

Inclusion complex of 4-hydroxycoumarin with cyclodextrins and its characterization in aqueous solution

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The physicochemical properties of 4-hydroxy-7-methoxy-3-phenyl-2H-chromen-2-one (4HC) and β -cyclodextrins (CDs) inclusion complexes were investigated. The phase solubility profile of 4HC with β -cyclodextrin derivatives was classified as AL-type. Stability constants for complexes with 1:1 molar ratios were calculated from the phase solubility diagrams and indicate the following trend: DM β CD > HP β CD > β CD. The highest value of the binding constant was for 4HC-DM β CD; the binding association constant (K_a) for this complex was determined at different temperatures and the thermodynamic data indicate that 4HC-DM β CD association is mainly an entropically driven process. ¹H NMR and ROESY were carried out, revealing that 4HC is embedded in the apolar cavity of DM β CD with the 4OH group buried in the cyclodextrin cavity with the phenyl group outside, near the primary rim. These results are in agreement with ORAC FL values; the decrease in the antioxidant activity of 4HC-DM β CD is explained by the e