

## **Workshop HTP Crystallisation and Information Management (BIOXHIT / TEACH-SG)**

**NKI Amsterdam, The Netherlands, June 18 – 20 2008**

**Organisers:** Patrick Celie and Anastassis Perrakis

**Number of Tutors:** 9

**Number of participants:** 13 (10 from European Institutes, 2 from Indian Universities and 1 from The Weizmann Institute, Israel)

The workshop was organized as a sequel to the course 'HTP Macromolecular Crystallisation', held at the NKI in December 2005. The first course mainly concentrated on the different robotics that were available for the preparation and imaging of crystallization trials at a nanoliter scale. In the recent workshop we focused more on different crystallization methods and their application in high-throughput crystallisation facilities. A substantial part of the program was reserved for an introduction to xtalPiMS, a protein crystallization information management system developed at the NKI, EMBL Grenoble and Oxford University as part of PiMS.

The workshop included both lectures and practicals. A very-well received part of the program was the 5- 10 minutes presentation of each individual participant. This format proved to be an excellent opportunity to get an impression of the techniques and methodologies used at different labs and provided a nice template for discussion among participants.

The lectures about Free Interface Diffusion (Eve Marquis, Fluidigm), In-situ crystal analysis (Jochen Müller-Dieckmann, EMBL Hamburg) and counter diffusion (José Antonio Gavira, University of Granada) were very informative and gave new insight in the current possibilities of crystallisation screening and optimization. The integration of these technologies including HTP nanodrop crystallisation at large crystallisation facilities was presented by Jochen Müller-Dieckmann, (EMBL Hamburg), José Antonio Marquez (EMBL Grenoble) and Ian Berry (OPPF). The presentations on (micro-) seeding in automated crystallisation (Patrick Shaw Stewart, Douglas Instruments) and computational classification of crystallisation images (Julie Wilson, university of York) were highly appreciated.

The combined tutorial and practical session on xtalPIMS (Ian Berry, OP PF) was very informative and allowed participants to get experience with this information management system.

The hands-on part of the workshop included practicals on capillary crystallisation, free interface diffusion microfluidics (TOPAZ), nanodrop crystallisation using the Mosquito (TTP Labtech) and the Oryx dispensing robot (Douglas Instruments) and a live demo on the Crystal Farm storage and imaging system (Bruker AXS).

During the general assembly at the end of the course the workshop was evaluated. Although the number of participants was somewhat lower than expected (the maximum was set to 20 participants), all contributing people were very motivated and communicative, resulting in a very lively and informal environment. Some of the participants are responsible or involved in setting up crystallisation facilities and they all found the information they obtained very useful for establishing their crystallisation setup.

All participant presentations and most of the lectures are available from [http://xtal.nki.nl/CW\\_0608/](http://xtal.nki.nl/CW_0608/)