

SPS-XRPD Workshop



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Characterization of Mesomorphous Pharmaceuticals Using Pair Distribution Function.

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Crystalline pharmaceuticals have long and short range three dimensional and translational symmetry order. However, these crystalline materials may lose one or even two-dimensional order to become mesophases (or commonly referred to as liquid crystals). Characterizing pharmaceutical mesophases using Bragg based X-ray powder diffraction has its limitation and generally is not enough to understand the molecular based structure of these unique phases. In this presentation a case study of using pair distribution function (a total scattering technique) calculated using Synchrotron X-ray powder diffraction to characterize lab generated thermotropic mesomorphous materials will be presented. The process used to analyze the synchrotron diffractogram and the techniques used to analyze the calculated pair distribution function and improve its resolution are outlined and discussed. The results of this work illustrate the power of pair distribution function in analyzing disordered pharmaceuticals in order to explore the molecular structures of these materials.

Primary author: Dr ATASSI, Faraj (Pulmatrix Inc)

Presenter: Dr ATASSI, Faraj (Pulmatrix Inc)

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