

SUPPORTING INFORMATION

Medicarpin and Homopterocarpin Isolated from *Canavalia lineata* as Potent and Competitive Reversible Inhibitors of Human Monoamine Oxidase-B

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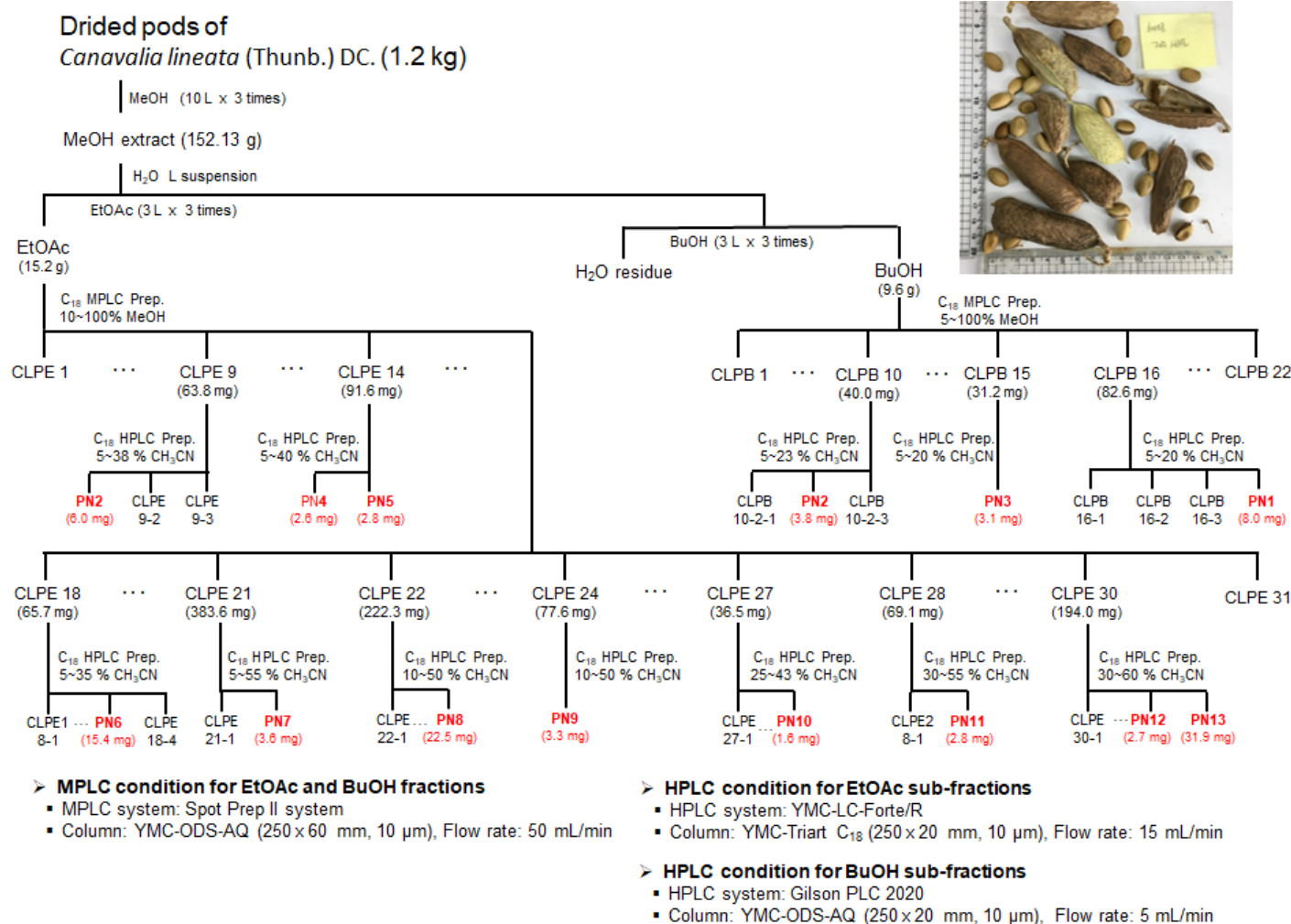


Figure S1. Separation scheme of compounds (PN1–PN13) from *Canavalia lineata* pods.

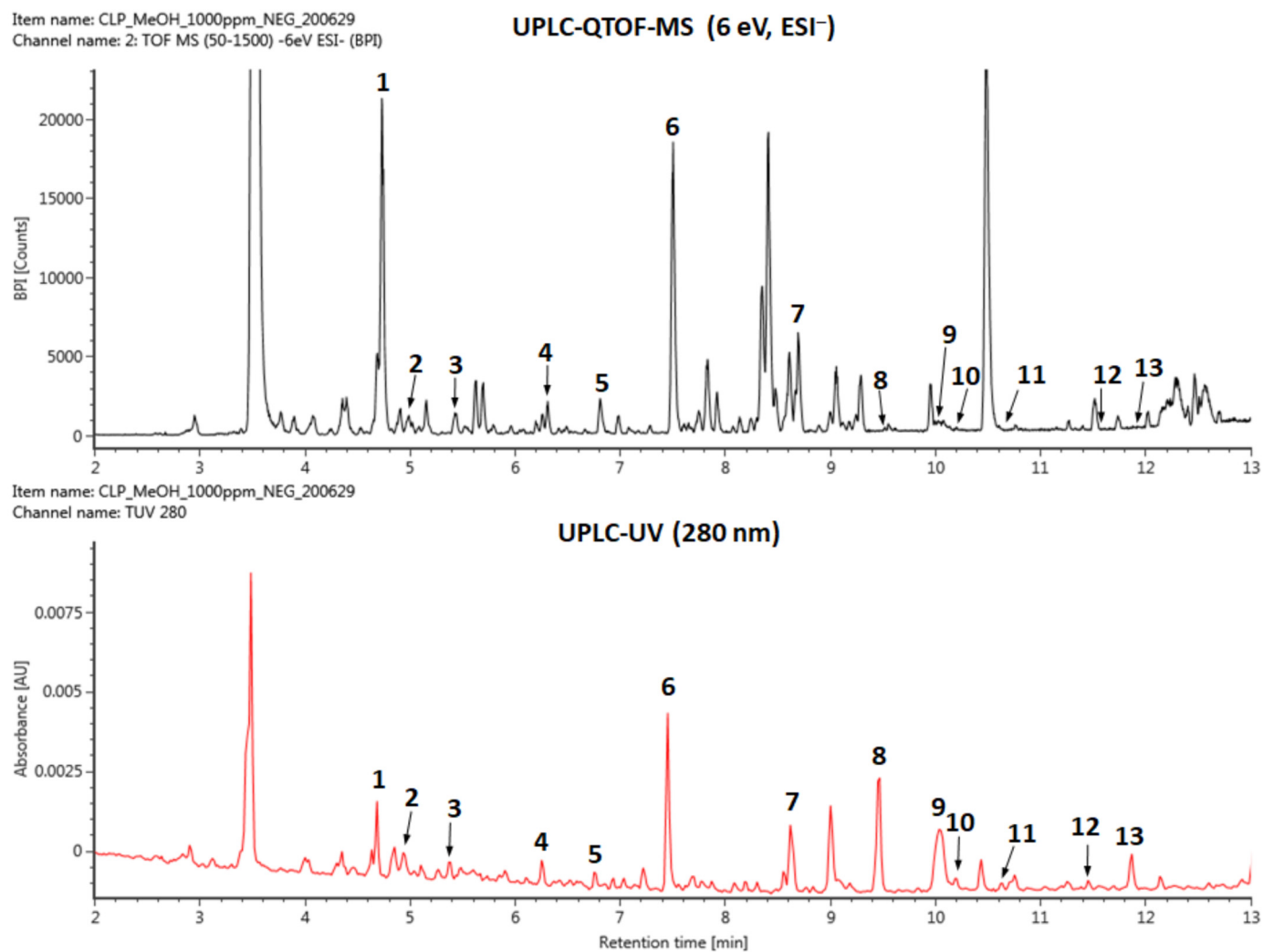


Figure S2. MS and UV chromatogram of *C. lineata* pod extract using UPLC-QTOF-MS.

PN 1. Rutin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
611.1608	611.1612	-0.4	-0.7	12.5	C27 H31 O16	27	31	16
	611.1647	-3.9	-6.4	34.5	C45 H23 O3	45	23	3
	611.1553	5.5	9.0	21.5	C34 H27 O11	34	27	11

CLPB_16_4_100ppm_POS_200628 1373 (4.721) Cm (1369:1379)

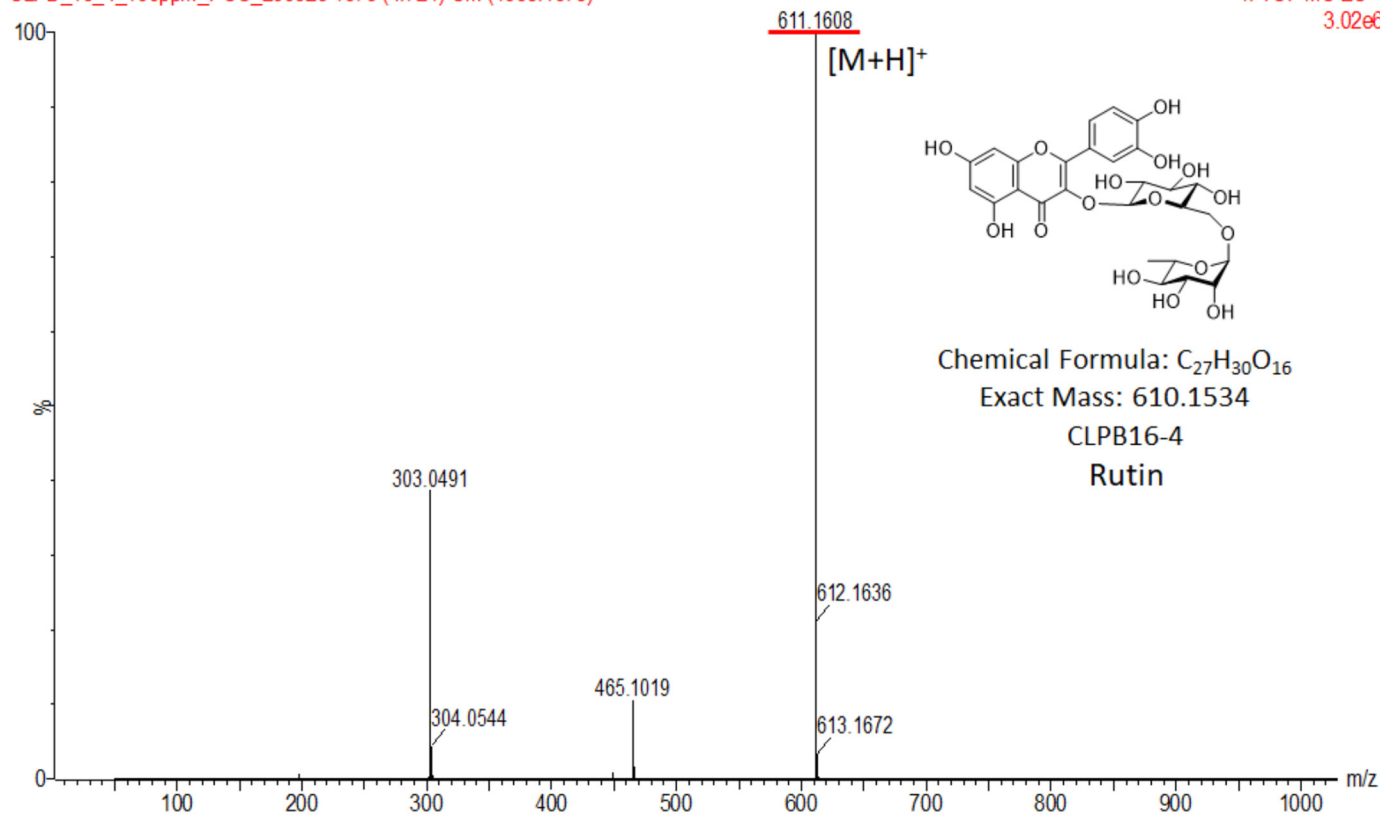
1: TOF MS ES+
3.02e6

Figure S3. UPLC-QTOF-MS spectrum of rutin (1).

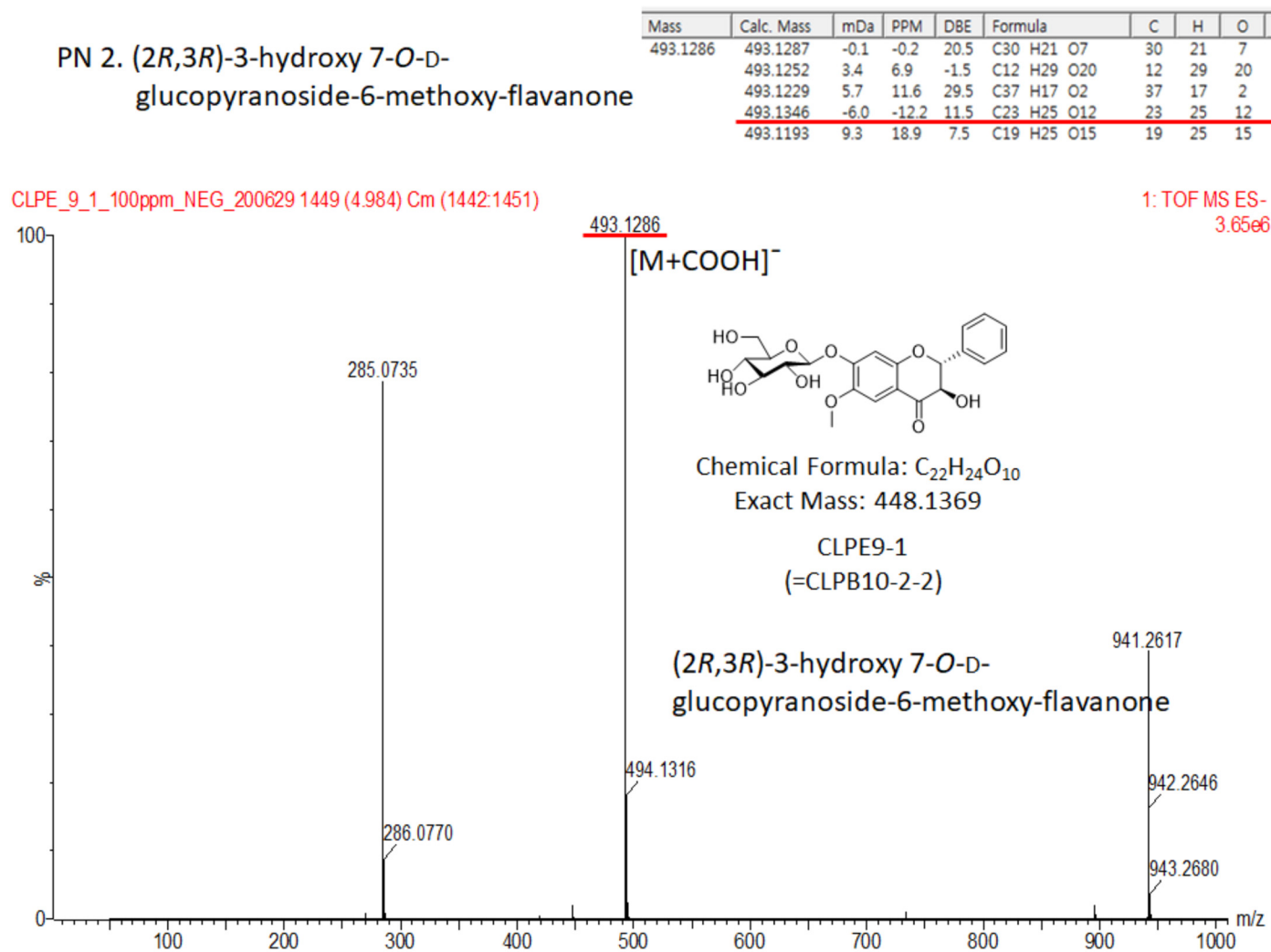
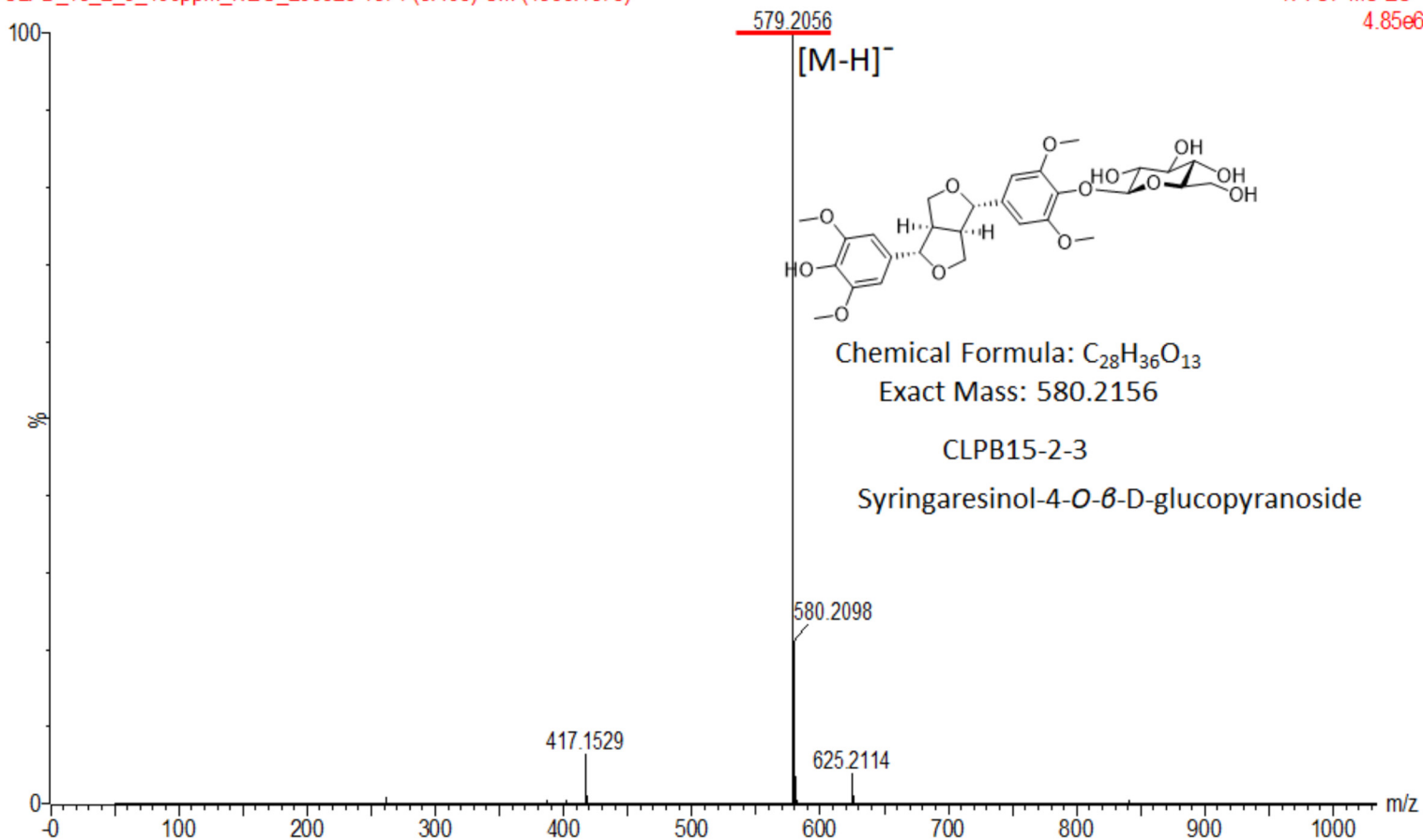


Figure S4. UPLC-QTOF-MS spectrum of (2*R*,3*R*)-3-hydroxy 7-*O*-β-D-glucopyranoside-6-methoxy-flavanone (2).

PN 3. Syringaresinol-4-*O*- β -D-glucopyranoside

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
579.2056	579.2078	-2.2	-3.8	11.5	C ₂₈ H ₃₅ O ₁₃	28	35	13

CLPB_15_2_3_100ppm_NEG_200629 1571 (5.409) Cm (1568:1579)

1: TOF MS ES-
4.85e6Figure S5. UPLC-QTOF-MS spectrum of (-)-syringaresinol-4-*O*- β -D-glucopyranoside (3).

PN 4. Ononin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
431.1305	431.1283	2.2	5.1	20.5	C29 H19 O4	29	19	4
431.1342	-3.7	-8.6	11.5		C22 H23 O9	22	23	9
431.1248	5.7	13.2	-1.5		C11 H27 O17	11	27	17
431.1401	-9.6	-22.3	2.5		C15 H27 O14	15	27	14
431.1190	11.5	26.7	7.5		C18 H23 O12	18	23	12

CLPE_14_1_100ppm_POS_200628 1833 (6.310) Cm (1827:1839)

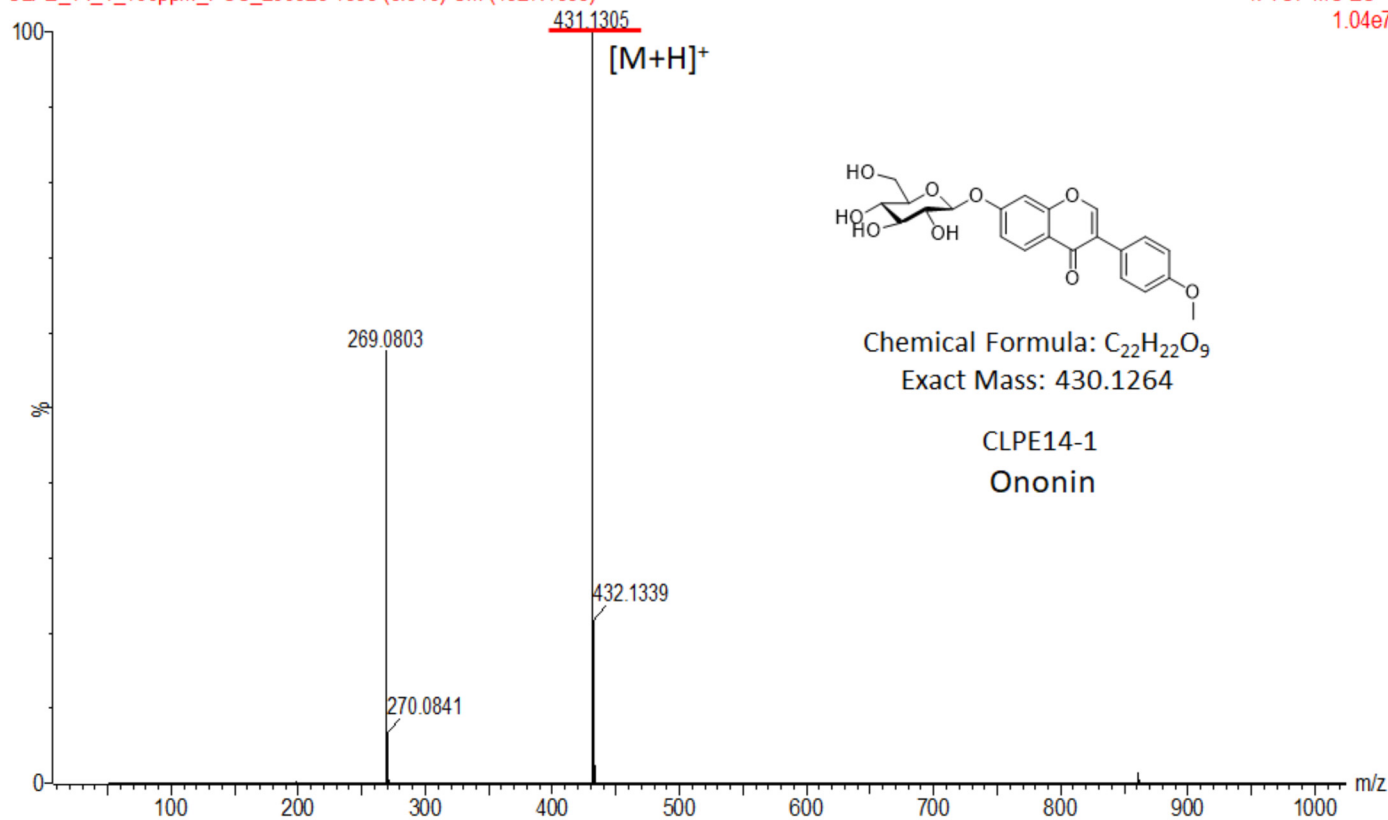
1: TOF MS ES+
1.04e7

Figure S6. UPLC-QTOF-MS spectrum of ononin (4).

PN 5. Syringaresinol

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
419.1668	419.1647	2.1	5.0	18.5	C29 H23 O3	29	23	3
	419.1706	-3.8	-9.1	9.5	C22 H27 O8	22	27	8
	419.1765	-9.7	-23.1	0.5	C15 H31 O13	15	31	13
	419.1553	11.5	27.4	5.5	C18 H27 O11	18	27	11

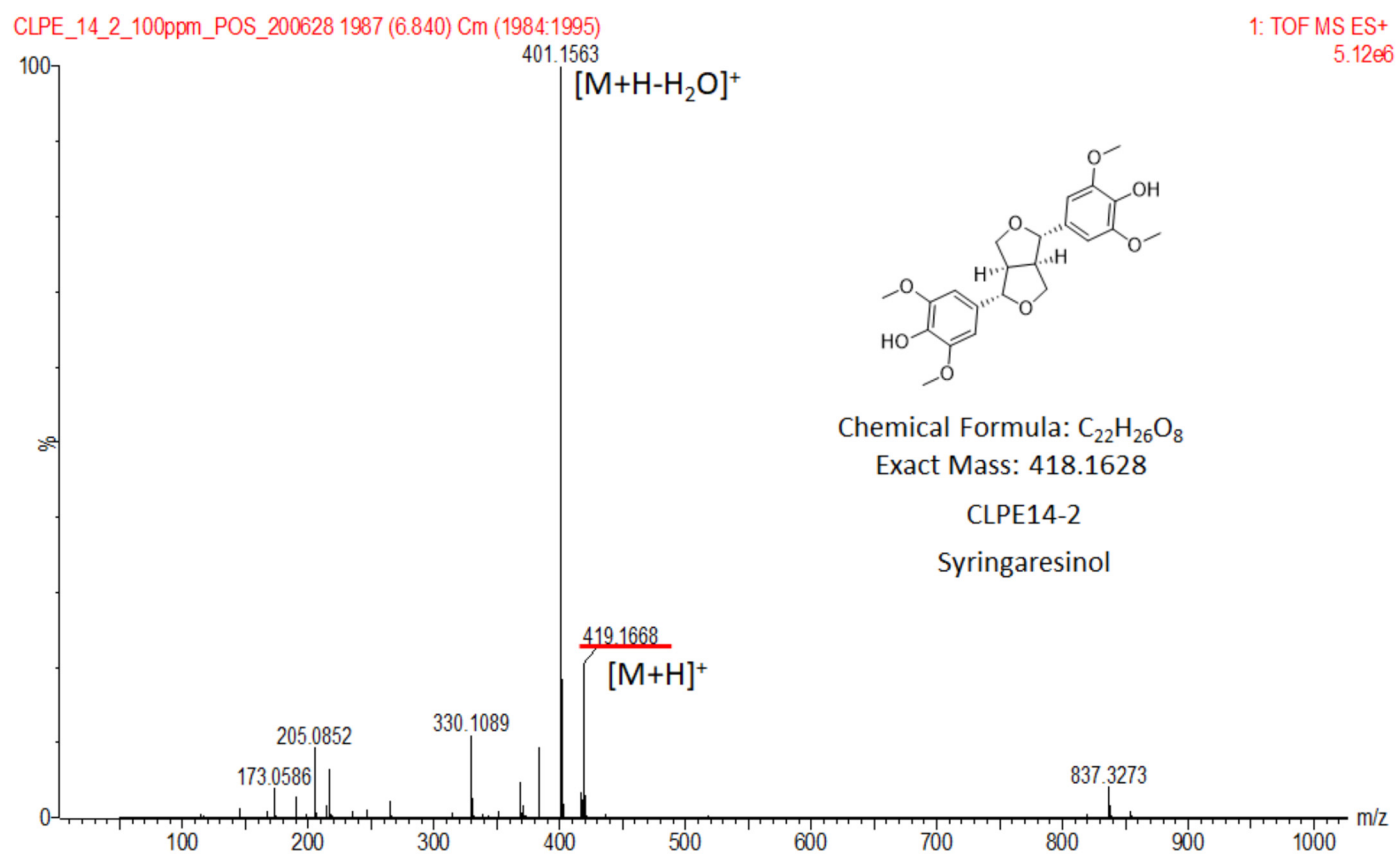


Figure S7. UPLC-QTOF-MS spectrum of syringaresinol (5).

PN 6. (2*R*,3*R*)-3,7'-Dihydroxy-6-methoxy-flavanone

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
287.0902	287.0919	-1.7	-5.9	9.5	C16 H15 O5	16	15	5
	287.0861	4.1	14.3	18.5	C23 H11	23	11	
	287.0978	-7.6	-26.5	0.5	C9 H19 O10	9	19	10

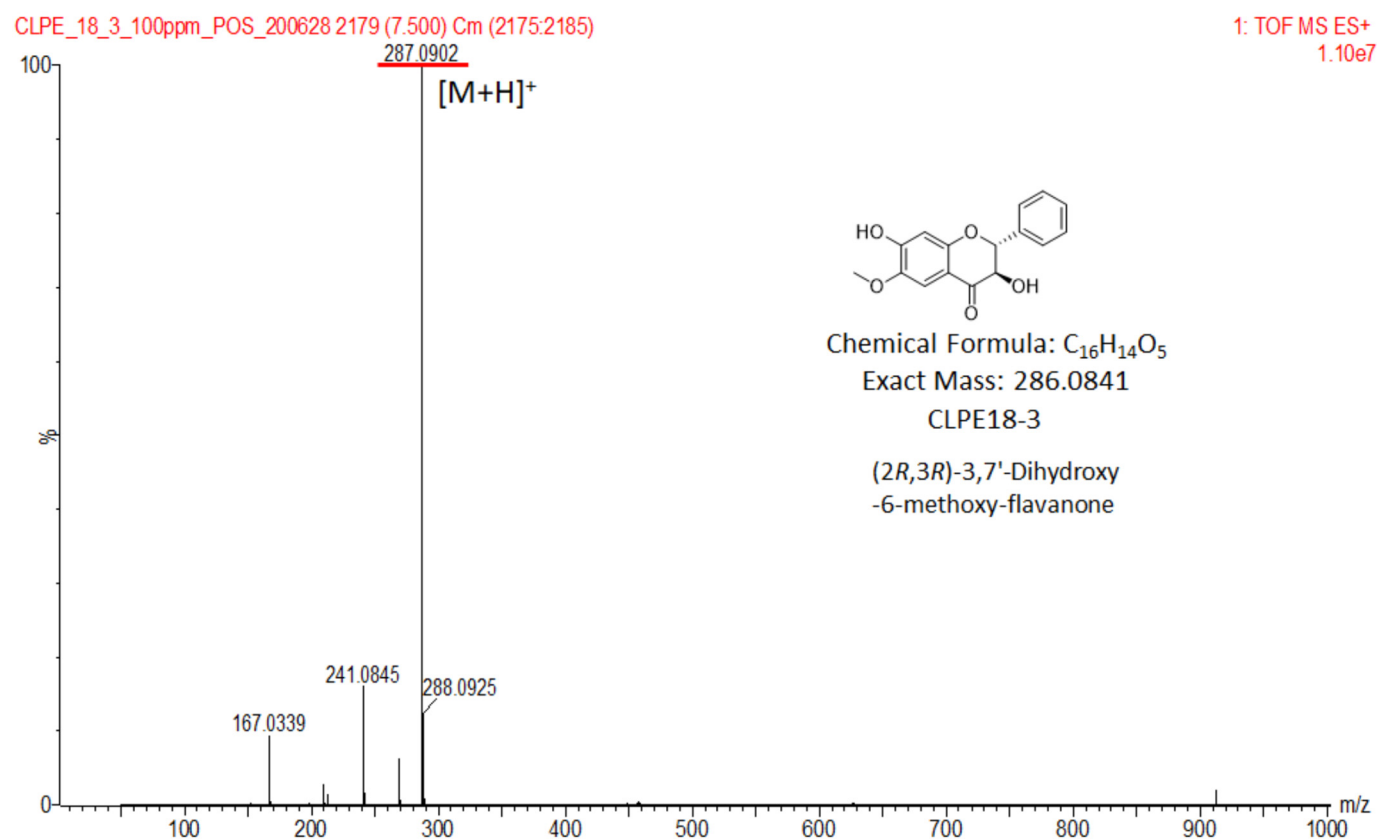


Figure S8. UPLC-QTOF-MS spectrum of (2*R*,3*R*)-3,7-dihydroxy-6-methoxyflavanone (6).

PN 7. Cajanin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
301.0555	301.0560	-0.5	-1.7	6.5	C12 H13 O9	12	13	9
		5.4	17.9	15.5	C19 H9 O4	19	9	4
		-9.8	-32.6	19.5	C23 H9 O	23	9	1
		14.8	49.2	2.5	C8 H13 O12	8	13	12
		-15.7	-52.1	10.5	C16 H13 O6	16	13	6

CLPE_21_M3_100ppm_POS_200727 2530 (8.708) Cm (2521:2535)

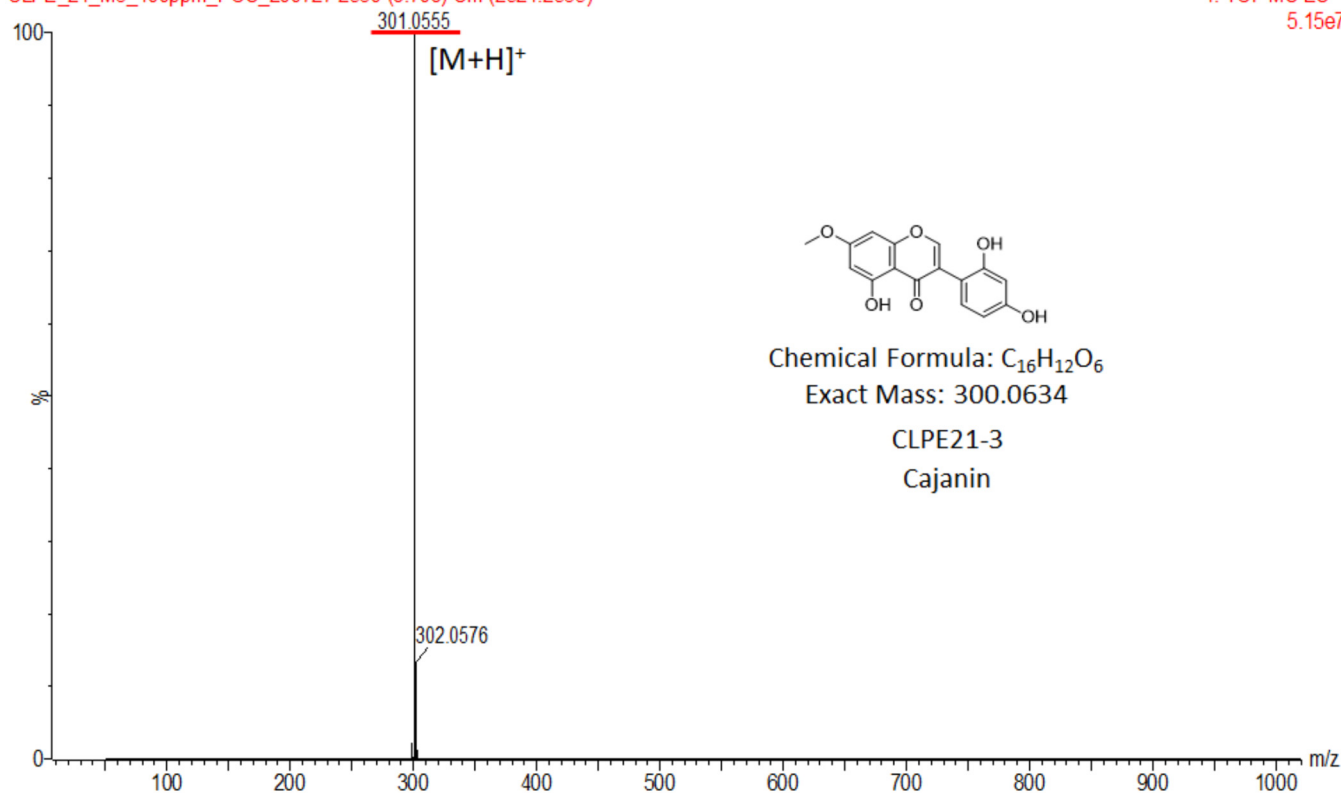
1: TOF MS ES+
5.15e7

Figure S9. UPLC-QTOF-MS spectrum of cajanin (7).

PN 8. Medicarpin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
271.0940	271.0970	-3.0	-11.1	9.5	C16 H15 O4	16	15	4
	271.1029	-8.9	-32.8	0.5	C9 H19 O9	9	19	9
	271.0818	12.2	45.0	5.5	C12 H15 O7	12	15	7

CLPE_22_3_100ppm_POS_200628 2762 (9.502) Cm (2757:2769)

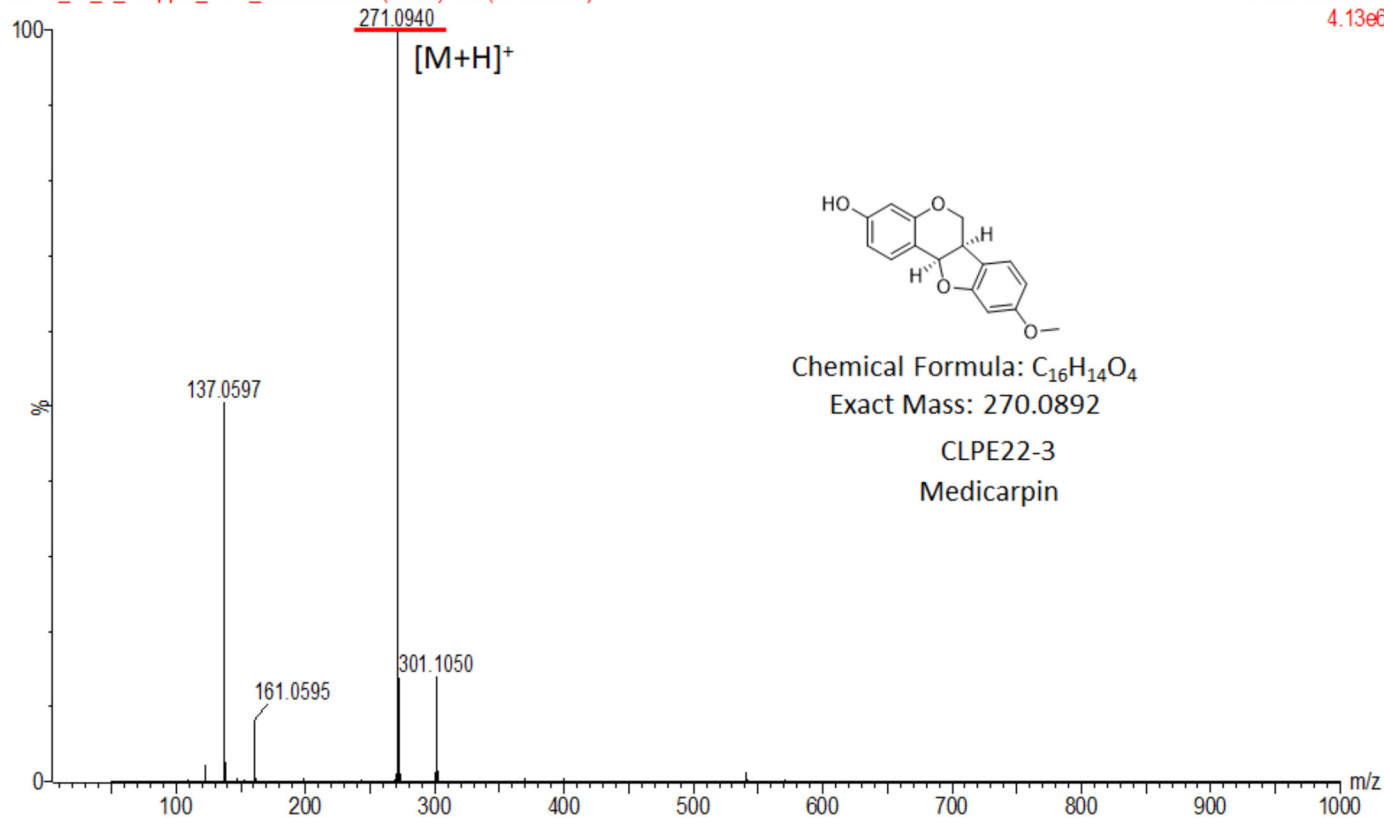
1: TOF MS ES+
4.13e6

Figure S10. UPLC-QTOF-MS spectrum of medicarpin (8).

PN 9. Prunetin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
285.0736	285.0763	-2.7	-9.5	10.5	C ₁₆ H ₁₃ O ₅	16	13	5
	285.0704	3.2	11.2	19.5	C ₂₃ H ₉	23	9	

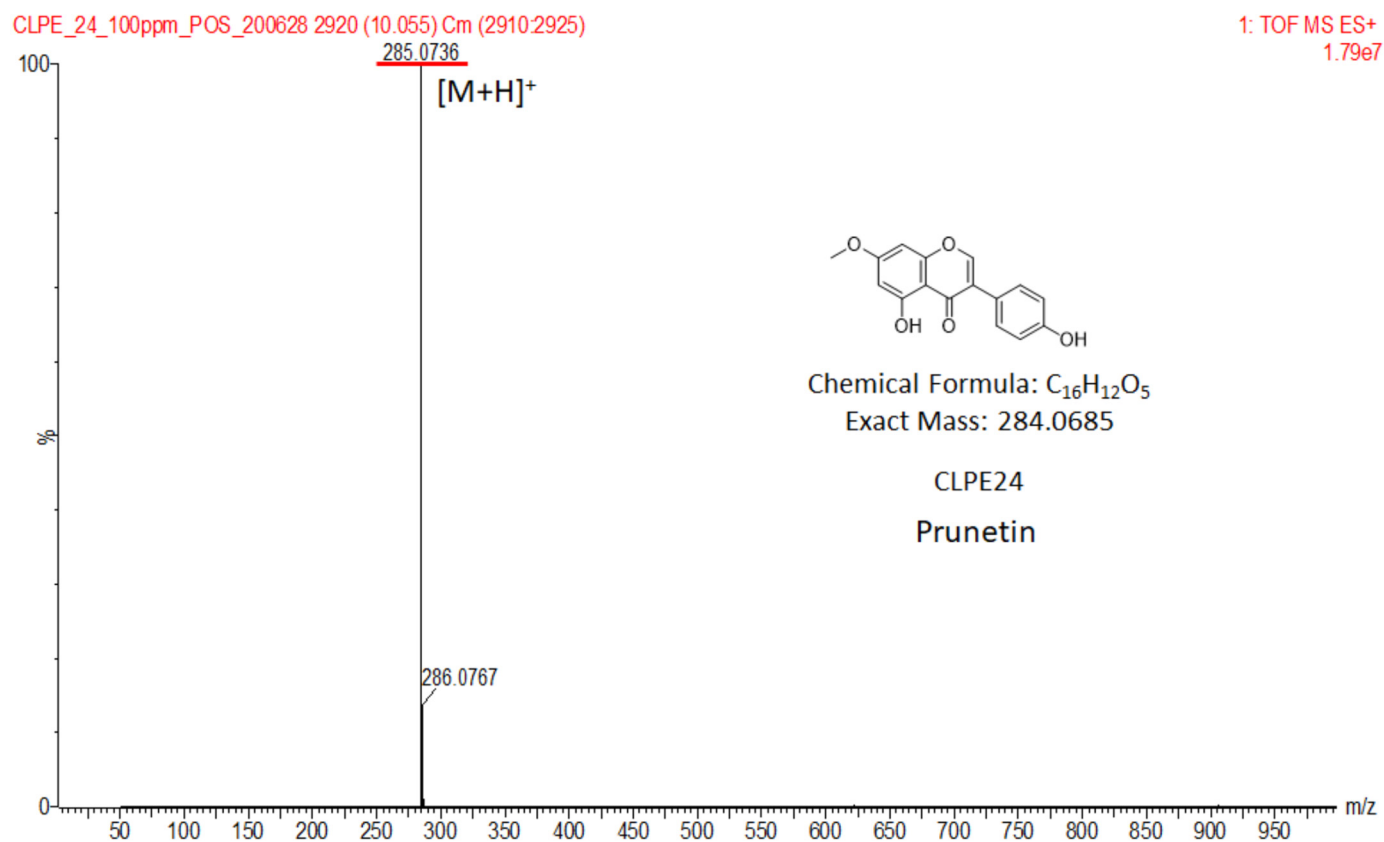


Figure S11. UPLC-QTOF-MS spectrum of prunetin (9).

PN 10. 7,4'-Dimethyl-3'-hydroxygenistein

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
315.0837	315.0810	2.7	8.6	19.5	C ₂₄ H ₁₁ O	24	11	1
315.0869	-3.2	-10.2	10.5		C ₁₇ H ₁₅ O ₆	17	15	6
315.0927	-9.0	-28.6	1.5		C ₁₀ H ₁₉ O ₁₁	10	19	11

CLPE_27_3_100ppm_POS_200628 2970 (10.225) Cm (2968:2981)

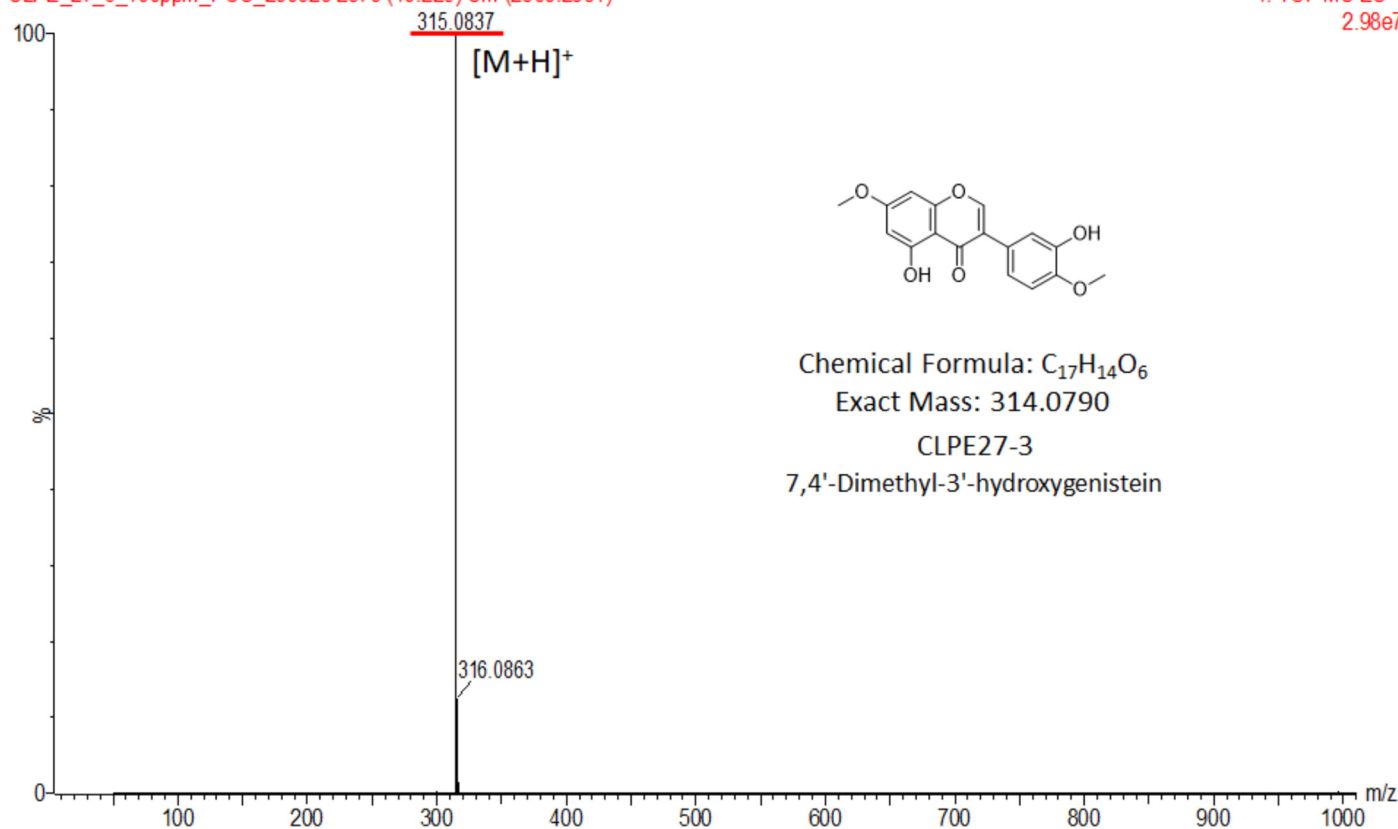
1: TOF MS ES+
2.98e7

Figure S12. UPLC-QTOF-MS spectrum of 7,4'-dimethyl-3'-hydroxygenistein (10).

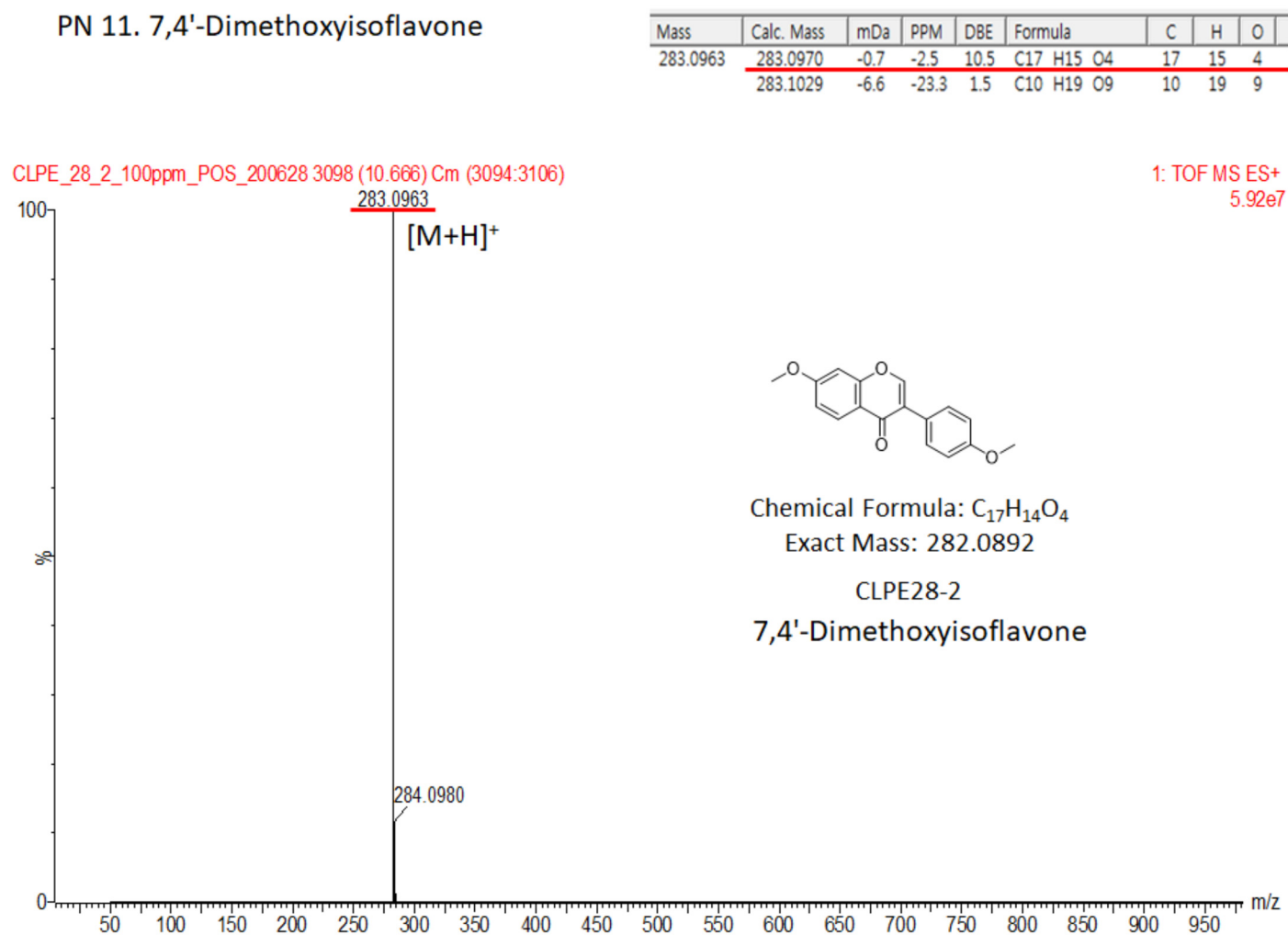


Figure S13. UPLC-QTOF-MS spectrum of 7,4'-dimethoxyisoflavone (11).

PN 12. Pterocarpin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
299.0903	299.0919	-1.6	-5.3	10.5	C17 H15 O5	17	15	5
	299.0861	4.2	14.0	19.5	C24 H11	24	11	

CLPE_30_5_100ppm_POS_200628 3367 (11.590) Cm (3359:3372)

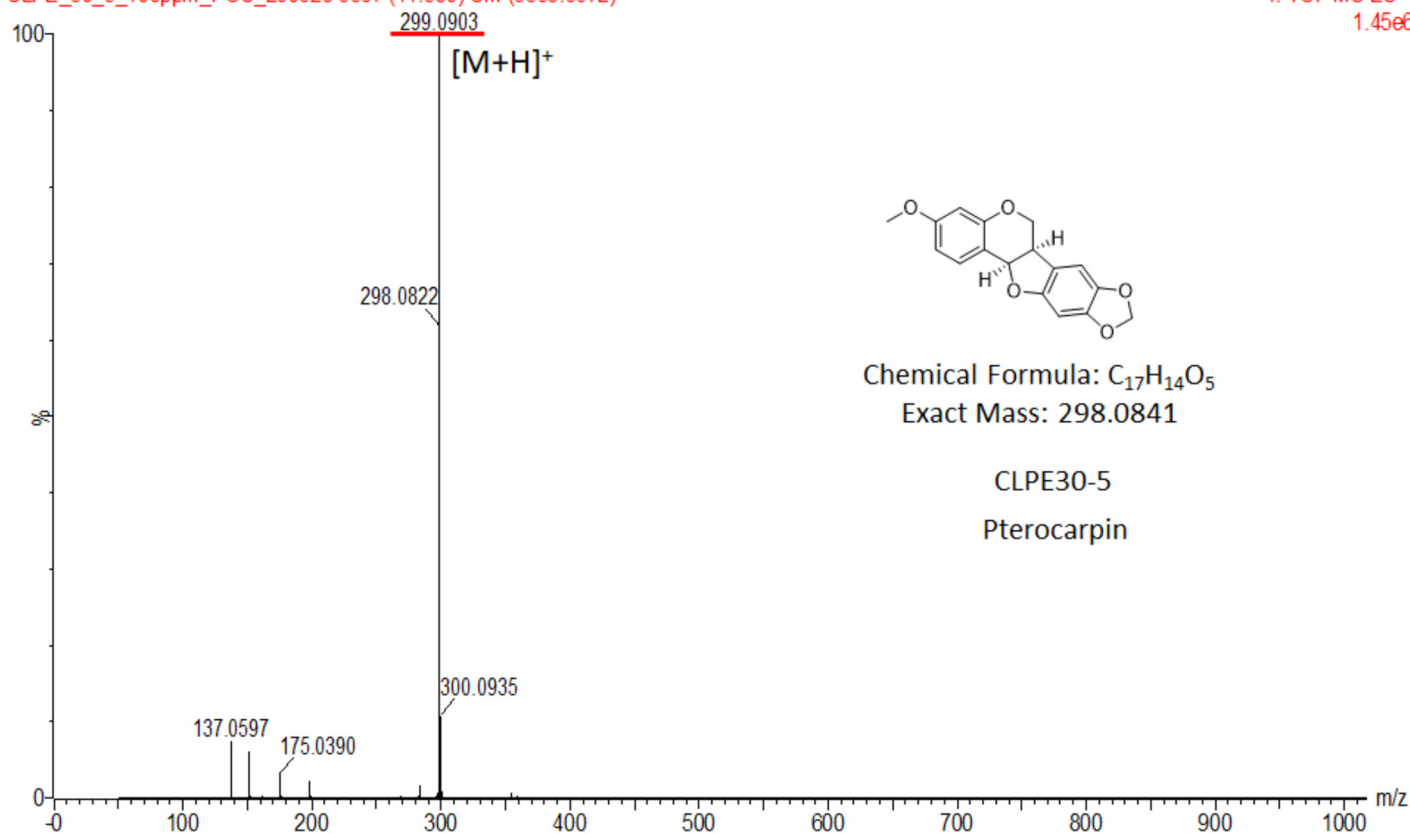
1: TOF MS ES+
1.45e6

Figure S14. UPLC-QTOF-MS spectrum of pterocarpin (12).

PN 13. Homopterocarpin

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O
285.1123	285.1127	-0.4	-1.4	9.5	C17 H17 O4	17	17	4
	285.1186	-6.3	-22.1	0.5	C10 H21 O9	10	21	9
	285.0974	14.9	52.3	5.5	C13 H17 O7	13	17	7
	285.1279	-15.6	-54.7	13.5	C21 H17 O	21	17	1

CLPE_30_6_100ppm_POS_200628 3456 (11.897) Cm (3453:3466)

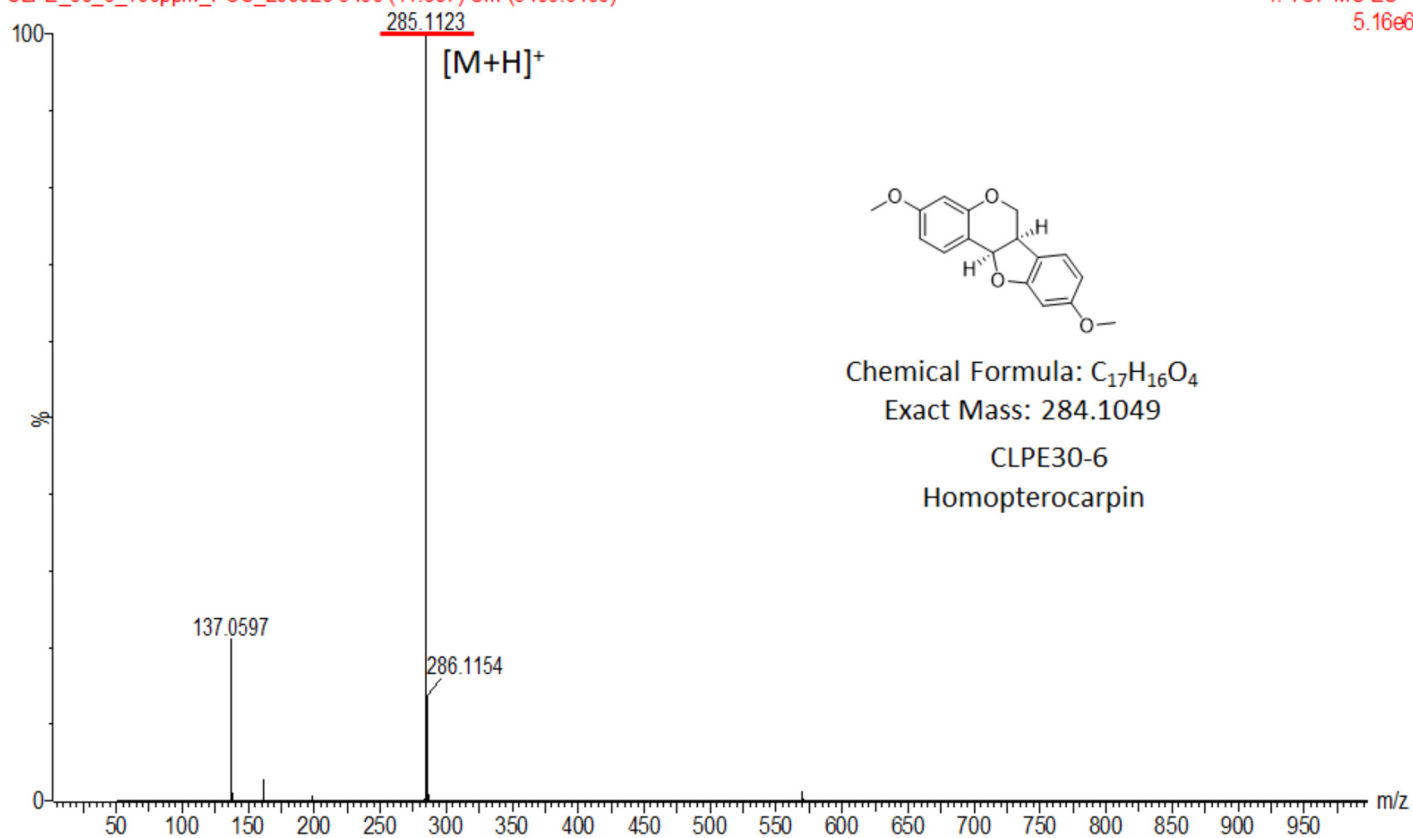
1: TOF MS ES+
5.16e6

Figure S15. UPLC-QTOF-MS spectrum of homopterocarpin (13).

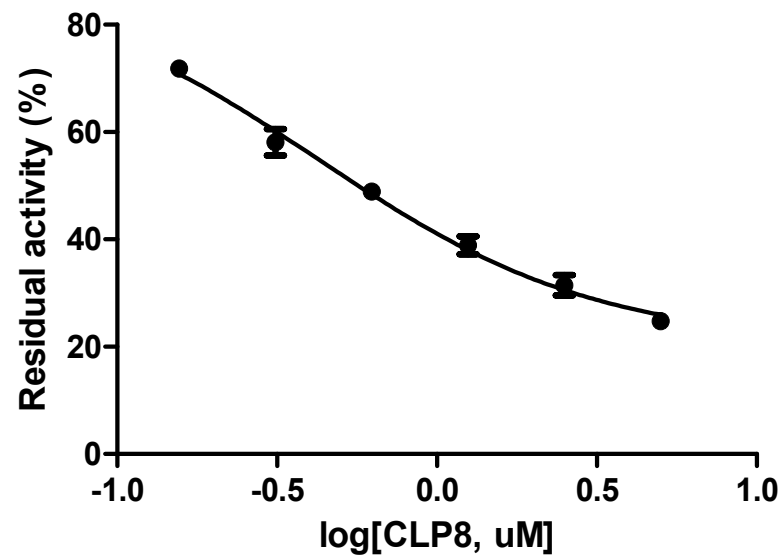


Figure S16. IC₅₀ curve of medicarpin (8) for hMAO-B.

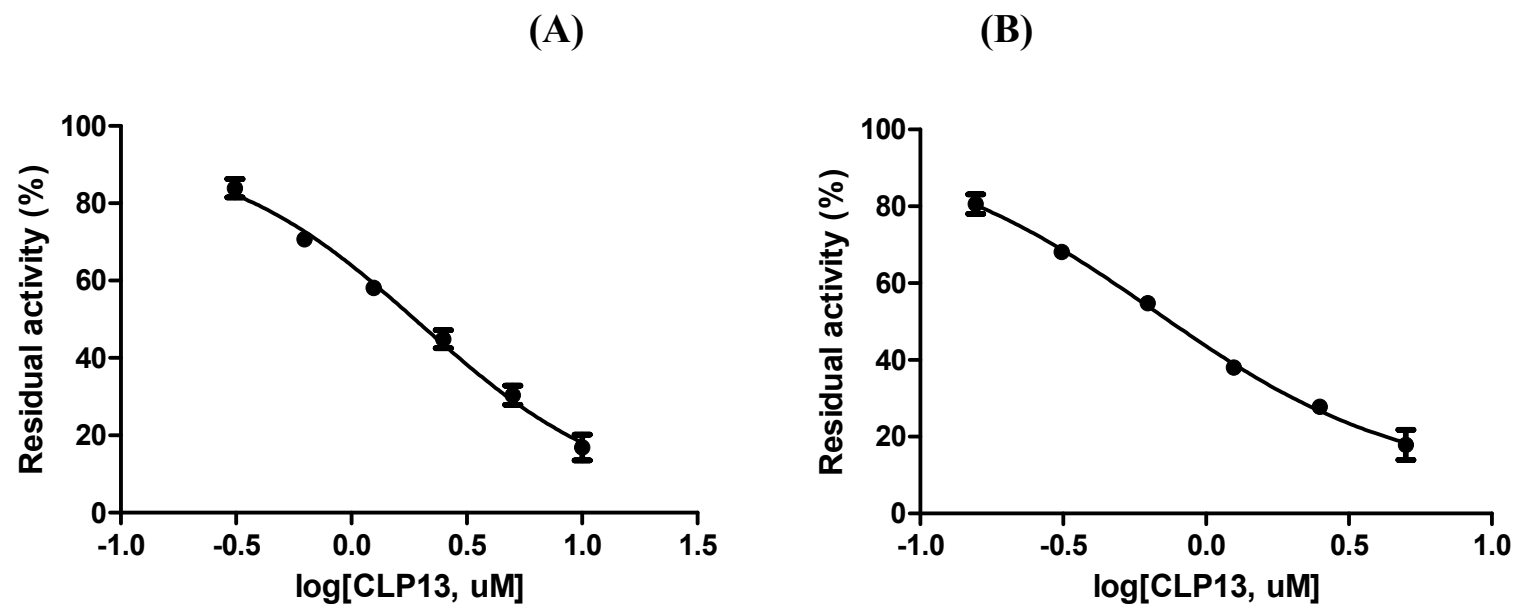


Figure S17. IC₅₀ curves of homopterocarpin (13) for hMAO-A (A) and hMAO-B (B).