



WK04: A Protein Crystallographic Toolbox: The CCP4 Software Suite

**ACA 2005 Orlando
May 28th 2005**

About this workshop ...

The objective of this one-day workshop is not to teach crystallography but to teach people how to use some of the programs distributed with the CCP4 package to do protein crystallography.

Thanks to ...

Maeri Howard (co-organiser)
The ACA (Ed Collins and Marcia Colquhoun)
Funding from CCP4

CCP4 in exhibition area ...

We're at Booth #604!

About CCP4 ...

CCP4 is the Collaborative Computational Project no.4

- UK-based initiative
- Provides software for Macromolecular X-ray Crystallography
- Educational remit to promote “good practice”
- Core funding from BBSRC
- Addition income from industrial receipts

Core staff based at CCLRC Daresbury Laboratory in UK

- Maintain, develop and release core software
- Make releases of the software suite
- Coordinate other activities including:
 - Annual study weekend
 - Newsletters
 - Maintain website, bulletin board, problems pages
 - Conferences, workshops (like this one!)



CCP4 funds other staff working on CCP4-related projects and programs across the UK

Software is also provided by developers not funded by CCP4

CCP4-related software developments

- CCP4 Molecular Graphics (CCP4mg)
- Refmac5
- Mosflm
- Phaser

Other projects

- CCP4 Automation effort
- Involvement in various European projects:
 - e-HTPX, SPINE, BIOXHIT, PIMS ...

Some general CCP4 resources ...

CCP4 website

- <http://www.ccp4.ac.uk/>
- Links to lots of useful information (downloads, documentation...)

Bulletin Board `ccp4bb`





- lively forum for discussing all aspects of protein crystallography
- “Sorry for the non-CCP4 related query...”
- To (un)subscribe: <http://www.ccp4.ac.uk/ccp4bb.php>

Newsletters

- *news@ccp4*
- “Journal style” newsletters
- Current and past issues:
<http://www.ccp4.ac.uk/newsletters.php>

Timetable		
8:30	Introduction and Welcome	
<i>Morning session: General</i>		
8:45	An Introduction to the CCP4 Suite: CCP4i, Files and Utilities	Peter Briggs
9:30	Overview of using CCP4 for PX	Johan Turkenburg
10:15	Help! Finding your way around CCP4	Maria Turkenburg
<i>10:45</i>	<i>Coffee</i>	
11:15	Data Processing and Reduction using MOSFLM & SCALA	Harry Powell
<i>12:45</i>	<i>Lunch</i>	
<i>Afternoon session</i>		
13:45	Refinement using REFMAC5	Roberto Steiner
<i>15:15</i>	<i>Coffee</i>	
15:45	CCP4 Molecular Graphics: Pictures and Movies with CCP4MG	Stuart McNicholas
16:15	Coot and Graphical Model Building Tools	Paul Emsley
<i>Summing Up</i>		
16:45	Summary, or: "if you don't remember anything else from today, remember this..." Questions and Answers	
<i>17:00</i>	<i>Close</i>	

Practical points ...

- Coffee breaks at 10:45am and 3:15pm A black silhouette of a coffee cup with steam rising from it.
- Lunch not provided
 - But there are places to eat nearby A red circle with a diagonal slash over a sandwich icon, indicating that food is not provided.
- Packs contain copies of all the talks *except* for Johan's presentation
 - Copies are be available
 - Please let me know if there other missing documents/other problems
 - There are also questionnaires in the packs – please give us feedback!
- Speakers
 - Please please please stick to time A yellow clock face with black hands and numbers.
 - Gather for photo at morning coffee A grey camera icon.