

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

August 3rd, 2007
Torino, Italy

Meeting Attendees: Sergey Bachurin, Eli Breuer, Janos Fischer, Robin Ganellin, A. Ganesan, Giovanni Gaviraghi and Jörg Senn-Bilfinger (pm). Mukund Chorghade was prevented from attending due to a flight cancellation.

Apologies for being unable to attend were received from: David Alker, John Bremner, Derek Buckle, Gerhard Ecker, Paul Erhardt, Javed Iqbal, Stefan Jaroch, Toshi Kobayashi, Per Lindberg, Yvonne Martin, Grzegorz Mloston, Antonio Monge, Tom Perun, John Proudfoot, Ferran Sanz, Giorgio Tarzia, Henk Timmerman, Mario Varasi.

In the absence of John Proudfoot, Janos kindly accepted to write draft minutes.

1. Minutes of the last meeting, which was held in London (7 October 2006), were accepted without revision. They have already been submitted for posting on the IUPAC home page, as draft minutes (since 11 March 2007). They will be confirmed.

2. Matters arising from the Minutes

2.1. IUPAC-Richter Prize

The first prize winner, Professor Malcolm Stevens from Nottingham (UK) will give a repeat lecture here in Turin.

Post-Meeting note: Professor Stevens gave a new lecture under the title: "Chemistry-driven Anticancer Drug Discovery" at the 41st IUPAC World Chemistry Congress as a Keynote Lecturer in the Symposium "Cancer Chemotherapeutic Agents" chaired by Robin Ganellin on August 8.

In his prize winner lecture in Istanbul (Sept 1, 2006) Stevens discussed his anticancer research achievements starting from the natural product necatorone.

In Istanbul, Stevens received a plaque as well as his cheque. The description of his recognised achievements were, however, missing from the plaque.

Therefore another plaque was ordered through the IUPAC Secretariat which contained the wording as agreed by the Selection Committee: "Presented to Professor Malcolm F.G. Stevens for his creative use of heterocyclic chemistry over a period of twenty five years applied to the invention of therapeutic agents which have been developed for the treatment of cancer." This second plaque was mailed to him.

The 2008 IUPAC-Richter Prize was discussed emphasizing the need to start publicity immediately. The ACS Med. Chem. Division meeting in Pittsburgh will host this ceremony in June 2008. Hopefully the ACS meeting will also be ready to pay the travel expenses of the prize winner.

A repeat lecture is planned. A possible site could be the EFMC meeting in Vienna. Giovanni contacted the EFMC President Prof R. Pellicciari, who will speak with the local organizer Peter Etmayer. The Lecture programme has, however, been finalized. Alternative venues will be investigated.

Post-Meeting note: Advertising activity started after the Subcommittee meeting. RG drafted a call for nomination and the Richter company prepared a final version with the logos of IUPAC and Richter. It was sent to IUPAC to be distributed at conferences. The Call for Nomination should be published on the home pages of the ACS and EFMC.

The previous Selection Committee will be invited to serve again, chaired by Prof Robin Ganellin. The nomination deadline is 31 December 2007.

2.2 IUPAC Emeritus fellows

Action at the Division committee is pending.

3. Membership

The following names were proposed: Noël J. de Souza (Mumbai, India) who stood for election to the DC should be invited to our Subcommittee. JF mentioned that Prof Peter Matyus (Hungary) would also be willing to participate.

Two former members have resigned: Derek Buckle (UK) and John Bremner (Australia). RG will invite Derek to participate as a project leader on the Glossary of Terms in Medicinal Chemistry.

Following a contact made by Tom Perun, Robin invited Yvonne Martin (retired from Abbott) to attend.

4. Projects

4.1. Nomenclature and Terminology

4.1.2. Glossary of Combinatorial Chemistry Terms (Arun Ganesan)

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

The project has two further members: Dr. Nunzio Sciametta (Pfizer, UK) and Prof Stefan Bräse (Karlsruhe).

An updated version of the glossary is planned by the next year.

4.1.3. Generic structures (Derek Maclean)

No new information. Following Ganesan's assessment, this item will be removed from the next agenda.

4.1.4. Glossary on Drug Metabolism Terms (Paul Erhardt)

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

Definitions are being adjusted to IUPAC format. The Glossary is planned to be available for public comment in 2008.

- 4.1.5. Compendium of Glossaries** (Robin Ganellin)
IUPAC Project [2002-001-1-700](#)
This project depends on some other ongoing glossary projects.
- 4.1.6. Glossary of Terms in Pharmaceutics** (Eli Breuer)
IUPAC Project [2001-049-2-700](#)
The definitions have been reformatted according to the IUPAC requirements but the references need to be numbered. Robin has produced a draft title page and will send this to Eli. When the foregoing has been completed the Glossary should be submitted using Manuscript Central for acceptance by the Secretary of ICTNS. If approved, it should then be sent out to 15 independent experts for review prior to becoming an IUPAC recommendation.
- 4.1.7. Glossary of Terms in Pharmaceutical Process Chemistry**
(Mukund Chorghade)
IUPAC Project [2001-049-2-700](#)
The formatting will be finished very soon. Robin will produce a draft title page and send it to Mukund.
- 4.1.8. Prototype Analysis of Molecular Biomarkers in Cancer**
(Michael Liebmann)
IUPAC Project [2005-050-0-700](#)
No new information.
- 4.1.9. Compendium of Molecular Targets for Drugs** (John Proudfoot)
This project was formally terminated at the last Division Committee meeting (Brussels, December 2007). John wrote an article about this for Chemistry International, published 2007, [29](#) (3) May/June, 23.
- 4.1.10. Glossary of terms for Biomolecular Screening** (John Proudfoot)
IUPAC Project [2004-019-3-700](#)
A draft document containing the definitions for approximately 150 terms has been sent to reviewers from the Society for Biomolecular Screening (SBS) for comment; it will also be posted on the SBS website for comment by SBS members. This phase should be completed by the end of September 2007. The document will then be formatted according to IUPAC guidelines.
- 4.1.11 Glossary of Terms in Medicinal Chemistry**
The 1998 medicinal chemistry glossary should be updated and Robin will contact Derek Buckle to see whether he is prepared to chair this. Robin will prepare a Project Submission form on his behalf in time to take advantage of the new budget in 2008.
- 4.2. Training and Development**
- 4.2.1. Research and Training in Medicinal Chemistry in Latin America.** (Antonio Monge)
Short courses have been organized in Habanah, Cuba (November 2006), Reynosa and Monterrey, Mexico (March 2007), on "R+D+I of Drugs in the Development of Societies. In Istmo, Guatamala (August 2007), and

Huancayo, Peru (November 2007). The courses are on “Functional Foods” and “Project Manager in Drugs”.

A future project (2007-2011), coordinated among 8 Latin American countries, involves new compounds for treating Chagas disease.

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 2008. The workshops will be sponsored by the Indian government with additional funding and facilities provided by ACS. Some of the Division and MC Subcommittee members will participate in the workshops.

Post-Meeting note: Several logistical problems were encountered in organizing the first of these in 2007. These problems centered on raising funds and organizing travel for all speakers. After extensive discussions with the representatives of the CSIR (an India govt. agency) and representatives from the Indian Pharma industry, a new date of February 2008 will be set. Mukund will have several meetings in Boston with ACS officials in August.

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

IUPAC Project 2004-028-1-700

The online book, edited by Antonio Monge and Robin Ganellin, has been freely available on the IUPAC web site since January 2007:

www.iupac.org/publications/cd/medicinal-chemistry/index.html

(see Chemistry International Vol 29 No 2 (March-April) 2007, 21).

The aim of this book is to provide developing countries with a practical text for studying medicinal chemistry. All the six chapters are written in English, and most are also presented in Spanish or Portuguese. Students taking courses in Medicinal Chemistry in academic institutions in the developed countries could pay a small fee for use of a prescribed text in courses. Further discussion with John Jost about the appropriate mechanism for doing so is suggested.

4.3. New Technologies and Special Topics

4.3.2. Human Drug Metabolism Database (Paul Erhardt)

IUPAC Project 2000-010-1-700

A prototype of the database has been assembled. A partner from the private sector is being sought to assist in fine tuning of the database. This will either occur in 2008 or the project will be made available to the public and IUPAC involvement will be terminated.

4.3.3. Natural Products with Medicinal and Nutritional Value

(Mukund Chorghade)

IUPAC Project 2001-050-2-700

Revision of the manuscript to conform to IUPAC guidelines and reviewer suggestions has been completed. An additional project is being written to survey the utility of plants for specific diseases such as diabetes and cancer. A review article or a monograph is planned.

4.3.4. Latin American Plants as Sources for Nutraceuticals

(Antonio Monge)

IUPAC Project 2005-031-2-700

The objectives of this project are to provide possible commercial opportunities for local industry in Latin American countries. Seventy pages of a draft have been circulated by Antonio Monge: some editing is required and is ongoing. Plants from Uruguay, Peru and Mexico are covered. The section on Uruguay needs to be expanded. An article in PAC is envisaged in the first instance; it could be followed up with articles per country and ultimately all these articles could be suitably edited and combined into a book.

The terms functional foods and nutraceuticals were discussed as alternatives. The majority of the members prefer the term “nutraceutical”. A more recent term is naturaceuticals.

4.3.5. Analogue-based Drug Discovery (Janos Fischer)

IUPAC Project 2002-051-1-700

Janos reported on the book “Analogue-based Drug Discovery” published in January 2006 by Wiley-VCH.

The Publisher wrote the following text:

“18 months ago the book was first published in Europe and then in the overseas markets of Americas, Australasia, and Africa. The market success was so great that the starting print-run of 800 copies is now completely sold out, and we have already been able to undertake a first reprint of the fine book.

That the demand for the book continues to be so high first of all testifies to its great concept and quality, which is the result of the dedication of the two editors (JF and RG), as well as the many authors who have contributed to it.

It also indicates for us that there is a great interest in the global drug development community to educate themselves from books like this one, and we have every reason to believe that a companion volume with new case studies of analogue-based drug development will enjoy the same outreach and popularity as did the first book.”

The Publisher is enthusiastic that we begin working on a follow-up volume.

Janos analyzed the success of the book. An important role was played by having a core-team consisting of several members of this IUPAC Subcommittee.

A new project proposal “Analogue-based Drug Discovery II” is under preparation. This step depends upon how quickly a new team (at least a core-team) can be set-up.

During the meeting Ganesan expressed his readiness to write on analogue-based drug discovery where natural product drugs are the lead molecules. Giovanni is ready to write on beta 2-agonists. Janos

would write two chapters : 1. Optimization of Drug Therapy by Analogues and 2. Analogues and Stand Alone Drugs.
 Prof. Rudolf Wiechert (Berlin) proposed by mail that diagnostics could be a chapter of a possible second volume, where he recommended to ask Bayer-Schering. Another idea by him is a chapter on prostanes, however, their commercial results are not very good.

4.3.6. Stand-alone Drugs (János Fischer)

IUPAC Project 2005-032-2-700

A drug classification based on analogy would differentiate analogues and stand-alone drugs. The definition of stand-alone drugs has been discussed. A possible definition is the following: a drug is a stand-alone when no successful optimizer drug, which acts by the same pharmacological mechanism, has been marketed. Therefore, such a drug does not belong to any analogue class. The interest is to discuss in each case why analogues have not been possible or successful.

This approach could afford a chapter of the new book (4.3.5 as above) and/or a review article.

Ganesan and Jörg would participate in the project.

4.3.7. Biological Context by Text Datamining (Michael Liebmann)

IUPAC Project 2005-049-1-700

No new information.

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

No new information.

4.3.9. Working Party on Chemistry for Biology (Robin Ganellin)

IUPAC Project 2005-042-1-300

The project belongs to the Division on Organic Chemistry.

No new information.

4.4. New Projects

Two new project proposals have been mentioned above:

1. Analogue-based Drug Discovery II
2. Glossary on Medicinal Chemistry

5. Division Committee

Paul Erhardt will finish his work as Division President at the end of 2007. Unfortunately Prof. Pedro Soares de Araujo is now unable to assume the position as the new President, because his country (Brazil) did not pay the membership fees due to IUPAC.

The result of the last election to the Division Committee is that the new Titular Members (TM's) for 2008-2011 are: Dr Ole Andersen (Denmark), Prof. Xavier Fuentes-Arderiu (Spain), Dr. Françoise Pontet (France) and

Prof. Giorgio Tarzia (Italy). They replace Dr. Derek Buckle, Prof. John Duffus, Dr. Janos Fischer and Prof. Henk Timmerman.

Post-meeting note: the Division Committee proposed Prof. Douglas M. Templeton (Canada) to be named as the new Division President for 2008-09.

6. EFMC (European Federation for Medicinal Chemistry)

No new information.

7. AFMC (Asian Federation for Medicinal Chemistry)

Toshi Kobayashi received a long-service award from the AFMC at the last meeting in Istanbul.

At the conference AIMECS 07 in Istanbul (July 8-11, 2007) 500 scientists from 42 countries participated.

The new President in 2008-09 is Prof. David Winkler (CSIRO, Clayton, South Australia) and the new President-elect is Prof. Masakatsu Shibasaki (Tokyo, Japan).

AIMECS 09 will be in Cairns, Australia and AIMECS 11 will be in Tokyo, Japan.

8. Other Business

a. 44th General Assembly and 41st IUPAC World Chemistry Congress in Torino, Italy.

In spite of many organizational problems the Chemistry and Human Health Division and the Subcommittees helped to organise and contributed to five symposia at the Congress:

- Analogue-based Drug Design (Chair: János Fischer)
- Nomenclature, properties and units in clinical chemistry (Chair: Françoise Pontet)
- Cancer Chemotherapeutic Agents (Chair: Robin Ganellin)
- Multitarget Drugs (Chair: Giuseppe Ronsisvalle)
- Prodrugs and Soft Drugs (Chair: Paul Erhardt)

b. Posters

Two posters have been prepared for display at the World Chemistry Congress to summarize the activities of the Division on Chemistry and Human Health and the Subcommittee on Medicinal Chemistry and Drug Development. Posters were also contributed by the other two Subcommittees.

c. Herbal medicines

Under this title a new project (2005-034-1-300) has been initiated by the Division on Organic Chemistry (see Chemistry International 2006, 28 (3), May/June Issue). This was assessed as a project and rejected at DC level. Mukund is aware of it. The Chair is Mohammed Mosihuzaman, Bangladesh.

9. Next meeting

April 6, 2008 in New Orleans (attached to the ACS meeting), or

possibly with a teaching school in India, or at the Jolly Beach Resort, Antigua in association with the Zing Drug Discovery Conference, 17-20 January 2008, that Ganesan is chairing. Pittsburgh in June 2008 would be too long to wait for.