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Supplementary information

3D-QSAR studies on structure-bitterness analysis of citrus flavonoids

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This material includes: The correlation between the training set and test set observed

value data and predicted value data (Figure S1) and bitterness threshold of 20 flavonoids (Table S1).

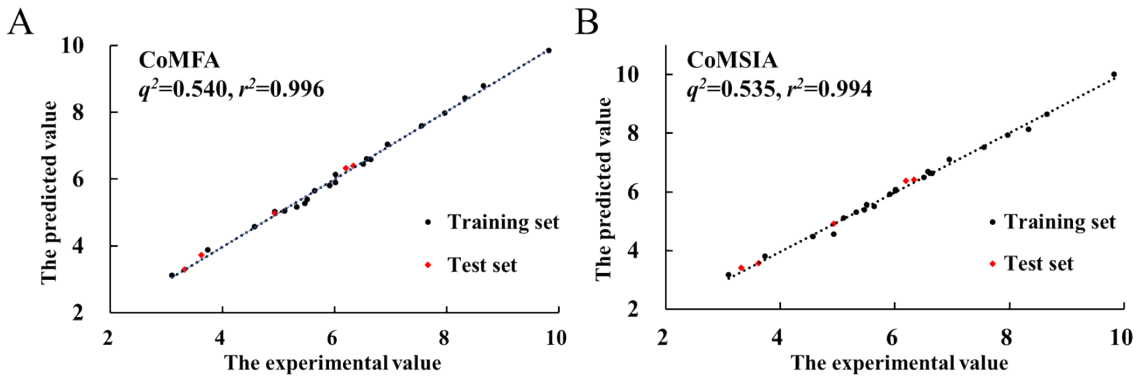
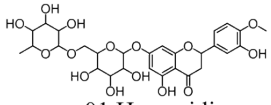
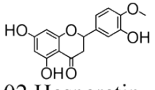
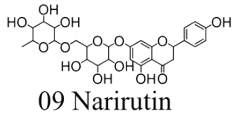
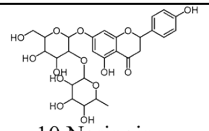
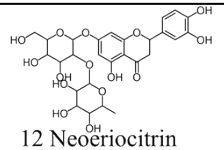
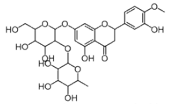
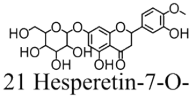
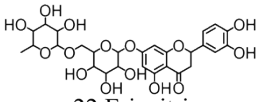
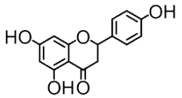
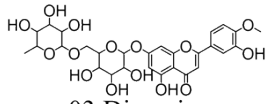
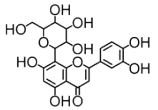
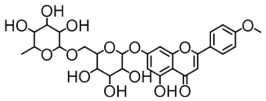
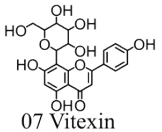
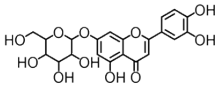
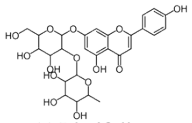
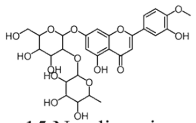
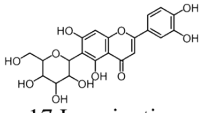
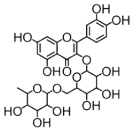
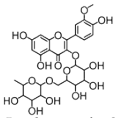
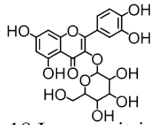
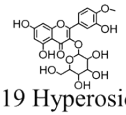
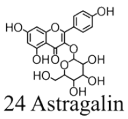
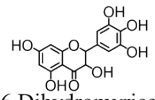
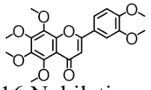
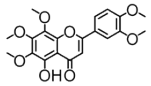
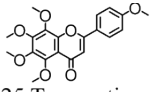


Figure S1. The correlation between the training set and test set observed value data and predicted value data. (A): CoMFA model results; (B): CoMSIA model results

Table S1 Bitterness threshold of 26 flavonoids

	Compound Structure	Bitterness Threshold	Compound Structure	Bitterness Threshold	Compound Structure	Bitterness Threshold	Compound Structure	Bitterness Threshold	Compound Structure	Bitterness Threshold
Flavanone	 01 Hesperidin	0.075	 02 Hesperetin	0.011	 09 Narirutin	0.042	 10 Naringin	0.015	 12 Neoeriocitrin	0.025
	 13 Neohesperidin	0.002	 21 Hesperetin-7-O-glucoside	0.010	 22 Eriocitrin	0.012	 23 Naringenin	0.033		
Flavone	 03 Diosmin	0.023	 04 Orientin	0.003	 06 Linarin	0.005	 07 Vitexin	0.001		
	 08 Luteoloside	0.017	 11 Rhoifolin	0.029	 15 Neodiosmin	0.022	 17 Isoorientin	0.016		
	 05 Rutin	0.117	 14 Isorhamnetin-3-O-rutinoside	0.033	 18 Isoquercitrin	0.011				
Flavonol	 19 Hyperoside	0.004	 24 Astragalin	0.014	 26 Dihydromyricetin	0.081				
PMF	 16 Nobiletin	0.008	 20 5-Demethylnobiletin	0.020	 25 Tangeretin	0.100				