

Supplementary data

Oxidation mechanism of black tea pigment theaflavin by peroxidase

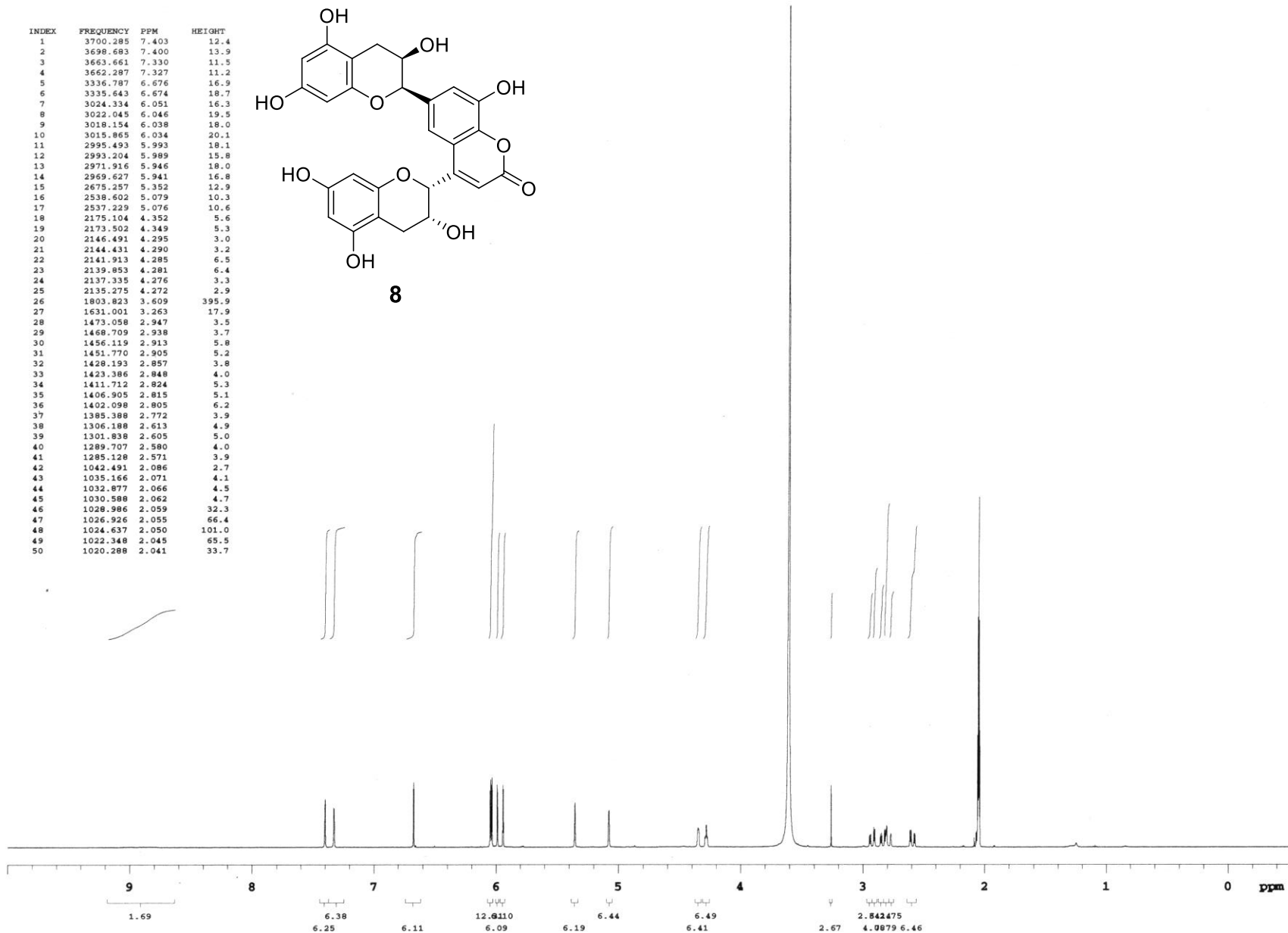
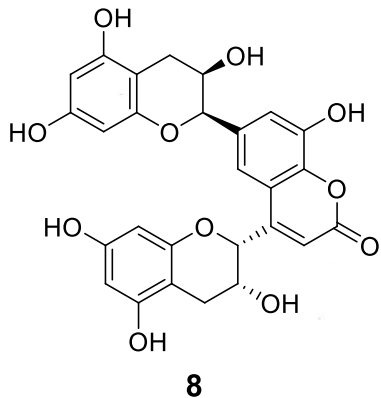
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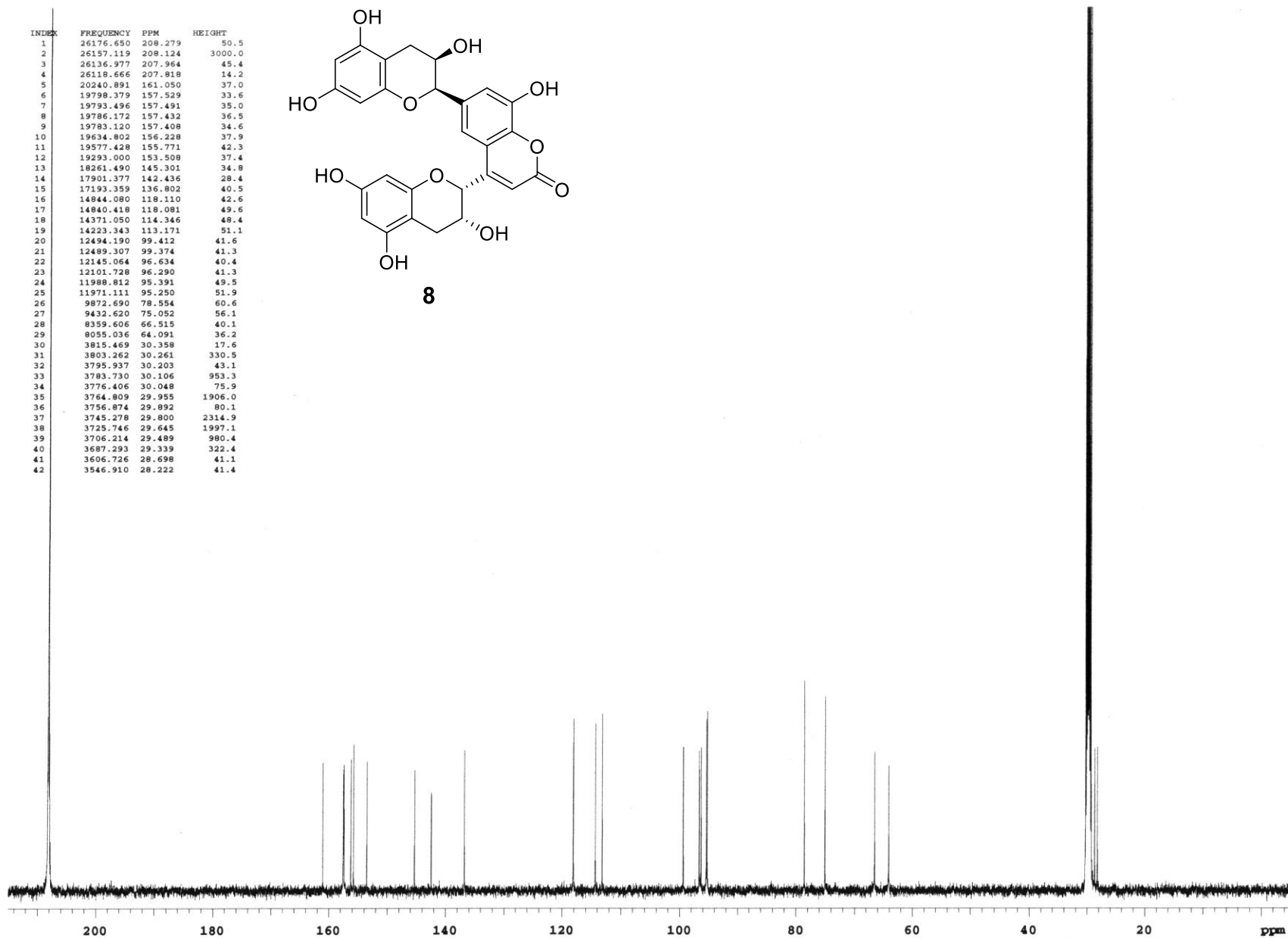
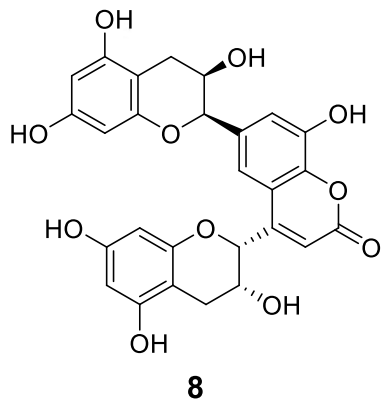
S1. ¹H NMR spectrum of 8 (acetone-d₆ + D₂O, 500 MHz).

INDEX	FREQUENCY	PPM	HEIGHT
1	3700.288	7.403	12.4
2	3699.883	7.400	13.9
3	3663.661	7.330	11.5
4	3662.287	7.327	11.2
5	3336.787	6.676	16.9
6	3335.643	6.674	18.7
7	3024.334	6.051	16.3
8	3022.045	6.046	19.5
9	3018.154	6.038	18.0
10	3015.865	6.034	20.1
11	2995.493	5.993	18.1
12	2993.204	5.989	15.8
13	2971.916	5.946	18.0
14	2969.627	5.941	16.8
15	2675.257	5.352	12.9
16	2538.602	5.079	10.3
17	2537.229	5.076	10.6
18	2175.104	4.352	5.6
19	2173.502	4.349	5.3
20	2146.491	4.295	3.0
21	2144.431	4.290	3.2
22	2141.913	4.285	6.5
23	2139.853	4.281	6.4
24	2137.335	4.276	3.3
25	2135.275	4.272	2.9
26	1803.823	3.609	395.9
27	1631.001	3.263	17.9
28	1473.058	2.947	3.5
29	1468.709	2.938	3.7
30	1456.119	2.913	5.8
31	1451.770	2.905	5.2
32	1428.193	2.857	3.8
33	1423.386	2.848	4.0
34	1411.712	2.824	5.3
35	1406.905	2.815	5.1
36	1402.098	2.805	6.2
37	1388.388	2.772	3.9
38	1306.188	2.613	4.9
39	1301.838	2.605	5.0
40	1289.707	2.580	4.0
41	1285.128	2.571	3.9
42	1042.491	2.086	2.7
43	1035.166	2.071	4.1
44	1032.877	2.066	4.5
45	1030.588	2.062	4.7
46	1028.986	2.059	32.3
47	1026.926	2.055	66.4
48	1024.637	2.050	101.0
49	1022.348	2.045	65.5
50	1020.288	2.041	33.7

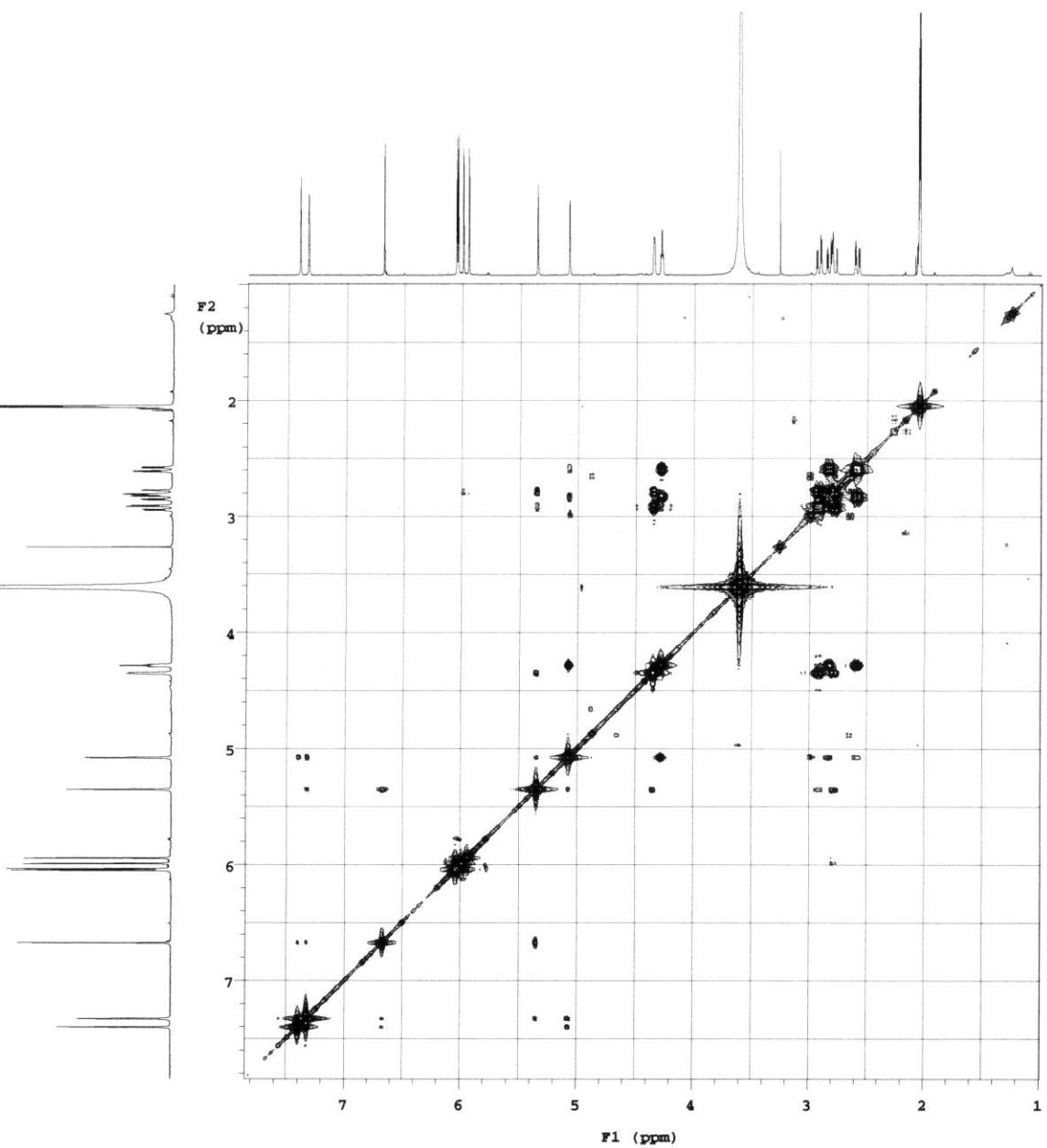
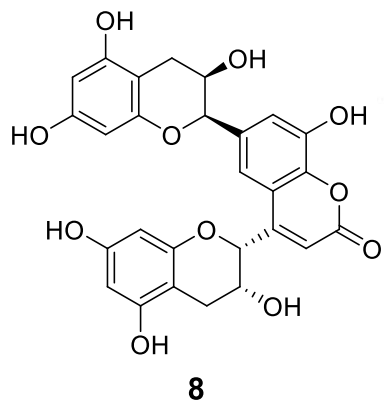


S2. ¹³C NMR spectrum of 8 (acetone-d₆ + D₂O, 125 MHz).

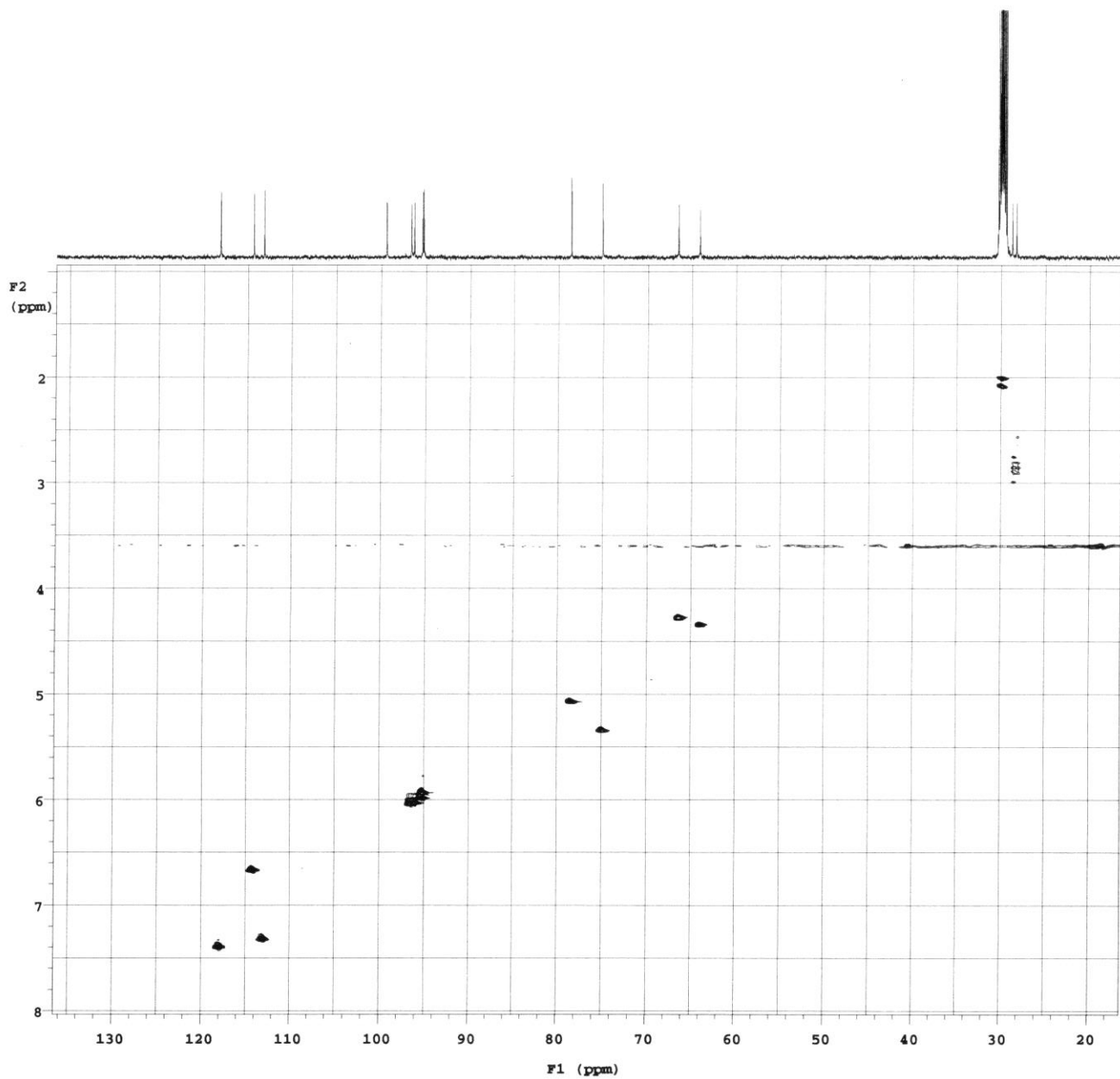
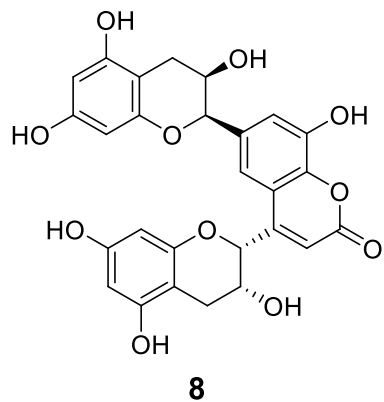
INDEX	FREQUENCY	PPM	HEIGHT
1	26176.650	208.279	50.5
2	26157.119	208.124	3000.0
3	26136.977	207.964	45.4
4	26118.666	207.818	14.2
5	20240.891	161.050	37.0
6	19798.379	157.529	33.6
7	19793.496	157.491	35.0
8	19786.172	157.432	36.5
9	19783.120	157.408	34.6
10	19634.802	156.228	37.9
11	19577.428	155.771	42.3
12	19293.000	153.508	37.4
13	18261.490	145.301	34.8
14	17901.377	142.436	28.4
15	17193.359	136.802	40.5
16	14844.080	118.110	42.6
17	14840.418	118.081	49.6
18	14371.050	114.346	48.4
19	14223.343	113.171	51.1
20	12494.190	99.412	41.6
21	12489.307	99.374	41.3
22	12145.064	96.634	40.4
23	12101.728	96.290	41.3
24	11988.812	95.391	49.5
25	11971.111	95.250	51.9
26	9872.690	78.554	60.6
27	9432.620	75.052	56.1
28	8359.606	66.515	40.1
29	8055.036	64.091	36.2
30	3815.469	30.358	17.6
31	3803.262	30.261	330.5
32	3795.937	30.203	43.1
33	3783.730	30.106	953.3
34	3776.406	30.048	75.9
35	3764.809	29.955	1906.0
36	3756.874	29.892	80.1
37	3745.278	29.800	2314.9
38	3725.746	29.645	1997.1
39	3706.214	29.489	980.4
40	3687.293	29.339	322.4
41	3606.726	28.698	41.1
42	3546.910	28.222	41.4



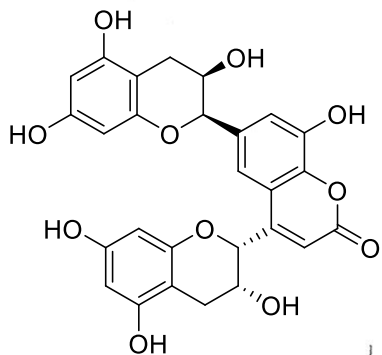
S3. ^1H - ^1H COSY spectrum of 8 (acetone- d_6 + D_2O).



S4. HSQC spectrum of 8 (acetone- d_6 + D_2O).



S5. HMBC spectrum of 8 (acetone- d_6 + D_2O).



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