Supplementary material

Morindaquinone, a new bianthraquinone from *Morinda coreia* roots

Suwadee Chokchaisiri, Yuttana Siriwattanasathien, Chopaka Thongbamrer, Apichart Suksamrarn and Thitima Rukachaisirikul*

Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand

ABSTRACT

Phytochemical investigation of the roots of *Morinda coreia* led to the isolation of one new bianthraquinone, morindaquinone (**1**), together with 12 known compounds, soranjidiol (**2**), rubiadin-1-methyl ether (**3**), 2-methoxy-1,3,6-trihydroxyanthraquinone (**4**), 1-hydroxy-2-methylanthraquinone (**5**), tectoquinone (**6**), nordamnacanthal (**7**), damnacanthal (**8**), 2-formylanthraquinone (**9**), 3-hydroxy-2-hydroxymethyl-anthraquinone (**10**), lucidin-ω-methyl ether (**11**), scopoletin (**12**) and (+)-mellein (**13**). The structures of these compounds were determined on the basis of extensive spectroscopic analyses, as well as by comparison with literature reports. Compound **1** was the first example of bianthraquinone found in the genus *Morinda*, whereas compound **13** was firstly isolated from this genus. Among them, compounds **2**, **7**, **8** and **10** exhibited moderate to weak cytotoxicity against human cervical (HeLa), human colon (HT 29) and human breast (MCF-7) cell lines, while compounds **6** and **9**–**11** showed weak anti-acetylcholinesterase activity.

Table of Contents **Page**

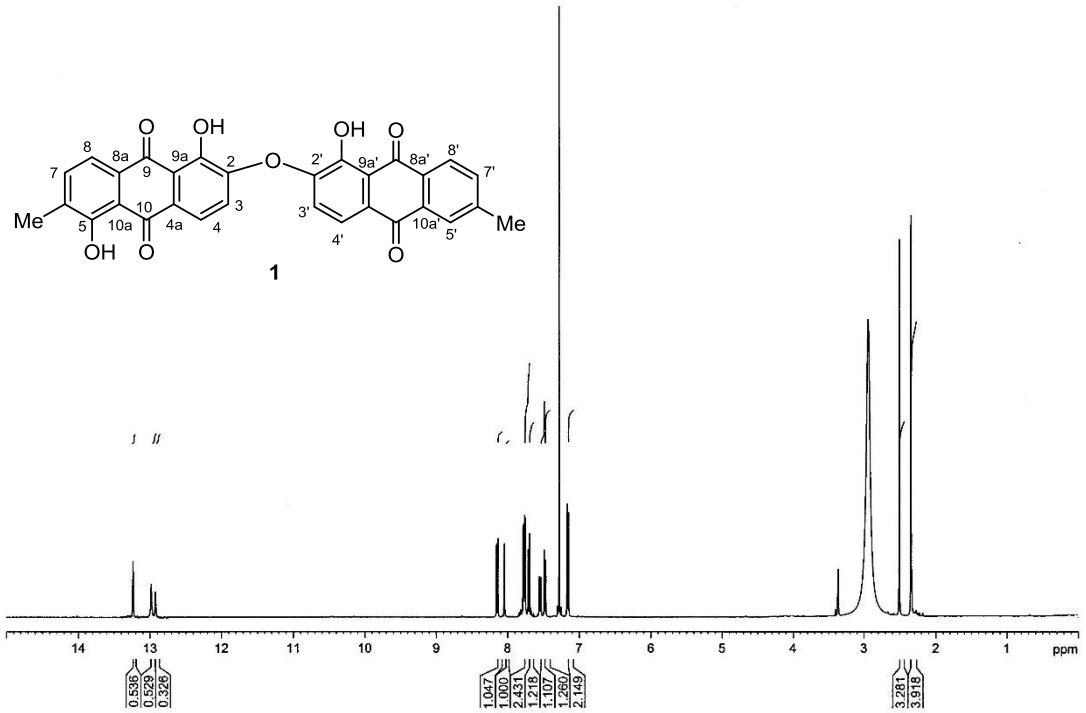


Figure S1. ^{1}H NMR spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

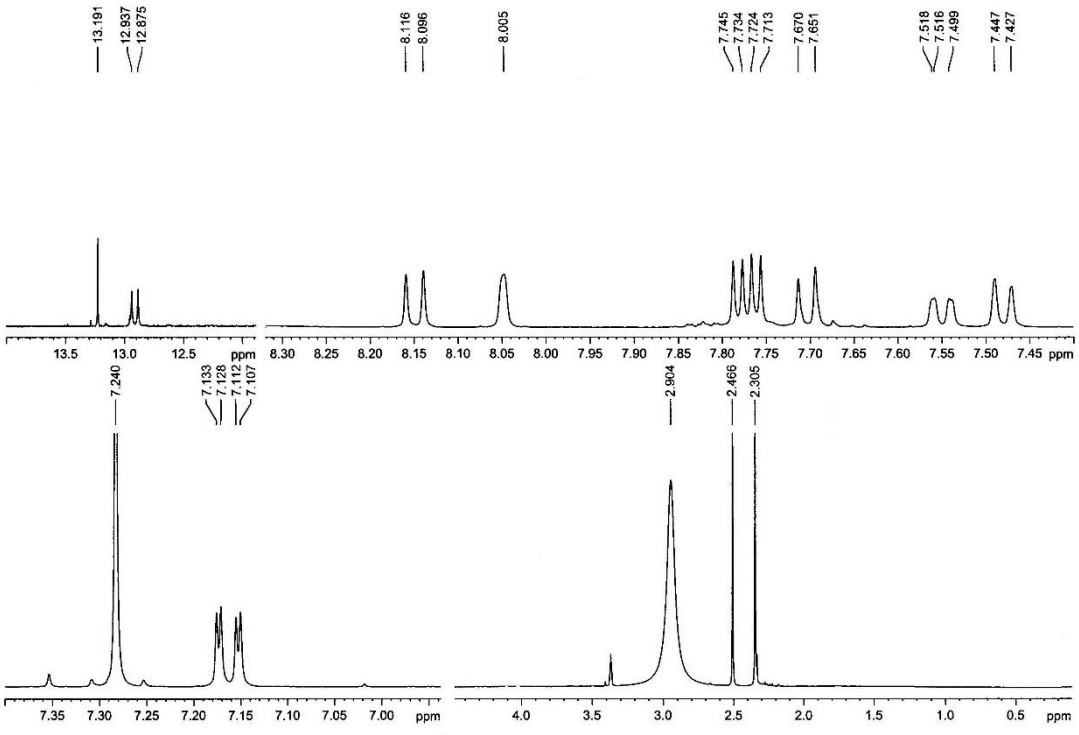


Figure S2. Expansion of ^{1}H NMR spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

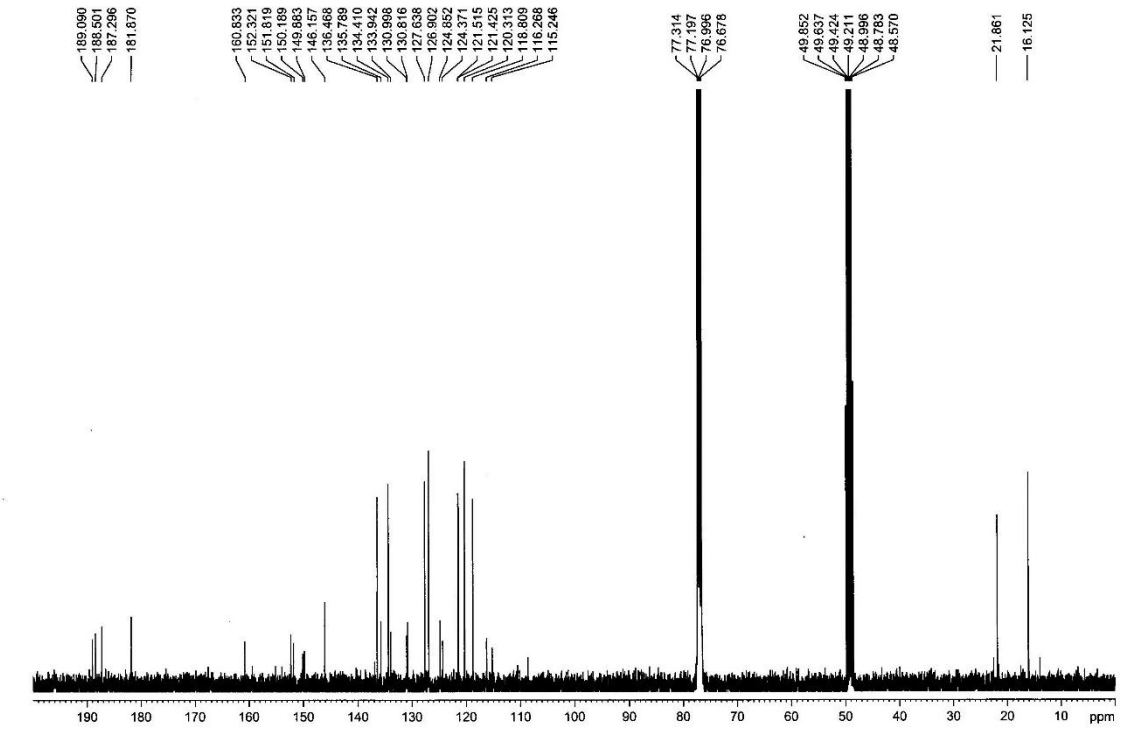


Figure S3. ^{13}C NMR spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

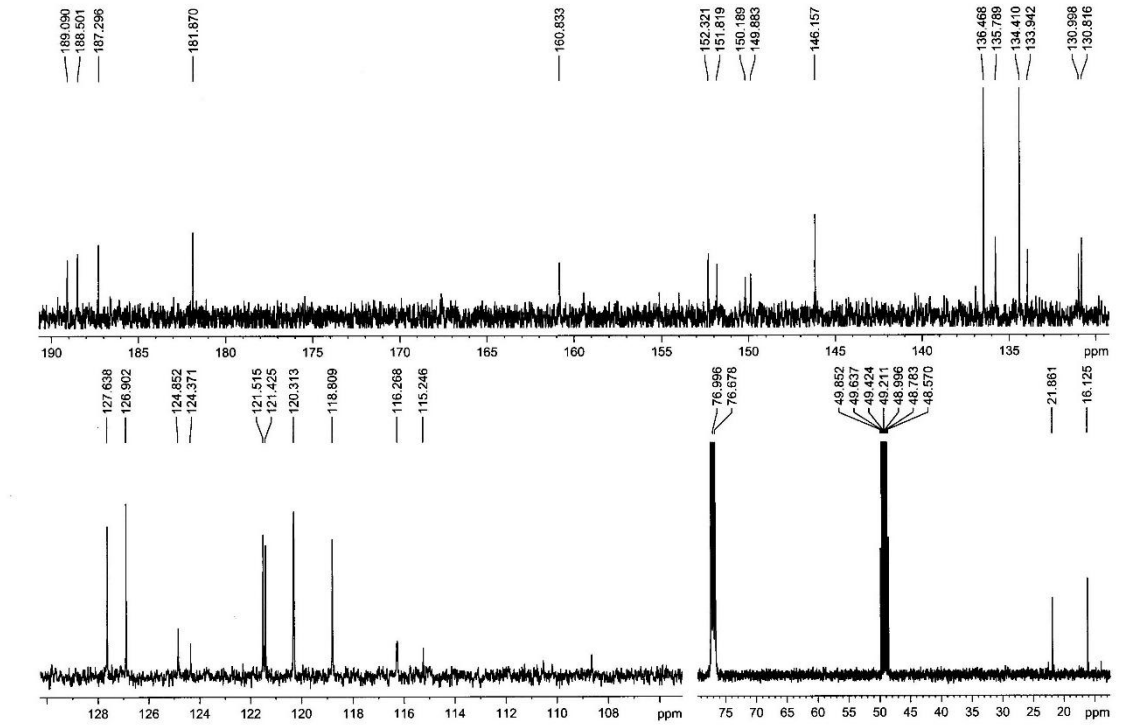


Figure S4. Expansion of ^{13}C NMR spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

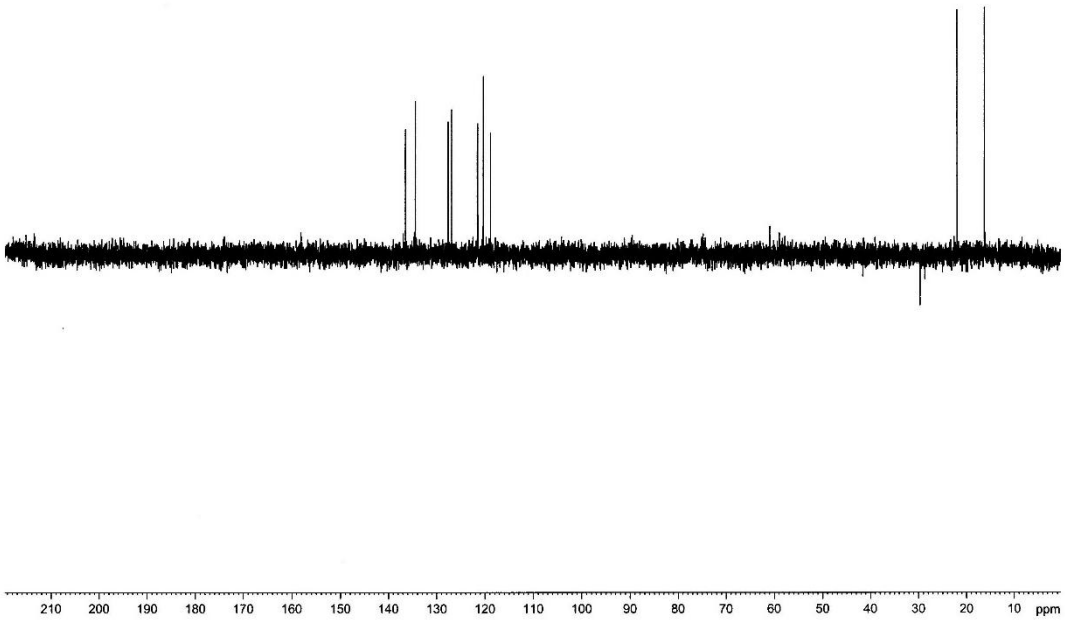


Figure S5. DEPT135 spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

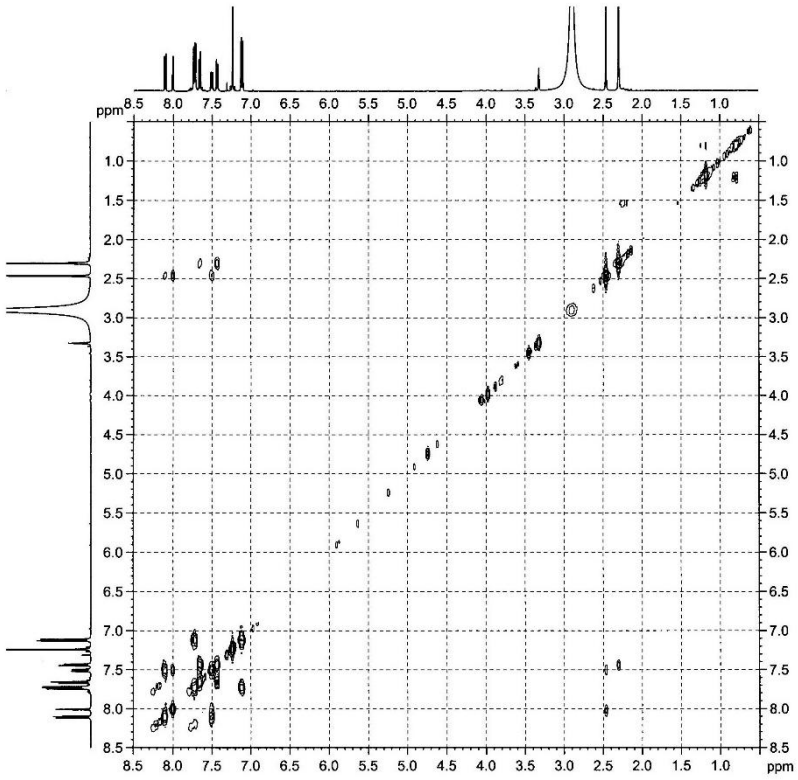


Figure S6. ^1H, ^1H-COSY spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

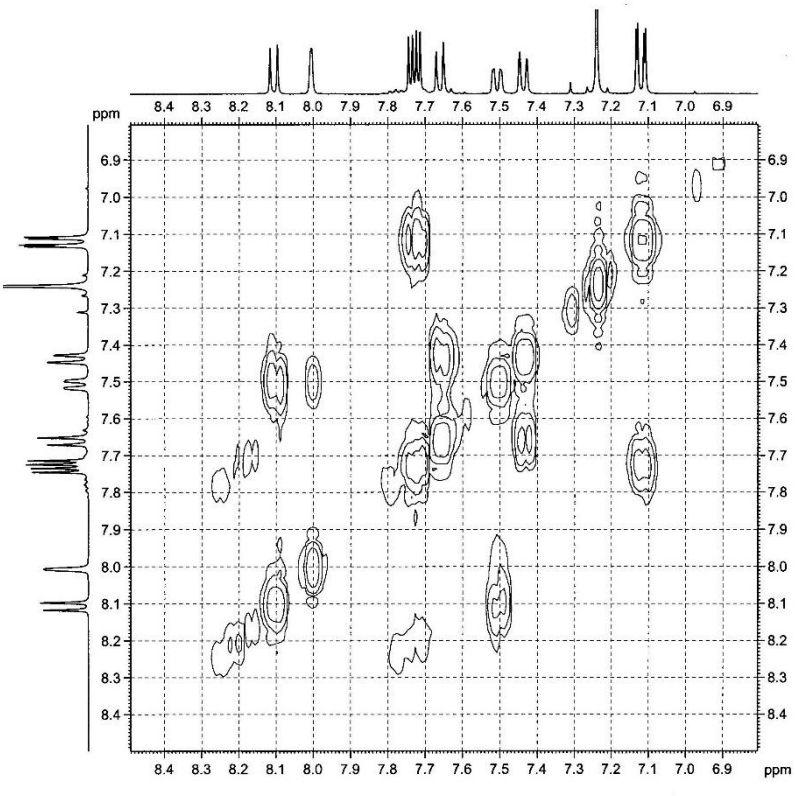


Figure S7. Expansion of ^{1}H, ^{1}H-COSY spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

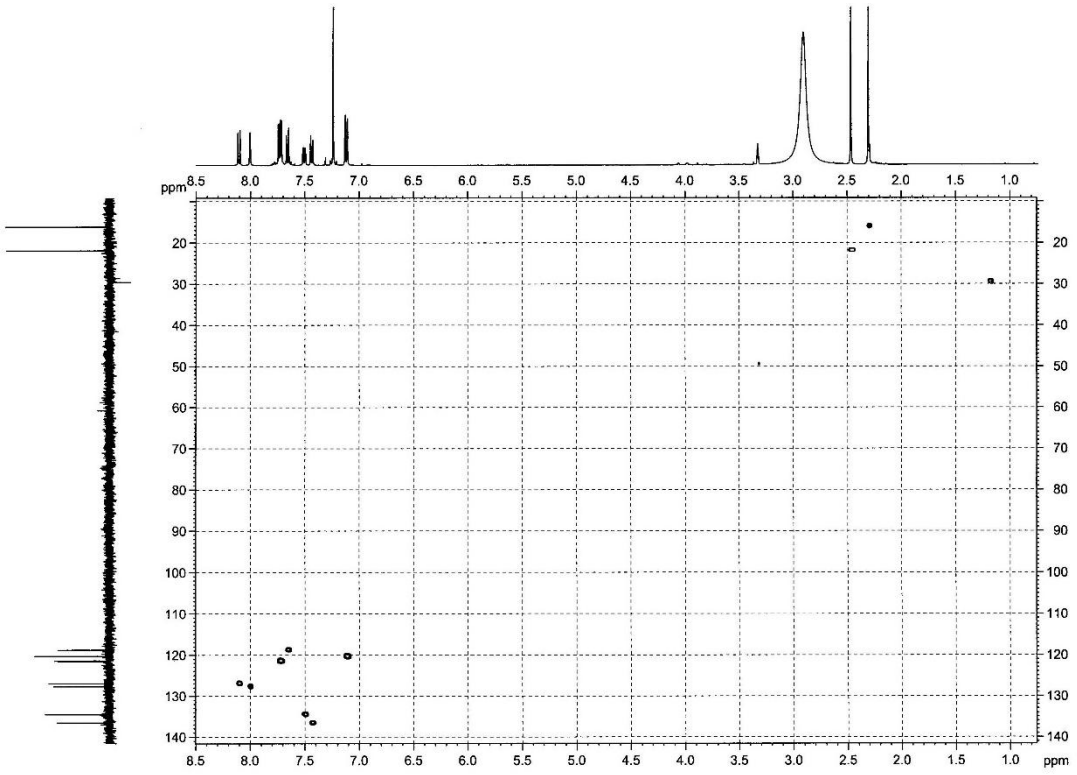


Figure S8. HSQC spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

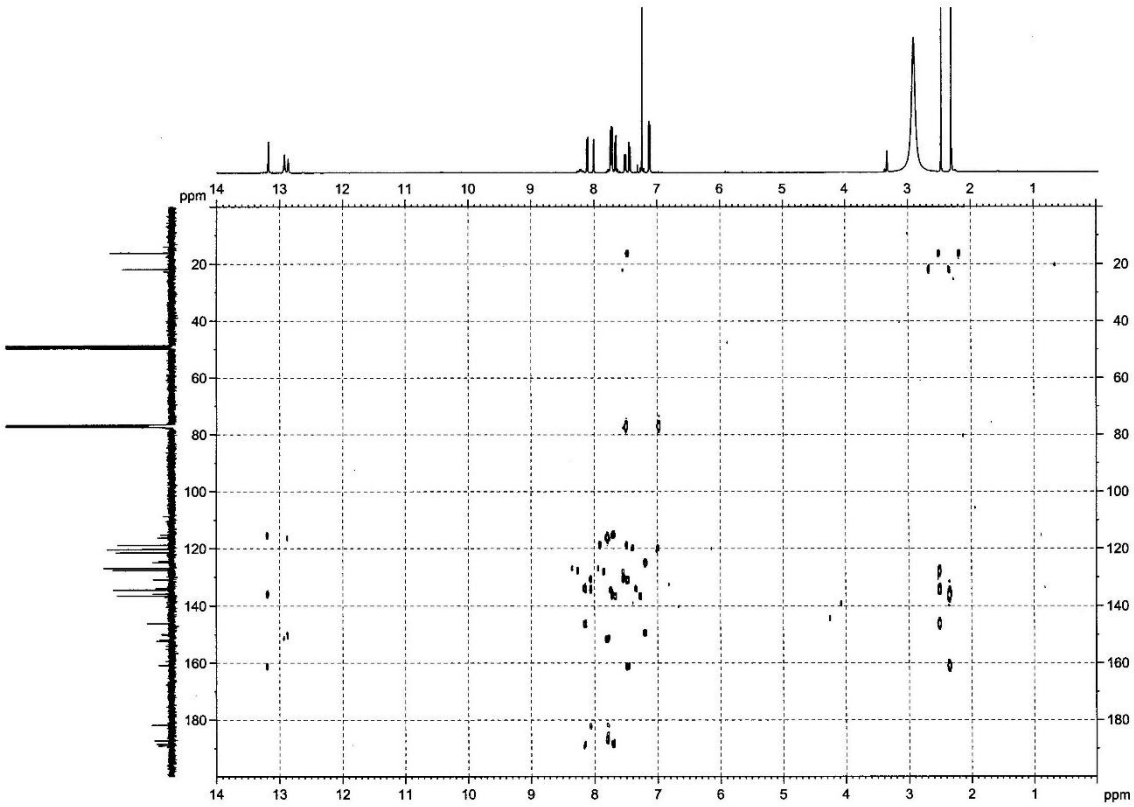


Figure S9. HMBC spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD

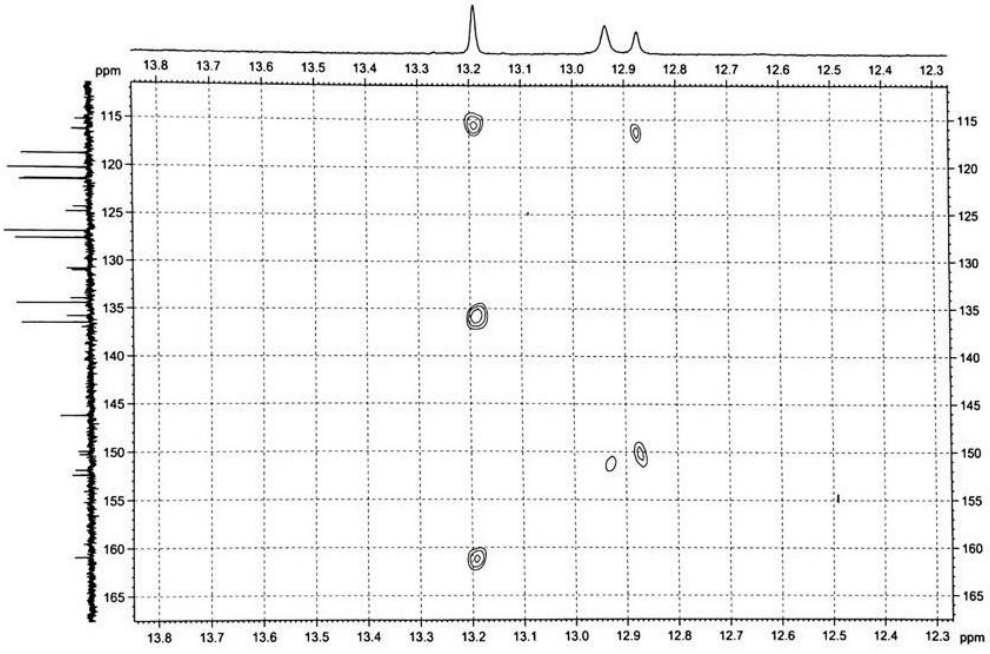
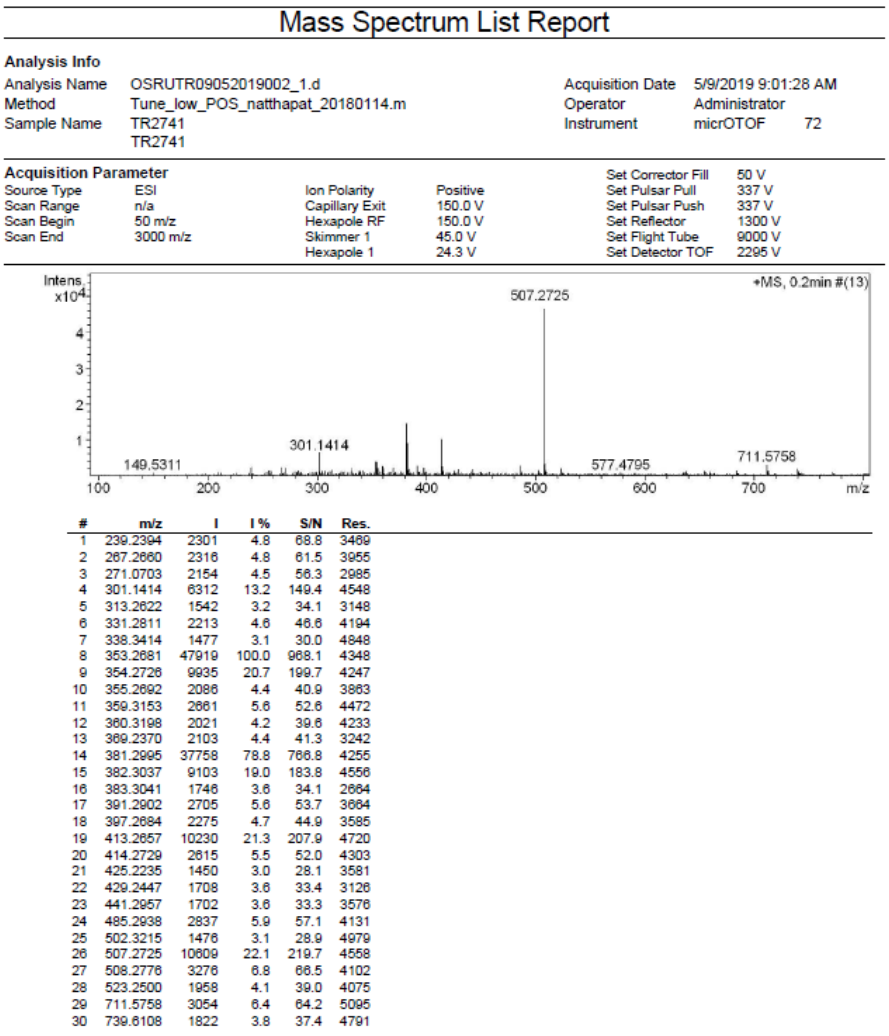


Figure S10. Expansion of HMBC spectrum of morindaquinone (**1**) in $CDCl_3$+1 drop of CD_3OD



Mass Spectrum List Report

Analysis Info

Analysis Name	OSRUTR09052019002_1.d	Acquisition Date	5/9/2019 9:01:28 AM
Method	Tune_low_POS_natthapat_20180114.m	Operator	Administrator
Sample Name	TR2741	Instrument	micrOTOF 72
	TR2741		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	50 V
Scan Range	n/a	Capillary Exit	150.0 V	Set Pulsar Pull	337 V
Scan Begin	50 m/z	Hexapole RF	150.0 V	Set Pulsar Push	337 V
Scan End	3000 m/z	Skimmer 1	45.0 V	Set Reflector	1300 V
		Hexapole 1	24.3 V	Set Flight Tube	9000 V
				Set Detector TOF	2295 V

#	m/z	I	I %	S/N	Res.
1	239.2394	2301	4.8	68.8	3469
2	267.2660	2316	4.8	61.5	3955
3	271.0703	2154	4.5	56.3	2985
4	301.1414	6312	13.2	149.4	4548
5	313.2622	1542	3.2	34.1	3148
6	331.2811	2213	4.6	46.6	4194
7	338.3414	1477	3.1	30.0	4848
8	353.2681	47919	100.0	968.1	4348
9	354.2726	9935	20.7	199.7	4247
10	355.2692	2086	4.4	40.9	3863
11	359.3153	2661	5.6	52.6	4472
12	360.3198	2021	4.2	39.6	4233
13	369.2370	2103	4.4	41.3	3242
14	381.2995	37758	78.8	766.8	4255
15	382.3037	9103	19.0	183.8	4556
16	383.3041	1746	3.6	34.1	2664
17	391.2902	2705	5.6	53.7	3664
18	397.2684	2275	4.7	44.9	3585
19	413.2657	10230	21.3	207.9	4720
20	414.2729	2615	5.5	52.0	4303
21	425.2235	1450	3.0	28.1	3581
22	429.2447	1708	3.6	33.4	3126
23	441.2957	1702	3.6	33.3	3576
24	485.2938	2837	5.9	57.1	4131
25	502.3215	1476	3.1	28.9	4979
26	507.2725	10609	22.1	219.7	4558
27	508.2776	3276	6.8	66.5	4102
28	523.2500	1958	4.1	39.0	4075
29	711.5758	3054	6.4	64.2	5095
30	739.6108	1822	3.8	37.4	4791

Figure S11. HR-ESI-MS spectrum of morindaquinone (**1**)

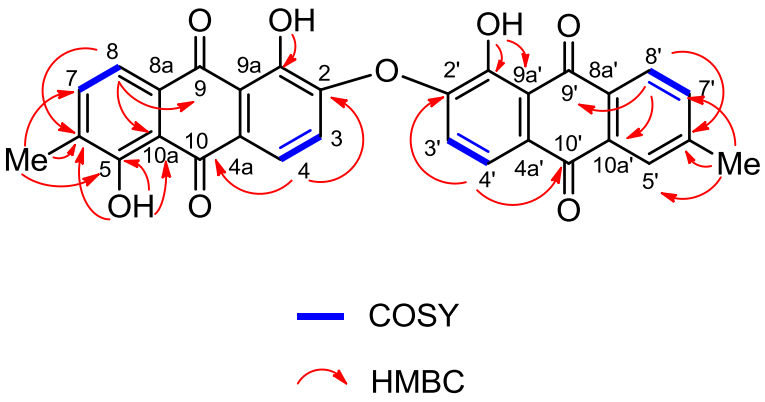


Figure S12. The key COSY and HMBC correlations for morindaquinone (**1**)

Table S1. Anti-acetylcholinesterase and cytotoxic activities of isolated compounds from *M. coreia*.

Compound	Anti-acetylcholinesterase Activity IC_{50} (μM)	Cytotoxicity (IC_{50}, μM)		
		HeLa[c]	HT 29[d]	MCF-7[e]
1	Inactive[b]	Inactive[f]	Inactive[f]	Inactive[f]
2	Inactive[b]	35.40	40.92	25.96
4	Inactive[b]	Inactive[f]	Inactive[f]	Inactive[f]
6	205.46 ± 1.72	-	-	-
7	Inactive[b]	25.78	21.17	35.67
8	Inactive[b]	30.56	37.01	40.63
9	216.00 ± 4.13	-	-	-
10	195.11 ± 3.34	7.89	56.74	10.88
11	304.90 ± 7.02	Inactive[f]	Inactive[f]	Inactive[f]
12	-	Inactive[f]	Inactive[f]	Inactive[f]
Galanthamine[a]	1.01 ± 0.09	-	-	-
Doxorubicin[a]	-	0.68	1.65	0.31

[a]Reference drug
[b]Inactive at 0.1 mg/ml
[c]Human cervical cancer cells
[d]Human colon cancer cells
[e]Human breast cancer cells
[f]Inactive at 50 μg/ml