



Fourth BIOXHIT/BCO COURSE: Remote datacollection at the ESRF and the CCP4 structure determination pipeline.

Time April 21 – April 25, 2008
Place Department of Biochemistry, University of Oulu, Linnanmaa
Credits 2.5 study points (ECTS units)
Organizers Rik Wierenga, Tuomo Glumoff, Antti Haapalainen, Kristian Koski, Markus Alahuhta, Miki Kallio. Department of Biochemistry and Biocenter Oulu Graduate School, University of Oulu, Oulu, Finland

Monday, April 21 (Linux class room)

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| 09.15-09.20 | Opening Rik Wierenga , University of Oulu |
| 09.20-09.25 | Welcome Kalervo Hiltunen , Head of the Department of Biochemistry, University of Oulu |
| 09.25-09.30 | Practical matters Tuomo Glumoff , University of Oulu The computing environment Miki Kallio , University of Oulu |
| 09.30-10.30 | Data collection at the ESRF, DNA, ISPyB Xavier Thibault , ESRF, Grenoble, F |
| 10.30-11.30 | eHTPX Ian Berry , OPF, University of Oxford, Oxford, UK |

11.30-12.30 *Lunch*

Monday April 21 (BK226)

12.30-14.30 Remote datacollection, with the students being present
Xavier Thibault

14.30-14.45 *Coffee*

Monday April 21 (Linux class room)

14.45-17.00 eHTPX, ISPyB tutorials
Xavier Thibault, Ian Berry

Tuesday, April 22 (Linux Class Room)

10.00-11.00 DNA tutorial, Discussion/Evaluation of the remote datacollection
Xavier Thibault, Ian Berry, Kristian Koski, Antti Haapalainen

11.00-11.15 *Coffee*

11.15-12.15 the CCP4i concept and the data checking tools of CCP4
Martyn Winn, Daresbury Laboratory, Daresbury, UK

12.15-13.15 *Lunch*

13.15-14.15 CCP4 molecular replacement tools
Martyn Winn

14.15-14.30 *Coffee*

14.30-17.00 Tutorial on MrBUMP, Molrep
Martyn Winn

18:00-20:00 extra time for teachers / students, for working with student data

Wednesday, April 23 (Linux Class Room)

09.00-10.00 Coot, the basics: how to built a model in a map
Paul Emsley, University of Oxford, Oxford, UK

10.00-10.15 *Coffee*

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| 10.15-12.00 | Coot tutorial: how to built a model in a map, structure validation Paul Emsley |
| 12.00-13.00 | <i>Lunch</i> |
| 13.00-14.00 | Experimental phasing, phase improvement and model building Kevin Cowtan , University of York, York, UK |
| 14.00-14.15 | <i>Coffee</i> |
| 14.15-17.00 | Tutorial on the map improvement CCP4 software Kevin Cowtan |
| 19.00-22.00 | Joint dinner in Sokeri-Jussi, Oulu |

Thursday, April 24 (Lecture Hall BK226 and Linux Class Room)

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| 09.30-10.15 | Crystal peculiarities. Pseudo translation, twinning: detection and handling. Garib Murshudov , University of York, York, UK |
| 10.15-11.00 | How to do TLS refinement and how to analyse the TLS description of a PDB-file Martyn Winn |
| 11.00-11.15 | <i>Coffee</i> |
| 11.15-12.00 | REFMAC5, the basics, scaling options, xloggraph etc Garib Murshudov |
| 12.00-13.00 | <i>Lunch</i> |
| 13.00-14.00 | REFMAC5 tutorial Garib Murshudov |
| 14.00-14.15 | <i>Coffee</i> |
| 14.15-17.00 | REFMAC5 tutorial Garib Murshudov |
| 18:00-20:00 | extra time for teachers / students, for working with student data |

Friday, April 25 (Lecture Hall BK226 and Linux Class Room)

- 09.00-10.00 New Ligands. Making own libraries, covalent links in case of modified residues, SMILES, etc)
Garib Murshudov
- 10.00-10.15 *Coffee*
- 10.15-12.00 REFMAC5/Coot advanced options tutorial
Garib Murshudov, Paul Emsley
- 12.00-13.00 *Lunch*
- 13.00-14.00 NCS, validation, scripting in Coot
Paul Emsley
- 14.00-14.15 *Coffee*
- 14.15-15.00 Practicing Coot and CCP4
Paul Emsley, Garib Murshudov, Kevin Cowtan, Martyn Winn