

W0439

Description of Software for the Planning, Execution, and Refinement of Crystallography Experiments. Paige N. Vinson, Thermo Electron Corporation, Brentwood, TN, USA 37027, E-mail: paige.vinson@thermo.com

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. Some key features include reagent/protein management, screen design, database query tools, and graphical image control. 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.

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