

**Confirmed Minutes of the Medicinal Chemistry Section
Chemistry and Human Health Division
San Diego, March 31st, 2001**

Meeting Attendees: Drs. C.R. Ganellin, B.K. Trivedi, T. J. Perun, J. Topliss, N. Koga, A. Monge, P. Erhardt, M. Chorghade, G. Gaviraghi, E. Kyburz, J. Fischer, M. Liebman, P. Woster.

Apologies were received from E. Breuer, J. Seydel, D. Maclean, A. Kallner, O. Kebir, T. Kobayashi, P. Lindberg, and C. M. de Sant'Anna.

1. Opening Remarks & Minutes of the Bologna Meeting

Robin opened the meeting at 9:00 AM by welcoming everyone, and asking everyone to introduce each other. The minutes of the Bologna meeting were approved.

2. Plans for Integration into the Division of Human Health

Tom Perun reviewed the plans for integration into the Division of Clinical Chemistry & Human Health. The plan is to merge in 2002. This means that the section of Medicinal Chemistry will be dissolved and all activities will be done at the project team level with allocated budget. The Division Committee will consist of 10 members. Four officers and six people at large representing different activities and discipline.

3. Future Committee Members & meeting participants

Tom Perun is appointed to nominating committee with four other members, three of which are not members of IUPAC. Two nominees for each of the 10 positions are due by April 2001. Members of each section will vote to elect members of the new committee. Question was raised as to who else should be nominated instead of Camille? The group did not have a final name.

Robin pointed out that Dave Wustrow from Pfizer, Ann Arbor, has been invited as an observer to the Brisbane section meeting. He was also invited to attend our meeting in San Diego. Tom Perun mentioned that he has identified Cardellina from Center for Responsible Nutrition to participate in topics related to Nutrition. Tom Perun also nominated Michael Liebman as Bioinformatics expert.

Commissions:

4.1 Commission on Nomenclature & Terminology: (Per Lindberg)

4.1.1 Patenting of Virtual Libraries

The topic of patenting virtual libraries was briefly discussed. BK will confirm with Per if he would take the responsibility of chairing a committee on Patenting Virtual Libraries. Paul Erhardt would work with the committee and may take the task if no one is available. The goal would be to have this project completed in about six months. A formal project submission would have to be made, however.

4.1.2 Working Party on Glossary of Combinatorial Chemistry Terms (D. Maclean)

Derek had communicated by e-mail regarding the topic of how to update the glossary. Robin suggested putting it on the web and updating it through small committee. Tom said it would have to go through the formation of a project team for a two-year basis. Originally published in P.A.C. 1999, 71, 2349-2635, it was republished in the ACS journal of J.Comb. Chem. 2000, 2, 562-578.

Derek had also made a suggestion to have the glossary on the web but revise it on a 2-year basis. He has been invited to Gordon Conference to talk about this topic. A question was asked regarding the possibility of a compendium of glossary of terms and have it refereed by other journals. Robin commented it would be significant work in terms of editorial response.

4.1.3 Glossary of Drug Metabolism Terms (P. Erhardt)

The working party was on hold for a while, which is now formally approved by the new process, and will move forward to complete the project. The group currently has 15 members, and they are planning to review approx. 150 terms.

Topliss pointed out that in the future we need to make sure that projects do not get held-up by formal approval process. Of course, the budget needs to be looked into for attendance at meetings etc. The group discussed the issues around the formal approval process. The part of the problem is that certain groups are not happy with the new process. (i.e. nomenclature group) It was pointed out that the approval process is on the web, and the forms are available to download. Paul Erhardt mentioned that he had requested funding for 2-years on the drug metabolism project under the new guidelines and procedure, which he has received.

4.1.4 Compendium of Glossaries (R. Ganellin)

Robin mentioned that Paul Erhardt had suggested that it should be done under each project rather than a global alphabetized one. A global compendium will not be user friendly. It will also be useful to have it separate such that we can annotate or cross-reference in the future. Kallner had offered to merge two glossaries but it was not completed. A question regarding the budget was raised for this project, which will be looked into.

4.1.5. Glossary of Terms in Pharmaceutical Technology (E. Breuer)

Eli Breuer had indicated that he would send an initial set of terms but Robin had not received it.

4.1.6 Pharmaceutical Process Chemistry (M. Chorghade and G. Gaviraghi)

M. Chorghade provided the update of this project. The working group has prepared a draft, which has been sent to technical experts from industry. The first draft will be completed by the end of April. A question was asked regarding the possible peer-reviewer. It was suggested that they should send the list of names to Per for formal approval. The plan is to complete this project by July of this year. Nothing had been put forward for the budget on this project yet.

4.2 Commission on Training and Development (A. Monge)

4.2.1. Research and Training in Medicinal Chemistry in South and Central American Countries

Antonio discussed the status of this project. He has established a society of medicinal chemistry for the Spanish speaking countries. First meeting of this group is scheduled in Cuba on April 16-19. The Cuban government provides the funding (\$5000). 80 Cuban researchers plan on participating in this meeting entitled: "R & D and development of New Drugs". Paul Erhardt pointed out that the cost to attend this meeting is very high for non-Cubans.

Another meeting is being organized in Brazil in collaboration with Brazilian Society of Medicinal Chemistry. The attendance is expected to be about 100 participants from 15 different Latin-American countries. Brazil (\$10,000) and Spain (\$10,000) will fund this meeting. The intent is to bridge the gap between Latin America and the western world. The course is being run in Rio de Janeiro 20-26 August 2001.

4.2.2. Training in Medicinal Chemistry in the Indian Subcontinent (M. Chorghade)

A document is ready for this group to review. Mukund commented on Training in medicinal chemistry courses in four different cities in India. The CSIR is to run courses in Mumbai, Delhi, Bangalore and possibly Hyderabad. Companies are looking for visitors to come as consultants for 2-3 months duration. He solicited support for participation from this group, as well as any ideas for faculty to teach the basic course. BK suggested contacting faculty at "Drew University" who teach the Medicinal Chemistry course during the summer. Topic of standardization of curriculum was briefly discussed, and it was concluded that standardization of such curriculum would benefit all of the developing countries. However, it would not work for Europe and North America.

4.2.3. Medicinal Chemistry in the Development of Societies. Biodiversity and Natural Products (A Monge)

Antonio reviewed activities regarding the Biodiversity and Natural Products in Developing Societies. Articles have been published in journals from various countries, which is important. Copies of these articles were provided to the group, eg. Eur. J. Med. Chem. 2000, 35, 1121-1125.

4.2.4 Patents and contracts in Developing countries: Medicinally active agents -

Preliminary document is in the draft stage. Mukund will provide input from India, China etc., which he will provide to Antonio. He will incorporate those into the document and will bring it for distribution in Brisbane. The issue of patenting was discussed at length. Paul encouraged Antonio to publish a suggestion for two levels of patenting costs, i.e. a lower level for the underdeveloped countries, to follow up on the Antonios first article. Much discussion ensued. Emilio commented on this topic as well.

4.3 Commission on New Technologies & special topics (B.K. Trivedi)

4.3.1 Pharmaceutically Acceptable salts (C. Wermuth)

The book is currently in proofing stage, and will be published soon.

4.3.2 Natural and non-natural substances related to human health (J. Topliss)

John briefly reviewed the genesis of the project. He has recruited five members to participate in this team. Most of the communication is accomplished by fax, e-mail etc. Two drafts have been prepared. Third draft will incorporate comments received from the team members. Michael Liebman commented on putting together a document for common people to clarify the confusion of terminology around natural vs unnatural. A suggestion was made to change "unnatural" to "synthetic". After a significant debate a word "non-natural" was proposed by John and was accepted. This project will be completed by the end of this year.

4.3.3 Compendium of Guidelines of Regulatory Agencies (T. Kobayashi)

Team deferred discussion on this topic since there was no additional information submitted by Toshi.

4.3.4 Human Drug Metabolism Database (P. Erhardt)

The previous project has been completed, and a book has been published "Drug Metabolism: Databases and High-Throughput Testing During Drug Design and Development." Ed. P.W. Erhardt. Blackwell, 1999. The cover of the book has been utilized by IUPAC in various PR brochures. Human drug metabolism database is once again supported by IUPAC and is funded. This is a joint venture with IUPHAR. It has been funded at the tune of \$50000 from ICSU. Paul Erhardt will net work with bioinformatics group as a part of the process. Tom Perun asked a question regarding the budget for this activity. Paul replied that the budget is primarily for travel to attend meetings with FDA. One of the group members is coordinating the European Regulatory Agency. ICSU money will be used in part as a salary for the Web activity. Thus, IUPHAR will be updated frequently.

4.3.5 Natural Products with Medicinal & Nutritional Value (M. Chorghade)

Not much has been done on this project. The plan is to initiate it soon.

4.3.6 Isotopically Labeled Compounds as Probes for Human Clinical Effectiveness

Giovanni Gaviraghi is leading the task, but he has had difficulty-recruiting members for this project. It was suggested that individuals from Schering (Germany) would be interested in participating in this project. Giovanni will follow up to see if there is enough interest to participate in this project. Emilio will provide additional names as possible participants. Paul will identify someone as well from metabolism point of view. The scope of this project would be broadened to include "Probes for Therapeutic and Diagnostic Effectiveness" instead of being restricted to isotopically labeled compounds for clinical use.

4.3.7 New Project: "Timing of Analogue Research" (J. Fischer)

J. Fischer discussed the initial idea of this proposal. A significant debate ensued following proposal on the "timing of analogues". During the discussion, a suggestion was made that this working group may consider the theme on "Evolution of Drug Discovery". It was decided that BK and J. Fischer would put forward a proposal to modify the theme, and provide it to this group. The output could be a book under the title of "The remarkable productivity of Me-too drug research."

4.3.8 Collaborations with WHO (T. Kobayashi)

Toshi has communicated to Robin about the project, but nothing has been formally submitted. The discussion was tabled till the Brisbane meeting.

5 New and Future Projects

5.1 Monograph on Pharmacokinetics

J. Seydel brought a proposal for a monograph on pharmacokinetics for medicinal chemists.

5.2 Bioinformatics (T.Perun)

This proposal originated from the Division meeting in Paris. Tom introduced the topic and the team leader Michael Liebman, who has been involved with this subject in his career. It was suggested that Michael should interface with groups having expertise in the area, and develop a proposal for consideration. Michael and Paul agreed to collaborate and draft a proposal for Kallner within a month based on an example of the progression for relating metabolism, diagnostics and clinical chemistry.

5.3 Predicting Drug Shelf -life (M. Chorghade)

A 4-6-page article will be prepared to summarize what software is being developed based on a consortium of companies that is involved in such a database of predicting shelf life.

5.4 Intellectual Property for University Research (H. Wikstrom)

Wikstrom has not provided any information on this project. Robin will get in touch with Hank to see if he still plans to work on this project.

5.5 IUPAC & Industry (Robin Ganellin)

During the Bologna meeting the extent of our contribution to industry was discussed. Robin was going to write a letter to identify such activities. A number of such activities were identified including formation of AFMC. A point regarding the membership to this committee from industry was highlighted.

6 Internet Home Page

Pat Woster of ACS has put together a web page. The intent was to put things on it including glossaries etc. Pat requested our input to define what is it that we need from such a web page. The question of section's identity was brought up. It was suggested that the activities related to Clinical Chemistry could be included here as well. We need to tell Pat what additional information we would like to include on the web page. BK will interface with Pat to initiate this activity.

7 AIMECS

Robin did not receive any information from Toshi regarding AIMECS. Paul Alewood had sent an e-mail to Robin highlighting difficulties organizing certain sessions at this meeting. Issues regarding communication from Brisbane were raised and discussed.

8 AFMC (N. Koga)

The fifth AIMECS meeting will be held in 2003 in Kyoto, Japan; :, and the secretariat will also move to Japan. Nao also discussed the structure of AFMC.

9 EFMC

Bologna meeting was a success. There were 1100 participants from 49 different countries. EFMC will stay in contact with various MED Chem. bodies such as ACS, AFMC and IUPAC. Next EFMC, meeting is in Barcelona in September of 2002. Emilio highlighted the new executive committee for EFMC, which was formed in January 2001 with Timmerman as chair.

10 Link to other bodies

The group discussed publications, and activities of other division. Pure and Applied Chemistry is published internally by IUPAC and not by Blackwell. Organic Division is working on preferred names for organic molecules, which will be completed by the Brisbane meeting. CAS would accept these "Preferred names". The IUBMB enzyme book is now on the web. (Classification of enzymes). The web address is: (www.chem.qmw.ac.uk/iubmb/enzyme).

11 General Assembly in Brisbane

The Section Meeting is on Friday 29th of June from 9:00 to 6:00PM. The Division Meeting is on Saturday morning and Monday afternoon. Division open meeting is on Tuesday afternoon.

(Post Meeting Note: The section meeting in Brisbane is now scheduled on Monday, July 2nd from 9:00 to 5:00 PM)

Finally, the group discussed the future of this section. Topliss suggested that the Project Team Review Meetings could be held twice a year in conjunction with ACS & EFMC meetings.

The meeting was adjourned at 6:16 PM.