

WK03: A Protein Crystallographic Toolbox: CCP4 Software Suite and PDB Deposition Tools

**ACA 2004 Chicago
July 17th 2004**

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, and how to get the best from the PDB when they deposit their structures.

Organised by ...

Maeri Howard-Eales, Judy Flippen-Anderson, Peter Briggs, John Westbrook

With financial assistance from ...

ACA, CCP4 and the RCSB-PDB

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
- CCP4 LIMS
- Involvement in various European projects:
 - e-HTPX, SPINE, BIOXHIT ...

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.html>

Newsletters

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

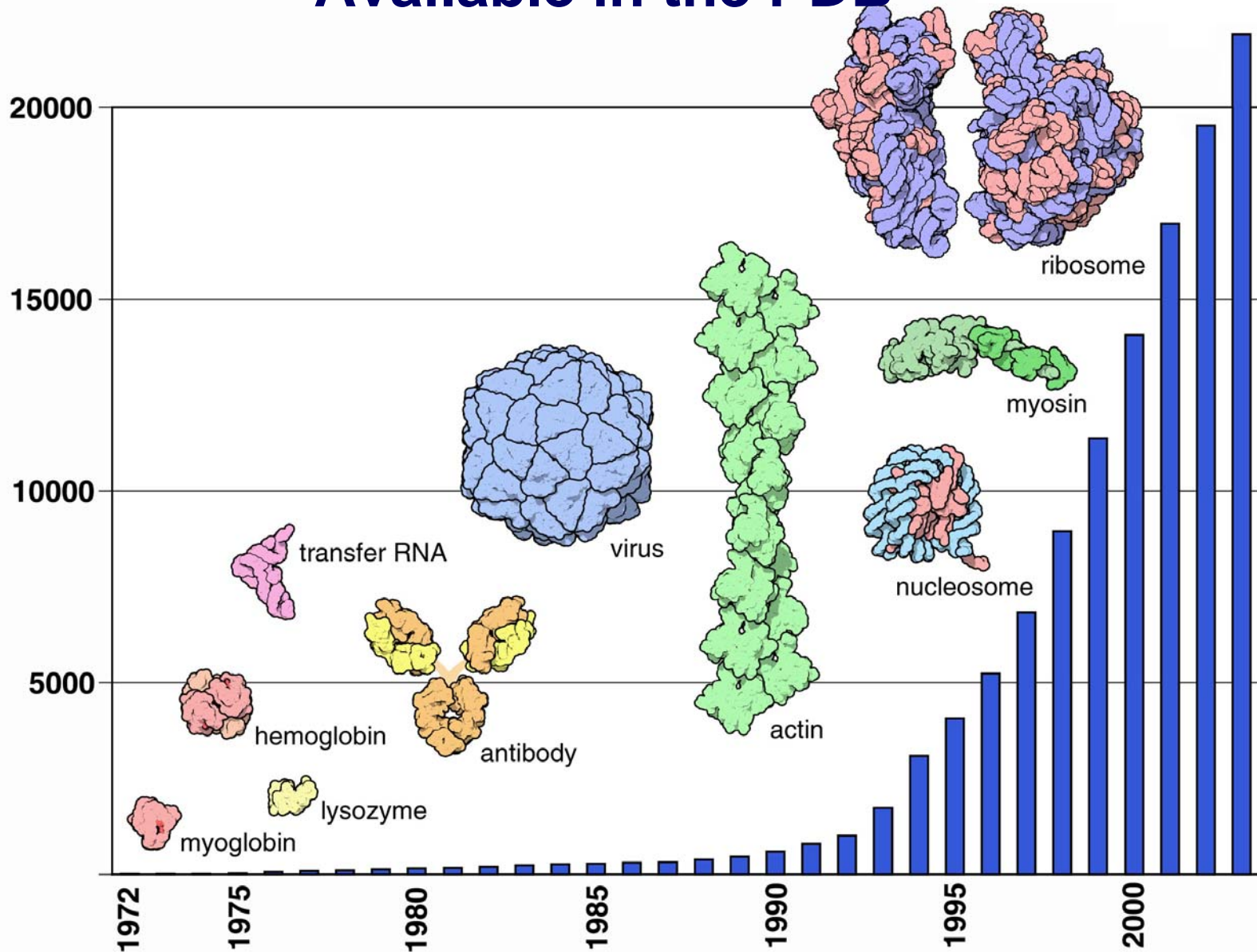


The Protein Data Bank is the single worldwide repository for the processing and distribution of 3-D biological macromolecular structure data.

The RCSB PDB's mission is provide the most accurate, well-annotated data in the most timely and efficient way possible to facilitate new discoveries and advances in science.

As of July 13, 2004, there are more than 26,000 structures available in the archive.

Growth in Number of Structures Available in the PDB



Workshop Timetable

8:30am	Introduction and Welcome	
<i>Morning session</i>		
8:35	Introduction to CCP4 and the PDB	Peter Briggs & Judith Flippen-Anderson
8:50	The CCP4 Package: General Overview: CCP4i, Files and Utilities	Peter Briggs
9:20	Overview of using CCP4 for PX	Martin Noble
10:20	<i>Coffee</i>	
10:40	PDB_EXTRACT and CCP4 - making deposition easier	Shuchismita Dutta
11:40	Data collection & data reduction using MOSFLM and SCALA	Gwyndaf Evans
12:20	<i>Lunch (provided onsite)</i>	
<i>Afternoon session</i>		
13:00	Data collection & data reduction using MOSFLM and SCALA (continued)	Gwyndaf Evans
13:40	Refinement using REFMAC5	Roberto Steiner
14:40	<i>Coffee</i>	
15:00	CCP4 Molecular Graphics: what can it do for you?	Stuart McNicholas
15:30	Data deposition using ADIT	Kyle Burkhardt
<i>Summing Up</i>		
16:30	Summary, or: "if you don't remember anything else from today, remember this..."	
16:40	Question and Answer Session	
17:00	<i>Close</i>	