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New insights on the spectrophotometric determination of melatonin pK_a values and melatonin- β CD inclusion complex formation constant

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Abstract

Using UV-Vis spectrophotometry a stability study of melatonin at different pH values was done in aqueous media, finding that at acidic pH melatonin is unstable when interacting with the environment, however it becomes stable protecting it from light and oxygen. From the UV-Vis spectra and SQUAD software, melatonin pK_a values, in a completely protected aqueous medium, were estimated as 5.777 ± 0.011 and 10.201 ± 0.024 . Using the same techniques, the melatonin and β -cyclodextrin inclusion complex formation constants were assessed at pH 3, 7 and 11.5, giving the values of $\log \beta = (3.07 \pm 0.06)$, (2.94 ± 0.01) and $(3.07 \pm 0.06) \text{ M}^{-1}$, respectively. From the global acidity formation constants and the complexes' formation constants, the molar fractions were determined for each species of MT and MT- β CD, to build the molar fraction- $[\beta\text{CD}]$ -pH 3D diagram and the molar fraction-pH 2D diagrams, where it was possible to observe the predominance of the MT species with and without β CD. A voltammetric study at pH 3, allowed obtaining a value of $\log \beta = (3.15 \pm 0.01) \text{ M}^{-1}$, which corroborates that obtained through UV-Vis spectrophotometry, supporting strongly the rationale behind using simple, straightforward techniques.

Keywords: Melatonin; acidity constants; β -cyclodextrin; inclusion complex.

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