

Supplementary Material

Preparation of Carotenoid-Flavonoid Hybrids and their Properties

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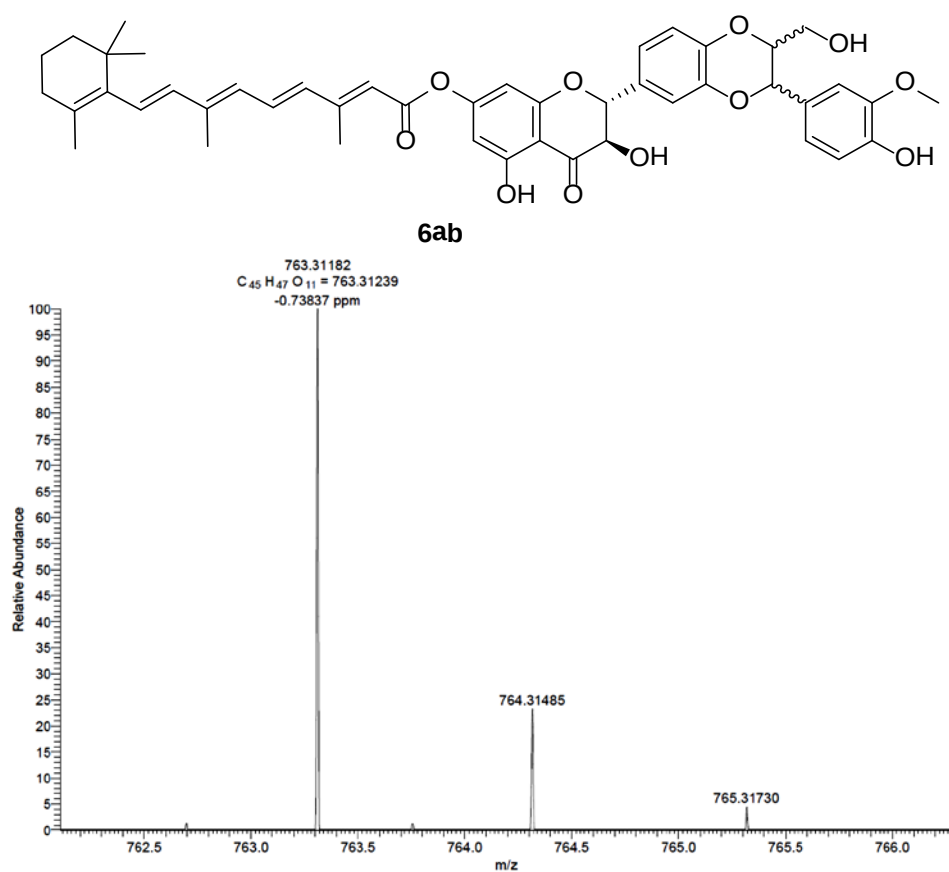
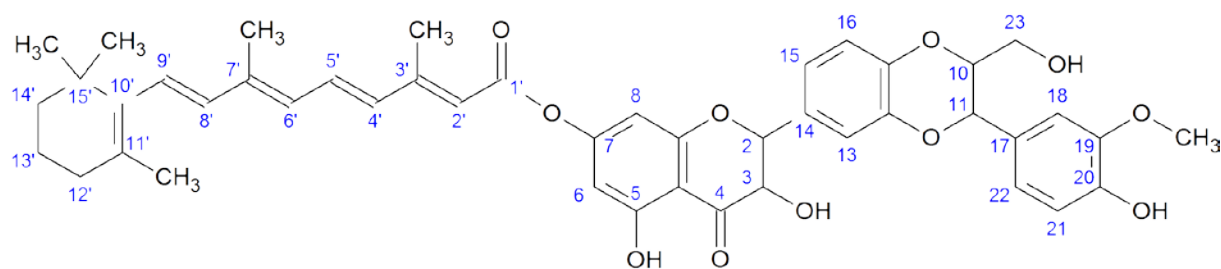


Figure S1. HRMS (ESI⁻) of compound **6ab** m/z [M - H]⁻ calcd for $C_{45}H_{47}O_{11}$ 763.31239; found 763.31182

Table S1. ^1H and ^{13}C NMR data of compound **6ab**.

Atom #	δ_{C}	m	δ_{H}	n_{H}	m	$J_{\text{H-H}}$ [Hz]
2	82.66 / 82.63	d	5.231 / 5.230	1	d	11.7 / 11.7
3	71.60 / 71.67	d	4.782 / 4.771	1	dd	11.7, 6.3 / 11.7, 6.3
4	199.39 / 199.37	s	-	-	-	-
4a	104.53	s	-	-	-	-
5	161.83 / 161.82	s	-	-	-	-
6	102.85	d	6.384	1	d	2.0
7	158.05	s	-	-	-	-
8	101.61	d	6.343 / 6.350	1	d	2.0 / 2.0
8a	161.69 / 161.68	s	-	-	-	-
10	78.02 / 78.04	d	4.177 / 4.171	1	m	-
11	75.75	d	4.916	1	d	7.9
12a	143.19	s	-	-	-	-
13	116.53 / 116.58	d	7.115 / 7.111	1	d	2.1 / 2.1
14	129.57 / 129.62	s	-	-	-	-
15	121.31 / 121.18	d	7.035 / 7.037	1	dd	8.4, 2.1 / 8.4, 2.1
16	116.24 / 116.28	d	6.983 / 6.984	1	d	8.4 / 8.4
16a	143.69 / 143.66	s	-	-	-	-
17	127.38	s	-	-	-	-
18	111.64 / 111.58	d	7.014 / 7.018	1	d	2.0 / 2.0
19	147.53 / 147.54	s	-	-	-	-
20	146.93 / 146.92	s	-	-	-	-
21	115.22 / 115.20	d	6.803 / 6.801	1	d	8.1 / 8.1
22	120.42 / 120.41	d	6.864 / 6.866	1	dd	8.1, 2.0 / 8.1, 2.0
23	60.07	t	3.543	1	ddd	12.2, 4.4, 2.6
			3.350	1	ddd	12.2, 6.4, 4.1
3-OH	-	-	5.927	1	d	6.3
5-OH	-	-	11.657	1	s	-
19-MeO	55.60	q	3.777 / 3.778	3	s	-
20-OH	-	-	9.110	1	s	-
23-OH	-	-	4.925	1	dd	6.4, 4.4
1'	163.43	s	-	-	-	-

2'	116.03	d	6.052	1	s	-
3'	156.44	s	-	-	-	-
4'	134.45	d	6.514	1	d	14.9
5'	132.90	d	7.190	1	dd	14.9, 11.4
6'	129.63	d	6.281	1	d	11.4
7'	140.49	s	-	-	-	-
8'	136.71	d	6.204	1	d	16.0
9'	128.55	d	6.325	1	d	16.0
10'	137.14	s	-	-	-	-
11'	129.74	s	-	-	-	-
12'	32.55	t	2.011	2	m	-
13'	18.61	t	1.577	2	m	-
14'	39.10	t	1.443	2	m	-
15'	33.77	s	-	-	-	-
3'-Me	13.84	q	2.343	3	s	-
7'-Me	12.61	q	2.015	3	s	-
11'-Me	21.42	q	1.695	3	m	-
15'-Me	28.71	q	1.021	3	s	-

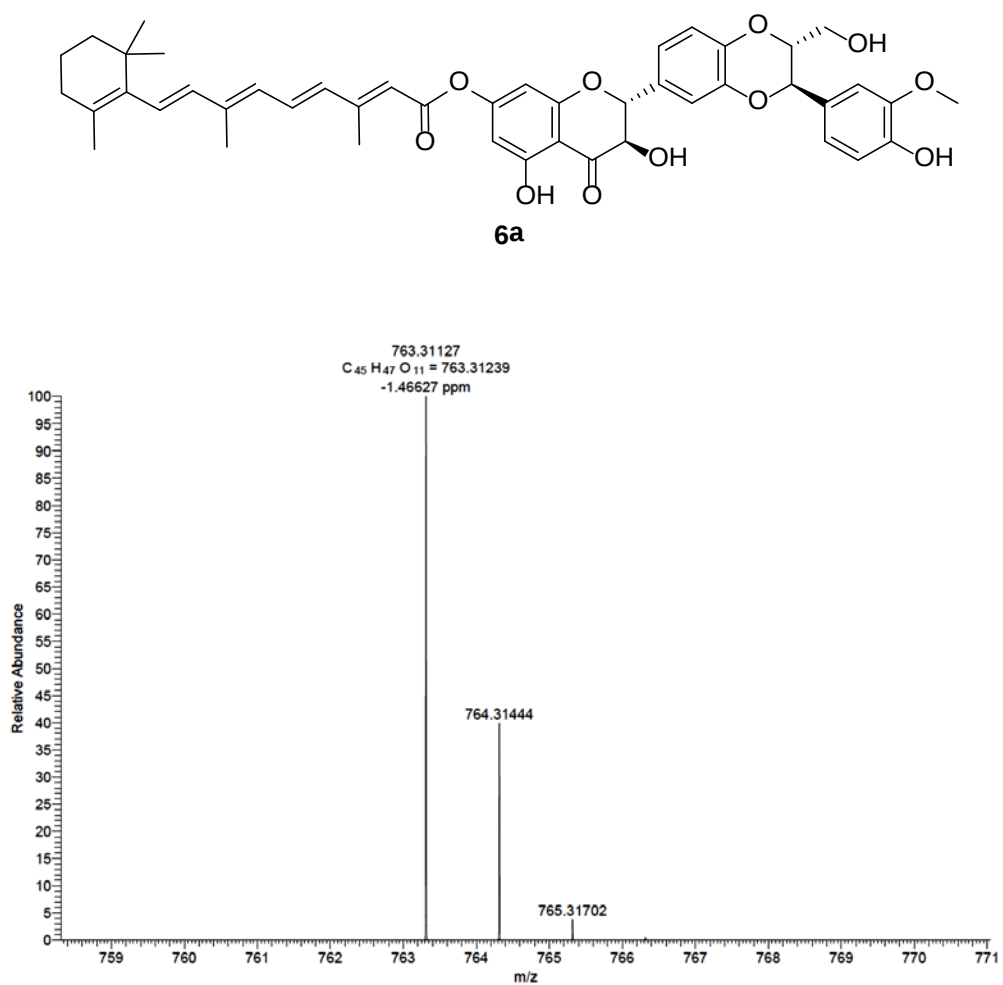
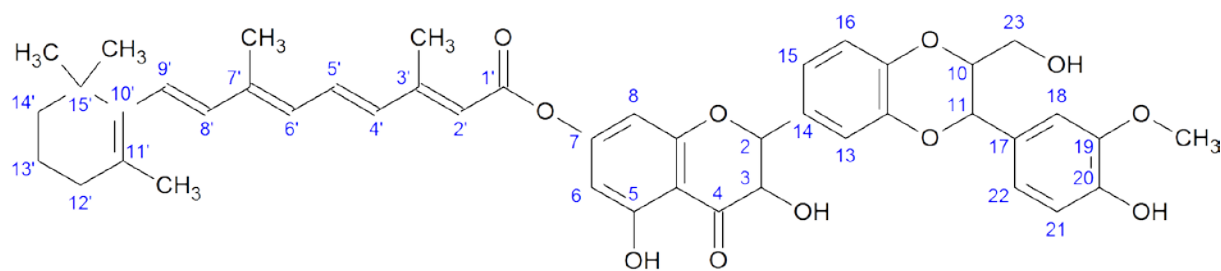


Figure S2. HRMS (ESI) of compound **6a** m/z $[M - H]^-$ calcd for $C_{45}H_{47}O_{11}$ 763.31239; found 763.31127

Table S2. ^1H and ^{13}C NMR data of compound **6a**.

Atom #	δ_{C}	m	δ_{H}	n_{H}	m	$J_{\text{H-H}}$ [Hz]
2	82.66	d	5.231	1	d	11.6
3	71.60	d	4.782	1	dd	11.6, 6.4
4	199.39	s	-	-	-	-
4a	104.53	s	-	-	-	-
5	161.83	s	-	-	-	-
6	102.85	d	6.384	1	d	2.1
7	158.05	s	-	-	-	-
8	101.61	d	6.343	1	d	2.1
8a	161.69	s	-	-	-	-
10	78.02	d	4.177	1	ddd	8.0, 4.5, 2.5
11	75.74	d	4.916	1	d	8.0
12a	143.19	s	-	-	-	-
13	116.54	d	7.115	1	d	2.0
14	129.57	s	-	-	-	-
15	121.31	d	7.035	1	dd	8.3, 2.0
16	116.24	d	6.983	1	d	8.3
16a	143.69	s	-	-	-	-
17	127.37	s	-	-	-	-
18	111.64	d	7.014	1	d	1.9
19	147.53	s	-	-	-	-
20	146.93	s	-	-	-	-
21	115.22	d	6.803	1	d	8.1
22	120.42	d	6.864	1	dd	8.1, 1.9
23	60.08	t	3.543	1	ddd	12.3, 4.6, 2.5
			3.350	1	ddd	12.3, 4.5, 6.1
3-OH	-	-	5.926	1	d	6.4
5-OH	-	-	11.681	1	s	-
19-MeO	55.61	q	3.777	3	s	-
20-OH	-	-	9.111	1	s	-
23-OH	-	-	4.923	1	dd	6.1, 4.6
1'	163.43	s	-	-	-	-

2'	116.03	d	6.051	1	s	-
3'	156.44	s	-	-	-	-
4'	134.45	d	6.513	1	d	15.1
5'	132.90	d	7.189	1	dd	15.1, 11.6
6'	129.63	d	6.280	1	d	11.6
7'	140.49	s	-	-	-	-
8'	136.71	d	6.204	1	d	16.0
9'	128.55	d	6.324	1	d	16.0
10'	137.14	s	-	-	-	-
11'	129.74	s	-	-	-	-
12'	32.55	t	2.012 ^J	2	m	-
13'	18.60	t	1.577	2	m	-
14'	39.10	t	1.443	2	m	-
15'	33.77	s	-	-	-	-
3'-Me	13.84	q	2.342	3	s	-
7'-Me	12.61	q	2.015	3	s	-
11'-Me	21.42	q	1.695	3	s	-
15'-Me	28.71	q	1.021	6	s	-

^J - *J*-resolved readout

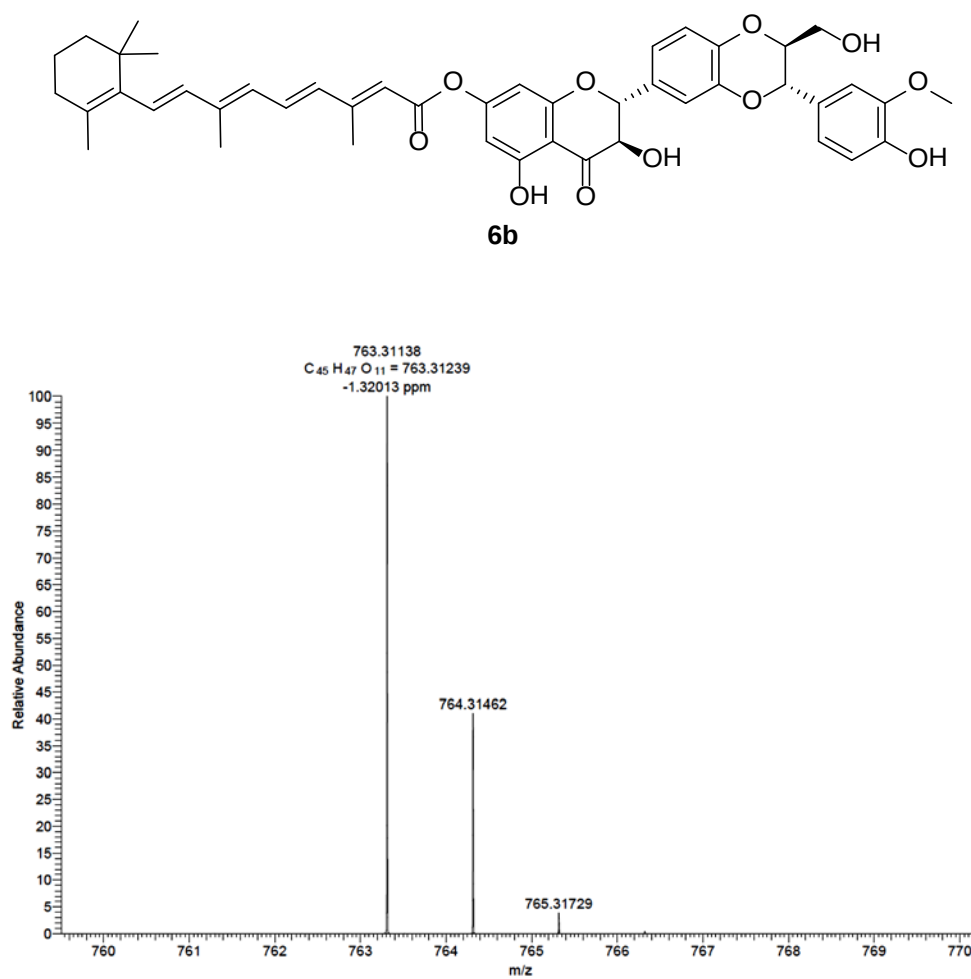
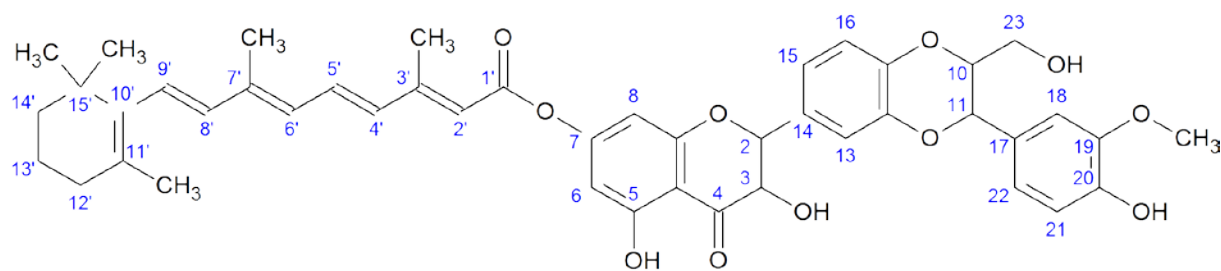


Figure S3. HRMS (ESI⁻) of compound **6b** m/z [M - H]⁻ calcd for C₄₅H₄₇O₁₁ 763.31239; found 763.31239

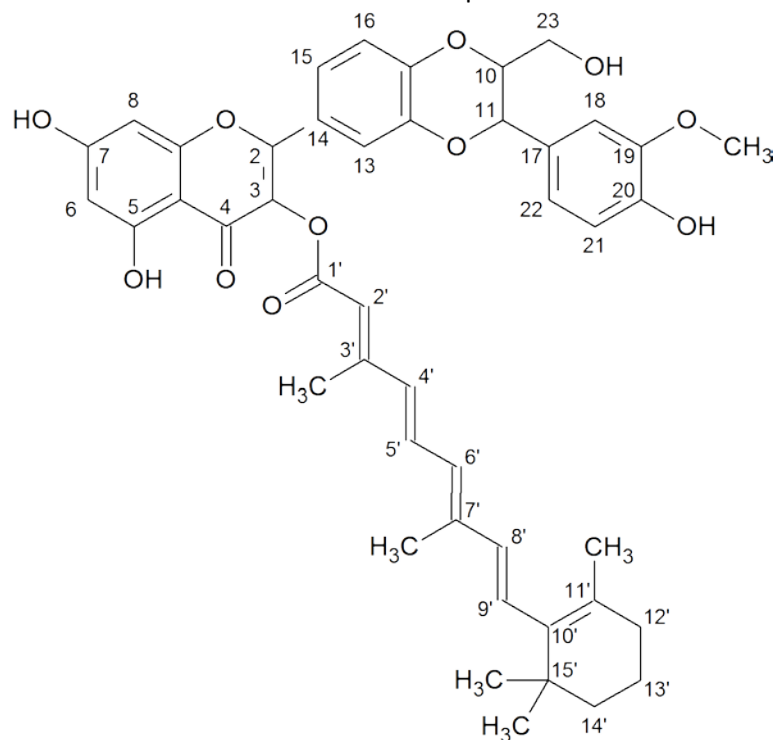
Table S3. ^1H and ^{13}C NMR data of compound **6b**.

Atom #	δ_{C}	m	δ_{H}	n_{H}	m	$J_{\text{H-H}}$ [Hz]
2	82.62	d	5.230	1	d	11.6
3	71.67	d	4.772	1	dd	11.6, 6.4
4	199.37	s	-	-	-	-
4a	104.53	s	-	-	-	-
5	161.82	s	-	-	-	-
6	102.85	d	6.384	1	d	2.0
7	158.05	s	-	-	-	-
8	101.62	d	6.350	1	d	2.0
8a	161.67	s	-	-	-	-
10	78.03	d	4.171	1	ddd	7.9, 4.5, 2.5
11	75.75	d	4.916	1	d	7.9
12a	143.18	s	-	-	-	-
13	116.58	d	7.111	1	d	2.0
14	129.62	s	-	-	-	-
15	121.18	d	7.037	1	dd	8.3, 2.0
16	116.28	d	6.985	1	d	8.3
16a	143.66	s	-	-	-	-
17	127.38	s	-	-	-	-
18	111.58	d	7.018	1	d	1.9
19	147.54	s	-	-	-	-
20	146.92	s	-	-	-	-
21	115.20	d	6.800	1	d	8.1
22	120.41	d	6.866	1	dd	8.1, 1.9
23	60.07	t	3.543	1	ddd	12.3, 5.0, 2.5
			3.349	1	ddd	12.3, 4.5, 6.0
3-OH	-	-	5.926	1	d	6.4
5-OH	-	-	11.684	1	s	-
19-MeO	55.60	q	3.778	3	s	-
20-OH	-	-	9.104	1	s	-
23-OH	-	-	4.925	1	dd	6.0, 5.0
1'	163.43	s	-	-	-	-

2'	116.03	d	6.053	1	s	-
3'	156.44	s	-	-	-	-
4'	134.44	d	6.515	1	d	15.0
5'	132.90	d	7.191	1	dd	15.0, 11.4
6'	129.63	d	6.281	1	d	11.4
7'	140.49	s	-	-	-	-
8'	136.71	d	6.205	1	d	16.0
9'	128.55	d	6.325	1	d	16.0
10'	137.13	s	-	-	-	-
11'	129.73	s	-	-	-	-
12'	32.55	t	2.014 ^J	2	m	-
13'	18.60	t	1.578	2	m	-
14'	39.10	t	1.444	2	m	-
15'	33.77	s	-	-	-	-
3'-Me	13.84	q	2.344	3	s	-
7'-Me	12.61	q	2.016	3	s	-
11'-Me	21.42	q	1.696	3	s	-
15'-Me	28.71	q	1.022	6	s	-

^J - J-resolved readout

Table S5. ^1H and ^{13}C NMR data of compound **7**.



Atom #	δ_{C}	m	δ_{H}	n_{H}	m	$J_{\text{H-H}}$ [Hz]
2	155.25	s	-	-	-	-
3	130.39	s	-	-	-	-
4	175.28	s	-	-	-	-
4a	103.59	s	-	-	-	-
5	161.25	s	-	-	-	-
6	99.33	d	6.233	1	d	2.0
7	165.27	s	-	-	-	-
8	94.42	d	6.492	1	d	2.0
8a	156.88	s	-	-	-	-
10	78.72	d	4.269	1	ddd	7.9, 4.8, 2.3
11	76.06	d	4.955	1	d	7.9
12a	143.88	s	-	-	-	-
13	116.66	d	7.461	1	d	2.0
14	121.97	s	-	-	-	-
15	121.85	d	7.452	1	dd	8.5, 2.0
16	117.40	d	7.118	1	d	8.5
16a	146.59	s	-	-	-	-
17	127.17	s	-	-	-	-
18	111.79	d	7.011	1	d	1.8
19	147.80	s	-	-	-	-
20	147.29	s	-	-	-	-

21	115.46	d	6.796	1	d	8.1
22	120.72	d	6.863	1	dd	8.1, 1.8
23	60.16	t	3.568	1	dd	12.4, 2.3
			3.358	1	dd	12.4, 4.8
5-OH	-	-	n.a.	-	-	-
7-OH	-	-	n.a.	-	-	-
19-MeO	55.72	q	3.761	3	s	-
20-OH	-	-	n.a.	-	-	-
23-OH	-	-	n.a.	-	-	-
1'	163.44	s	-	-	-	-
2'	115.41	d	6.154	1	s	-
3'	157.30	s	-	-	-	-
4'	134.59	d	6.526	1	d	15.0
5'	133.38	d	7.185	1	dd	15.0, 11.5
6'	129.81	d	6.267	1	d	11.5
7'	140.85	s	-	-	-	-
8'	136.98	d	6.189	1	d	16.1
9'	128.86	d	6.321	1	d	16.1
10'	137.37	s	-	-	-	-
11'	129.98	s	-	-	-	-
12'	32.76	t	1.994	2	m	-
13'	18.84	t	1.571	2	m	-
14'	39.3 ^H	t	1.434	2	m	-
15'	33.97	s	-	-	-	-
3'-Me	13.94	q	2.317	3	s	-
7'-Me	12.67	q	2.003	3	s	-
11'-Me	21.54	q	1.689	3	s	-
15'-Me	28.83	q	1.011	6	s	-

^H - HSQC readout

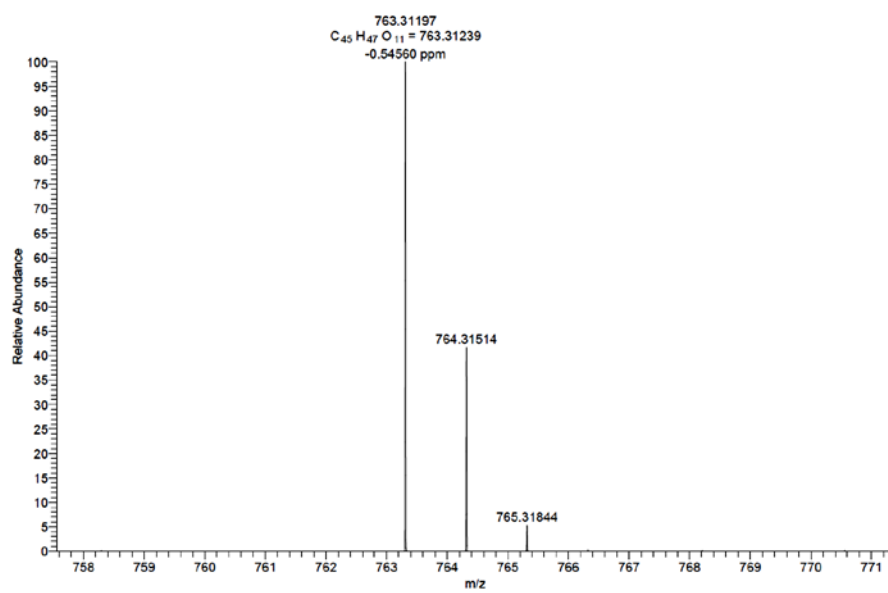
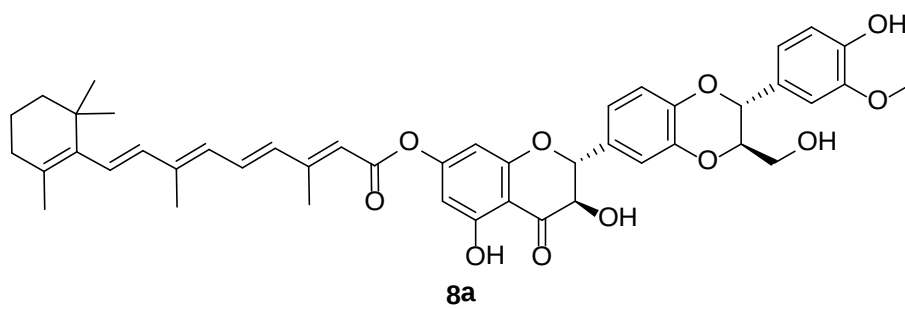
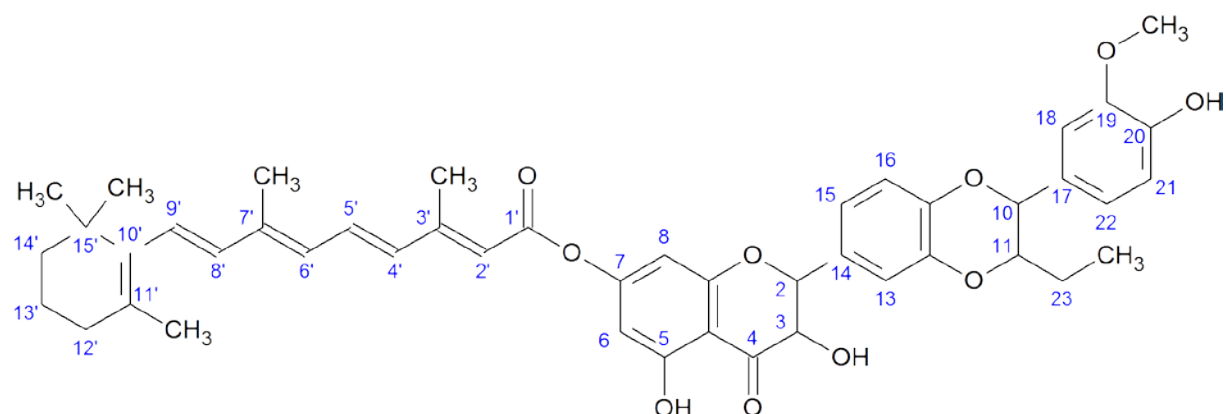


Figure S5. HRMS (ESI⁻) of compound **8a** m/z $[M - H]^-$ calcd for $C_{45}H_{47}O_{11}$ 763.31239; found 763.31197

Table S5. ^1H and ^{13}C NMR data of compound **8a**



Atom #	δ_{C}	m	δ_{H}	n_{H}	m	$J_{\text{H-H}}$ [Hz]
2	82.63	d	5.252	1	d	11.5
3	71.69	d	4.759	1	dd	11.5, 6.3
4	199.25	s	-	-	-	-
4a	104.53	s	-	-	-	-
5	161.82	s	-	-	-	-
6	102.81	d	6.391	1	d	2.0
7	158.04	s	-	-	-	-
8	101.59	d	6.361	1	d	2.0
8a	161.66	s	-	-	-	-
10	75.72	d	4.926	1	d	7.6
11	77.89	d	4.168	1	ddd	7.6, 4.6, 2.7
12a	142.82	s	-	-	-	-
13	116.39	d	7.125	1	d	1.8
14	129.79	s	-	-	-	-
15	120.86	d	7.014	1	dd	8.4, 1.8
16	116.34	d	6.945	1	d	8.4
16a	143.90	s	-	-	-	-
17	127.36	s	-	-	-	-
18	111.71	d	7.007	1	d	1.8
19	147.49	s	-	-	-	-
20	146.91	s	-	-	-	-
21	115.24	d	6.806	1	d	8.1
22	120.34	d	6.861	1	dd	8.1, 1.8
23	60.06	t	3.548	1	ddd	12.2, 4.6, 2.7
			3.357	1	ddd	12.2, 5.6, 4.6
3-OH	-	-	5.924	1	d	6.4
5-OH	-	-	11.678	1	s	-
19-MeO	55.62	q	3.780	3	s	-

20-OH	-	-	9.082	1	s	-
23-OH	-	-	4.901	1	dd	5.6, 4.6
1'	163.40	s	-	-	-	-
2'	115.99	d	6.056	1	s	-
3'	156.40	s	-	-	-	-
4'	134.41	d	6.518	1	d	15.1
5'	132.86	d	7.194	1	dd	15.1, 11.6
6'	129.70	d	6.284	1	d	11.6
7'	140.46	s	-	-	-	-
8'	136.66	d	6.206	1	d	16.1
9'	128.53	d	6.33 ^H	1	m	-
10'	137.11	s	-	-	-	-
11'	129.58	s	-	-	-	-
12'	32.52	t	2.01 ^H	2	m	-
13'	18.58	t	1.582	2	m	-
14'	39.11	t	1.448	2	m	-
15'	33.74	s	-	-	-	-
3'-Me	13.83	q	2.349	3	d	0.8
7'-Me	12.57	q	2.018	3	s	-
11'-Me	21.37	q	1.698	3	s	-
15'-Me	28.68	q	1.024	3	s	-

^H - HSQC readout

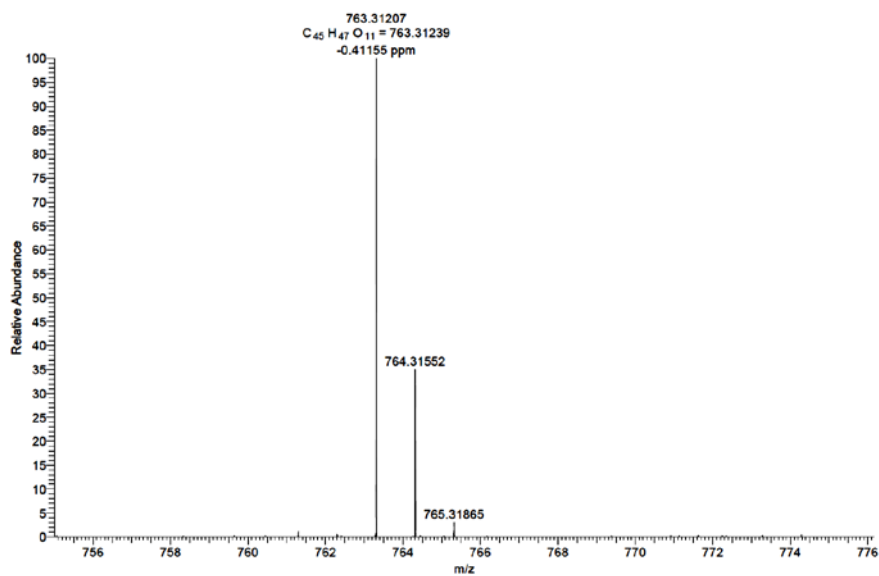
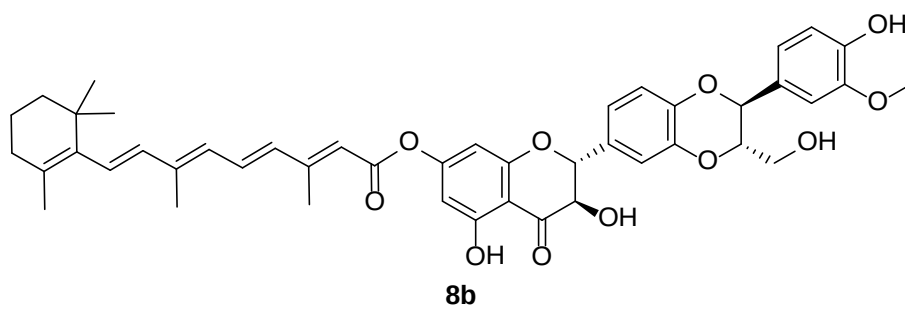
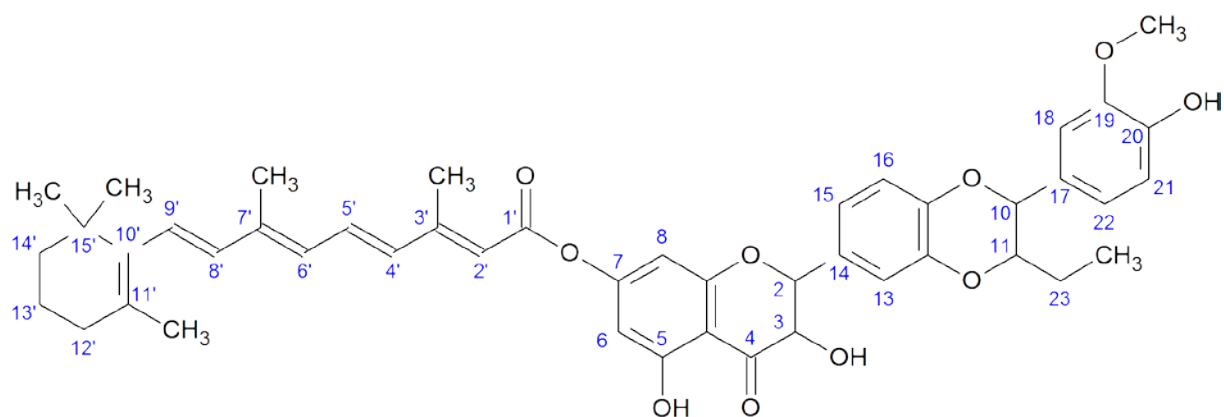


Figure S6. HRMS (ESI⁻) of compound **8b** m/z [M - H]⁻ calcd for C₄₅H₄₇O₁₁ 763.31239; found 763.31197

Table S6. ^1H and ^{13}C NMR data of compound **8b**.



Atom #	δ_{C}	m	δ_{H}	n_{H}	m	$J_{\text{H-H}}$ [Hz]
2	82.60	d	5.254	1	d	11.5
3	71.67	d	4.775	1	dd	11.5, 6.3
4	199.34	s	-	-	-	-
4a	104.56	s	-	-	-	-
5	161.85	s	-	-	-	-
6	102.86	d	6.393	1	d	2.0
7	158.06	s	-	-	-	-
8	101.63	d	6.362	1	d	2.0
8a	161.68	s	-	-	-	-
10	75.74	d	4.928	1	d	7.9
11	77.92	d	4.172	1	ddd	7.9, 4.7, 2.7
12a	142.88	s	-	-	-	-
13	116.45	d	7.133	1	d	2.0
14	129.82	s	-	-	-	-
15	120.91	d	7.011	1	dd	8.3, 2.0
16	116.38	d	6.947	1	d	8.3
16a	143.92	s	-	-	-	-
17	127.38	s	-	-	-	-
18	111.66	d	7.007	1	d	1.9
19	147.51	s	-	-	-	-
20	146.92	s	-	-	-	-
21	115.24	d	6.805	1	d	8.1
22	120.36	d	6.859	1	dd	8.1, 1.9
23	60.09	t	3.547	1	ddd	12.3, 4.9, 2.7
			3.350	1	ddd	12.3, 5.9, 4.7
3-OH	-	-	5.944	1	d	6.3
5-OH	-	-	11.691	1	s	-
19-MeO	55.61	q	3.778	3	s	-

20-OH	-	-	9.108	1	s	-
23-OH	-	-	4.922	1	dd	5.9, 4.9
1'	163.44	s	-	-	-	-
2'	116.03	d	6.057	1	s	-
3'	156.46	s	-	-	-	-
4'	134.45	d	6.519	1	d	15.1
5'	132.91	d	7.195	1	dd	15.1, 11.7
6'	129.63	d	6.283	1	d	11.7
7'	140.50	s	-	-	-	-
8'	136.71	d	6.206	1	d	16.1
9'	128.55	d	6.326	1	d	16.1
10'	137.14	s	-	-	-	-
11'	129.74	s	-	-	-	-
12'	32.55	t	2.01 ^H	2	m	-
13'	18.61	t	1.578	2	m	-
14'	39.10	t	1.444	2	m	-
15'	33.77	s	-	-	-	-
3'-Me	13.85	q	2.349	3	d	0.8
7'-Me	12.61	q	2.018	3	s	-
11'-Me	21.42	q	1.697	3	s	-
15'-Me	28.71	q	1.022	3	s	-

^H - HSQC readout