

Minutes
IUPAC Division of Chemistry and Human Health
Subcommittee for Medicinal Chemistry and Drug Development

August 10, 2003
Ottawa, Canada.

Meeting Attendees: Mukund Chorghade, Paul Erhardt, Janos Fischer, Robin Ganellin, Stefan Jaroch, Michael Liebman, Per Lindberg, Tom Perun, John Proudfoot, Jeorg Senn-Bilfinger.

1. Robin welcomed the members attending.

Pierre Bost, Eli Breuer, Edmond Differding, Giovanni Gaviraghi, Osama Kebir, Toshi Kobayashi, Nao Koga, Chris Lipinski, Henk Timmerman, and John Topliss conveyed apologies at being unable to attend.

Robin thanked Per Lindberg who had hosted a very enjoyable dinner for the Subcommittee members on the previous evening.

2. **Matters arising from the Minutes.** Minutes of the previous Subcommittee meeting held in New Orleans (March 22 2003) were approved, pending correction of two typographical errors. It was agreed that minutes for this meeting and future meetings will be posted on the IUPAC website as soon as Subcommittee members have approved the draft document by e-mail and prior to final approval at the following Subcommittee meeting.

3. **Membership.** Robin welcomed Stefan Jaroch (Schering AG) and Michael Liebman (University of Pennsylvania) as new members of the Subcommittee.

It was noted that there is no limit placed on the number of Subcommittee members, and new contributors to projects should be invited to participate at Subcommittee meetings.

Henk Timmerman, John Duffus and Janos Fischer have been elected as new members of the Chemistry and Human Health Division Committee. Robin and Tom have ended their terms as members of the Division Committee but will continue as members of the Subcommittee.

John Bremner (Australia) who was a candidate for election to the Division Committee should be invited to join our Subcommittee.

- 4.1.1 **Legal implications of Patenting Virtual Libraries** (Paul Erhardt, Per Lindberg).

Paul shared the replies he had received in response to the letter (attached below) expressing IUPAC concern over the patenting of virtual libraries. The World Trade Organization will include the IUPAC position statement

in a monthly list of position papers circulated to members. The committee agreed that it would be worthwhile to also send a copy to the major law firms involved in patent litigation to familiarize them with the IUPAC position on this subject.



Acrobat Document



Acrobat Document



Acrobat Document

IUPAC cover letter

IUPAC position statement

Recipients

In follow up discussions, Per agreed to look into the feasibility of generating a project proposal around this topic. In addition, it was suggested that a session on "Patenting for medicinal chemists" at the upcoming EFMC meeting (or a future ACS meeting) would be of general interest to the medicinal chemistry community. Robin to inform Per about the EFMC meeting draft programme.

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

Derek could not attend and Robin presented Derek's update in this area. Some progress has been made in the glossary revision. A new project submission has been prepared, to be submitted in the near future, with the aims of updating the [1999 technical report](#) and providing an authoritative on-line resource for combinatorial chemistry nomenclature. Task group members, in addition to Derek, include Eric Gordon, Arun Ganesan, Eric Martin and Mario Geysen. The members of the Subcommittee reiterated the previously expressed opinion that addition of participants to balance geographical, technical and professional expertise and opinion is desirable. Robin will let Derek know of Prof. Wili Bannwarth at University of Freiburg as a potential project member from Germany.

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

The manuscript titled "On the representation of Combinatorial Libraries" by Derek and co-author Eric Gordon has been accepted for publication by the Journal of Combinatorial Chemistry.

The committee concurred with Robin that expansion of this manuscript could form the basis for a project, possibly integrated with the [IUPAC chemical identifier](#) project. Robin agreed to broach these possibilities with Derek.

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

IUPAC Project [2000-009-1-700](#).

Paul projected that the glossary will be complete by the end of 2003 and expects the review process to be complete in Q1 2004.

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

IUPAC Project [2002-001-1-700](#)

Robin is currently reformatting the various glossaries to a consistent appearance. Robin noted that there will need to be a discussion on the harmonization and refinement of the definitions of various terms at a future Subcommittee meeting. Michael pointed out that terms that are duplicated in separate glossaries should not be removed because this indicates their contextual relevance. It was suggested that the title be changed to "Compendium of Terms Associated with Drug Discovery and Development" (i.e. dropping "for Chemists").

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

IUPAC Project [2001-049-2-700](#)

Eli was unable to attend the meeting but Robin relayed that suggestions received from reviewers have been incorporated into the glossary and that it is ready to be sent to John Jost for a formal review process. Robin had annotated a hard copy version for the Compendium and would send this to Mukund.

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

IUPAC Project [2001-049-2-700](#) (shares the project number of 4.1.6 above).

Mukund reported that the glossary is complete and that he will send Robin a copy for circulation to the Subcommittee members. As above, this glossary will be sent to John Jost to initiate formal review.

4.1.8 Glossary of Chemical Biomarkers for Therapeutic and Diagnostic Use. (Giovanni Gaviraghi).

Giovanni communicated to Robin that his interest in this topic is limited to radioisotope diagnostics. Paul noted that a broader scope would be more "cutting edge" and the committee members concurred. Michael and Paul volunteered to try and identify a suitable individual to champion this potential project.

4.2.1 Research and Training in Medicinal Chemistry in Latin America. (Antonio Monge).

Robin noted that Antonio had sent the following information for dissemination at the Subcommittee meeting.

The following courses have been presented.

Benchmarking in R+D+i in medicaments, May 21-24, Peru and June 23-24, Bolivia.

Project Management in R+D+i in Medicaments, May 27-30, Columbia.

A course on the discovery of new medicines for parasitic diseases will be presented in September.

Mukund noted that the 26th Latin American Chemistry Congress (Congreso FLAQ 2004) will take place in Salvador, Bahia, Brazil in May 2004.

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

IUPAC project [2001-048-2-700](#)

Circulation of the finalized report from the survey is scheduled for September. In brief, it was noted that there is no formal academic training in medicinal chemistry and that medicinal chemists learn “on the job”.

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

Antonio relayed to Robin prior to the meeting that he is assembling a working group on the topic of “Nutraceuticals and Functional Foods for Developing Countries.” The intention is to present a project proposal in Q1 2004.

4.2.5 Practical Studies for Medicinal Chemistry Students. (A. Monge).

The book / web based source would provide low cost practical studies in medicinal chemistry spanning synthesis, measurement of biological activity, calculation of ADME properties etc.

Antonio has received favourable responses from a number of potential contributors. The general utility of this potential project was reiterated by several committee members.

A project proposal is in preparation for submission in Q1 2004.

4.3.1 Natural and Synthetic Substances Related to Human Health (Tom Perun).

J.G. Topliss et al [Pure and Applied Chemistry \(2002\) 74 1957-1985](#).

<http://www.iupac.org/publications/pac/2002/7410/7410x1957.html>

An official summary of this has been written by Thomas Perun, Paul Erhardt, James McAlpine and the EurekaAlert service (a press service created by the AAAS) has helped to distribute it by providing a link to the article on its website.

http://www.eurekaalert.org/pub_releases/2003-04/iuop-irn041803.php.

This was effected through the help of Laura Abernathy of the IUPAC.

The summary article has appeared at :

http://www.brightsurf.com/news/april_03/IUPAC_news_042303.html

[Chimia, 57 \(6\), 364, 2003](#) (the Swiss Chemical Society);

[Environmental Science and Pollution Research, 10 \(3\), 201, 2003.](#)

It was noted that there may be additional projects / technical reports where a similar summary document would be useful as a general source of topical information. It was also suggested that use of the document could be increased by the generation of a number of related documents with specific titles such as "Natural and synthetic substances related to Breast Cancer" or "Natural and synthetic substances related to prostate cancer" etc. Tom agreed to contact Laura to explore the potential usefulness of these suggestions.

4.3.2 Project on Human Drug Metabolism Database (Paul Erhardt).
IUPAC project [2000-010-1-700](#)

Paul noted with regret that an earlier verbal commitment for funding to support the database had been withdrawn. He is currently exploring other opportunities to fund the set-up of the database.

4.3.3 Natural Products with Medicinal and Nutritional Value (M. Chorghade).

IUPAC project [2001-050-2-700](#)

The project has been focussed to a discussion of natural products with therapeutic use only.

It was agreed that a draft of the document would be circulated to the Subcommittee members for evaluation and that there would be further discussion at the next Subcommittee meeting.

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

IUPAC project [2002-051-1-700](#)

Janos has completed classification of the 500 most frequently used drugs as analogs or pioneer drugs. There was a debate on whether drugs could be categorized as analogs based on similar pharmacological effects as opposed to a classification based only on structure. Janos has received draft manuscripts from several contributors to date and is expecting to have completed chapters in hand before the end of the year.

Post meeting: Janos circulated an updated structure for the book.

- I Introduction (Robin Ganellin)
- II Optimizing Drug Therapy by Analogs (János Fischer)
- III Analogs as Means of Discovering New Drugs (Camille Wermuth)
- IV Drug Likeness and Analog-Based Drug Discovery (John Proudfoot)
- V Case Studies
 - 1. Lacidipine (Giovanni Gaviraghi)
 - 2. Pantoprazole (Jörg Senn-Bilfinger)
 - 3. Esomeprazole (Per Lindberg)
 - 4. Moxifloxacin (Uwe Petersen)

- 5. Drospirenone (Rudolf Wiechert)
- 6. Bisphosphonates (Eli Breuer)
(further case studies are planned)
- VI Tables of Analog-Groups (János Fischer)
generic name + chemical structure +therapeutic field+
mechanism of action+ basic patent (year) and first launch (year)
- VII. Subject Index

4.3.7 **Bioinformatics.** (Michael Liebman).

Mike presented the outline of a project designed to evaluate a text data mining tool (Leximine) as a means of identifying the different contexts in which glossary terms can appear in the scientific literature. Such a data mining tool can abstract concepts and collections of concepts from the text of many thousands of articles, not just the article abstracts.

The initial prototype project will use a text data mining tool in conjunction with specific glossaries to abstract the concepts associated with the glossary terms from two journals spanning the period 1998-2003.

Mike will disseminate a detailed description of the proposal to the Subcommittee members along with three proposed areas for evaluation.

Post Meeting. Mike proposed the following as topics for the prototype study and asked each Subcommittee member to indicate a preference.

Scenario 1: Environmental factors in association with breast cancer.

Scenario 2: Toxicological impact of natural products with estrogen-like activity

Scenario 3: Metabolic factors and processes relevant to estrogen and estrogen-like compounds

5 **European Federation for Medicinal Chemistry (EFMC).**

Next EFMC meeting: [18th International Medicinal Chemistry Symposium, Copenhagen and Malmo, August 15-19 2004.](#)

6 **Asian Federation for Medicinal Chemistry (AFMC).**

Next AFMC meeting: [5th AFMC International Medicinal Chemistry Symposium](#), AIMECS 03, October 14-17 2003, Kyoto Park Hotel, Kyoto, Japan. Robin has been invited to represent the Subcommittee (and Division) but the cost is a problem. It was also noted that in the process for seeking IUPAC sponsorship one of the referees had complained that the AFMC was still rather narrowly based since they did not include Societies from South East Asia or the Indian subcontinent; they should be encouraged to expand.

7 **Links with other bodies.**

9 **Next Meeting.**

London, Friday December 12th 2003.

