

Towards a Structural Biology Work Bench

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Structural biologists now target larger, multi-component biological objects. In parallel, the focus is shifting from the macromolecules produced by simpler prokaryotic organisms to the macromolecules from higher organisms. Researchers now use multiple techniques and visit multiple experimental facilities/infrastructures to collect their data. Structural biologists are each expert in one or more techniques but they now often need to use complementary techniques in which they are less expert.

The various individual experimental infrastructures have developed different solutions to their requirements. There are some technique-specific pipelines that are largely automated for data analysis and/or structure determination, but integrated management of structural biology data from different techniques is lacking.

Repositories exist for the final structural data, but the provenance and integrity of such data are often an issue and metadata is often incomplete. The best way to acquire accurate metadata is to integrate data management infrastructure with data processing infrastructure.

There are no common strategies to address or support the storage of structural biology raw data, after the end of the SB project/grant within which the data were generated.

The presentation will discuss ways to address these challenges.

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