

## Practical course

# CcpNMR Analysis: Macromolecular NMR assignment

*University of Queensland, Brisbane, Qld, Fri 12 & Sat 13 December 2008*

Dear Colleagues and NMR Afficionados,

We are pleased to announce a practical course into "CcpNMR Analysis: Macromolecular NMR assignment" to be held at the University of Queensland, Brisbane, from 12-13 December 2008, immediately after the ANZMAG 2008 conference.

CcpNMR analysis is a leading new program for the analysis and interpretation of multidimensional NMR spectra, developed by the Collaborative Computational Project for NMR Spectroscopy (CCPN) at the University of Cambridge, and inspired partly by the programs ANSIG and Sparky. Analysis runs under Linux, Unix, and MacOSX, with a preliminary Windows version available. CcpNMR Analysis includes a completely new graphical user interface, support for automatic assignment, Python as a scripting and macro language, and a number of features similar to Sparky.

We are pleased to welcome Tim Stevens, one of the head developers, for a two-day course on CcpNMR Analysis, version 2. The course is split into two days, covering basic and more advanced topics. Course participants can elect if they want to attend either or both days. The course will be held hands-on in a computer lab at the University of Queensland.

## Course Outline

<u>Day 1 - Introduction &amp; Basics:</u>	<u>Day 2 - Advanced Topics:</u>
<ul style="list-style-type: none"><li>• Loading spectra</li><li>• Peak picking</li><li>• Entering residue sequences</li><li>• Navigating in windows</li><li>• Resonances &amp; basic assignment</li><li>• Working with variable chemical shifts</li><li>• Protein backbone assignment</li><li>• Protein side chain assignment</li><li>• Making distance constraints</li><li>• Structures and violations</li><li>• NOE assignment/refinement</li><li>• Assignment quality control</li></ul>	<ul style="list-style-type: none"><li>• Titrations - following chemical shifts</li><li>• Relaxation rates</li><li>• Scalar and dipolar couplings</li><li>• Entering non-standard molecules</li><li>• Isotope labeling schemes</li><li>• Dihedral constraints</li><li>• Writing Python "macro" scripts (can do this to different levels)</li><li>• Interfacing with CYANA and ARIA2</li><li>• PRODECOMP</li></ul>

## Fees

As ANZMAG and the CCPN project will sponsor Tim Steven's visit, there is no registration fee, but you will have to pay for accommodation at St John's College (see below).

## Accommodation

We have arranged accommodation for course participants at St John's College. The college charges \$67.70 per person and day/night for breakfast and dinner for single-room college accommodation. Lunches will be held on campus (not included in accommodation charge). Accommodation is available Thursday and Friday night for people attending the ANZMAG conference. Course participants not attending the ANZMAG conference can arrive on Friday morning in time for the CCPN course. For participants living in Brisbane, there is the option of staying off-site.

The course will start on Friday morning (9:30 am) and end Saturday evening. Accommodation for an additional night after the course can be arranged upon request for participants wishing to fly out on Sunday morning instead of Saturday evening (\$58.20 for bed & breakfast or \$67.70 for dinner, bed & breakfast).

## Registration

PhD students, post-docs, or anyone with basic knowledge of biomolecular NMR and an interest in learning CcpNMR is encouraged to attend. Please send registration requests by e-mail to: [h.schirra@uq.edu.au](mailto:h.schirra@uq.edu.au)

**Please indicate which days you are attending and if you need accommodation for Saturday night.**

Deadline for registrations: 31 October 2008. Registrations after this date can be considered only if spaces are still available.

**We hope to see you all in Brisbane!**  
*Horst Joachim Schirra*