Contribution ID: **28** Type: **not specified**

In house and synchrotron based atomic PDF studies on non-crystalline drugs: is there room for both ?

Monday, 7 May 2018 16:00 (25 minutes)

Pharmaceutical industry is entering a new era in drugs development involving a transformation from crystalline to non-crystalline drug formulations. The driving force of the transformation is the largely improved bioavailability of the latter in comparison to the former. Non-crystalline drugs, however, are both an opportunity and challenge for pharmaceutical research and development (R&D). In particular, assessing the quality of a non-crystalline drug requires precise information about its 3D structure type, phase content, amount of different non-crystalline ingredients eventually present, stability, and others. With crystalline drugs, such information is almost straightforward to obtain by traditional powder x-ray diffraction (XRD). A non-traditional "powder XRD-type"technique using x-rays of higher (> 15 keV) than usual (Cu Kα ˜ 8 keV) energy, often referred to as total x-ray scattering coupled to atomic pair distribution function (PDF) analysis, is emerging as a powerful analytical tool for structural characterization of non-crystalline drugs [1]. We will present results from recent total x-ray scattering studies utilizing in house equipment (Panalytical XRD instrument) and state-of-the-art synchrotron x-ray sources. Examples will include indomethacin, aspirin and ingredients used in non-crystalline drugs, such as starch, trehalose, polyvinylpolypyrrolidone, and others. Special attention will be given to demonstrating the viability of in house PDF studies on non-crystalline drugs since experiments at National Synchrotron Radiation Facilities are not necessarily an affordable (e.g. proprietary issues) and/or time-efficient pharmaceutical R&D option.

`Figure 1. Comparison between atomic PDFs for indomethacin and Polyvinylpyrrolidone (PVP) obtained on an in-house XRD instrument (Ag K ) and using high-energy x-rays (115 keV) at the 11-ID-C beamline, Argonne.`

1. Petkov, V., Ren, Y., Kabekkodu, S., Murphy, D., PhysChemChemPhys 15, 8544-8554 (2013).

Presenter: Dr PETKOV, Valeri (Dept. Physics, Central Michigan university)

Session Classification: Lab. vs S-XRPD

Track Classification: Monday, May 7th Afternoon (Day 1 Workshop)