

Continuous improvement in a crystallization laboratory at AstraZeneca

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Reconstruction of ACTOR robots

Our laboratory has two in-house X-ray generators (FRE and FRE+) equipped with ACTOR robots. We use our equipment for in-house data collection and pre-screening of crystals prior to data collection at ESRF. The robots were converted to accept SPINE pucks a few years ago leading to:

- Compatibility with ESRF
- Enable easy prescreen in house
- A user friendly system
- Reduced handling with precious crystals



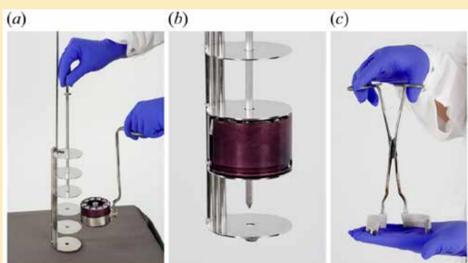
Development of a storage rack for SPINE pucks

Long-term storage of SPINE pucks became necessary after re-construction of the ACTOR robots but there was no commercial SPINE racks available. The only way to store these pucks was in transport dewar canisters which is undesirable for several reasons:

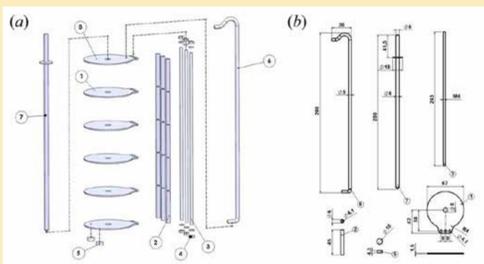
1. Multiple users, multiple projects → many crystals → many transport canisters/dewars required
2. Pucks can not be taken out without removing pucks stored above
3. Cumbersome to keep transport dewars cold compared to larger variants

The solution was to develop ourselves a simple affordable rack for SPINE pucks. Instead of stacking pucks on top of each other the pucks sits on individual shelves in our rack.

The rack consists of **five shelves** and a removable **locking pin** that is inserted through all shelves and pucks to secure them in place.



To handle the pucks into and out of the racks a pair of Actor puck **tongs** where **modified** by incorporating callipers to grip the puck.



Solutions for the storage and handling of SPINE standard pucks. C. Bodin, et.al, J. Synchrotron Rad., (2012), 19, 288-289

With increasing number of challenging and diverse crystallization targets and the never ending demands on shorter delivery times of structures in complex with ligands for structure based drug design there is a need to work smarter, faster and more organized.

The implementation of automation during the last ten years has completely changed the way of working and increased the crystallization throughput dramatically, but it also created gaps where there are no good commercial solutions.

In our crystallization lab at AstraZeneca we are constantly developing the infrastructure of the laboratory to optimize the workflow and also produce tools that can help us, always with a mindset of continuous improvement.

For us, simple, technical and logistical innovations in the lab have been the key to fully benefit from the development in automation of all aspects of crystallography.

In this poster we present a few examples.

Tracking system for pucks

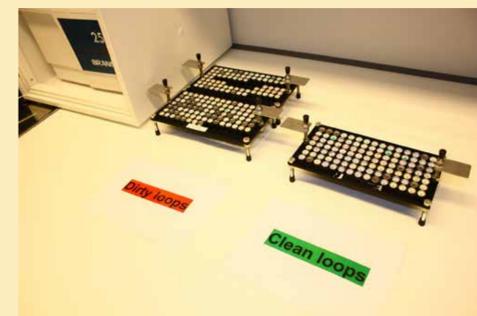
To keep track of all pucks we have developed a tracking system. Each puck is represented by a white board magnet labeled with the unique puck number. When the puck is in use, its location is updated by transferring the magnet between boards representing our various storage and transport dewars, which in turn contain visualization of the racks within each dewar.

Cap holder

When working with iterative soaking/seeding systems the Qiagen 15-well tool plate with screw caps is commonly used since it is very easy to handle. We have developed a tool for easy handling of the screw caps when transferring crystals from drop to drop enabling full focus on the crystal and transfer. The cap holder is simply made by drilling two wholes into a thick piece of plastic.



Wash rack for loops – a time saver



The number of crystals tested for diffraction has increased due to automation of both crystal setup and diffraction screening. Commercial solutions for storage and handling of loops has not followed in the same pace.

To handle dirty loops more systematically we designed a loop rack that wash 7x15 loops simultaneously. When the rack is filled up the loops are washed effectively in an ultrasonic bath for only a few minutes and then left to dry on the bench.

→ Puck barcode

→ Position of the puck

→ Owner

→ Content

→ Date

Jenny I SD5 pos. 5		Annemarie I SD1 pos. 1	
5		5	
4		4	
3		3	P2 26/8-13
2		2	P1 20/8-13
1	P3 16/8-13	1	P1 20/8-13

