Automated Single Crystal Structure Determination – A Tool for Synthetic Chemists?

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During recent years large improvements in software functionality and its ease-of-use have made single crystal X-ray structure determination easier than ever. These days most structures can be measured, processed, solved and refined using well selected defaults with no or little crystallographic knowledge. Recently, microfocus sources and CCD detectors both air-cooled, have entered the marketplace. Combining these innovations with an automated sample loader and an intelligent graphical user interface allows for the design of a table top single crystal diffractometer, which only requires a standard single phase power connection and no cooling water at all. An instrument taking advantage from these software and hardware developments would enable synthetic chemists or pharmacists to perform a complete single crystal structure analysis almost next to the reaction flask.

Performance analysis results

To compare the system performance a family of p38 MAP kinase inhibitors was crystallized and measured on the SMART X2S. Data were collected on a state of the art research instrument (SMART APEXII) and a previous generation rotating anode instrument (CAD4). The data collection time and the resulting quality can be gleaned from the tables below. All structures were solved and refined automatically by the SMART X2S diffractometer. It is clear that the SMART X2S has a superior performance over the previous generation system and shows very competitive performance in comparison to the state-of-the-art research instrument.

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