

IUPAC Division of Chemistry and Human Health  
Subcommittee on Medicinal Chemistry and Drug Development  
September 1, 2012 Berlin, Germany

**Meeting Attendees:** Robin Ganellin, Chair, Tom Perun (Acting Secretary), Janos Fischer, Joerg Senn-Bilfinger, David Alker (morning), Henk Timmerman (morning).

**Apologies:** John Bremner, Eli Breuer, Mukund Chorghade, Paul Erhardt, Chris Hill, Toshi Kobayashi, Yvonne Martin, Peter Matyus, Serge Mignani, Antonio Monge, John Proudfoot, Anjali Rahatgoankar, Ferran Sanz, Giorgio Tarzia, Johan Ulander, Mario Varasi.

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

Robin welcomed the Sub-committee members to the meeting and asked for any comments or changes to the minutes for the last MCDD meeting in San Diego. The minutes of the last meeting held on March 29, 2012 were accepted and will be sent to the Secretariat for posting on the IUPAC home page.

### **2. Matters arising from the Minutes**

#### **IUPAC-Richter Prize**

The Richter Prize for 2012 was awarded to Professor Stephen Hanessian at the National Medicinal Chemistry Symposium held in Tucson, Arizona in May, and Professor Hanessian also delivered an award address at the ISMC meeting in Berlin.

The funding for the 2014 prize is being discussed with the Richter Company, and a new agreement between IUPAC and Richter must be worked out to continue the prize beyond 2014. Negotiations are also underway between the EFMC and Richter for a continuation of this prize as part of the ISMC meeting program in future years.

#### **IUPAC Emeritus Fellows**

The recommendation has been made to award Emeritus Fellow status to Nao Koga, for his many years of service to the Medicinal Chemistry Section and his founding of the Asian Federation of Medicinal Chemistry. The Award and Plaque is scheduled to be presented to Nao at the Pharmaceutical Society of Japan meeting, in November 2012 by Toshi Kobayashi.

### **3. Membership**

The matter of appointment of a new Chair and Secretary for the Subcommittee was discussed, but with only a few members present, it was not resolved. Tom Perun will chair the next meeting, which will be held at the ACS meeting in New Orleans in April, 2013. The following subcommittee meeting will be held in conjunction with the Division meeting at the IUPAC General

Assembly in Istanbul, in August, with the Chair to be determined. The Secretary for these meetings has not yet been determined.

There was considerable discussion of the need to attract new members to the subcommittee if it will continue to meet twice a year. The decrease in company funds for industrial members, and the cost of travel for retired members were given as reasons for the low turnout. Younger members using newer communication techniques like Skype may be necessary to enlarge the participants.

New individuals have been suggested for addition to the invitation list for future subcommittee meetings. Those expressing an interest are: Helmut Buschmann, Edmond Differding, Rob Leurs and Brian Rees.

In a post-meeting discussion with the President of EFMC, it was resolved that the EFMC will encourage members to attend the MCDD meeting prior to its next ISMC meeting in Lisbon, 2014, and will begin the Council Meeting at mid-day to allow members to attend the subcommittee meeting in the morning.

#### **4. Projects/Working Parties**

##### **Nomenclature and Terminology**

4.1.2 Glossary of Combinatorial Chemistry Terms. Project 2003-044-1-700 (A.Ganesan). No new information

4.1.4 Glossary of Drug Metabolism Terms. Project 2000-009-1-700 (P. Erhardt). This project is essentially completed but has been on hold for number of years. It is now high on Paul's list of priorities to bring to conclusion.

4.1.11 Glossary of Terms in Medicinal Chemistry. Project 2008-010-1-700 (D. Buckle). This project is complete and the glossary was sent out to external reviewers. The comments from the reviewers have been collected by Derek and are being considered for minor changes. It was recommended that the glossary should be considered as final and no additional terms be added unless there were major omissions.

4.1.12 Glossary of Terms used in Computational Drug Design. Project 2010-057-3-700 (Y. Martin). This glossary is also essentially complete and should be sent to the committee for review.

##### **Training and Development**

4.2.1 Research and Training in Medicinal Chemistry in Latin America. (Antonio Monge). Antonio has scheduled a video conference in Peru, Guatemala, Honduras, and Mexico on Project Management, Benchmarking and Outsourcing in the Discovery of New Drugs in the 21<sup>st</sup> Century

4.2.5 Practical Studies for Medicinal Chemistry Students. Project 2004-028-1-700(Antonio Monge). The book that resulted from this project has been very successful, and an attempt will be made to determine how many hits have been made for the web edition. Robin will ask Paul Erhardt if he is willing to write a review of the book for Chemistry International.

4.2.6 A Survey of Research into New Drugs for Neglected Diseases in Latin America. Project 2009-033-1-700 (Antonio Monge). The initial survey of research being conducted in 30 research centers needs to be expanded to include more information, and the results should be published in appropriate publications outside Latin America. Post meeting note: An article, jointly authored by Monge and Ganellin, was submitted to Fabienne for publication in CI.

### **New Technologies and Special Topics**

4.3.2 Human Drug Metabolism Database. Project 2011-018-1-700 (P. Erhardt). This revitalized project is growing in momentum aided by new funding, a new software platform and new informatics personnel.

4.3.3 Natural Products with Medicinal and Nutritional Value. Project 2001-050-2-700 (M. Chorghade). An article describing this work is planned for submission to Pure and Applied Chemistry.

4.3.7 Biological Context by Datamining. Project 2005-049-1-700 (M. Liebman). No further information on the completion of this project.

4.3.8 Trends in Patenting Drug-Related Technologies. (P. Erhardt and P. Lindberg). A proposal for this project was never completed and nothing is planned.

4.3.9 Analogue-based Drug Discovery III. Project 2011-011-1-700 (J. Fischer). The book has been completed with 15 chapters and 40 authors, and includes chapters on five drug classes and six case studies. It is scheduled for publication in December 2012. Wiley has suggested combining Vols I, II, and III into a paperback book for students.

### **New Projects**

4.4a Physicochemical Properties and SAR analysis. (J. Ulander). The project proposal needs to be resubmitted after discussions with task group members.

4.4b Neglected Diseases (P. Woster). A project proposal has not been submitted yet.

4.4c Rare Diseases (R. Muthyala). A first draft of a project proposal has been submitted. Suggestions have been made for improving the proposal, but questions on its feasibility have not yet been resolved.

4.4e Analogue-based Drug Discovery, Vol IV (J. Fischer). A fourth volume of this successful series has been suggested. Subjects for this volume have

arisen from the previous volumes, and will be considered for another one. The publisher has recommended a change in the title.

4.4f Medicinal Chemistry in India (B. Balasubramanian). This project is based on the successful medicinal chemistry course at Drew University, held once a year. The project proposal has been completed and submitted for approval.

Post meeting note: The reviews have been completed and the project has received an official number: 2012-032-2-700. The course will be held in Chennai, India on Feb 11-14, 2013.

## **5. Division Committee**

Elections will be held later this year for the term beginning in 2014. Three of the current TMs will complete their four year terms at the end of 2013. Four others will complete two years and are eligible for re-election. Doug Templeton will finish his two year term as Past President. Candidates will be chosen by the Nominating Committee for the four open positions.

The next Division Committee meeting will be held in Istanbul during the IUPAC General Assembly in August 2013.

## **6. EFMC**

The next EFMC-ISMIC meeting will be held in Lisbon, Portugal in 2014.

## **7. AFMC**

The next AIMECS meeting will be held in Taiwan in 2013.

## **9. Next Meeting**

The next meeting of the MCDD subcommittee meeting will be held in New Orleans at the spring ACS meeting.

