Evaluation of Solid Structure using Pair Distribution Function (PDF) and Principal Component Analysis (PCA)

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This study aimed to investigate the usefulness of the pair distribution function (PDF) and principal component analysis (PCA) to detect the amorphousness of a pharmaceutical solid, and to determine the optimal experimental conditions to achieve good amorphous pharmaceutical solid. The PDF was obtained from the powder X−ray diffraction (PXRD) pattern of the samples via a Fourier transform directly. Moreover, the PDF analysis can achieve the structure information of the pharmaceutical solid. PCA was used to visualize the differences in the PXRD and PDF data of different samples. The PCA approach revealed that PDF is more efficient in assessing the degree of disorder in the amorphous pharmaceutical solid than PCA of the corresponding PXRD diffractograms. The PDF analysis was able to determine the optimal experimental conditions that facilitated the highest degree of disorder in the samples. Therefore, it is concluded that the PDF technique may be used as a complementary tool to other solid state methods and that further investigations are warranted to elucidate the capabilities of this technique.