Application Note SMX018

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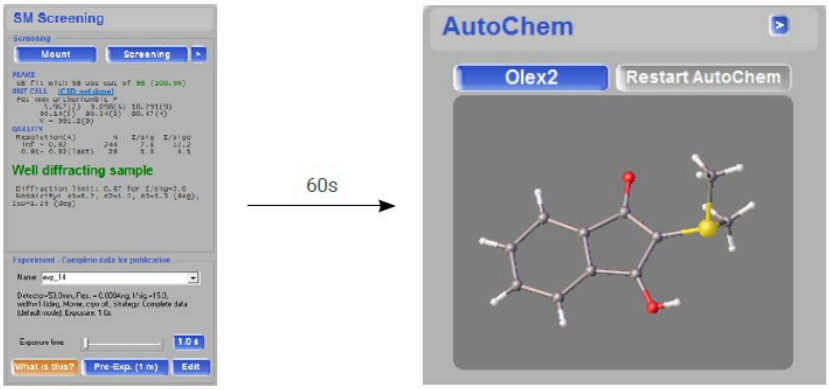
SMX018 - Structures in seconds with What Is This

A new tool for ultrafast sample identification

Sometimes it is useful to understand a molecular structure without delay before you need to collect full publication-quality data. This is especially true in today's fast-paced research programs, where molecular connectivity of intermediates in a synthetic pathway are required before moving on to the next stage. The new "What is this?" (WIT) tool is designed to provide a structure as fast as possible. Using the latest AutoChem2.1 and Rigaku Oxford Diffraction's advanced hardware, it is often possible to identify a sample with a fully determined structure in under a minute.

Features

- Save instrument time by identifying structures before full data collection
- Generate data collection strategy based on a structure for more accurate predictions
- Be sure of symmetry and structure before you collect data

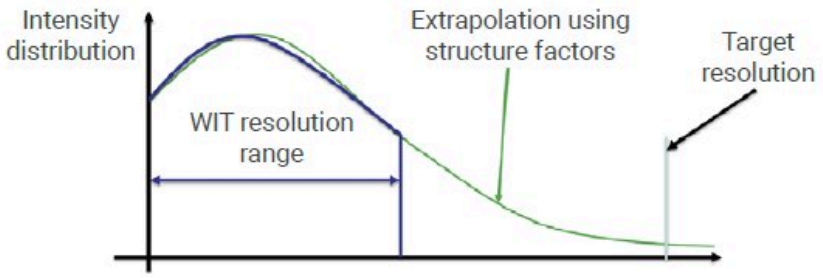


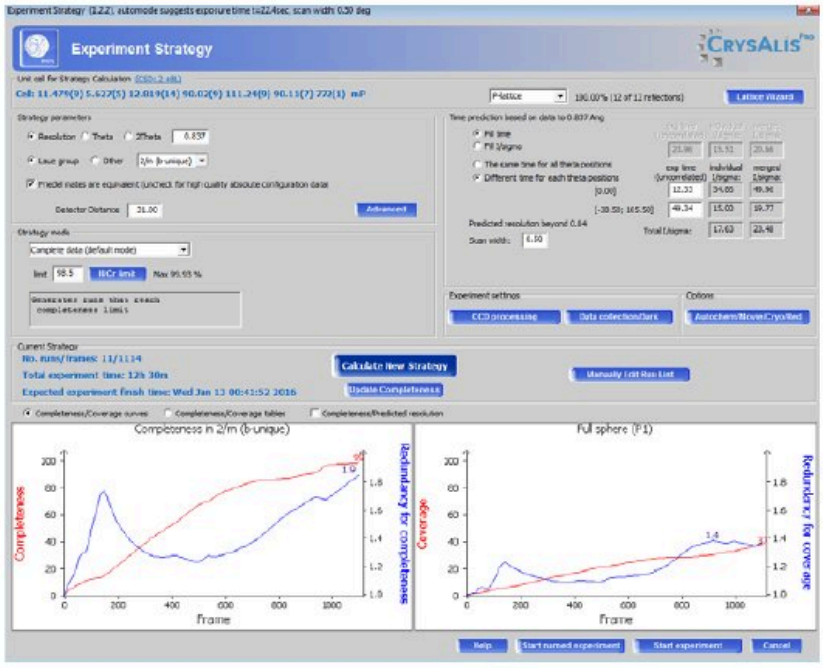
How it works

Using carefully selected strategies, the WIT tool allows for the fast collection of a minimal dataset solely aimed at providing a structure. Following sample screening, the WIT tool becomes available for fast sample identification. The user may choose to continue with a traditional pre-experiment or attempt to identify the structure using WIT. The tool requires only a list of elements present in the structure and an exposure time.

Using diffraction observations from the screening experiment as a basis, appropriate exposure times will be recommended by the software, although the user may choose their own as desired. The list of elements is optional but recommended for the best success rate. A solved structure is typically available within a few minutes, but can take less than a minute for strongly diffracting crystals.

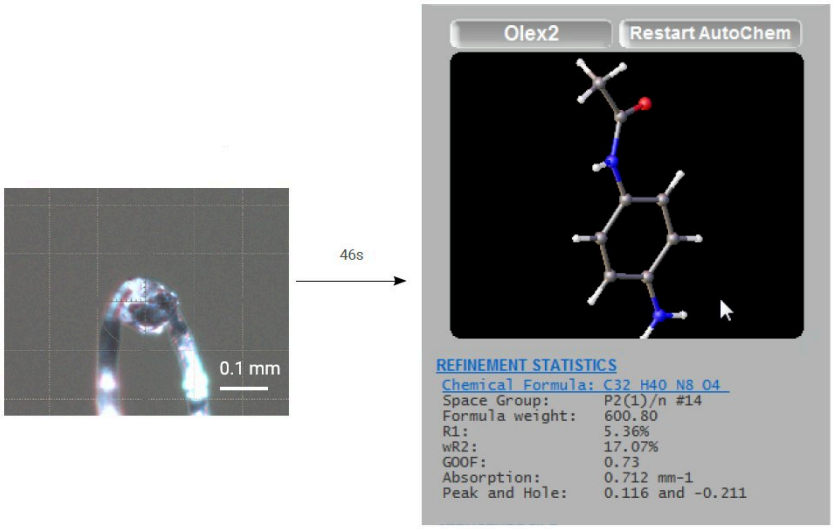
The symmenty and unit cell are known with more certainty when even a rudimentary structure is available, reducing the chance of erroneous or duplicate data collection. Once structure factors are known, the strategy module can use them to extrapolate to target resolution for full experiments, giving better predictions of reflection intensities and thus calculated exposure times leading to higher-quality, efficient data collection.





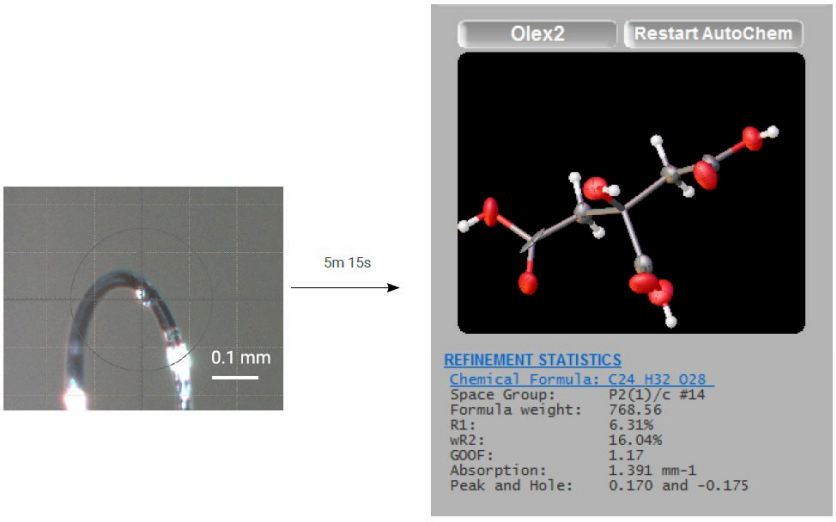
Example 1: Ultrafast identification of a small organic

For well-diffracting samples, WIT is frequently able to solve the structure in under a minute, well before the short data collection has completed. In this example, a full structure, complete with hydrogen atoms and a low R1 of 5.36%, was available in only 46 seconds, providing clear identification of the material.



Example 2: Identification of a weakly diffracting citric acid crystal

Even for more weakly diffracting samples, WIT can provide a structure in minutes. In this example collection, a full dataset took 12 h 30 m. WIT provided a structure in only 5m 15s. Atom types, connectivity and hydrogen positions were all correct and ADPs were mostly reasonable. A low R1 of 6.31% was achieved.



Summary

The ability to identify samples prior to full publication-quality data collection is invaluable in a busy lab. When even challenging samples take only minutes to identify, users are better informed and can focus their attention on the samples of greatest interest, avoiding wasted instrument time.

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