

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

December 12, 2003
 London, England.

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

1. Robin welcomed the members attending and gave a short account of the history of the Chemistry Department in University College London.

Pierre Bost, Gerhardt Ecker, Giovanni Gaviraghi, Osama Kebir, Toshi Kobayashi, Derek Maclean, Antonio Monge, Henk Timmerman, John Topliss and Camille Wermuth conveyed apologies at being unable to attend.

2. **Matters arising from the Minutes.** Some members noted difficulties in printing the minutes from the Ottawa meeting So they will be sent out again without the attachment. They have already been posted on the IUPAC website.
3. **Membership.** Professor John Bremner from the University of Wollongong has accepted an invitation to become a member of the subcommittee.

Bost, Pierre	Institut Pasteur, France
Bremner, John	University of Wollongong, Australia
Breuer, Eli	Hebrew University of Jerusalem, Israel
Chorghade, Mukund	Chorghade Enterprises, USA
Ecker, Gerhard	University of Vienna, Austria
Erhardt, Paul	University of Toledo, USA
Fischer, Janos	Gedeon Richter, Hungary
Ganellin, Robin	University College London, United Kingdom
Gaviraghi, Giovanni	Sienabiotech, Italy
Jaroch, Stefan	Schering AG, Germany
Kallner, Anders	Karolinska Hospital, Sweden
Kebir, Osama	Scientific & Trading Co., Egypt
Kobayashi, Toshi-hiko	Japan-based Technical Committee, Pharmaceutical Research and Manufacturers of America (PhRMA)
Koga, Naofumi	Daiichi Pharmaceutical Co, Japan
Liebman, Michael	Windber Research Institute, USA
Lindberg, Per	AstraZeneca, Sweden
Lipinski, Christopher A	Pfizer, USA (retired)

Maclean, Derek	Kai Pharmaceuticals, USA
Monge, Antonio	Universad de Navarra, Spain
Nifantiev, Nikolay	Zelinsky Institute of Organic Chemistry, Russia
Perun, Tom	Abbott Labs, USA (retired)
Proudfoot, John	Boehringer Ingelheim Pharmaceuticals, USA
Senn-Bilfinger, Joerg	Altana Pharma, Germany
Timmerman, Henk	Universiteit Leiden, The Netherlands
Topliss, John	University of Michigan, USA
Wermuth, Camille G	Prestwick Chemical, France
Wikstrom, Henk	University of Groningen, The Netherlands

- 4.1.1 Legal implications of Patenting Virtual Libraries** (Per Lindberg).
Per emphasized the need to increase patent knowledge within the medicinal chemistry community. Per agreed to follow up on a preliminary communication with the chairman of the organising committee for the upcoming International Medicinal Chemistry Symposium to determine whether a session on this topic is feasible. Per is also interested in generating a formal proposal related to this topic and will circulate a draft outlining scope and objective to the subcommittee for discussion.
- 4.1.2 Glossary of Combinatorial Chemistry Terms** (Derek Maclean).
Derek could not attend the meeting and Robin presented Derek's update in this area and in regard to 4.1.3 below. A new project proposal to update the [1999 technical report](#) and provide an authoritative on-line resource for combinatorial chemistry nomenclature has been submitted – project number 2003-04-1.
Dr Yos Kato (Japan) has joined the working group.
- 4.1.3 Generic Structures** (Derek Maclean).
The manuscript titled "On the representation of Combinatorial Libraries" by Derek and co-author Eric Gordon is "in press", Journal of Combinatorial Chemistry. An immediate goal of this work is to enable an "electronic supplementary material section" in journals publishing in the combinatorial chemistry fields. A broader aim is to standardize computational recording of chemical libraries so that a database of libraries, analogous to those for crystal structures and protein sequences, might be envisioned.
Post Meeting Note. The article has been published. J. Comb. Chem. 6 (1), 1 -11, 2004.
- 4.1.4 Glossary of Drug Metabolism Terms.** (Paul Erhardt).
IUPAC Project 2000-009-1-700
Paul projected that the glossary will soon be completed and plans to circulate a copy to subcommittee members in the near future.
- 4.1.5 Compendium of Glossaries.** (Robin Ganellin).
IUPAC Project [2002-001-1-700](#)

A suitable consistent format has been identified for the compendium and progress is being made on harmonization of the various glossaries. Robin noted that the medicinal chemistry glossary needs to be updated and Mukund volunteered to identify potential contributors to this task. Robin will also distribute a list of missing terms. Paul Erhardt has produced a composite list of merged terms from six of the glossaries.

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

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

The glossary, containing more than 150 terms, is complete. A final draft was circulated to subcommittee members prior to the meeting and sent to referees. See also 4.1.7 below.

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).

The glossary, containing more than 800 terms, is complete. The glossary has been circulated to the editor and editorial board of Organic Process Research for comment. The intention is to publish this glossary along with the glossary of terms in pharmaceutical technology back-to-back in the same journals since they target similar audiences. Both glossaries will be sent for final review by the end of January.

4.1.8 Glossary of Chemical Biomarkers for Therapeutic and Diagnostic Use. (Michael Liebman).

Mike discussed the relevance of biomarkers to diagnosis, therapeutic choices and genetic risk, and agreed to spearhead efforts on this potential project.

4.1.9 Project Proposal on a Glossary on Molecular Targets for Drugs. (John Proudfoot).

John introduced a proposal to generate a glossary of the protein targets of marketed drugs. Stefan, Mike, Susan and Tom indicated an interest in contributing to this proposal. John agreed to generate a formal project proposal and circulate to subcommittee members by end of January.

4.1.10 Project Proposal on a Glossary of Terms for Biomolecular Screening (John Proudfoot).

The glossary would provide standardized definitions of terms used in biomolecular screening and also to provide descriptions of the technologies used in the high throughput and routine molecular screening processes. John agreed to generate a formal project proposal and circulate to subcommittee members by end of January.

- 4.2.1 Research and Training in Medicinal Chemistry in Latin America.** (Antonio Monge).
No new information.
- 4.2.2 Research and Training in Medicinal Chemistry in the Indian Subcontinent.** (Mukund Chorghade).
IUPAC project [2001-048-2-700](#).
As a follow up to the results of the survey indicating a lack of academic sources of medicinal chemistry training in the Indian subcontinent, Mukund discussed the idea of organizing a formal medicinal chemistry short course to be taught in India. The course would be based on the syllabus for an introductory medicinal chemistry short course generated as part of this project. Mukund will explore the possibility of a project proposal based on this short course idea.
- 4.2.3 Medicinal Chemistry in the Development of Societies. Biodiversity and Natural Products.** (Antonio Monge).
No new information.
- 4.2.5 Practical Studies for Medicinal Chemistry Students.** (Antonio Monge).
No new information. At the last meeting it was noted that a project proposal was in preparation for submission in Q1 2004.
- 4.3.1 Natural and Nonnatural Substances Related to Human Health.** (Tom Perun).
[Pure and Applied Chemistry \(2002\) 74 1957-1985.](#)
<http://www.iupac.org/publications/pac/2002/7410/7410x1957.html>
(Official summary by Thomas Perun, Paul Erhardt, James McAlpine).
A portuguese translation of the article has appeared on the web. Members expressed an interest in knowing how many "hits" the article had generated on the IUPAC website and at the Eureka Alert service.
- 4.3.2 Project on Human Drug Metabolism Database** (Paul Erhardt).
IUPAC project [2000-010-1-700](#)
Paul indicated that additional work on the database is on hold until significant funding is obtained. He will have an opportunity to explore potential funding sources while on sabbatical next year but there is no expectation for substantial progress until 2005 at the earliest.
Paul noted that seed funding from IUPAC for this project has been acknowledged in a recent article: Paul W. Erhardt, "A Human Drug Metabolism Database: Potential Roles in the Quantitative Predictions of Drug Metabolism and Metabolism-Related Drug-Drug Interactions" Current Drug Metabolism, 2003, 4, 411-422. The acknowledgement is on page 421.

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

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

A multiauthored 104 page article has been produced in draft. After appropriate editing it will be submitted for publication as a Monograph and also as an article in J.P.A.C.

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

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

Janos expects to complete classification of the 1000 most frequently used drugs as analogs or pioneer drugs in the near future. Most contributors have provided draft manuscripts of their chapters and Janos anticipates that the complete manuscript will be in hand by next June.

Miljenko Dumic has agreed to contribute a chapter on azithromycin.

4.3.7 Bioinformatics (Michael Liebman).

A prototype project proposal is in preparation. A text data mining tool in conjunction with specific glossaries will be used to abstract the concepts associated with the glossary terms from two journals spanning the period 1998-2003. Mike noted that the group favoured the topic "Metabolic factors and processes relevant to estrogen and estrogen-like compounds" for this exploratory project.

A formal project proposal will be circulated in the near future.

4.4 New Projects

Mukund is interested in revisiting the idea of a project on predicting the storage life and stability of drugs, and compound libraries.

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).

Tom attended AIMECS 03, October 14-17 2003, Kyoto Park Hotel, Kyoto, Japan and represented IUPAC and the ACS at the management committee meeting. Tom noted that the Turkish Association of Pharmaceutical and Medicinal Chemistry has requested membership in the Asian Federation.

Next AFMC meeting will take place in Korea, 2005.

Dr Ho Koon Park, Minister of Science and Technology, Republic of Korea, is president-elect of the AFMC.

7 Links with other bodies.

9 Next Meeting.

Saturday, March 27th 2004, 9:00 am - 6:00 pm, Anaheim Convention Center, Room 211A.