

Supplementary Information

Effect of pH on the chemical modification of quercetin and structurally related flavonoids characterized by optical (UV-visible and Raman) spectroscopy

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Figure S1

FT-Raman spectra of structurally related flavonols (kaempferol, KPF; galangin, GAL; morin, MOR), flavanone (taxifolin, TAX) and flavone (apigenin, APG) in absolute ethanol (EthOH) and in 0.5 M NaOH aqueous solution (NaOH); 20mg/mL. The excitation line was 1064 nm. The spectra have been normalized to the intensity of the band at $\approx 600\text{ cm}^{-1}$.

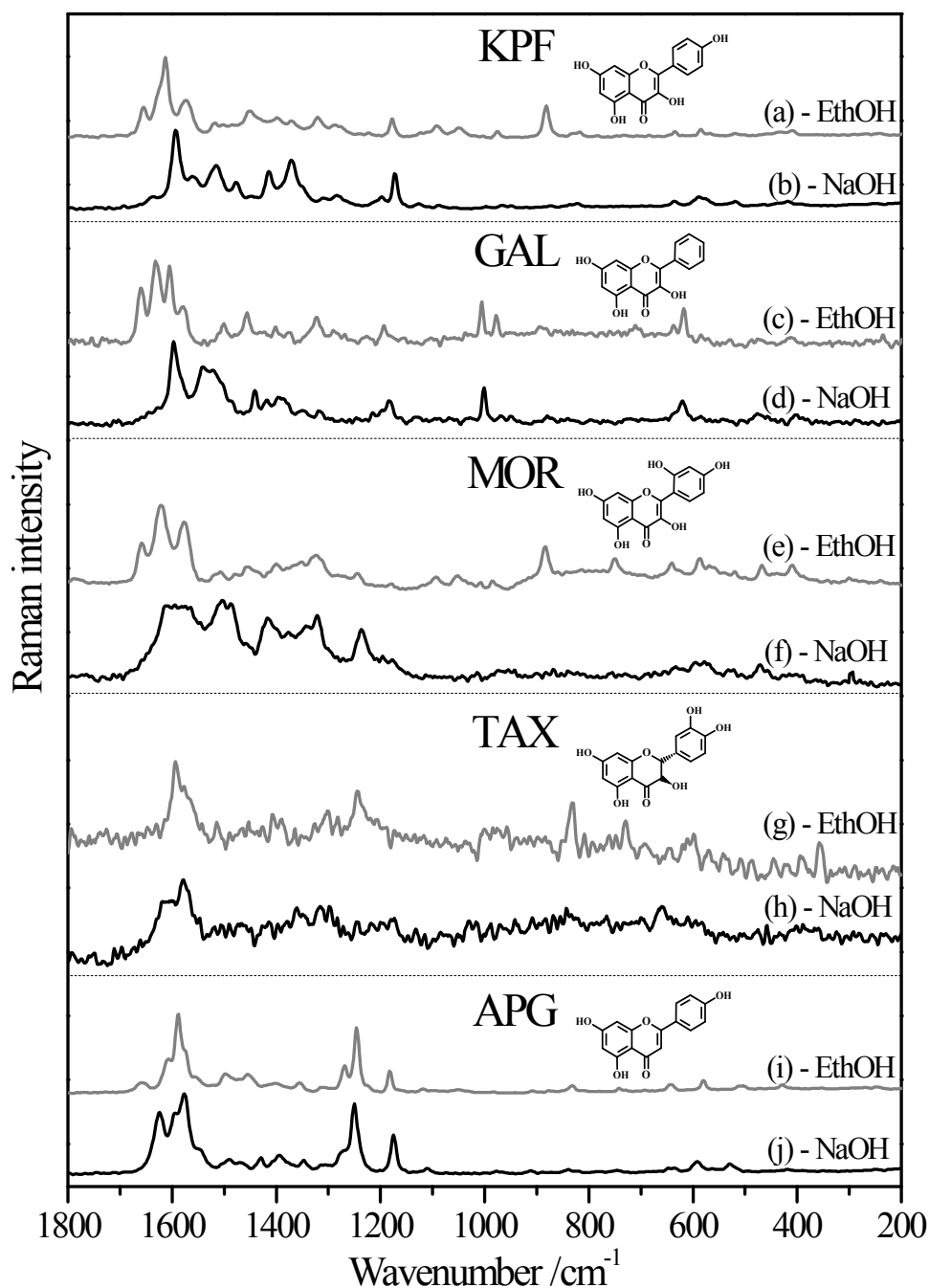


Figure S2

(a) FT-Raman spectrum of quercetin (QUC) in 0.5 M NaOH aqueous solution (NaOH); 20mg/mL, $\lambda_{\text{exc}} = 785\text{nm}$; and (b) calculated Raman spectrum of QUC* ($\approx$ benzofuranone) obtained at PCM/B3LYP/6-311++G** level theory with the applied scale-factor: 0.941. Inset: The optimized structure of benzofuranone in calculated in water (front and lateral view).

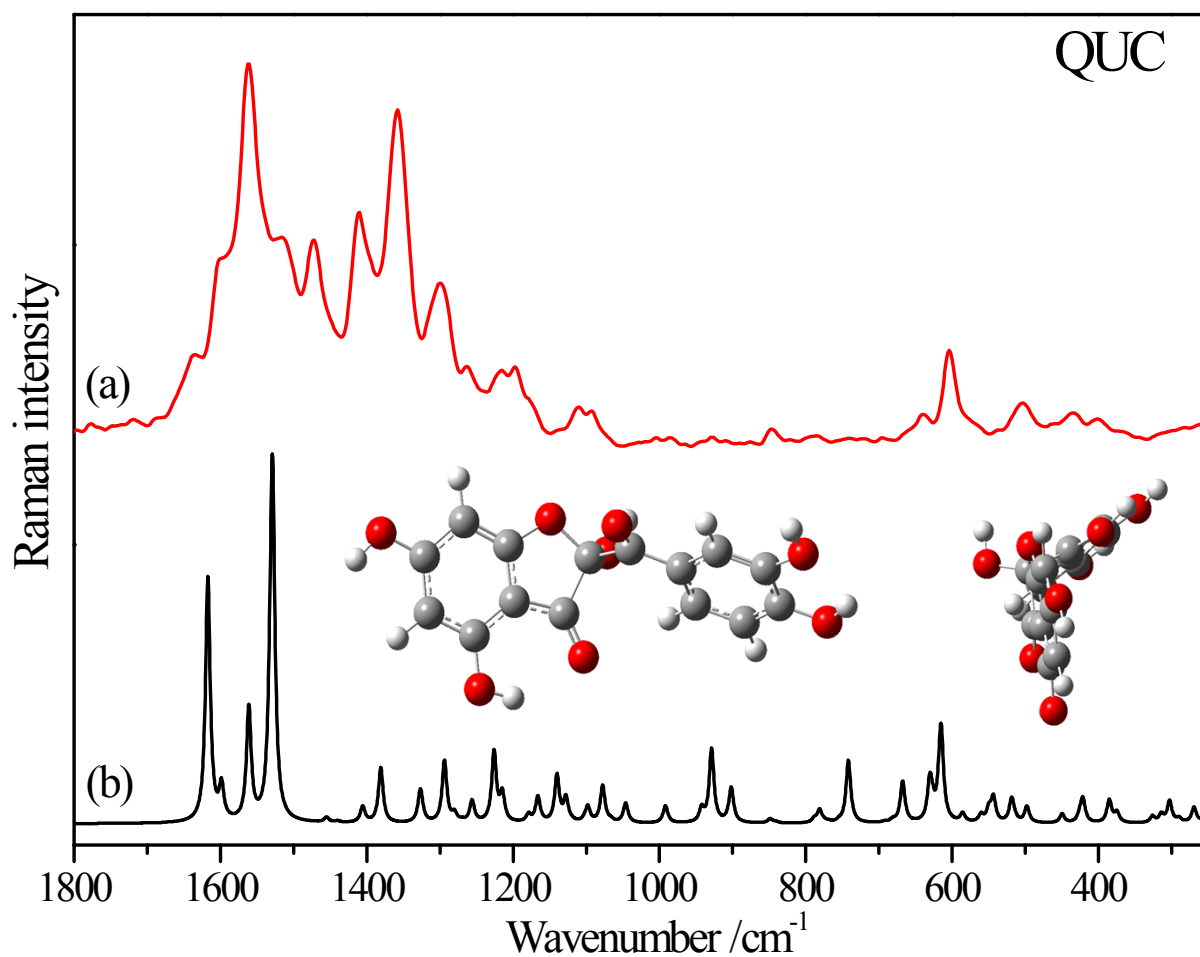


Figure S3

(a) FT-Raman spectrum of fisetin (FIS) in 0.5 M NaOH aqueous solution (NaOH); 20mg/mL, $\lambda_{\text{exc}} = 785\text{nm}$; and (b-f) calculated Raman spectra of different conformers of FIS* obtained at PCM/B3LYP/6-311++G** level theory without any scale-factor.

