Supporting information

Benzophenones and Biflavonoids from *Rheedia edulis*

Ulyana Muñoz-Acuña,[†] Mario Figueroa,[†] Adam Kavalier,[†] Nikola Jancovski,[†] Margaret J. Basile,[§] and Edward J. Kennelly[*,†]

[†]Department of Biological Sciences, Lehman College and The Graduate Center, The City University of New York, New York 10468, USA, and [§]Department of Neurology, University of Miami School of Medicine, Florida 33136, USA

Table of contents **Page**

Table S1. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **1a**. S3

Table S2. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **1b**. S5

Table S3. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **1c**. S7

Table S4. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **2a**. S9

Table S5. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **2b**. S11

Table S6. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **2c**. S13

Table S7. Calculated CD Data for Compounds **1** and **2** at the B3LYP/6-31G++(d,p) Level in MeOH S15

Figure S1. Compounds identified from *R. edulis* S16

Figure S2. ^{1}H NMR (300 MHz, d_4-MeOH) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**) S19

Figure S3. ^{13}C NMR (300 MHz, d_4-MeOH) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**) S19

Figure S4. HMBC NMR (300 MHz, d_4-MeOH) of the new compound 32- S20

hydroxy-*ent*-guttiferone M (**1**)

Figure S5. HSQC NMR (300 MHz, d_4-MeOH) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**) S20

Figure S6. ^{1}H NMR (300 MHz, d_4-MeOH) of the new compound 6-*epi*-guttiferone J (**2**). S21

Figure S7. ^{13}C NMR (300 MHz, d_4-MeOH) of the new compound 7-*epi*-guttiferone J (**2**). S21

Figure S8. DPPH and $ABTS^{\bullet+}$ scavenging activity plots of compounds **1–4** (A and C), and extracts (B and D) from *R. edulis*. S22

Table S1. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **1a**.

Number	Atom	X	Y	Z
1	H	-5.8776	0.4556	-0.9208
2	C	-5.0305	0.2041	-1.5746
3	C	-2.8587	-0.4365	-3.2252
4	C	-3.7474	0.0933	-1.0317
5	C	-5.2311	-0.0047	-2.9403
6	C	-4.1397	-0.3252	-3.7789
7	C	-2.6749	-0.2316	-1.8645
8	H	-1.6619	-0.3342	-1.4420
9	H	-1.9980	-0.6893	-3.8680
10	O	-6.4679	0.0930	-3.5345
11	H	-7.0995	0.2630	-2.8471
12	O	-4.2303	-0.5373	-5.1251
13	H	-5.1408	-0.4714	-5.3831
14	C	-1.9491	-1.3143	1.5090
15	O	-2.7947	-2.1794	1.3785
16	C	-0.5935	-1.6071	2.1906
17	C	0.1389	0.7997	1.6308
18	C	0.7905	2.0623	2.2392
19	H	0.0484	2.6118	2.8536
20	H	1.5872	1.7415	2.9520
21	C	-0.7727	-2.6433	3.3184
22	H	0.2258	-2.8420	3.7852
23	H	-1.0809	-3.6116	2.8578
24	C	-1.7671	-2.2750	4.3584
25	H	-2.7002	-1.8199	3.9998
26	C	-1.5963	-2.4995	5.6688
27	C	-2.6527	-2.1370	6.6519
28	H	-3.5925	-1.8344	6.1712
29	H	-2.3180	-1.3020	7.2827
30	H	-2.8765	-2.9839	7.3145
31	C	-0.3711	-3.1075	6.2494
32	H	-0.0081	-2.5192	7.1024
33	H	0.4463	-3.1699	5.5121
34	H	-0.5772	-4.1252	6.6073
35	C	1.0685	0.2158	0.5535
36	C	-0.0304	-0.2841	2.7201
37	O	0.2815	-0.0951	3.8742
38	C	0.5971	-1.1249	-0.0053
39	C	0.4369	-2.1627	1.1356
40	C	-1.2496	1.0393	1.0617
41	C	-2.1870	0.0585	0.9982
42	O	-1.6091	2.2442	0.5510
43	H	-0.8785	2.8503	0.6227
44	C	-3.5510	0.3306	0.4295
45	O	-4.4460	0.7275	1.1504
46	H	2.0784	0.0843	1.0098
47	H	1.1932	0.9508	-0.2746

48	C	1.7935	-2.4065	1.8068
49	H	1.6789	-2.9264	2.7717
50	H	2.3186	-1.4548	1.9955
51	H	2.4500	-3.0173	1.1729
52	C	-0.0663	-3.4859	0.5554
53	H	-0.2620	-4.2159	1.3569
54	H	0.6750	-3.9143	-0.1396
55	H	-0.9997	-3.3592	-0.0097
56	C	1.3944	2.9997	1.2519
57	C	2.7041	3.2606	1.1385
58	C	3.2219	4.2662	0.1252
59	H	0.6967	3.5495	0.5944
60	C	3.7505	2.6081	1.9651
61	H	4.4650	2.0673	1.3290
62	H	3.3221	1.8858	2.6800
63	H	4.3124	3.3550	2.5422
64	C	3.6252	3.5683	-1.1902
65	C	2.4874	2.8833	-1.8544
66	C	2.1006	3.0834	-3.1217
67	C	0.9503	2.3291	-3.6883
68	H	1.2655	1.6862	-4.5300
69	H	0.1777	3.0131	-4.0621
70	H	0.4811	1.6593	-2.9454
71	C	2.7586	4.0419	-4.0454
72	H	3.1774	3.5166	-4.9141
73	H	3.5797	4.5893	-3.5539
74	H	2.0377	4.7819	-4.4176
75	C	1.5523	-1.6011	-1.1083
76	H	2.6006	-1.3255	-0.8760
77	H	1.5388	-2.7191	-1.1617
78	C	1.1674	-1.0161	-2.4196
79	H	1.0586	0.0839	-2.4423
80	C	0.9348	-1.7237	-3.5336
81	C	0.5081	-1.0408	-4.7860
82	H	0.8501	-1.5777	-5.6796
83	H	0.8869	-0.0050	-4.8514
84	H	-0.5947	-0.9903	-4.8239
85	C	1.0450	-3.2026	-3.6128
86	H	1.8875	-3.4925	-4.2550
87	H	0.1329	-3.6397	-4.0401
88	H	1.2052	-3.6593	-2.6215
89	H	-0.4144	-0.9848	-0.4801
90	H	1.9531	2.1454	-1.2287
91	H	4.0833	4.3151	-1.8781
92	H	4.4141	2.8195	-0.9770
93	H	4.1046	4.7994	0.5511
94	O	2.3374	5.3361	-0.1024
95	H	1.5194	4.9571	-0.4108

Table S2. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **1b**.

Number	Atom	X	Y	Z
1	H	5.9029	-0.1173	-0.4074
2	C	5.1039	-0.0011	-1.1528
3	C	3.0461	0.2906	-3.0351
4	C	3.7682	-0.1073	-0.7567
5	C	5.4137	0.2534	-2.4899
6	C	4.3811	0.3961	-3.4449
7	C	2.7511	0.0498	-1.7004
8	H	1.6950	-0.0035	-1.3862
9	H	2.2302	0.4045	-3.7702
10	O	6.7055	0.3659	-2.9470
11	H	7.2790	0.3207	-2.1925
12	O	4.5805	0.6315	-4.7743
13	H	5.5115	0.7185	-4.9338
14	C	1.8377	1.3712	1.4906
15	O	2.7203	2.1955	1.3401
16	C	0.4460	1.7651	2.0325
17	C	-0.3054	-0.6801	1.7179
18	C	-1.0335	-1.8512	2.4139
19	H	-0.3586	-2.3257	3.1536
20	H	-1.8894	-1.4402	3.0000
21	C	0.5710	2.9288	3.0365
22	H	-0.4532	3.2028	3.3975
23	H	0.9396	3.8273	2.4874
24	C	1.4731	2.6729	4.1884
25	H	2.4100	2.1454	3.9653
26	C	1.2184	3.0765	5.4409
27	C	2.1879	2.8221	6.5403
28	H	3.1052	2.3293	6.1916
29	H	1.7380	2.1799	7.3098
30	H	2.4806	3.7639	7.0241
31	C	-0.0199	3.7939	5.8409
32	H	-0.7754	3.7909	5.0375
33	H	0.2021	4.8408	6.0879
34	H	-0.4734	3.3296	6.7265
35	C	-1.1345	-0.2184	0.5064
36	C	-0.1895	0.5266	2.6763
37	O	-0.5901	0.4906	3.8176
38	C	-0.5954	1.0385	-0.1726
39	C	-0.4915	2.2044	0.8447
40	C	1.1162	-1.0088	1.3001
41	C	2.0738	-0.0546	1.1530
42	O	1.3245	-2.3208	1.0431
43	H	2.2499	-2.4771	0.8902
44	C	3.4515	-0.3999	0.6697
45	O	4.2562	-0.9244	1.4185
46	H	-2.1726	-0.0195	0.8644
47	H	-1.2131	-1.0485	-0.2330

48	C	-1.8867	2.5484	1.3790
49	H	-1.8302	3.1746	2.2840
50	H	-2.4484	1.6339	1.6345
51	H	-2.4791	3.0931	0.6319
52	C	0.0854	3.4391	0.1496
53	H	0.2416	4.2578	0.8700
54	H	-0.5934	3.7924	-0.6445
55	H	1.0534	3.2293	-0.3252
56	C	-1.5409	-2.9024	1.4913
57	C	-2.8342	-3.2024	1.3067
58	C	-3.2522	-4.3198	0.3681
59	H	-0.7830	-3.4953	0.9532
60	C	-3.9541	-2.4950	1.9771
61	H	-4.6416	-2.0645	1.2360
62	H	-3.5961	-1.6749	2.6214
63	H	-4.5297	-3.1867	2.6070
64	C	-3.5447	-3.7753	-1.0459
65	C	-2.3562	-3.1619	-1.6907
66	C	-1.8925	-3.4774	-2.9076
67	C	-0.6938	-2.7925	-3.4616
68	H	-0.9349	-2.2480	-4.3924
69	H	0.0986	-3.5157	-3.6937
70	H	-0.2777	-2.0451	-2.7625
71	C	-2.5077	-4.5043	-3.7864
72	H	-2.8931	-4.0451	-4.7064
73	H	-3.3461	-5.0204	-3.2903
74	H	-1.7698	-5.2642	-4.0754
75	C	-1.4631	1.3944	-1.3879
76	H	-2.5282	1.1474	-1.2048
77	H	-1.4352	2.5000	-1.5610
78	C	-0.9916	0.6711	-2.5978
79	H	-0.8744	-0.4230	-2.4884
80	C	-0.6979	1.2537	-3.7684
81	C	-0.1891	0.4442	-4.9096
82	H	-0.4995	0.8629	-5.8751
83	H	-0.5360	-0.6039	-4.8716
84	H	0.9150	0.4277	-4.8886
85	C	-0.8178	2.7125	-4.0200
86	H	-1.6343	2.9153	-4.7259
87	H	0.1077	3.1117	-4.4554
88	H	-1.0256	3.2762	-3.0949
89	H	0.4424	0.8272	-0.5557
90	H	-1.8480	-2.3818	-1.0947
91	H	-3.9495	-4.5962	-1.6805
92	H	-4.3450	-3.0111	-0.9810
93	H	-4.1659	-4.8192	0.7685
94	O	-2.3424	-5.3927	0.3314
95	H	-1.4887	-5.0223	0.1238

Table S3. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **1c**.

Number	Atom	X	Y	Z
1	H	3.3754	0.9066	2.6193
2	C	4.1746	0.1528	2.5059
3	C	6.2127	-1.7482	2.2011
4	C	4.3645	-0.4850	1.2787
5	C	5.0053	-0.1561	3.5839
6	C	6.0327	-1.1166	3.4369
7	C	5.3846	-1.4267	1.1329
8	H	5.5381	-1.9156	0.1632
9	H	7.0088	-2.4917	2.0769
10	O	4.8767	0.4322	4.8194
11	H	4.1734	1.0747	4.7671
12	O	6.8890	-1.4937	4.4321
13	H	6.6937	-0.9875	5.2101
14	C	1.7269	1.5731	0.6603
15	O	2.5347	2.4502	0.4151
16	C	0.3283	1.9021	1.2254
17	C	-0.3317	-0.5538	0.8282
18	C	-1.0372	-1.7622	1.4871
19	H	-0.3567	-2.2481	2.2160
20	H	-1.8962	-1.3846	2.0910
21	C	0.4443	3.0225	2.2762
22	H	-0.5758	3.2485	2.6809
23	H	0.7685	3.9570	1.7598
24	C	1.3920	2.7308	3.3824
25	H	2.3034	2.1696	3.1117
26	C	1.2046	3.1278	4.6486
27	C	2.2128	2.8366	5.7027
28	H	3.0948	2.3062	5.3098
29	H	1.7780	2.2121	6.4950
30	H	2.5680	3.7660	6.1679
31	C	0.0036	3.8747	5.1028
32	H	-0.7964	3.8599	4.3435
33	H	0.2544	4.9245	5.3052
34	H	-0.4036	3.4429	6.0266
35	C	-1.1597	-0.0861	-0.3795
36	C	-0.2657	0.6236	1.8261
37	O	-0.6617	0.5340	2.9669
38	C	-0.6892	1.2278	-1.0018
39	C	-0.6370	2.3520	0.0686
40	C	1.1142	-0.8302	0.4470
41	C	2.0564	0.1479	0.4289
42	O	1.5394	-2.0773	0.1260
43	H	0.7975	-2.6740	0.1226
44	C	3.4898	-0.1679	0.1113
45	O	3.8952	-0.1761	-1.0327
46	H	-2.2129	0.0403	-0.0319
47	H	-1.1803	-0.8870	-1.1540

48	C	-2.0383	2.6016	0.6391
49	H	-1.9901	3.1673	1.5840
50	H	-2.5600	1.6499	0.8379
51	H	-2.6629	3.1714	-0.0616
52	C	-0.1341	3.6466	-0.5731
53	H	0.0046	4.4331	0.1856
54	H	-0.8490	4.0093	-1.3303
55	H	0.8282	3.5082	-1.0845
56	C	-1.5410	-2.7914	0.5351
57	C	-2.8294	-3.1224	0.3732
58	C	-3.2635	-4.2099	-0.5937
59	H	-0.7779	-3.3350	-0.0458
60	C	-3.9454	-2.4692	1.1045
61	H	-4.6898	-2.0701	0.4015
62	H	-3.5977	-1.6348	1.7358
63	H	-4.4540	-3.1910	1.7581
64	C	-3.5895	-3.6167	-1.9797
65	C	-2.4172	-2.9587	-2.6108
66	C	-1.9040	-3.2792	-3.8065
67	C	-0.7317	-2.5403	-4.3471
68	H	-0.9895	-2.0172	-5.2854
69	H	0.0993	-3.2241	-4.5626
70	H	-0.3642	-1.7666	-3.6492
71	C	-2.4395	-4.3595	-4.6733
72	H	-2.7800	-3.9513	-5.6341
73	H	-3.2930	-4.8776	-4.2059
74	H	-1.6658	-5.1095	-4.8843
75	C	-1.6046	1.6044	-2.1743
76	H	-2.6614	1.3570	-1.9432
77	H	-1.5851	2.7145	-2.3213
78	C	-1.2191	0.9186	-3.4349
79	H	-0.9685	-0.1543	-3.3496
80	C	-1.1775	1.5191	-4.6326
81	C	-0.8188	0.7628	-5.8628
82	H	-1.5186	0.9893	-6.6783
83	H	-0.8307	-0.3308	-5.7111
84	H	0.1881	1.0403	-6.2032
85	C	-1.4755	2.9600	-4.8420
86	H	-2.4491	3.0852	-5.3342
87	H	-0.7153	3.4289	-5.4804
88	H	-1.5068	3.5180	-3.8911
89	H	0.3477	1.0900	-1.4027
90	H	-1.9687	-2.1345	-2.0261
91	H	-3.9874	-4.4203	-2.6405
92	H	-4.4026	-2.8713	-1.8748
93	H	-4.1653	-4.7231	-0.1825
94	O	-2.3568	-5.2817	-0.6762
95	H	-1.5823	-4.9626	-1.1266

Table S4. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **2a**.

Number	Atom	X	Y	Z
1	H	2.9767	4.6446	0.7723
2	C	3.7262	3.8578	0.6225
3	C	5.6318	1.8535	0.2160
4	C	3.4894	2.8361	-0.2961
5	C	4.9287	3.8575	1.3405
6	C	5.8906	2.8573	1.1388
7	C	4.4385	1.8356	-0.5003
8	H	4.2406	1.0225	-1.2096
9	H	6.3664	1.0546	0.0571
10	O	5.2434	4.8176	2.2637
11	H	4.5118	5.4197	2.3191
12	C	1.3195	0.7026	-0.0322
13	O	1.6654	1.0385	1.0846
14	C	0.7702	-0.7139	-0.3049
15	C	-0.2089	0.1732	-2.5024
16	C	-0.3629	-0.0695	-4.0224
17	H	-0.8572	0.8109	-4.4955
18	H	0.6397	-0.1493	-4.4889
19	C	1.7318	-1.7454	0.3217
20	H	1.3815	-2.7686	0.0499
21	H	1.6509	-1.6931	1.4380
22	C	3.1554	-1.6020	-0.0777
23	H	3.3502	-1.2331	-1.0934
24	C	4.1810	-1.9277	0.7224
25	C	5.5877	-1.8049	0.2546
26	H	6.0582	-2.7949	0.1860
27	H	6.1824	-1.2013	0.9554
28	H	5.6637	-1.3282	-0.7329
29	C	4.0057	-2.4306	2.1095
30	H	4.7187	-1.9587	2.7979
31	H	4.1687	-3.5157	2.1503
32	H	2.9896	-2.2291	2.4890
33	C	-1.6085	0.1968	-1.8685
34	C	0.6586	-0.8990	-1.8235
35	O	1.2138	-1.7830	-2.4386
36	C	-1.6890	0.1009	-0.3435
37	C	-0.6872	-0.9195	0.2633
38	C	0.5335	1.4805	-2.2498
39	C	1.3682	1.6554	-1.1700
40	O	0.3192	2.4152	-3.1821
41	H	0.8086	3.2201	-2.9650
42	C	2.2370	2.8517	-1.1019
43	O	1.9551	3.8477	-1.7698
44	H	-2.1887	-0.6463	-2.3027
45	H	-2.1437	1.1203	-2.1929
46	C	-1.1460	-2.3326	-0.1428
47	H	-2.0691	-2.6234	0.3844

48	H	-0.3773	-3.0839	0.1042
49	H	-1.3461	-2.4111	-1.2211
50	C	-0.6973	-0.8294	1.8053
51	H	-0.4292	0.2059	2.1148
52	C	-1.1309	-1.2983	-4.3631
53	C	-2.0578	-1.3613	-5.3299
54	C	-2.7497	-2.6409	-5.6434
55	H	-2.5833	-2.9217	-6.6922
56	H	-2.4042	-3.4748	-5.0182
57	H	-0.8783	-2.2041	-3.7939
58	C	-2.4666	-0.2014	-6.1637
59	H	-3.5600	-0.1079	-6.1994
60	H	-2.1084	-0.3240	-7.1946
61	H	-2.0604	0.7489	-5.7798
62	H	6.8286	2.8679	1.7050
63	H	-3.8338	-2.5418	-5.4953
64	H	-2.7069	-0.3108	-0.1106
65	C	-1.6608	1.5005	0.2860
66	H	-1.5274	1.4261	1.3934
67	H	-0.7941	2.0897	-0.0765
68	C	-2.9008	2.2467	-0.0562
69	H	-3.1087	2.3013	-1.1384
70	C	-3.7224	2.8149	0.8354
71	C	-3.5080	2.7544	2.3047
72	H	-4.4005	2.3665	2.8136
73	H	-3.3013	3.7548	2.7077
74	H	-2.6597	2.1016	2.5724
75	C	-4.9321	3.5629	0.3989
76	H	-4.8934	4.6010	0.7560
77	H	-5.8409	3.1045	0.8122
78	H	-5.0419	3.5913	-0.6931
79	H	0.1041	-1.4857	2.2113
80	C	-2.0256	-1.1928	2.4590
81	H	-2.4292	-2.1433	2.0307
82	C	-2.7931	-0.4189	2.2449
83	H	-1.8703	-1.3006	3.9333
84	H	-1.3417	-0.4667	4.4144
85	C	-2.3314	-2.3187	4.6722
86	C	-2.1505	-2.3403	6.1489
87	H	-1.6516	-1.4388	6.5282
88	H	-1.5457	-3.2061	6.4516
89	H	-3.1213	-2.4211	6.6565
90	C	-3.0508	-3.4889	4.1054
91	H	-4.1040	-3.4829	4.4164
92	H	-2.6052	-4.4297	4.4543
93	H	-3.0270	-3.4937	3.0031

Table S5. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **2b**.

Number	Atom	X	Y	Z
1	H	4.5043	3.0731	0.8392
2	C	4.8754	2.0742	0.5798
3	C	5.8391	-0.4675	-0.0850
4	C	4.2067	1.2876	-0.3543
5	C	6.0341	1.5657	1.1843
6	C	6.5233	0.2958	0.8536
7	C	4.6862	0.0192	-0.6885
8	H	4.1440	-0.6030	-1.4112
9	H	6.2010	-1.4703	-0.3423
10	O	6.6432	2.3859	2.0951
11	H	7.3950	1.9246	2.4454
12	C	1.4186	0.1048	0.0248
13	O	1.9560	0.1939	1.1122
14	C	0.3509	-0.9760	-0.2499
15	C	-0.3912	0.3893	-2.2871
16	C	-0.7641	0.3452	-3.7876
17	H	-0.9232	1.3821	-4.1656
18	H	0.0834	-0.0701	-4.3693
19	C	0.8907	-2.3410	0.2251
20	H	0.1548	-3.1301	-0.0570
21	H	0.9219	-2.3552	1.3452
22	C	2.2250	-2.7108	-0.3126
23	H	2.4680	-2.3544	-1.3224
24	C	3.1053	-3.4675	0.3587
25	C	4.4118	-3.8428	-0.2456
26	H	4.4572	-4.9257	-0.4220
27	H	5.2435	-3.5790	0.4234
28	H	4.5926	-3.3387	-1.2054
29	C	2.8554	-3.9871	1.7280
30	H	3.7467	-3.8897	2.3613
31	H	2.5828	-5.0502	1.6940
32	H	2.0313	-3.4453	2.2228
33	C	-1.6088	0.9011	-1.4986
34	C	0.0525	-0.9819	-1.7542
35	O	0.1769	-1.9562	-2.4639
36	C	-1.5905	0.7144	0.0202
37	C	-1.0220	-0.6634	0.4593
38	C	0.8193	1.2895	-2.0675
39	C	1.7375	1.0559	-1.0699
40	O	0.9125	2.2966	-2.9433
41	H	1.6858	2.8410	-2.7433
42	C	3.0004	1.8283	-1.0405
43	O	3.0722	2.8993	-1.6447
44	H	-2.5090	0.3870	-1.9009
45	H	-1.7558	1.9770	-1.7323
46	C	-2.0244	-1.7518	0.0306
47	H	-2.9380	-1.7210	0.6469

48	H	-1.5860	-2.7577	0.1432
49	H	-2.3333	-1.6444	-1.0191
50	C	-0.8781	-0.7264	1.9958
51	H	-0.1659	0.0587	2.3356
52	C	-1.9735	-0.4705	-4.0839
53	C	-2.9400	-0.0992	-4.9359
54	C	-4.0983	-0.9912	-5.2141
55	H	-4.1567	-1.2240	-6.2860
56	H	-4.0410	-1.9434	-4.6706
57	H	-2.0364	-1.4476	-3.5842
58	C	-2.9461	1.1923	-5.6705
59	H	-2.7484	1.0275	-6.7381
60	H	-2.1786	1.8874	-5.2920
61	H	-3.9207	1.6904	-5.5848
62	H	7.4291	-0.1005	1.3266
63	H	-5.0403	-0.5027	-4.9298
64	H	-2.6667	0.6975	0.3400
65	C	-0.9557	1.9352	0.7040
66	H	-0.5174	1.6543	1.6882
67	H	-0.1040	2.3280	0.1026
68	C	-1.9662	3.0022	0.9368
69	H	-2.7965	2.7254	1.6024
70	C	-1.9118	4.2349	0.4145
71	C	-0.8334	4.7011	-0.4952
72	H	-0.3093	5.5656	-0.0670
73	H	-1.2493	5.0079	-1.4642
74	H	-0.0837	3.9152	-0.6867
75	C	-2.9571	5.2471	0.7263
76	H	-3.4370	5.6051	-0.1948
77	H	-2.5130	6.1178	1.2278
78	H	-3.7466	4.8547	1.3807
79	H	-0.4095	-1.6967	2.2736
80	C	-2.1849	-0.5562	2.7611
81	H	-2.9837	-1.2036	2.3220
82	C	-2.5589	0.4854	2.6670
83	H	-1.9908	-0.8588	4.2033
84	H	-1.1291	-0.3691	4.6765
85	C	-2.7864	-1.6603	4.9241
86	C	-2.5324	-1.8958	6.3712
87	H	-1.6681	-1.3326	6.7471
88	H	-2.3428	-2.9610	6.5624
89	H	-3.4056	-1.6026	6.9697
90	C	-3.9677	-2.3684	4.3660
91	H	-4.8959	-1.9728	4.7994
92	H	-3.9244	-3.4418	4.5929
93	H	-4.0357	-2.2589	3.2709

Table S6. DFT B3LYP/6-31G++(d,p) atomic Cartesian coordinates (Å) for conformer **2c**.

Number	Atom	X	Y	Z
1	H	-3.7111	-1.4591	0.1761
2	C	-3.9135	-2.5362	0.0365
3	C	-4.4583	-5.2584	-0.3216
4	C	-2.9058	-3.4832	0.2052
5	C	-5.2003	-2.9720	-0.3082
6	C	-5.4797	-4.3322	-0.4920
7	C	-3.1795	-4.8422	0.0284
8	H	-2.3830	-5.5813	0.1744
9	H	-4.6651	-6.3248	-0.4599
10	O	-6.1461	-1.9930	-0.4558
11	H	-6.9710	-2.4132	-0.6647
12	C	-1.1878	-0.5504	0.7141
13	O	-1.5536	-0.5799	1.8749
14	C	-0.8986	0.7810	-0.0095
15	C	0.0984	-0.5653	-1.9469
16	C	0.1090	-0.7652	-3.4810
17	H	0.6861	-1.6887	-3.7377
18	H	-0.9260	-0.9390	-3.8401
19	C	-1.9916	1.7999	0.3804
20	H	-1.7968	2.7675	-0.1494
21	H	-1.8869	2.0349	1.4657
22	C	-3.3839	1.3478	0.1230
23	H	-3.5899	0.2703	0.2504
24	C	-4.3760	2.1806	-0.2230
25	C	-5.7620	1.6833	-0.4292
26	H	-6.0791	1.8457	-1.4685
27	H	-6.4659	2.2213	0.2200
28	H	-5.8631	0.6107	-0.2146
29	C	-4.1835	3.6403	-0.4254
30	H	-4.5661	4.2034	0.4363
31	H	-4.7174	3.9909	-1.3181
32	H	-3.1179	3.8976	-0.5479
33	C	1.5096	-0.1732	-1.4847
34	C	-0.8994	0.5215	-1.5189
35	O	-1.6135	1.1024	-2.3056
36	C	1.6721	0.3765	-0.0639
37	C	0.5269	1.3507	0.3434
38	C	-0.3652	-1.8360	-1.2450
39	C	-1.0158	-1.8070	-0.0551
40	O	-0.1434	-3.0600	-1.7907
41	H	0.3576	-2.9519	-2.5939
42	C	-1.5215	-3.0651	0.5860
43	O	-0.8378	-3.7049	1.3576
44	H	1.8939	0.5947	-2.1914
45	H	2.1811	-1.0531	-1.6151
46	C	0.7376	2.6538	-0.4517
47	H	1.6217	3.1980	-0.0795

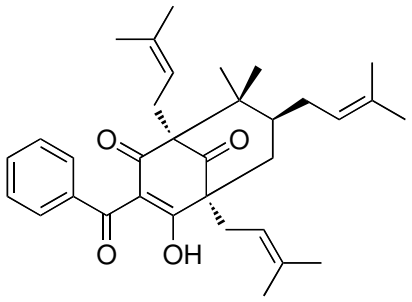
48	H	-0.1291	3.3283	-0.3540
49	H	0.8870	2.4677	-1.5245
50	C	0.5821	1.7109	1.8438
51	H	0.3514	0.8177	2.4606
52	C	0.6729	0.3825	-4.2411
53	C	1.5584	0.2663	-5.2410
54	C	2.0351	1.4664	-5.9808
55	H	1.8034	1.3763	-7.0509
56	H	1.5778	2.3972	-5.6198
57	H	0.2914	1.3758	-3.9637
58	C	2.1288	-1.0256	-5.7034
59	H	3.2251	-0.9783	-5.7453
60	H	1.7664	-1.2675	-6.7116
61	H	1.8550	-1.8630	-5.0410
62	H	-6.4867	-4.6690	-0.7633
63	H	3.1245	1.5727	-5.8856
64	H	2.6023	1.0050	-0.0943
65	C	1.9841	-0.7212	0.9607
66	H	2.1386	-0.2507	1.9663
67	H	1.1366	-1.4270	1.0759
68	C	3.1973	-1.5027	0.6017
69	H	3.2904	-1.7746	-0.4624
70	C	4.1295	-1.8982	1.4789
71	C	4.0740	-1.5818	2.9289
72	H	5.0716	-1.3611	3.3305
73	H	3.6665	-2.4320	3.4921
74	H	3.4284	-0.7047	3.1358
75	C	5.2978	-2.7110	1.0458
76	H	5.3362	-3.6572	1.6024
77	H	6.2368	-2.1744	1.2394
78	H	5.2710	-2.9564	-0.0241
79	H	-0.2401	2.4320	2.0587
80	C	1.9183	2.2822	2.3005
81	H	2.3198	2.9900	1.5411
82	C	2.6610	1.4494	2.3775
83	H	1.7755	2.9925	3.5979
84	H	1.1249	3.8771	3.5816
85	C	2.3725	2.6236	4.7389
86	C	2.1847	3.4056	5.9910
87	H	1.5500	4.2900	5.8478
88	H	3.1521	3.7508	6.3805
89	H	1.7176	2.7847	6.7677
90	C	3.2525	1.4334	4.8655
91	H	2.8952	0.7689	5.6639
92	H	4.2789	1.7338	5.1158
93	H	3.2945	0.8377	3.9321

Table S7. Calculated ECD Data for Compounds **1** and **2** at the B3LYP/6-31G++(d,p) Level in MeOH.

Compound	E (eV)[a]	λ (nm)[b]	f[c]	R_{vel}[d]	R_{len}[e]
1	3.1589	375	0.0044	2.3453	2.6372
	3.5168	320	0.2301	-54.4440	-58.5969
	3.5533	305	0.1119	25.9726	27.8688
	3.6055	297	0.0005	-0.2355	-0.2706
	3.708	265	0.0041	-67.7400	-68.9112
	3.7113	220	0.0199	48.3241	48.5721
2	3.0787	360	0.0023	8.8453	9.1721
	3.4961	310	0.017	-89.4750	-93.8963
	3.5291	299	0.3185	-54.8550	-53.0833
	3.5912	275	0.0117	60.9575	59.1011
	3.6248	240	0.0003	-45.9574	-47.8510
	3.7059	220	0.0119	108.4650	111.7348

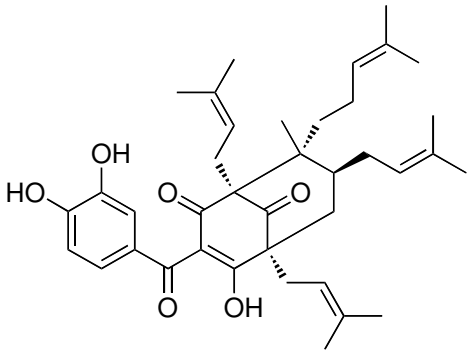
[a] Excitation energy.
[b] Wavelength.
[c] Oscillator strength.
[d] Rotatory strength in velocity form (10^{-40} cgs).
[e] Rotatory strength in length form (10^{-40} cgs).

Figure S1. Compounds identified from *R. edulis*



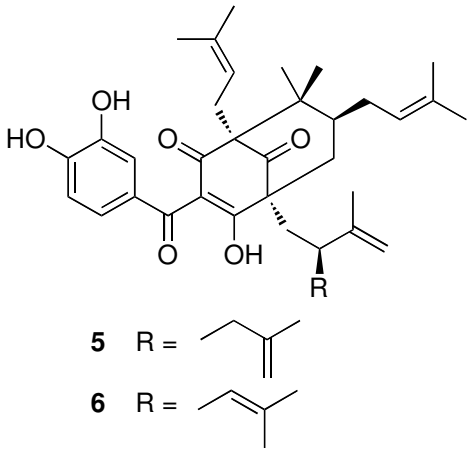
3

6-*epi*-Clusianone (3): yellow oil; , $[\alpha]_{25}^{D}$ +15.6 (*c* 0.1, MeOH); UV (MeOH) λ_{max} 248, 280 nm; HRESIMS (negative ion) *m/z* 501.2924 $[M - H]^-$ (calcd for $C_{33}H_{41}O_4$, 501.3005). NMR, MS and UV data are consistent with published data.[1]



4

Guttiferone A (4): yellow oil; $[\alpha]_{25}^{D}$ +31.4 (*c* 0.1, MeOH); UV (MeOH) λ_{max} 233, 279 nm; HRESIMS (negative ion) *m/z* 601.3441 $[M - H]^-$ (calcd for $C_{38}H_{49}O_6$, 601.3529). NMR, MS and UV data are consistent with published data.[2]

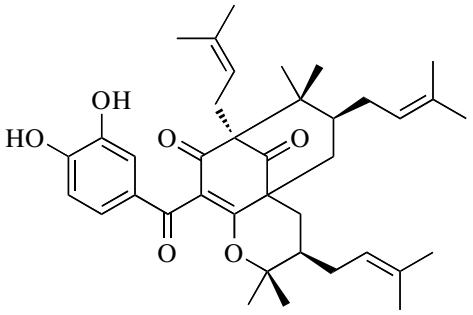


5 R =

6 R =

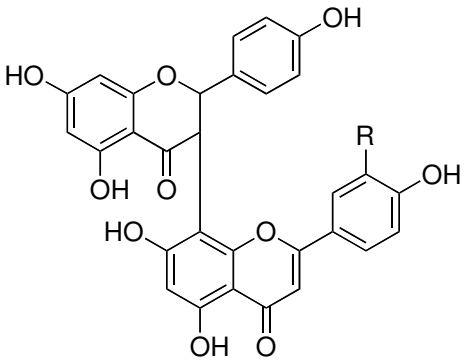
Xanthochymol (5): UV (MeOH) λ_{max} 241, 279 nm; HRESIMS (negative ion) *m/z* 601.3145 $[M - H]^-$ (calcd for $C_{38}H_{49}O_6$, 601.3163). MS and UV data are consistent with published data.[3]

Guttiferone E (6): UV (MeOH) λ_{max} 241, 279 nm; HRESIMS (negative ion) *m/z* 601.3548 $[M - H]^-$ (calcd for $C_{38}H_{49}O_6$, 601.3516). MS and UV data are consistent with published data.[3]



7

Isoxanthochymol (7): UV (MeOH) λ_{max} 233, 279 nm; HRESIMS (negative ion) *m/z* 601.3511 $[M - H]^-$ (calcd for $C_{38}H_{49}O_6$, 601.3492). MS and UV data are consistent with published data.[3]



8 R = H

9 R = OH

(+)-Volkensiflavone (8): UV (MeOH) λ_{max} 215, 288, 323 nm; HRESIMS (positive ion) *m/z* 541.1132 $[M + H]^+$ (calcd for $C_{30}H_{21}O_{10}$, 541.1156). MS and UV data are consistent with published data.[3]

(+)-Morelloflavone (9): UV (MeOH) λ_{max} 214, 289, 329 nm; HRESIMS (positive ion) *m/z* 557.1089 $[M + H]^+$ (calcd for $C_{30}H_{21}O_{11}$, 557.1067). MS and UV data are consistent with published data.[3]

Figure S2. ^{1}H NMR (300 MHz, MeOH-d_4 + 0.1% TFA) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**)

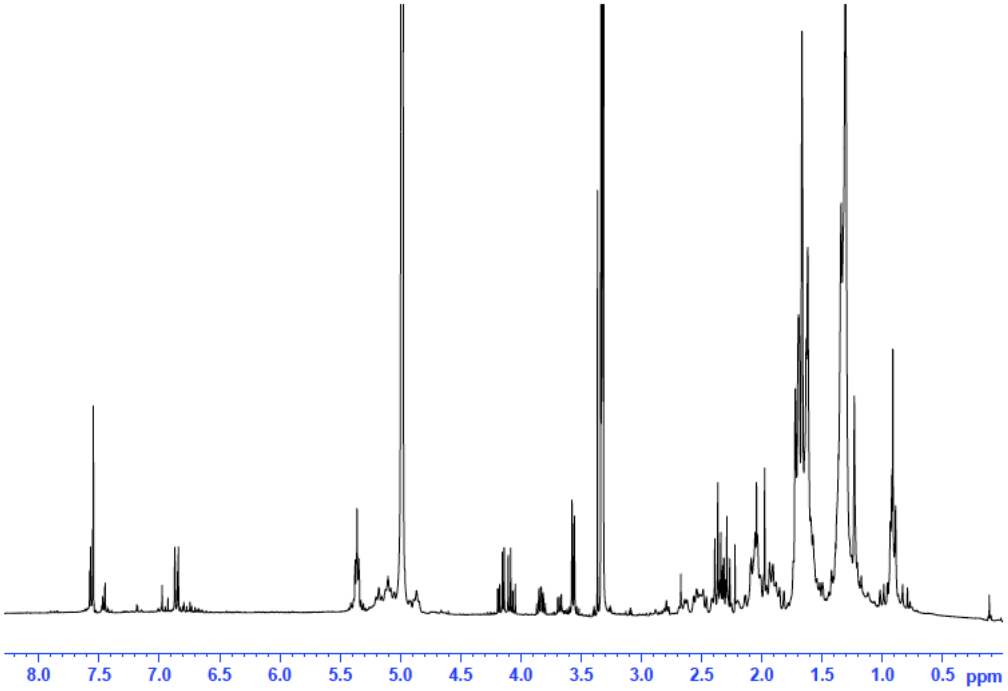


Figure S3. ^{13}C NMR (300 MHz, MeOH-d_4 + 0.1% TFA) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**)

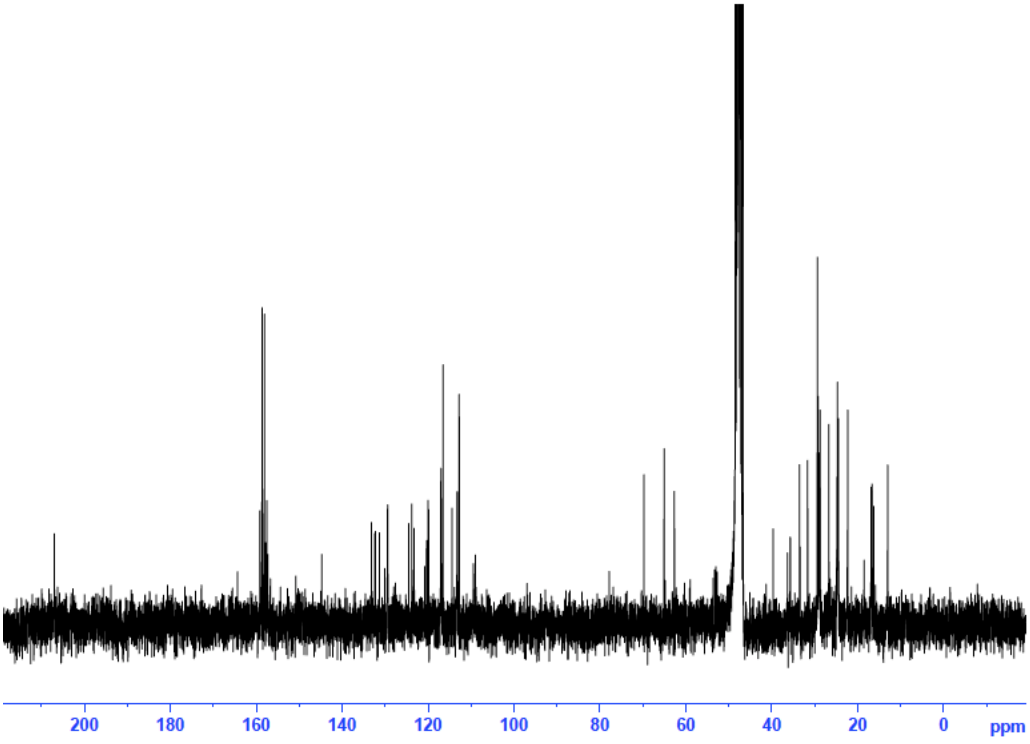


Figure S4. HMBC NMR (300 MHz, MeOH-d_4 + 0.1% TFA) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**)

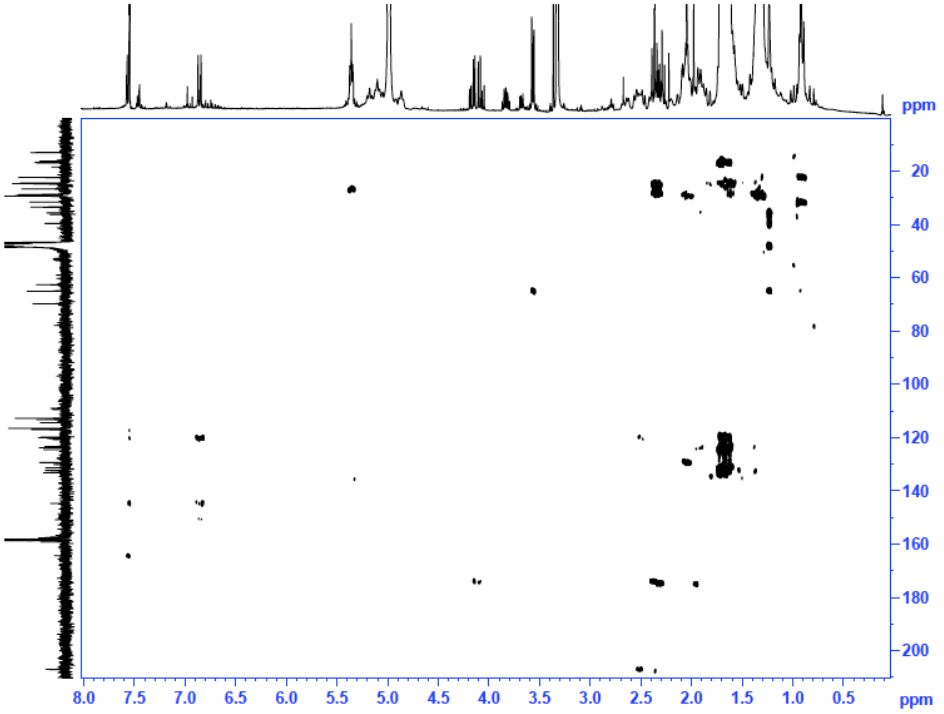


Figure S5. HSQC NMR (300 MHz, MeOH-d_4 + 0.1% TFA) of the new compound 32-hydroxy-*ent*-guttiferone M (**1**)

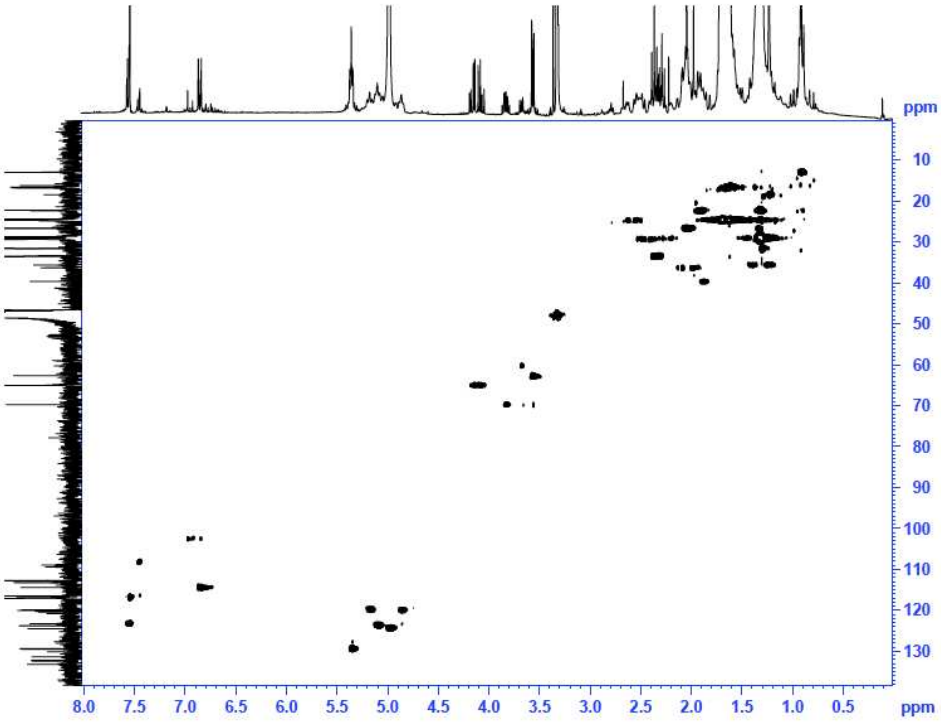


Figure S6. ^{1}H NMR (300 MHz, MeOH-d_4 + 0.1% TFA) of the new compound 7-*epi*-guttiferone J (**2**)

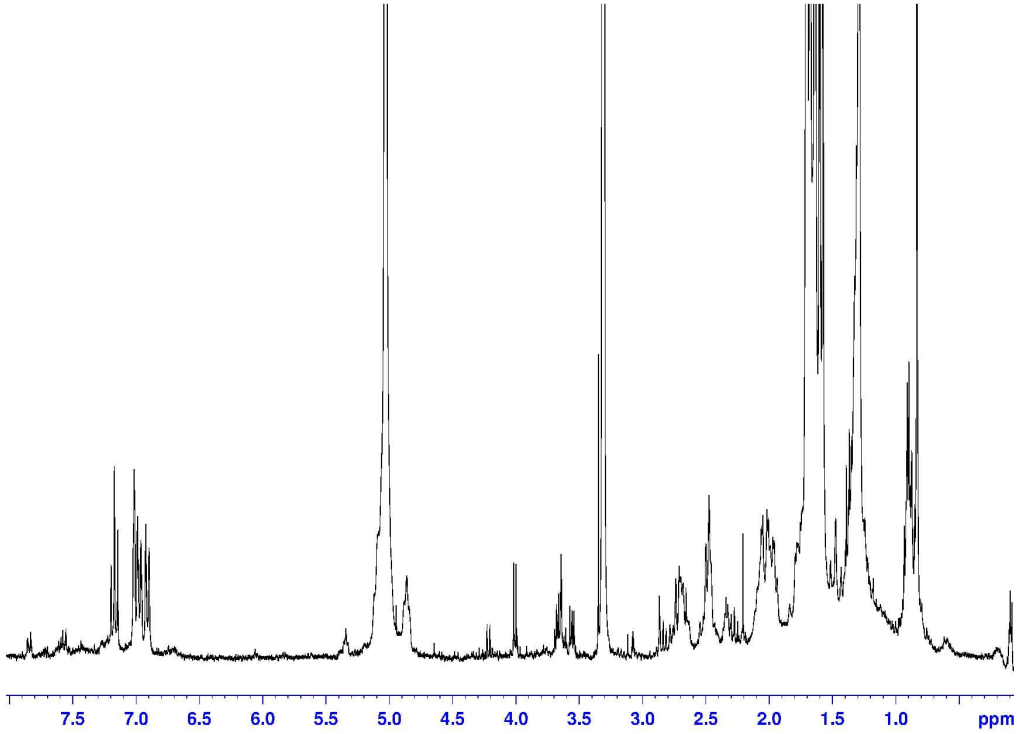


Figure S7. ^{13}C NMR (300 MHz, MeOH-d_4 + 0.1% TFA) of the new compound 7-*epi*-guttiferone J (**2**).

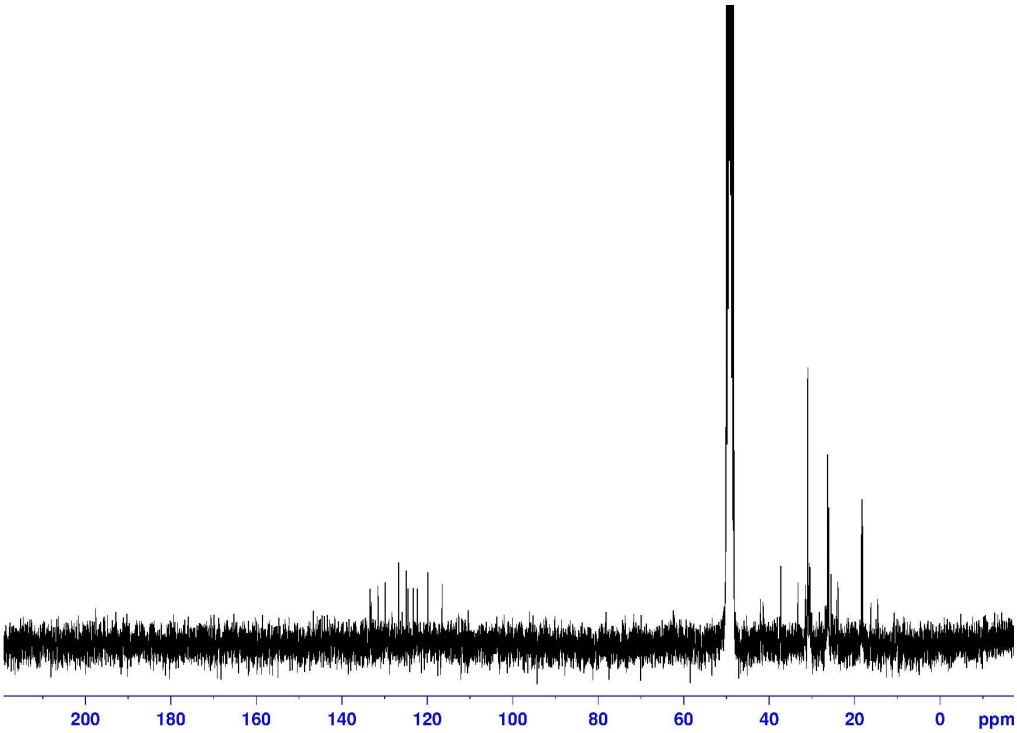
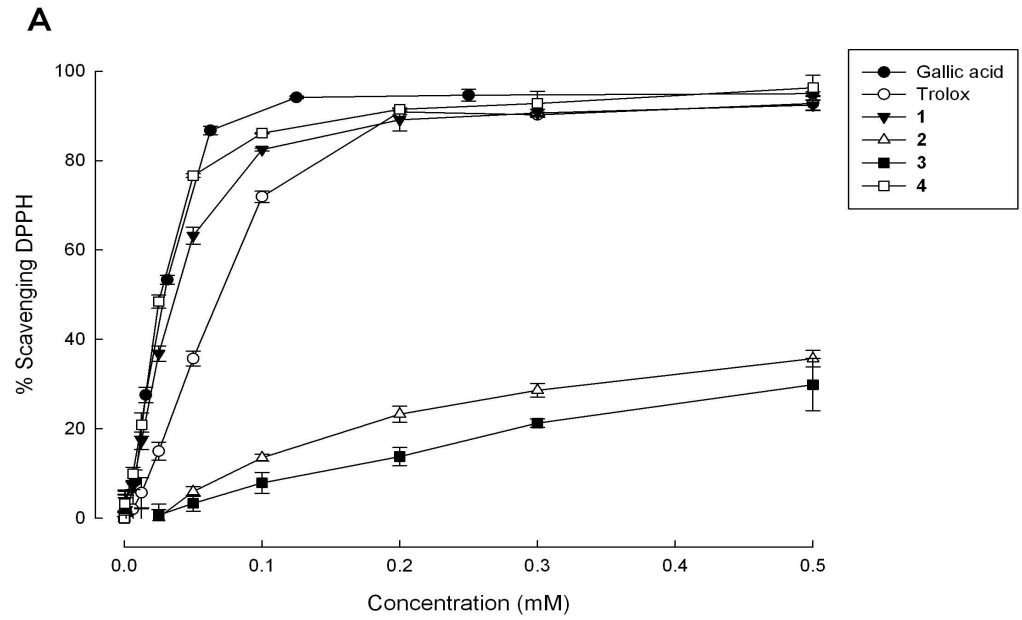
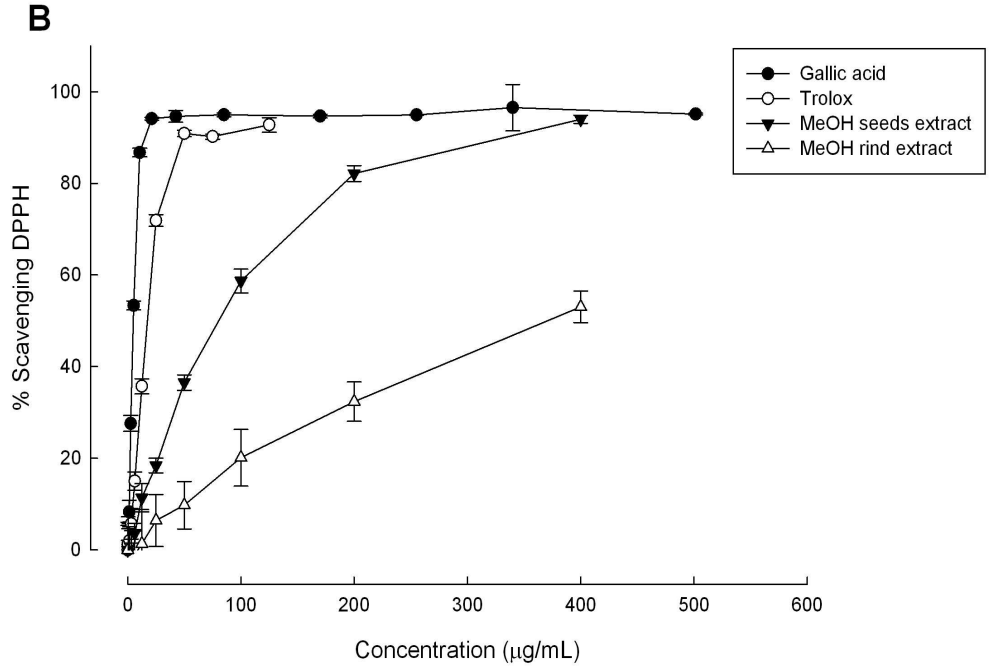
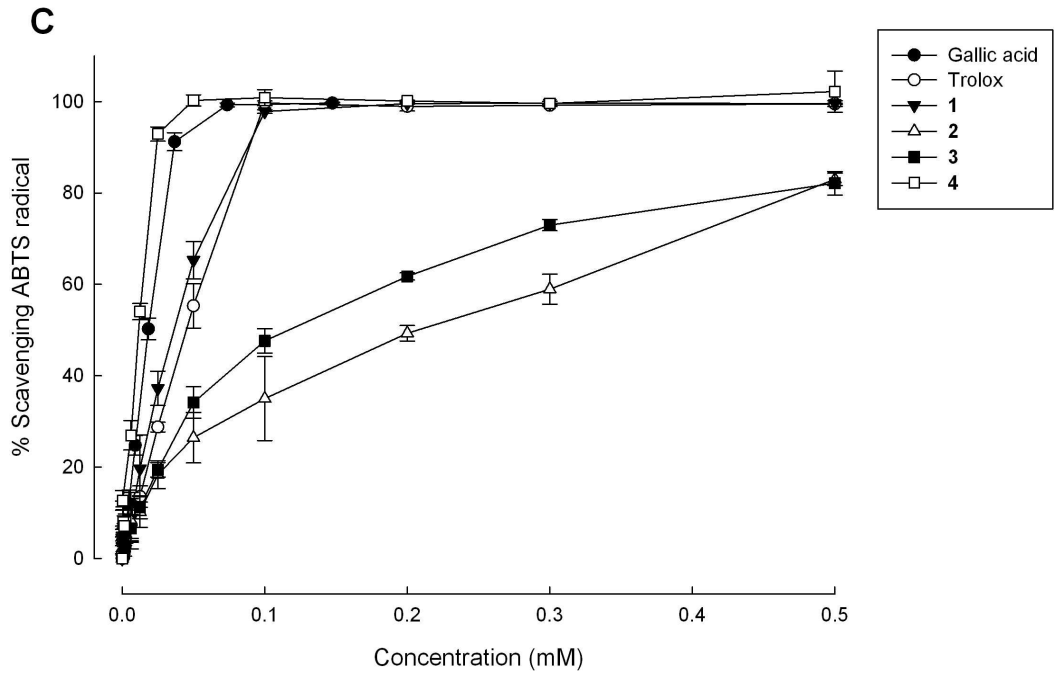
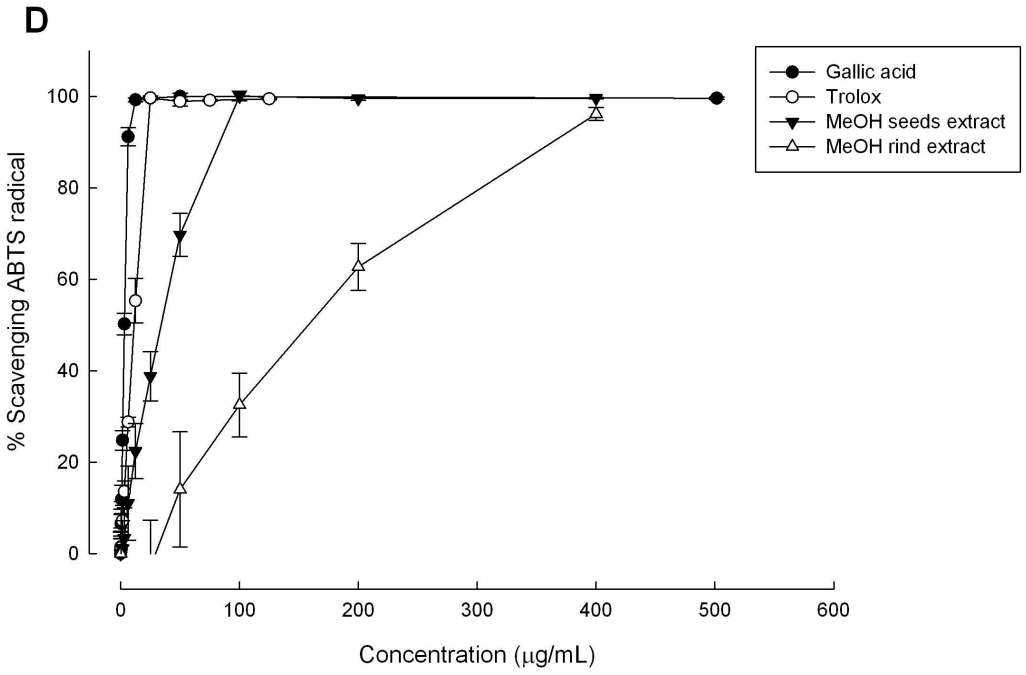


Figure S8. DPPH and ABTS scavenging activity of compounds **1–4** (A and C), and extracts (B and D) from *R. edulis*.






C
Gallic acid
Trolox
1
2
3
4
% Scavenging ABTS radical
0
20
40
60
80
100
0.0
0.1
0.2
0.3
0.4
0.5
Concentration (mM)


D
Gallic acid
Trolox
MeOH seeds extract
MeOH rind extract
% Scavenging ABTS radical
0
20
40
60
80
100
0
100
200
300
400
500
600
Concentration (μg/mL)

References and Notes

(1) Piccinelli, A. L.; Cuesta-Rubio, O.; Chica, M. B.; Mahmood, N.; Pagano, B.; Pavone, M.; Barone, V.; Rastrelli, L. *Tetrahedron* 2005, *61*, 8206-8211.

(2) Gustafson, K. R.; Blunt, J. W.; Munro, M. H. G.; Fuller, R. W.; McKee, T. C.; Cardellina, J. H.; McMahon, J. B.; Cragg, G. M.; Boyd, M. R. *Tetrahedron* 1992, *48*, 10093-10102.

(3) Yang, H.; Figueroa, M.; To, S.; Baggett, S.; Jiang, B.; Basile, M. J.; Weinstein, I. B.; Kennelly, E. J. *J. Agric. Food Chem.* 2010, *58*, 4749-4755.