

CCP4 WG1 Meeting January 2015 Minutes

Present: Dave Brown (Kent, Chair), Arnaud Basle (Newcastle), Ben Bax (GSK), Katherine Brown (Cambridge), Randy Cambridge (Cambridge), Atlanta Cook (Edinburgh), Kevin Cowtan (York), Judit Debreczeni (AZ), Eleanor Dodson (York), Phil Evans LMB (Cambridge), Ralf Flaig (Diamond), Vilmos Fulop (Warwick), Elspeth Garman (Oxford), Stephen Graham (Cambridge), Mike Hough (Essex), Nick Keep (Birkbeck), Eugene Krissinel (CCP4), Dave Lawson (John Innes Centre), Ed Lowe (Oxford), Peter Moody Leicester), Garib Murshudov (LMB Cambridge), Arwen Pearson (Hamburg), Steve Prince (Manchester), Andrew Purkiss (CRUK/LRI), Daniel Rigden (Liverpool), Pierre Rizkallah (Cardiff), Paula Salgado (Newcastle), Ivo Tews (Southampton), Johan Turkenburg (York), Frank von Delft (Diamond), Martin Walsh (Diamond), Keith Wilson (York), Martyn Winn (Daresbury).

1. Chair's report. DB.

Thanks to Airlie and Thomas for organising SW2015. Core team and ccp4 staff for distribution, bug fixes etc. KW and MN for all their work in running CCP4 and i2. Thanks to non-CCP4 funded developers for continuing hard work.

2. Finance. KW and CB.

Finance report circulated. Most posts assumed to continue. CCP4 contribution to PIMS will be terminated. Currently have a surplus of £500K. CB: over the next 3-year period we could fund an additional 5 man years, to be steered towards non-grant fundable activities. £90k spending on workshops. SW £130k outgoings, £60k income, 391 attendees. Hardware expenditure minimal. Project reports for CCP4 funded posts will be circulated at Cosener's. One saving going forwards for SW is that there will no longer be hard copies of the proceedings, but they will be open access. The cost of this shot up to £36K. Reversed post meeting due to lower offer.

3. CCP4 BBSRC/MRC grant 04/2014-2019. DB

Positions filled: Two positions requested in the grant have been already filled, the remaining three start in April 2015 with identified candidates.

Future remit of CCP4. Discussion about whether we need have more bioinformatics/construct design developed or integrated into the suite.

- Should CCP4 be looking pre crystal (molecular biology, bioinformatics) and/or post crystal (validation, deposition, added value).
- Steve: something for construct design would be very useful - Oxford has some nice tools for construct design linked to PIMS that were never rolled out.
- Garib expresses concerns that we might become too disperse.
- DB: do we develop this or look for tools that we can link into CCP4. Judit/FvD: there are already tools for a lot of this that we could just link in. Randy: we should talk to EBI.
- Eleanor: by having to leave CCP4 for bioinformatics we lose that information in the experiment data base run by CCP4. i2 is keeping a proper report of the experiment, and it would be good to get external programme information linked into it.
- Eugene talked about the EBI deposition tool, comments that the useful fields for us in the cheminformatics/ligand sides for us were not being included.
- Ben Bax: the validation tool from PDB is still not picking up incorrect ligand structures (especially the density fit part of things). PDB were discussing something like a ligand wiki - keeping crystallographic restraints in the PDB deposition. Garib: thinks this is something ccp4 should take the lead on.

General feeling that there is support from WG1 to extend the ccp4 remit, but not by reinventing existing wheels.

Action: RR to talk to GK Deposition tool being developed with EBI. Ligand validation at the PDB a problem. WG1 suggest look for existing tools.

4. i2. KSW and DB

- There are now steering groups that report directly back to Exec on a quarterly basis for key projects, currently i2 and ligands.
- Not in a position to roll out i2 in 2014. Lots of work at York, Newcastle.
- i2 is in the 6.4.5 release and available to friendly testers. Will very soon be made available to be tested by the wider community. Testing and further release will be coordinated with WG2.
- CCP4 Annual Review meeting at Cosener's will focus on GUI2.
- A new 3-year post has been assigned to the core team to work on i2. Second 2-year position for development of a GUI interface to DIALS.

5. WG2 and SW 2016 topic. Ivo Tews

Ivo has done a great job at rejuvenating WG2, with new remit and improved attendance, plus improvements on the website. Plan user interaction and outreach, workshops and study weekends. Next meeting 28th Jan. All welcome.

2016 SW will be at about the same time and probably in Nottingham. Topics proposed.

- Phasing/extremes of resolution
- Crystal to structure
- Bioinformatics (linking in with people with useful software)
- Ligands (chemoinformatics).
- Complexes

IT: Crystal to structure is timely with i2, as is a session on ligands. GK/FvD: Ligands is more timely. WG2 to make final decision.

Could bioinformatics and ligands be linked in one meeting? Garib: no - both topics too big. Judit: ligands would be a good meeting to highlight the developments in ligands. KW: could this be part of "from crystal to structure". Ben Bax suggests "crystals to liganded structures". KW: an overview meeting gives us a route to get current CCP4 literature updated in the proceedings. DB: quite likes idea of "crystal to liganded structure". Eleanor: should there be a forum for getting all the other tool users to come and talk to us and to each other. DB: this should be a separate meeting. Peter Moody: you could do "gene to liganded structure" to give a taster for bioinformatics. Garib: CCP4SW should be crystallography focused.

Summary: Ivo: very pro "from crystal to structure" to link to the roll out of i2, with a ligand session. Garib very strongly for ligands. FvD suggests a session on i2 in a liganded focus meeting.

Infrastructure: implemented a new management structure, i2 additional project and ligands additional project. Short reports will be provided at CCP4dev and lunchtime bytes at the SW are a key possibility to get information on the developments in the package. Lunchtime bytes are reformatted. Looking for feedback on whether the new format works to Keith.

6. Elections

No elections required this year for Exec. All people in post with running terms.

7. Infrastructure

Management structure formalised. Minutes now on the web, including Chair's report.

8. AOB

None.