

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

October 7th, 2006
London, UK

Meeting Attendees: Sergey Bachurin, Derek Buckle, Mukund Chorghade, Janos Fischer, Robin Ganellin, A. Ganesan, Michael Liebman, Per Lindberg, Antonio Monge, Tom Perun, John Proudfoot, Jörg Senn-Bilfinger, Henk Timmerman, Mario Varasi.

Apologies for being unable to attend were received from: David Alker, John Bremner, Eli Breuer, Paul Erhardt, Giovanni Gaviraghi, Stefan Jaroch, Brigitte Lesur, Derek Maclean, Ferran Sanz, John Topliss, Georgio Tarzia,

- 1. Minutes of the last meeting**, which was held in Atlanta (25 March 2006) were accepted without revision. 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 first IUPAC Richter prize was awarded to Professor Malcolm Stevens during the recent ISMC meeting held in Istanbul. The award recognises Professor Stevens' many contributions in the area of anticancer therapeutics. Several of Professor Stevens' drug molecules have progressed to clinical trials and Temozolomide reached the market in 1999.

Since the prize does not at present include travel expenses for the winner the subcommittee recommends that the Division make appropriate arrangements to budget additional funds to support travel expenses for future prize winners. The amount should be consistent with the original intention that the recipient should present a plenary lecture at both an EFMC and ACS sponsored meeting.

The next prize will be awarded during the ACS medicinal chemistry Symposium at Pittsburgh in June 2008. If possible a repeat lecture will take place at the EFMC Symposium in Vienna, Austria, August/September 2008

Information on the prize has been linked to the ACS medicinal chemistry division website.

2.2 Honorary membership

Action at the division level is pending.

3. Membership.

Following contacts made by Tom Perun at the EFMC meeting in Istanbul, Robin invited Brigitte Lesur (Servier, France) and David Alker (David Alker Associates) to attend this subcommittee meeting. They expressed continued interest in the activities of the subcommittee but unfortunately were unable to attend the meeting.

David Alker	David Alker Associates, UK
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
Ganesan	University of Southampton, United Kingdom
Gaviraghi, Giovanni	Siena Biotech, Italy
Han, So-Yeop	Ewha Womans University, South Korea
Iqbal, Jayed	Dr. Reddy's Laboratories, India
Jaroch, Stefan	Schering AG, Germany
Kobayashi, Toshi	Pharmaceutical Manufacturers Association (Japan) Technical Committee
Lesur, Brigitte	Servier, France
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, Arun Ganesan).

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

At the last subcommittee meeting Derek had conveyed his intention to step down as leader of this project. Robin invited Dr. Ganesan who has a longstanding interest in the area of combinatorial chemistry to take over this responsibility. The subcommittee members welcomed Ganesan to this new role. Derek will stay on as a member of the team.

4.1.3 Generic Structures (Derek Maclean).

No new information. Since this topic is linked historically to the project above, Ganesan will contact Derek to determine whether it is worth pursuing as a possible project.

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](#)

Ongoing, definitions are being adjusted to IUPAC format. Appropriate references are being added.

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).

Ongoing, definitions are being adjusted to IUPAC format. Appropriate references are being added.

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

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

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.

Michael indicated that the project was underway and that initial progress would be presented at the Division meeting scheduled for December.

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

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

This project will be formally terminated at the next Division Committee meeting. John will write an article about this for Chemistry International.

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

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

The glossary sections prepared by the three sub-teams have been recompiled into one document and this is undergoing internal review by the team members. The current document contains draft definitions of approximately 150 terms related to biomolecular screening.

Reviewers for the final glossary have been identified.

Estimated date for project completion is mid-2007.

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

Mukund is preparing a project proposal aimed at updating this glossary and other glossaries related to the subcommittee's activities. Mukund agreed to circulate a draft project proposal to members after the meeting.

4.2 Training and Development.

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

Antonio has presented or will present the following courses/lectures:
"Research a Necessity for the Development of Society. A Reflexion on the R&D of Drugs in Developing countries". Buenos Aires. Argentina, 4/27/06
"Research and Drugs Cooperation: Challenge and Opportunity for Developing Countries". University of Navarra. Pamplona, Spain, 9/21/06
"Scientific Research. A necessity for the Development of Societies. Reflexions on Cooperation in R&D of Drugs". Havana, Cuba, 10/17/2006
"Advanced course in the Directing and Management of Research, Development and Innovation Projects" Tacna, Peru, 11/6-9/2006.
"Role of Scientific Journals in Education and for Progress in Scientific Research" Lima, Peru, 11/6-9/2006.

The subcommittee members expressed their continued interest in and commitment to contributing to medicinal chemistry training in underdeveloped countries. Henk and Mukund expressed a willingness to identify available funding to support such training events. During the discussion on medicinal chemistry in underdeveloped countries, Antonio's article on "Natural Products, a Possibility for the R&D of Drugs for Developing Countries" (Chemistry International 2005, vol 27 (6), 21-22) was cited.

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 is in the late stages of organizing the first of two projected four day workshops on the basic aspects of Medicinal Chemistry to take place in India during 2007. The workshops will be sponsored by the Indian government with additional funding and facilities provided by some of the leading Indian pharmaceutical companies.

Some of the subcommittee members will participate in the workshops and there was a discussion on whether the next subcommittee meeting could be held in India in conjunction with the first workshop.

4.2.5 Practical Studies for Medicinal Chemistry Students. (Antonio Monge). IUPAC project [2004-028-1-700](#).

The current document contains 41 experiments contributed by authors from nine countries and provided in Spanish or Portuguese with an accompanying English version. Antonio expressed thanks to Fabienne Meyers and Cheryl Wurzbacher for assistance in editing the current document. Robin noted that some additional “polishing” of the English scientific terminology would be helpful and several subcommittee members volunteered to help with this.

Following a suggestion from Mukund, it was agreed that we should explore the possibility for users to have a voluntary option of paying for the book.

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](#).

Revision of the manuscript has been completed

4.3.4 Latin American Plants as Sources for Nutraceuticals (Antonio Monge) IUPAC Project [2005-031-2-700](#)

This project has been approved.

Antonio has identified contributors from most Central and South American countries with the exception of Argentina, Honduras, Nicaragua and Venezuela

Bolivia:	Dr. Teresa Cardozo
Brazil:	Dr. Eliezer Barreiro
Chile:	Dr. Patricio Huenchunir
Colombia:	Dr. Roberto Pinzón
Costa Rica:	Dr. Gerardo Mora
Cuba:	Dr. Alberto Núñez Selles

Ecuador: Dra. Ximena Chiriboga
Guatemala: Dr. Armando Cáceres
Mexico: Dr. Gildardo Rivera
Panama: Dr. Mahabir Gupta
Paraguay: Dr. Esteban Ferro
Prof. Inocencia Peralta
Peru: Dr. Olga Lock
Dr. Diana Flores
Salvador: D.^a Ligia E. Salazar, D. Oscar D. Guzmán Julián
Uruguay: Dr. Hugo Cerecetto

The contributors have provided lists of locally used potential nutraceutical plants. The assessment of which are appropriate for inclusion in the project is in progress.

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

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

The book was published by VCH-Wiley in January and has been described in Chemistry International 2005, vol 27 (6), 26. It has received almost 40 positive reviews to date including one in J Med Chem 49 (15), 4799, 2006. Sales are sufficiently robust that the publisher has contacted Janos to propose a 2nd edition for 2009. Janos outlined a proposed structure for the next edition and there was some discussion on whether a second volume would be more appropriate than a revised or updated edition.

It was suggested that a project proposal could be submitted to support work on this next edition.

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 perspective on situations where it has not proven possible to improve an existing drug with an analog based approach. There was a spirited debate among the members on the nature and scope of structural and pharmacological “analogy” and the ultimate scope of the project is still under discussion.

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.

The project is underway and initial progress will be presented at the Division meeting scheduled for December.

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

No new information.

4.3.9 Working Party on Chemistry for Biology.

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

No new information.

4.4 New Projects.

- 4.4.1** No additional communication from John Bremner on possible new projects related to “antimicrobial drug resistance” or a “compendium of natural products”. Tom Perun mentioned that Yvonne Martin at Abbott is writing a book on Molecular Modeling for Medicinal Chemists and will submit a project proposal to IUPAC.

5 Division Committee

A nominating committee for upcoming elections to the Division Committee is being organized by Tom Perun

6 European Federation for Medicinal Chemistry (EFMC).

Professor Roberto Pellicciari is the new president of the EFMC.

The next Symposia will take place in Vienna (2008) and Brussels (2010).

7 Asian Federation for Medicinal Chemistry (AFMC) (Toshi Kobayashi).

AIMECS 07 will take place in Istanbul, July 7-8 2007 (<http://aimecs07.org>).

Robin will contact Prof. Ismail Yalcin, Ankara, to offer 3 or 4 speakers. Dr. Dave Winkler, CSIRO Clayton South, Australia, is President Elect for 2008-2009

8 Other Business

For the General Assembly in Torino, August 4-12, 2007, Robin is to explore further the possibility of including speakers from our Division VII.

9 Next Meeting

Turin, Italy, 3 August 2007