

**MS3-P3** Key metrics for single crystal 2D X-ray area detector systems. Zoltán Gál,<sup>a</sup> Alex Griffin,<sup>a</sup> Fraser White,<sup>a</sup> Oliver Presly,<sup>a</sup> Damian Kucharczyk,<sup>b</sup> and Mathias Meyer,<sup>b</sup>  
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The advent of electronic 2D area detector systems for small molecule and protein crystallography has revolutionized the diffraction experiment.

Depending of the application such as ‘standard structure solution’, ‘absolute structure’, ‘charge density’, ‘screening’, ‘SAD-phasing’ or ‘molecular replacement’ experiments, the requirements placed on the detection system will vary. In all cases the goal of the technology optimization is to minimize the influence of the electronics on the actual raw data with the aim of measuring optimal data quality in a given unit of time.

This poster will present some of the key metrics of modern 2D area detector design with relevance to the above applications and it will also show how the user can significantly influence data quality for the given experiment.

**Keywords:** area detectors; data quality; efficiency

**MS3-P4** XDSAPP - A graphical user interface for processing diffraction data using XDS. Uwe Mueller<sup>a</sup>, Michael Krug<sup>b</sup>, Manfred S. Weiss<sup>a</sup> and Udo Heinemann<sup>b</sup>  
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Today’s third generation synchrotrons allow the collection of diffraction images of protein crystals using typical exposure times of less than one second per image. Since the corresponding end stations for macromolecular crystallography (MX) are equipped with fast detector hardware, the time necessary to collect a complete diffraction data set has decreased from hours a few years ago to minutes.

In order to enable the synchrotron users to analyse all diffraction data during the data collection at the beamline, we have developed the program XDSAPP (XDS Automation and Plotting Protocols) [1] which mainly utilizes the diffraction data processing program XDS [2], but also other software like POINTLESS of the CCP4 software suite [3], XDSSTAT [4], SFCHECK [5] and PHENIX.XTRIAGE [6]). XDSAPP is a Tcl/Tk based graphical user interface for processing diffraction data sets using XDS. It provides easy access to all XDS functionalities, automatizes the data processing and generates graphical plots of various data set statistics provided by XDS. By incorporating additional software, further information on certain features of the data set, such as for instance radiation decay during data collection or the presence of pseudo translational symmetry and/or twinning can be obtained. Intensity files suitable for CCP4, CNS and SHELX are generated.

- [1] Krug, M. et al, (2012). *J. Appl. Cryst.* **45**, 568-572
- [2] Kabsch, W. (2010). *Acta Cryst.* **D66**, 125-132
- [3] Collaborative Computational Project, N. (1994). *Acta Cryst.* **D50**, 760-763.
- [4] Diederichs, K. (2006). *Acta Cryst.* **D62**, 96-101
- [5] Vaguine, A. et al. (1999). *Acta Cryst.* **D55**, 191-205
- [6] Adams, P. D. et al. (2010). *Acta Cryst.* **D66**, 213-221

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