Optimization and Standardization of Structure Determination Workflow in a Service Facility Using Home-Built Software

Paul Boyle   Canada   University of Western Ontario

This talk will present how the structure determination workflow may be standardized and optimized through the use of a number of home-built software programs. Such standardization is particularly important when the laboratory has multiple student users as well as full time staff. Adoption of home-built software allows the workflow to be optimized for the laboratory's particular computational environment as well as fulfilling the needs and expectations of end users. These programs are written in a variety of languages which fit the problem being addressed: from Unix shell scripts to interpreted languages such as Python and compiled programming languages used to solve particular programs and provide specialized calculations. Some tasks which are automated using home-built software include transfer of data files from diffractometer control computers to data processing workstations, standard laboratory specific edits to CIFs, customized report writing software, marshaling files from the finished structure for distribution to end users, and standardized data archiving.