# PDF “feat” solid-state NMR: a combined approach for crystal structure determination of organic compounds

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The properties of solid compounds are determined by their solid-state structures. This is of particular relevance in the development of new materials, i.e., drugs and organic pigments. For nanocrystalline organic compounds (ordering lengths of 5–40 nm), the standard methods for structure determination fail. In the last decades a new technique has been established for the analysis of nanocrystalline substances: the analysis of the pair distribution function (PDF). Whilst being well established for inorganic compounds, organic compounds are rarely investigated by PDF analysis. Schmidt and co-workers developed a method called ‘Global-PDF-Fit’, which allows for the determination and refinement of crystal structures of organic compounds from scratch by a global fit to the pair distribution function (PDF), without prior knowledge of lattice parameters and space group [1]. Nevertheless, there are cases for which the Global-PDF-Fit method does not yield a unique solution, but several different structures, which all fit the experimental PDF data equally well [2]. Thus, we are developing a method to determine the crystal structures of organic compounds by combining a PDF fit with solid-state nuclear magnetic resonance (SSNMR), to achieve a faster and more reliable method than the existing ones to apply to such systems. 1D and 2D SSNMR experiments can provide precise information on the local structure, such as tautomeric character, hydrogen-bond network, intra- and intermolecular atom-atom proximities and precise atom-atom distances [3]. All this information can be used as restraints for the generation of the structures, for the PDF fit and as additional parameters for the selection of the correct structure. Here we are presenting the results obtained so far for crystalline organic compounds of pharmaceutical interest.

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[3] Rossi, F., Vioglio, P. C., Chierotti, M. R., Gobetto, R. (2018) Solid-State NMR in the Study of Intermolecular Interactions. In *Understanding Intermolecular Interactions in the Solid State: Approaches and Techniques*, edited by D. Chopra, pp. 243-284. The Royal Society of Chemistry.

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