

Confirmed Minutes

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

March 26th, 2009, Salt Lake City, Utah, USA

Meeting Attendees: Mukund Chorghade, Janos Fischer, Robin Ganellin (Chair), Tom Perun, John Proudfoot (Secretary). Michael Liebman participated by teleconference for a discussion on his projects

Apologies for being unable to attend were received from: David Alker, Sergey Bachurin, John Bremner, Eli Breuer, Derek Buckle, Noel De Souza, Paul Erhardt, A. Ganesan, Giovanni Gaviraghi, Toshi Kobayashi, Per Lindberg, Yvonne Martin, Antonio Monge, Jörg Senn-Bilfinger, John Topliss, Mario Varasi.

1. Minutes of the last meeting, which was held in Vienna (August 30-31, 2008) were accepted without revision. They will be sent to the secretariat for posting on the IUPAC home page.

2. Matters arising from the Minutes

2.1 [IUPAC Richter Prize](#)

The current prize winner Jan Heeres (Janssen, retired) presented award lectures in 2008 at the following meetings.

1. National Medicinal Chemistry Symposium (Pittsburgh)
2. XXth International Symposium on Medicinal Chemistry (Vienna).
3. 2nd Coast to Coast Medicinal and Synthetic Chemistry Symposium (Torquay, UK).

The next IUPAC Richter prize will be awarded in 2010. The announcement of the prize and solicitation for nominations will be made towards the middle of the year with a closing date for nominations of December 31st. A number of candidates from the previous cycle will be encouraged to resubmit applications for consideration during this round. RG will contact the EFMC to confirm that there will be a lecture slot available for the winner at the next International Symposium on Medicinal Chemistry, August 2010, in Brussels.

2.2 Emeritus Fellows

The proposed title has been modified to Distinguished Fellow and draft guidelines for the nomination process have been provided by the Division Chair. Since the Subcommittee would like to recognise a number of former members, nomination packages will be provided for consideration to the Division Committee as soon as possible. It is possible that the nomination and approval process might not be completed in time for a recognition ceremony the IUPAC National Assembly in Glasgow and

Mukund will explore the possibility of holding an event at the next ACS meeting in Washington DC.

3. Membership.

Sergei Bachurin and Tetsuo Nagano were elected to the Division committee from the National Representatives. Derek Buckle, Yvonne Martin and Michael Schwenk have also been elected to the Division Committee with terms starting in 2010. Janos Fischer will continue as an Associate Member of the Division Committee. Mukund Chorghade will stand down as Secretary at the end of 2009 but can continue as an AM.

4. Projects / Working Parties

4.1 Nomenclature and Terminology

4.1.2 **Glossary of Combinatorial Chemistry Terms** (A Ganesan).

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

Ganesan met recently with Stefan Braese to discuss addition and modification of a number of terms. It is expected that a working draft of the document will be available by the summer.

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](#)

The current intention is to provide an online collection of glossaries. The next step is to identify which glossaries are available as editable text documents.

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

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

Feedback on this glossary and the glossary of terms in pharmaceutical process chemistry (4.1.7 below) was recently obtained from the USP and FDA and resulted in the addition and modification of a few terms. The glossary is now ready for dissemination and will be published in PAC. The recent interactions with the FDA and USP in relation to this glossary should result in closer ties between these two organizations and IUPAC. The FDA will promulgate the glossary in their guidance and the USP has indicated that IUPAC representation will be welcome at future USP meetings.

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).

See 4.1.6 above.

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

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

A comparison among biomarkers under development and in use, both clinically and “off-label”, to categorize and evaluate the relevance of such biomarkers in both pharmaceutical development and healthcare decision support has been completed.

A publication that summarizes this study is being prepared and has been solicited by several journals for potential publication. The targeted submission date for this paper is 8/09.

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

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

Since the last meeting in Vienna, the draft glossary has been reviewed by members of IUPHAR, has been formatted according to IUPAC guidelines and was reviewed by members of the Subcommittee. It has been forwarded to the Division with the expectation that the final required IUPAC review process will be completed over the next couple of months.

4.1.11 Glossary of Terms in Medicinal Chemistry. (Derek Buckle).

IUPAC Project [2008-010-1-700](#)

The project announcement was published in [Chemistry International, 2009, 31, \(March/April\), p20.](#)

Derek provided the following status update by e-mail before the meeting. A compilation of approximately 150 suggested additions to the Glossary has been prepared. It has been circulated to both the Task Group members and the Subcommittee on Medicinal Chemistry and Drug Development. Definitions have been proposed for many of the new terms based on input from experts, primary journals, the internet (particularly Wikipedia), other IUPAC Glossaries, and Subcommittee Members. Input has also been requested from the three main editors of the Journal of Medicinal Chemistry, although comments were received only from Carlo Melchiorre. Suggestions have also been sought from the RSC Bioorganic & Medicinal Chemistry Sector Committee.

Next Steps:

Decide on which of the added terms should be retained for inclusion in the updated Glossary and ensure that no major omissions exist.
Check, and if necessary amend, all proposed definitions.
Suggest definitions of those terms for which none is currently proposed.
Amend as necessary existing Glossary definitions.

The Subcommittee members in attendance spent a full hour towards the end of the meeting editing the new definitions from A-C and Robin will forward the collated comments to Derek.

4.2 Training and Development.

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

Antonio has presented lectures on drug discovery related to neglected diseases in Buenos Aires (Argentina), Guatemala City, Mexico, Cuzco (Peru) and San Juan (Puerto Rico) over the past six months. In particular, "New quinoxalines for the treatment of Chagas". There was some discussion on the possibility of generating a project related to Antonio's ongoing activities, perhaps in the area of identifying opportunities for productive collaboration for research on neglected diseases.

It was also suggested that the Subcommittee could assist in Antonio's efforts, possibly in a manner similar to the course given in Rio de Janeiro in 2005.

4.2.2 Research and Training in Medicinal Chemistry in the Indian Subcontinent. (Mukund Chorghade). IUPAC project [2001-048-2-700](#).

Training of medicinal chemists is currently a national priority in India and Mukund is involved in planning a five day Medicinal Chemistry workshop to take place in India during January 2010.

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

A printed version (539 pages) of the text, generated directly from the web version, is expected to be available soon, courtesy of Dr. Rosa Cattana, Universidad Nacional de Rio Cuarto, Cordoba, Argentina.

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 - 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](#).

A review of the top 100 medicinal plants in India is ready for publication in either PAC or Natural Products Reviews.

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

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

Antonio has written a project related article entitled "Functional Foods, Reflections on an Expanding Market" which appeared in [Chemistry International, 2008, 30\(September-October\) N° 5, 9-13](#). The same article has also been published in Revista de la Asociación de Química y Farmacia de Uruguay, 2008, [53](#), 16-23; in Cuba in CENIC. Ciencias Químicas, 2008, [39](#), 81-85; and in Sociedad Química del Perú, 2008, [74](#) (2), 138-147. He has also reviewed a book on Functional Food and Health in Chemistry International, 2009, [31](#), (March-April) N°2, p26. Articles on Functional Foods in Mexico, Functional Foods in Uruguay and Functional Foods in Perú are in preparation by Drs G. Rivera, H. Cerecetto, and D. Flores respectively.

The original idea of compiling a number of contributions into book format is unlikely to happen given the insufficient number of articles / chapters available.

4.3.5 Analogue-based Drug Discovery II(Janos Fischer).

IUPAC project [2008-013-1-700](#)

A project announcement appeared in [Chemistry International, March/April, 2009, 31, p20-21](#).

Commitments for 26 chapters have been obtained. A number of manuscripts have been received already with a target date of May 31st for receipt of all manuscripts from the authors.

In addition to Chapters on the general aspects of analogue-based approaches to drug discovery and general discussions of a number of analogue classes, chapters will include case studies on the following drugs:

Eplerenone (J. Kalvoda and M. De Gasparo)

Lapatinib (K. Lackey)

Dasatinib (J. Das and JC Barrish)

Conazoles (J. Heeres, P. Lewi, and L. Meerpoel)

Clevudine (CK. Chu)

Rasagiline (M. Youdim)

Liraglutide (LB. Knudsen)
Tipranavir (S. Thaisrivongs, J. Strohbach, and S. Turner)
Rilpivirine (J. Guillemont)

4.3.6 Stand-Alone Drugs. (Janos Fischer).
IUPAC Project [2005-032-2-700](#)

A progress report on this project appeared in [Chemistry International, Sept/Oct 2008](#), 30, p20-21. This project will be rolled into a chapter for Analogue-Based Drug Discovery II above.

4.3.7 Biological Context by Data Mining (Michael Liebman).
IUPAC Project [2005-049-1-700](#)

This study is nearing completion and a publication is currently being developed to report on the results of the application of text datamining to the identification and evaluation of biological context vs biological content. This topic has gained significant relevance with the increased efforts to develop electronic medical records, etc and the publication is being planned for submission to the Journal of the American Medical Informatics Association with the intent to extend the activity and seek external funding to support a larger project. The targeted submission for this paper is 8/09

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.

4.3.10 Introduction to Computer-Assisted Drug Design.
Project [2007-006-1-700](#) (Yvonne Martin, Tom Perun).

Since no funding is associated with this project, it will be allowed to expire at the end of March.

4.4 New Projects.

5 Division Committee

6 European Federation for Medicinal Chemistry (EFMC).
3rd International Symposium on Advances in Synthetic and Medicinal Chemistry, will take place during August 23 - 27, 2009 Kiev, Ukraine

XXIst International Symposium on Medicinal Chemistry will take place during September 5-9, 2010 Brussels, Belgium

- 7 Asian Federation for Medicinal Chemistry (AFMC)** (Toshi Kobayashi). AIMECS 2009 will be held August 23 – 27 in Cairns, Australia. AIMECS 2011 will take place in Tokyo or Yokohama, hosted by N Shibasaki.

8 Other Business

9 Next Meeting

Glasgow, in conjunction with the General Assembly. Date and location have been requested from John Jost via the Secretariat. Our meeting will be on Sunday 2 August 2009.