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New results, Directions and Opportunities

Book of Abstracts

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Amorphous pharmaceuticals and biopharmaceuticals - physical and chemical stability

Invited talk

AP-BioP-1

Molecular dynamics potentially relevant to the physical stability of amorphous pharmaceutical drugs

Correia, Natália[1]; Silva, Cindy G[3]; Rodrigues, Andreia C.[3]; Viciosa, Maria Teresa[2]; Danède, Florence[1]; Ottou, Thierry[1]; Affouard, Frédéric[1]; Dionísio, Madalena[3]
(1) Univ Lille 1; (2) Universidade Técnica de Lisboa; (3) Universidade Nova de Lisboa

Until now, many substances of pharmacy have been developed especially in the crystalline state for obvious reasons of stability. Either by accident or design, they may also exist in a total or partially amorphous state. Due to its higher free energy, the amorphous form of a drug often shows an improved solubility, accelerated dissolution and bioavailability promoting therapeutic activity when compared to its crystalline state. The development of active substances in the amorphous form thus offers an interesting route and has motivated a strong interest in the last decade. However, these forms are inherently unstable physically which is a significant concern from a pharmaceutical perspective. Molecular mobility is generally recognized to be a key parameter governing physical stability. It can be assessed *in situ* by dielectric relaxation spectroscopy, a powerful and non invasive tool. We will discuss some of the most relevant aspects characterizing the complex dynamics of amorphous pharmaceuticals belonging to the family commonly referred to as *profens* which can have a significant influence on crystallization processes and stability.

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Invited talk

AP-BioP-2

Proteins in amorphous disaccharides: insights on bioprotection from Molecular Dynamics simulations and FTIR experiments.

Cottone, Grazia[1]; Giuffrida, Sergio[1]; Cordone, Lorenzo[1]
(1) University of Palerm

Bioprotection by sugars is a relevant topic due to its implications in many fields. Here we report on results obtained on binary water/sugar and ternary protein/water/sugar systems, in a wide range of temperature, at different water content and homologues disaccharides. The data presented come from a complementary set of Molecular Dynamics simulations and FTIR measurements. The peculiar effect of trehalose on protein and matrix dynamics, and the key role of the residual water in regulating both of them, are pointed out. Results are also discussed in the light of data from a larger set of experimental techniques, on different time and space scales, providing a consistent picture of bioprotection from the atomistic to the macroscopic level.

Invited talk

AP-BioP-3