The handling of cryo-cooled protein crystals has been automated by robotics systems, where samples are kept in liquid-nitrogen storage, to be loaded on the goniometer for the experiment and retrieved afterwards. Crystals are automatically centered in the X-ray beam by means of an automated goniometer head and software that applies algorithms that determine the crystal position in three-dimensional space from images taken with high resolution digital microscopes. For the steps that follow, we report on the development of XPRESSO, a new crystal screening and data collection system for macromolecular samples.

The screening process starts out by taking short series of X-ray diffraction images from which the general quality of the crystal is judged by the resolution limit, the mosaicity, the ability to find the unit cell, and the presence of ice rings. User input limits for the unit cell help distinguish between the actual sample and unwanted crystals, such as from buffers or salts co-crystallized with a protein.

For the data collection a strategy is determined based on the screening results. It takes into account the exposure time, sample to detector distance, scan width, and resolution limit, among others. The data is integrated in parallel to the data acquisition, followed by data scaling. Space group determination is the final step. Results are provided as HTML reports, including Matthews coefficient probabilities.

Keywords: automation, protein, software

MS72.P06

Acta Cryst. (2011) A**67,** C660

New Tools for Biological Crystallography in the Home Lab.

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Advances in crystallographic hardware and software have enabled structural biologists to investigate more challenging projects. Recent developments have greatly increased the capabilities of in-house diffraction systems providing increased productivity for synchrotron trips and home-lab studies.

We have made recent improvements in source and detector technology which have significantly improved the capability of home-lab systems for both screening and data collection. Developments include next generation microfocus sources which exhibit significantly higher intensity as well as enhanced beam stability. Combined with a new sensor-based active pixel detector, these systems provide a significant improvement in overall performance while offering extremely low maintenance and cost of ownership. A new feature in our PROTEUM software, XPRESSO, offers a completely automated data acquisition and analysis pipeline for macromolecular crystallography. New developments in hardware and software will be discussed.

Keywords: microfocus source, detector, automated data acquisition

MS72.P07

Acta Cryst. (2011) A**67,** C660

Graphical user interface for automated crystallography data reduction.

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With the advances in throughput at synchrotron facility sites capable of yielding up to 15 data sets an hour the automatic reduction of single crystal diffraction data is becoming a routine component on synchrotron beamlines. For the past three years at Diamond Light Source, packages such as fast_dp (in house development) and xia2[1] have been employed to carry out data reduction immediately after data collection and are automatically triggered without user interaction. Here we describe how our first implementation which was geared towards processing single sweeps of data with no user interaction has been integrated with a graphical user interface that provides finer control to these programs and the ability to process multiple or partial sweeps of data.

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Keywords: data processing, automation, GUI

MS72.P08

Acta Cryst. (2011) A**67,** C660

Readiness evaluation method for X-ray difraction data collection systems

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High quality diffraction data is critical for structure determinations. For macromolecular crystallography, there are many factors that may compromise the final data quality. In addition to crystal quality and data collection strategy, the instrumentation factors, such as x-ray beam quality, goniometry and the quality of detectors, are important for data quality too. Since the data collection systems are composed of many electronic and mechanical units and they have to work synegically at their at least normal performance. But this may not always be true.

In order to develop a quick and simple method to access the overall performance of the X-ray data collection system, we proposed a protocol to test X-ray diffraction facilities' readiness. In this protocol, cubic insulin crystals are used to quickly collect anomalous data at long wavelength such 1.54Å. The weak anomalous signals from the 3 disulfide bonds are used to indicat the acuracy of the whole data collection system. This method has been tested at different data collection systems including both rotating anode based home labs and synchrotron beam lines. The detailed results and analysis will be presented.

Keywords: data collection, readiness

MS72.P09

Acta Cryst. (2011) A**67,** C660-C661

New version of CrysAlisPro optimized for automatic macromolecular data collection and processing

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While the majority of macromolecular X-ray data are currently collected using highly-efficient beam lines on an ever increasing number of synchrotrons, there is still a need for low-maintenance, reliable systems for in-house experiments. In addition to crystal screening and optimization of x-ray experiments before a successful synchrotron trip,

the home system allows collection of data as soon as the crystals are produced to get the initial solution of novel structures and is invaluable in the quick turnover often required in ligand-binding studies.

We will describe how the combination of the updated Agilent Technologies SuperNova, a highly efficient compact diffractometer, with the new version of fully automated CrysAlisPro data collection and processing software, optimized for macromolecular crystallography, makes an ideal home lab solution complementing synchrotron data collection.

New unique features of CrysAlisPro and several examples of high quality results obtained with the system will be presented.

Keywords: macromolecular, experiment, software

MS73.P01

Acta Cryst. (2011) A**67,** C661

Fluorine determines the aggregation of pyridines. Experiment vs. theory

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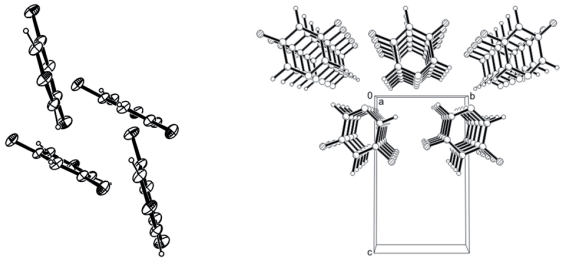
Fluorine is a unique element. The question about the role of Fluorine in intermolecular interactions is discussed controversially. Well known is the influence of fluorine on the electronic structure of aromatic backbones and therefore on the entire molecules. On the other hand, fluorine forms only weak intermolecular interactions and seems to have no influence on the crystal packing. Pauling's definition of the hydrogen bond would imply that fluorine, as the most electronegative atom, should be a stronger hydrogen-bond acceptor then oxygen and nitrogen. But the C-F group, the so-called "organic fluorine", does not form hydrogen bonds commensurate with electronegativity considerations in contrast to the C-O and C-N groups.

We investigated a range of partially fluorinated pyridines and analysed their crystal packings experimentally and theoretically. Low temperature *in situ* crystallisation on the diffraktometer was used to investigate crystal structures of low melting fluorinated pyridines followed by analysis of the crystallisation behavior. Interesting tendencies were observed in crystal packings depending on the fluorination degree.

But still the general question we are interested in, is: what determines the crystal packing in the absence of strong intermolecular interactions? Theoretical study of the energies of weak intermolecular interactions is an innovative method for research of the basic motives in the solid state. The comparison of our experimental and theoretical findings shows how fluorine atoms influence the aggregation of substituted pyridines. The picture below shows the difference between basic structural motives in the experimental (a) and theoretical (b) crystal packing of 3,5-difluoropyridine.



[1] V. Vasylyeva, K. Merz, *J. Fluorine Chem.* **2010**, *131*, 446-449. [2] V. Vasylyeva, K. Merz, *Cryst. Growth Des.* **2010**, *10*, 4250-4255. [3] K. Merz and V. Vasylyeva, *CrystEngComm* **2010**, *12*, 3989-4002. [4] V. Vasylyeva, O.V. Shishkin, K. Merz *Cryst. Growth Des*. **2011,** submitted.

Keywords: crystal engineering, fluorine, halogen bonding

MS73.P02

Acta Cryst. (2011) A**67,** C661

TMA alcohol solvates: filling the gaps and increasing the dimensionality

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Benzene-1,3,5-ticarboxylic acid, or trimesic acid (TMA), has been the focus of research interest for many years due to its symmetry, hydrogen bonding ability, ability to form salts and solvates, and use as an organic linker in metal organic frameworks. We have previously reported 1:1 and 1:2 TMA:MeOH solvates that demonstrated the stepwise dissolution of TMA via disruption by methanol of the $R^2_2(8)$ head-to-tail carboxylic acid dimer H-bonding pattern. This common pattern is seen in many pure carboxylic acids including the three-fold interpenetrated honeycomb lattice of pure TMA [1]. The disruption occurs via the insertion of an alcohol OH group into the $R^2_2(8)$ ring to generate an expanded $R^3_3(10)$ motif. More recently, the related structures of the higher alcohol homologues 1-butanol, 1-pentanol, and 1-hexanol were reported by Perepichka and Rosei [2]. This work revealed a structural dependence on the length of the alcohol's alkyl chain.

We are now able to report the intervening 'missing' TMA–alcohol solvate crystal structures with EtOH, 1-propanol, and 2-propanol, two of which are twinned. Their structures are placed in the context of the preceding work and our new findings plug the gap in current knowledge. We also report the structures of two diols which extend the dimensionality from 1D ladders (Fig. 1) to 2D sheets. The diol solvates/co-crystals exhibit further disruption of the $R^2_2(8)$ rings.

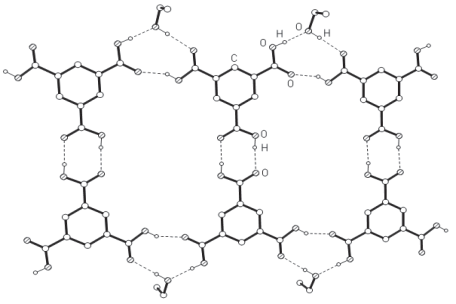

Fig. 1. 1D ladder structure adopted by TMA·EtOH with $R^2_2(8)$ and $R^3_3(10)$ H-binding motifs.

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Keywords: hydrogen bonding, crystal engineering, trimesic acid

MS73.P03

Acta Cryst. (2011) A**67,** C661-C662

Hydrogen bonding, Z' and stability of diclofenac amine salts

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