EMBO'07 – A course on Exploiting Anomalous Scattering in Macromolecular Structure Determination

EMBO'07 – A course on Exploiting Anomalous Scattering in Macromolecular Structure Determination was held in Grenoble France June 18-22, 2007. The workshop was arranged with collaboration with ESRF and EMBL. Normally for these courses applications have arrived 200, but this time these were only 50 and therefore it was easier to get in. Number of participants was limited to 20 persons. Days were mostly long starting from 8:45 to 10:00 and ending between 17:00 and 21:00.

It was promised that course content is following. "This practical course addresses young scientists who intend to apply single- and multiple-wavelength anomalous scattering (SAD & MAD) methods in macromolecular structure determination. The course aims to impart the theoretical and practical basis for the 3-dimensional structure determination of bio-macromolecules using these techniques. Through a series of lectures, software demonstrations, practicals and tutorials, participants will get insights into all aspects of the structure determination process including beamline instrumentation, data collection and processing, heavy atom substructure determination, phasing and model building. There will also be sessions focusing on automated structure solution procedures and newer methods which exploit small anomalous scattering signals from crystals of native macomolecules." Course really came up with the goods.

There were presented three automated pipelines for experimental phasing, CRANK, AutoRickshaw and Phenix. In most cases it is enough if you have reasonable good data with anomalous signal, like 2.5 Å diffracting SeMet peak data and protein sequence. All pipelines were tested with students own data and it was shown that XDS prosessed data with autoRickshaw works best. AutoRickshaw was only one which solved data where was pseudotranslation. With autoRickshaw you can know after few minutes if your structure will be solved most probable or not. After two or three hours you might have first ARP/wARP structure which has structured almost all amino acids. One good hint was that it is always good to collect long wavelength data set if it is possible. It gives anomalous information of many metals. In many structures there is build waters even there really is metal ions.

Course was very good. I had possibility to meet people how have developed most of programs which we are using in protein X-ray crystallography. I got also my phases solved for my structure.

We had chance to familiarize ourselves to French midsummer party on Thursday night. It differs much from Finnish one. There were all around in French cities musicians playing and singing all kind of music. At the end we had excursion to Monteynard Lake where was farewell dinner. It was nice to have chance to go first time to Alps in Grenoble where you normally on data collection trips work inside long days and around are beautiful views of Alps.

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