Incorporation of Pharmaceutical API's into the PDF® Databases

Amy Gindhart[1], Tom Blanton[1], Jim Kaduk[2]
International Centre for Diffraction Data, Newtown Square, PA, U.S.A
Illinois Institute of Technology, Chicago, IL, U.S.A.

The International Centre for Diffraction Data (ICDD®) continues to extend the coverage of the Powder Diffraction File™ (PDF®) databases with comprehensive data and subfile systems, greatly enhancing the database analysis capabilities. As the X-ray diffraction method is more actively used in the pharmaceutical area, an even more enhanced database is required for the analysis of pharmaceutical materials. The "Pharmaceutical Project" grew out of the need to acquire more pharmaceutical diffraction patterns and crystal structures in the PDF databases for phase identification and quantitative analysis, particularly for analysis performed at room temperature. After reviewing the lists of the top 200 pharmaceutical drugs by U.S. sales and prescription in 2011 and 2012, ICDD found 97 pharmaceutical API materials had not been reported as being analyzed by X-ray diffraction based on a search of published literature. A collaboration was proposed between ICDD-Argonne National Laboratories-Illinois Institute of Technology to collect synchrotron diffraction data for these materials. Once collected, the diffraction data were analyzed for structure elucidation, and all pharmaceutical diffraction patterns were analyzed at ICDD using a comprehensive, three-tier editorial review before their incorporation into the PDF products. Due to the nature of the project with potentially hygroscopic materials, some of the samples were found to not be the exact API expected. In addition, it was observed that some of the materials received were not the phase claimed by the supplier. This information has been used as a learning mechanism to further study the complexity of these materials by looking at other aspects of their physical properties. To date, 88 entries have been published in the PDF database with 9 additional entries to be published in Release 2019. Notable inclusions of Tamiflu, Zoloft and Nexium will be discussed. This research program has also enhanced the understanding of pharmaceutical materials leading to 25 papers being published in *Powder Diffraction*, with additional manuscripts in progress. Highlights of the technical results of this project will be discussed, including the next stage of targeting the top drugs by application in disease-focused categories (i.e. respiratory system drugs, oncological drugs, nervous system drugs, etc.).