Supplementary Information (ESI)

Antioxidant mechanisms and products of four 4',5,7-trihydroxyflavonoids with different structural types

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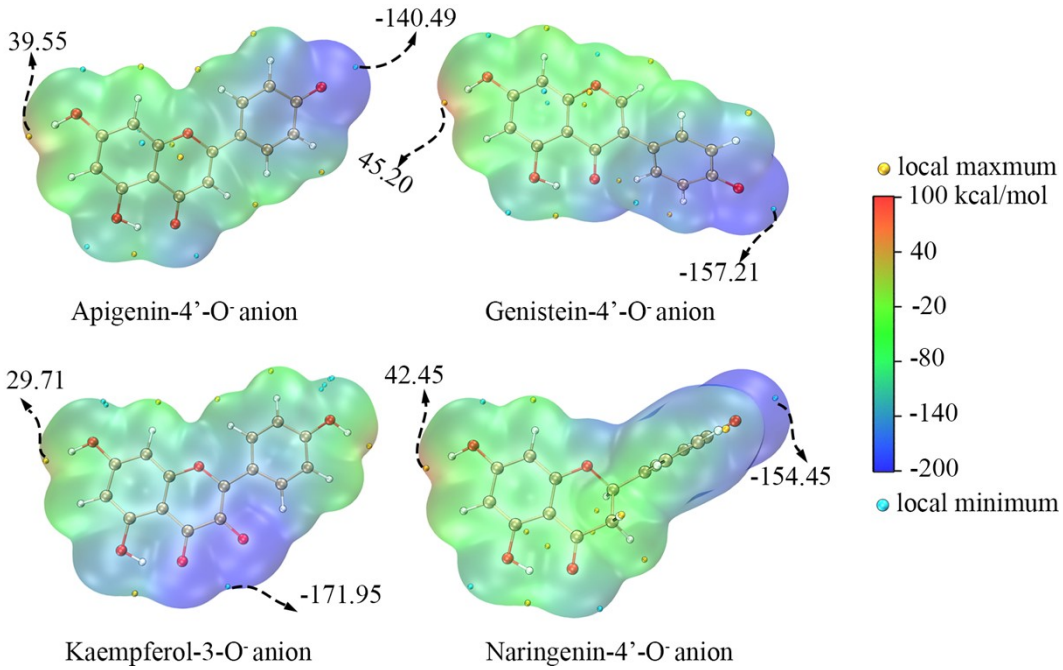

Fig. S1 The electrostatic potential of the four flavonoid anions.

Table S1 The atomic charges and bond dipole moments (Debye) of hydroxyls of the four flavonoids

Molecule	Site of the hydroxyl	Charge of the O atom	Charge of the H atom	Charge of the hydroxyl	bond moment of the O-H
AP	C_5	-0.414	0.280	-0.134	0.83087
	C_7	-0.408	0.317	-0.091	0.66642
	$C_{4'}$	-0.413	0.315	-0.098	0.66393
GE	C_5	-0.410	0.282	-0.128	0.82867
	C_7	-0.407	0.318	-0.089	0.66790
	$C_{4'}$	-0.429	0.310	-0.119	0.65531
KA	C_3	-0.413	0.293	-0.120	0.72244
	C_5	-0.408	0.284	-0.124	0.79888
	C_7	-0.407	0.318	-0.089	0.66698
	$C_{4'}$	-0.417	0.313	-0.104	0.66174
NA	C_5	-0.405	0.282	-0.123	0.81699
	C_7	-0.403	0.318	-0.085	0.66712
	$C_{4'}$	-0.429	0.310	-0.119	0.65572

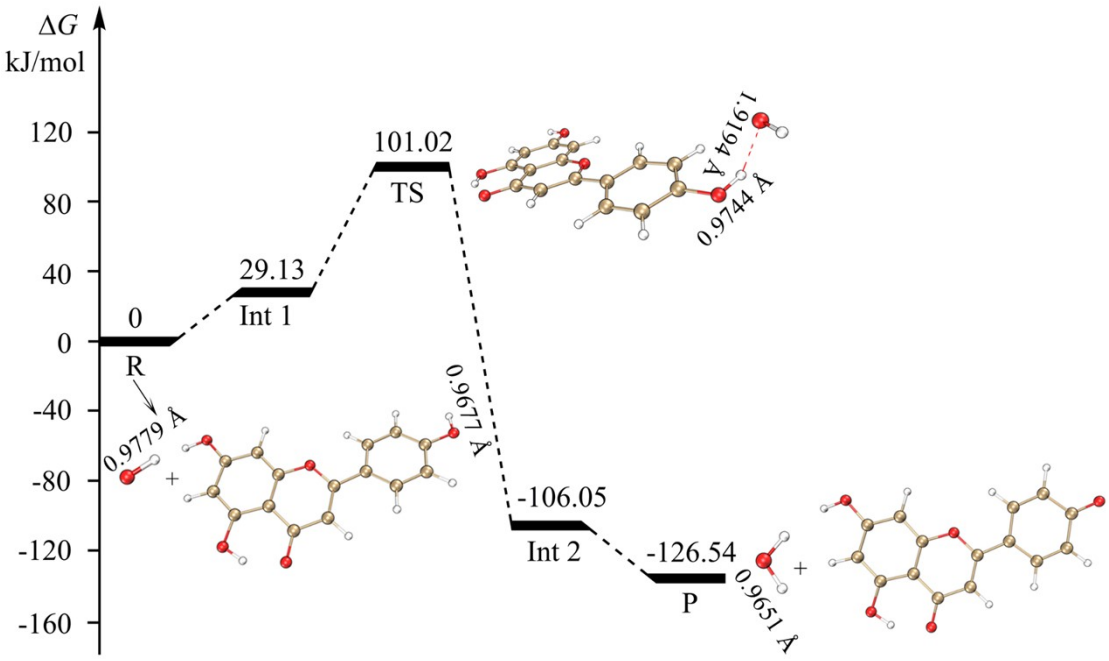

Fig. S2 The intrinsic reaction coordinates of apigenin to scavenging •OH (R: reactants; Int: intermediates; TS: transition state; P: products).

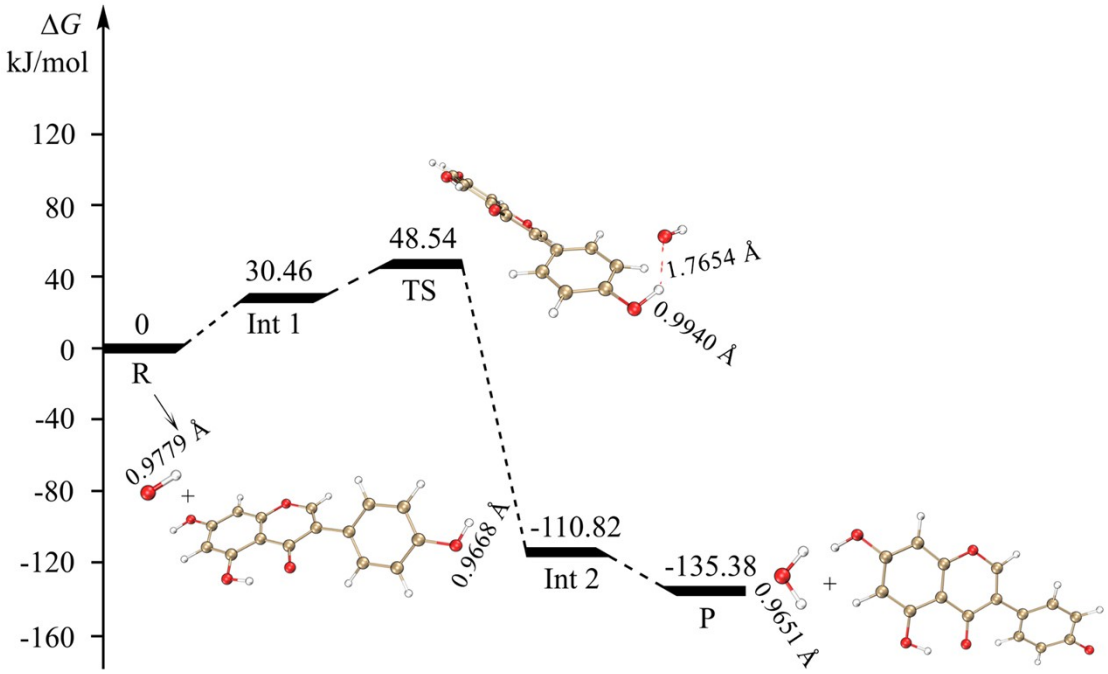

Fig. S3 The intrinsic reaction coordinates of genistein to scavenging •OH (R: reactants; Int: intermediates; TS: transition state; P: products).

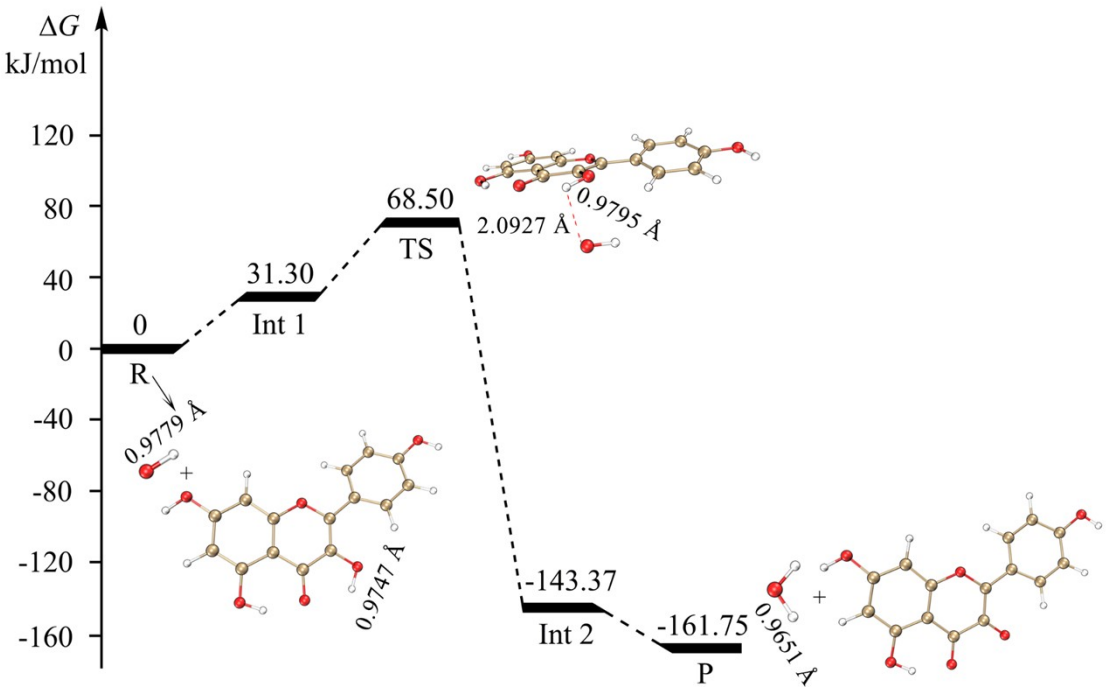

Fig. S4 The intrinsic reaction coordinates of kaempferol to scavenging •OH (R: reactants; Int: intermediates; TS: transition state; P: products).

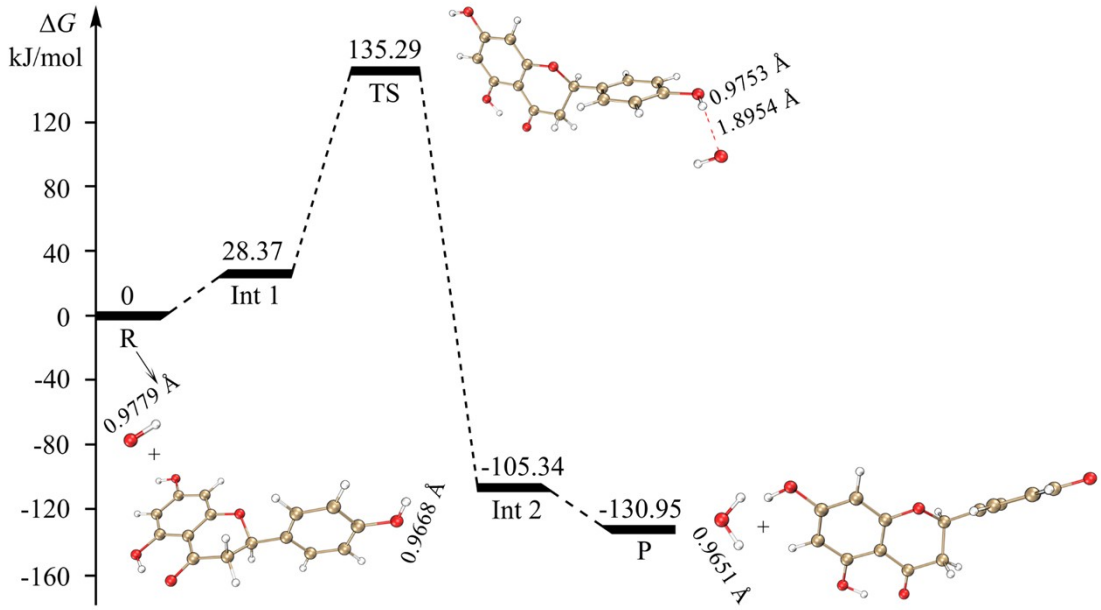

Fig. S5 The intrinsic reaction coordinates of naringenin to scavenging •OH (R: reactants; Int: intermediates; TS: transition state; P: products).

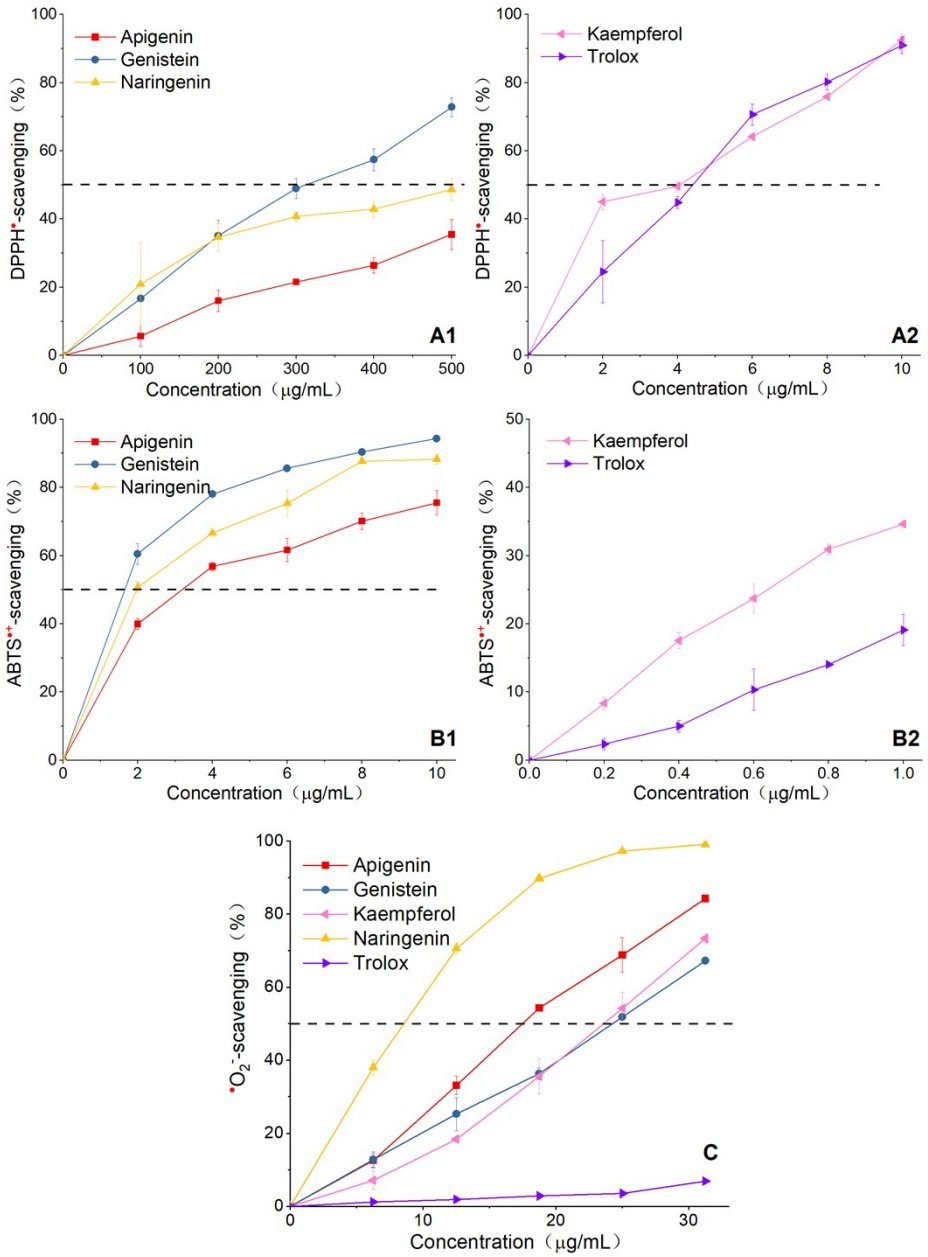

Fig. S6 The dose-response curves of the four flavonoids in DPPH•-scavenging (**A**), ABTS•+-scavenging (**B**), and •O_2^--scavenging (**C**) assays.