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Abstract

Solvatochromism of Norfloxacin and Sulfadiazine †

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Abstract: Fluoroquinolones (FQ) and sulfonamides (SA) are antibacterial substances used in therapeutics. Both are Active Pharmaceutical Ingredients (APIs) of low solubility. The solute-solvent interactions allow understanding drug´s absorption and the interactions involved in molecular recognition. This research aims to study Norfloxacin (NOR) and Sulfadiazine (SDZ) solvent interactions in pure solvents through experimental solvatochromism. Three apolar aprotic and six polar protic solvents were selected for this study. Multiparametric statistical analysis was performed with the method of linear solvation energy relationship of Kamlet and Taft, Catalan, and Laurence method. The results were analyzed by taking as reference the aprotic solvent, acetonitrile. In the case of SDZ, a shift towards shorter wavelengths (hypsochromic shifts) was observed when switching to nonpolar aprotic solvents, whereas in polar and some nonpolar protic solvents, the shifts were bathochromic (towards longer wavelengths). In the case of NOR, hypsochromic shifts were observed in most of the solvents tested, except 1-propanol, which exhibited a bathochromic shift. The Catalan and Laurence equation revealed that the highest relative contribution to NOR's behavior was attributed to the polarizability (π parameter), while for SDZ, it was the b parameter, representing hydrogen bond accepting capacity towards functional groups such as $–NH_2$, $–SO_2NH$, and –N, as indicated by the Kamlet and Taft and Catalan equations. The identification of key parameters contributing to these behaviors enhances our understanding of the solubility and molecular recognition of these antibacterial compounds.

Keywords: solvatochromism; norfloxacin; sulfadiazine; multiparametric analysis

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