

Poster Presentation

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Area Detector Systems: Setting Higher Standards for Data Quality

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At least four major factors affect single-crystal diffraction data quality: 1) Hardware (source, goniometer and detector), 2) the sample, 3) the data collection procedure and strategy, and 4) the integration and data reduction software. Three of these factors can be carefully designed by the instrument manufacturer, and the other (the sample) can be chosen to optimize interaction with the instrument. We can define important hardware factors to allow quantification, such as absolute detectivity, overhead, readout speed, minimizing dead time and diffractometer access. Advances in area detector technology (including the new S2 generation of area detectors) and data collection approaches will be presented. The experimental procedure includes the choice of wavelength and the geometric strategy. Details of the detector operation (gain, bin-mode) can be optimized to fit the experiment. Agilent's latest CrysAlisPro software implements the 4th generation of strategy software and includes new on-the-fly detector optimization to provide significant gains in data quality. Integration software must be flexible in order to extract consistently good intensities from excellent samples and also from those that suffer from real-life flaws. Twinned samples represent an additional challenge. Agilent's new data reduction approach for twins significantly improves the data quality of both small molecule and protein twins.

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