

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

March 27, 2004
 Anaheim, California, USA.

Meeting Attendees: Eli Breuer, Mukund Chorghade, Paul Erhardt, Janos Fischer, Robin Ganellin, Michael Liebman, Tom Perun, John Proudfoot, Jörg Senn-Bilfinger.

1. John Bremner, Giovanni Gaviraghi, Stefan Jaroch, Toshi Kobayashi, Per Lindberg, Derek Maclean, Antonio Monge, Henk Timmerman, John Topliss and Camille Wermuth conveyed apologies at being unable to attend.
2. **Matters arising from the Minutes.**
3. **Membership.**

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	Pharmaceutical Manufacturers Association (Japan) Technical Committee
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, Jörg	Altana Pharma, Germany
Timmerman, Henk	Universiteit Leiden, The Netherlands
Topliss, John	University of Michigan, USA

[Wermuth, Camille G](#)
[Wikstrom, Henk](#)

Prestwick Chemical, France
University of Groningen, The Netherlands

4.1 Nomenclature and Terminology.

4.1.2 Glossary of Combinatorial Chemistry Terms (Derek Maclean).

IUPAC Project 2003-044-1.

Post meeting note: A working draft of the revised Glossary has been completed. It has many new terms and substantial modification of existing terms. It is being circulated to three members of the working party.

4.1.3 Generic Structures (Derek Maclean).

No new information.

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

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

Paul noted that the glossary is almost complete, only some ten or so terms remain to be defined. He noted that new terms continue to arise illustrating this with the examples of "Phase 0" and "Phase 4" which relate to nonmetabolic processes of absorption, distribution and excretion.

4.1.5 Compendium of Glossaries. (Robin Ganellin).

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

No new information. Robin has been contacted by Professor Aubrey Jenkins to suggest terms from the Medicinal Chemistry Glossary for inclusion in the Gold Book (IUPAC Compendium of Chemical Terminology). This has been done.

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

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

The review process has been completed and the glossary is ready for publication. It will be published back-to-back with the "Terms in Pharmaceutical Process Chemistry" (see 4.1.7 below). Robin to write to John Jost to recommend publication of these Glossaries.

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 has been extensively reviewed. Forty or so additional terms have been suggested by reviewers. Incorporation of these terms would require substantial revision and the intention is to reserve them for a future update. Mukund proposed the idea of a project to service this and other glossaries in need of updating and will formulate a project proposal, see 4.4 below. The glossary will be published along with 4.1.6 above as "compendia of terms".

4.1.8 Glossary of Chemical Biomarkers for Therapeutic and Diagnostic Use.

Prototype Analysis of Molecular Biomarkers in Cancer. (Michael Liebman).

A project proposal to compile existing breast cancer biomarkers and classify them in terms to disease progression and research and clinical use is ready for submission.

Post meeting note. A copy of the proposal was circulated to Subcommittee members 3/29/04.

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

Based on a suggestion from Stefan, the initial idea has been modified to prototype project to compile a compendium of the targets for the top 100 drugs and a project proposal on these lines will be prepared.

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

A project proposal was circulated to members before the meeting and will be submitted to IUPAC. A project team has been assembled with assistance from The Society for Biomolecular Screening.

Post meeting note. The project proposal was submitted to the secretariat 4/9/04.

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

Robin relayed that Antonio intends to organize a medicinal chemistry course in Rio De Janiero in February 2005. Robin agreed to follow up with Antonio to determine whether there are opportunities for Subcommittee members to contribute to this endeavor.

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

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

Mukund is in the process 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. The current proposal is for a five day course to be offered at different locations in India where a vibrant drug discovery industry is emerging (e.g. New Delhi, Hyderabad, Bombay, Pune or Bangalore). Mukund has obtained agreement that interested scientists from Pakistan would be also be allowed to attend the course. Several members of the Subcommittee expressed an interest in contributing, and Mukund requested that they forward to him topics from the proposed syllabus that they would be willing to cover.

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).

Robin relayed that a draft project proposal has been prepared under the title "Practical Studies for Medicinal Chemistry Students: An Integrated Approach for Developing Countries." The intention is to provide a book of practical medicinal chemistry experiments that can be carried out at low cost with easily accessible local materials. It was noted that such a book could be of value in developed as well as developing countries. Several members noted that the proposed timeframe for completion of this project - 18 months from Jan '04 - is very ambitious. The project submission form requires some amendments. Robin will liaise with Antonio to achieve this.

4.3.1 Natural and Synthetic 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).

Tom noted that the article has appeared on the web at the following websites: scienceblog.com and brightsurf.com.

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

Paul relayed that he is currently putting copyright protection in place for the database. A draft copyright agreement has been accepted by the University of Toledo and IUPAC and is under evaluation by IUPHAR (International Union of Pharmacology). Once the agreement is in place, Paul intends to seek additional funding to enable completion of the project.

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

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

The manuscript is essentially complete aside from some minor editing of graphics. Since the file is too large to distribute by e-mail, Mukund agreed to send Subcommittee members a copy on CD after the meeting. Robin to then collate their responses.

Mukund is exploring the possibility of analogous projects focused on "Disease Specific Uses of Plant Natural Products or Extracts" or on "Natural Products with Medicinal and Nutritional Value from the Americas."

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

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

The current projection for completion of the manuscript is December 2004. Janos reported that, in addition to the specific case history studies noted in previous minutes, he has arranged for contributors to provide introductions to the following sections of the book.

Statins	J. Fischer, S. Kerpel-Fronius
ACE-inhibitors	J. Fischer, S. Kerpel-Fronius
AT1-antagonists	J. Fischer, S. Kerpel-Fronius
Calcium channel blockers	G. Gaviraghi
Beta-blocking agents	L. Matos
Organic nitrates	L. Dezsi
Heparin-analog:	
pentosan polysulfate sodium	A.J. Domb and A. Label
H2 antagonists	R. Ganellin
Opiates	S. Furst
Quinolones	U. Petersen
From Erythromycin to	M. Domic, S. Mutak, M. Bukvic
Azithromycin and Newer Analogs	Krajacic
Platinum Compounds	S. Kerpel-Fronius
Bisphosphonates	E. Breuer
Corticosteroids	Z. Tuba

In addition, contributions on "Chemogenomics in Drug Discovery" from Hugo Kubinyi and "CNS Related Pharmacophore Modeling Studies" by R. A. Glennon were proposed for inclusion.

Paul volunteered to contribute to the section on beta-blocking agents.

4.3.7 Bioinformatics (Michael Liebman).

A project proposal "Prototype Analysis of Glossary Terms to Establish Biological Context by Text Datamining" has been prepared. The project will specifically examine the Journal of Medicinal Chemistry and Biochemistry (years 1998-2003) for concepts related to "metabolic factors and processes related to estrogen and estrogen like compounds" and relate the concepts to the use of glossary terms. Mike estimated that the prototype project would be complete within three months of initiation.

Post meeting note. A copy of the proposal was circulated to Subcommittee members 3/29/04.

4.3.8 Project on Patents (Paul Erhardt, Per Lindberg).

Paul presented a project proposal titled "IUPAC Survey and Discussion Group on Present Trends in Patenting Drug-Related Technologies." Initially, the project goal would be to survey a variety of different perspectives (e.g. inventor, patent attorney, patent regulatory offices, pharmaceutical industry, less industrially developed nations) on current and possible future patent practices. Analysis of the survey results could lead to downstream proposals aimed at improving general awareness of

intellectual property issues and the education of medicinal chemists in the role of inventor.

A formal project proposal will be submitted to the secretariat in the near future.

4.4 New Projects.

Mukund noted that glossaries are in continual need of updating and revision, and has undertaken to prepare a project proposal to provide support for glossary updates commencing with the Medicinal Chemistry Glossary.

5 European Federation for Medicinal Chemistry (EFMC).

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

6 Asian Federation for Medicinal Chemistry (AFMC).

Next AFMC meeting will take place in Korea, 2005.

7 Links with other bodies.

8 Other Business.

Mukund proposed that the Subcommittee organize a half day symposium on "Recent Advances in Medicinal Chemistry" to take place in conjunction with the 2005 meeting of the general assembly in Beijing.

Tom solicited suggestions for individuals to serve on the Division nominating committee. The nominating committee is responsible for identifying candidates for the next round of Division committee elections scheduled to take place next year.

The Subcommittee members expressed their appreciation for the support given by the ACS in providing facilities for the Subcommittee meeting. John expressed his thanks, in particular, to Susanne Beckley for assistance in making arrangements for the meeting.

9 Next Meeting.

Robin to determine whether the suggested date of Saturday 14 August 2004 in Copenhagen or Malmoe (immediately before the 18th International Symposium on Medicinal Chemistry) will be sufficiently supported by our members.