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

J.Y. Xu ¹, H.Y. Xu ¹, X.D. Zou ¹, C.C. Sun ² ¹Stockholm University - Stockholm (Sweden), ²University of Minnesota - Minnesota (United States)

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.

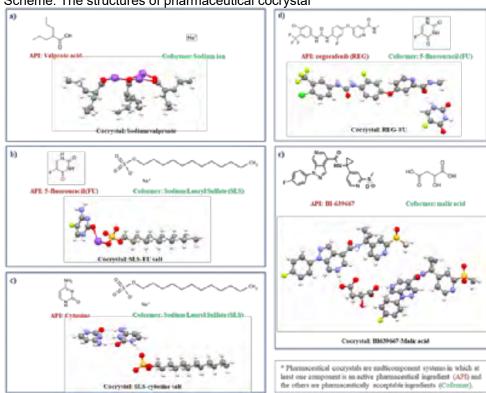
References

1.Gruene, T. etal. Rapid Structure Determination of Microcrystalline Molecular Compounds Using Electron Diffraction. Angew. Chemie - Int. Ed. (2018).

2. Jones, C. G. etal. The CryoEM Method MicroED as a Powerful Tool for Small Molecule Structure Determination. ACS Cent. Sci. (2018).

3.Wan, W., Sun, J., Su, J., Hovmöller, S. & Zou, X. Three-dimensional rotation electron diffraction: software RED for automated data collection and data processing. J. Appl. Crystallogr. (2013).

4.Cichocka, M.O., Ångström, J., Wang, B., Zou, X. & Smeets, S. High-throughput continuous rotation electron diffraction data acquisition via software automation. J. Appl. Crystallogr. (2018).



Scheme. The structures of pharmaceutical cocrystal