

Poster Presentations

[MS10-P13] Advances in Data Quality in Area Detector Diffraction Experiments.

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The data quality of single crystal diffraction experiments depends on several factors: a) The diffractometer and the area detector hardware, b) the sample, c) the experimental procedure/strategy and d) the data reduction approach and software. The talk will highlight key aspects of each of these factors. The hardware revolves around the notions of absolute detectivity, overhead, readout speed, minimizing systematic errors and diffractometer access. Advances in area detector technology and data collection approaches will be presented. The sample choice, mounting, protection environment is controlled within reason by the user. The experimental procedure comprises the choice of wavelength, the geometric strategy, the mode of scan and detector operation and the decision on absolute detectivity vs. redundancy. Agilent's CrysAlis^{Pro} software implements the 4th generation of strategy software with new features for data quality. The data reduction software has to be optimized at extracting consistently area detector data not only under good conditions, but also under real life flaws of the practical experimental procedure. Especially twinned samples represent a challenge. The new data reduction approach for twins significantly improves the data quality of small molecule and protein twins.

Keywords: Data quality, area detectors, strategy, twins