

CONFIRMED MINUTES

IUPAC Division of Chemistry and Human Health
Subcommittee on Medicinal Chemistry and Drug Development
September 3-4th 2010, Brussels, Belgium

Meeting Attendees: Sergey Bachurin, Derek Buckle, Janos Fischer, Robin Ganellin, A. Ganesan, Per Lindberg, Peter Matyus, Tom Perun, Joerg Senn-Bilfinger, Giorgio Tarzia, Henk Timmerman, Johan Ulander

Apologies: Dave Alker, John Bremner, Eli Breuer, Mukund Chorghade, Paul Erhardt, Toshi Kobayashi, Yvonne Martin, Antonio Monge, John Proudfoot, Ferran Sanz, Noel de Souza, Mario Varasi, Yao Zhu-Jun

1. Introductions and Minutes of the last Meeting.

RG welcomed our potential new member Johan Ulander.

The minutes of the last meeting held in San Francisco (29th March 2010) 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 for 2010

It was noted that Professor Arun K Ghosh (Purdue University, USA), the recipient of the 2010 IUPAC- Richter Prize, had already presented one lecture on the 9th June at the 31st National Medicinal Chemistry Symposium in Minnesota at which Paul Erhardt presided. A second lecture will be presented at the current XXIst EFMC Symposium in Brussels on 7th September during which RG would preside and present him with his plaque.

RG would investigate the possibility of using IUPAC publicity concerning the award lecture in MedChemComm, the newly introduced journal jointly published by the RSC and EFMC. He also reported that we should try to ensure a proportionate allocation of space in Chemistry International for reporting on these awards to that provided for other IUPAC Divisions (i.e. a full page). For example, see CI 2010, 32, N^o 3 (May-June), pp 14-17 and back cover.

2.2 IUPAC Emeritus Fellows

Despite considerable delays, production of suitable plaques for the three Medicinal Chemistry and Drug Development Emeritus Fellow awardees, Les Mitcher, John Topliss and Camille Wermuth, is underway. Camille Wermuth will be the first to receive his during his Nauta Award presentation on Sunday 5 September. RG will present him with his plaque just prior to his giving the opening Plenary Lecture. This will give excellent exposure of IUPAC to an audience of over 1100 medicinal chemists. Opportunities to present the other plaques have yet to be identified.

3. Membership

It was noted that Giovanni Gaviraghi stepped down from the Subcommittee and that Pat Woster had accepted an invitation to join. There is an urgent need to identify a Secretary to replace JP. Johan Ulander will also join.

Other names were suggested as possible new members of the Subcommittee and RG will contact them.

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](#)

On account of major restructuring changes taking place at the University of Southampton AG reported that he had been unable to devote time to this Project over the last year. He now hoped to move it forward. He noted, however, that the term 'Combinatorial' is no longer in vogue and that the title of the Project would have to change. It was not clear at this time what terminology was appropriate and AG was awaiting a decision by the ACS regarding the renaming of their combinatorial journal.

4.1.4 Glossary of Drug Metabolism Terms (Paul Erhardt)

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

While progressing very slowly it was reported that this Project is still active and that PE hopes to complete it by 1Q11.

4.1.5 Compendium of Glossaries (Robin Ganellin)

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

This Project is currently on hold.

4.1.7 Glossary of Terms in Pharmaceutical Process Chemistry

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

No new information is available.

4.1.8 Prototype Analysis of Molecular Markers of Cancer (Michael Liebman)

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

Status not known and no new information is available.

4.1.10 Glossary of Terms for Biomolecular Screening (John Proudfoot)

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

This Glossary was approved for publication in PAC on 18 August subject to minor revision. This has now been done and the document was submitted on 29 August.

4.1.11 Glossary of Terms in Medicinal Chemistry (Derek Buckle)

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

This Project is progressing well having had considerable input from various members of the Subcommittee. All of the newly considered terms have now been reviewed and revisions are in hand.

4.1.12 Glossary of Terms in Computational Drug Design (Yvonne Martin)

Four additional Task Group members have been identified for this new Project; making a total of three from the USA, one from Australia and one from the UK. Other possibilities include Ferran Sanz, Peter Etmayer, Gjörgy Ferenczy, and Brigitte Lesur. Three potential referees have been identified and Hugo Kubinyi has also accepted.

4.2 Training and Development

4.2.1 Research and Training in Medicinal Chemistry in Latin America

(Antonio Monge)

No new information available.

4.2.2 Research and Training in Medicinal Chemistry in the Indian Sub-continent

IUPAC Project [2001-048-2-700](#) (Mukund Chorghade)

Two medicinal chemistry workshops are planned to run consecutively in 2011; 4-7th February in Rajkot and 9-10th February in Nagpur. MC is the international advisor and he is currently seeking both speakers and finance. Steve Ley, George Fleet, Bill Greenlee and Janos Fischer are among the confirmed speakers.

4.2.5 Practical Studies for Medicinal Chemistry Students

IUPAC Project [2004-028-1-700](#) (Antonio Monge)

Publication of the first dual language book (English and Spanish or Portuguese) is imminent following resolution of a number of administrative issues and money is now available to continue the initiative. Copies of the book will be sent to AM and made available to authors. TP requires a picture of the cover to add to his PR material.

4.2.6 A Survey of Research into New Drugs for Neglected Diseases in Latin America

IUPAC Project [2009-033-1-700](#) (Antonio Monge)

A questionnaire was sent to key institutions in Latin America and replies have been received from 15 countries detailing their interests, specific skills, needs and existing collaborations. From these responses AM hopes to clarify

individual areas of strength and weakness and further develop collaborative effort.

4.3 New Technologies and Special Topics

4.3.2 Project on Human Drug Metabolism Database (Paul Erhardt)

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

More funding is needed for this Project to continue but it was noted that considerable compilation had already been done. DB asked whether this potentially very useful embryonic database could be made available to the subcommittee.

It was suggested that the Project might be restarted by means of funding via a Project extension.

4.3.3 Natural Products with Medicinal and Nutritional Value

(Mukund Chorghade) IUPAC Project [2001-050-2-700](#)

No new information available.

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

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

A review has now been published under the title Traditional Foods as a Source of Functional Foods in *Cyta*, **8**(2) 159-167, 2010.

4.3.5 Analogue-based Drug Discovery II (Janos Fischer)

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

This second book in the series (Editors JF and RG) was published in July and involved 41 contributors from 10 countries. It is of similar size to volume I which was published in 2006. Thanks to JF and Fabienne Meyers it was nicely reported in C.I. 2010, 32, N°4 (July-August) pp 12-15 and appeared on the front cover.

4.3.6 Standalone Drugs (Janos Fischer)

IUPAC Project [2005-032-2-700](#)

From a survey of the top 100 best selling drugs, nine were identified as standalone drugs. The results were published in Analogue-based Drug Discovery II, as Chapter 2, pp 29-59. Greater impact would result from publication in a journal, rather than a book, and opportunities to do this would be sought. ChemMedChem was suggested as a possible journal. A new project is being considered to extend this to the next 100 or so drugs. AG will draft a new Project Submission Form.....

4.3.7 Biological Context by Text Datamining (Michael Liebman)

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

No new information available.

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

PL discussed problems that have arisen from broad-based patents that can subsequently interfere with more focused and important later applications. He particularly stressed the need for chemists to be more aware of patenting implications when they make new filings. Particular areas of concern were the broad filing that accompanies chemical libraries, especially those containing a large virtual content, since selection patents on specific optimised compounds then become very difficult to achieve. The primary goal of this new Project would be to send out a questionnaire to identify key issues of concern and to collate subsequent findings. The next stage would be a document intended to educate medicinal chemists on best practices. One specific area of need relates to compounds that are of potential or proven benefit yet for which no strong patent position is possible. Currently such compounds are usually abandoned. A further aim would be to enhance the lay public appreciation of the patenting process and its value to the development of drugs and hence its contribution to human health. PL was asked to complete a Project Submission Form for Subcommittee review. Possible Task Group members include Steve Smith and Paul Bartlett.

4.4 New Projects

4.4a Physicochemical Properties and SAR-analysis (Johan Ulander & Per Lindberg)

JU outlined current thoughts on the use of lipophilic ligand efficiency (LLE, defined as $p\text{LogIC}_{50} - \log D$) as a more accurate parameter for SAR analysis. He proposed a Project that to some extent would be of educational value to medicinal chemists as well as attempting to collate and unify modern practices. A draft Project Submission Form would be prepared detailing the objectives and outcomes of the Project for which PM, AG and possibly JP might contribute. The ACS Boston meeting had a session on this topic. TP to advise.

4.4b Neglected Diseases (Pat Woster)

PW planned to extend the survey of research into new drugs for neglected diseases to areas outside of Latin America and hopes to put forward a proposal for consideration by the Subcommittee. It was noted that Dundee has an active unit focused on 3rd World Diseases in which Paul Wyatt is a senior scientist and he might wish to contribute. He had been one of the referees identified in the Project Submission. (It was also suggested that Paul Wyatt might be a possible speaker for Puerto Rico).

4.4c Analogue-based Drug Discovery III (Janos Fischer)

Following the success of the two earlier volumes in this series, JF proposed a third volume based on the same broad structure. He currently has 64 potential

case studies from which to choose and hopes to complete the proposal by the next Subcommittee meeting. The estimated date of publication is 2013..

4.4d Possible Project to highlight specific IUPAC activities (Johan Ulander)

In discussions JU identified a need to raise broader awareness of IUPAC activities, especially via the existing web site which is not always easy to navigate. In particular, he mentioned IUPAC's access to Google and Wikipedia. He volunteered to review the issue to see whether a Project submission might be appropriate.

5 Division Committee

It was noted that Francoise Pontet will be the new Divisional President following the retirement of Doug Templeton at the end of 2011 and that Michael Schwenk was the new Divisional Secretary.

TP is collating the names of potential new Titular Members; three of whom are required for the next four year term beginning in 2012. He emphasised that thoughts should be given to succession planning for the next Divisional President since following normal rotation he/she would come from our Subcommittee. DB agreed to contact Chris Hill as a possible Division Committee nominee.

6 European Federation for Medicinal Chemistry (EFMC)

The EFMC XXIst ISMC Symposium in Brussels follows on the 5-9th September 2010 (www.ismc2010.org). The Emeritus Fellow Plaque would be presented to Camille Wermuth on 5th September. The IUPAC Richter Prize would be presented to Arun K Ghosh before his Plenary Lecture on 7th September.

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

The next AIMECS 11 meeting will be held in Tokyo, November 29th to December 2nd 2011 (www.aimecs11.org). A brochure was circulated to the Subcommittee.

8. IYC 2011 and IUPAC World Chemistry Congress

Doug Templeton suggested that IUPAC- Richter Prize recipients might be willing to provide some video input for the International Year of Chemistry (2011) and RG had contacted Professor Ghosh and previous recipients in the hope that they might be able to provide a CD of their talks, simplified for a less specialised audience, especially schools. The response was encouraging, but highly dependent on the amount of time available in which to prepare something appropriate. In a similar vein DB suggested that a CD from the Royal Society of Chemistry, Biological and Medicinal Section, BMCS, that had been circulated to British schools, might also be suitable.

Other ideas included approaching David Phillips, formerly of the Royal Institution and current RSC President, who had presented numerous educational lectures in the hope that he could provide something suitable. (There is an article on David Phillips in the September 2010 RSC News in which he states that he is keen to be actively involved in IYC. Contact at president@rsc.org). John Topliss might also be in a position to provide something on the relationship of natural products to small molecules based on his article in PAC. RG would make enquiries.

The previous Subcommittee Meeting in San Francisco was followed by the second IUPAC-ACS Collaboration Summit meeting to discuss IYC and the IUPAC World Chemistry Congress in Puerto Rico; RG and MC attended. RG made contact with Prof. Kathy Kantardjieff to plan for a day's Symposium on Structure-based Drug Design (see the minutes from San Francisco, item 8) Subsequently, however, neither RG nor MC were able to elicit a response from her after sending several e-mails. Consequently, other plans have been made and MC managed to obtain a one-day symposium slot in Puerto Rico allocated to Medicinal Chemistry and Drug Development for which the focus would be The Search for Drugs for Orphan Diseases. RG has put together a skeleton programme and will now start to contact potential speakers. It was suggested that the EU initiative on neglected diseases and recent related symposia organised by the Gordon Research Conference and EFMC might identify additional speakers and topics.

9 Any Other Business

None to report

10 Date of Next Meeting

The next meeting will coincide with the Anaheim ACS meeting next March. Possible dates are 25th March or 1st April 2011 (this is well before Easter). The Subcommittee members would be canvassed for their preference.