New insights on the spectrophotometric determination of melatonin pKa values and melatonin-βCD inclusion complex formation constant

A. Zafra-Roldán, S. Corona-Avendaño, R. Montes-Sánchez, M. Palomar-Pardavé, M. Romero-Romo, M.T. Ramírez-Silva

PII:	S1386-1425(17)30770-9
DOI:	doi: 10.1016/j.saa.2017.09.042
Reference:	SAA 15476
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	1 May 2017
Revised date:	###REVISEDDATE###
Accepted date:	15 September 2017

Please cite this article as: A. Zafra-Roldán, S. Corona-Avendaño, R. Montes-Sánchez, M. Palomar-Pardavé, M. Romero-Romo, M.T. Ramírez-Silva , New insights on the spectrophotometric determination of melatonin pKa values and melatonin-βCD inclusion complex formation constant, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2017), doi: 10.1016/j.saa.2017.09.042

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

A. Zafra-Roldán[a], S. Corona-Avendaño[a,*], R. Montes-Sánchez[a], M. Palomar-Pardavé[a], M. Romero-Romo[a], M.T. Ramírez-Silva[b,*]

[a]Universidad Autónoma Metropolitana–Azcapotzalco, Departamento de Materiales, Área Ingeniería Materiales. C.P. 02200, Ciudad de México, México.
[b]Universidad Autónoma Metropolitana–Iztapalapa, Departamento de Química, Área de Química Analítica, C.P. 09340, Ciudad de México, México.
*Corresponding authors emails:
scav@correo.azc.uam.mx (SCV) and mtrs218@xanum.uam.mx (MTRS)

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 β = (3.07 ± 0.06), (2.94 ± 0.01) and (3.07 ± 0.06) 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−βCD, to build the molar fraction–[βCD]–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 βCD. A voltammetric study at pH 3, allowed obtaining a value of log β = (3.15 ± 0.01) 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.