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Advances in the quantification of amorphous pharmaceuticals via Multivariate Analysis of Synchrotron X-Ray Powder Diffraction Patterns

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In recent years, novel amorphous dosage forms have increasingly been developed by the pharmaceutical industry due to their improved solubility compared to their crystalline counterparts. Because the accurate control of drug phase composition is crucial in pharmaceutical development, researchers face challenges finding suitable analysis techniques to assess this issue when one or more component phases in the formulated samples lack long-range order such as amorphous, mesomorphous, nanocrystalline compounds and solid dispersions. Additionally, quantification via conventional XRPD methods such as Rietveld method becomes impossible since no structural model is available. Rietveld-like methods in which a poorly crystalline or amorphous phase is described mimicking a crystalline phase can result viable, but if more than one non-crystalline phase is present, the accuracy of the quantitative analysis is compromised.
Over the last decade, the fast development of synchrotron sources and instrumentation has enabled a more systematic use of Synchrotron X-Ray Powder Diffraction (S-XRPD) to analyze solid forms at several stages of the industrial drug development process, and enabled more specifically the generation of Pair Distribution Function (PDF) curves of amorphous organic samples.
In this work, we combined the power of S-XRPD in both real and reciprocal space with multivariate analysis methods to achieve reliable quantification of the individual amorphous phases of pharmaceutical mixtures via dual space analysis.

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