



Chemical Database Service

Management Advisory Panel Meeting

Minutes of the meeting held on the 20th December 2004 at Daresbury Laboratory

Present:

Dr. A.J.(Sandy) Blake (Nottingham)
Dr. Kathy A. Johnson (Liverpool)
Dr. Nick Greeves (Liverpool)
Prof. Martyn F. Guest (DL)
Prof. Rod E. Hubbard (Chairman) (York and Vernalis)
David. Osa-Edoh (CDS)
Dr. (Bob) R.F. McMeeking (CDS)
Dr. Don Parkin (Secretary) (CDS)
Dr. David A. Fletcher (CDS)
Dr. Wendy A. Warr (Wendy Warr & Associates)
Dr. Jeremy Frey (Southampton)
Dr. William (Bill) G. Town (Kilmorie Consultants)
Dr. Mark J. Biggs (Edinburgh)
Prof. Chick C. Wilson (Glasgow)

Apologies for absence were received from:

Dr. Carmine Ruggiero (EPSRC)
Dr. Andy Whiting (Durham)

The meeting started with an introduction by each person present, as four members were new to the panel.

1. [Minutes of Previous Meeting \(held on 30th March 2004\)](#)

The minutes previously circulated, were agreed to be an accurate record of the previous meeting.

1.1 Matters arising – most issues would be covered by agenda items. It was agreed to review and identify any actions outstanding at the end of the meeting

2. **New Membership Switch Over**

RFM started by presenting an overview of CDS which included the funding cycle (3 years – 1st April 2004 to 31st March 2007) with a review after one year. (There was some discussion on the EPSRC Review at this stage – see Agenda Item 4)

A slide showed the MAP members (old and new) of which four were due to retire from the MAP, namely Sandy Blake, Kathy Johnson, Wendy Warr and Andy Whiting.

The new Terms of Reference for the Map (as shown in 'Material relating to Agenda Item 4') now state

The composition of the MAP will be based on the following criteria:

- a) MAP membership should be for a fixed three year term.
- b) New MAP members to be chosen in consultation with EPSRC.
- c) MAP to have at least one member from industry.
- d) MAP to have a member from the UK academic library community
- e) MAP to include no more than one member from any single institution.

It was noted that there was not a UK academic librarian present on the panel. After an extensive discussion of possible candidates [Linda Humphreys (Bristol), Joanne Yoemans (Leeds), Denise Harrison (Sheffield), Dinah Northall (Nottingham) and Fred Friend (UCL)], it was agreed that none were appropriate for the CDS MAP. Increasingly, the responsibility for coordinating access to chemical information has been devolved to Departments. NG has such a role at Liverpool. The MAP therefore suggest that Terms of Reference d) is modified to be:

d). MAP to have at least one member who coordinates chemical information provision at a major UK university.

During the discussion, it was suggested that somebody from JISC (Dr. Alan Robiette - Programme Director, Authentication and Security, John Blundell-Ellis or with a biological background (Philip Judson) should be considered.

3. CDS Road Show Update

DAF showed statistics related to the road shows that have taken place. 18 Visits have taken place so far, mainly in October and November, with 283 registrations resulting from the visits. The figures showed a substantial increase in the number of registrations, with some departments more than doubling in the number of users. These figures can be used to support progress towards meeting EPSRC's criteria (see Agenda item 6).

Although the sheet showed which department was visited, it did not show how many from different department turned up at the stand or the lecture (a later remark suggested displaying only the University and not the department). MJB therefore suggested that a short questionnaire be handed out at the lecture. AJB asked about feedback and suggested sending a questionnaire to newly registered users. It would also be useful to know if potential users are using some other service instead.

JF stated that User Representatives were crucial and should help to provide user feedback. It was suggested that CDS should check how active the Rep. is and get the 'department' to sign up.

The MAP congratulated the CDS team on this successful run of road shows and recognise that these events take a considerable amount of time and effort to organise and execute. CDS are encouraged to review the comments made by MAP and the experiences of the first set of visits and consider whether it is possible to improve the format for the visits, and incorporate a useful level of feedback through questionnaires etc.

The number of registrants for the service is one measure of the success of the service. However, CDS should consider how to assess what proportion of possible users this represents and also what kind of measure would demonstrate extended usage of the service.

4. Recent EPSRC Review (2004 Renewal Report and Cross-Service Review)

The review gave CDS an overall amber grade (performing well, but with a few minor issues). Publicity was given a red grade but with the acknowledgement that *the service was making great efforts to engage with the community through a new visit schedule*. The cross-service review was just a 'light touch' this time but will be a full review next time. The review of the service will probably coincide with this cross-service review, which should happen around May 2005. An annual report would be needed by this time (which should be more of a grant application rather than a review of the year). The research highlights from previous reports were commended.

WW wondered if there was a PR problem or just one of perception – for instance that the service was skewed towards crystallography. She suggested that CDS should be promoting use of the data rather than promoting helping people.

The review stated that the Service was still primarily used by crystallographers though DP disagreed with this, stating that around 50% of the active users accessed Organic or Spectroscopy databases. Therefore use outside of Crystallography must be demonstrated more.

JF suggested that the web site should be updated as often as possible so that people would keep looking at the 'What's New' section (drip feed) with removal of stale items quickly. NG said he would like to see a button or more prominent information on the home page for 'Latest News'.

5. E-Science – Development and Involvement with CCLRC E-Science Centre

DP gave a short review of the interactions of CDS with the e-science centre at Daresbury such as 'web services' and linking / harvesting data. JF explained more about linking to other data like CrystalGrid and how this would be seen as a good thing. The data holders would be willing as they could say 'we link our data through CDS' – which would also raise the profile.

CDS should engage with the current set of e-science projects to explore whether the service is an appropriate outlet for deploying data and systems developed through e-science projects, possibly in collaboration with other data services.

If an appropriate set of products from the e-science projects can be identified, then the service should explore whether there are e-science translational funds available.

With some caution, the service should also explore whether the e-science initiatives could provide additional recognition and opportunities for the service in coordinating research and development of novel methods for deploying chemical information services through the GRID.

6. Progress Towards Meeting Criteria Fixed for April 2005 Review

The discussions centred on the Executive summary of the full panel report issued on 23rd September 2003. Item xi. of that report recommended a review one year into the grant. CR has confirmed the review will be in (late) May 2005.

The report identified a number of issues that had to be addressed. If not satisfied, the Review panel will have the option of closing the current CDS one year before the end of the grant and putting the service out to tender.

The issues are (item numbering refers to panel report):

iv. - Concern that staff are not totally suited to current and potential future needs of the service.

Staff must demonstrate that they have the required (new) skills to carry forward the mission of the CDS. MAP considers this is a communication issue. It is clear that the roadshow programme, the interactions on e-science and initiatives in new areas (Detherm) demonstrate that a breadth and depth of experience is required.

iii. and vii. - Lack of awareness, low use in certain areas and restriction of feedback.

The CDS has begun to address this through the series of roadshows and the iterative assessment of their effectiveness and feedback mechanisms. It will be important for CDS to gather whatever quantitative evidence it can on the extent and effectiveness of uptake of the service in the chemical community. It is considered unrealistic to have a comprehensive survey. Instead, CDS should focus on 2-3 major universities and carry out an in-depth analysis. This should include an analysis of who should be using chemical information services (both numbers, departments, disciplines), how many are, where they are getting the services from and what additional services are required.

WW suggested interaction with organisations in the chemistry/biology area such as the RSC Chemical Biology Forum and the Pro-Bio Faraday Partnership [DARTS is a member and CDS has links from the Pro-Bio site (<http://www.pro-bio-faraday.com/links.htm>)]

To raise the awareness of the service an article should be written for a periodical such as the RSC's Chemistry World, EPSRC's Connect, Scientific Computing World and The Chemical Engineer. As the review is in May, the article should be done as soon as possible, preferably with the help of a publicity/scientific writer.

The use by other departments such as chemical engineering (especially since the introduction of Detherm) could be used to show awareness in other areas.

Although citations could be used to show awareness, not all users cite the service in their publications. It was suggested that a questionnaire be sent to users asking 'how many papers have you published in the last 5 years that have made use of CDS'. The answers should be restricted to groups like 1-5, 6-10 etc.

A count should also be made of how many links there were from web sites to CDS. Users should be encouraged to add a link from their own home page – an icon could be produced for users to download with the appropriate link to CDS home page.

7. DETERM Update

It was noted that the service has been upgraded with a new PC client (version 2). MJB offered to help publicise the database.

8. Accelrys Trial

DP showed results of the recent trial of databases from Accelrys (Failed Reactions, Bioster and Metabolism) in terms of accesses (web vs client) and users followed by the questionnaire. Although not many replies were received, most were very favourable.

MAP felt that the low response was probably because these databases are for different groups of scientists. The failed reactions database would be of most value to synthetic organic chemists, whereas the other two would be of most value to the pharmacology / medicinal chemistry communities. The discussion highlighted that this was a high priority area for extending the take up of CDS. First, the types of databases of most value to these communities should be established. It was proposed that CDS performs a survey of suitable departments (e.g . Pharmaceutical Science) and circulates the list to WW and REH so that they could pick out a few names so that their opinion could be sought.

9. **Any Other Business**

All actions from the previous meeting of 30th Mar 2004 were either completed or covered in the agenda for this meeting.

There was a discussion on whether other databases in non-core areas should be investigated such as an adsorption database. This can be considered as part of the strategy to be proposed at the review in 2005.

List of Actions from the meeting

		<u>Action</u>
2	Future handouts to be numbered globally. EPSRC to comment on proposed change to MAP membership requirement If seemed appropriate, JISC member to be invited	RFM CR RFM
3a	Questionnaire to be produced for distribution at Road Shows to obtain feedback and an idea of which departments attended.	DAF
3b	The activity of the Rep. should be checked.	CDS
3c	Follow up new registrations with a questionnaire.	DAF/DOE
3d	Consider what metrics will demonstrate uptake / penetration of CDS amongst chemical community	???
4	Update website as often as possible. Add 'latest news' information regularly.	DP
5	Explore e-science more and develop link to other datasets.	DP
6a	Conduct in-depth study of two or three Universities	RFM
6b	Write article for periodical such as Chemistry World (identify writer).	RFM/MFG
6c	Send questionnaire to users asking about number of publication that made use of CDS in the last 5 years.	CDS
6d	Icon to be produced for users to download with the appropriate link to CDS home page. Count how many links there are from other web sites to CDS.	DP
8a	Produce list of suitable people in Bio/Pharm. area and circulate to WW and REH.	CDS
8b	Pick out a few names from above list (8a) and contact them	WW and REH

These minutes will also be available on-line at: -

<http://cds.dl.ac.uk/report/minutes-dec04.pdf>

Some of the handouts of the meeting can also be seen on-line by following the links in the minutes.