

Supplementary Information

Some absorption spectra of mangiferin in water at several pH values. Gibbs free energies of the mangiferin conformers. Gibbs free energies of reaction for successive deprotonations in aqueous solution. Gibbs free energies of activation. Imaginary frequencies of the TS. Gibbs free energies of activation.

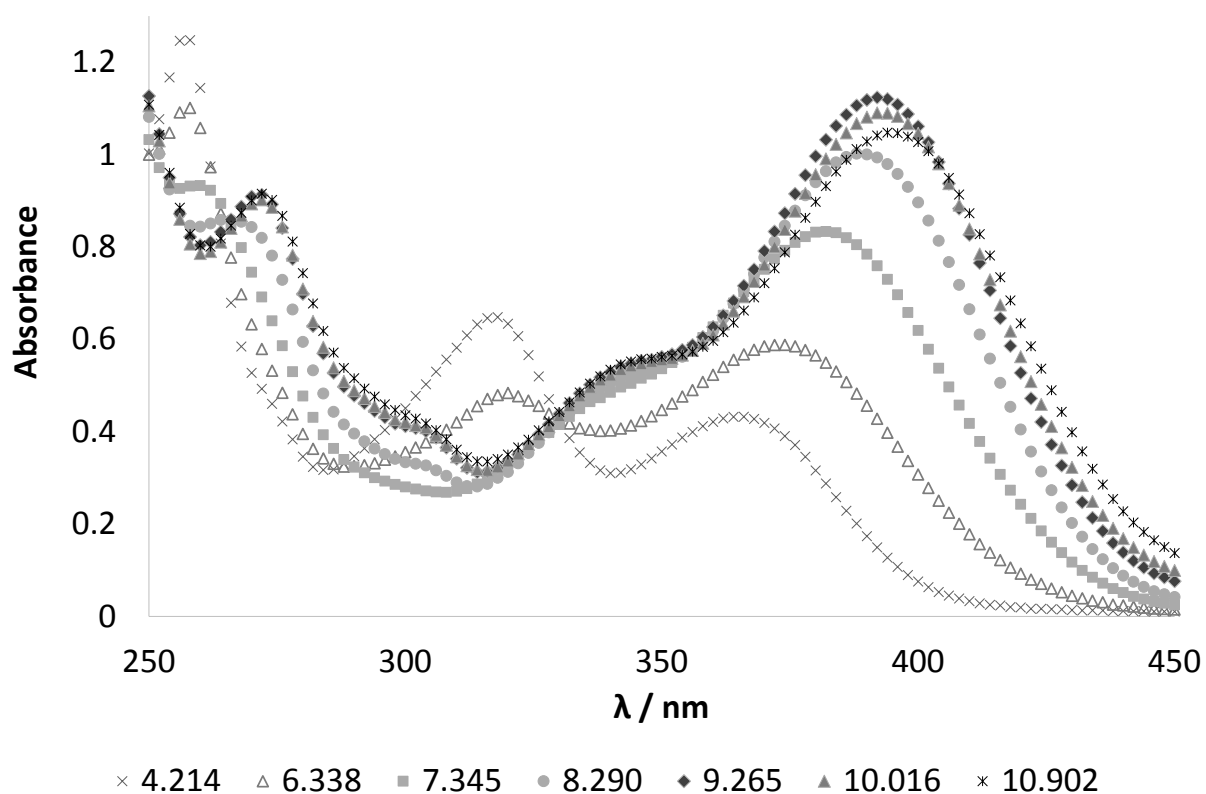


Figure 1S. UV-Visible absorption spectra for $4.17 \times 10^{-5} \text{ M}$ mangiferin solution in aqueous solution.

Table 1S. Relative Gibbs energies (ΔG) corresponding to the studied conformations of mangiferin, at 298.15 K.

Dihedral angle (2',1', 2, 3)	ΔG (Kcal/mol)	Population (%)
-90.98	0.00	99.65
79.02	14.44	0.00
179.02	3.35	0.35

Table 2S. Gibbs free energies (ΔG , in kcal/mol) of reaction for each possible successive deprotonation of mangiferin in aqueous solution, at 298.15 K.

Deprotonation Site	First deprotonation	Second deprotonation	Third deprotonation
1	8.56	3.17	1.58
3	9.08	0.00	
6	0.00		
7	8.37	4.22	0.00

Table 3S. Gibbs free energies of activation (kcal/mol), at 298.15 K.

	PE H ₄ M	Water H ₄ M	Water H ₃ M ⁻	Water H ₂ M ²⁻	Water HM ³⁻
SET	144.63	39.98	15.21	10.90	0.41
SPLET	39.98	15.21	10.90	0.41	0.01
HT					
site 7	14.57	16.46	13.96	0.00	
site 1					0.00
RAF					
site 4b					5.54
site 8					3.32