

Confirmed Minutes

IUPAC Division of Chemistry and Human Health Subcommittee on Medicinal Chemistry and Drug Development June 14th, 2008, Pittsburgh, USA

Meeting Attendees: Mukund Chorghade, Paul Erhardt, Janos Fischer, Robin Ganellin, Yvonne Martin, Tom Perun, John Proudfoot.

Apologies for being unable to attend were received from: John Bremner, Eli Breuer, Derek Buckle, Ganesan, Toshi Kobayashi, Per Lindberg, Antonio Monge, Feran Sanz, Joerg Senn-Bilfinger, Henk Timmerman, Mario Varasi.

1. Introductions, Opening Remarks, and Minutes of the Previous Meeting in Turin.

The minutes from the previous meeting in Torino (August, 2008), were accepted and will be confirmed and submitted for display on the IUPAC web site.

2. Matters arising from the Minutes

2.1. IUPAC-Richter Prize

Malcolm Stevens, the 2006 recipient, received his Prize at the Istanbul EFMC meeting where he also presented his lecture. The lecture was repeated at the IUPAC General Assembly in Turin.

Seven nominations for the 2008 IUPAC-Richter Prize were received before the nomination deadline of December 31st, 2007. The Prize Committee selected Jan Heeres, (Janssen, retired), notably for his contributions to the invention of ketoconazole and the conazole class of antifungal agents. He has subsequently worked on various other projects, including Rilpivirine, an antiviral agent that is currently being assessed in Phase 3 clinical trials for the treatment of AIDS. The award was presented during a special awards session at the ACS 31st National Medicinal Chemistry Symposium on June 18th 2008, in Pittsburgh. Jan received his plaque and cheque and presented the IUPAC - Richter Award Lecture entitled: "Progress in the Development of Non-nucleoside Reverse Transcriptase Inhibitors: From TIBO to Rilpivirine", and was joined by Professor Edward Arnold (Rutgers University) who lectured on "High-Resolution Structures of HIV-I RT / Rilpivirine complexes."

Two repeat lectures are planned; the first at the [XXth International Symposium on Medicinal Chemistry](#) (Vienna) in September, and the second at the 2nd [Coast to Coast Medicinal and Synthetic Chemistry Symposium](#) (Torquay, UK) in October 2008.

We are grateful to all the conference organizers for providing sponsorship covering travel expenses to the award winner.

2.2 IUPAC Emeritus Fellows

After discussion of this topic at the Secretariat, any action on the matter of Emeritus Fellows has reverted to the subcommittee level. The Subcommittee intends to recognize the service of Camille Wermuth, John Topliss and Les Mitscher with the Distinguished Fellow Award of a suitably engraved plaque at the Divisional Meeting of the IUPAC Congress in Glasgow, Scotland, 2009. This recognition could be linked to the medicinal chemistry technical session at the Congress, perhaps with the awardees chairing the session.

Mukund, who is organizing the technical session, will look into the available options.

This proposition has to be ratified by discussion at the Division Committee level, especially to allow the other Subcommittees to act if they wish to. Robin will notify Doug Templeton, the Division President, of our Subcommittee's intentions.

3. Membership

Prof Peter Matyus (Hungary) and Noël J. de Souza (Mumbai, India) accepted invitations to join the Subcommittee.

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

No additional information.

4.1.4. Glossary on Drug Metabolism Terms (Paul Erhardt)

IUPAC Project 2000-009-1-700

Adjustment of formatting to IUPAC requirements is ongoing. Completion of the Glossary is still targeted for the end 2008, with publication in PAC as part of a thematic issue on "Metabolism Issues in Drug Design".

4.1.5. Compendium of Glossaries (Robin Ganellin)

IUPAC Project 2002-001-1-700

There was some debate on the relevance of publishing a collection of Glossaries in book form, given the growing use of internet resources for information retrieval. One suggestion is to provide this collection of Glossaries online, rather than as a published manuscript.

Robin will determine which of the glossaries is already available online and/or text-searchable and will decide on a strategy for the project based on this information.

4.1.6. Glossary of Terms in Pharmaceutics (Eli Breuer)

IUPAC Project 2001-049-2-700

The draft glossary was circulated to twenty referees and many of the suggestions returned were incorporated into the document.

A communication from the US Pharmacopoeia indicated concern regarding some definitions that differ from those of the Pharmacopoeia. The Subcommittee recommendation is to incorporate the Pharmacopoeia's definition into the glossary in cases where it is clearly superior. However, there may be instances where the IUPAC definition is more suitable for a chemistry audience. In these cases, the IUPAC definition should be retained.

Mukund will meet with Pharmacopoeia representatives to attempt to resolve the differences.

4.1.7. Glossary of Terms in Pharmaceutical Process Chemistry (Mukund Chorghade)

IUPAC Project 2001-049-2-700

See 4.1.6 above. Mukund has submitted this glossary to the US Pharmacopoeia and asked them to review the terms.

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

IUPAC Project 2005-050-0-700

No new information. JP will organize an internet conference with Michael and Robin to discuss this project.

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

IUPAC Project 2004-019-3-700

A draft version of the glossary, containing 152 terms, has been reviewed by members of the SBS and has been adjusted to IUPAC formatting requirements. There was some discussion on the merits of disseminating the work as a "compendium of terms" rather than an IUPAC recommendation and it was suggested that Jack Lorimer be contacted for advice.

Post meeting note. Feedback from Professor Lorimer encouraged publication as a joint recommendation from IUPAC, SBS and IUPHAR. Olivier Nosjean, a task group subteam leader, had already initiated this contact. The formatting generally complies with IUPAC standards and once input is obtained from IUPHAR the document will be submitted for formal IUPAC review. The document has been circulated to all Subcommittee members.

4.1.11 Glossary of Terms in Medicinal Chemistry (Derek Buckle)

IUPAC Project 2008-010-1-700

This project has been approved with Derek Buckle as project leader and Robin Ganellin, Joerg Senn-Bilfinger, Tom Perun, John Proudfoot and Paul Erhardt as task group members. Derek is actively seeking to identify additional team members. Meanwhile Subcommittee members are requested to propose new terms for definition.

The Subcommittee and task group members gratefully acknowledge the financial support (\$2500) provided by the American Chemical Society for this project.

Post meeting note: Toshi Kobayashi will participate as a project team member.

4.2. Training and Development

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

Antonio has provided medicinal chemistry courses in Puerto Rico and Peru. Antonio has expressed an interest in setting up a global network to promote the study of new drugs for the treatment of neglected diseases.

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

IUPAC Project 2001-048-2-700

No new information.

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

IUPAC Project 2004-028-1-700

www.iupac.org/publications/cd/medicinal_chemistry/

A printed version of the book will be produced by Dra Rosa Cattana, Universidad Nacional de Rio Cuarto, Cordoba, Argentina. It will be dedicated to Prof. Dr. Liliana Giacomelli who was a co-author of exercises (I.6, I.7, and VI.2) and who, sadly, died in an accident at work last December.

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 drug metabolism database has been assembled. Paul is pursuing opportunities for public funding to complete the project through the end of this year. One company from the private sector has expressed an interest in the database and discussions are ongoing.

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

IUPAC Project 2001-050-2-700

No new information, editing is ongoing and the final article is planned for publication in PAC.

4.3.4. Latin American Plants as Sources for Functional Foods (Antonio Monge)

IUPAC Project 2005-031-2-700

The initial plan for an article covering plants from Uruguay, Peru and Mexico has been modified. The current intention is to generate three individual articles, each concentrating on a single country. The first article, which is general and will act as an introduction, is completed and is ready for submission. The collection of the articles generated by this project could be combined eventually into a book.

An announcement of progress in the project is in preparation for Chemistry International.

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

IUPAC Project 2008-013-1-700

The book "Analogue-based Drug Discovery" published in January 2006 by Wiley-VCH generated significant interest in the drug discovery and development community and the intention is to provide a second volume of equivalent quality. Janos has decided on an outline for the book, and identified authors and topics. Chapter outlines are in progress and expected from the authors within the next few months.

The draft outline of the new volume is as follows:

I. Introduction

II. General Aspects

1. Optimizing Therapy by Analogues (J. Fischer, EM. Alapi)
2. Analogues and Standalone Drugs (J. Fischer, R. Ganellin, Ganesan, J. Proudfoot)
3. Molecular Modeling in ABDD (G. Ferenczy)
4. The Impact of Natural Products upon Modern Drug Discovery (Ganesan)
5. Monoterpenoid Indole Alkaloids (Nemes)
6. Paclitaxel analogue (Erhardt)
7. Issues for Patenting of Analogues (Smith)

III. Analogue Classes

1. Beta2 agonists (Gaviraghi)
2. M3 muscarinic antagonists (Grauert)
3. SSRIs (Rotella and Childers)
4. Progestogens (Tuba)
5. DPP-IV inhibitors (Peters and Mattei)
6. PDE5 inhibitors (Haning and Bischoff)
7. CB1 antagonists (Carpino and Griffith)

IV. Case Studies

1. Eplerenone (Kalvoda and De Gasparo)
2. Lapatinib (Lackey)
3. Dasatinib (Das)
4. Conazoles (Heeres, Lewi and Meerpoel)
5. Clevudine (Chu)
6. Rasagiline (Youdim)

V. Table of Analogue Classes and Standalone Drugs (EM. Alapi and Fischer)

4.3.6. Stand-alone Drugs (János Fischer)

IUPAC Project 2005-032-2-700

An assessment of the stand-alone drugs that are present in the top 400 of the IMS list has been completed. Janos and Robin have drafted a preliminary report for Chemistry International that describes the stand-alone drugs in the top 100 of the IMS 2006 list.

The current plan is to provide a chapter on this topic for project 4.3.5 above.

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.

4.3.10. Introduction to Computer-Assisted Drug Design (Yvonne Martin, Tom Perun)

IUPAC Project 2007-006-1-700

Work on this project is slated to begin in September, with a timeframe for completion of 18 months. However, since Yvonne already had a signed contract in place with Wiley prior to project approval, the status of this project (which carries no funding allotment) will need to be reconsidered.

4.4. New Projects

No new information.

5. Division Committee

Professor Douglas M. Templeton (Canada) was named as the new Division President (term 2008-11).

Prof. Pedro Soares de Araujo was unable to assume the position as new President, because his country (Brazil) did not pay the membership fees due to IUPAC.

6. EFMC (European Federation for Medicinal Chemistry)

XXth International Symposium on Medicinal Chemistry will take place in Vienna, Austria from August 31 to September 4, 2008.

XXIst International Symposium on Medicinal Chemistry will take place in Brussels, Belgium in September, 2010

7. AFMC (Asian Federation for Medicinal Chemistry)

AIMECS 09 will take place in Cairns, Australia from August 23 to 27, 2009.
AIMECS 11 will be in Tokyo, Japan.

8. Other Business

The Subcommittee expresses its thanks and appreciation to Professor Barry Gold (University of Pittsburgh) for arranging meeting facilities.

9. Next meeting

Vienna, August 30th - 31st in conjunction with the EFMC XXth ISMC.