CCP4 Release 5.0

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Core libraries provide common functions to the programs:
• CCP4 environment (e.g. keyworded input)
• Read/write standard file formats (e.g. MTZ, PDB, maps)
• Basic crystallographic functions (e.g. symmetry info)

New CCP4 libraries:
• Support the existing Fortran77 “legacy” programs
• Make functions available to different programming languages
• Provide basis for improved software infrastructure in future

Useful for software developers, of little interest to general users!
New Programs

• **topdraw** - sketchpad for drawing protein topology cartoons *(Charlie Bond)*

• **dtrek2scala** - convert unmerged D*TREK data to input into scala *(Gwyndaf Evans)*

• **bulk** - bulk-solvent correction for translation search in AMoRe *(Andrei Fokine, Cuido Capitani, Marcus Grütter, Alexandere Urzhumtsev)*

• **ncont** - search for protein contacts

• **pdbcur** - manipulate PDB files *(Eugene Krissinel)*
Updated Programs and Other Changes

Updated programs include:
• **REFMAC5.2** (plus major updates to the monomer library)
• **ACORN, AMORE, MOLREP, SCALA, OASIS, SFCHECK** …
• many other minor updates

New supported platforms:
• Intel compilers on Linux
• Itanium systems (SGI, Hewlett-Packard)

Updated documentation:
• New CCP4i-based tutorials (*Maria Turkenburg, Eleanor Dodson*)
• “Maths for crystallographers”
Updates to CCP4i

New interfaces:
• Mosflm - batch mode integration
• AreaIMol - solvent accessible area calculation
• PolarRFn - rotation function calculation
• ClustalW* - sequence alignments

Other changes:
• Significantly updated Refmac interface
• Help text also displayed as “balloon help”
• New module Graphics and Viewing Utilities
• plus many other more minor updates and bugfixes

* ClustalW program not distributed as part of CCP4.
Updates to Data Harvesting (Pryank Patel)

• Data Harvesting now enabled under Windows

• New harvesting based applications include:
  • **cif2xml** - convert CCIF harvest files into XML format
  • **cross_validate** - check harvest files for consistency
  • **PDB_EXTRACT** - generate harvesting information from CCP4 logfiles (RCSB)

• **Data Harvesting Management Tool**
  • CCP4i-based
  • manage/review harvesting files
  • interface to **pdb_extract, cif2xml, cross_validate**
CCP4 5.0 - when will it be available?

- Target release date end of September 2003
- Watch for announcements on “ccp4bb”

For more information: come and see our poster (#8)

or

Talk to us at the CCP4 stand in the marquee
Developments within the CCP4 software suite beyond 5.0

CCP4 Molecular Graphics CCP4mg
- aims to produce graphics package for solution and analysis of macromolecular structures
- [http://www.ysbl.york.ac.uk/~lizp/molgraphics.html](http://www.ysbl.york.ac.uk/~lizp/molgraphics.html)

CLIPPER-based Crystallographic Applications
- *Clipper* = Kevin Cowtan’s advanced software libraries for crystallographic computation
- Forthcoming applications PIRATE (phase improvement) and BUCCANEER (automatic chain tracing)
- [http://www.ysbl.york.ac.uk/~cowtan](http://www.ysbl.york.ac.uk/~cowtan)
CCP4 Version 5.0: Acknowledgements

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• Pryank Patel
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