

# 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 Workshop ACA 2005 Orlando FL





# 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

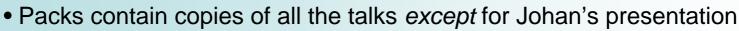


Timetable		
8:30	Introduction and Welcome	
Morning session: General		
8:45	An Introduction to the CCP4 Suite: CCP4i, Files and Utilities	Peter Briggs
9:30	Overview of using CCP4 for PX	Johan Turkenburg
10:15	Help! Finding your way around CCP4	Maria Turkenburg
10:45	Coffee	
11:15	Data Processing and Reduction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



# Practical points ...

- Coffee breaks at 10:45am and 3:15pm
- Lunch not provided
  - But there are places to eat nearby



- 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
  - Gather for photo at morning coffee

