

Poster Presentation

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Strategies for high-throughput ligand screening - automated co-crystallisation and soaking

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Growing protein-ligand complex crystals can be challenging, especially in cases where the affinity is poor and the solubility of the ligand in the crystallisation condition is low. Various methodologies are often trialled before obtaining a diffraction-quality protein-ligand crystal.

Co-crystallisation is a common method for producing protein-ligand complex structures. It is especially useful when drug-like compounds trigger conformational changes in proteins. This can result in variations in the growing conditions or crystal forms, and may necessitate wider screening strategies for co-crystallisation in general.

Alternatively, soaking protein crystals with ligands is the fastest route to produce highthroughput structures, as long as the starting crystal form is easy to grow reproducibly, able to accommodate the desired ligand and, is robust to physical and chemical changes.

This poster will describe automated low-volume, high-throughput techniques for both types of crystallisation methods.

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