

Supporting Information

Biological Activity of Natural Flavonoids as Impacted by Protein Flexibility: An

Example of Flavanones

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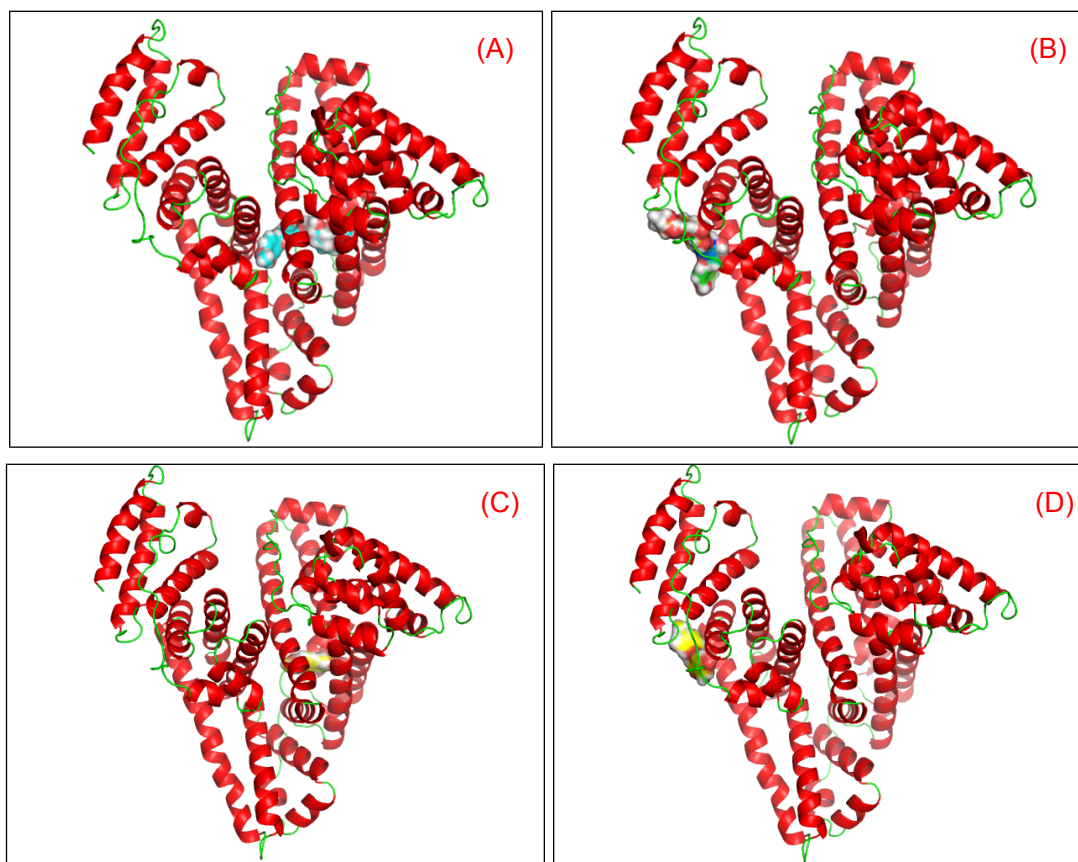


Fig. S1. The pattern shows docked flavanones in HSA at subdomains IIA and IIIA, HSA displayed in surface colored in red, to flavanones, colored as per the atoms and endowed with opaque surface of electron spin density. Panel (A): HSA-hesperidin (subdomain IIA); Panel (B): HSA-hesperidin (subdomain IIIA); Panel (C): HSA-hesperetin (subdomain IIA); and Panel (D): HSA-hesperetin (subdomain IIIA). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

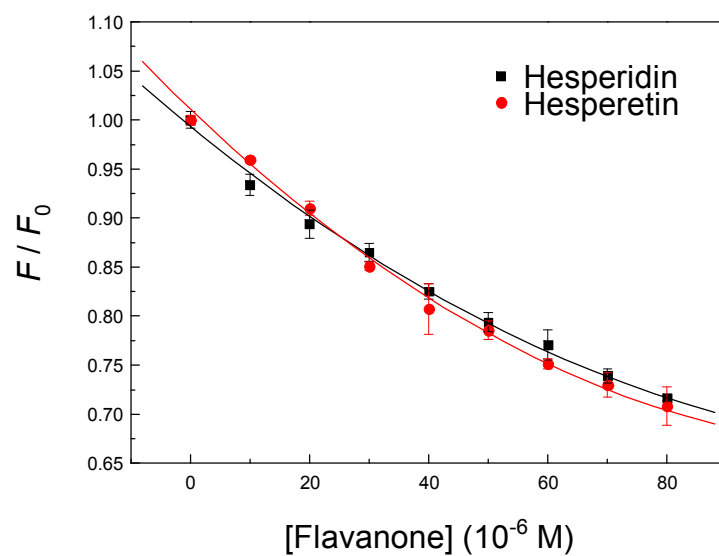


Fig. S2. Trp residue quenching of HSA (1.0 μM) at $\text{pH}=7.4$ and $T=298\text{ K}$, plotted as disappearance of fluorescence intensity (F/F_0) versus flavanones concentrations.

The λ_{em} maximum emerged at 334 nm and all data were corrected for quencher fluorescence. Each point was the average of three independent determinations \pm S.D. ranging 0.22%–2.58%.

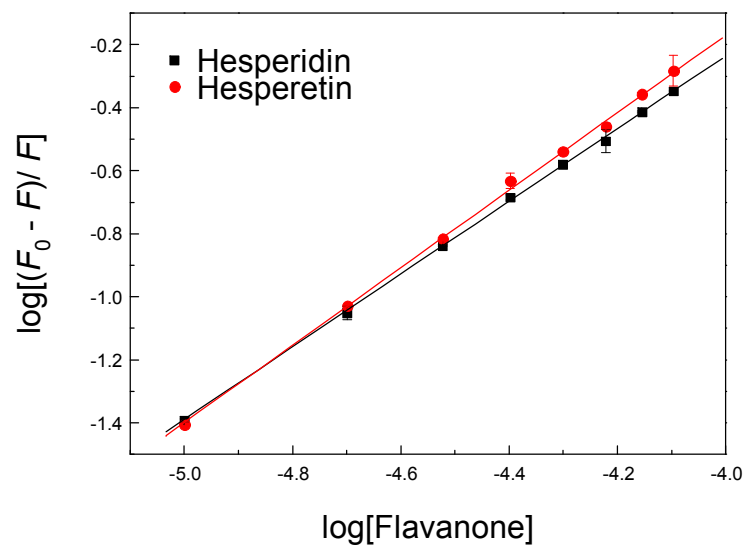


Fig. S3. Molecular recognition capacity plot narrating HSA Trp residue quenching induced by flavanones at pH=7.4 and $T=298$ K. (■) Hesperidin, $y=1.16x+4.392$, $R=0.9998$; (●) hesperetin, $y=1.24x+4.774$, $R=0.9995$, based upon equation (3). Fluorescence emission intensity was registered at 334 nm and all data were corrected for quencher fluorescence. Each value was the mean of three separate measurements \pm S.D. ranging 0.2%–4.86%.