

Administrative Contact

SPECTRa Workshop
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The **SPECTRa** Workshop

*Capture of Primary Chemistry
Research Data
in Digital Repositories*

Supported by funding from the
Joint Information Systems Committee

JISC



Cambridge UK
September 2008

<http://www.lib.cam.ac.uk/spectra/>

Where and When

The **SPECTRa** tools workshop will be held in the teaching laboratory at the Unilever Centre, Department of Chemistry, Cambridge University, UK. It will be led by Peter Murray-Rust and Jim Downing.

There is a registration fee of £100 for the two-day course (18-19 September 2008) to include 2 nights accommodation, workshop dinner and refreshments. Attendees will have to arrange and pay for their own travel.

There will be a limit of 20 attendees.

Who should come

This workshop is aimed at chemists, crystallographers, developers and research managers who want to set up digital repositories at a departmental level in order to capture, preserve and enable re-use of their primary research data.

Institutional departments would optimally be represented in pairs (e.g. chemist or crystallographer and support developer) to get maximum value from the presentations.

What you will get out of the workshop

- Sustainable methods for data preservation and re-use
- Well-engineered, distributable, repository-agnostic components
- Presentations from leading figures in digital curation and publication of supplementary data

What you will be doing

- Download and install SPECTRa software from SourceForge
- Review file formats and convert to CML:
 - General NMR spectroscopic data (JCAMP-DX; MDL molfiles)*
 - Small molecule crystallography (CIF)*
 - Computational Chemistry (Equilibrium geometry GAUSSIAN calcs.)*
- Use search (metadata/substructure) & display (2D/3D structure) tools
- Application to: thesis/publication authoring; dynamic web page update

Registration

First Name	
Surname	
Position / job title	
Institution	
Address	
Country	
email	

*Payment by Sterling cheque for £100 included.
Please make payable to 'University of Cambridge'.*

Please invoice me for £100

***Payment to be received by 20th.August 2008
We will confirm your place on receipt of payment***

Please note:

- We are unable to accept payment by debit/credit card
- Full fee will be charged for cancellations notified after 20th.August
- On-site parking is not available at the Chemistry Department