validation. New interfaces for the ranking and evaluation of Pipedream results were developed within the Crystallization Information Management System (CRIMS) in order to support rapid analysis and decision making in the context of large-scale compound and fragment screening campaigns. The use of a small number of "Club Class" datasets (manually collected on the ESRF ID30B and SLS PX-III beamlines) led to a significant increase in the number of hits and enabled a complete elucidation of initially ambiguous binding modes for a number of challenging fragments. The approach described here is widely applicable and illustrates the potential of the combined use of "Club Class" data collection strategies and of fully automated protein-to-structure X-ray crystallography pipelines to achieve higher performance in large-scale compound and fragment screening campaigns.

Keywords: Fragment screening, multi-axis goniometry, ligand detection sensitivity

MS02-O2

The ultimate experiment

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Data collection is often described as the last experimental step in crystallographic experiments. The reason is that the choice of data collection parameters and strategy will influence the quality of the data which in turn will determine the amount of information that subsequent data processing and phasing software can be extract from the data, the quality of electron density maps and, ultimately, the failure or success of the experiment.

Unfortunately there is not a simple one-fits-all recipe to collect good data. The optimal strategy depends on the experimental purpose, the characteristics of the X-ray beam and instrumentation used to collect data and the samples properties. Radiation damage is often a critical factor limiting data quality and being able to predict the absorbed dose and mitigate the effects of exposure to X-rays is very important to a successful experiment.

While some general principles and guidelines to obtain good data are often successfully followed, blind application of rules of thumb can sometimes result in suboptimal experiments due to the conflicting effects of different data collection practices. Strategy programs developed over the last decade are in use at many dedicated macromolecular crystallography beamlines provide good guidance; however human experience is still beneficial to interpret software output and make the best decicions in difficult cases. Understanding the role of all the different factors on data quality is key to designing a reasonable data collection strategy that offers the best compromise between conflicting requirements and facilitates data processing and structure solution.

Keywords: Data collection, experimental strategy, radiation damage