Retrospect and Prospect of Small Molecule Microcrystal Electron Diffraction for Pharmaceutical Industry

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Microcrystal electron diffraction (MicroED) is a novel experimental method for elucidating the three-dimensional structures of molecules ranging from organic compounds1 to protein complexes.2 Understanding the molecular structures of active pharmaceutical ingredients (APIs) is a prerequisite for the design and synthesis of novel chemical entities for development as new medicines. It is essential for assessing their phase purity (polymorphs, salts, solvates etc.) in order to ensure product quality during API synthesis, formulation development and product manufacture.3 Though MicroED is a relatively new technology, since its initial demonstration, it has enabled structure elucidation for a variety of samples that were intractable by other techniques, but its adoption across the pharmaceutical industry is rather slow. In this presentation, we will summarize the lessons we have learnt from our attempts at structure determination from MicroED and retrospection of the considerations in choosing the appropriate candidates for MicroED and for extracting the most meaning out of measured data.

References:

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