

*Minutes of the Medicinal Chemistry Section
Division of Chemistry and Human Health
San Francisco
March 25, 2000*

Meeting Attendees: Drs. N. Koga, C.R. Ganellin, T.J. Perun, C.G. Wermuth, A. Monge, M. Chorghade, P. Lindberg, D. Maclean, J.G. Topliss, P.W. Erhardt, B.K. Trivedi, J.K. Seydel.

Apologies for Absence received from E. Breuer, J. Fischer, G. Gaviraghi, M.K Gurjar, O. Kebir, T. Kobayashi, E. Kyburz, L. Mitscher.

Opening Remarks and the Minutes of the Berlin Meeting: Robin opened the meeting by introducing everyone. Minutes were reviewed. Per commented on a request for financial assistance for travel to attend these committee meetings for someone from academia. The procedure should be to contact Linda Tapp at North Carolina for funding request, and it will be forwarded to Camille for his approval.

Chemistry and Human Health Division Report:

Camille commented on the meeting of the Evaluation Committee in Frankfurt. This group needs to determine the value of new projects when completed. Newly proposed projects will be reviewed by external reviewers for approval. Image of IUPAC needs to be considered in these projects. Companies have stopped funding IUPAC in France since they do not know what is happening within IUPAC that concerns their interest. Camille commented that the name IUPAC should be clearly indicated on projects eg IUPAC Handbook of Pharmaceutical Salts. We should also aim to implement projects with worldwide implications, and utility within the Industrial sector.

A question was asked if IUPAC has chosen a publisher yet? No- we can publish with any publisher we deem appropriate. John Jost signs a contract with the publisher so we need to contact him first. List of possible projects, prepared by Camille after the Berlin meeting, was shared and discussed. We have to submit new projects and create new task forces. Funding is now available to support such activities.

It was mentioned that including the IUPAC name for the book is an excellent idea.

Paul Erhardt brought up the issue with Blackwell publishing that they are not advertizing properly the Drug Metabolism Book. It was agreed that Paul would contact John Jost to discuss this issue, and advertise on his own.

3.0 Section Membership: We welcomed Dr Jo Seydel who is replacing Dr Engel as the National Representative from Germany.

Robin had been unable to make contact with the Associate Member from Russia; Camille suggested – Contact Russian Academy of Science – to contact Luk'yanets or get a suggestion for another member! Robin will first check on the e-mail address with Fabienne Meyers. Post-meeting: a fax was successful and we now have the correct e-mail address.

There appears to be some confusion over who is the National Representative for Brazil. The IUPAC handbook lists Eliezer Barreiro but our last minutes (Berlin meeting) listed Ricardo Bicca. Antonio Monge will write to Barreiro for clarification.

4.0 Commissions and Working Parties

4.1 Commission on Nomenclature and Terminology (VII.M.1)- P. Lindberg

4.1.1 Working Party on Nomenclature and Publication Guidelines for Combinatorial Chemistry in the Synthesis and Screening of Compound Libraries (D. Maclean)

D. Maclean reviewed the activities of this working group. Derek commented on the meeting that he attended in Washington D.C. IUPAC Strategy Round Table Representation of Molecular Structure: Nomenclature and its alternatives, March 10-11, 2000. Participants from various organizations: Patents, Registry, Software/Internet and Nomenclature - The group was pleased to see that the activity is happening. Derek attended this meeting on his own. It was somewhat independent of this section's activity, but to learn where combichem is going- and how does IUPAC view this field. One of the key topics was the registration of combi chem compounds. Derek commented, Affymax made a million and a half compounds last year. Certainly, this is an issue with regards to registering these compounds. People are patenting large virtual libraries. However, serious discussion followed this comment, and suggestion was made to recommend not to register such libraries. It was also suggested that this group should provide a scientific opinion on this matter.

Robin suggested discussing forming a task force. Per suggested keeping it within the commission. This could be an industry driven project.

John suggested keeping it within the section. The aim would be to create an opinion document, that would advise patent lawyers on how to regard virtual libraries with respect to novelty as it affects future patents.

Following Members were identified-

Derek Maclean, BK Trivedi, Per Lindberg, Paul Erhardt: Recall the similarity with the 1970's pronouncements on QSAR predictions and patent problems for as yet unmade compounds, and the J.Med. Chem. statement made by Portuguese

Check feasibility of this with John Jost before starting this project. -BK Trivedi

John and Robin complemented Derek on his work so far.

4.1.2 Glossary of Combinatorial Chemistry Terms (A. Czarnik/D. Maclean)

Derek Maclean reported that the glossary was now on its 10th and final revision. It has been cleared through IDCNS and was due to be published as a Technical Report (not yet as a “Recommendation”) in Pure and Applied Chemistry in December. Czarnik will also publish it in the Journal of Combinatorial Chemistry. Note that it should be titled: the “IUPAC Glossary of.....

It should also have reference to the Pure & Applied Chemistry article and it should include a footnote regarding the division name and the group’s involvement. It was suggested that the timing is of the essence, and we should publish this ASAP.

4.1.3 Working Party on Glossary of Drug Metabolism Terms (P. Erhardt)

Submit a copy of the article (Paul shared it with the team) to John Jost and President Alan Hayes.

Paul distributed a copy of the article “Metabolism Special Report” by MDL’s “Molecular Connection” which was highlighted as an IUPAC article. Which supported the thinking of IUPAC. He also commented on membership of the “Drug Metabolism Terms” Project- Journal editors etc. The working party had compiled a considerable number of terms and he agreed to have a more focused glossary on Drug Metabolism Terms.

Camille asked Paul to fill out the project request form for this project

4.1.4 Compendium of Glossaries (R. Ganellin)

Number of problems encountered. The question was raised of how can one merge two glossaries? Robin has asked John Jost regarding this to see if things published in PAC can be captured and integrated as one document and sorted. One suggestion was made to use “endnote” to sort references. Paul Erhardt suggested as an alternative that we could have a series of “chapters” with an index for definitions.

4.1.5 Working Party on Glossary of Terms in Pharmaceutics (G. Gaviraghi)

This will be split into two glossaries: Pharmaceutical Process Chemistry led by G. Gaviraghi and Mukund Chorghade and Pharmaceutical Technology led by Eli Breuer. The working party is to be expanded to include more industrial people and then both

will submit a form to John Jost regarding these projects. It was suggested that they consider Prof. Howard Stevens from Strathclyde.

4.2 Commission on Training and Development (VII.M.2)- A. Monge

4.2.1 Working Party on Medicinal Chemistry Curriculum (R. Ganellin

Robin commented on the project which was discussed last time and published in the European Journal of Medicinal Chemistry 1st issue this year. It came out about two weeks ago in the January issue. Reprints will be distributed to the authors. European Journal of Med Chem, 35, 163-174, 2000.

4.2.2 Working Party on Research and Training in Medicinal Chemistry in South and Central American Countries and Sub-Saharan Africa (A. Monge)

Antonio discussed the status of this project and its membership. Last year in Uruguay, a course was presented. This was a four-day program, which included participants from Industry and academia. It was truly an international participation from various countries.

At the end of this program, a proposal was made to organize a "Latin American Medicinal Chemistry Society". Antonio was encouraged by the team members to continue the work, which is important for this region.

Question was asked re-funding of such projects. In part supported by companies in Argentina ?? Funding can be obtained in part from IUPAC, but one may consider ICSU for additional funding – suggested by Paul. However, it must go to IUPAC first who will forward it to ICSU.

4.2.3 Research and Training in Medicinal Chemistry in the Indian Subcontinent (M. Chorghade)

Mukund Chorghade has mailed 65 letters to institutions in India. No one is offering Med Chem courses but there are institutions offering pharmaceutical chemistry. A report will be prepared by next meeting. Mukund has also suggested the IUPAC Curriculum in Medicinal Chemistry as the basis for a course in India. He is also investigating the setting up of a web site for long-distance learning.

4.2.4 Research and Training in Medicinal Chemistry in China.

Antonio contacted Dr. Wang by letter. Their response was good, but they wanted to be paid for writing an article. This poses problems.

4.2.5 Medicinal Chemistry in the Development of Societies – Biodiversity and Natural Products

Antonio reviewed the status of this project first by reviewing the list of authors from various countries. Highlighted key features of

the article. Antonio, plans to distribute it to different companies, and may consider publishing in journals.

Paul commented- we need to decide as a group, if we support the concept? We do.

Parallel activity by Fischli and Pandit. Camille will contact them to see if this project can be integrated with theirs, since they are involved in discussions on biodiversity. John Topliss suggested changes in language and that the document should make some specific recommendations. Post meeting note: M. Chorghade has drafted a revised version which is extremely helpful.

4.2.6 Research and Development in Medicinal Chemistry in Developing Countries- Patents and Contracts (The Researcher's View)

The report was distributed to the group last December for comments and/or suggestions. Antonio wishes to keep this back pending progress on 4.2.5.

4.3 Commission on New Technology and Special Topics (VII.M.3)- B. Trivedi

4.3.1 Working Party on Pharmaceutically Acceptable Salts of Drug Substances (C. Wermuth)

One of the main co-authors has recently moved, which made it difficult to complete the project. The book will be ready by the middle of May, and will go to the printer, Verlag Helvetica Chimica Acta which is now owned by Wiley ! Nine of the ten chapters are almost ready. It will be identified as "IUPAC Handbook of Pharmaceutical Salts".

4.3.2 Natural and Unnatural Substances Related to Human Health (J. Topliss)

JT- the group has completed the first draft of all the sections. John has written the introduction and conclusion. Several sections have been prepared with six different authors. Details are being looked at by John and then sent back to the participants for their final review. The goal is to complete this by the end of this year. Use as a source article to disseminate it to a more general public. JT will contact John Jost in this regard. It will be initially published in Pure and Applied chemistry. It should go out in the primary form then consider the secondary publication in the public domain. Total length of 20-25 printed pages.

5 New and Future Projects

5.1 Human Metabolism Database with IUPHAR (P. Erhardt)

This is a joint project with IUPHAR. Funding is being transferred to University of Toledo, which will support a bioinformatics person. This will be a compilation of human bio metabolism of standard drugs.

5.2 Chemical, Pharmacological and Toxicological Aspects of Nutraceuticals (M. Chorghade)

Contacts have been made in Industry, but which Nutraceuticals to include remains a question. Camille suggested contacting individuals at AAPS. Mukund will think about this project and see if he wants to continue doing it. Tom Perun shared an ad for PDR of Herbal Medicine !!

5.3 Isotopically Labeled Compounds as Probes for Human Clinical Effectiveness (G. Gaviraghi)

Dr Gaviraghi could not attend but will report in writing.

5.4 Other Possible Projects:

Camille reviewed the list that he had put together. NPU will be under PL's commission. A suggestion was made to contact Peter Andrews for considering Proceedings of his AFMC symposium in 2001, which is sponsored by IUPAC. BK will contact Peter regarding this.

Another project is to write an opinion document on drug likeness criteria. Possibility: Mark Divers (Astra-Zeneca), Mark Murecko (Vertex), Wiese (Halle University), Bicca (Rio de Janeiro), Revah (Cerep, France), Lipinsky (Pfizer), Kubinyi (BASF).

For Biomarkers identify possible participants from Parke-Davis.

For Pharmaceutics add Polymorph, hydrate crystallinity etc.

A critical review of emerging technologies to assess "drug-likeness" was proposed by Camille.

6 Home Page

The home page needs to be revised. Tom contacted Pat Wooster from Wayne State who could not attend the meeting. He will prepare a proposal for this project. This page should have links to both ACS and IUPAC. It should also mention our books that are being published.

7 AIMECS IUPAC Symposium 2001 (P. Andrews):

No news from Peter on this symposium. Post-meeting note: Prof. Paul Alewood (University of Queensland) contacted some of us for suggestions regarding names of invited speakers. Remember that the AIMECS meeting opens in Brisbane on the evening of Tuesday 3 July 2001 and lasts for the following three days.

8 European Federation of Medicinal Chemistry

Program for the Meeting in Bologna, Italy, 18-22 September 2000 is prepared and distributed.

For information see:

Symposium website: <http://www.scfarm.unibo.it/bo2000/>

Conference Centre website: <http://www.bolognacongressi.it>

Bologna website: <http://www.nettuno.it/bologna/TouringBologna>

Registration and administration:

Planning Congressi Srl, via S., Stefano 97, IT-40125 Bologna, Italy, Tel. +39 051 302 980-981, Fax +39 051 309 477, e-mail: info.planning@planning.it

The XVIIth ISMC will be held in Barcelona (Spain) 1-5 September, 2002. The congress hall has been booked.

9 Asian Federation of Medicinal Chemistry (AFMC) (N. Koga)

Two symposia in AFMC. Nao reported that 15 Societies are involved from Japan, Korea, China and Australia April 11-13. in Tokyo 100 scientists. Melbourne meeting will be held in May 14-18, The 4th Australian Japan joint symposium on Drug design and Development

10 Symposium Sponsorship

11 Links with other bodies

IDCNS next meeting in August 28-29 in France. Robin cannot attend this meeting, but he will submit a written report.

12 Other Business: Mukund Chorghade suggested that he could invite an IUPAC speaker to address the ACS Northeast Section, eg in Boston in the fall (Autumn) 2000.

13 Next Meeting: The next section meeting will be scheduled on Sunday the 17th of September at 9: 00 AM. Before the International Medicinal Chemistry Symposium in Bologna, Italy. Robin to make appropriate arrangements.

Meeting was adjourned at 6:00 PM.