MS33 Supramolecular recognition

MS33-2-3 The interplay of strong and weak intra and intermolecular hydrogen bonds in Sparfloxacin multicomponent forms: how it affects stability and solubility #MS33-2-3

M.T.T. Duarte ¹, M. Djaló ¹, M. Arpacıoğlu ¹, T. Neuparth ¹, A. Cunha ¹, V. André ¹ ¹Centro Quimica Estrutural, Dept. Engenharia Química - LISBOA (Portugal)

Abstract

Hydrogen bonds are known to be determinant in the supramolecular arrangement of multicomponent drug crystal forms. The main goal of the present study is to correlate these crystal engineering principles with the improvement of Sparfloxacin (SPAR) stability and solubility.1 SPAR is an antibiotic from the class of the fluoroquinolones, used in the treatment of bacterial infections.

Stable homo and hetero synthons between SPAR carboxylic acid moiety and carboxylic acid/amides/amines/ moiety's of some generally recognized as safe(GRAS) co-formers led to the formation of cocrystals and salts.

Attempts were performed in order to rationalize the formation of strong and directing intermolecular interactions with shelf and room humidity stability as well as solubility. SPAR molecules present a strong intramolecular pattern, N-H...O(C=O)...H-O(COOH), maintained in the majority of the supramolecular arrangements, promoting or preventing further SPAR-SPAR intermolecular contacts. 2,3

Results will be present and discussed here.

Acknowledgement: FCT - Project UID/QUI/00100/2019 and PTDC/QUI-OUT/30988/2017

References

[1] Desiraju, G. R., JACS, 2013, 135, (27), 9952-9967.

[2] Shemchuk, O.; Andre, V.; Duarte, M. T.; Taddei, P.; Rubini, K.; Braga, D.; Grepioni, F., Crystal Growth & Design 2017,176, 3379-3386

[3] Djaló, M.; Cunha, A., Luís, João; Quaresma, S.; Fernandes, A.; André, V.; Duarte, M. T., Crystal Growth & Design, 2021, 21, 2, 995–1005

Figure 1. The illustration of SPAR:AA crystal struc



