

Encapsulated Nanodroplet Crystallisation of Small Molecules (Enact): High-Throughput Small-Scale Crystallisation Methods Direct To Single Crystal XRD

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Accessing single crystals of small molecules is critical to facilitate structural analysis by diffraction methods. However, successful crystallisation, including access to different polymorphs, hydrates and solvates can only be achieved through the rigorous exploration of large areas of experimental space. Achieving this through classical methods is extremely challenging, in part due to the need for both large quantities of sample and extensive operator time.

We have developed Encapsulated Nanodroplet Crystallisation (ENaCt) which employs high-throughput liquid handling robotics to rapidly screen hundreds of crystallisation conditions in parallel, with only a few milligrams of sample.^[1,2] We have successfully applied this technology to a wide range of problems in the crystallography of small molecules, including high-throughput structural elucidation of unknowns (e.g. natural products) and new polymorph discovery for active pharmaceutical ingredients (e.g. CBD).^[3,4,5] In this talk we will present the newest developments in ENaCt, including seeding, co-crystallisation and even more polymorphs of ROY (e.g. O22).

References:

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