

CCP4 WG1 Meeting 9th January 2016

Apologies – Kevin Cowtan, Keith Wilson, Ivo Tews

1. Minutes of last meeting – have been on website.

Accept – Prop DB, seconded EG, agreed, no objections

2. Thanks (DB)

Thanks to Judit and Paul for organising this year's CCP4 SW, excellent speaker list and an oversubscribed meeting (405 attendees).

3. Finance (CB/DB)

Finance is going to plan, spending down as planned and bringing our reserves down to a level that is commensurate with our income. We have used our reserves to recruit new strategic posts.

License fee: Proposal to increase to £10,500k (first increase for 7 years).

Proposed DB, Seconded Kate Brown, agreed, no objections

4. CCP4 grant 04/2014-02/2019

Updates from the WP leaders on the grant. All WPs have now started. See attached slides for summary reports.

- WP0 –STFC also running its own cloud computing initiative. So have taken advantage of this to make things more efficient.
- WP1 – assembling an annotated archive/database of test datasets that will be available to the wider methods development community. Will also be approaching users for datasets to go into the archive. Agreement to use the WG1 list request datasets.
- WG2 – Quark in place of Rosetta has made a big difference to how easy it is to run/install Ample. No licensing issues for industrial users with Quark. MN asks if there are IP issues (linked to sequences being released to an external server). DB says this is something the industrialists work out for themselves.
- WP3 now starting (as scheduled) and on track
- WP4 on track

5. i2 (MN)

i2 now in good shape, all essential modules in place. Now included in the CCP4 7.0 release that has just come out.

Show of hands ~ 50% of people in the room have used i2.

ED – suggests that a link to the bug reporting reporting be made clear – include this in the minutes. There is a bug reporter in the GUI – please use!

6. WG2 – SW2017 (Phil in place of Ivo)

Ivo's been doing a great job stimulating WG2 activities and workshops. These have been useful (DIALS, i2 demos etc.). Request to WG1 to please interact with WG2.

Paul & Garib have been running a ligands group to promote development in this area.

Please contact Ivo, Paul/Garib if you or your group would like to be involved in any of these activities.

SW2017 topic – proposed from Exec is “From Crystals to Structures” linked to i2 release – proceedings will include the i2 publications and provide an enhanced user manual. Haven't had a “from crystals to structures” for 5 years so it's timely. Suggestion for 2018 to have a focus on multi-crystal approach to solving structure (linked to maturation of grant WPs).

Full support from WG1 for “From Crystals to Structures”.

Keith Wilson has offered to be one of the organisers for that. If anyone else is interested in co-organising SW2017, please email Dave Brown and Keith Wilson to express interest.

7. Executive Elections

FvD stepping down this year. 4 people (EG, AP, IT and BB) due to step down next year so would like to recruit two additional this year to ensure continuity.

David Brown nominates Roberto Steiner – unanimously supported

Arwen Pearson nominates Paula Salgado – unanimously supported

8. AOB

MN: Research Fish for the grant starts in February – so WP leaders should be prepared for reporting/papers etc.

EG: Thanks to DB for his continuing service as Chair

In attendance:

Who	Where
Dave Brown	U of Kent
Martin Noble	Newcastle U
Phil Evans	MRC LMB
Ed Lowe	Oxford
Simon Newstead	Oxford
Paula Salgado	Newcastle U
Ehmke Pohl	Durham
Vilmos Fulop	Warwick
Elsbeth Garman	Oxford
Katy Brown	Cambridge

Arnaud Basle	Newcastle U
Johan Turkenburg	York
Daniel Rigden	Liverpool
Dave Lawson	John Innes
Gwyndaf Evans	Diamond
Thomas Sorensen	Diamond
Pierre Rizkallah	Cardiff
Svetlana Antonyuk	Liverpool
Garib Murshudov	MRC-LMB
Eleanor Dodson	York
Jennifer Littlechild	Exeter
Ben Bax	GSK
Alun Coker	UCL
Judit Debreczeni	Astra Zeneca
Eugene Krissnel	CCP4
Frank von Delft	Oxford/Diamond
Arwen Pearson	Hamburg