

Description of Software for the Planning, Execution, and Refinement of Crystallography Experiments

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A modular and highly integrated software package will be described which takes the crystallographer from the planning stage through to the refinement of the experimental process. This includes configuration and control of automation used to execute the experiment. Some key elements include reagent/protein management, screen design, database query tools, imaging, and real-time monitoring of automation and experiment status. Each application is specialized for a specific function but provides input to other applications. For example, while viewing experimental images, a user may choose an image deemed “interesting” and have the conditions for that site sent to the screen designer application for the starting conditions of a fine screen. Data generated from experiments can be mined using a novel, graphical query tool. Query results may be sent to the image viewing and analysis application for further study, as well as to the screen design application for use in designing additional rounds of refined experiments. This technology is highly data-driven and is enabled through the use of a centralized database. This single point of data management promotes efficient viewing, sharing, and mining of information.

These and other features of the software will be presented in a format describing typical scenarios and methods of use.

Keywords: software for crystallography, application software, databases