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Evaluation of spectroscopic and solvatochromic properties of Quinquangulin and Rubrofusarin: Comparative analysis with data from Density Functional Theory.

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Introdução

Quinguangulin and Rubrofusarin (figure 1) are two well known naphthopyrones employed for several pharmacological purposes. Naphthpyrones are compounds with interesting biochemical actions, such as potential to modify the enzyme regulator properties of the Calmodulin (CaM). In this work, excitation and emission spectra are evaluated in order to elucidate the properties of these compounds in several solvent systems.[1]

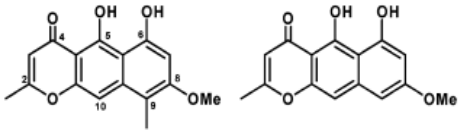
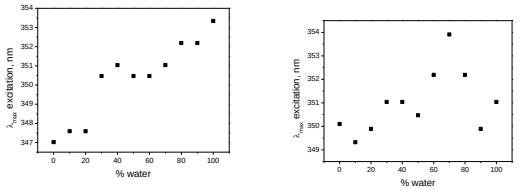


Figure 1 - Molecular Structures of Quinquangulin and Rubrofusarin

Resultados e Discussão

Each solvent system (water/ethanol and water/acetonitrile) has peculiar characteristics regarding physico-chemical properties. The quantum yield of these naphthopyrones obtained in “pure” water is low, being higher in several “pure” organic solvents. This data reinforces the relevance of tests involving mixtures of solvents, since the water, inhibits the quantum yield of the naphthopyrones. In this way, mixtures of solvents could to promote an optimum condition in order to obtain a maximum quantum yield. It demonstrated that maximum excitation wavelength can be significantly modulated changing the proportion of organic solvent in the water/organic solvent system. Quinquangulin, for example, presented the higher wavelength of maximum excitation in an ethanol-water mixture containing 70% of water (figure 2). [2]

Probably, the organization between ethanol and water molecules in this condition favors the formation of strong polar interactions with the π^* orbitals of naphthopyrones. This kind of spectral shift is lower for acetonitrile-water system, probably due to the lower capability of acetonitrile to form hydrogen bonds when compared with ethanol. Furthermore, the acetonitrile molecule can act only as base of Lewis, while the ethanol, due to its amphipatic character can develop actions as base or acid of Lewis, depending of the chemical neighborhood.



(a) **(b)**

Figure 2 - Variation in the maximum excitation as function of the water percentage of quinquangulin **(a)** and rubrofusarin **(b)** in water/acetonitrile mixture.

The additional methyl group in quinquangulin seems to develop a decisive function related to the ability to formation of hydrogen bonds, altering significantly the solute-solvent interaction, which can be related to this difference in terms of acid-base behavior, between acetonitrile and ethanol. The present data are discussed in details in agreement with recent literature, contributing to elucidate several physico-chemical properties of these compounds.[3]

Conclusões

The present results demonstrate that the organization between ethanol and water molecules as well as acetonitrile and water affects significantly the photophysical properties of the quinquangulin and rubrofusarin. The difference between the solvatochromic and spectroscopic profiles of these compounds in the solvent systems evaluated is associated to the lower capability of the acetonitrile to form hydrogen bonds when compared to ethanol.

Agradecimentos

Fapesp, CNPq.

[1] J.G. Graham, H. Zhang, S.L. Pendland, B.D. Santarsiero, A.D. Mesecar, F. Cabieses, N.R. Farnsworth, J. Nat. Prod. 67 (2004) 225-227.
[2] H.P.M. de Oliveira, A.Machulek Junior, A. O. Legendre, M.H. Gehlen, Quím. Nova, 26 (2003) 564-569.
[3] A.E.H. Machado, D. Severino, J. Ribeiro, R. De Paula, M.H. Gehlen, H.P.M. de Oliveira, M.S. Matos, J.A. Miranda, Photochem. Photobiol. Sci., 3 (2004) 79-84.