

Minutes of the meeting held on the 16th September 2005 at Daresbury Laboratory

Present:

Dr. Nick Greeves (Liverpool)
Prof. Martyn F. Guest (DL)
Prof. Rod E. Hubbard (Chairman) (York and Vernalis)
Dr. William (Bill) G. Town (Kilmorie Consultants)
Dr. Mark J. Biggs (Edinburgh)
Dr. Carmine Ruggiero (EPSRC)
Dr. (Bob) R.F. McMeeking (CDS)
Dr. Don Parkin (Secretary) (CDS)
Dr. David A. Fletcher (CDS)
David. Osa-Edoh (CDS)

Apologies for absence were received from:

Dr. Jeremy Frey (Southampton) – [sent an e-mail with comments]
Prof. Chick C. Wilson (Glasgow)

1. [Minutes of Previous Meeting \(held on 20th December 2004\)](#)

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

1.1 It was agreed to review and identify any actions outstanding at the end of the meeting

2. **EPSRC Review held May 13th-14th 2005**

CR outlined the background to the Review. In the past, there had been *ad-hoc* panels convened to review performance of the Services separately, and these may not have used the Annual Reports. Now, an annual review will be undertaken as a light touch health check (early warning system) using the Annual Report. All Services will undergo the same sort of review with grading under the various assessment criteria.

MFG expressed his concern about the ethos of the Review panel. A new panel brought together in the short term for the review would only look at the last annual report. He stated that it would be better if some of the panel remained longer for subsequent reviews to give some sort of continuity. CR said that panels would have extra 'experts' in the field and 2 to 3 members would be carried over to the next review.

The [Review Report](#) was then considered under the various graded criteria, as it would be these areas that would be examined at the next health check.

2.3 Demand

CR explained that the view was that the crystallography databases are well used by most crystallographers but that the message about the wide usage of the other databases was not coming across. In particular, it was felt that more usage by organic chemists could be obtained, especially after the Road Shows.

He stated that the Service would **not** continue if it was purely crystallography.

DP explained that the crystallography database, as a whole, were indeed the most used in terms of accesses (~3,200 accesses/month) and users (~410 unique users/month) but that the ISIS databases weren't that far behind (~2,500 accesses/month from nearly 300 users/month). Unlike the crystallography area, there were other sources of organic synthesis data available and users had to be taught that the CDS data was complementary to that in Beilstein and SciFinder Scholar.

The overall number of accesses to the ISIS databases has remained fairly static, but **the number of users has gone up**.

Re: "The overall usage appears static despite the extensive publicity effort." NG stated that this statement was not correct and not substantiated, judging by the statistics he had seen. DP showed that usage had gone up **every month** over the last year, showing an average increase in users over the previous year of 10%. A graph needs to put in the next report showing clearly the rise in usage.

RFM pointed out that usage usually lags behind publicity (e.g. from the Road Shows) as users may not find a use for the data immediately.

It was suggested that the ISIS figures be compared to Beilstein statistics. It would show not only trends but also the percentage of ISIS vs. Beilstein usage for each University and give an indication of the possible penetration of organic synthesis in Universities. It is difficult in this area to come up with the metric as to how much people should be using the databases.

DP stated that he had tried to contact MIMAS to try and get figures but had obtained no reply. Figures were available on the MIMAS web site but only registered users could obtain these figures and only for their own University (CCLRC is not registered for Beilstein).

Therefore, it was suggested that the help of user representatives be elicited to obtain the information.

2.4 Research Quality

CR said that other services now showed Research Highlights and also quite extensive Publications Lists of papers which referenced use of their services.

It was recognised by the review panel that it was difficult to obtain the true number of users who should have cited the CDS in their publications. A large fraction omit to cite the Service even though they have used the CDS. It was suggested that large users of the Service should be targeted, and their publications checked so that an estimate could be made of the number of where it would have been appropriate to cite the Service.

When they publish articles which have made significant use of the Service, users should cite a specific article (J. Chem. Inf. Comput. Sci. (1996), 36, 746-749.). DP stated a search in the WoS indicated that, in 2004, 55 articles had cited this paper and, so far, 44 articles had cited the paper in 2005. These were in quality journals with good impact factors.

There was a discussion as to what could be done to ensure that users cite the Service more. It would be nice if authors provide feedback and actually let us know if they do cite the service. CDS will soon be sending out a questionnaire which asks about citations (see 6. Online Survey). The aim should be to demonstrate that CDS has made an effort to get users to cite the Service and obtain an indication of the potential number of publications.

NG thought the figures were quite impressive, considering the above, and asked if EPSRC could provide a tick box on the Grant Report form to indicate if the grant holder had used any of the Services but CR replied that this would be difficult. EPSRC will be targeting first grant holders to recognise the Services but it is difficult for them to collect data about citations. CR recognised that we were not like some of the experimental services who could provide a carrot and stick to users as a lack of publications may stop them using the service. It would be inappropriate for CDS to use a similar stick (e.g. only those that cite the Service could continue using it!).

2.5 Management / 2.6 Performance

CR stated that the previous report was a little opaque regarding the management structure. The review panel thought the individual roles needed to be clarified, and were unclear as to whether the level of support (4 people) was appropriate. If the review panel had indeed studied the grid chart shown in Appendix 2 of the annual report, it would appear that the management structure was not displayed in the form they wanted.

It was agreed to supply a list of key roles for each individual team member along with time spent on these tasks and identify who was the lead person in various areas. A more formal structure should be presented (Director, Service Manager?) and how this relates to the Service.

Although the panel were presented with extensive performance statistics, CR thought important trends needed clearer emphasis. He believed that key statistics should be highlighted and possibly given in the main report rather than added to all the other statistics in the appendices (Key figures are demand - across the whole service – and the impact since the last renewal).

2.7 Training

It was assumed that the review panel had focused on ‘hands on’ training and not the availability of electronic material demonstrating package use, such as flash movies, on the CDS web pages. CDS should aim for 4 or 5 hands-on training sessions over the year.

DP stated that a number of the user representatives run their own training course and had been trained by CDS for this. This was probably not apparent to the panel and should be highlighted in the next Annual Report.

[CDS supply a number of exercises that can be used on these courses – see for example:- <http://cds.dl.ac.uk/cds/datasets/orgchem/isis/exercises/webexercises.html>]

More visibility of the reps. was desired (e.g. email all internal users that they are the rep.)

2.8 Publicity

NG asked if more laptops could be taken to Road Shows to give a more interactive element. CDS replied that normally two laptops are taken along which are used for demonstrations and registrations but often it is very difficult to obtain an internet connection.

Usage figures should be shown that indicate the impact of the Road Shows.

It was stated that this could be difficult as a lot of users do not use the service straight away but wait until they need to use it – which could be several months. A follow up survey of the newly registered users in January 2005 showed about two thirds had not used the databases but this was mainly due to lack of time and they had not got around to it yet! (see Appendix 7 of the Annual Report).

Questionnaires handed out at the Road Shows indicated that the visits were helpful (32% very helpful) and would increase their use of the Service (34% probably, 47% yes).

DOE asked if the reduced number of Road Shows planned for this year would be an issue, as it is less than the previous year, but the amount is OK when teamed with possible training courses. Other departments have been targeted more in the next year (see section 5)

The overall conclusion is that this set of criteria used in the Review Report should be used as a template for the next Annual Report.

It was not considered appropriate that we produce a formal response.

3. Future Refunding Schedule

CR explained that, in the past, reviews had been conducted by *ad hoc* panels for individual services with little or no overview of the services as a whole. This has been replaced by a combined panel that will convene and review all services (including routine “health checks” and funding renewals). In the future the format will be the same (over two days), but there will be more expertise on the panel and a greater breadth (increase in the number of panel members).

The review date means that there is an issue with synchronisation (CDS funding is out of sync with other services). If the health check gives a thumbs-up in May 2006 then the Service will go out to tender in May 2007 and CDS will receive bridging funding up to November 2007 while the tender is resolved. Two (maximum) proposals would be considered in May 2007.

The health check in May 2006 will be in the form of a case made for “Do we need a Service”.

This caused quite a bit of discussion as to who should put the case for a Service. There were concerns that even if there was a need for the Service, the case may not be made well by the appropriate person(s). Should the case be made by the funding agency, the provider/stake holder or by the users? If a vision document was produced by CDS, would it be the same vision as EPSRC?

CDS should not be the driver but, along with users, should provide the steer. A vision document should be sent to the panel and any input from users should first be seen by Daresbury so that they can add comments.

NG/MJB enquired about the input from the chemical engineering area and how much, if any comes out of the Chem. Eng. programme, and should they be involved? CR replied that he couldn't go to another programme and ask for funding as this is a ‘chemistry’ national service. However they would support chemistry at the interface.

CR was asked if the report should contain recommendations on the size of the group and the budget but he suggested that the wording should be perhaps more like the ‘level of is appropriate’.

It was agreed that one, coherent (vision) document should be available before the May 2006 meeting. There will be consultations with the MAP in producing this – interactions should be off-line and electronic rather than via physical meetings.

4. Format for Future Annual Reports

The various set of graded criteria, already discussed above, should be used as a template for the format of future Annual Reports.

5. CDS outreach for 2005/6

a) Bioscience Contacts

DOE outlined the outreach effort with regard to biosciences departments – more to gain information rather than give Road Shows. Librarians seem to be good contacts.

MJB pointed out that not all bioscience departments were the same, much like Chem. Eng. departments where Detherm wouldn't be of used much.

CDS should be supporting chemistry at the interface with the present set of databases, not trying to find extra biosciences data.

It was suggested that CDS should investigate which 'Chemical Biology' departments exist and what is being funded. CDS should also look at other initiatives such as Selective Chemical Intervention in Biological Systems (SCIBS) from the BBSRC.

Recommendations for outreach to biosciences departments should be available by the end of March 2006.

b) DETHERM letter to department heads, etc.

A letter had been drafted by MJB and was presented to the MAP. It included an image of a Detherm poster available for download.

c) Promoting non-crystallographic aspects of Service and d) Training courses

This will take the form of hands-on training for the ISIS databases and could involve training the trainers (user representatives or a more appropriate local person). Training should be done by April/May so that the trainers are ready for the new intake in October.

6. Online Survey planned for Sept/Oct 2005

The proposed questionnaire for the planned survey was shown to the MAP. The panel agreed that the number of questions was appropriately short but it was suggested that the first two questions regarding citations should be put at the end. A preamble about the importance of citing the Service should be added.

It was also suggested that SCOPUS be added to the list of other chemical information sources that people may use (question 4).

WGT asked about how the survey would be promoted to which the reply was via email to all users and via the web site.

7. The CDS Website

DP outlined that a new design with different content was being prepared. The original 4 areas would be split into 5 areas to match the exhibition material and talks. 'Dead wood' such as information about old packages like ELYS or PLUTO would also be removed.

It was stressed that the new site should either be ready by the beginning of the new academic year, so that road shows could point to it, or at a point where a switch over isn't so noticeable, such as over the Christmas/New Year break. If the site was available as a trial then it should be circulated to MAP members to try out.

8. SciFinder Scholar and other major external packages

DP had discussions with Dr. Barry Dunne, the CAS Marketing Manager for the UK. He was keen to look into a deal for the UK (CDS could not host the data). Hopefully, the UK community would get a cheaper deal per seat (increased number of seats) and the CDS could act as a help service and possibly give training courses. NG said that this role may not look like much but it would be extremely valuable to the academic community and also help promote CDS. It would be expected that each Institution would pay for seats but these would be at a reduced cost compared to the present cost (cheaper deal per seat, increased number of seats). This cost should be set against what the EPSRC already makes by indirect contributions to such licences via items within funding grants.

A meeting should be put together involving representatives from CAS, EPSRC, JISC and CDS.

9. E-science related developments

DAF outlined the developments of a Molecule Database which would integrate all our present databases and provide a common front end. It would promote the whole range of the databases as a search for a structure may point to other data available in the other databases that the user hadn't considered. The Molecule Database may include structures as InChI files. A bid for funding is also underway which involves incorporating Shibboleth into the project as the means of authentication.

CR was concerned about the amount of time this would take up but DAF replied that we should be doing more as CDS should not remain static and this will be an added feature to CDS, making it easier to use and ultimately benefit the community (cf. CrystalWeb). The database could also be extended by pointing to external data held in archives at Institutes as more and more archives are being set up (such as eMinerals and CrystalGrid).

The work is being scoped out at present and CDS are collaborating with people from IBM, hopefully leading to a proof of concept soon. This would then give an indication of how much work it would involve.

10. Any Other Business

Actions from the previous meeting of 20th December 2004 were considered. The following have been completed or covered in the agenda of this meeting, with the rest ongoing.

2. New members of the MAP were considered such as a member from JISC and another synthetic organic chemist or from the biosciences (REH could be considered to represent this area). A larger MAP membership would also mean that potentially more people could be present at meetings. A list of the MAP membership with length of tenure should be available for the next meeting.

3a., b., and c. Results of questionnaires distributed at Road Shows and for new users are available in Appendix 7 and 8 of the Annual Report (see 2.2.8). The questionnaires were of some use but were not telling us anything that was unexpected. DP reported that around half of the reps. were also active users of the Service. However, reps should be made more visible (see 2.2.7).

3d. Someone needs to be tasked with this important issue and come up with some justifiable numbers.

4. 'Latest news' on the web site had been automated such that, as soon as the new information is entered in the News section, an entry appears in the latest news section, which then points to this new information.

5. Links with e-science have been established and two members are included in the IBM collaboration concerning the Molecule Database.

6b. RFM has written a letter to Chemistry World (no response yet). NG suggested writing a letter in the form of a plea to users to acknowledge the Service and MJB suggested a chemical engineer could write an article for The Chemical Engineer. A list of top Detherm users should be made available to MJB so that he can then ask one of them to write the article.

6d. An icon had been produced (available on the Links page) for linking to CDS (favicon.ico, which is downloaded when you bookmark the home page and then appears in your favourites list, has been available for some time)

8a, b. This was considered as part of new MAP membership.

The next meeting (Physical or virtual?) should be in 6 months time (mid March 2006).

List of Actions from the meeting

	<u>Action</u>
1	Future handouts to be numbered globally. RFM
2	Beilstein access figures to be obtained from either MIMAS or via user reps. DP
3	Large users of the Service to be approached to obtain: CDS (a) an idea of the percentage of publications that could have cited the Service but didn't. (b) an estimate of the potential user base and CDS take-up (c) a strategy for increasing usage of the service by synthetic organic chemists If current 5* departments are not large users – find mechanism for understanding their needs and how to recruit as major users
4	A list of key roles for each individual CDS team member to be produced. CDS
5	A list of 4 or 5 sites for hands-on training to be produced. DP User reps to be encouraged to email all internal users at the start of the academic year so that they are known to them. DP CDS Training exercises to be sent to REH for him to try out. DP
6	Usage figures to be produced to show the impact of the Road Shows. DP/DAF
7	EPSRC to decide who produces the case for database services for May 2006 review CR If CDS, then first draft by March 2006 to be discussed by MAP RFM/MFG
8	Investigate which 'Chemical Biology' departments exist and what is being funded. Look at SCIBS. CDS
9	Send Detherm letter to department heads. RFM Send list of top Detherm users to MJB to pick out someone who could write an article in The Chemical Engineer. DP/MJB
10	Identify trainers at various Universities and check they can be used for training courses. CDS
11	Replace old web site with new one either before start of the academic year or at start of New Year (2006). DP/DAF
12	Meeting to be organised between CAS and interested parties (EPSRC, JISC etc.) CR
13	List of MAP members and terms to be available at next meeting. RFM Possible new members (JISC, organic chemist) to be identified. RFM

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

http://cds.dl.ac.uk/map/MinutesMAP_Sep05.pdf

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