

**Confirmed Minutes of the Medicinal Chemistry Section  
Chemistry and Human Health Division  
Brisbane, July 2<sup>nd</sup>, 2001**

Meeting Attendees: Tom Perun, Dave Wustro, Osama Kebir, Mukund Chorghade, Antonio Monge, Nao Koga, B.K. Trivedi, Paul Erhardt, Anders Kallner, Toshi Kobayashi, Robin Ganellin.

Robin welcomed everyone, and introduced Dave Wustro as a young observer from Pfizer. Dr. Kebir requested a copy of the San Diego Meeting minutes. Paul Erhardt requested a change in the minutes for item 5.2 where a timeline was attached. It was accepted that the timeline will be removed from the minutes, and Paul will work with Michael Liebman to prepare a proposal. The minutes were accepted.

- A. Kallner introduced the project driven process to the group. This is a computer-based process in which anyone can propose a project, and send it to the IUPAC Secretariat to pass it onto the respective division. The division will identify three reviewers for approval. Following approval, money will be appropriated for the project. Subcommittees, reporting to the Division Committee, will be formed to represent particular groupings of expertise. Clinical chemistry, for example, has two subcommittees, one on Nomenclature, Properties and Units, and the other on Toxicology. Limiting factor is a budget, approx. \$50k/ year, which limits us to 8-10 projects. The Division Committee met previous week. During that meeting project listing was shared with request for specific funding. Robin asked, what is the implication of a sub-committee? None as far as the finance is concerned? They can request funding for meeting to review incoming proposal, which can be approved from the division sub-committee. Robin suggested that we form a sub-committee to represent our expertise and interest under the title "Drug Discovery and Development". What is considered a fundable project was briefly discussed. Projects #7 and #18 need to be looked at. Mukund will combine project #12, with pharmaceutical technology as a one-project submission.
- B. Nominations for the new organization are in, but not ready for balloting because some CV's have yet to come in. 5 nominations for the 4 Officer positions, and 10 for 6 additional members. All Titular Members will be able to vote by e-mail ballot by 15 September. A question was raised about the basis on which we will be able to vote? Nominating Committee were asked to nominate based on 10 different areas of expertise. Tom commented on the fact that the Organic Division is appointing 5 Associate Members as a part of their Division. Kallner, had to attend another meeting, and he stepped out, and joined later in the afternoon.

#### **4.1 Commission on Nomenclature and Terminology:**

##### **4.1.1. Legal implications of patenting virtual libraries (Paul Erhardt)**

Paul updated the group on this project and presented a draft position paper coauthored by Erhardt, Lindberg and Trivedi. The central issue concerns the request by some companies to have Chemical Abstracts registry numbers assigned to virtual compounds in libraries, which are proposed to have 'drug-like' properties and are being claimed for patent protection. The perceived danger is that this could inhibit future patent protection for real compounds as drugs. Explained the status of it. Robin asked if we needed a

formal approval for such a document for publication ? A significant discussion ensued on this topic. It was decided that Robin would take this project to IDCNS meeting next day for approval process and endorsement by IUPAC. Paul will then finalize the document ASAP to publish. Paul will provide the names of the referees for this project. Post meeting note: Discussion at IDCNS suggested that there is no requirement to obtain approval through IDCNS since the document will not involve nomenclature, symbols or units. It would just have to be approved by the Division Committee.

**4.1.2. Glossary of Combinatorial Chemistry Terms (Derek Maclean)**

Derek Maclean is to make a project submission for updating the Glossary of Combinatorial Chemistry Terms. This is already available electronically on the web and could be kept up to date if there were a project team in existence to attend to it.

**4.1.3. Generic Structures (Markush)(Derek Maclean)**

Not discussed.

**4.1.4. Glossary of Drug Metabolism Terms (Paul Erhardt)**

Paul has recruited 15 experts on this project. Paul shared the list of the participants, and highlighted the process in which he used statistical tools to identify top 150 terms from the list of about 600 terms. It is now reduced to 210 terms. Paul will crosscheck the terms previously defined, and incorporate them accordingly.

**4.1.5. Compendium of Glossaries (Robin Ganellin)**

This is an ongoing project, and Robin will continue.

**4.1.6. Glossary of Terms of Pharmaceutical Technology (Eli Breuer)**

He has put together a 15-page document of such terms. The group will provide comments and feedback to Robin, who will compile it and give it to Eli Breuer, hopefully by the end of July.

**4.1.7. Glossary of Terms in Pharmaceutical Process Chemistry (Mukund Chorghade)**

Mukund has a rough draft ready, which he will circulate to the experts for their comments in July. He plans on having a group meeting in September for final version. Mukund has not submitted this as a project for funding approval from this year's pool. There are 285 terms in this document. OPRD, Organic Process Research and Development is a possible journal site for publication of these terms. Paul suggested that Mukund might want to reduce number of terms to make it tractable. Mukund also agreed that the group has raised the same concern, and he will follow up on it. The group is due to meet on November 7 in London at the CPHI meeting.

**4.2. Commission on Training and Development – A. Monge**

**4.2.1. Working Party on Research and Training in Latin America (Antonio Monge)**

Antonio reviewed the activities in different countries. He presented our work on biodiversity and Natural Products in developing country during the 4<sup>th</sup> international congress on chemistry in Havana, in April 2001. The next such meeting is in Brazil in August. Antonio also provided copies of the article published in South American journals this year, including Anales Quimica and Anales de la Real Academia de Farmacia. Tom asked what is the recommendation for the future of this project. Antonio plans to discuss this with another group, i.e. Interdivisional Commission on Biotechnology.

#### **4.2.2. Research and Training in Medicinal Chemistry in the Indian Subcontinent (Mukund Chorghade)**

Mukund has prepared a document, which he will finalize soon, on "Medicinal chemistry courses for industry in India, assessing the current situation and identification of the needs". It will be submitted to this group for review. The issue of who will be the faculty and what they will do, was debated. It was suggested that we need to wait and see if the government shows interest in implementing such curriculum, and then participate in helping to establish it in India.

Dr. Osama Kebir discussed education in Egypt. MSI (Molecular Simulation Inc.) was invited to the Faculty of pharmacy in Egypt to teach molecular modeling packages. The university teaches ADME, pharmaceutical chemistry etc. However, they do not have the exposure to computational modeling. It was suggested to tap into the curriculum and faculty at Drew University. Dave Wustro agreed on providing him with the information regarding Drew University.

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

Antonio will resubmit this project following the meeting with the Interdivisional Commission on Biotechnology, and with Division III (Organic).

#### **4.2.4. Research and Development in Medicinal Chemistry in Developing countries (II) – Patents and Contracts: (Antonio Monge)**

It was suggested that we have to submit it through IUPAC, and this means first sending it to referees. Also Paul Erhardt indicated that he should not be a coauthor since he is a patent agent and this could put him in a compromising position.

#### **4.3. Commission on New Technologies & Special Topics (B.K. Trivedi)**

##### **4.3.1 Pharmaceutically Acceptable Salts (C. Wermuth)**

It has not yet been finalised and submitted to John Wiley for publication, but is expected soon.

##### **4.3.2 Natural and Non-natural Substances Related to Human Health (John Topliss)**

John is expecting to get feedback from his collaborators. He plans to submit the final article for publication in the 4<sup>th</sup> quarter.

##### **4.3.3 Project on Human Drug Metabolism Database (Paul Erhardt)**

It is a joint project with IUPHAR, which is funded by ICSU, and it is now funded by IUPHAR, as well, as a 2-year project. It will be a web-based database available to everyone. The model will be initiated in 2002. Information about the project has been presented as an IUPAC poster at the Brisbane meeting. The ICSU funding will be used to mount a model system on the web, on a not-for-profit basis, to identify metabolites. Paul is seeking help from computational experts in his Department in order to explore conformational aspects. Paul is also submitting a letter to ICSU to request an extension of funding for the project.

##### **4.3.4 Natural Products with Medicinal and Nutritional Value (Mukund Chorghade)**

Mukund will submit this as a new project. The aim is still to produce a selective compendium of activities and toxicities (the latter to come from John Duffus) using sources from India on non-conventional medicine based on a CD produced by the Indian Government. During this discussion, a concern was raised regarding the content of this

document, and a suggestion was made not to consider it as a compendium. It was agreed that the project will be for 5 or 6 people to produce a "Technical Report".

**4.3.5 Probes for Therapeutics and Diagnostic Effectiveness: (Giovanni Gaviraghi)**

Giovanni had originated the idea, but is looking for someone to lead the task. Paul will identify names from Schering AG to participate in this project. The suggestion was to change the topic to "Biomarkers for Therapeutic and Diagnostic Effectiveness", and BK will initiate the task to write a proposal.

**4.3.6 Evolution of Drug Discovery (Janos Fisher)**

The budget estimate is not appropriate, and there is a need to revise it to \$5000 maximum. It was also suggested that BK would provide the feedback and comment on this project. The aim would be possibly to produce a book. Various titles were suggested such as: "The productivity of analogue drug research" or "Ligand-based drug design" or "Analogues in drug discovery".

**4.3.7 Predicting Drug Shelf-life: (Mukund Chorghade)**

The project is put on hold and will be revisited later at an appropriate time.

**4.3.8 IUPAC and Industry (Robin Ganellin)**

Robin is writing a letter on "IUPAC and Industry", and plans to get input from John and Camille. Mukund wishes to use this as a basis for requesting funding assistance from Biotech companies.

**5.0 Internet Home page:**

Tom Perun will contact Pat Woster to let him know that there is no need to maintain this page since the section will be dissolved at the end of this year. A link is needed from the ACS to IUPAC.

**6.0 AIMECS – IUPAC Symposium 2001**

Currently being held in Brisbane. Not discussed.

**7.0 AIMECS 2003**

Toshi is the Symposium Chair. Due to take place in June/July 2003, probably in Tokyo.

**8.0 Links with other Bodies**

Robin will attend the IDCNS meeting this week. There is no other new information.

**9.0 Any other business**

**10.0 Next meeting**

We will meet again as the Sub-committee for Drug Discovery and Development on Saturday, April 6<sup>th</sup> in Orlando, Florida, before the ACS meeting.