

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

March 25th, 2006
Atlanta, USA

Meeting Attendees: Mukund Chorghade, Paul Erhardt, Janos Fischer, Robin Ganellin, Giovanni Gaviraghi, Tom Perun, John Proudfoot, Jörg Senn-Bilfinger, Ferran Sanz, Henk Timmerman.

Apologies for being unable to attend were received from: Sergey Bachurin, John Bremner, Eli Breuer, Derek Buckle, Stefan Jaroch, Per Lindberg, Antonio Monge, John Topliss, Georgio Tarzia, Mario Varasi.

1. **Minutes of the last meeting**, which was held in Modena (11 September 2005) were accepted pending minor typographical correction. They will be sent to the secretariat for posting on the IUPAC home page.

We encourage subcommittee members to respond to the circulated draft minutes in a timely fashion, otherwise posting of the final document is delayed.

2. **Matters arising from the Minutes**

2.1 **IUPAC Richter Prize**

The prize, \$10,000 including travel expenses (when with academic background), will recognise a scientist's outstanding contributions in medicinal chemistry and drug discovery. The first prize will be awarded during the medicinal chemistry symposium in Istanbul (August 29 to September 2). Over the next 10 years the prize will be granted 5 times.

The call for nominations was announced on the IUPAC website and in the IUPAC journal "Chemistry International". It was also announced in Chemical and Engineering News, the Journal of Medicinal Chemistry, AACP news and in the ACS Medicinal Chemistry Division electronic newsletter. Because of the slow international delivery of printed material carrying the prize announcement, the deadline for nominations was extended to April 20th.

The committee to evaluate the nominations and award the prize has been finalized and will comprise: R. Ganellin, P. Lindberg, G. Tarzia, T. Kobayashi, T. Perun, W. Nelson, R. Pellicciari, and D. Winkler. J. Fischer will participate as a non-voting member.

2.2 **Honorary membership**

The Subcommittee would like to honor the IUPAC services of Mitscher, Topliss, Koga and Wermuth with an Emeritus Fellowship. Action at the division level is required to pursue this further and this topic is an agenda item for the division meeting following this subcommittee meeting.

3. Membership.

The following individuals, Sergey O. Bachurin, (Russia), So-Yeop Han (South Korea), Javed Iqbal (India), Grzegorz Mloston (Poland), Derek Buckle and Mario Varasi have accepted invitations to join the subcommittee and are added to the membership list below.

Bachurin, Sergey O.	Inst. of Physiologically Active Compounds, Russia
Bremner, John	University of Wollongong, Australia
Breuer, Eli	Hebrew University of Jerusalem, Israel
Buckle, Derek	GSK, UK (retired)
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	Siena Biotech, Italy
Han, So-Yeop	Ewha Womans University, South Korea
Iqbal, Javed	Dr. Reddy's Laboratories, India
Jaroch, Stefan	Schering AG, Germany
Kobayashi, Toshi	Pharmaceutical Manufacturers Association (Japan) Technical Committee
Liebman, Michael	Windber Research Institute, USA
Lindberg, Per	AstraZeneca, Sweden
Maclean, Derek	Kai Pharmaceuticals, USA
Mloston, Grzegorz	University of Lodz, Poland
Monge, Antonio	Universidad de Navarra, Spain
Nifantiev, Nikolay	Zelinsky Institute of Organic Chemistry, Russia
Perun, Tom	Abbott Labs, USA (retired)
Proudfoot, John	Boehringer Ingelheim Pharmaceuticals, USA
Sanz, Ferran	IMIM/Universitat Pompeu Fabra, Spain
Senn-Bilfinger, Joerg	Altana Pharma, Germany
Tarzia, Giorgio	University of Urbino, Italy
Timmerman, Henk	Universiteit Amsterdam, The Netherlands
Topliss, John	University of Michigan, USA
Varasi, Mario	Genextra Group, Milano, Italy
Wermuth, Camille	Prestwick Chemical, France

4. Projects

4.1 Nomenclature and Terminology

4.1.2 Glossary of Combinatorial Chemistry Terms (Derek Maclean).

IUPAC Project [2003-044-1-700](#).

Because of work commitments, Derek has suggested that an alternate leader for this effort be identified for this project. The committee supports Derek's proposal to identify an alternate project leader and thanks him for all his hard work on this project.

Robin agreed to contact Dr. Ganesan, Southampton University as a possible candidate(s) to gauge the level of interest in taking over this project.

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](#)

Ongoing, definitions are being adjusted to IUPAC format.

4.1.5 Compendium of Glossaries. (Robin Ganellin).

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

Ongoing, definitions are being adjusted to IUPAC format

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

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

Drafting of a final document was previously complicated by editorial issues including IUPAC incompatible formatting. Mukund is attending to this.

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).

Same issues as above.

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

IUPAC Project [2005-050-1-700](#)

The project has been approved. The objective of the project is to identify the existing biomarkers in breast cancer and classify them in terms of disease progression and also as to their clinical vs. research use. No new information from Michael.

4.1.9 Compendium of Molecular Targets for Drugs. (John Proudfoot).

IUPAC Project [2004-025-1-700](#)

The intention of this project was to provide a resource containing a variety of information on commercially important drug targets. Recently it has become apparent that this substantial portion of this material is now readily available on the world-wide-web, eg <http://redpoll.pharmacy.ualberta.ca/drugbank>. Rather than duplicate the efforts of others in this area, it was recommended that this project be terminated.

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

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

Team leaders (Jan Blanchard, Olivier Nosjean and John Wang) for the three subsections of the glossary are progressing towards readying the sections for internal review within the team. It is anticipated that this will take place within the next few months.

Olivier identified several reviewers for the final glossary at the last Society for Biomolecular Screening Meeting in Geneva.

4.1.11 Glossary of Terms in Medicinal Chemistry. (Mukund Chorghade).

No new information.

4.2 Training and Development.

4.2.1 Research and Training in Medicinal Chemistry in Latin America. (Antonio Monge). Nothing further to add since Modena.

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

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

Medicinal chemistry and drug discovery are currently key growth areas in India. Mukund has arranged for, and is currently organizing, workshops on Medicinal Chemistry to take place in Pune and Hyderabad in early 2007.

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

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

A draft printed version has been produced and was provided at the last subcommittee meeting. On Robin's suggestion information on safety and hazards has since been added in the local language (Spanish or Portuguese). Some of this information was rather general and has since been refined to address specific issues.

4.3 New Technologies and Special Topics.

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

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

The project is on hold pending procurement of additional funding.

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

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

The final document is intended for publication in Pure and Applied Chemistry. Revision of the manuscript has been completed and takes into account the comments of J. Lorrimer and suggestions by Paul and Robin. The document should come back to the Subcommittee before being resubmitted to the Secretariat.

4.3.4 Latin American Plants as Sources for Nutraceuticals (Antonio Monge)

IUPAC Project [2005-031-2-700](#)

This project has been approved.

Henk Timmerman suggested a rearrangement of the title to "Latin American Plants as Sources for Nutraceuticals" as more reflective of the project intent. Some members expressed concern about the potential for possible misuse and misrepresentation of the project results by commercial interests.

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

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

The book was published by VCH-Wiley in January. All the subcommittee members applauded Janos on his diligence and hard work over the past three years in seeing this project to conclusion. It is important that the book is reviewed in medicinal chemistry journals.

4.3.6 Stand-Alone Drugs. (Janos Fischer).

IUPAC Project [2005-032-1-700](#)

This project has been approved.

The project will study drugs having no structural and pharmacological analogues with the intention of providing a review article.

4.3.7 Biological Context by Data Mining (Michael Liebman).

IUPAC Project [2005-049-1-700](#)

This project has been approved with the title "Prototype analysis of glossary terms to establish biological context by text data mining."

The intention is to explore methods for identifying the various contexts in which glossary terms appear in the scientific literature.

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

A project proposal had been prepared but has not been submitted.

4.3.9 Working Party on Chemistry for Biology.

IUPAC Project [2005-042-1-300](#)

This is an interdivisional project of the Organic and Biomolecular Chemistry and the Physical and Biophysical Chemistry Divisions. The

intention is to make a feasibility study and an inventory of current and planned IUPAC activities in the area of Biological Chemistry and also to suggest and initiate new activities

Robin agreed to act as a liaison between the subcommittee and this project group

4.4 New Projects.

- 4.4.1** After the Copenhagen subcommittee meeting, John Bremner was considering new projects on “antimicrobial drug resistance” and a possible “compendium of natural products”. Robin agreed to follow up with John as to the status.

5 Division Committee

No new information.

6 European Federation for Medicinal Chemistry (EFMC).

Professor Roberto Pellicciari is the new president of the EFMC.

The next Symposia will take place in Istanbul (August 27 to September 2, 2006) and Vienna (2008).

- 7 Asian Federation for Medicinal Chemistry (AFMC)** (Toshi Kobayashi). Following the problems with Korea, Prof. Ismail Yalcin, Ankara University, Turkey has become the new AFMC President for 2006-2007 and AIMECS 07 will be in Istanbul in July 2007. Dr. Dave Winkler, CSIRO Clayton South, Australia, becomes President Elect for 2008-2009

8 Other Business

9 Next Meeting

London, October 7th 2006.