

MS28-2-2 Structure Determination of Pharmaceutical Cocrystals by Three-dimensional Electron Diffraction #MS28-2-2

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Abstract

Three-dimensional Electron Diffraction (3D ED), also known as MicroED, is becoming a powerful method for structure determination of nano-/micro- sized crystals. Owing to the strong interaction between electrons and matters, crystals that are too small for single-crystal X-ray diffraction and too complex for powder X-ray diffraction, can be studied by 3D ED. Thanks to the ease of beam manipulation, fast rotation as well as sensitive detectors, low-dose 3D ED becomes possible. With the assistance of a cryo-holder, further protection of the specimen against vacuum and electron beam damage can be achieved, which extends the application of electron crystallography to the structure determination of beam-sensitive crystals^{1,2}.

Herein, we show a series of pharmaceutical cocrystals solved by 3D ED^{3,4}. With this method, more structures of pharmaceutical crystals can be solved efficiently, which will accelerate the development of structural pharmacology and drug discovery.

References

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Scheme. The structures of pharmaceutical cocrystal

