



# 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 1m<sup>2</sup> 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.



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## 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

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