

Supplementary Information

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1 Supplementary Tables

Table S1 Calculated Secondary Structure Fractions

C3A (μM)	C3Ga (μM)			Pn3A (μM)			Pn3Ga (μM)					
	0	100	200	0	100	200	0	100	200	0	100	200
α-helix	0.49	0.46	0.18	0.48	0.47	0.39	0.51	0.52	0.50	0.41	0.50	0.53
β-strand	0.00	0.03	0.08	0.01	0.00	0.03	0.01	0.00	0.00	0.00	0.01	0.00
β-turn	0.16	0.15	0.16	0.15	0.17	0.16	0.14	0.17	0.14	0.19	0.15	0.12
β-total	0.16	0.17	0.25	0.16	0.17	0.18	0.16	0.17	0.15	0.19	0.16	0.13
unordered	0.35	0.37	0.58	0.36	0.36	0.43	0.34	0.30	0.35	0.40	0.34	0.34

Table S2 Summary of fluorescence spectroscopy statistics

		C3A		C3Ga	Pn3A	Pn3Ga
Temperature (K)	310	320	330	310	310	310
K_q (10¹³ L/mol·s)	5.72	3.14	4.32	4.51	5.20	4.32
K_a (10⁴ L/mol)	80.2	47.8	18.8	2.98	9.98	68.5
n	1.03	1.03	0.93	0.80	0.90	1.03
ΔH (kJ/mol)		-61.5		-	-	-
ΔS (J/mol)		-84.9		-	-	-
ΔG (kJ/mol)	-35.2	-34.4	-33.5	-	-	-

2 Supplementary Figures

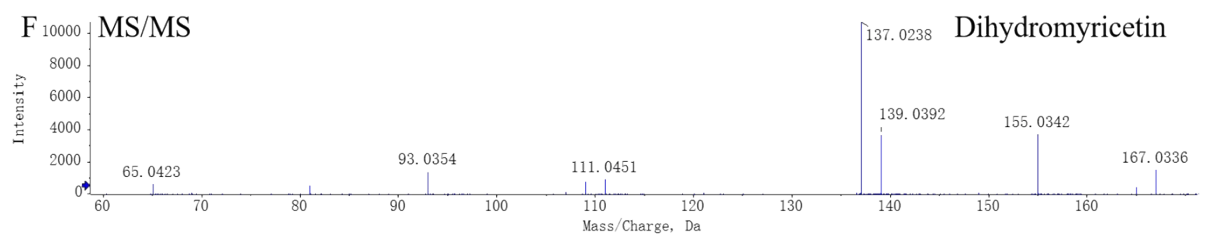
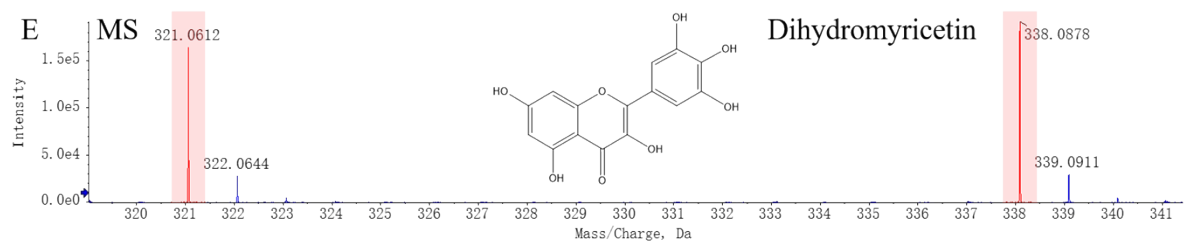
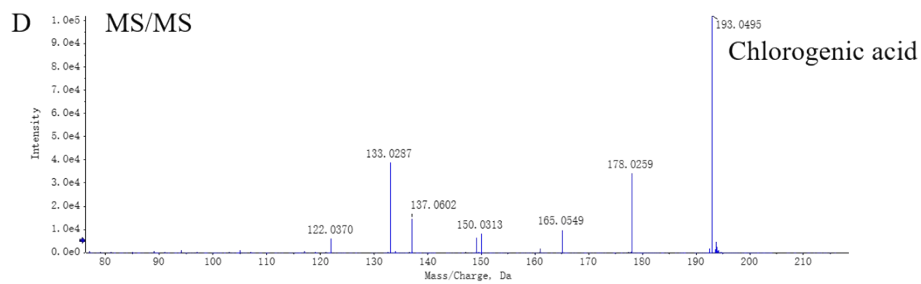
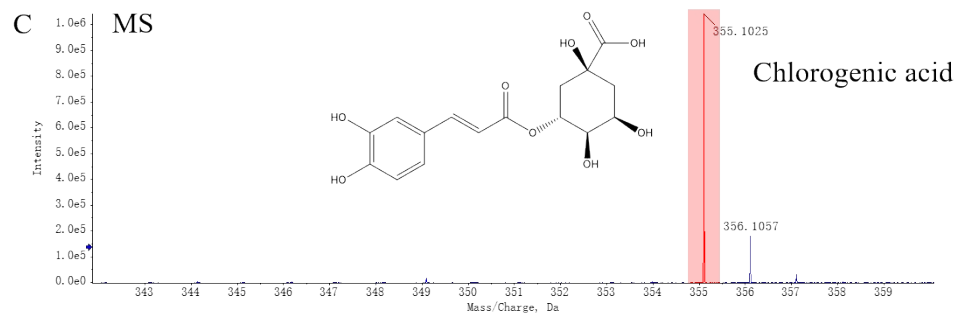
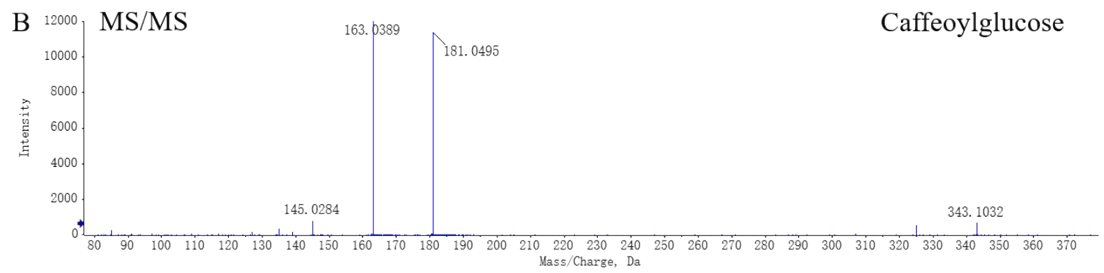
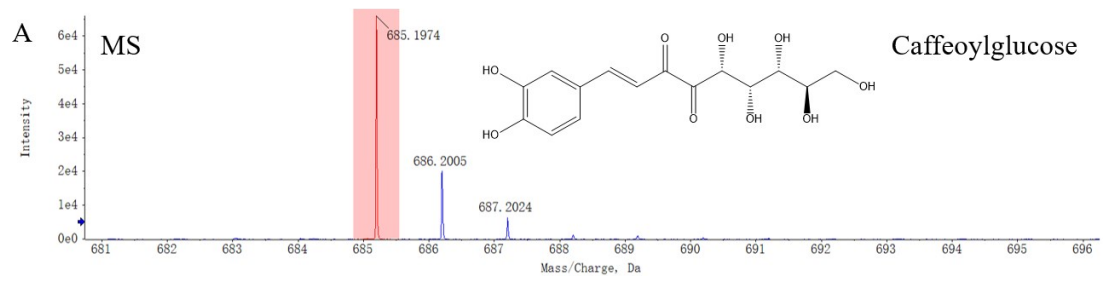


Figure S1. LC-MS/MS chromatograms of compound 2, 4 and 17 in Table 1. A. MS chromatogram of compound 2 (identified as caffeoylglucose). B. MS/MS chromatogram of compound 2 (identified as caffeoylglucose). C. MS chromatogram of compound 4 (identified as chlorogenic acid). D. MS/MS chromatogram of compound 4 (identified as chlorogenic acid). E. MS chromatogram of compound 17 (identified as dihydromyricetin). F. MS/MS chromatogram of compound 17 (identified as dihydromyricetin).

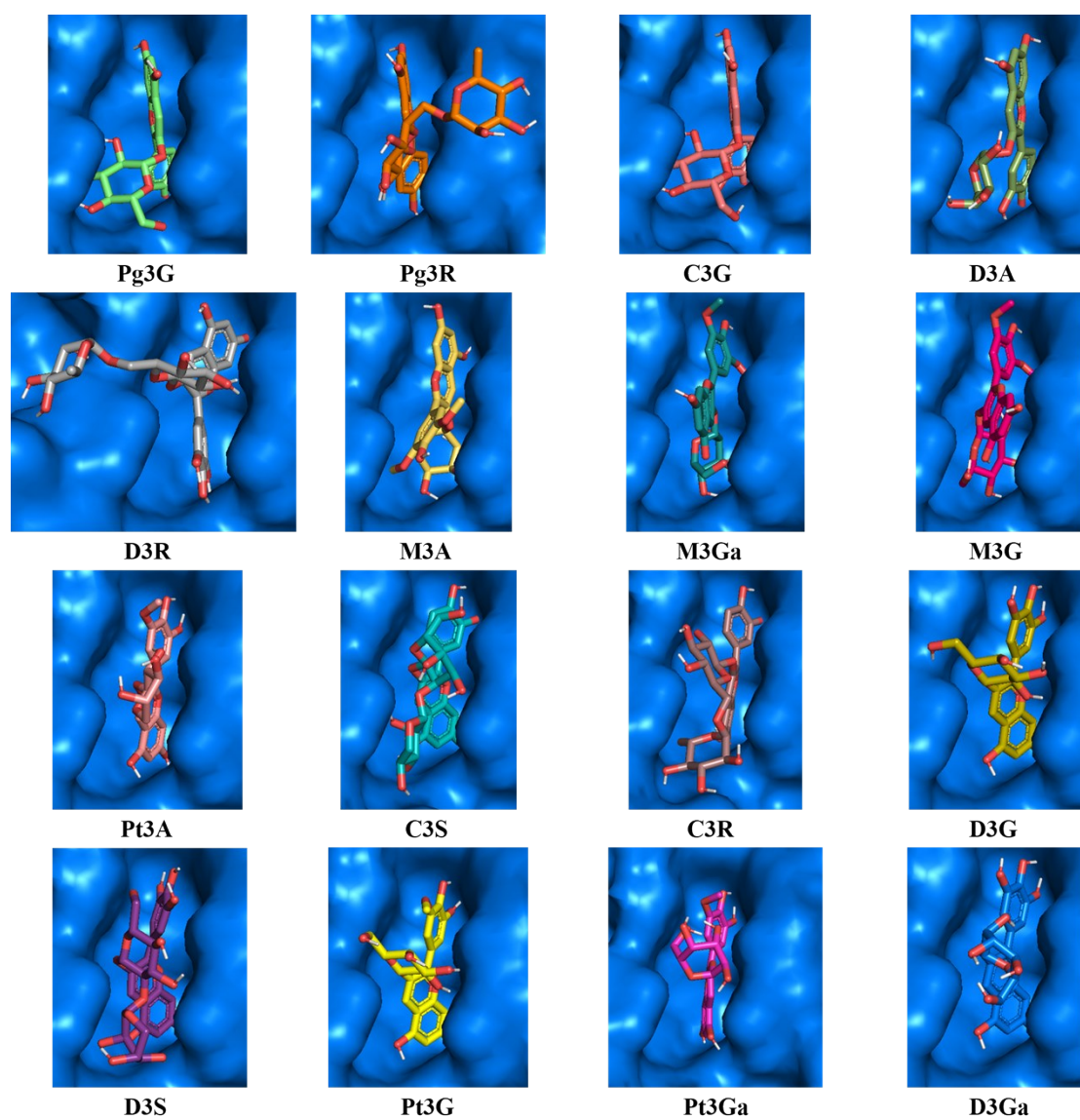


Figure S2. Binding Conformations of 16 anthocyanin analogues with the pancreatic lipase. Type A conformation: Pg3G, Pg3R, C3G, D3A and D3R. Type B conformation: M3A. Type C conformation: M3Ga and M3G. Type D conformation: Pt3A, C3S, C3R, D3G, D3S, Pt3G, Pt3Ga and D3Ga.