The inclusion of the half-millionth structure into the Cambridge Structural Database highlights the rate of growth of the CSD in recent years, the growing body of structural knowledge this provides, and the challenges this amount of information represents in terms of validation and maintenance. This talk will describe the processing and validation of X-ray crystal structures at the CCDC and the development of tools to enhance this process. These tools include assigning chemistry to crystal structure data, indicating reliability of assignments, and the use of the existing database to enhance future processing. Further developments that will aid this growing body of structural knowledge to be exploited in a range of external applications and the provision of additional services that can assist the scientific community will also be illustrated.

Keywords: Cambridge Structural Database, validation

FA5-MS44-T04

CATS & G-ROB: 6-AXIS robotic-arm-based AUTOMATED systemS for crystallography.

Jean-Luc Ferrer[a], Xavier Vernede[a], Pierre Mazel[c], Pierrick Rogues[c], Florian Bouis[a], Jacques Joly[a], Matthieu Privas[b], Jean-Loup Rechatin[b,] Nathalie Ferrer[c]. [a]*Institut de Biologie Structurale CEA-CNRS-UJF, Grenoble, France.* [b]*Irelec, Saint Martin d'Hères, France.* [c]*NatX-ray SAS, Grenoble, France.*
E-mail: jean-luc.ferrer@ibs.fr

CATS and G-Rob systems were developed on protein crystallography beamline FIP-BM30A at the ESRF. CATS [1] is a sample changer currently now installed on various synchrotrons (SLS, BESSY, DLS, APS, ...). G-Rob, also a 6-axis robotic arm based system, is a fully integrated device for crystallography beamlines and laboratories. G-Rob is an "all in one" system, since it integrates the following functions:

- sample changer,
- goniometer for frozen samples, capillaries, … [2],
- crystallization plates/micro-chips screening for *in situ* analysis of diffraction condition and data
- collection [3],
- goniometer for non-classical sample environments (high pressure cells, …),
- beam monitoring.

G-Rob provides unique features. It is automated: thanks to its tool changer, it goes automatically from one application to another. CATS and G-Rob are also highly flexible: if a new application or a new sample format emerges in the community, a new tool can be designed to implement it. They are highly reliable systems, based on well-known, industrial quality equipments, with reduced maintenance.
They are currently in use on beamline FIP-BM30A. It was made available to the research community in 2005 and up to now, users have expressed an unprecedented high degree of satisfaction. The crystallization plates screening capability for example appears to be a precious tool in several cases (crystals too small to be fished, or too fragile, of when there is no good cryoprotectant).
Several results obtained on FIP-BM30A are presented, such as *in situ* screening of membrane proteins, ribosome, high pressure protein diffraction, etc. Recent experiments demonstrated also the possibility of the automated structural screening for the Fragment Based Drug Design strategy: the same crystal was reproduced in presence of a library of fragments. Systematic *in situ* data collection has shown some of the fragments present in the active site, without having to manipulate the crystals individually. Movies are available on www.natx-ray.com.

[1] Jacquamet *et al.*, *JSR*, 2009, 16, 14. [2] Jacquamet *et al.*, *Acta Cryst.,* 2004, D60, 888. [3] Jacquamet *et al.*, *Structure,* 2004, 12, 1219.

Keywords: robot goniometer, X-ray screening automation

FA5-MS44-T05

What can the Bruker SMART X2S do for me?

Simon Lawrence[a], Kevin Eccles[a], Anita Maguire[b]. [a]*Department of Chemistry, Analytical and Biological Chemistry Research Facility, University College Cork, Cork, Ireland.* [b]*Department of Chemistry and School of Pharmacy, Analytical and Biological Chemistry Research Facility, University College Cork, Cork, Ireland.*
E-mail: s.lawrence@ucc.ie

The Bruker Smart X2S is a completely automated instrument designed for routine chemical crystallography for the non-specialist, encompassing all stages of data collection, structure solution and refinement.
Advances in automation can lead to greater awareness and uptake of a technique, although this can come at a cost, namely, reduction in the practical knowledge and understanding of the underlying scientific theory, as well as in the awareness of the difficulties and limitations of the technique in question. Indeed, a major criticism of such advances is that they often lead to a "black box" philosophy, characterized by a non-critical appraisal and over reliance on the results obtained.
In this presentation we wish to discuss our experiences with the Bruker SMART X2S, by presenting data for a representative range of samples in inorganic, organic and pharmaceutical chemistry, highlighting its successes and challenges.

Keywords: chemical crystallography, automation