

Potentialities in amorphous drugs characterization by pair distribution function method

Vinicius D. N. Bezzon

Department of Physics, Federal University of Ouro Preto, Rua Quatro, Campus Universitário
Morro do Cruzeiro, Ouro Preto - MG, Brazil.

e-mail: vinicius.bezzon@ufop.edu.br

Active pharmaceutical ingredients (APIs) are typically obtained in their crystalline form due to its favorable stability under environmental conditions. However, a major limitation of many crystalline APIs is their poor aqueous solubility. One effective strategy to overcome this challenge is to convert the API into the amorphous state, either in its pure form or stabilized within polymeric matrices, for example. The amorphous state possesses higher inner energy, which frequently translates into significantly enhanced solubility. Characterizing the local atomic structure of these amorphous materials is crucial, and the Pair Distribution Function (PDF) method has emerged over recent decades as a particularly powerful tool for this purpose in pharmaceutical research. Since amorphization can be achieved through various processing routes, such as ball-milling, melt-cooling, spray-drying, among others, PDF analysis is highly effective in detecting the subtle structural variations induced by each method [1-2]. This capability is valuable for both industrial development and fundamental academic research. In this talk, I will present key advances in the characterization of amorphous drugs using the PDF method with high- and medium-energy radiation data and discuss the promising potentialities for the future.

References:

[1] MARTINS, I. C. B. et al. ChemRxiv. Cambridge: Cambridge Open Engage **1**, 1 (2023).

[2] BEZZON, V.D.N. et al.. J. Pharm. Sci. **111**, 3054 (2022).

The author would like to thank the National Council for Scientific and Technological Development (CNPq) for funding resources (project numbers 405362/2023-4 and 310961/2023-8).