

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

August 14th, 2004
 Copenhagen, Denmark.

Meeting Attendees: John Bremner, Gerhard Ecker (in part), Janos Fischer, Robin Ganellin, Giovanni Gaviraghi, Toshi Kobayashi, Antonio Monge, Nikolai Nifantiev, John Proudfoot, Jörg Senn-Bilfinger, Henk Timmerman (in part).

1. Philippe Barthelemy, Eli Breuer, Mukund Chorghade, Paul Erhardt, Per Lindberg, Derek Maclean, Tom Perun, 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
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
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	Prestwick Chemical, France

4.1 Nomenclature and Terminology.

- 4.1.2 Glossary of Combinatorial Chemistry Terms** (Derek Maclean).
IUPAC Project [2003-044-1-700](#).
The project proposal has been approved (project number above). Although Derek was unable to attend this meeting, he circulated an e-mail message the subcommittee members indicating that work on the project had begun. Currently the team comprises four US, one UK, two Japanese representatives and Derek would like to expand membership to include more European representation.
- 4.1.3 Generic Structures** (Derek Maclean).
No new information. Derek is focusing on making progress on 4.1.2 above before committing to a proposal on generic structures.
- 4.1.4 Glossary of Drug Metabolism Terms.** (Paul Erhardt).
IUPAC Project [2000-009-1-700](#)
No new information.
- 4.1.5 Compendium of Glossaries.** (Robin Ganellin).
IUPAC Project [2002-001-1-700](#)
Robin is waiting for completion of current glossary projects before additional substantial work is done on the compendium.
- 4.1.6 Glossary of Terms in Pharmaceutical Technology.** (Eli Breuer).
IUPAC Project [2001-049-2-700](#)
No new information.
- 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).
No new information.
- 4.1.8 Glossary of Chemical Biomarkers for Therapeutic and Diagnostic Use.**
Prototype Analysis of Molecular Biomarkers in Cancer. (Michael Liebman).
A copy of the proposal was circulated to Subcommittee members 3/29/04.
No additional information.
- 4.1.9 Compendium of Molecular Targets for Drugs.** (John Proudfoot).
IUPAC Project [2004-025-1-700](#)
The project proposal was submitted (6/4/2004) and approved (7/21/2004, project number above). Work has begun on compiling a list of the targets for the top 100 drugs.

4.1.10 Glossary of Terms for Biomolecular Screening (John Proudfoot).

IUPAC Project [2004-019-3-700](#)

Project proposal was submitted (4/9/04) and approved (6/18/2004). A project announcement has been forwarded to Fabienne Meyers for publication in Chemistry International. A list of some 200 terms has been compiled by the task force and the next step will focus on deciding which of these terms should progress to definitions.

4.2 Training and Development.

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

Antonio has taught the following courses over the past 6 months:

Feb 11-14 2004 Summer Medical School, Rio de Janeiro, Brazil.
June 21-23, 2004 Outsourcing in the research of Medicaments, Lima, Peru.

The following courses are planned for the future:

Oct 11-18, 2004 Benchmarking in R+D+I in Medicaments, Lima, Peru.
Oct 28, 2004 Research for Medicaments for forgotten diseases, Spanish Royal Academy of Pharmacy.
Feb 14-18, 2005 Summer Medicinal Chemistry School, Rio de Janeiro.

The Subcommittee members agreed to participate in the Summer Medicinal Chemistry school, Federal University, Rio de Janeiro, Feb 14-18 2005. Members will forward proposed lecture topics to Robin.

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

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

Mukund has reached agreement with the Indian government to fund a medicinal chemistry course at four locations on the Indian subcontinent, Mumbai, New Delhi, Hyderabad, and Pune or Bangalore. Planning for the time and location of the first course is under way.

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

Antonio agreed to draft a project proposal on the topic of "Nutraceuticals and Functional Foods" with the objectives of providing appropriate definitions and illustrating the importance of nutraceuticals and functional foods in healthcare and nutrition in developing countries.

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

IUPAC project [2004-028-1-700](#).

This proposal has been approved. The objective is to provide a source of practical and low cost experiments that can be used for medicinal chemistry training in developing countries. Antonio would like to broaden

task group representation to include members from Australia, Japan, China and India.

4.3 New Technologies and Special Topics.

4.3.2 Project on Human Drug Metabolism Database (Paul Erhardt).

IUPAC project [2000-010-1-700](#)

No new information.

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

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

No new information.

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

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

Janos reported that the 13 of the manuscripts for the book chapters / sections have been received and are under review. An additional 11 manuscripts are expected by the end of October.

The table of structural and functional analogs from the top 500 drugs along with the relevant information has been compiled and will be circulated to the subcommittee members and co-authors for review.

4.3.7 Bioinformatics (Michael Liebman).

No new information. Robin will follow up with Mike to see whether Mike's project proposals were submitted to the secretariat.

4.3.8 Trends in Patenting Drug-Related Technologies (Paul Erhardt, Per Lindberg).

No new information.

4.4 New Projects.

John Bremner initiated discussion on the following ideas for projects.

A compendium of natural products available in quantity as starting points for synthesis along with illustrations on the opportunities available for modification.

Antimicrobial drug resistance.

Extremophiles in drug discovery.

Research training for postgraduates in medicinal chemistry.

After discussion among the group he agreed to further explore the possibility of project proposals on the compendium of natural products and antimicrobial drug resistance. Antimicrobial drug resistance will comprise a compilation of terms relating to molecular targets and mechanisms that could be attacked for potential drugs.

5 European Federation for Medicinal Chemistry (EFMC).

The present EFMC meeting in Copenhagen-Malmö is very successful and has drawn an attendance of approximately 1200. The next Symposia will be in Istanbul (2006) and Vienna (2008). Also, next year a joint meeting of the Medicinal Chemistry Societies of Austria, Germany, Hungary, Poland, Italy and Spain will be held in Vienna (20-23 June 2005) under the auspices of the EFMC

- 6 Asian Federation for Medicinal Chemistry (AFMC)** (Toshi Kobayashi). AIMECS 03, October 14-17 2003, was very successful with 650 participants from 29 countries. The 6th Australia / Japan Symposium on Drug Design and Development, hosted by the AFMC and the Royal Australian Chemical Institute was held in Sydney, June 27-30 2004. The 10th Japan – Korea Joint Symposium on Drug Design and Development was held in Tokushima, April 21-23, 2004. Future planned conferences: A joint China / Japan Symposium is planned for 2005. The next AFMC meeting will take place in Korea, 2005.
- 7 Workshop on DNA Supramolecular Assembly, University of Avignon, May 5th – 6th 2004.** (Philippe Barthelemy). *Post meeting. Robin circulated a report from Philippe on the workshop which was sponsored in part by IUPAC. Twenty five attendees presented their work on supramolecular chemistry related to DNA. The meeting provided an opportunity for specialists in the field to interact and forge new collaborations. Philippe is working toward having the workshop's papers appear in Pure and Applied Chemistry.*
- 8 Other Business.**
- 8.1 General Assembly in Beijing.** The Subcommittee proposed that project [2002-051-1-700](#), Analogue-based Drug Discovery (Janos Fischer) and project [2000-010-1-700](#), Human Drug Metabolism Database (Paul Erhardt) be highlighted, either as oral or poster presentations, during the overview of divisional activities at the General Assembly. Robin will convey the recommendation to Paul.
- 8.2 Division Nominating Committee** (Tom Perun). Nominations for candidates to serve on the Division Nominating Committee were solicited. Names suggested were: Peter Andrews (University of Queensland), Peter Matyus (Med. Chem. Professor and Director in Semmelweiss University, Budapest) and Giorgio Tarzia (Dean of Pharmacy at the University of Urbino). Robin will forward the suggested names to Tom.
- 9 Next Meeting.**

Rio De Janiero, Sunday, Feb13th, in conjunction with the Medicinal Chemistry Summer School, Feb 14th-18th.