

## Confirmed Minutes

### IUPAC Division of Chemistry and Human Health Subcommittee on Medicinal Chemistry and Drug Development March 29<sup>th</sup> 2012, San Diego, USA

**Meeting Attendees:** Tom Perun (acting chair for this meeting), John Proudfoot (acting secretary for this meeting), Janos Fischer, Toshi Kobayashi, Mukund Chorghade, Yvonne Martin, Sergey Bachurin, Balu Balasubramanian, Anita Mehta, William Greenlee, Anjali Rahatgaonkar, Johan Ulander.

**Apologies:** Robin Ganellin, Paul Erhardt, Per Lindberg, Jörg Senn-Bilfinger, Henk Timmerman Peter Matyus, Camille Wermuth.

#### 1. Introductions and Minutes of the last Meeting.

Tom welcomed Professor Anjali Rahatgaonkar, National Representative from India to Division VII. Also attending for the first time were Dr William Greenlee, Dr Balu Balasubramanian and Dr Anita Mehta.

Tom Perun provided an introduction to the workings of IUPAC, Division VII and the subcommittee for the new members present for the first time: He emphasized the central importance of projects and project funding to the framework of our activities.

Minutes from the Puerto Rico meeting were not available for comment. Minutes from the [Anaheim meeting](#) (Spring 2011) are now posted on the IUPAC web site.

#### 2. Matters arising from the Minutes

##### 2.1 IUPAC Richter Prize for 2012

The winner of the 2011 prize was announced at the meeting to be Professor Stephen Hanessian.

An [announcement](#) appeared concurrently on the IUPAC website. The award announcement highlighted the outstanding achievements of Professor Hanessian in natural product chemistry, his Chiron Approach to chiral compound synthesis, and his many seminal contributions that have facilitated the synthesis and discovery of medicinally active compounds and novel drug prototypes.

The IUPAC-Richter Prize, comprising a plaque and a cheque for USD 10,000, will be presented on May 21, 2012, at the 33rd ACS National Medicinal Chemistry Symposium in Tucson, Arizona. The plaque will be signed by Prof. Kazuyuki Tatsumi, President of IUPAC, Erik Bogisch, Chief Executive Officer of Gedeon Richter plc (Budapest, Hungary), and Prof. Robin Ganellin, Chair of the IUPAC-Richter Prize Selection Committee.

Prof. Hanessian will present his award lecture at this symposium and also at the XXII EFMC International Symposium on Medicinal Chemistry in Berlin, Germany, 2-6 September 2012

## 2.2 IUPAC Emeritus Fellows

Plaques recognizing the contributions of subcommittee emeritus fellows, Camille Wermuth, John Topliss and Les Mitscher have now been presented. The plaque awarded to Camille Wermuth was presented by Robin Ganellin at the EFMC meeting in Brussels September 5, 2010. The plaque for Les Mitscher was presented by Tom Perun at the ACS Medicinal Chemistry Division Hall of Fame reception in Denver last August . The plaque for John Topliss was accepted at the same meeting by Steve Munk on his behalf. Emeritus Fellow status for Nao Koga has also been proposed and Toshi Kobayashi agreed to identify a suitable forum for the presentation.

## 3. Membership

Robin Ganellin, the current subcommittee chair has reiterated his intention to step down from this position. See Section 8 below for discussions and planning in relation to this.

The process of selecting candidates for Titular Members of the Division of Chemistry and Human Health will begin again this year. A Nominating Committee will be assembled, and candidates will be selected from individuals proposed by the National Adhering Organizations and from Division members. Since the terms have been shortened to two years each, a total of eight positions will be open. Current TMs who have not used up their eligibility can be nominated for re-election.

## 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 new information available. Professor Ganesan has recently moved to a new academic position.

#### 4.1.4 Glossary of Drug Metabolism Terms (Paul Erhardt)

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

The glossary is still at the stage of adjusting to IUPAC format and is a top priority for completion by Paul.

#### 4.1.5 Compendium of Glossaries (Robin Ganellin)

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

This Project is on hold.

#### **4.1.7 Glossary of Terms in Pharmaceutical Process Chemistry**

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

The glossary is almost complete and just awaiting some responses from the FDA. It is expected that the glossary will be ready for publication by year end. The exact timing will likely depend on the extent of external review still required.

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

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

Publication of the project results was delayed since approval from a co-sponsoring organization was not forthcoming. Approval is now available to publish a portion of the results.

#### **4.1.11 Glossary of Terms in Medicinal Chemistry** (Derek Buckle)

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

The document is formatted and is ready for review at the Division level. Preparation for external review is in progress.

In addition to publication in PAC, Tom noted that it is scheduled for publication in Annual Reports in Medicinal Chemistry (2013). It was also suggested that a link to the glossary (perhaps the PAC publication itself) be placed on the ACS MedChem Division home page.

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

Approximately 250 terms have been collected and these are being culled to the most relevant. Around 20% of the terms in the original glossary are also found to be in need of updating.

### **4.2 Training and Development**

#### **4.2.1 Research and Training in Medicinal Chemistry in Latin America**

(Antonio Monge)

See 4.2.5

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

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

A joint meeting with the RSC, IUPAC and the ACS was held in Rajkot in January/February 2011. No funding for travel is presently available. If we are to participate in future meetings it is very important to have clear planning in good time beforehand and to know what the programme will be.

#### 4.2.5 Practical Studies for Medicinal Chemistry Students

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

This project was completed with the publication of the book, Practical Studies for Medicinal Chemistry, An Integrating Approach for Developing Countries. The book was published in three languages, Spanish, Portuguese and English, (ISBN 978-950-665-570-9) and is also available in a web edition. It has been very well received by the intended audience, and the web edition is being used extensively.

#### 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 network of 30 research centers in ten countries has been identified, with the names of the researchers and the diseases being studied. The next stage is to determine the nature of the research program, and to make this information available to government, industry and philanthropic organizations.

### 4.3 New Technologies and Special Topics

#### 4.3.2 Project on Human Drug Metabolism Database (Paul Erhardt)

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

A new project to continue development of the database has been approved.

IUPAC Project [2011-018-1-700](#)

Paul has identified an informatics/database core group on UT's health sciences campus that is willing to assist him on the project. The project will move from the original Oracle platform to a common desk-top platform.

The complete project submission/description is available on the IUPAC Projects website via the hyperlink above.

The project announcement was published: [Chem. Int. Jan-Feb 2012, p. 22](#)

#### 4.3.3 Natural Products with Medicinal and Nutritional Value

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

An article has been submitted to PAC.

#### 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)

Activities on this potential project are on hold and at this point it is unlikely a project proposal will be prepared unless a new sponsor is forthcoming.

#### 4.3.9 Analogue-based Drug Discovery III. (J. Fischer)

IUPAC Project [2011-011-1-700](#)

The book is scheduled for publication in Q3 2012. Reviews for the selected chapters are completed. The book includes contributions from 39 authors from 9 countries.

Some of the chapters deemed not ready for this volume may be appropriate for a fourth volume.

#### 4.4 New Projects

4.4a: Physicochemical properties and SAR-analysis (J. Ulander, P. Lindberg).

A project proposal has been prepared and is ready for submission.

4.4b: Neglected diseases (P. Woster).

Project proposal has not been submitted yet

4.4c: Rare Disease (Ramaiah Muthyala)

A project proposal was submitted. Feedback from the review process is awaited.

4.4d: Tutorials on Neglected Diseases (Y. Martin)

This project proposal will not be submitted

4.4e: Analogue-based Drug Discovery, Vol IV (J. Fischer)

Janos has identified more than 30 possible topics for a fourth Volume. Once activities on ABDD-III are completed, a new project for Vol IV will be proposed.

4.4f: DMPK certified course in India (B. Balasubramanian).

The objective is to provide, in India, advanced training along the lines of that provided by the Drew University course in Medicinal Chemistry and Drug Discovery. The course is planned for 2013 with facilities and infrastructure to be provided by Sri Ramachandra University in Madras and would take place over 3-4 days. Faculty/speakers have been identified and up to 100 attendees are expected. Sponsorship is being sought from IUPAC and the ACS Med Chem Division.

The objective of this course fits well with the goals of the subcommittee on Research and training in medicinal chemistry and it was recommended that a project proposal, with requested funding at the \$5000 level, be submitted.

#### 5 Division Committee

It was noted that Françoise Pontet would be the next Divisional President and that Michael Schwenk will continue as the Divisional Secretary. The next meeting is in Budapest, Hungary, June 22-23, 2012. .

## **6 European Federation for Medicinal Chemistry (EFMC)**

The next EFMC ISMC Symposium would be held in Berlin on the 2-6<sup>th</sup> September 2012 (<http://www.ismc2012.org/>). The IUPAC Richter Prize award winner, Professor Hanessian will present a lecture at the meeting.

## **7 Asian Federation for Medicinal Chemistry (AFMC)**

More than 1000 attendees participated at the AIMECS 11 meeting held in Tokyo on November 29<sup>th</sup> to December 2<sup>nd</sup> 2011, and two sessions were organized by the ACS and EFMC medicinal chemistry societies.

The next AIMECS meeting will be held in Taiwan in 2013 followed by South Korea in 2015.

## **8 Any Other Business**

### **8.1 Succession for subcommittee Chair and Secretary.**

The subcommittee members held a prolonged discussion on succession plans for the chair and secretary positions for the subcommittee. As background it was noted that funding is not provided to either the chair or secretary for travel expenses to subcommittee meetings and this directly or indirectly had led to the current chair and secretary being unable to attend this particular meeting. It was also noted that subcommittee meetings tend to alternate between European and US locations which potentially is a significant expense burden to these individuals. It was also noted that the input and guidance that these individuals provide to the project task leaders is of significant value, and that in the future one or other of these individuals should be included on the project teams where applicable.

The following proposals were advanced and agreed by the members present to address this situation for the future.

1. For the future, the subcommittee will have a chair and a vice chair.
2. The chair and the vice-chair will alternately be resident in either North America or Europe.
3. The vice-chair will automatically succeed to the chair after a two year term, at which time a new vice-chair will be identified.
4. In the event that the chair cannot attend a subcommittee meeting, the vice-chair will preside.
5. Tom Perun will continue as acting chair for the Americas through Spring 2013, at which point a vice chair representing the Americas should be identified.
6. Selection of a vice chair representing Europe will be an agenda item for the meeting in Berlin.
7. A similar process will be followed for succession planning for the subcommittee secretary.
8. Derek Buckle, (pending agreement) may continue as secretary for meetings in Europe through 2013
9. A vice-secretary representing the Americas should be identified at either the Fall meeting in Berlin or at latest by the next meeting in North America.

## 8.2

Tom presented a poster on Division activities at the MedChem poster session.

## 9 Date of Next Meeting

The next meeting will be held in Berlin on Saturday, September 1 before the XXII EFMC International Symposium on Medicinal Chemistry, 2-6 September 2012.

Location to be provided at a later date.

