

**Confirmed Minutes**  
**IUPAC Division of Chemistry and Human Health**  
**Subcommittee for Drug Discovery and Development**

April 6, 2002  
Orlando, Florida

**Meeting Attendees:** Robin Ganellin, Mukund Chorghade, Paul Erhardt, Janos Fischer, Nao Koga, Chris Lipinski, Tom Perun, Camille Wermuth

1. Robin welcomed everyone to the first meeting of the Subcommittee for Drug Discovery and Development. As the former Medicinal Chemistry Section of IUPAC no longer exists, this Subcommittee will offer an opportunity for the medicinal chemistry members of IUPAC to meet and discuss activities, and for the Project Leaders to review the progress of their project teams. Robin discussed the Composition of the Subcommittee, and the Terms of Reference which were submitted to Anders Kallner, the Division President. The National Representatives were also invited to attend, but none of them chose to do so. B.K. Trivedi has had to resign from the Subcommittee because of increasing time commitments at work and with the ACS Division of Medicinal Chemistry. Robin mentioned the need to find new people to participate in the activities of the Subcommittee and also the need for a new secretary. He also discussed the changes in personnel at the Secretariat offices. Janos suggested Dr. Joerg Senn-Bilfinger of Altana (Byk-Gulden) as a potential new member of the subcommittee.  
The Minutes of the last Medicinal Chemistry Section meeting in Brisbane were approved.

2. Matters arising from the minutes:  
The book "Pharmaceutical Salts: Properties, Selection, and Use- A Handbook", Eds. C.G. Wermuth and P.H. Stahl was published by Wiley in April 2002. \$ 120, € 149, £ 85. ISBN 3906-39026-8. It has been announced in Chem. Internat. 2002, 24, N°3, 20.

3. Changes have been made to some of the National Representatives. Joe Seydel is no longer the representative from Germany, and has been replaced by Klaus Frobels from Bayer AG.  
The representative from the EFMC, Emilio Kyburz has retired. The new Secretary of the EFMC is Edmund Differding, who is at UCB. Zhongliang Chen (China) has resigned and No-Sang Park (South Korea) has retired.

- 4.1.1 **Legal Implications of Patenting Virtual Libraries.** (Paul Erhardt)  
Paul reviewed the position statement that he drafted on behalf of the IUPAC Division of Chemistry and Human Health. This document discusses the intellectual property concerns with the attempts to patent virtual libraries, or

specific compounds contained in them without a *reduction to practice*. Approval had been sought from the Organic Chemistry Division but they had not responded. The document has been sent to the heads of the U.S., European and International patent organizations, to the WTO, to intellectual property organizations and to the editors of prominent scientific journals (in March 2002).

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

Derek has moved to a new location, and was unable to attend. It is important to maintain a project in this area to provide updates when necessary, and a possible development of an electronic version.

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

As Derek was not present, there was little discussion. If Derek cannot participate in the future, a new Project Leader will be needed.

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

The Project Team of 15 members has pared down the original list of 600 terms to about 170. This list has been divided up among the members who are providing definitions to be discussed and finalized by the entire team. It is anticipated that the project will be completed by the end of this year.

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

A task force has been assembled to review the 10 glossaries selected for the compendium, and to determine if some of the older ones need to be updated. The goal would be to produce a hard copy and an electronic version. Members of the task force include: Robin Ganellin, Paul Erhardt, Eli Breuer, Mukund Chorghade, John Duffus and Andes Kallner.

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

A draft document is ready to be sent to reviewers, but we await formal acceptance from the secretariat.

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

The eight members of this Project Team had reduced the original list to 150 terms but the reviewers have requested that it be increased again to 600 terms. Most of the definitions have been written. Mukund mentioned that the editor of the process chemistry journal Organic Process Research & Development (jointly between ACS & RSC) has agreed to publish the glossary.

4.2.1 **Research and Training in Medicinal Chemistry in Latin America.**

(Antonio Monge)

Antonio submitted a report indicating that he is working on a project entitled "Manager; Outsourcing and Benchmarking in Research, Development and Innovation of New Drugs in the developing countries."

He has carried this out in Cuba (Oct 2001), Bolivia (Nov 2001), Ecuador (March 2002) and El Salvador (March 2002).

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

Contact has been made with Bangla Desh, Sri Lanka, and Pakistan. A response is still awaited from the former two countries. The current aim is to publish an article.

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

There is the potential here for a new project based on listing the pharmaceutical and nutraceutical materials which are derived from plant byproducts. This could also encompass the cultivation of medicinal plants. It was suggested that we might contact John Cardelina (nutraceuticals) and Jim McAlpine (plant sources).

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

The document presented in Brisbane has been shelved. Information is being collected on the current situation in various Latin American countries.

#### **4.2.5 Practical Studies for Medicinal Chemistry Students.** (Antonio Monge)

This is a suggestion for a new project to produce a textbook containing descriptions of practical studies for medicinal chemistry students especially in less advanced countries. The suggestions should be multifaceted (representing the interdisciplinary nature of medicinal chemistry) and low cost. One useful suggestion made was to calculate the properties of sets of molecules using QSAR software.

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

John submitted a final copy of this document to ICTNS for clearance for publication. As the document has 59 pages and 108 references, it was felt that a condensed version would be necessary for the lay press. John indicated that he was finished with the project. Tom Perun offered to read it and work on producing a shorter version.

#### **4.3.2 Human Drug Metabolism Database.** (Paul Erhardt)

The project is funded by a \$50 K grant from ICSU. Although a single bioinformatic/chemoinformatic expert could not be hired to provide direct assistance with this project, the required expertise was identified through a number of individuals at the University of Toledo. A preliminary skeleton of the information to be included in the database has been assembled, and the programs for the actual database construction are starting to be written. A prototype with a limited amount of data is expected to be available by mid-year. After refinement and finalization of the prototype's features, mass input

of human drug metabolism data will commence. It will be concerned only with intact human data; in vitro or isolated tissue studies will not be included.

- 4.3.3 **Natural Products with Medicinal and Nutritional Value.** (Mukund Chorghade)  
Information on homeopathic medicine is being obtained from Indian sources, and some is being provided by Dr. Zhang in China. A contact person in Brazil has been identified. Six participants are working on this project so far, but the referees suggested more diversity among the participants. Antonio Monge will be contacted for other possible participants in South America.
- 4.3.4 **Biomarkers for Therapeutic and Diagnostic Effectiveness.**  
Not discussed.
- 4.3.5 **Analogue Research in Drug Discovery.** (Janos Fischer)  
Janos led a discussion of this proposed project as a start to redefining the objectives. A suggested outline was developed that included sections on Drug Likeness, Analog Types (chemical and pharmacological) and Classification of Drugs. The project proposal will be resubmitted and discussed at the Barcelona meeting.
- 4.3.6 **Predicting Drug Shelf Life.** (Mukund Chorghade)  
This is suggested to be a very difficult area because the data is not good. For example, the solubility may appear to change, so falsely suggesting decomposition. The project will be abandoned.
- 4.3.7 **IUPAC and Industry Letter.** (Robin Ganellin)  
The letter has been drafted and circulated and is now available as a reference source for a letter requesting funds from industry. It should also be published as a record of the achievements of the Medicinal Chemistry Section during the past decade.
5. **European Federation of Medicinal Chemistry (EFMC)**  
As mentioned earlier, the new representative is Edmund Differding. The next ISMC meeting will be held in Barcelona on Sept. 1-5, 2002.
6. **Asian Federation of Medicinal Chemistry (AFMC)**  
The next AIMECS meeting will be held in Kyoto, Japan on October 14-17, 2003.

#### **Next Meeting**

The next meeting of the Drug Discovery and Development Subcommittee will be on Saturday, August 31, 2002 in Barcelona.