4466	H	-8.7178	-2.3325	-0.6728
H	-7.374	-2.4249	0.8684	H	-7.2903	-2.261	0.3569
H	-9.0619	-2.8169	1.1657	H	-8.848	-2.7099	1.037
H	-6.6631	0.0406	0.4318	H	-6.8397	0.2029	-0.359
H	-7.7642	-0.0049	-0.9366	H	-8.2008	0.007	-1.4526
H	-7.8961	1.2782	0.2363	H	-8.1619	1.3618	-0.3555

Continued table S4.

1-E				1-F			1-G		
C	-10.1369	1.5903	2.6744	C	-10.4744	1.411	2.7294	C	-10.3408
C	-9.9568	0.1025	2.3043	C	-10.2539	-0.0422	2.2583	C	-10.194
C	-10.1233	-0.2672	0.8226	C	-10.1183	-0.2652	0.7442	C	-10.1685
C	-10.8698	0.8005	0.0138	C	-10.6504	0.9067	-0.0895	C	-10.7266
C	-11.2868	1.9451	0.6033	C	-11.1547	2.0087	0.5131	C	-11.1571
O	-11.0663	2.3351	1.8921	O	-11.2117	2.2592	1.8532	O	-11.1094
C	-11.167	0.5658	-1.4001	C	-10.6691	0.8099	-1.5499	C	-10.8458
C	-11.8421	1.4522	-2.1888	C	-11.1535	1.791	-2.3651	C	-11.3735
C	-12.3856	2.6989	-1.6184	C	-11.6298	3.0666	-1.8025	C	-11.8111
C	-12.0789	3.035	-0.1289	C	-11.7361	3.2031	-0.2544	C	-11.7619
C	-13.4474	3.2063	0.5913	C	-13.248	3.3141	0.0841	C	-13.2285
C	-11.2326	4.3395	-0.1299	C	-10.9328	4.4759	0.1467	C	-10.8741
O	-13.0784	3.4674	-2.2895	O	-11.931	4.0184	-2.5264	O	-12.2051
C	-12.0195	1.1455	-3.6263	C	-11.2116	1.5458	-3.8233	C	-11.5082
O	-12.23	-0.0081	-4.0111	O	-10.2758	0.9833	-4.3985	O	-10.6608
C	-11.7948	2.2394	-4.6976	C	-12.504	1.8703	-4.623	C	-12.7972
C	-13.1078	2.5414	-5.459	C	-13.6986	1.0354	-4.0985	C	-13.4974
C	-10.6339	1.8604	-5.655	C	-12.3237	1.7241	-6.1607	C	-12.58
C	-10.167	3.018	-6.5534	C	-13.4845	2.3026	-6.9878	C	-11.6528
O	-10.7316	-0.6177	-1.9118	O	-10.1855	-0.3473	-2.0787	O	-10.4068
C	-8.7541	2.2444	2.5253	C	-9.0765	2.0197	2.9242	C	-8.9164
C	-7.7385	1.1076	2.6835	C	-8.1393	0.833	3.1738	C	-7.9986
C	-8.4462	-0.1792	2.2161	C	-8.7639	-0.3771	2.4518	C	-8.7044
C	-10.7001	1.7539	4.0953	C	-11.3098	1.4659	4.0185	C	-11.0871
C	-8.595	-0.5034	0.7048	C	-8.6055	-0.5587	0.9179	C	-8.6554
C	-8.2429	-1.9702	0.3802	C	-8.2319	-2.0052	0.5316	C	-8.3466
C	-7.8452	0.4215	-0.2838	C	-7.6441	0.4158	0.1959	C	-7.72
H	-8.0959	-1.0182	2.8214	H	-8.5637	-1.2803	3.0325	H	-8.4907
H	-10.5193	-0.5375	2.9851	H	-10.9585	-0.7188	2.7433	H	-10.8825
H	-10.6933	-1.192	0.703	H	-10.6738	-1.148	0.4184	H	-10.7677
H	-14.0631	3.9793	0.1268	H	-13.7213	4.1546	-0.4278	H	-13.2741
H	-14.0283	2.2819	0.5898	H	-13.7968	2.4112	-0.1907	H	-13.7165
									4.2233
									-0.2611

H	-13.3168	3.5012	1.6334	H	-13.4043	3.4716	1.1523	H	-13.8369	2.4989	0.0744
H	-11.0305	4.6837	0.8853	H	-11.0101	4.6798	1.2154	H	-11.2502	5.3305	-0.4932
H	-10.2668	4.2002	-0.6195	H	-9.8706	4.3776	-0.0856	H	-10.8396	4.7044	1.0852
H	-11.7433	5.1598	-0.6387	H	-11.2967	5.3707	-0.3624	H	-9.844	4.2899	-0.3001
H	-11.4941	3.1445	-4.1708	H	-12.7224	2.9207	-4.441	H	-13.4893	2.1774	-3.7896
H	-13.4332	1.6883	-6.0567	H	-13.5573	-0.0304	-4.2848	H	-14.4207	0.8403	-5.6619
H	-12.9951	3.3919	-6.1306	H	-14.6331	1.3307	-4.5748	H	-13.7609	-0.179	-4.394
H	-13.9209	2.7907	-4.775	H	-13.8478	1.1664	-3.0256	H	-12.8651	0.0518	-5.8892
H	-9.7731	1.5193	-5.0753	H	-11.4099	2.2377	-6.469	H	-13.5521	3.2277	-5.9674
H	-10.9255	1.0123	-6.279	H	-12.175	0.6748	-6.424	H	-12.195	3.8108	-5.0733
H	-9.3079	2.7207	-7.1557	H	-13.2635	2.251	-8.0544	H	-12.015	1.7402	-7.3361
H	-10.9495	3.3356	-7.2428	H	-14.4129	1.7555	-6.8248	H	-11.5877	3.4404	-7.4494
H	-9.8703	3.885	-5.962	H	-13.6637	3.3497	-6.7402	H	-10.6382	2.3691	-6.435
H	-11.0977	-0.6806	-2.8062	H	-10.1577	-0.2199	-3.0375	H	-10.4482	-0.3671	-2.9775
H	-8.6634	2.6935	1.5378	H	-8.7765	2.5504	2.0222	H	-8.6624	2.5416	1.8702
H	-8.5851	3.049	3.2413	H	-9.0395	2.7502	3.7326	H	-8.8047	2.8095	3.5855
H	-7.482	1.0064	3.7397	H	-8.106	0.6272	4.2453	H	-7.8994	0.6787	4.1147
H	-6.8038	1.2965	2.1542	H	-7.1124	1.0308	2.864	H	-6.9896	1.0019	2.6566
H	-10.066	1.2615	4.8322	H	-10.8476	0.8833	4.8153	H	-10.5904	1.0415	4.8539
H	-10.7776	2.8057	4.3712	H	-11.4197	2.4902	4.3749	H	-11.1435	2.6484	4.3901
H	-11.6986	1.3232	4.1704	H	-12.3115	1.07	3.851	H	-12.1087	1.2388	3.9803
H	-8.5447	-2.2301	-0.6355	H	-8.3234	-2.1592	-0.5445	H	-8.5148	-2.2672	-0.5428
H	-7.1705	-2.1488	0.4638	H	-7.2048	-2.2383	0.814	H	-7.3092	-2.3299	0.74
H	-8.7435	-2.667	1.0535	H	-8.8786	-2.736	1.0185	H	-8.9776	-2.772	1.0743
H	-6.7655	0.3486	-0.1534	H	-6.6162	0.2804	0.5319	H	-6.6757	0.161	0.3266
H	-8.0679	0.1492	-1.3159	H	-7.6593	0.2501	-0.8819	H	-7.8107	0.1071	-1.0135
H	-8.1216	1.4672	-0.1755	H	-7.9071	1.4594	0.3494	H	-7.9462	1.3674	0.1833

Continued table S4.

1-H			1-I			1-J					
C	-10.0278	1.6192	2.5466	C	-10.5583	1.3543	2.7642	C	-10.2502	1.4059	2.7188
C	-9.8493	0.1347	2.1626	C	-10.1169	-0.0385	2.2644	C	-9.7393	0.0672	2.1435
C	-10.1123	-0.2371	0.6954	C	-10.1146	-0.3135	0.7517	C	-9.9927	-0.243	0.6594
C	-10.9274	0.82	-0.0585	C	-10.677	0.8367	-0.0866	C	-10.8494	0.8052	-0.0536
C	-11.3201	1.9584	0.5591	C	-10.9864	2.0212	0.485	C	-11.1907	1.956	0.5662
O	-11.0219	2.3485	1.832	O	-10.8991	2.3516	1.8025	O	-10.8893	2.3303	1.8395
C	-11.3091	0.5851	-1.4514	C	-10.8601	0.6603	-1.5287	C	-11.2574	0.5825	-1.4417
C	-12.0334	1.4706	-2.1947	C	-11.3031	1.6478	-2.3583	C	-11.9297	1.5058	-2.1865
C	-12.5514	2.7114	-1.5926	C	-11.5615	3.0025	-1.8436	C	-12.3744	2.7763	-1.5897
C	-12.1673	3.0418	-0.1199	C	-11.4872	3.2378	-0.3058	C	-11.9867	3.0792	-0.1122
C	-13.4956	3.1887	0.6762	C	-12.9287	3.5729	0.1673	C	-13.3139	3.2785	0.6744
C	-11.34	4.3581	-0.1592	C	-10.4883	4.4099	-0.0738	C	-11.1033	4.3592	-0.1362
O	-13.2785	3.4809	-2.2252	O	-11.8239	3.9408	-2.6005	O	-13.0497	3.5873	-2.2289

C	-12.2767	1.1722	-3.6233	C	-11.5246	1.3367	-3.7841	C	-12.2024	1.2152	-3.6077
O	-12.5724	0.0281	-3.9791	O	-10.7145	0.6538	-4.4158	O	-12.5625	0.0929	-3.9723
C	-12.0279	2.2617	-4.7048	C	-12.8495	1.7449	-4.476	C	-11.8853	2.2748	-4.69
C	-12.3041	1.7751	-6.1502	C	-13.8727	0.5902	-4.4001	C	-13.1418	2.6123	-5.5236
C	-10.6305	2.9364	-4.5946	C	-12.6629	2.2247	-5.9405	C	-10.7029	1.86	-5.6044
C	-9.4181	1.9898	-4.7016	C	-11.7871	3.4824	-6.0874	C	-9.364	1.6586	-4.8688
O	-10.8988	-0.594	-1.9936	O	-10.5701	-0.5741	-2.0244	O	-10.9249	-0.6234	-1.979
C	-8.6697	2.2961	2.3016	C	-9.3118	1.8884	3.4798	C	-8.9677	2.1066	3.1827
C	-7.6269	1.1764	2.387	C	-8.1385	1.3494	2.6592	C	-7.9138	1.6992	2.1511
C	-8.3441	-0.1221	1.9688	C	-8.5783	-0.0796	2.2816	C	-8.2334	0.2184	1.8624
C	-10.4924	1.7732	4.0037	C	-11.8015	1.3124	3.6637	C	-11.2852	1.2323	3.8391
C	-8.5923	-0.4491	0.4713	C	-8.5862	-0.5838	0.8169	C	-8.4585	-0.316	0.4259
C	-8.2408	-1.9104	0.1219	C	-8.2445	-2.0853	0.7113	C	-7.954	-1.7643	0.2523
C	-7.9279	0.4872	-0.5668	C	-7.7092	0.203	-0.187	C	-7.8999	0.5524	-0.7276
H	-7.9384	-0.955	2.5476	H	-8.1584	-0.7757	3.0112	H	-7.5969	-0.4035	2.4958
H	-10.3525	-0.5149	2.8798	H	-10.5798	-0.8243	2.8627	H	-9.9753	-0.755	2.8204
H	-10.6754	-1.1702	0.6137	H	-10.6948	-1.2037	0.4975	H	-10.4926	-1.2051	0.5233
H	-13.311	3.4781	1.7115	H	-12.951	3.8141	1.2309	H	-13.1252	3.5554	1.7124
H	-14.1467	3.9558	0.252	H	-13.3408	4.4378	-0.3568	H	-13.9284	4.0745	0.2488
H	-14.0628	2.2561	0.6999	H	-13.6147	2.7378	0.0131	H	-13.9201	2.3706	0.6891
H	-11.8895	5.1745	-0.6327	H	-9.4779	4.1543	-0.399	H	-11.6126	5.2016	-0.6089
H	-11.0861	4.6989	0.8454	H	-10.426	4.6814	0.9808	H	-10.8427	4.6825	0.8725
H	-10.4015	4.235	-0.703	H	-10.7838	5.3157	-0.607	H	-10.1663	4.1987	-0.6729
H	-12.7699	3.0354	-4.5116	H	-13.2741	2.5816	-3.9245	H	-11.5862	3.1891	-4.1788
H	-12.1703	2.5798	-6.8735	H	-14.0644	0.2889	-3.3687	H	-12.937	3.4034	-6.2454
H	-13.329	1.4157	-6.2574	H	-13.5281	-0.2911	-4.9443	H	-13.9572	2.9638	-4.8885
H	-11.6417	0.9578	-6.4388	H	-14.831	0.8848	-4.8294	H	-13.506	1.7458	-6.0783
H	-10.5481	3.7052	-5.3649	H	-12.2468	1.4195	-6.5502	H	-10.9577	0.9509	-6.1543
H	-10.5661	3.4876	-3.6547	H	-13.6414	2.4438	-6.3708	H	-10.5586	2.6297	-6.3646
H	-8.4837	2.5488	-4.6441	H	-11.7412	3.8096	-7.1264	H	-9.0789	2.5529	-4.3133
H	-9.4039	1.2543	-3.8966	H	-12.1813	4.3101	-5.496	H	-9.4082	0.8286	-4.1627
H	-9.4154	1.4478	-5.6476	H	-10.7633	3.3012	-5.7576	H	-8.5619	1.4394	-5.5743
H	-11.3192	-0.6562	-2.8635	H	-10.6202	-0.5021	-2.9879	H	-11.3533	-0.6648	-2.846
H	-8.6557	2.7463	1.3105	H	-9.3045	2.9767	3.5521	H	-8.6793	1.7497	4.1724
H	-8.4643	3.1036	3.0047	H	-9.265	1.5	4.4981	H	-9.0843	3.1886	3.2547
H	-7.2954	1.0795	3.4226	H	-7.1982	1.3637	3.2121	H	-6.895	1.8425	2.5137
H	-6.7347	1.3807	1.7938	H	-8.003	1.9841	1.7846	H	-8.0286	2.3261	1.2681
H	-9.8	1.2912	4.6936	H	-12.6734	0.9806	3.0999	H	-10.9087	0.5932	4.6374
H	-10.5678	2.8234	4.2859	H	-11.6661	0.6311	4.5033	H	-11.5519	2.1929	4.2799
H	-11.4759	1.3258	4.1482	H	-12.0264	2.299	4.0691	H	-12.1991	0.7818	3.4519
H	-8.6085	-2.1752	-0.8705	H	-8.4482	-2.4638	-0.2914	H	-8.2976	-2.1883	-0.6922
H	-7.1626	-2.0722	0.1305	H	-7.1915	-2.2686	0.9272	H	-6.8646	-1.8087	0.2594
H	-8.6825	-2.6146	0.8279	H	-8.8304	-2.6849	1.4088	H	-8.3128	-2.4169	1.0492

H	-6.8408	0.4315	-0.512	H	-7.8081	-0.2054	-1.1934	H	-6.8155	0.6425	-0.6638
H	-8.2175	0.2111	-1.5812	H	-7.9829	1.2546	-0.2574	H	-8.1373	0.1116	-1.6964
H	-8.2126	1.5285	-0.4389	H	-6.6551	0.1533	0.0861	H	-8.3148	1.5591	-0.7408

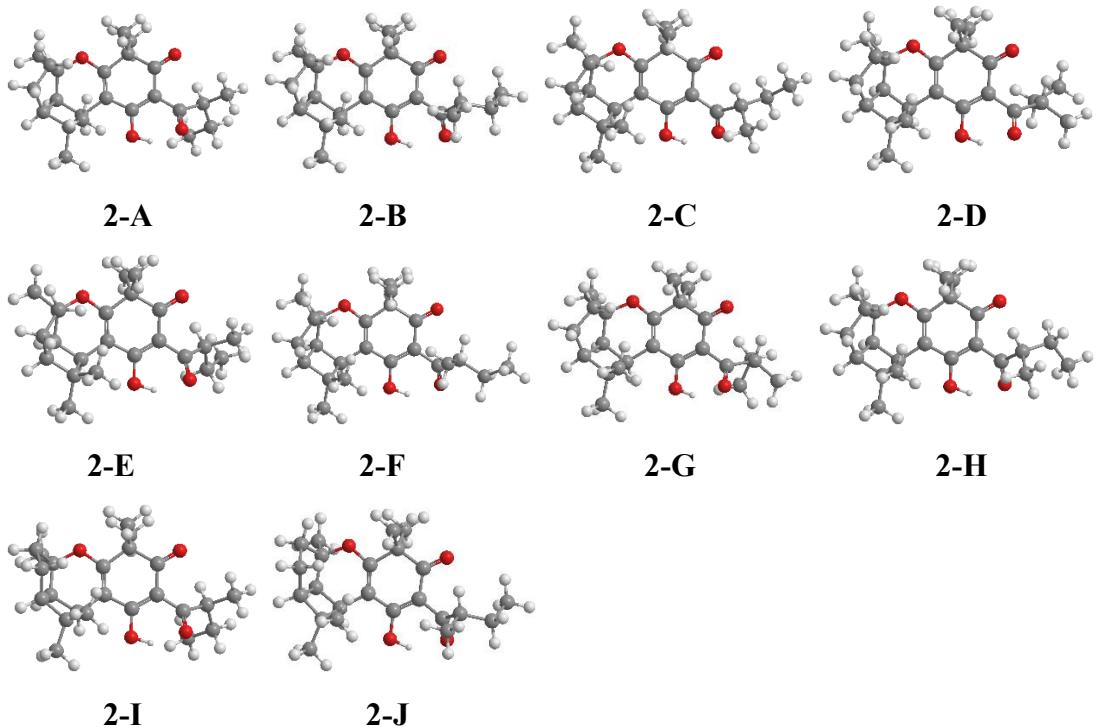


Figure S5. Conformers of isomer 2 for NMR calculation.

Table S5. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **2** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	ΔG (kcal/mol)	%	Number of imaginary frequencies
2-A	-1196.706294	0	21.47%	0
2-B	-1196.706287	0.004078812	21.32%	0
2-C	-1196.705759	0.335592081	12.18%	0
2-D	-1196.705758	0.335968586	12.17%	0
2-E	-1196.705247	0.656751443	7.08%	0
2-F	-1196.705245	0.657818209	7.07%	0
2-G	-1196.704507	1.12092022	3.23%	0
2-H	-1196.704502	1.124183269	3.22%	0
2-I	-1196.704435	1.166351908	2.99%	0
2-J	-1196.704434	1.166916666	2.99%	0

Table S6. Optimized Z-matrixes of isomer **2** in the gas phase (\AA) at B3LYP/6-31G* level.

2-A				2-B			
C	-1.9856	5.9803	-0.1638	C	-2.0825	5.679	-0.1887
C	-1.4892	6.3813	1.2417	C	-1.4884	5.9644	1.2073

C	-2.5657	6.6973	2.2913	C	-2.4534	6.5057	2.2729
C	-3.9402	6.9907	1.678	C	-3.7391	7.0935	1.6799
C	-4.123	6.9357	0.338	C	-3.9523	7.0784	0.3432
O	-3.203	6.5763	-0.6033	O	-3.1539	6.5183	-0.611
C	-5.0517	7.389	2.543	C	-4.7318	7.7078	2.5626
C	-6.2922	7.714	2.0766	C	-5.8933	8.2655	2.116
C	-6.6045	7.6155	0.6398	C	-6.1805	8.3587	0.6746
C	-5.4567	7.2549	-0.3493	C	-5.191	7.6896	-0.3249
C	-5.2504	8.4899	-1.2696	C	-4.7142	8.7985	-1.3067
C	-5.9146	5.9898	-1.1327	C	-5.9763	6.5525	-1.0372
O	-7.7469	7.8041	0.214	O	-7.1715	8.9597	0.2517
C	-7.3188	8.1782	3.034	C	-6.8607	8.7817	3.1031
O	-7.4233	7.6697	4.1535	O	-6.4839	9.4514	4.068
C	-8.1874	9.4181	2.7106	C	-8.3515	8.3689	3.0205
C	-9.6864	9.0461	2.6597	C	-8.6069	7.1088	3.8767
C	-7.9417	10.5968	3.6889	C	-9.3344	9.508	3.4028
C	-6.5007	11.1413	3.6856	C	-9.2607	10.7411	2.4838
O	-4.7835	7.4388	3.8764	O	-4.437	7.7061	3.8916
C	-2.1802	4.456	-0.1355	C	-2.5955	4.2306	-0.1533
C	-1.2595	3.9416	0.9765	C	-1.7897	3.5321	0.9475
C	-1.119	5.0906	1.9943	C	-1.3925	4.6248	1.9592
C	-0.9952	6.413	-1.2568	C	-1.0416	5.8933	-1.2993
C	-2.2367	5.3759	3.0335	C	-2.4085	5.1434	3.0128
C	-1.6758	5.6137	4.4512	C	-1.7907	5.2523	4.4225
C	-3.3894	4.3467	3.1181	C	-3.7553	4.3877	3.1139
H	-0.1109	5.0725	2.4145	H	-0.4057	4.392	2.3656
H	-0.7022	7.1335	1.1756	H	-0.5591	6.5294	1.1254
H	-2.3021	7.5778	2.8822	H	-1.9946	7.3073	2.8571
H	-4.9175	9.3663	-0.7101	H	-4.1602	9.5872	-0.7938
H	-4.4981	8.2935	-2.0348	H	-4.0571	8.3945	-2.0779
H	-6.166	8.7655	-1.797	H	-5.5481	9.2722	-1.8287
H	-6.8618	6.1475	-1.6526	H	-6.8742	6.924	-1.5356
H	-5.189	5.7067	-1.8962	H	-5.3709	6.0729	-1.8076
H	-6.0425	5.1274	-0.4756	H	-6.2867	5.7713	-0.3407
H	-7.907	9.7669	1.7173	H	-8.5694	8.1012	1.9882
H	-9.8777	8.2569	1.9303	H	-9.6389	6.7697	3.7796
H	-10.05	8.6951	3.6271	H	-7.9682	6.2781	3.5715
H	-10.2966	9.9017	2.3692	H	-8.423	7.2966	4.9362
H	-8.6136	11.4169	3.4297	H	-10.3551	9.1237	3.3693
H	-8.2182	10.303	4.7042	H	-9.1695	9.8161	4.4376
H	-6.4105	12.0066	4.343	H	-10.0131	11.4808	2.7585
H	-5.784	10.396	4.0324	H	-8.2873	11.2296	2.5425
H	-6.1982	11.4544	2.6856	H	-9.4291	10.4679	1.4411

H	-5.6285	7.6035	4.3193	H	-5.1126	8.247	4.324
H	-3.2172	4.2212	0.0983	H	-3.6555	4.2213	0.0946
H	-1.9707	3.9827	-1.0949	H	-2.504	3.7238	-1.1141
H	-0.2781	3.7235	0.5513	H	-0.8835	3.1101	0.509
H	-1.6153	3.0142	1.4271	H	-2.328	2.7018	1.406
H	-1.3249	6.0832	-2.242	H	-1.4499	5.6415	-2.2781
H	-0.0036	5.9969	-1.0802	H	-0.1573	5.277	-1.138
H	-0.9024	7.4986	-1.2908	H	-0.7221	6.9348	-1.3378
H	-2.446	6.0072	5.1161	H	-2.4481	5.8031	5.0968
H	-1.3001	4.6887	4.8895	H	-1.6183	4.2675	4.8575
H	-0.8544	6.3311	4.4483	H	-0.8335	5.7749	4.4073
H	-3.0292	3.3744	3.4542	H	-3.6089	3.3596	3.4447
H	-4.1521	4.6738	3.8254	H	-4.4186	4.8701	3.8324
H	-3.8956	4.2009	2.1671	H	-4.294	4.3581	2.1702

Continued table S6.

2-C				2-D			
C	-2.073	5.6567	-0.2065	C	-1.9398	6.0656	-0.1325
C	-1.4575	5.9273	1.1831	C	-1.4673	6.3422	1.3106
C	-2.4012	6.4784	2.2627	C	-2.5614	6.5782	2.363
C	-3.6855	7.0881	1.6882	C	-3.9226	6.9317	1.7516
C	-3.9144	7.0822	0.3542	C	-4.0805	6.9909	0.4088
O	-3.1361	6.5145	-0.612	O	-3.1434	6.7094	-0.5422
C	-4.6572	7.7151	2.5856	C	-5.0474	7.2663	2.6265
C	-5.8142	8.2984	2.1572	C	-6.2822	7.6226	2.1669
C	-6.1191	8.3932	0.7179	C	-6.5733	7.6186	0.7221
C	-5.1509	7.7151	-0.2961	C	-5.4008	7.3717	-0.273
C	-4.6693	8.8223	-1.2775	C	-5.1853	8.6985	-1.0516
C	-5.9606	6.5932	-1.0057	C	-5.8284	6.1926	-1.1967
O	-7.1109	9.0012	0.3078	O	-7.7155	7.7966	0.2934
C	-6.7613	8.8348	3.1587	C	-7.3184	8.0341	3.1421
O	-6.3584	9.4187	4.1683	O	-7.4417	7.429	4.2106
C	-8.2775	8.5545	3.0322	C	-8.1725	9.3099	2.8935
C	-8.7957	7.7384	4.2413	C	-9.2976	9.4996	3.9445
C	-9.071	9.871	2.8244	C	-7.2781	10.5744	2.7717
C	-10.5356	9.6543	2.4093	C	-8.0138	11.8061	2.2178
O	-4.3456	7.6967	3.9103	O	-4.7963	7.2266	3.9636
C	-2.608	4.2164	-0.1703	C	-2.1479	4.5463	-0.2359
C	-1.7991	3.5009	0.9172	C	-1.2525	3.9312	0.8452
C	-1.3726	4.5831	1.9283	C	-1.1211	4.9894	1.9582
C	-1.0425	5.8592	-1.3289	C	-0.925	6.5784	-1.1668
C	-2.3673	5.1125	2.9966	C	-2.2551	5.1971	2.9983
C	-1.7302	5.2064	4.3988	C	-1.7179	5.3118	4.4403

C	-3.7237	4.3764	3.1118	C	-3.4166	4.1746	2.9772
H	-0.3844	4.3336	2.3213	H	-0.1209	4.9264	2.3928
H	-0.5208	6.4786	1.0921	H	-0.6737	7.0902	1.3227
H	-1.9233	7.2706	2.8444	H	-2.3031	7.4044	3.0299
H	-4.0277	8.4126	-2.0587	H	-4.4133	8.5891	-1.8146
H	-5.5022	9.3112	-1.787	H	-6.0913	9.0214	-1.5686
H	-4.0972	9.5996	-0.7672	H	-4.874	9.5132	-0.3949
H	-6.8587	6.9801	-1.4918	H	-6.7648	6.3971	-1.7198
H	-5.371	6.1093	-1.7855	H	-5.0835	5.9968	-1.969
H	-6.2743	5.8126	-0.3099	H	-5.963	5.2648	-0.6374
H	-8.4141	7.9376	2.1445	H	-8.6712	9.1593	1.9381
H	-9.8315	7.4304	4.1011	H	-9.9667	10.317	3.6775
H	-8.214	6.8272	4.3899	H	-9.9171	8.6049	4.0287
H	-8.747	8.3147	5.1669	H	-8.8932	9.7115	4.9354
H	-9.034	10.4787	3.7311	H	-6.8421	10.8181	3.7428
H	-8.5918	10.4712	2.0469	H	-6.4332	10.3788	2.1082
H	-11.0267	10.6071	2.2093	H	-7.3257	12.6406	2.079
H	-10.6026	9.0541	1.5009	H	-8.4695	11.5916	1.2501
H	-11.1089	9.1518	3.1883	H	-8.801	12.1465	2.8904
H	-5.0115	8.2397	4.3565	H	-5.6476	7.3554	4.4062
H	-3.6647	4.2224	0.0912	H	-3.191	4.3029	-0.0411
H	-2.5368	3.7123	-1.1343	H	-1.9247	4.153	-1.2279
H	-0.905	3.067	0.4655	H	-0.2652	3.7398	0.4206
H	-2.3443	2.6769	1.3791	H	-1.6244	2.9729	1.2097
H	-1.4668	5.6179	-2.3036	H	-1.2387	6.3358	-2.1822
H	-0.7071	6.8957	-1.3674	H	-0.8219	7.6619	-1.1078
H	-0.1661	5.2285	-1.181	H	0.0595	6.1387	-1.0078
H	-2.3708	5.7642	5.0835	H	-2.4969	5.6559	5.1221
H	-1.5672	4.2174	4.8278	H	-1.3571	4.3504	4.8069
H	-0.7656	5.7147	4.3736	H	-0.8912	6.0196	4.511
H	-3.5883	3.3447	3.436	H	-3.07	3.1751	3.2396
H	-4.3704	4.8651	3.8411	H	-4.1905	4.4501	3.6945
H	-4.2751	4.3593	2.1751	H	-3.9053	4.1111	2.0082

Continued table S6.

2-E				2-F				2-G			
C	-1.9641	5.8988	-0.1988	C	-2.1507	5.5303	-0.2105	C	-1.9645	6.0816	-0.1253
C	-1.4388	6.2571	1.2077	C	-1.4942	5.9035	1.136	C	-1.5078	6.4434	1.304
C	-2.4922	6.5919	2.2747	C	-2.4003	6.5556	2.1911	C	-2.6137	6.6958	2.3402
C	-3.8622	6.9444	1.6825	C	-3.6898	7.139	1.6016	C	-3.9819	6.9775	1.7078
C	-4.061	6.9195	0.3441	C	-3.956	7.0271	0.2792	C	-4.1351	6.9661	0.3632
O	-3.1644	6.5449	-0.6138	O	-3.2151	6.3661	-0.6566	O	-3.1866	6.6643	-0.57
C	-4.9497	7.3662	2.567	C	-4.6286	7.8513	2.4696	C	-5.1209	7.3176	2.5617

C	-6.1843	7.7426	2.1223	C	-5.7827	8.4252	2.0223	C	-6.3609	7.6241	2.0809
C	-6.5138	7.6786	0.6862	C	-6.1139	8.4268	0.5869	C	-6.6408	7.5642	0.6354
C	-5.3897	7.297	-0.322	C	-5.1999	7.6273	-0.3884	C	-5.4621	7.2761	-0.3409
C	-5.1502	8.5408	-1.2223	C	-4.727	8.6196	-1.4904	C	-5.2708	8.5534	-1.2049
C	-5.8993	6.063	-1.1231	C	-6.0619	6.4646	-0.9549	C	-5.8666	6.032	-1.1853
O	-7.6528	7.9112	0.2746	O	-7.0827	9.0515	0.1487	O	-7.7787	7.7329	0.1909
C	-7.1862	8.2228	3.1016	C	-6.7057	9.0333	3.0052	C	-7.4169	8.0357	3.0344
O	-7.2705	7.72	4.2256	O	-6.2669	9.7242	3.9287	O	-7.5314	7.4624	4.1213
C	-8.0544	9.4671	2.796	C	-8.2221	8.6964	2.9667	C	-8.3079	9.2759	2.7379
C	-9.5506	9.0832	2.6995	C	-8.4526	7.181	3.19	C	-9.3579	9.5632	3.8414
C	-7.8039	10.5975	3.8294	C	-9.0651	9.563	3.9444	C	-7.4936	10.554	2.3885
C	-8.4069	11.9532	3.4249	C	-10.5845	9.4538	3.7309	C	-6.5084	11.0372	3.4713
O	-4.6628	7.3822	3.8973	O	-4.2916	7.9214	3.7865	O	-4.8794	7.3332	3.9011
C	-2.2119	4.382	-0.195	C	-2.701	4.105	-0.0441	C	-2.1225	4.5531	-0.1553
C	-1.298	3.8159	0.8974	C	-1.8729	3.4688	1.0776	C	-1.2132	4.0209	0.9577
C	-1.1062	4.941	1.9334	C	-1.4073	4.6234	1.9862	C	-1.122	5.1356	2.0183
C	-0.971	6.3162	-1.2953	C	-1.1491	5.6279	-1.3724	C	-0.9621	6.5767	-1.1803
C	-2.202	5.2467	2.99	C	-2.3677	5.2525	3.0316	C	-2.2679	5.357	3.0424
C	-1.6179	5.4394	4.4052	C	-1.6947	5.448	4.4063	C	-1.7428	5.5573	4.4795
C	-3.3893	4.2572	3.0696	C	-3.7311	4.5498	3.2377	C	-3.3965	4.2983	3.0656
H	-0.0949	4.8801	2.3417	H	-0.4127	4.3924	2.3741	H	-0.1228	5.1262	2.4595
H	-0.6266	6.9823	1.1457	H	-0.5528	6.4306	0.9758	H	-0.7383	7.216	1.2819
H	-2.191	7.4519	2.8779	H	-1.8954	7.3836	2.6949	H	-2.3844	7.5607	2.9675
H	-4.4141	8.3323	-1.9999	H	-4.1184	9.427	-1.0786	H	-4.4965	8.4095	-1.9598
H	-6.0614	8.8582	-1.7337	H	-4.1244	8.1184	-2.249	H	-6.182	8.8252	-1.7419
H	-4.7801	9.3945	-0.6512	H	-5.5654	9.0795	-2.0176	H	-4.9753	9.4147	-0.6027
H	-6.8455	6.2629	-1.63	H	-5.5122	5.8893	-1.7011	H	-6.8065	6.1845	-1.7198
H	-5.1918	5.7689	-1.8995	H	-6.3702	5.7661	-0.1746	H	-5.117	5.8007	-1.9432
H	-6.0506	5.1936	-0.4804	H	-6.9666	6.8274	-1.4472	H	-5.9837	5.14	-0.5669
H	-7.7388	9.8453	1.8243	H	-8.5665	8.9448	1.9647	H	-8.8846	9.0146	1.8518
H	-10.1588	9.9228	2.3646	H	-9.5	6.9117	3.0569	H	-9.9958	10.406	3.574
H	-9.7135	8.2759	1.9832	H	-7.8881	6.5739	2.4805	H	-10.0119	8.7038	3.9982
H	-9.945	8.7513	3.6613	H	-8.1592	6.8732	4.1949	H	-8.8901	9.7939	4.7995
H	-8.1946	10.3043	4.8066	H	-8.8222	9.3082	4.9781	H	-6.9456	10.3935	1.4583
H	-6.7298	10.7382	3.97	H	-8.7892	10.6139	3.8273	H	-8.1887	11.3629	2.1566
H	-8.1453	12.7264	4.148	H	-11.1181	10.1463	4.3828	H	-6.0006	11.9487	3.1544
H	-8.0394	12.2762	2.4501	H	-10.858	9.6946	2.7028	H	-7.0196	11.2588	4.4084
H	-9.4951	11.9131	3.3753	H	-10.9558	8.4532	3.9516	H	-5.7379	10.2943	3.6802
H	-5.4959	7.5683	4.3545	H	-4.9345	8.5126	4.2031	H	-5.7372	7.4591	4.3319
H	-3.254	4.1794	0.0463	H	-3.7506	4.1464	0.2416	H	-3.1581	4.2856	0.0472
H	-2.0294	3.9188	-1.1648	H	-2.6602	3.5236	-0.9654	H	-1.8813	4.1196	-1.1261
H	-0.3295	3.5713	0.4573	H	-0.9961	2.9871	0.6408	H	-0.218	3.8413	0.5467
H	-1.6813	2.8936	1.3357	H	-2.4158	2.6928	1.6186	H	-1.5557	3.0698	1.3673

H	-1.3228	6.0159	-2.2824	H	-0.2761	4.9997	-1.197	H	-1.263	6.2749	-2.1837
H	-0.8404	7.3982	-1.3113	H	-0.8036	6.6534	-1.5035	H	-0.8949	7.6646	-1.1737
H	0.0073	5.8625	-1.1375	H	-1.6025	5.3143	-2.3129	H	0.0354	6.1777	-0.9971
H	-2.3666	5.8479	5.0855	H	-2.3101	6.0688	5.059	H	-2.5361	5.9089	5.1407
H	-1.2704	4.4942	4.8231	H	-1.5349	4.4939	4.9094	H	-1.3542	4.6264	4.8933
H	-0.7718	6.1276	4.4055	H	-0.7239	5.9371	4.3176	H	-0.9391	6.2934	4.5197
H	-3.0599	3.2671	3.3845	H	-3.6022	3.5447	3.6393	H	-3.0199	3.3236	3.3756
H	-4.1324	4.598	3.7912	H	-4.3522	5.1046	3.9415	H	-4.182	4.5821	3.7667
H	-3.9105	4.1463	2.1221	H	-4.3065	4.4679	2.3191	H	-3.8786	4.1742	2.0992

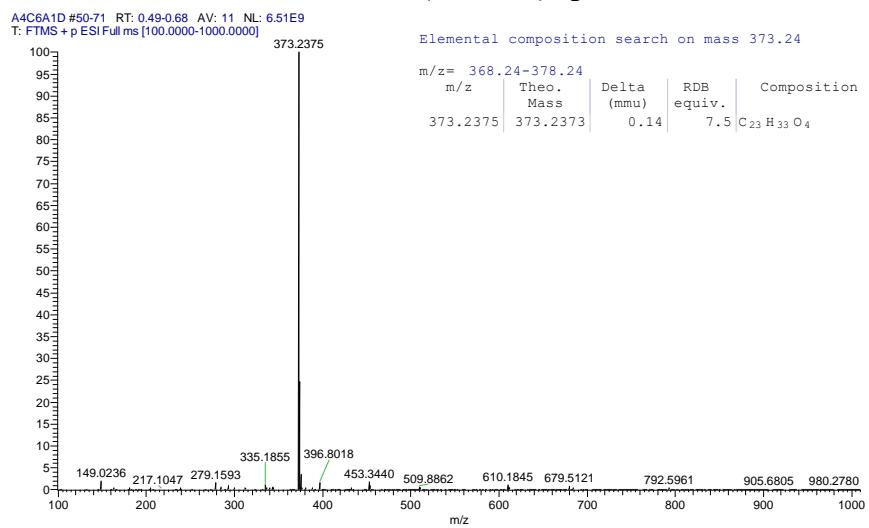
Continued table S6.

2-H				2-I				2-J			
C	-2.0497	5.6651	-0.2034	C	-1.8434	6.2127	-0.1505	C	-1.8859	5.8527	-0.1742
C	-1.4585	5.9828	1.1867	C	-1.4684	6.2733	1.3461	C	-1.4889	5.8553	1.3179
C	-2.4326	6.5186	2.2469	C	-2.5665	6.6055	2.3695	C	-2.478	6.4322	2.3437
C	-3.7325	7.0707	1.6493	C	-3.9159	6.9544	1.7375	C	-3.7243	7.0592	1.7153
C	-3.9475	7.0319	0.3141	C	-4.1119	6.8166	0.408	C	-3.9618	6.9443	0.3902
O	-3.1392	6.476	-0.6343	O	-3.205	6.417	-0.5248	O	-3.1792	6.3318	-0.5398
C	-4.7345	7.6797	2.5258	C	-5.0151	7.4193	2.5862	C	-4.6956	7.7485	2.5668
C	-5.9092	8.2135	2.0783	C	-6.2655	7.6987	2.1172	C	-5.8751	8.2542	2.1063
C	-6.2057	8.2605	0.634	C	-6.5984	7.4868	0.6981	C	-6.2021	8.2186	0.6713
C	-5.1996	7.6064	-0.3587	C	-5.4569	7.0827	-0.2812	C	-5.2197	7.4944	-0.2959
C	-4.7501	8.7176	-1.3506	C	-5.2756	8.2657	-1.2724	C	-4.7752	8.5398	-1.3592
C	-5.9557	6.4433	-1.0614	C	-5.9081	5.7693	-0.9858	C	-6.0012	6.3011	-0.9152
O	-7.2215	8.8088	0.2005	O	-7.7515	7.6185	0.2798	O	-7.2189	8.7583	0.2272
C	-6.8824	8.7396	3.0652	C	-7.2798	8.2331	3.051	C	-6.8193	8.849	3.0707
O	-6.4999	9.3173	4.0866	O	-7.3592	7.8204	4.2113	O	-6.4235	9.6126	3.9549
C	-8.3939	8.4281	2.9215	C	-8.1675	9.4331	2.6403	C	-8.3045	8.409	3.0756
C	-8.9413	7.6585	4.1472	C	-9.6628	9.0431	2.6457	C	-8.5084	7.2225	4.0436
C	-9.2574	9.6764	2.582	C	-7.9198	10.6917	3.513	C	-9.2945	9.5615	3.3938
C	-9.3139	10.783	3.6536	C	-6.4852	11.2479	3.4409	C	-9.2743	10.7118	2.3706
O	-4.4315	7.6961	3.8523	O	-4.7255	7.5774	3.9069	O	-4.3637	7.8694	3.8817
C	-2.5321	4.207	-0.1462	C	-1.5277	4.7634	-0.5392	C	-1.8858	4.3637	-0.54
C	-1.7092	3.5412	0.9622	C	-1.8834	3.9469	0.7048	C	-2.3933	3.6595	0.72
C	-1.3326	4.6563	1.9572	C	-1.4027	4.8291	1.8747	C	-1.7277	4.4393	1.8721
C	-1.016	5.8854	-1.3196	C	-1.0979	7.2456	-1.0071	C	-0.9509	6.6932	-1.0551
C	-2.3566	5.1683	3.006	C	-2.3323	5.2278	3.0479	C	-2.5426	5.0457	3.0417
C	-1.7377	5.3106	4.4123	C	-1.5715	5.3473	4.3855	C	-1.766	5.017	4.3753
C	-3.6867	4.3856	3.1219	C	-3.5881	4.3482	3.2609	C	-3.9574	4.4613	3.2712
H	-0.3401	4.4501	2.3641	H	-0.4006	4.505	2.1643	H	-0.8149	3.915	2.1636
H	-0.5416	6.5662	1.0945	H	-0.5411	6.8304	1.4862	H	-0.4623	6.2033	1.4398
H	-1.9895	7.3379	2.8184	H	-2.2884	7.4481	3.007	H	-2.0164	7.203	2.9655
H	-4.2151	9.5241	-0.8453	H	-4.5315	8.0336	-2.0355	H	-4.2219	9.3675	-0.9113

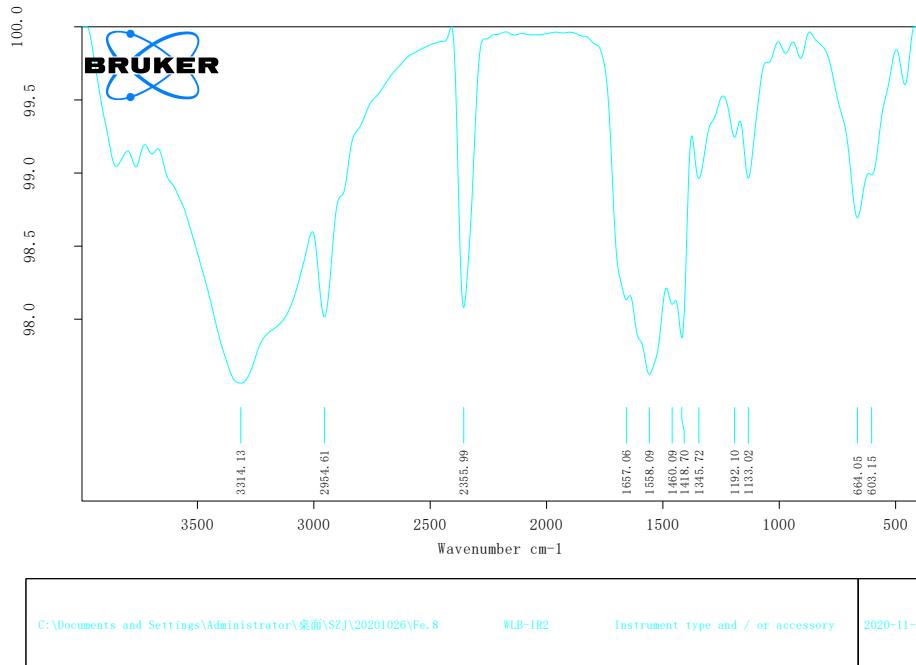
H	-4.0834	8.3224	-2.1181	H	-6.201	8.5018	-1.8019	H	-4.1275	8.0919	-2.114
H	-5.5953	9.166	-1.8769	H	-4.9448	9.1755	-0.7677	H	-5.6247	8.9675	-1.8958
H	-6.8621	6.7872	-1.5642	H	-6.8626	5.8854	-1.503	H	-5.4022	5.7774	-1.6615
H	-5.338	5.9718	-1.8269	H	-5.1874	5.4507	-1.7399	H	-6.2881	5.5654	-0.1614
H	-6.2472	5.661	-0.3579	H	-6.0177	4.9447	-0.2788	H	-6.9126	6.6253	-1.4217
H	-8.4867	7.7458	2.0771	H	-7.9071	9.701	1.617	H	-8.5516	8.0511	2.0778
H	-9.9964	7.4145	4.0202	H	-10.2873	9.8655	2.2958	H	-9.5366	6.8604	4.0109
H	-8.4089	6.7181	4.2973	H	-9.8568	8.1943	1.9873	H	-7.8648	6.3788	3.788
H	-8.8476	8.2362	5.0682	H	-10.0069	8.7697	3.6447	H	-8.2933	7.5026	5.0765
H	-8.9067	10.1179	1.6472	H	-8.6047	11.4807	3.1974	H	-10.3086	9.1602	3.4293
H	-10.2749	9.3476	2.3655	H	-8.1774	10.4809	4.5537	H	-9.1003	9.96	4.3921
H	-9.9642	11.5978	3.3344	H	-6.3945	12.1662	4.0219	H	-10.0304	11.4608	2.6072
H	-9.7022	10.4087	4.6007	H	-5.7552	10.5413	3.8376	H	-8.3085	11.2184	2.3532
H	-8.33	11.2128	3.8435	H	-6.2013	11.4789	2.4135	H	-9.4725	10.3472	1.3616
H	-5.1225	8.2205	4.2839	H	-5.5644	7.7731	4.3491	H	-5.0319	8.4425	4.2828
H	-3.591	4.1789	0.1048	H	-2.0778	4.4377	-1.4229	H	-2.5004	4.1477	-1.4147
H	-2.4323	3.6886	-1.1	H	-0.4661	4.6558	-0.7659	H	-0.8728	4.032	-0.7713
H	-0.7954	3.1319	0.5275	H	-1.4167	2.9609	0.707	H	-2.143	2.5979	0.7362
H	-2.229	2.7065	1.434	H	-2.9609	3.7891	0.7226	H	-3.4796	3.7308	0.7465
H	-1.4214	5.6115	-2.2937	H	-1.3196	7.1114	-2.066	H	-1.0255	7.7495	-0.7966
H	-0.1188	5.29	-1.1521	H	-1.3942	8.2582	-0.7335	H	-1.2085	6.5926	-2.1095
H	-0.7184	6.9327	-1.3735	H	-0.0184	7.1667	-0.881	H	0.0896	6.392	-0.9368
H	-2.4049	5.8569	5.0805	H	-2.193	5.8172	5.149	H	-2.2664	5.6213	5.1332
H	-1.5433	4.336	4.861	H	-1.2701	4.3683	4.7593	H	-1.6808	4.0016	4.7633
H	-0.7919	5.8531	4.3869	H	-0.6688	5.9513	4.2862	H	-0.7548	5.4103	4.2641
H	-3.5175	3.3656	3.4665	H	-3.3144	3.3207	3.5003	H	-3.9103	3.4021	3.5243
H	-4.3581	4.8637	3.8358	H	-4.194	4.728	4.0843	H	-4.4613	4.9741	4.0911
H	-4.2274	4.3315	2.1804	H	-4.2411	4.3217	2.3899	H	-4.6053	4.5651	2.4022

4. Spectral information of 1

4.1 HR-ESI-MS, IR and UV (CH₃OH) spectrum of 1b



HR-ESI-MS of compound 1b



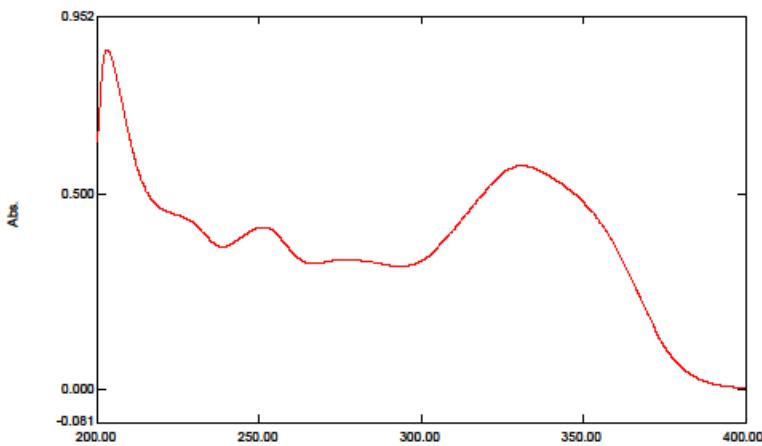
Page 1 of 1

IR spectrum of compound 1b

Spectrum Peak Pick Report

2020-11-02 19:44:46

Data Set: A4C6A1D 0.04mg ml - RawData



[Measurement Properties]
Wavelength Range (nm.): 200.00 to 400.00
Scan Speed: Medium
Sampling Interval: 0.5
Auto Sampling Interval: Disabled
Scan Mode: Single

No.	P/I/V	Wavelength	Abs.	Description
1	●	332.00	0.571	
2	●	276.50	0.332	
3	●	251.00	0.414	
4	●	203.00	0.866	

[Instrument Properties]
Instrument Type: UV-1600 Series
Measuring Mode: Absorbance
Slit Width: 2.0
Accumulation time: 0.1 sec.
Light Source Change Wavelength: 323.0 nm
Detector Unit: Direct
S/R Exchange: Normal
Stair Correction: OFF

[Attachment Properties]
Attachment: None

[Operation]
Threshold: 0.0010000
Points: 4
Interpolate: Disabled
Average: Disabled

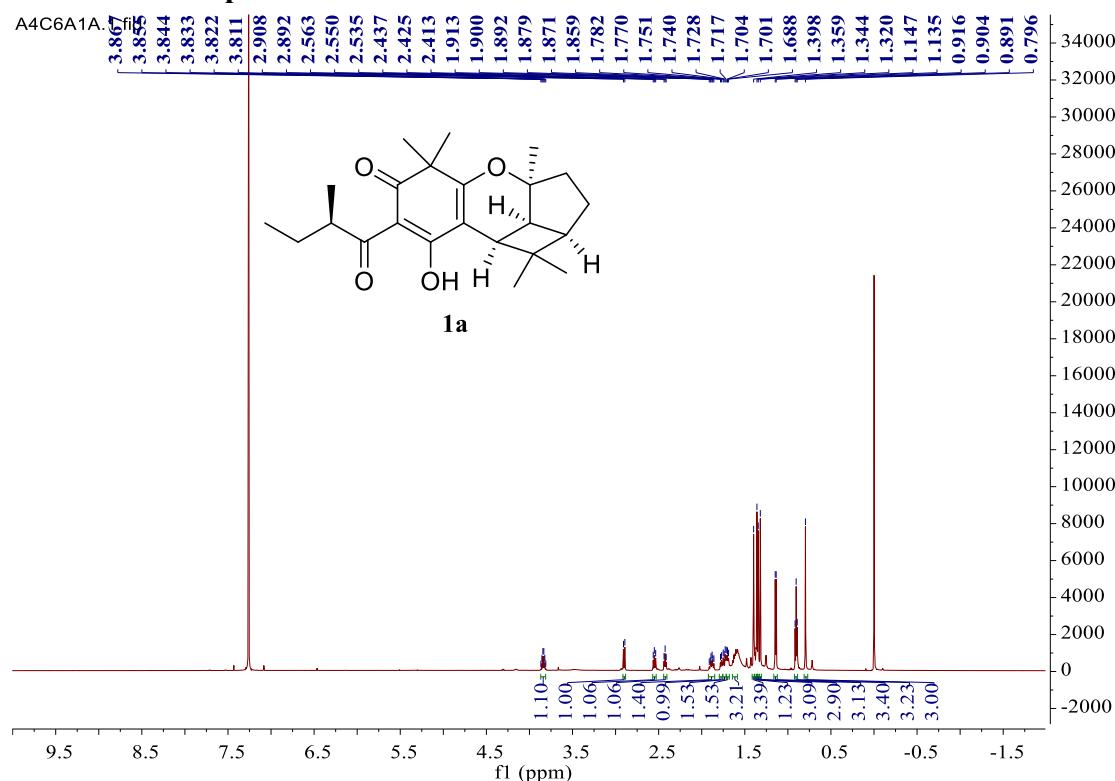
[Sample Preparation Properties]
Weight:
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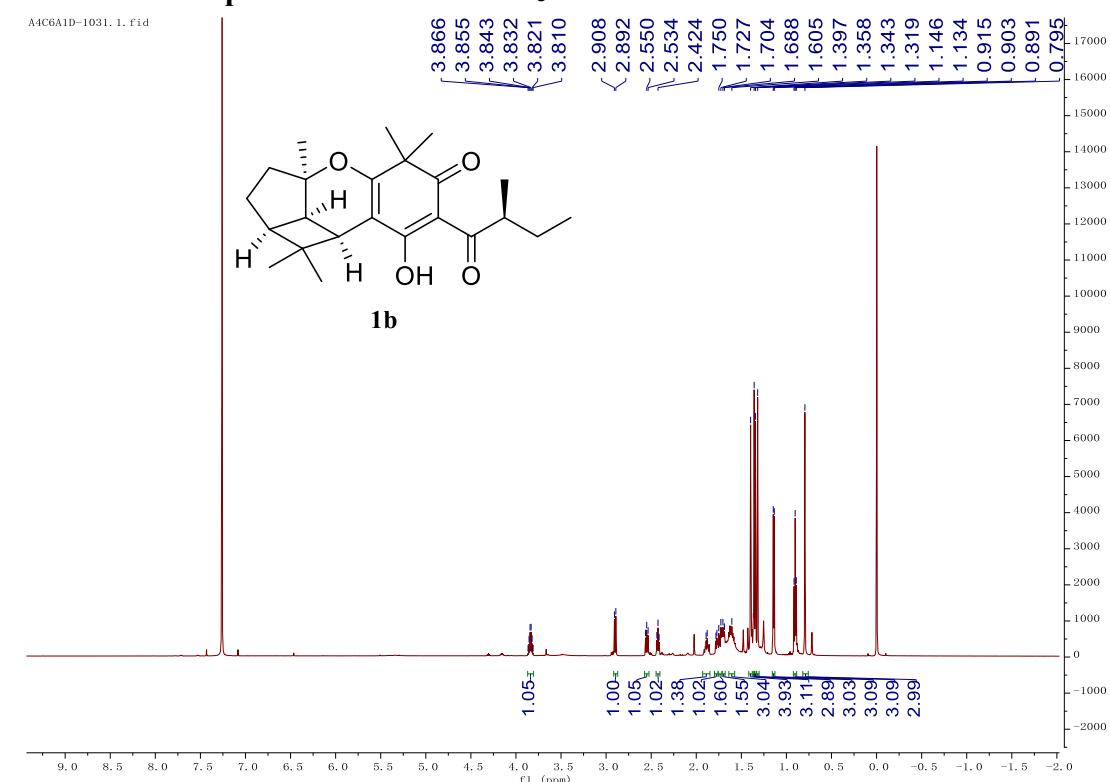
UV spectrum of compound 1b

4.2 1D and 2D NMR spectra of 1 in CDCl_3

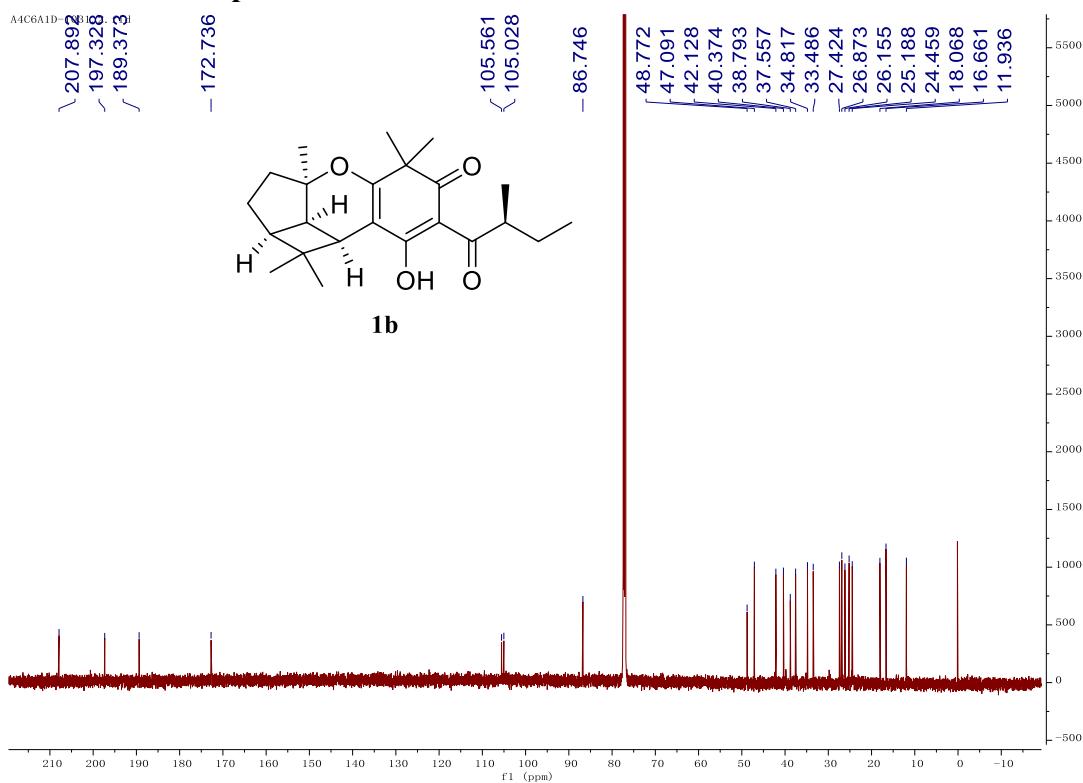
4.2.1 ^1H NMR spectrum of 1a in CDCl_3



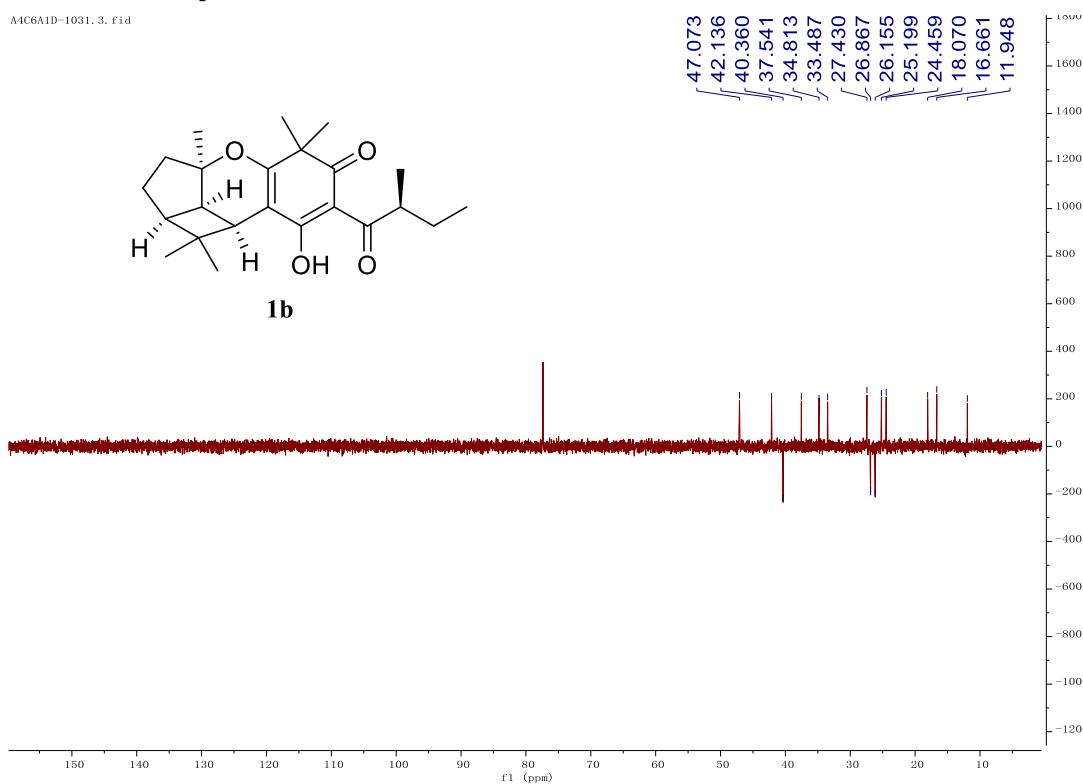
4.2.2 ^1H NMR spectrum of 1b in CDCl_3



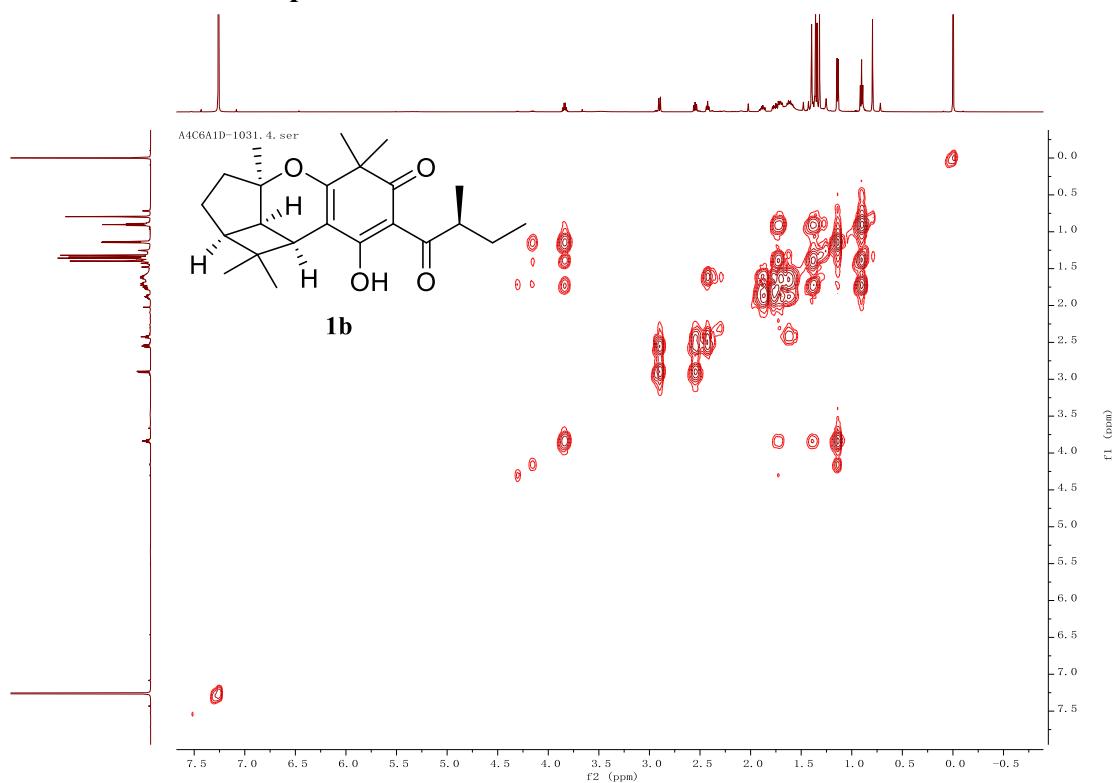
4.2.3 ^{13}C NMR spectrum of **1b** in CDCl_3



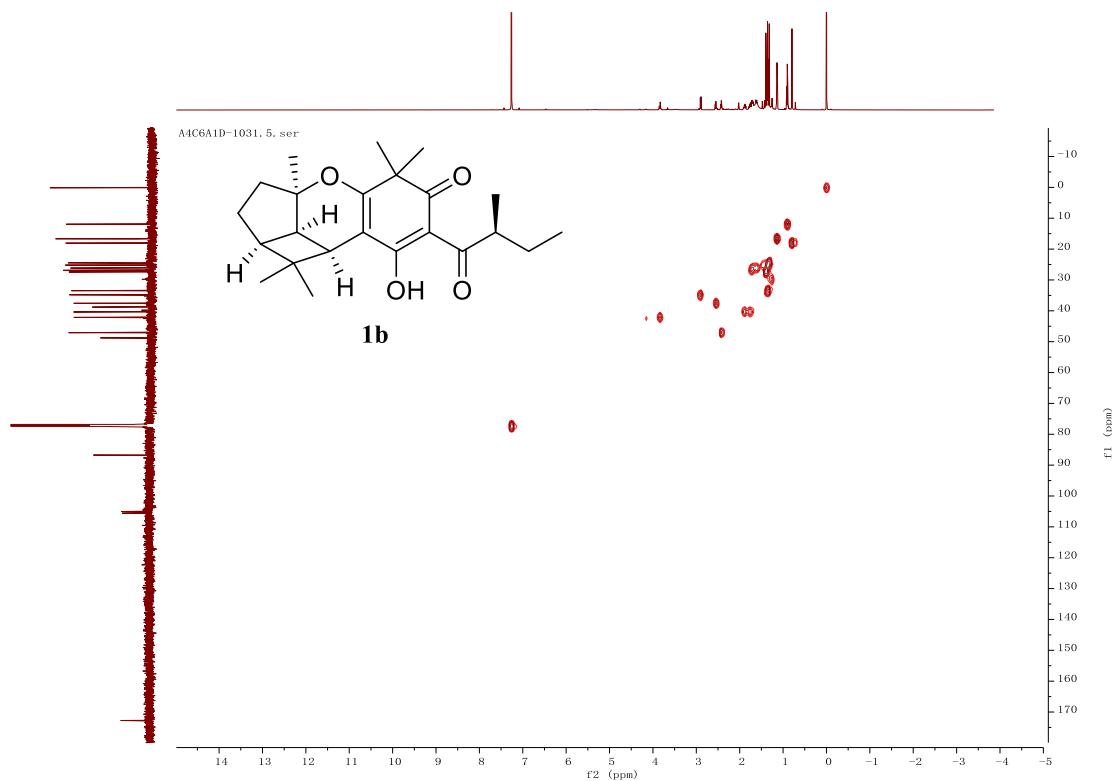
4.2.4 DEPT-135 spectrum of **1b** in CDCl_3



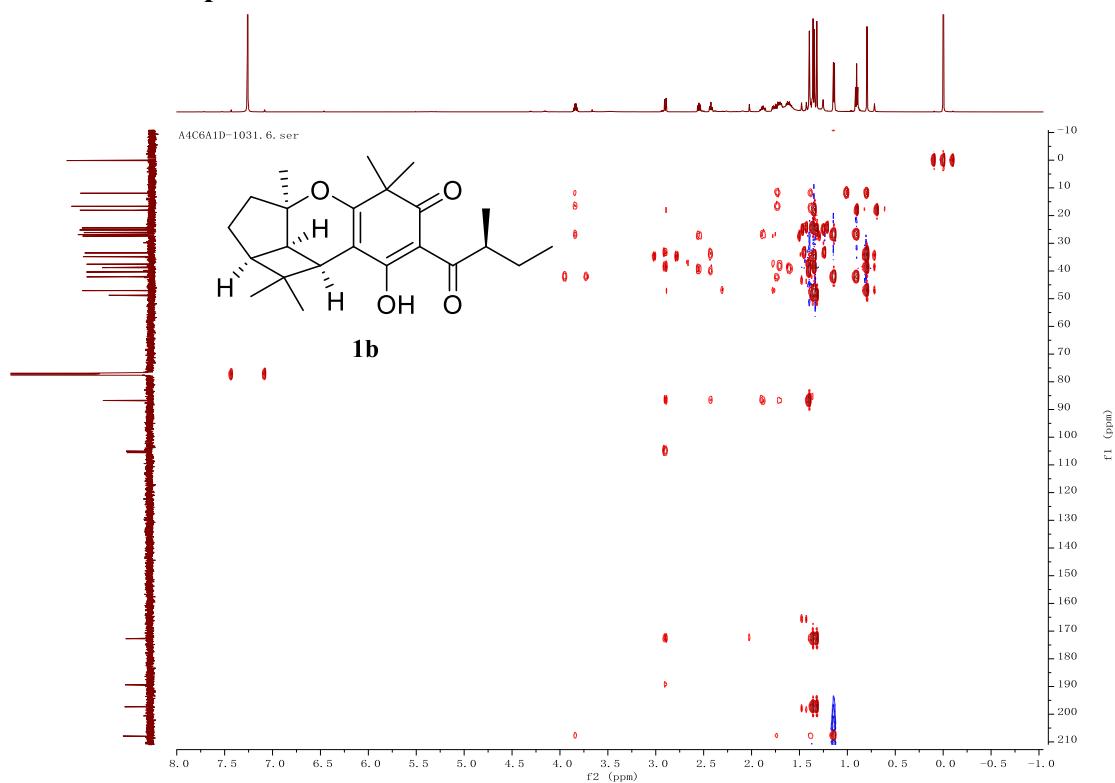
4.2.5 ^1H - ^1H COSY spectrum of **1b** in CDCl_3



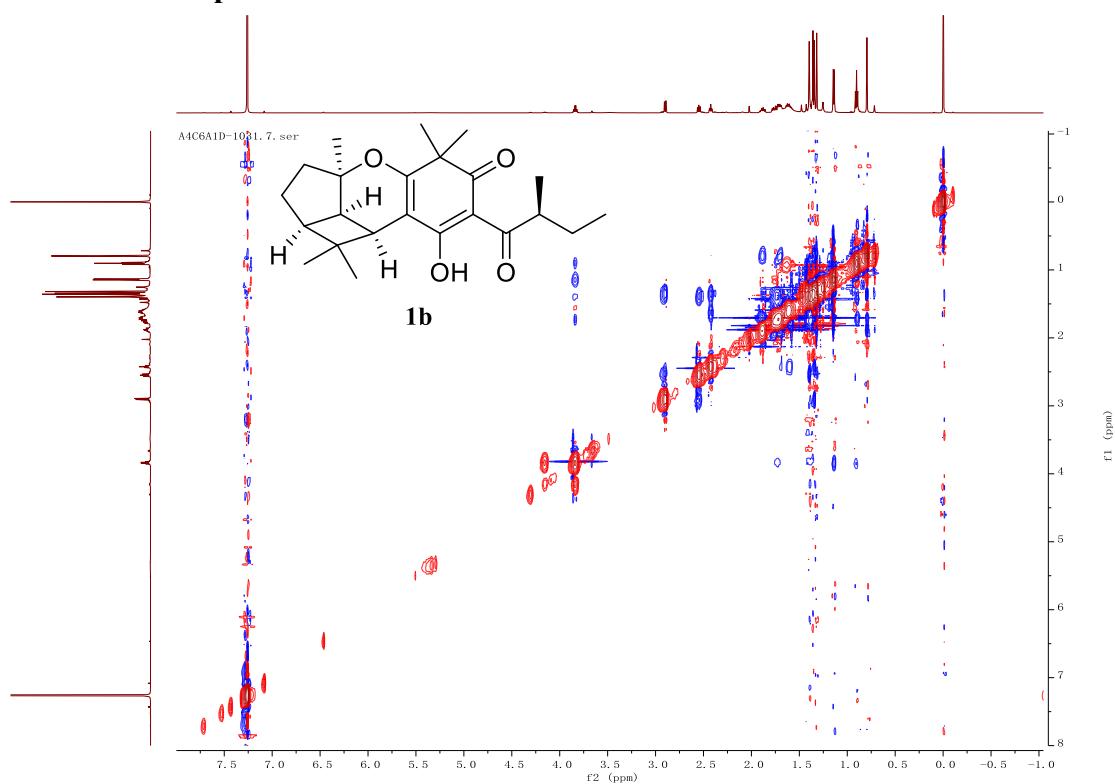
4.2.6 HSQC spectrum of **1b** in CDCl_3



4.2.7 HMBC spectrum of **1b** in CDCl_3

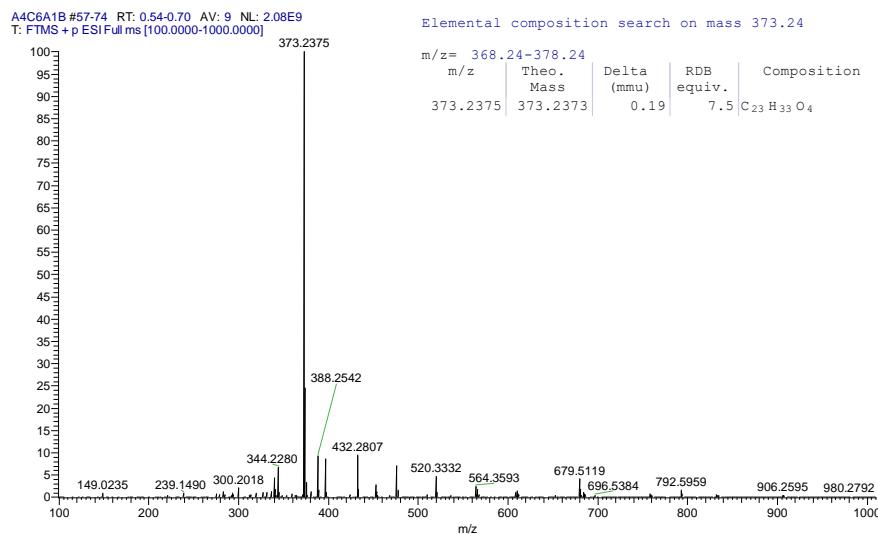


4.2.8 NOESY spectrum of **1b** in CDCl_3

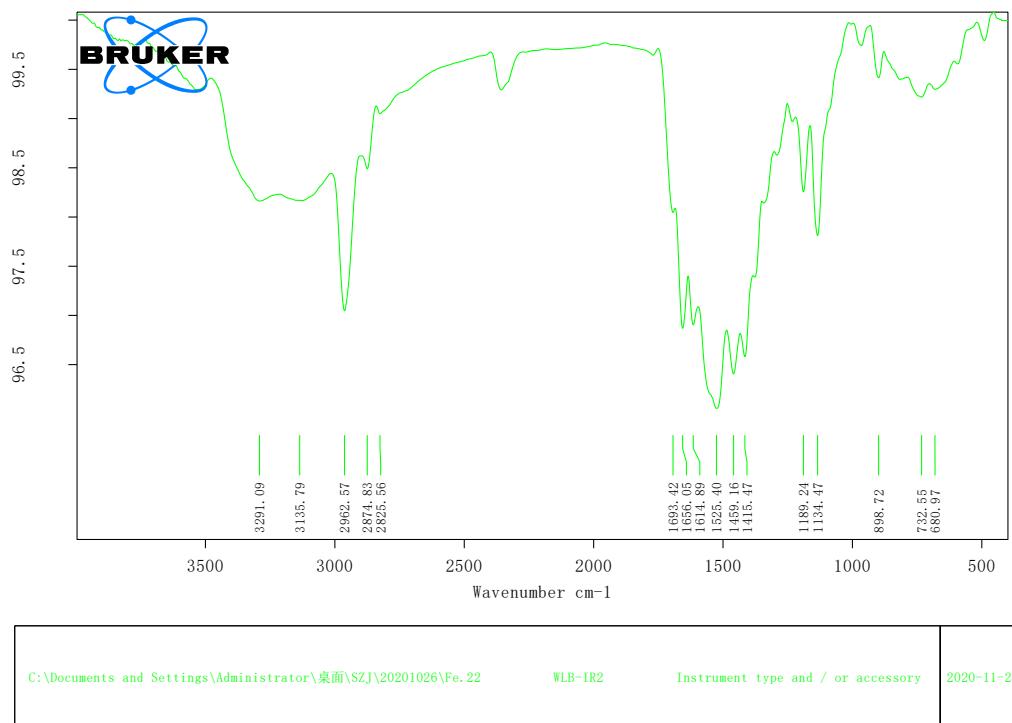


5. Spectral information of 2

5.1 HR-ESI-MS, IR and UV (CH_3OH) spectrum of 2a



HR-ESI-MS of compound 2a



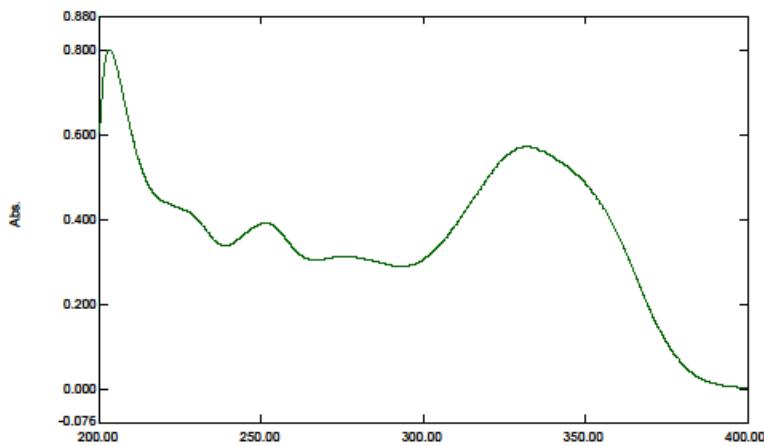
Page 1 of 1

IR spectrum of compound 2a

Spectrum Peak Pick Report

2020-11-02 19:43:19

Data Set: A4C6A1C 0.04mg ml - RawData



[Measurement Properties]

Wavelength Range (nm.): 200.00 to 400.00
Scan Speed: Medium
Sampling Interval: 0.5
Auto Sampling Interval: Disabled
Scan Mode: Single

No.	P/I/V	Wavelength	Abs.	Description
1	●	332.00	0.572	
2	●	276.00	0.313	
3	●	251.50	0.392	
4	●	203.00	0.800	

[Instrument Properties]

Instrument Type: UV-1600 Series
Measuring Mode: Absorbance
Slit Width: 2.0
Accumulation time: 0.1 sec.
Light Source Change Wavelength: 323.0 nm
Detector Unit: Direct
S/R Exchange: Normal
Stair Correction: OFF

[Attachment Properties]

Attachment: None

[Operation]

Threshold: 0.0010000
Points: 4
Interpolate: Disabled
Average: Disabled

[Sample Preparation Properties]

Weight:

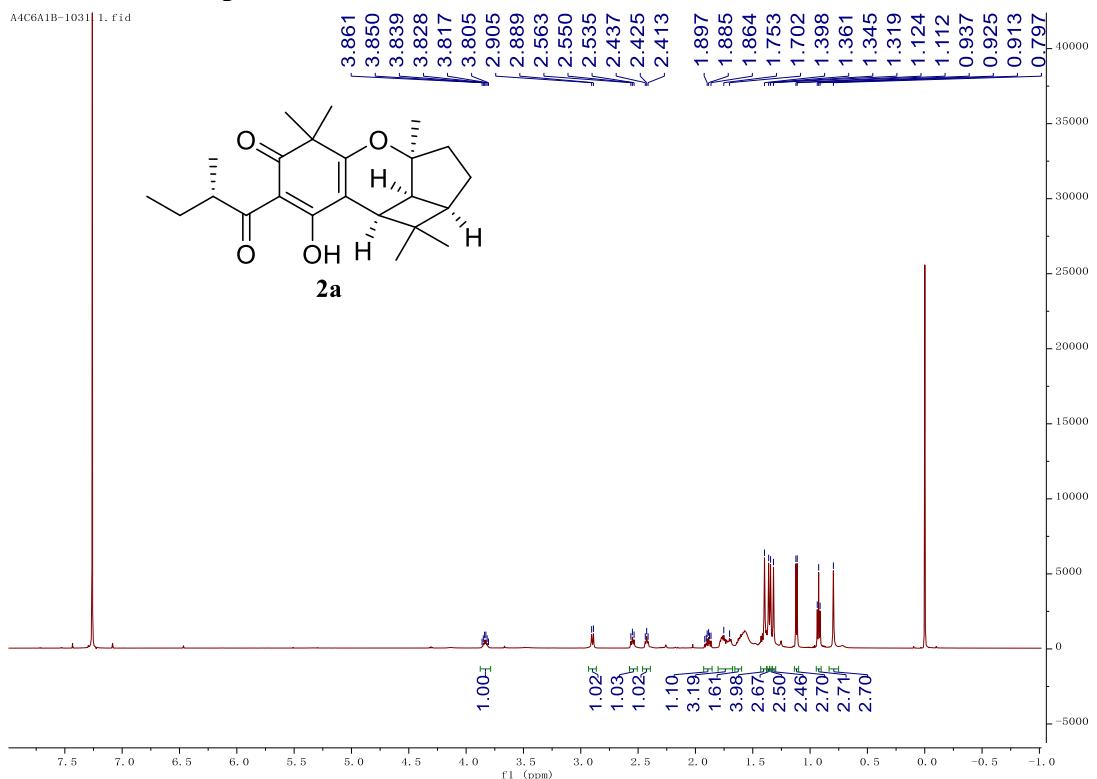
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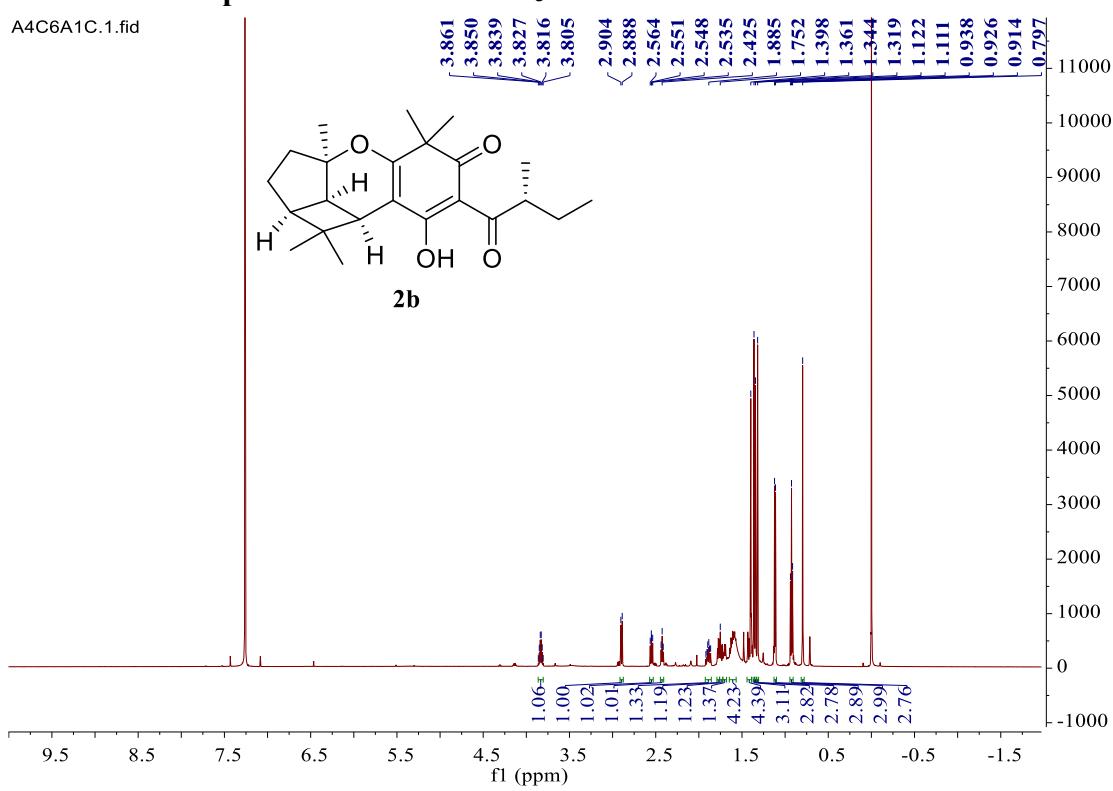
UV spectrum of compound 2a

5.2 1D and 2D NMR spectra of 2 in CDCl₃

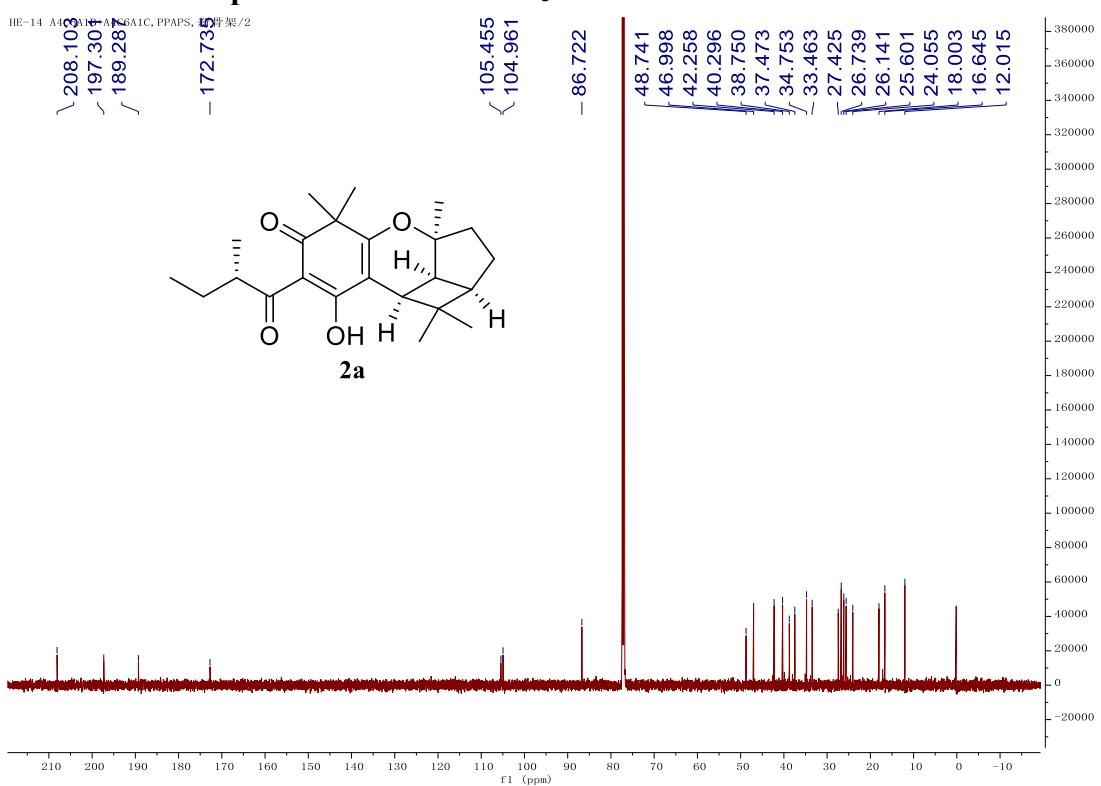
5.2.1 ^1H NMR spectrum of 2a in CDCl_3



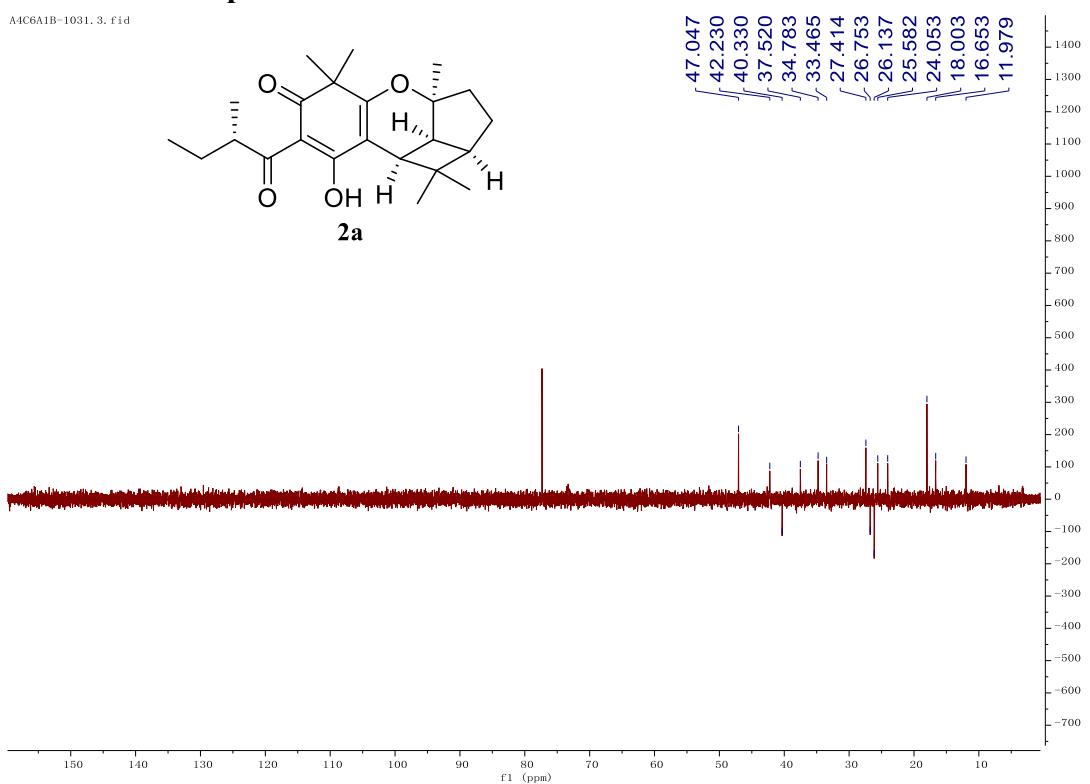
5.2.2 ^1H NMR spectrum of 2b in CDCl_3



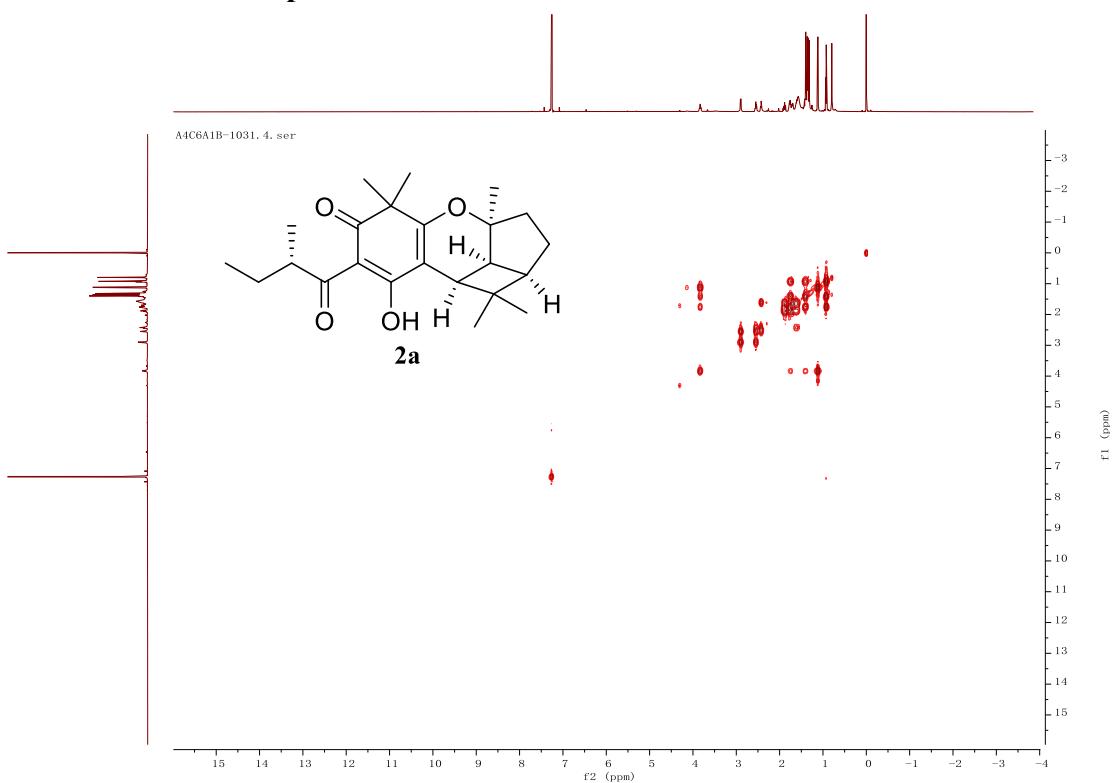
5.2.2 ^{13}C NMR spectrum of 2a in CDCl_3



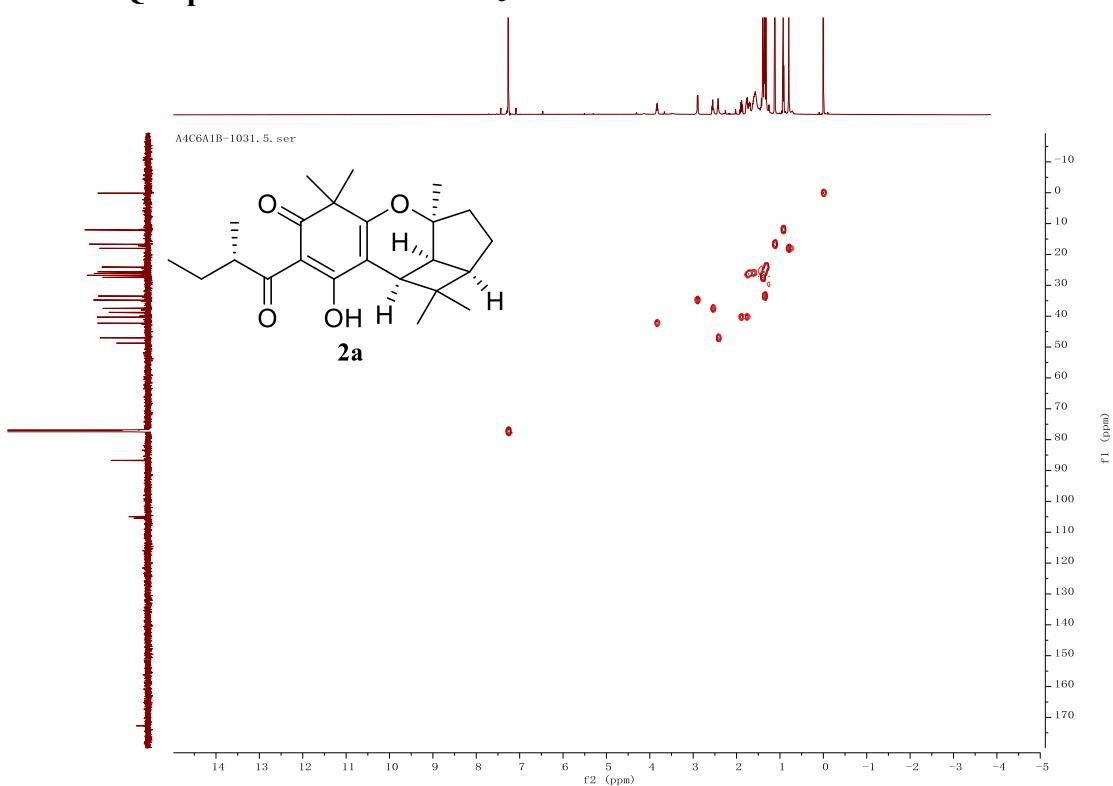
5.2.3 DEPT-135 spectrum of 2a in CDCl_3



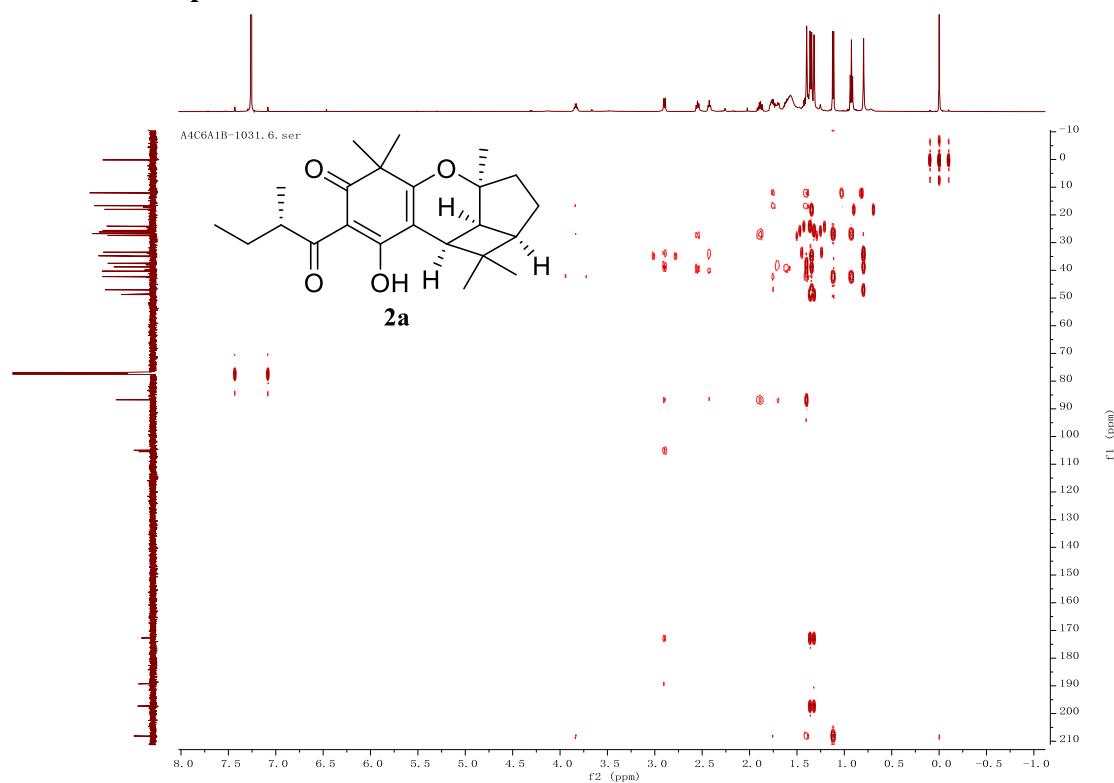
5.2.4 ^1H - ^1H COSY spectrum of **2a** in CDCl_3



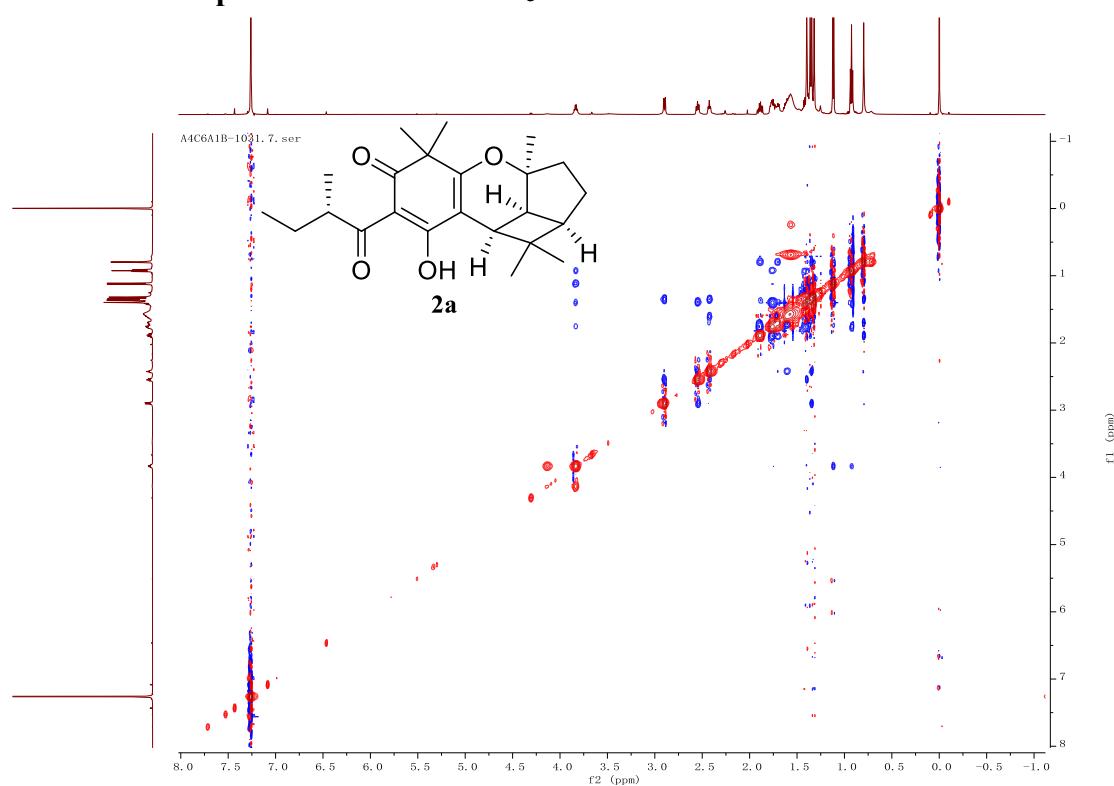
5.2.5 HSQC spectrum of **2a** in CDCl_3



5.2.6 HMBC spectrum of 2a in CDCl_3

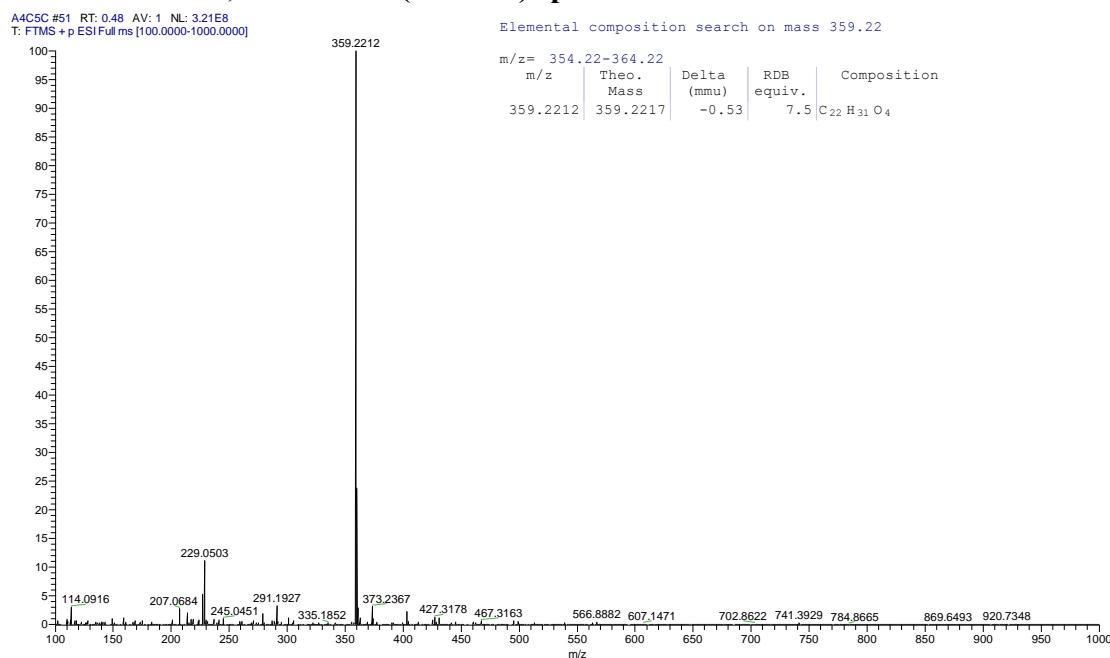


5.2.7 NOESY spectrum of 2a in CDCl_3

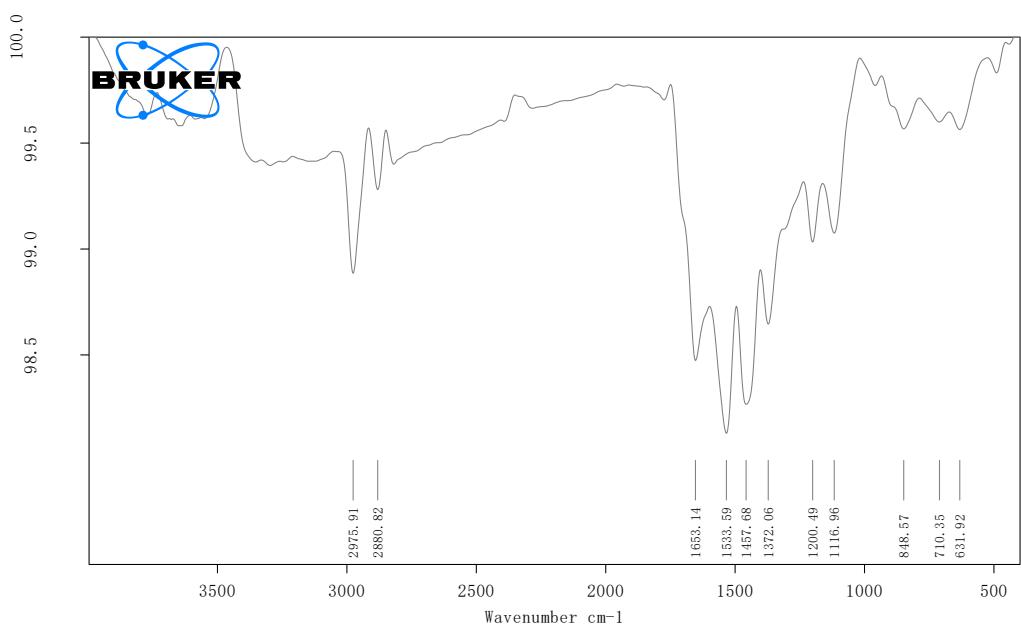


6. Spectral information of 3a

6.1 HR-ESI-MS, IR and UV (CH₃OH) spectrum of 3a



HR-ESI-MS of compound 3a



C:\Documents and Settings\Administrator\桌面\SZJ\20201026\Fe.26	WLB-IR2	Instrument type and / or accessory	2020-11-2
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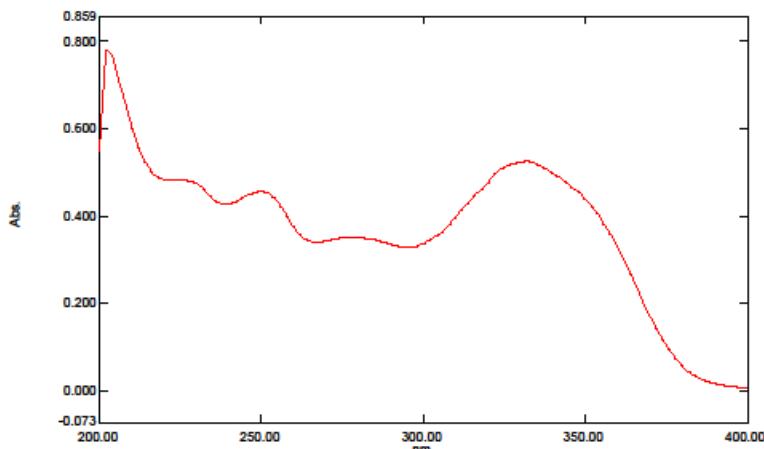
Page 1 of 1

IR spectrum of compound 3a

Spectrum Peak Pick Report

2020-11-17 21:30:56

Data Set: A4C5C2 0.08 - RawData



[Measurement Properties]
Wavelength Range (nm.): 200.00 to 400.00
Scan Speed: Medium
Sampling Interval: 2.0
Auto Sampling Interval: Disabled
Scan Mode: Single

No.	P/I/V	Wavelength	Abs.	Description
1	●	332.00	0.526	
2	●	278.00	0.350	
3	●	250.00	0.456	

[Instrument Properties]
Instrument Type: UV-1600 Series
Measuring Mode: Absorbance
Slit Width: 1.0
Accumulation time: 0.1 sec.
Light Source Change Wavelength: 323.0 nm
Detector Unit: Direct
S/R Exchange: Normal
Stair Correction: OFF

[Attachment Properties]
Attachment: None

[Operation]
Threshold: 0.0010000
Points: 4
Interpolate: Disabled
Average: Disabled

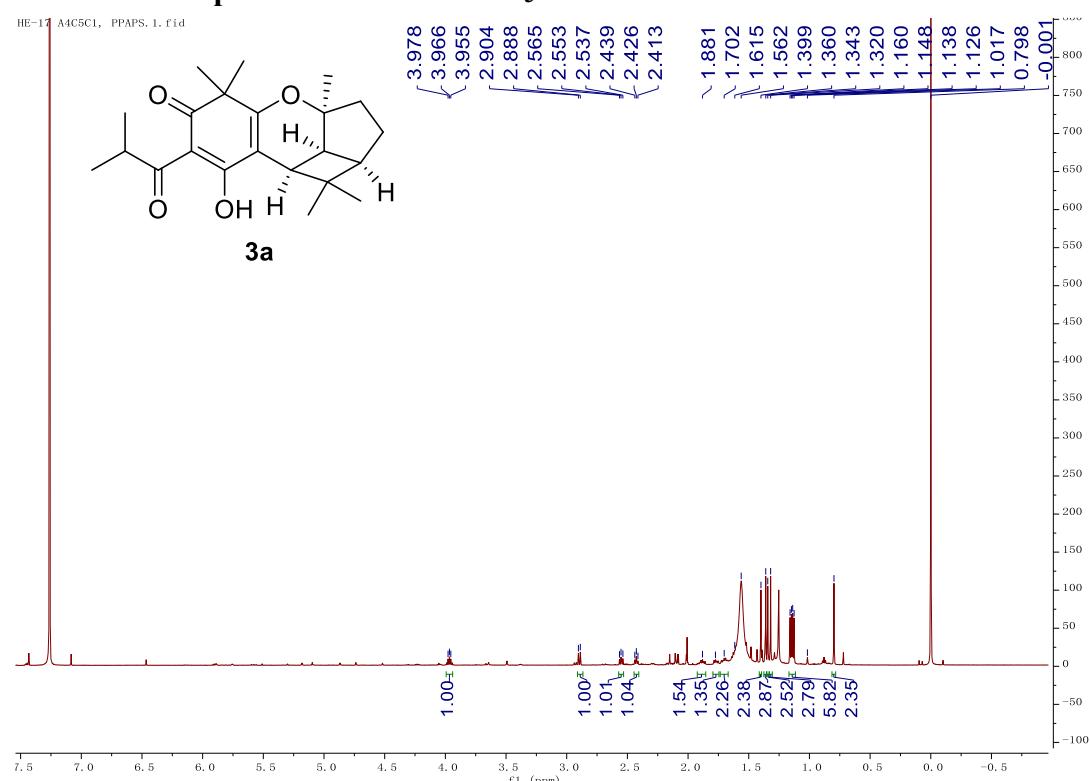
[Sample Preparation Properties]
Weight:
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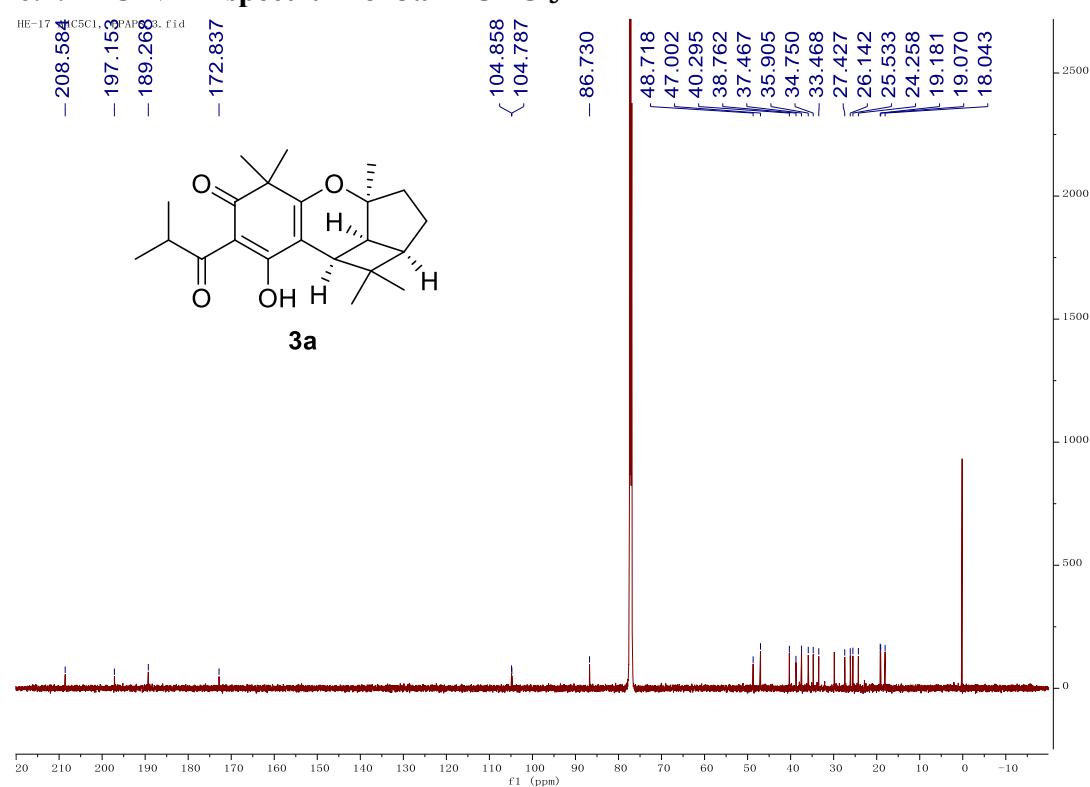
UV spectrum of compound 3a

6.2 1D and 2D NMR spectra of 3a in CDCl₃

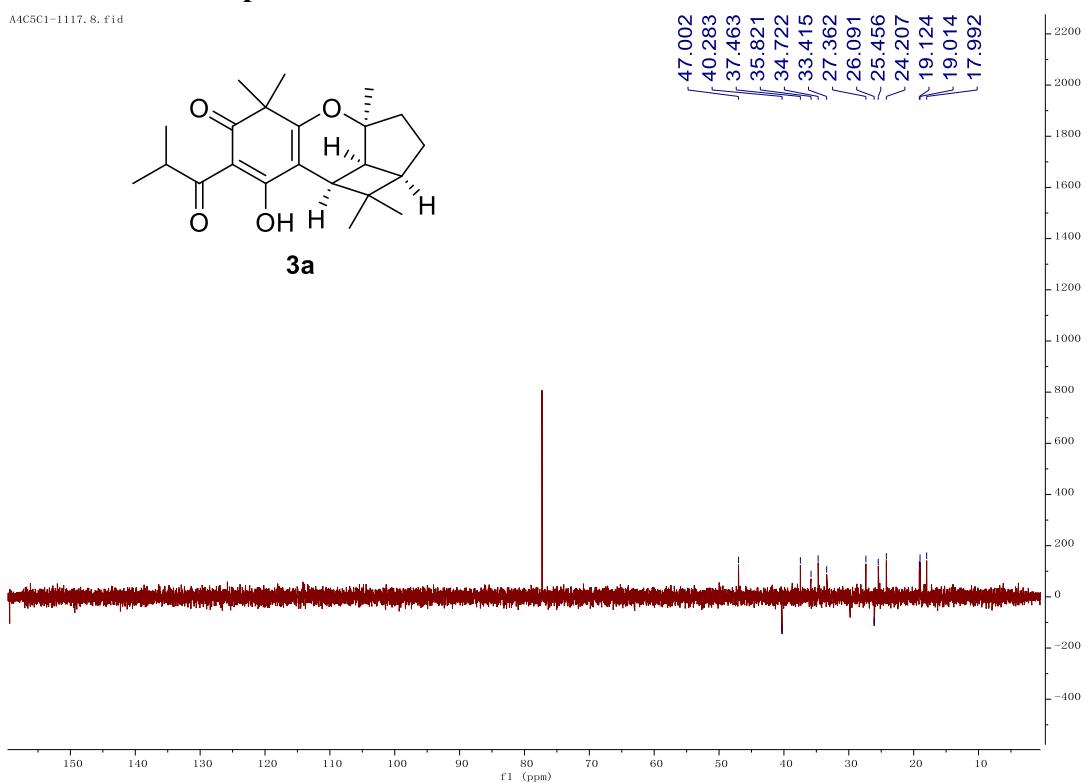
6.2.1 ¹H NMR spectrum of 3a in CDCl₃



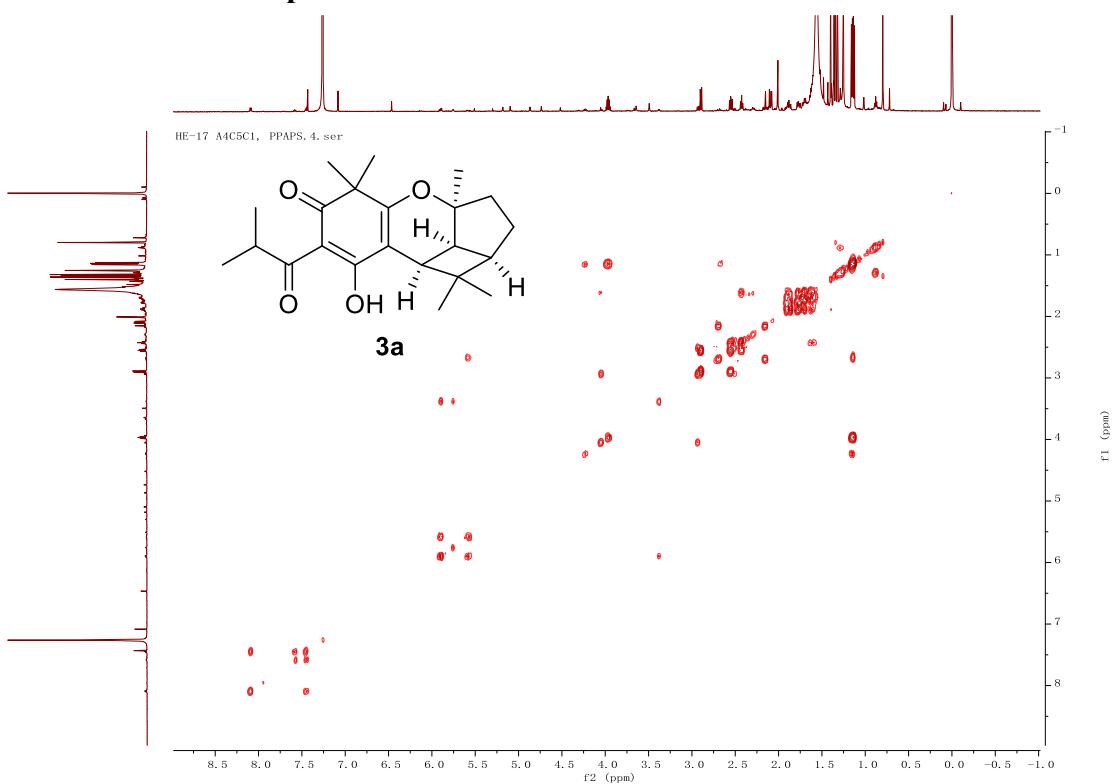
6.2.2 ¹³C NMR spectrum of 3a in CDCl₃



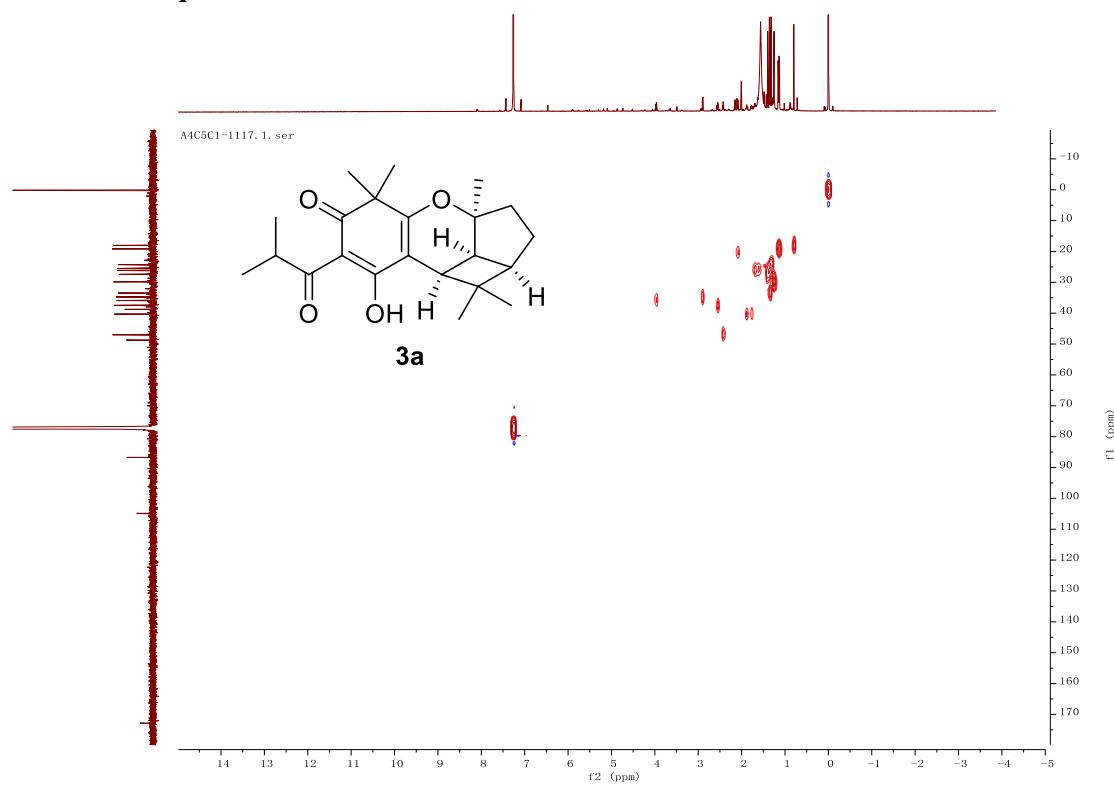
6.2.3 DEPT-135 spectrum of 3a in CDCl₃



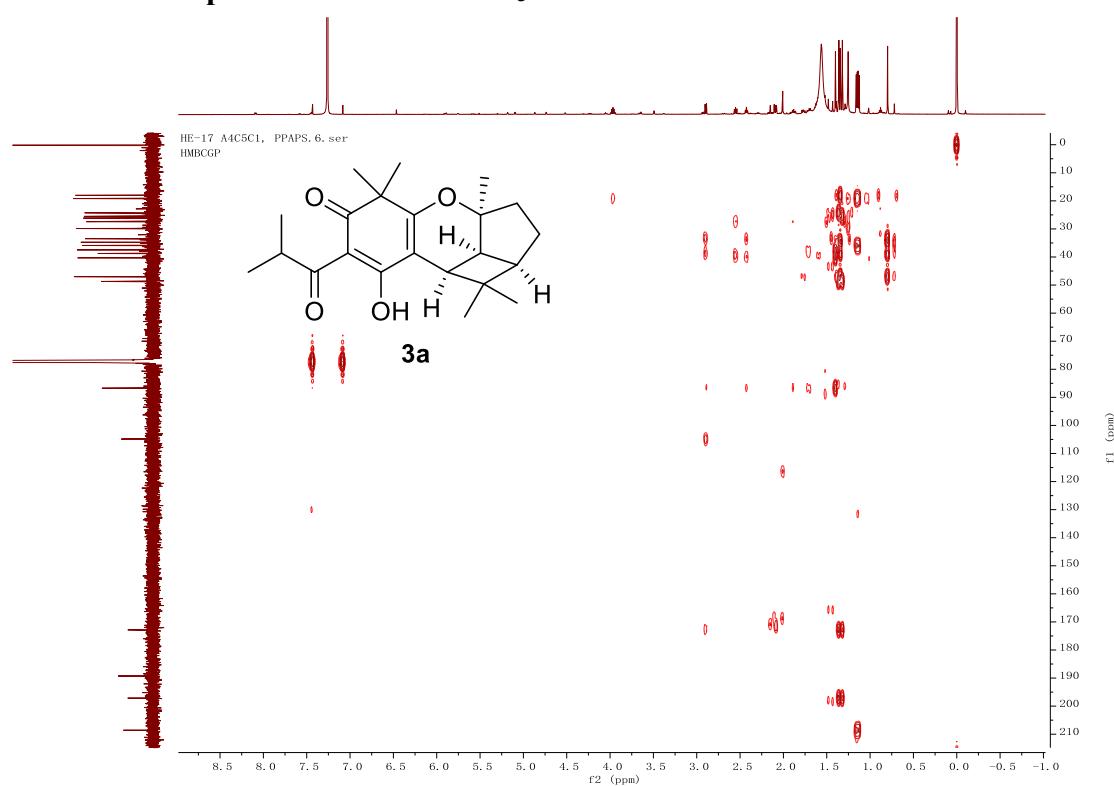
6.2.4 ¹H–¹H COSY spectrum of 3a in CDCl₃



6.2.5 HSQC spectrum of 3a in CDCl₃



6.2.6 HMBC spectrum of 3a in CDCl₃



6.2.7 NOESY spectrum of 3a in CDCl_3

