SUPPLEMENTARY MATERIAL

A new diarylhexane and two new diarylpropanols from the roots of *Knema globularia*

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Abstract: A new diarylhexane, kneglobularone B (**1**) and two new diarylpropanols, kneglobularols A–B (**2–3**) along with seven known compounds (**4–10**) were isolated and characterized from the roots of *Knema globularia*. It is the first time to find arylpropyl quinone (**4**) and isoflavone (**8**) in Myristicaceae family. In addition, **5** was found for the first time in *Knema* genus. Their structures were elucidated by UV, IR, MS, 1D and 2D NMR techniques. Compound **4** exhibited strong cytotoxicity against the NCI–H187 and MCF–7 cell lines with IC_{50} values of 3.08 and 6.68 µg/mL, respectively.

Keywords: *Knema globularia*, cytotoxicity, diarylhexane, diarylpropanol

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Table S1. ^{1}H NMR spectroscopic data of **1–3 [**400 MHz, (δ_{H}, mult. and *J* in Hz)**]**

Position	**1** ($CDCl_3$)	**2** ($CDCl_3$+CD_3OD)	**3** ($CDCl_3$)
1	2.52, t (8.0)	4.87, dd (10.0, 2.0)	5.08, dd (10.0, 2.8)
2	1.50–1.64, m	1.94–2.14, m	2.12–2.30, m
3	1.22–1.44, m	2.62–2.70, m	2.76–2.86, m
		2.80–2.90, m	2.89–3.02, m
4	1.22–1.44, m		
5	1.50–1.64, m		
6	2.80, t (8.0)		
1'			
2'			
3'		6.32, d (2.0)	6.46, d (2.4)
4'	6.26, s		
5'		6.34, dd (8.4, 2.0)	6.53, dd (8.4, 2.4)
6'	6.26, s	6.85, d (8.4)	7.00, d (8.4)
1"			
2"	6.66, s	6.83, s	
3"			6.49, s
4"		6.83, s	
5"	6.72, d (8.0)		
6"	6.60, d (8.0)	6.89, s	6.63, s
OCH_2O	5.92, s		5.91, d (1.6)
CH_3	2.63, s		
OH–3'	13.00, s		
OH–5'	5.78, br s		
OH–2',2"			6.65, br s
OCH_3–4'			3.76, s
OCH_3–3"		3.84, s	

Table S2. ^{13}C NMR spectroscopic data of **1–3** [100 MHz, (δ_C, Type)]

Position	**1** ($CDCl_3$)	**2** ($CDCl_3$+CD_3OD)	**3** ($CDCl_3$)
1	35.5, CH_2	78.0, CH	78.0, CH
2	31.5, CH_2	30.1, CH_2	27.9, CH_2
3	28.8, CH_2	24.6, CH_2	24.4, CH_2
4	29.4, CH_2		
5	32.1, CH_2		
6	36.2, CH_2		
1'	147.7, C	113.1, C	114.0, C
2'	115.3, C	155.6, C	154.4, C
3'	161.0, C	103.2, CH	101.8, CH
4'	101.7, CH	155.9, C	159.1, C
5'	165.9, C	108.2, CH	108.5, CH
6'	110.6, CH	129.9, CH	130.2, CH
1"	136.4, C	133.4, C	117.2, C
2"	109.0, CH	119.1, CH	150.0, C
3"	147.4, C	147.1, C	99.4, CH
4"	145.4, C	114.6, CH	148.0, C
5"	108.1, CH	145.5, C	141.3, C
6"	121.1, CH	109.2, CH	106.3, CH
CO	204.2, C		
OCH_2O	100.7, CH_2		101.2, CH_2
CH_3	32.1, CH_3		
OCH_3–4'			55.4, CH_3
OCH_3–3"		55.8, CH_3	

Table S3. Cytotoxicity of selected compounds

Compound	Cytotoxicity (μg/mL)		
	KB	MCF-7	NCI-H187
1	17.48	inactive [a]	18.42
4	8.47	6.68	3.08
5	inactive [a]	inactive [a]	18.09
7	29.79	ND[b]	30.11
8	inactive [a]	inactive [a]	inactive [a]
9	25.16	33.50	24.94
10	25.61	43.55	9.20
Ellipticine	3.27	–	3.70
Doxorubicin	0.658	9.72	0.087
Tamoxifen	–	8.45	–

[a] Inactive at > 50 μg/mL

[b] No Data

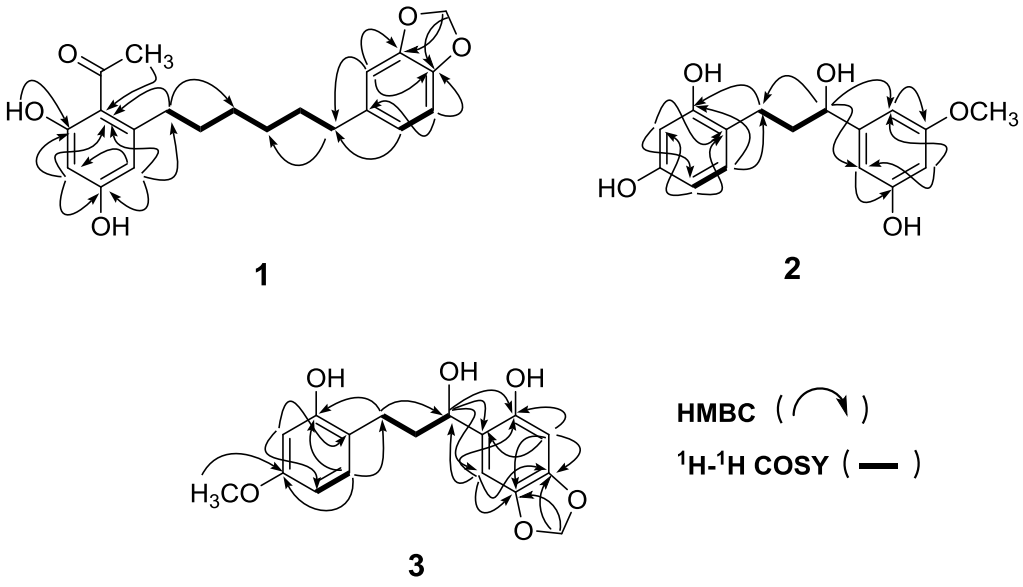


Figure S1 Key HMBC and ^{1}H–^{1}H COSY correlations of **1–3**

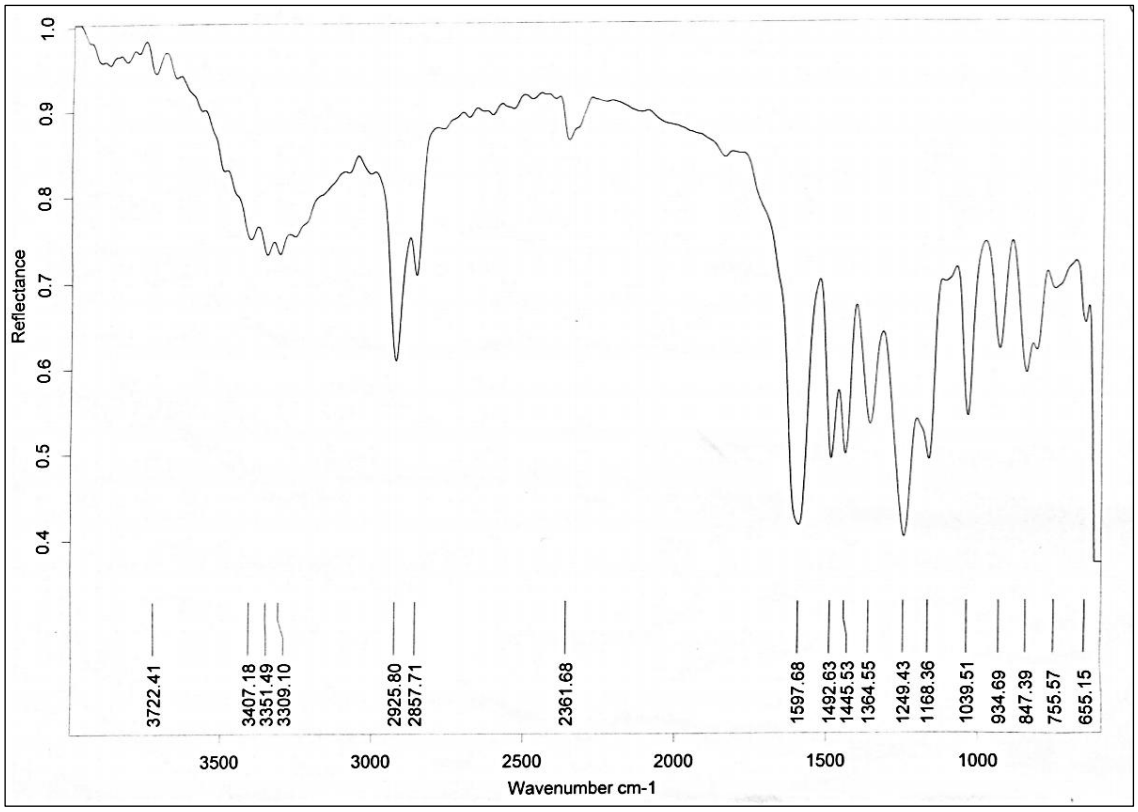


Figure S2 IR spectrum of **1**

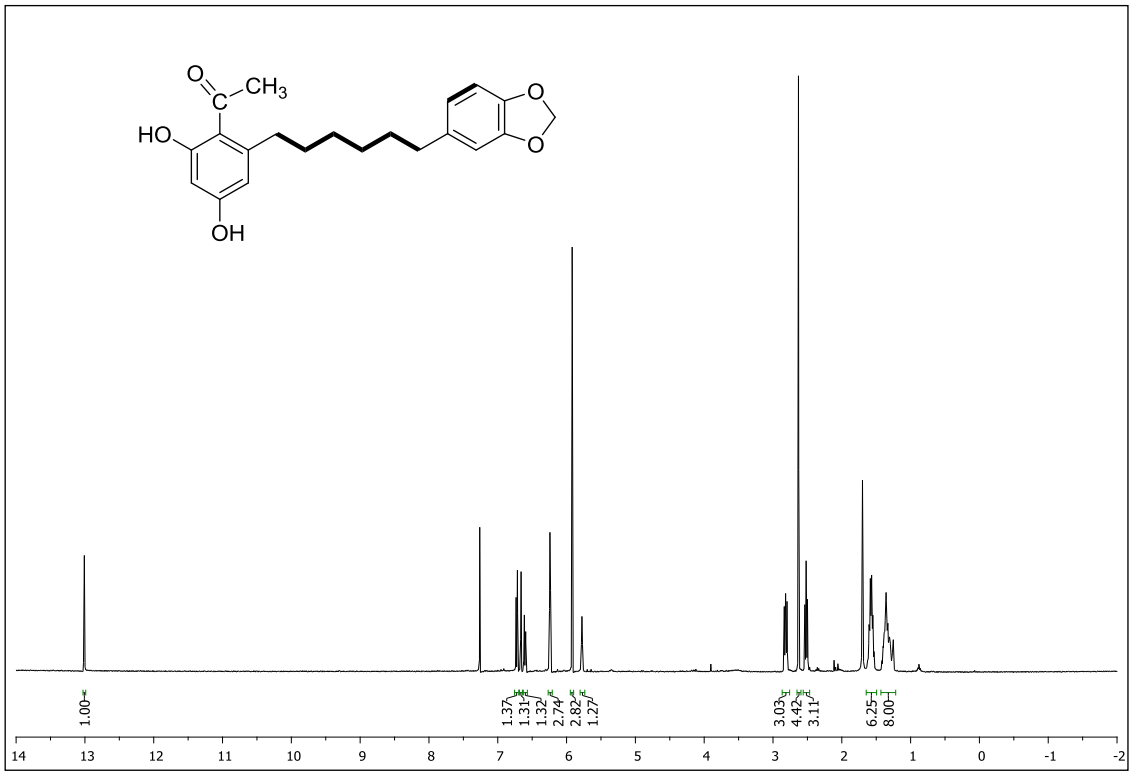


Figure S3 ^{1}H NMR spectrum of **1**

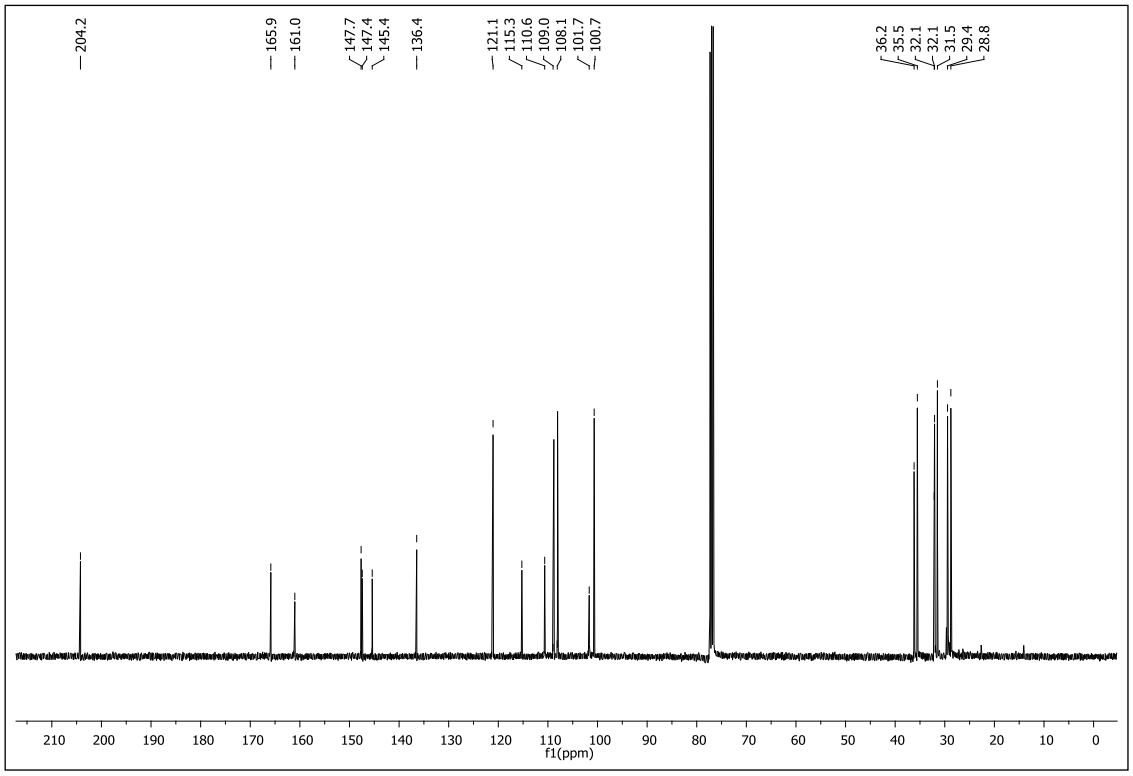


Figure S4 ^{13}C NMR spectrum of **1**

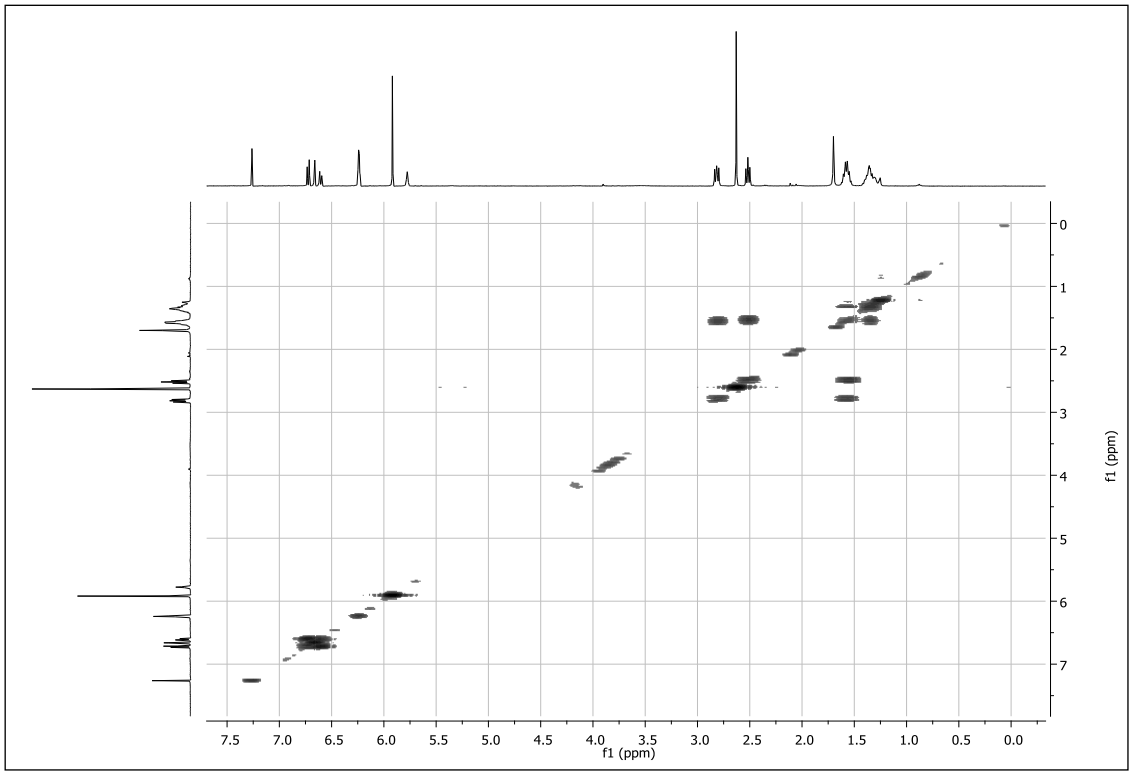


Figure S5 ^{1}H–^{1}H COSY spectrum of **1**

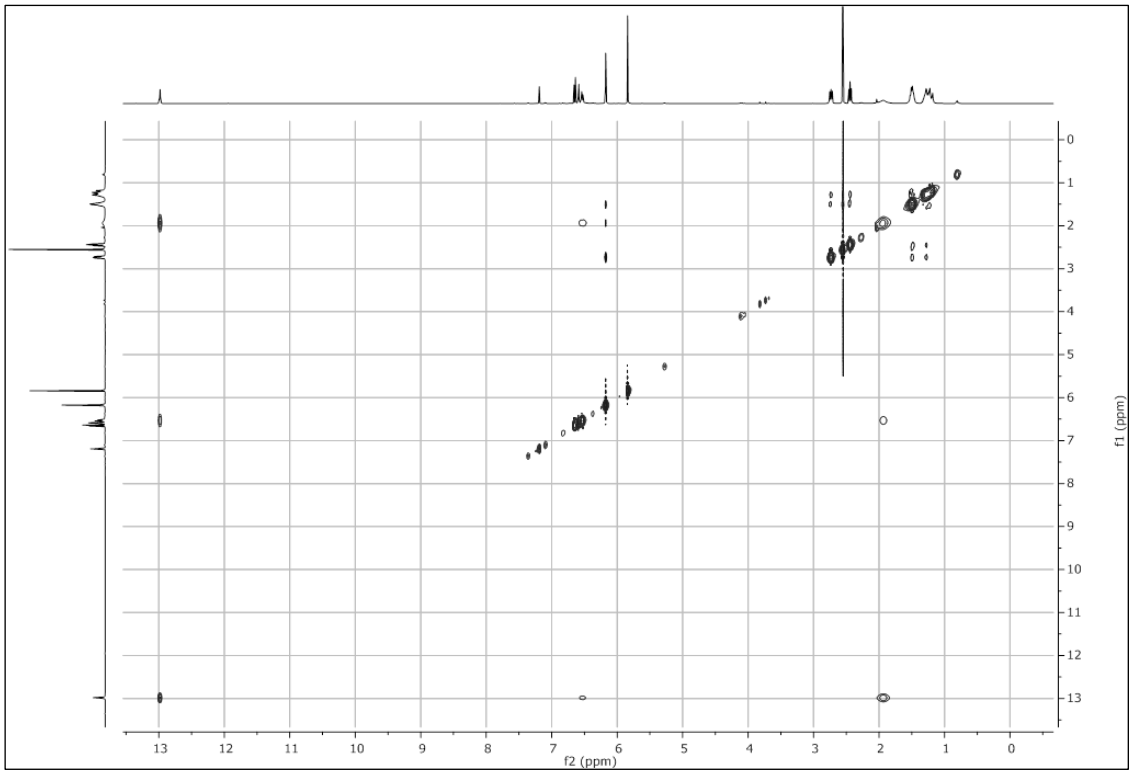


Figure S6 NOESY spectrum of **1**

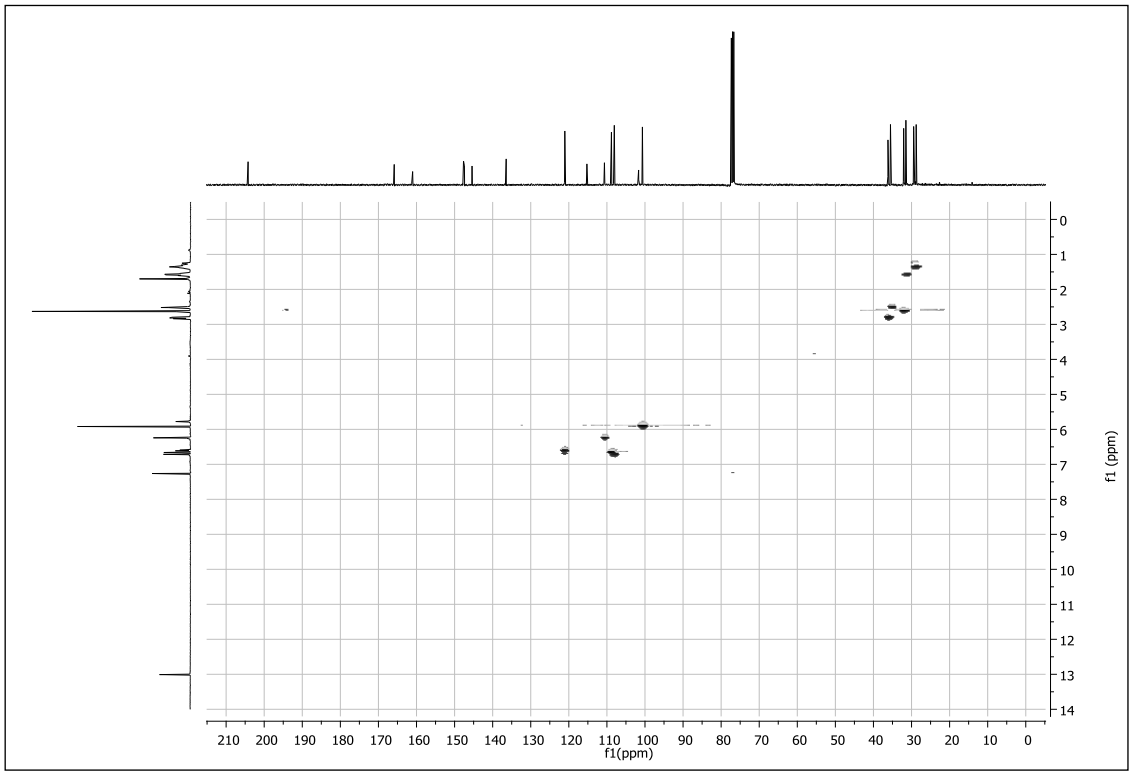


Figure S7 HMQC spectrum of **1**

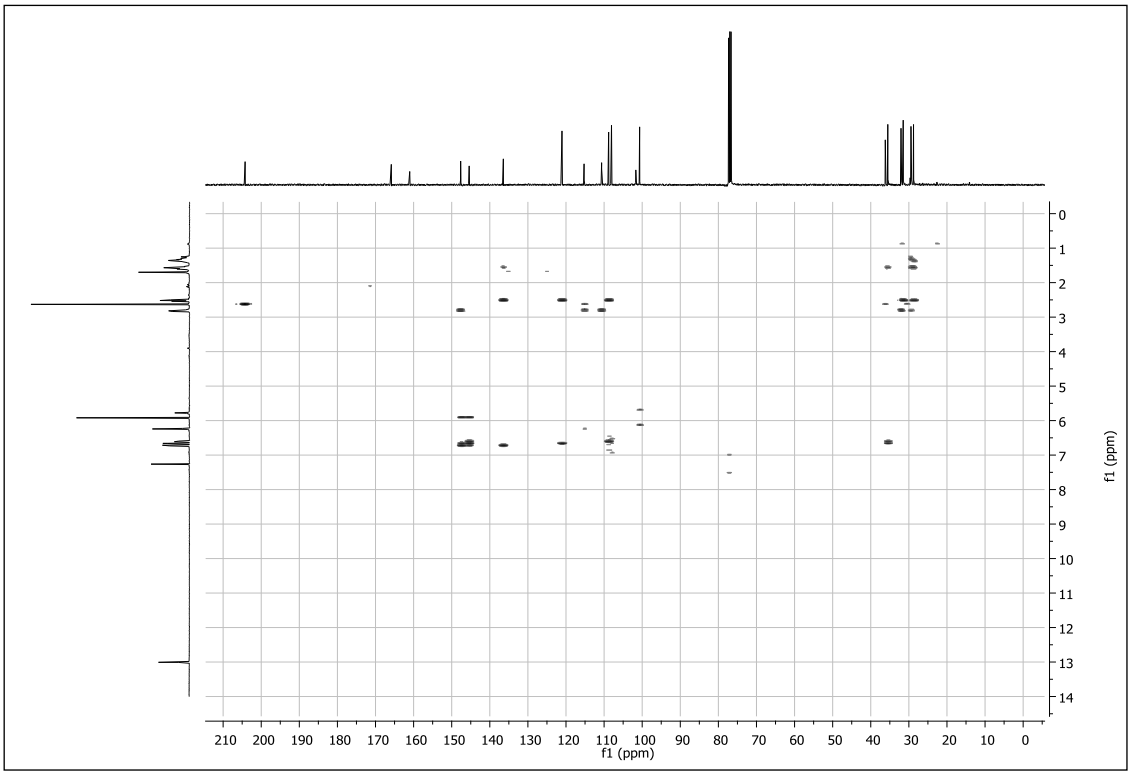
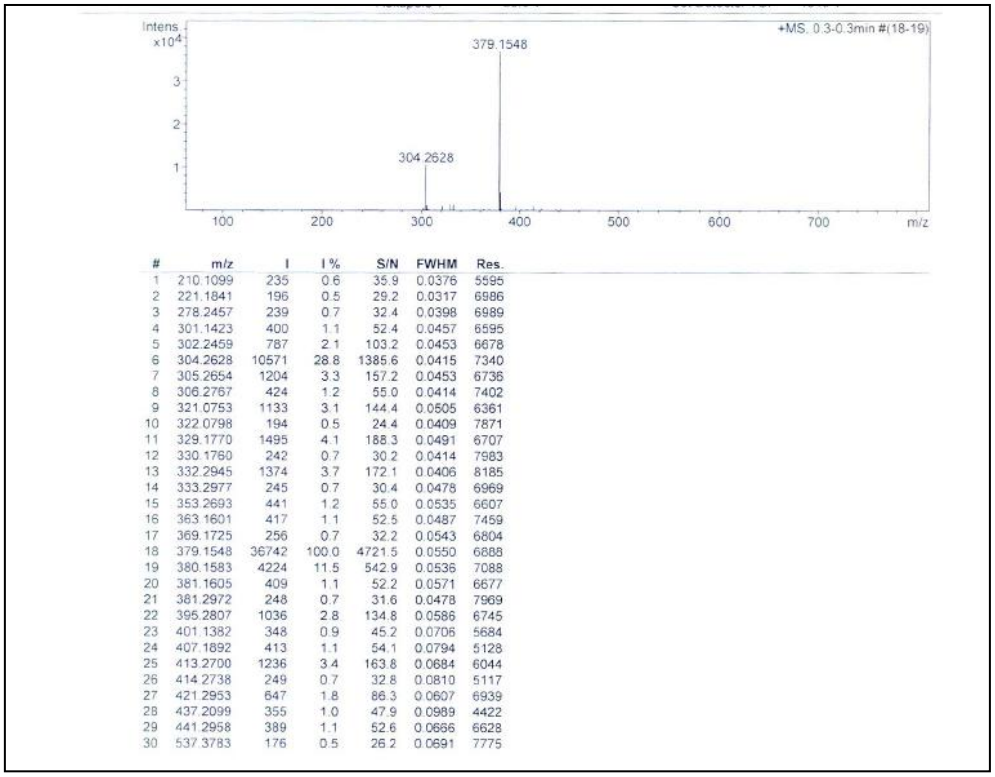


Figure S8 HMBC spectrum of **1**



#	m/z	I	I %	S/N	FWHM	Res.
1	210.1099	235	0.6	35.9	0.0376	5595
2	221.1841	196	0.5	29.2	0.0317	6986
3	278.2457	239	0.7	32.4	0.0398	6989
4	301.1423	400	1.1	52.4	0.0457	6595
5	302.2459	787	2.1	103.2	0.0453	6678
6	304.2628	10571	28.8	1385.6	0.0415	7340
7	305.2654	1204	3.3	157.2	0.0453	6736
8	306.2767	424	1.2	55.0	0.0414	7402
9	321.0753	1133	3.1	144.4	0.0505	6361
10	322.0798	194	0.5	24.4	0.0409	7871
11	329.1770	1495	4.1	188.3	0.0491	6707
12	330.1760	242	0.7	30.2	0.0414	7983
13	332.2945	1374	3.7	172.1	0.0406	8185
14	333.2977	245	0.7	30.4	0.0478	6969
15	353.2693	441	1.2	55.0	0.0535	6607
16	363.1601	417	1.1	52.5	0.0487	7459
17	369.1725	256	0.7	32.2	0.0543	6804
18	379.1548	36742	100.0	4721.5	0.0550	6888
19	380.1583	4224	11.5	542.9	0.0536	7088
20	381.1605	409	1.1	52.2	0.0571	6677
21	381.2972	248	0.7	31.6	0.0478	7969
22	395.2807	1036	2.8	134.8	0.0586	6745
23	401.1382	348	0.9	45.2	0.0706	5684
24	407.1892	413	1.1	54.1	0.0794	5128
25	413.2700	1236	3.4	163.8	0.0684	6044
26	414.2738	249	0.7	32.8	0.0810	5117
27	421.2953	647	1.8	86.3	0.0607	6939
28	437.2099	355	1.0	47.9	0.0989	4422
29	441.2958	389	1.1	52.6	0.0666	6628
30	537.3783	176	0.5	26.2	0.0691	7775

Figure S9 Mass spectrum of **1**

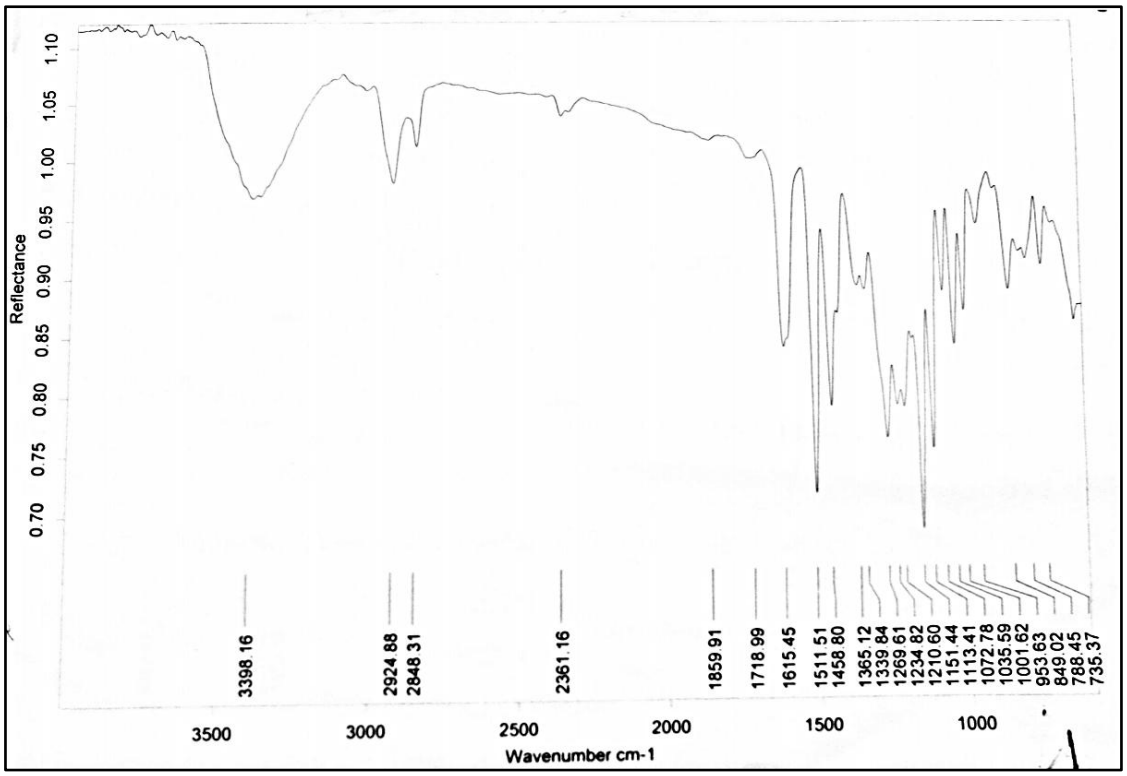


Figure S10 IR spectrum of **2**

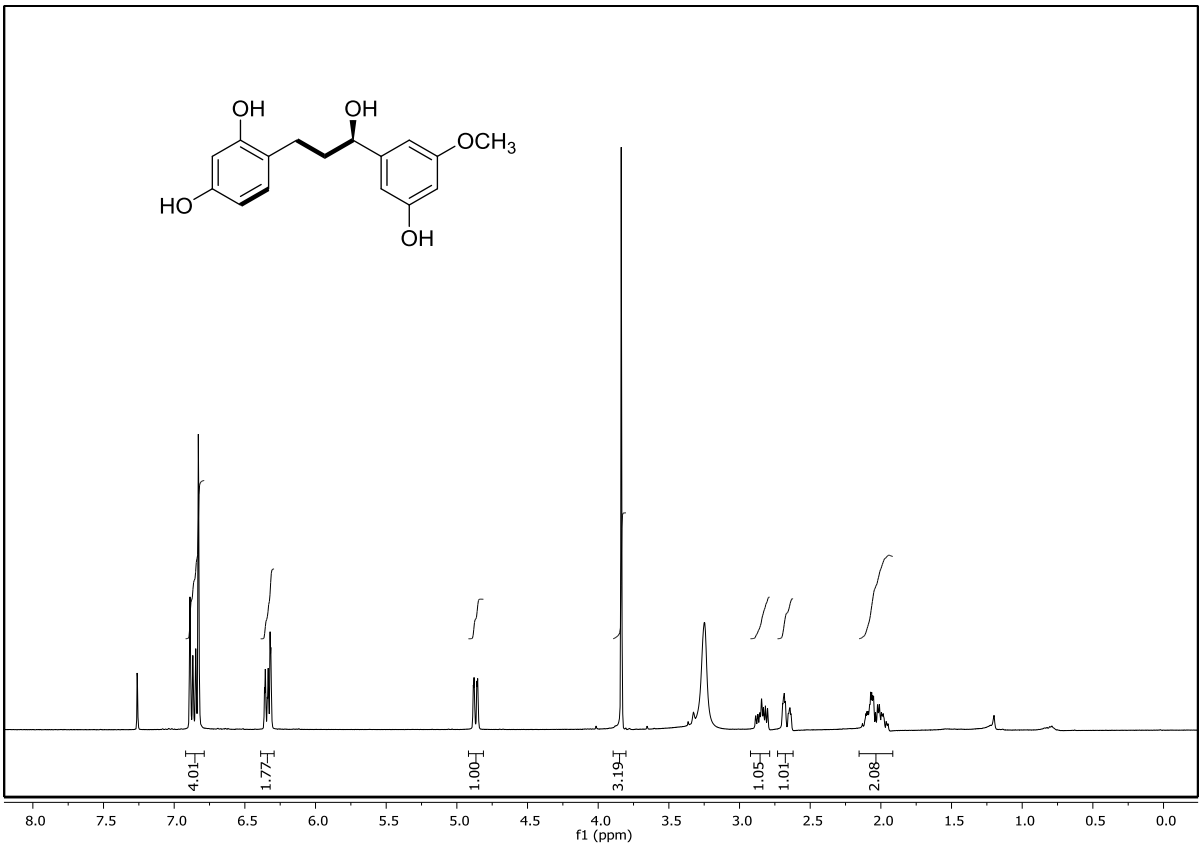


Figure S11 ^{1}H NMR spectrum of **2**

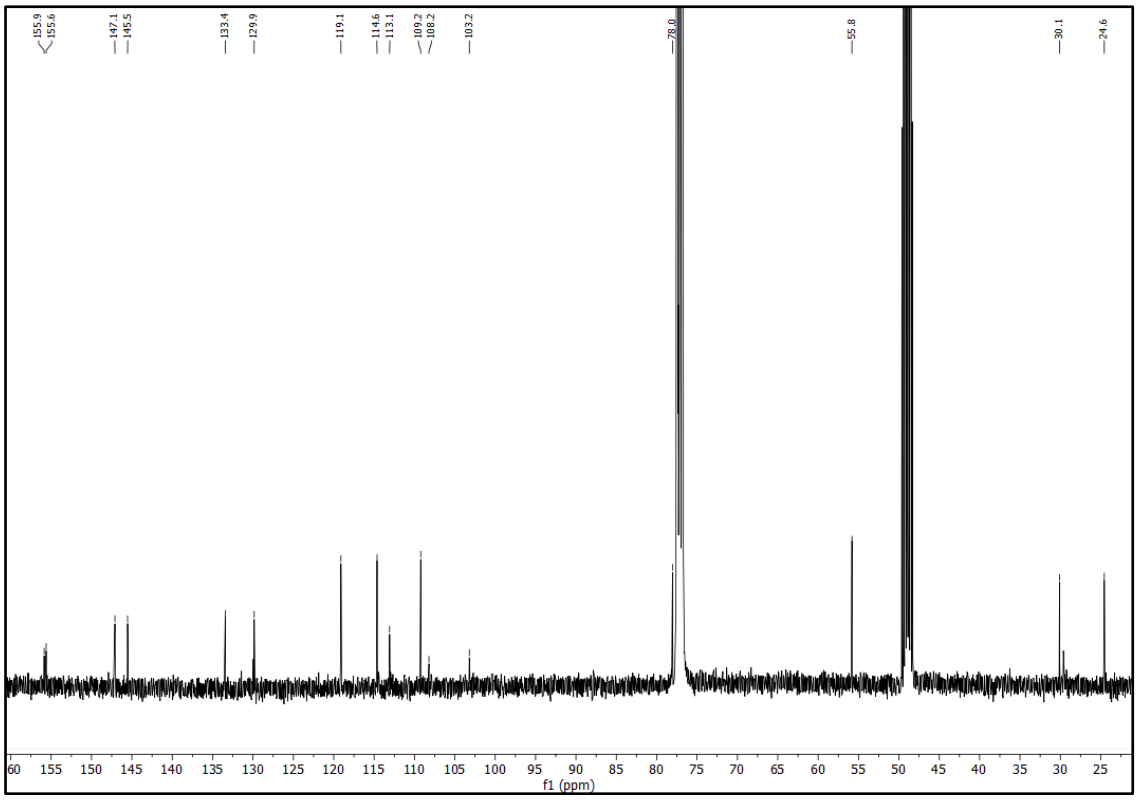


Figure S12 ^{13}C NMR spectrum of **2**

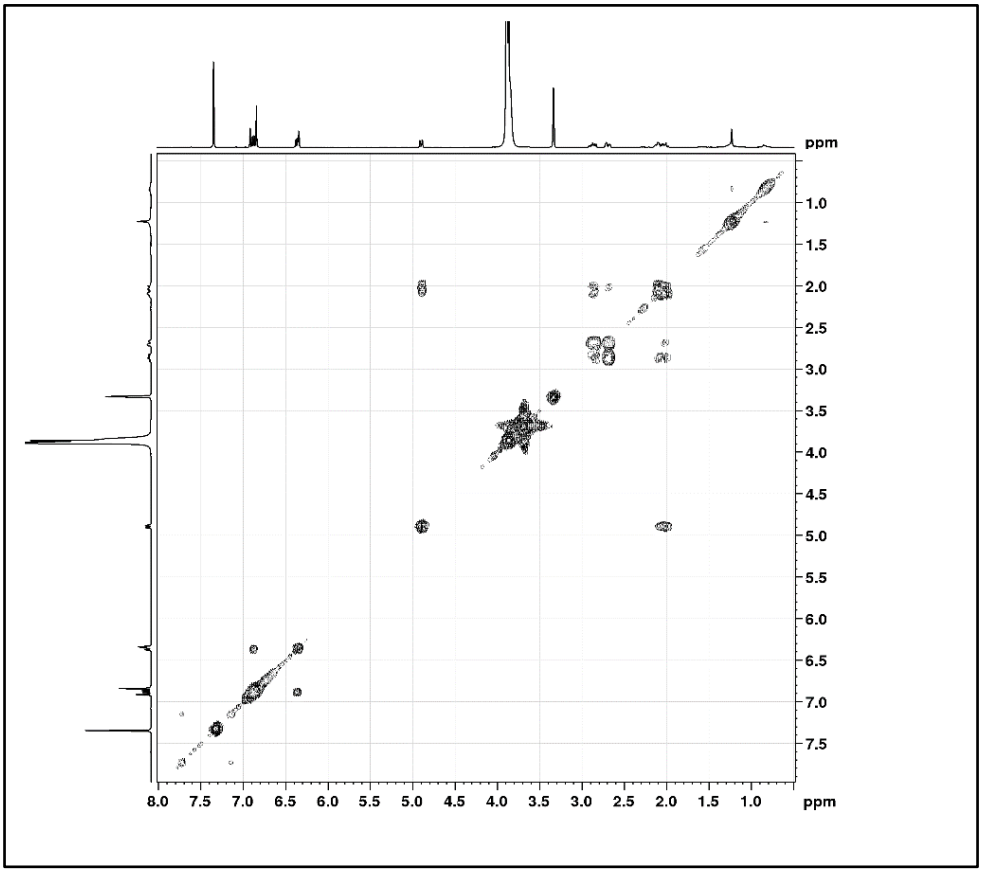


Figure S13 ^{1}H–^{1}H COSY spectrum of **2**

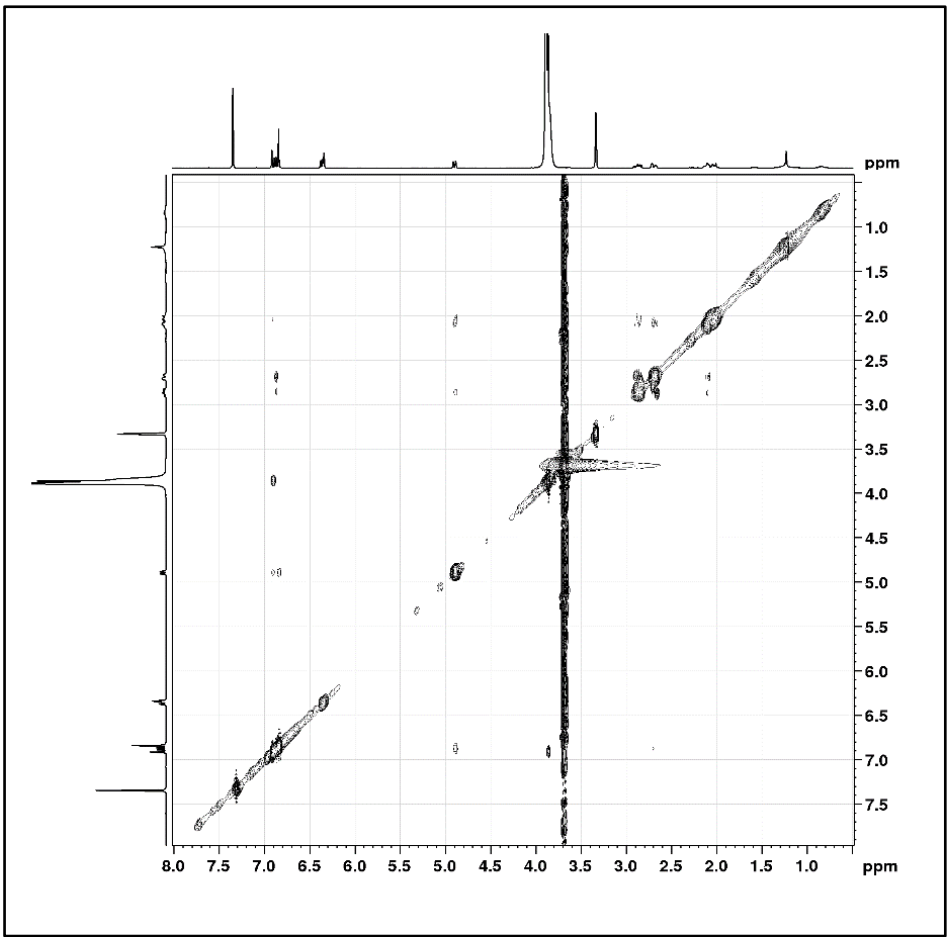


Figure S14 NOESY spectrum of **2**

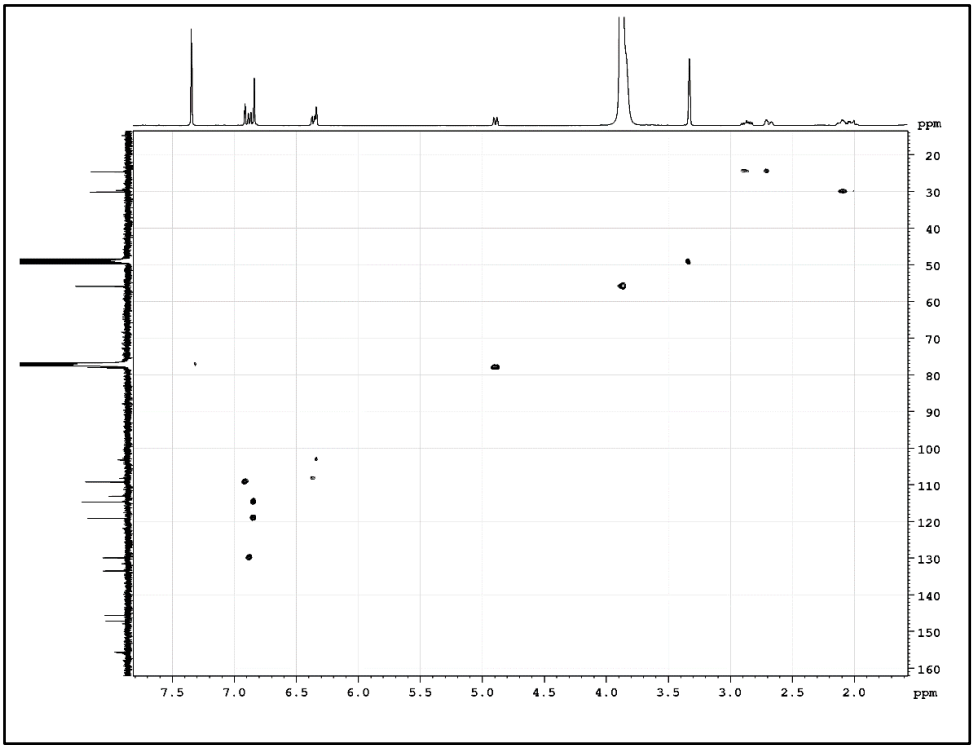


Figure S15 HMQC spectrum of **2**

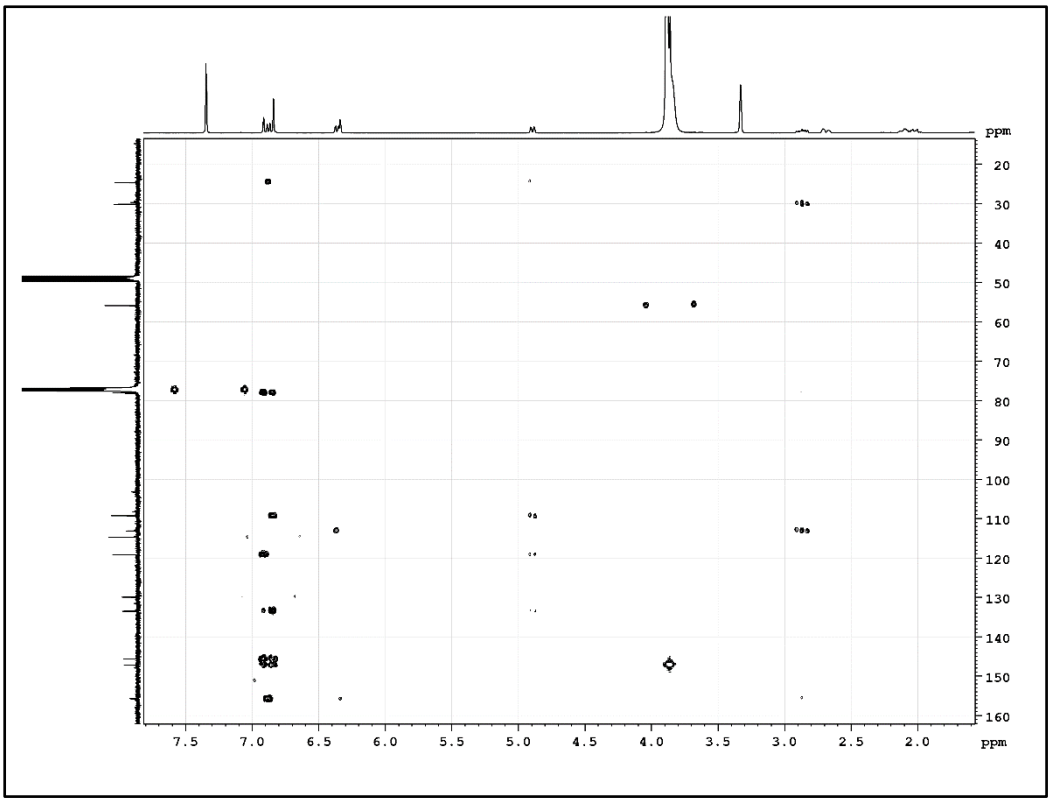
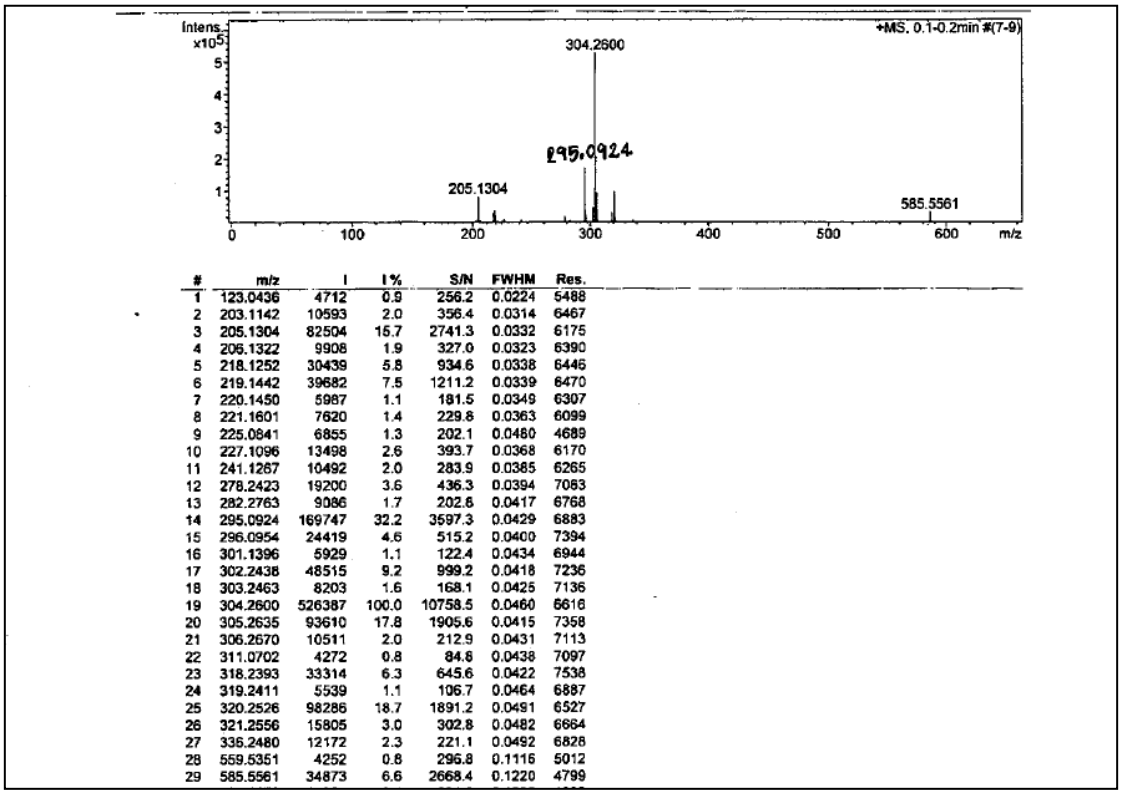


Figure S16 HMBC spectrum of **2**



#	m/z	I	I %	S/N	FWHM	Res.
1	123.0436	4712	0.9	256.2	0.0224	5488
2	203.1142	10593	2.0	356.4	0.0314	6467
3	205.1304	82504	15.7	2741.3	0.0332	6175
4	206.1322	9908	1.9	327.0	0.0323	6390
5	218.1252	30439	5.8	934.6	0.0338	6446
6	219.1442	39682	7.5	1211.2	0.0339	6470
7	220.1450	5987	1.1	181.5	0.0349	6307
8	221.1601	7620	1.4	229.8	0.0363	6099
9	225.0841	6855	1.3	202.1	0.0480	4689
10	227.1096	13498	2.6	393.7	0.0368	6170
11	241.1267	10492	2.0	283.9	0.0385	6265
12	278.2423	19200	3.6	436.3	0.0394	7083
13	282.2763	9086	1.7	202.6	0.0417	6768
14	295.0924	169747	32.2	3597.3	0.0429	6883
15	296.0954	24419	4.6	515.2	0.0400	7394
16	301.1396	5929	1.1	122.4	0.0434	6944
17	302.2438	48515	9.2	999.2	0.0418	7236
18	303.2463	8203	1.6	168.1	0.0425	7136
19	304.2600	526387	100.0	10758.5	0.0460	6616
20	305.2635	93610	17.8	1905.6	0.0415	7358
21	306.2670	10511	2.0	212.9	0.0431	7113
22	311.0702	4272	0.8	84.8	0.0438	7097
23	318.2393	33314	6.3	645.6	0.0422	7538
24	319.2411	5539	1.1	106.7	0.0464	6887
25	320.2526	98286	18.7	1891.2	0.0491	6527
26	321.2556	15805	3.0	302.8	0.0482	6664
27	336.2480	12172	2.3	221.1	0.0492	6828
28	559.5351	4252	0.8	296.8	0.1116	5012
29	585.5561	34873	6.6	2668.4	0.1220	4799

Figure S17 Mass spectrum of **2**

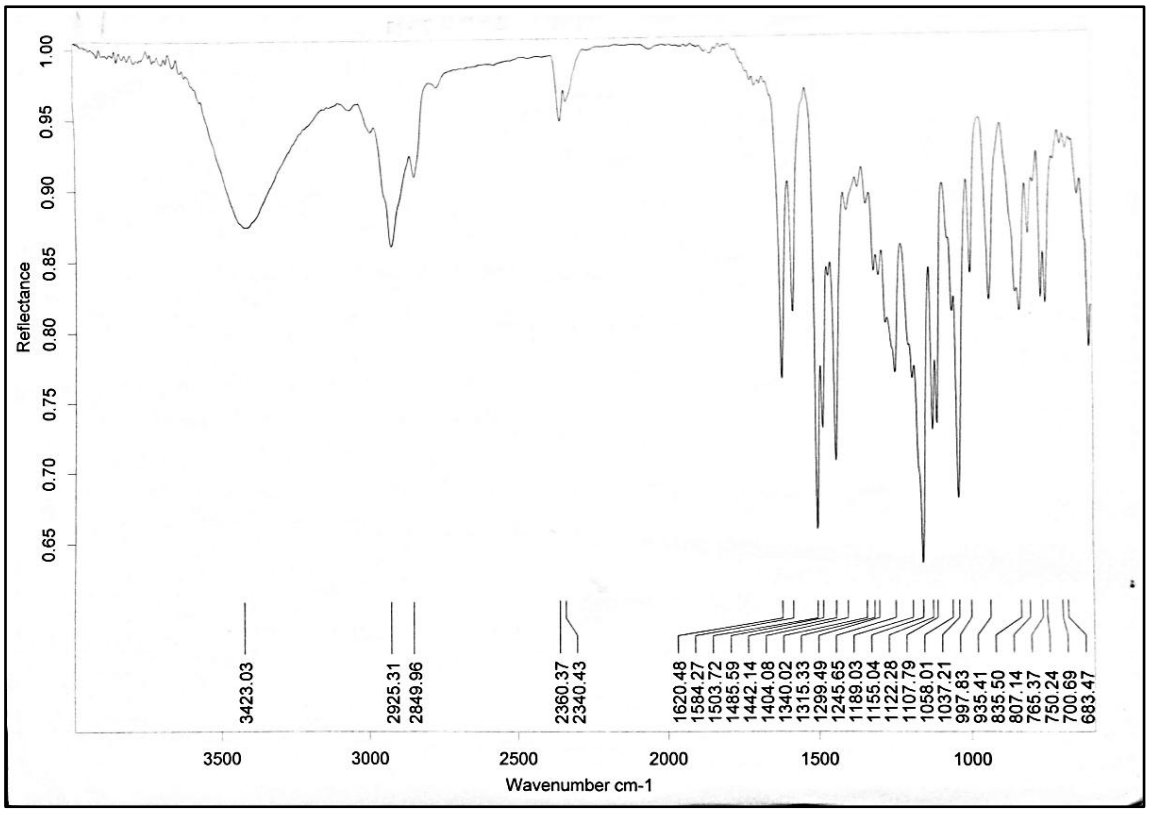


Figure S18 IR spectrum of **3**

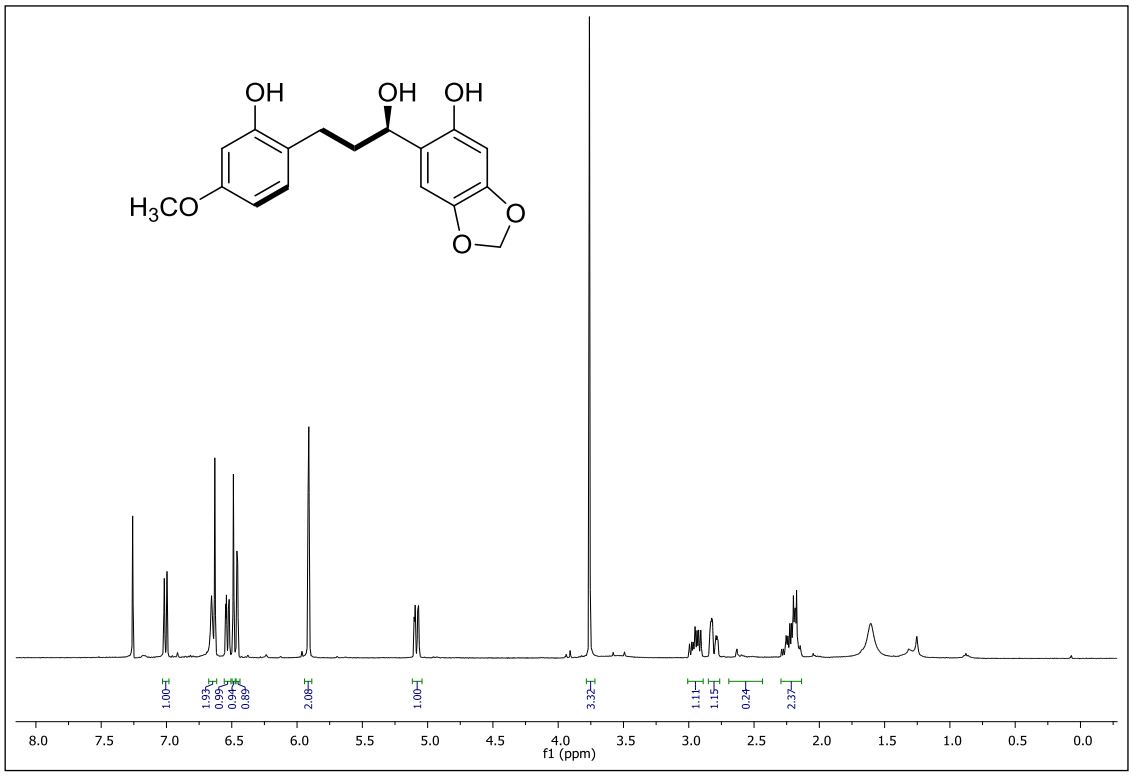


Figure S19 ^{1}H NMR spectrum of **3**

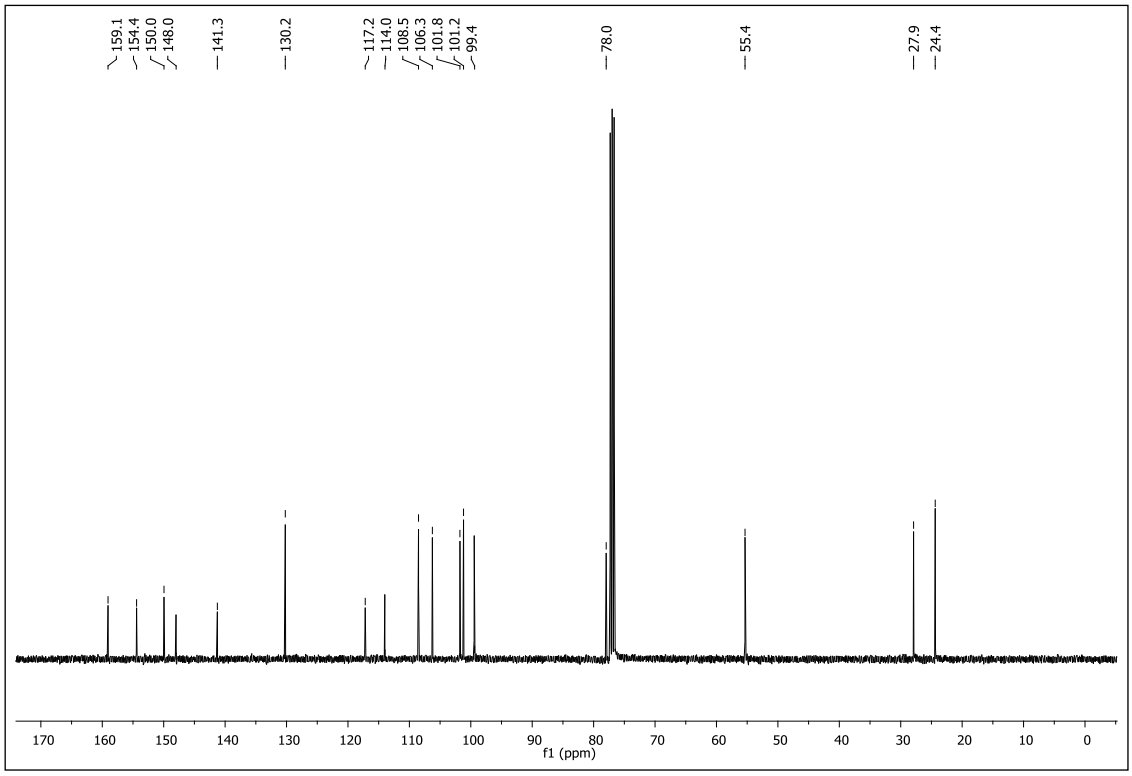


Figure S20 ^{13}C NMR spectrum of **3**

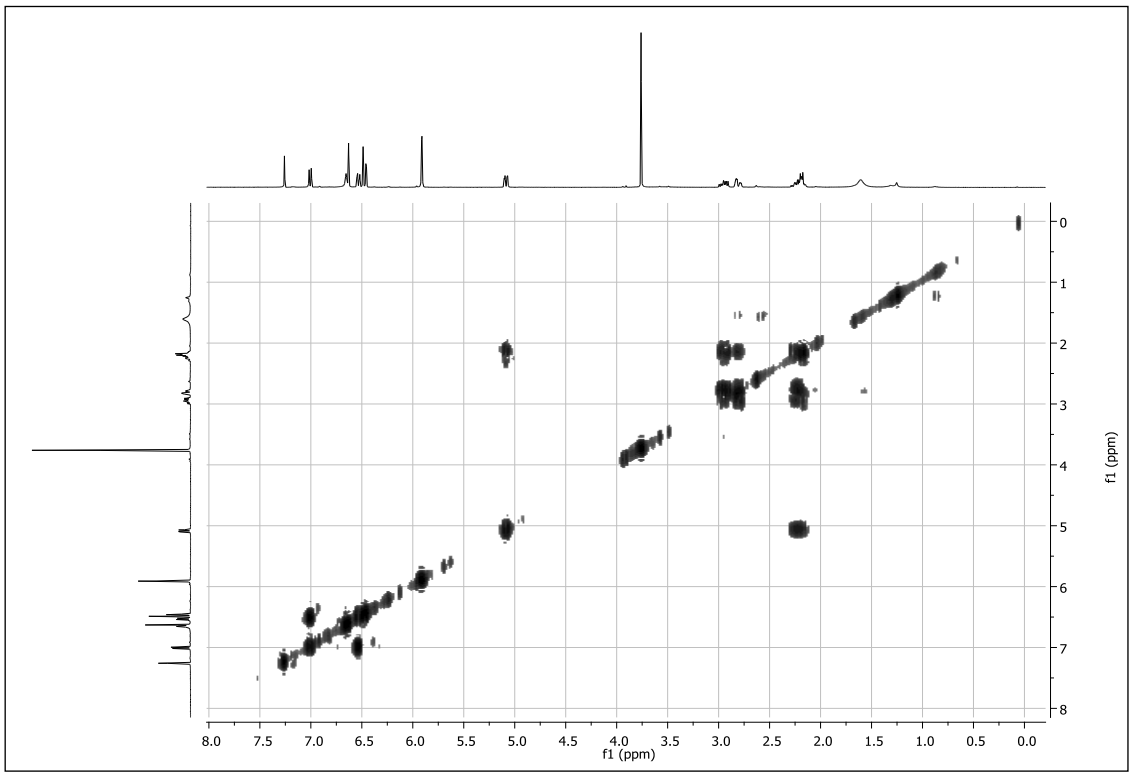


Figure S21 ^{1}H–^{1}H COSY spectrum of **3**

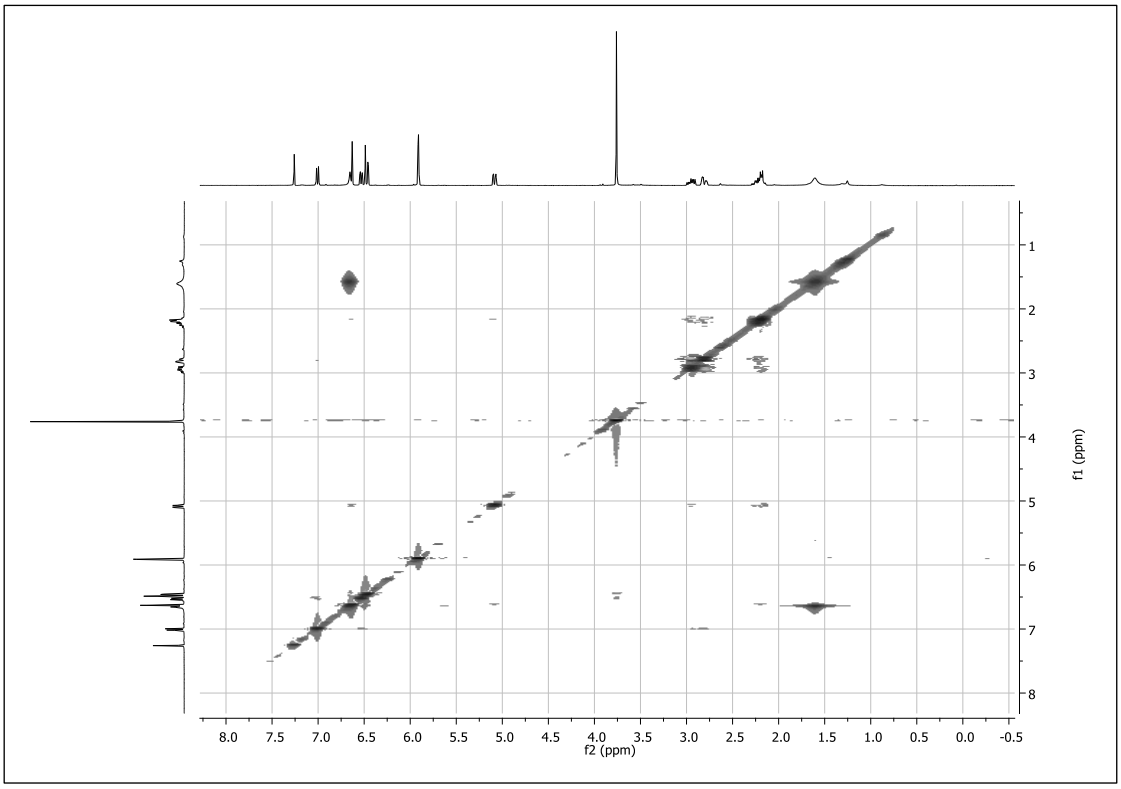


Figure S22 NOESY spectrum of **3**

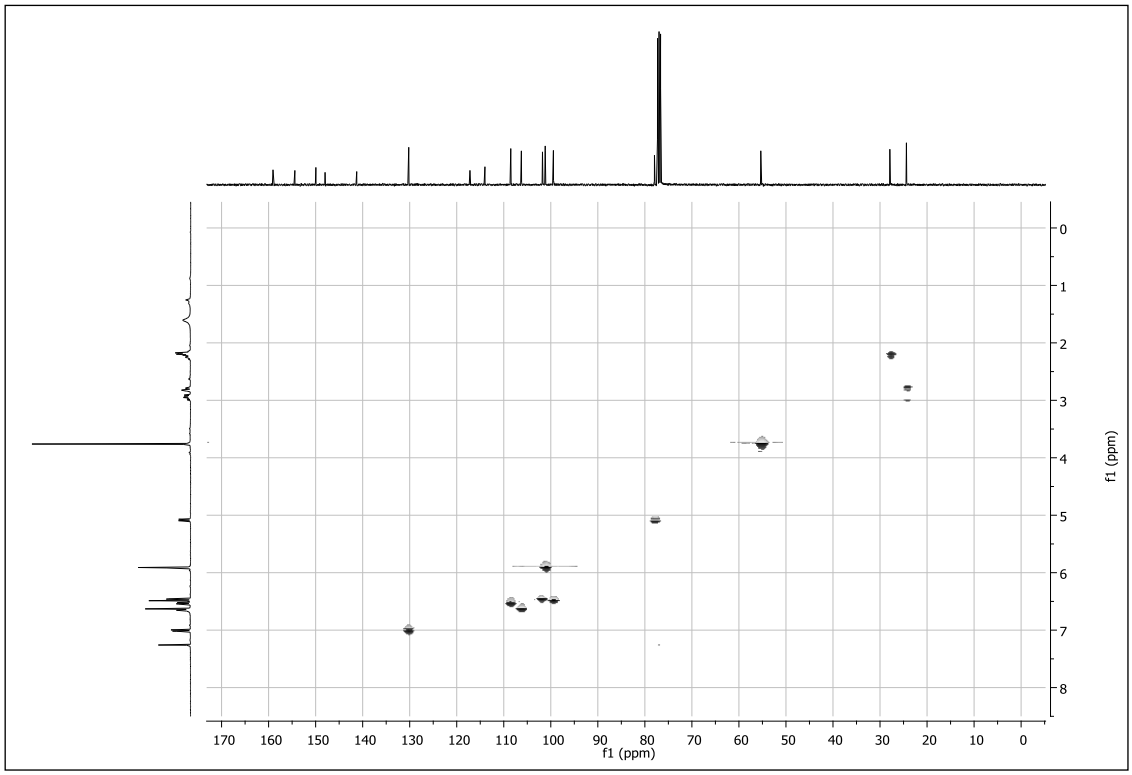


Figure S23 HMQC spectrum of **3**

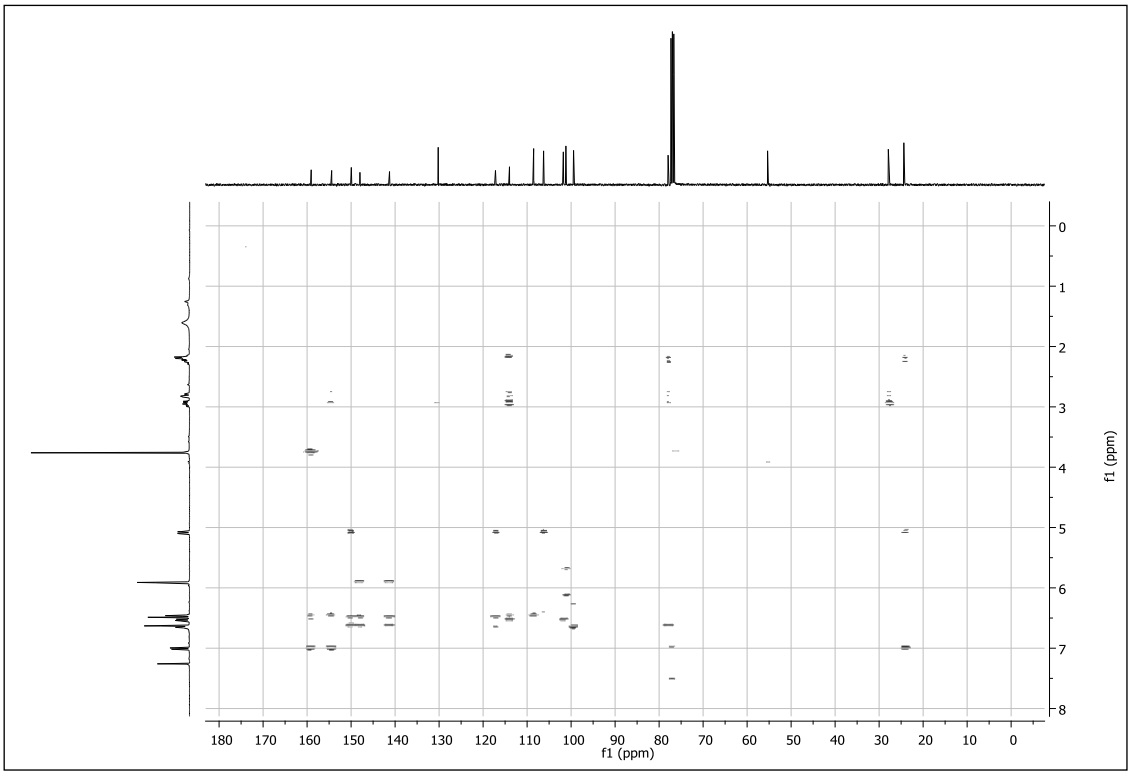
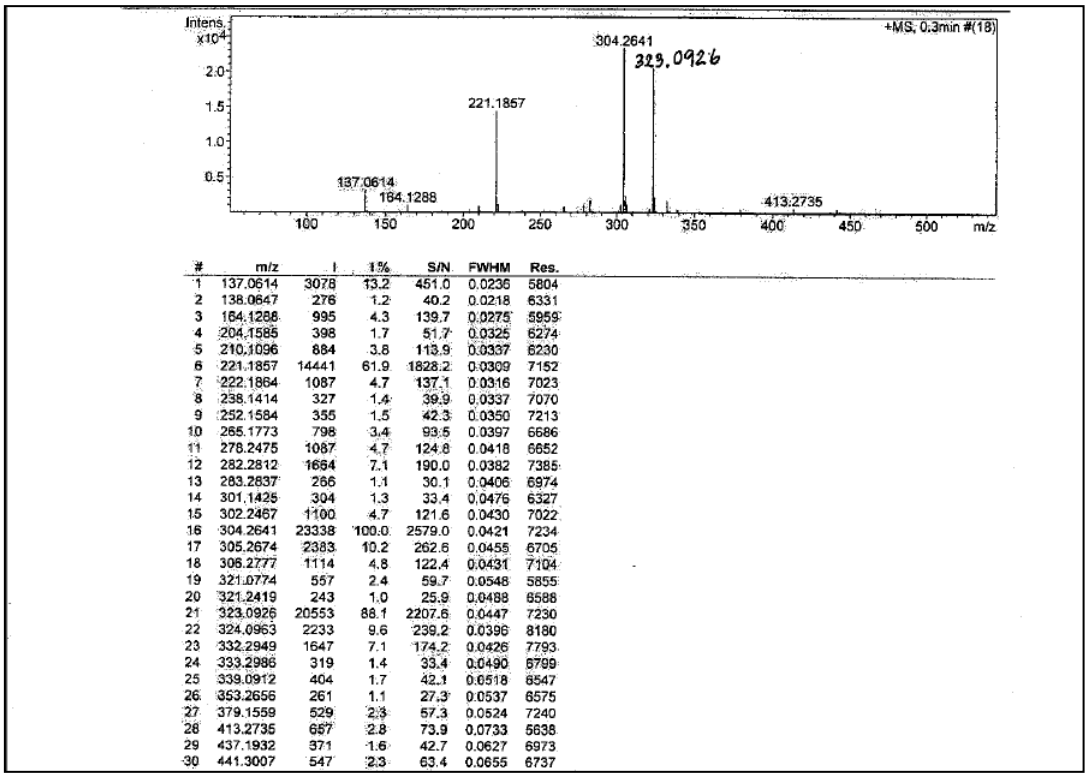


Figure S24 HMBC spectrum of **3**



#	m/z	I	I%	S/N	FWHM	Res.
1	137.0614	3078	13.2	451.0	0.0236	5804
2	138.0647	276	1.2	40.2	0.0218	6331
3	164.1288	995	4.3	139.7	0.0275	5959
4	204.1585	398	1.7	51.7	0.0325	6274
5	210.1096	884	3.8	113.9	0.0337	6230
6	221.1857	14441	61.9	1828.2	0.0309	7152
7	222.1864	1087	4.7	137.1	0.0316	7023
8	238.1414	327	1.4	39.9	0.0337	7070
9	252.1584	355	1.5	42.3	0.0350	7213
10	265.1773	798	3.4	93.5	0.0397	6686
11	278.2475	1087	4.7	124.8	0.0418	6652
12	282.2812	1684	7.1	190.0	0.0382	7385
13	283.2837	266	1.1	30.1	0.0406	6974
14	301.1425	304	1.3	33.4	0.0476	6327
15	302.2467	1100	4.7	121.6	0.0430	7022
16	304.2641	23338	100.0	2579.0	0.0421	7234
17	305.2674	2383	10.2	262.6	0.0455	6705
18	306.2777	1114	4.8	122.4	0.0431	7104
19	321.0774	557	2.4	59.7	0.0548	5855
20	321.2419	243	1.0	25.9	0.0488	6588
21	323.0926	20553	88.1	2207.6	0.0447	7230
22	324.0963	2233	9.6	239.2	0.0396	8180
23	332.2949	1647	7.1	174.2	0.0426	7793
24	333.2986	319	1.4	33.4	0.0490	6799
25	339.0912	404	1.7	42.1	0.0518	6547
26	353.2656	261	1.1	27.3	0.0537	6575
27	379.1559	529	2.3	57.3	0.0524	7240
28	413.2735	657	2.8	73.9	0.0733	5638
29	437.1932	371	1.6	42.7	0.0627	6973
30	441.3007	547	2.3	63.4	0.0655	6737

Figure S25 Mass spectrum of **3**