Poster

New hydrated salts of Sparfloxacin: a supramolecular synthon analysis

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The modulation of physicochemical properties of an Active Pharmaceutic Ingredient (API) by means of prospection of new solid forms, such as salts, cocrystals, eutectics, among other, is of great interest to the pharmaceutical industry [1]. The design of a new Multicomponent Pharmaceutic Material (MPMs) can be carried out by means of crystal engineering strategies, once this approach covers the understanding of the intermolecular interactions towards the crystal packing, thus enabling the design of new solid materials with specific physicochemical properties[2].

In this work, we reported a supramolecular synthon analysis of three new hydrated salts of sparfloxacin (SPA), a fluoroquinolone derivative drug with a broad-spectrum antibacterial activity, belonging the class II (low solubility, high permeability) of the Biopharmaceutical Classification System (BCS) [3,4]. These organic salts were obtained by slurry and mechanochemical methods, using 3-aminobenzoic acid (3ABA), 4-aminobenzoic acid (4ABA) and 5-aminosalicylic acid (5ASA) as hydrogen bond donors. The SPA:4ABA trihydrate and SPA:4ASA dihydrate salt are packing in the monoclinic system in the $P2_1/n$ space group, while SPA:3ABA dihydrate packing as orthorombic system in the *Pbcn* space group, and all salts comprising one molecule in the asymmetric unit with multiple intra and intermolecular hydrogen bonds including in their crystal packing. In addition to the interaction between SPA^+ and the anionic coformers, the supramolecular synthon analysis showed that the architectures of salts were governed by hydrogen bonds linking SPA and coformers through $D^1(2)$ motifs. All compounds present the typical $S^1(6)$ intramolecular synthon (N-H···$O_{(C=O)}$···H-$O_{(COOH)}$) in the SPA molecule. A robust $R^2(14)$ motif forming dimers between 3ABA molecules and $C^1(8)$ chains was found in the SPA:3ABA dihydrate salt. Additionally, as previously reported[3], in the SPA:4ABA trihydrate salt an extended supramolecular tape of hydrogen-bonded water slightly pentagonal along the *a* axis was also found (Fig. 1). Further characterization by TGA, DSC, solubility and stability tests are ongoing to enable the establishment of structure−property relationships of these compounds.

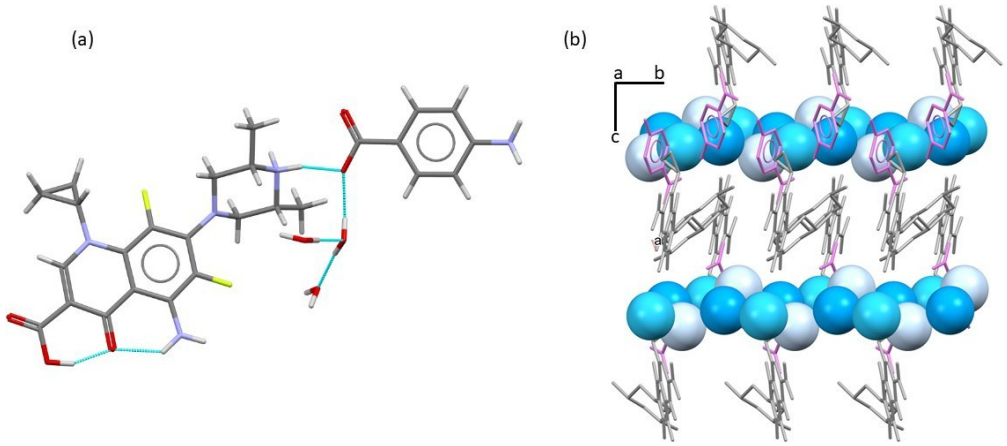

Figure 1: Asymmetric unit of SPA:4ABA (a) and crystal packing along of *a* axis.

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