

Preserving and publishing crystallographic fragment-screening data

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Fragment-screening by crystallography has recently skyrocketed. Many synchrotrons around the world have built or are in the process of building specialized screening platforms, established workflows, and assembled compound libraries. Crystallographic fragment screening is now widely accessible to research groups that had previously not considered the approach. While hundreds of crystallographic fragment-screening campaigns have been conducted in the last few years, most of the underlying data have neither been published nor made publicly accessible. In the presentation I will highlight the challenges imposed by the growing volume of fragment-screening data as well as the importance of establishing effective mechanisms for preserving large and often heterogeneous groups of datasets intrinsic to crystallographic fragment-screening campaigns. The overarching goal is to ensure their accessibility for advancing research and enabling applications such as training AI-based models for future discovery.