

Xcalibur E Fully Automated Crystal to Structure

Application Note

X-ray Crystallography



Fully Automated and User-Friendly

Automatic chemical structure determination using the Xcalibur E and AutoChem is simple and user-friendly. Designed for use by the chemist, the Xcalibur E allows for fast, highest publication quality structures with the minimum of user intervention in the minimum of time.

Full Sample Capability

Unlike other bench-top instruments which are limited to the study of only routine large crystals, the Xcalibur E has been designed to deal with crystals small or large, routine or problematic. With a footprint of just 1m² the Xcalibur E is fully prepared for dual wavelength and/or CCD upgrades should your future research focus or application change.

Three Clicks from Sample to Final Crystal Structure

Once the crystal is mounted the process is entirely software controlled and fully automated. As few as 3 mouse clicks are necessary to take the user from sample to final crystal structure.



Three Clicks from Sample to Final Crystal Structure

Click 1 - Start

The user clicks start.

Click 2 - Input Chemical Formula and OK

The user inputs chemical formula information if available and clicks to start pre-experiment. The Xcalibur then automatically measures a short (< 5 min) data sample from the crystal before automatically suggesting the best "full" experiment setup.

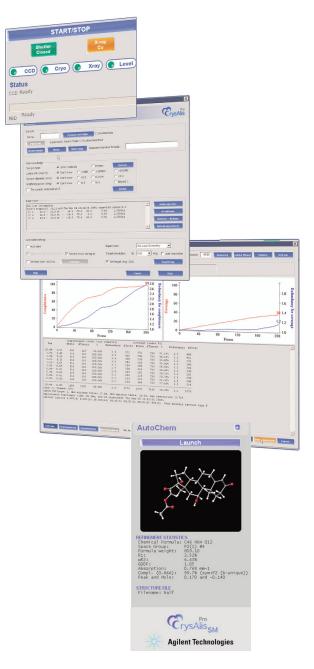
Click 3 - Start Full Experiment

The user simply reviews the setup (if required) and clicks start. Alternatively the user can elect for this to be automatic. The full crystal experiment is then automatically measured and the crystal data is automatically processed in the best possible manner, whether it is a routine or problematic crystal.

Throughout the experiment the software automatically solves and refines the crystal structure through to final publication quality, displaying a rotatable and editable structure on screen for user review.

For More Information

For more information on our products and services, visit our Web site at www.agilent.com/chem



www.agilent.com/chem

Agilent shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance, or use of this material.

Information, descriptions, and specifications in this publication are subject to change without notice.

© Agilent Technologies, Inc., 2009 Printed in the USA November 1, 2010 SI-A-1393

