

Expanding the Crystallographer's Toolbox

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Although the crystal structures of small molecule compounds are often determined from single crystal X-ray diffraction (scXRD), recent advances in three-dimensional electron diffraction (3DED) and crystal structure prediction (CSP) methods promises to expand the structure elucidation toolbox available to the crystallographer. This talk will discuss a comparative assessment of scXRD, 3DED, and CSP in combination with powder X-ray diffraction with case studies on two former drug candidate compounds and a multicomponent crystal of a key building block in the synthesis of gefapixant citrate.