

**Almost at the end ...**

***“If you don’t remember anything else,  
remember this”***

## **CCP4 and wwPDB have booths in the exhibition area**

- Please come and visit for software demos, questions, freebies
- Opportunities to talk to the people at the workshop

## **Follow-up for this workshop**

- Please fill in and return the questionnaires in the CCP4 packs
- If you have anything missing from the packs or want copies of the slides please let us know
- Materials will be posted on the web shortly after the conference

# Take home points from Peter's talk (CCP4 overview)

- Binary installations good for fast start up
- Add project, crystal and dataset information in MTZ and switch on data harvesting
- Use CCP4i project management tools to help organise your work

# Take home points from Martin Noble's talk (CCP4 for PX)

- CCP4 offers “cradle to grave” coverage of structure determination process
  - Some areas stronger than others ...
  - Well-integrated with other (non-CCP4) software
  - Easy to switch back and forth
- CCP4i makes it easy to work quickly on multiple projects
- Lots of good stuff still to come
  - Molecular graphics, Phaser, Pirate, BP3 ...

# Take home points from Gwyndaf's talk (using MOSFLM and SCALA)

- Collect the best data possible (no software can rescue bad data)
- Check logfile output and graphs for indications of things going wrong (and advice on how to fix)
  - look for sudden deviations from smoothly-varying behaviours
  - programs offer ways to correct for many of these
- Run SCALA immediately after MOSFLM
  - ideally during data collection

# My take home points from Martyn Winn's talk (REFMAC5 and TLS)

- It's always worth trying TLS (nothing to lose)
  - only adds 20 extra parameters per group
  - often works better for low/medium resolution data
- It's worth experimenting with assignment of TLS groups
  - analysis tools can help optimise
- Analysis of TLS parameters may suggest biologically significant protein motions

# Take home points from Liz's talk (CCP4 Molecular Graphics)

- Structure/map viewer with CCP4 look-and-feel
- Easy menu-driven way of creating complex diagrams
  - review structure (surfaces, accessible surfaces...)
  - superposition of structures
  - electron density maps ...
- See <http://www.ysbl.york.ac.uk/~ccp4mg>
- *It's also going to be in next CCP4 release*

# Take home points from Paul's talk (Coot)

- Coot: a powerful integrated system for building/refinement and validation (in development)
- Remember the “A” key when Real Space Refining
- *It's also in the next release of CCP4*



# Take home points from Kyle's talk (Validation and Deposition)

- Validate
- Validate ...
- Validate!
- Remember to keep talking!
  - *depositors and annotators are on the same side*

# And finally ...

- Thanks to the speakers
- Thanks to Claudio for dealing with A/V
- Thanks to the organisers
- Thanks to you for coming
  - please return your questionnaires
- **And ... please come and visit the CCP4 and wwPDB booths in the exhibition!**