

IUPAC Division VII Chemistry and Human Health
Medicinal Chemistry and Drug Development Sub-committee

Marriott Convention Center Hotel, New Orleans
April 6, 2013 9:00 am – 5:00 pm

Members present: Tom Perun, Balu Balasubramanian, Janos Fischer, Yvonne Martin

Regrets from: Paul Erhardt, William Greenlee, John Proudfoot, Dave Rotella, Johan Ulander, Edmund Differding, Sergey Bachurin, Derek Buckle, Mukund Chorghade, Antonio Monge, Robin Ganellin

Minutes of the last meeting: Approved.

Matters arising from the Minutes:

IUPAC-Richter Prize: In 2014 the awardee will receive his prize and present a lecture at the European Federation of Medicinal Chemistry, EFMC-ISMC meeting. He/she will also give a lecture at the ACS MedChem Symposium. Richter will provide travel funds for the awardee to attend the EFMC-ISMC meeting. Negotiations are in progress in the hopes that Gedeon Richter Plc will continue to support the IUPAC-Richter prize beyond 2014.

Post meeting note: Robin Ganellin has agreed to chair the selection committee for the 2014 prize this year for one more time.

Emeritus Fellows: Nao Koga was presented with his recognition plaque in November 2012 at a meeting of the Pharmaceutical Society of Japan.

Membership:

Recent Division elections for the 2014 – 2016 term saw the election of Tom Perun, Rita Cornelis, Helle Johannessen, and Linda Johnston as Titular Members, and the re-election of Janos Fischer, Chris Hill, Paul Illing, and Wayne Temple, with Françoise Pontet and Mike Schwenk continuing as officers of the Division. Yvonne Martin, Sergey Bachurin and Derek Buckle will exit the Division Committee as Titular Members.

The MCDD subcommittee will next meet August 11, 2013 as part of the IUPAC General Assembly in Istanbul. Balu has volunteered to organize a Skype teleconference of the meeting of the subcommittee at the 2014 Spring ACS meeting, as a way to include more members in the discussions.

Nomenclature and Terminology Projects:

The members expressed concern about some of the projects that are not completed and for which no progress report was submitted. For many of these the budget has been spent.

Glossary of Combinatorial Chemistry Terms. Project 2003-044-1 (A. Ganesan). Although there is money left, there has been no activity for several years.

Glossary of Drug Metabolism Terms. Project 2000-009-1-700 (P. Erhardt). No report. The project is near completion and the money has been spent, but the status is unclear.

Glossary of Terms in Pharmaceutical Process Chemistry. Project 2001-049-2-700 (M. Chorghade). The money has been spent, and the project is awaiting publication of the glossary.

Prototype Analysis of Molecular Biomarkers in Cancer. Project 2005-050-1-700 (M. Liebman). The money has been spent, and the investigator reports that a manuscript has been submitted. However, Google Scholar identifies no publication by this author with the keywords “biomarker, cancer, IUPAC”.

Glossary of Terms in Medicinal Chemistry. Project 2008-010-1-700 (D. Buckle). This project is essentially complete and is awaiting final approval for publication in Pure and Applied Chemistry. It will also be published in Annual Reports in Medicinal Chemistry.

Glossary of Terms in Computational Drug Design. Project 2010-057-3-700 (Y. Martin). The glossary has been completed and is under review.

Training and Development Projects:

Research and Training in Medicinal Chemistry in Latin America. (A Monge) This project has resulted in a successful textbook on practical studies in medicinal chemistry which is co-authored by Robin Ganellin. A review of the book has been written by Paul Erhardt which will be published in Chemistry International. The review has also been put on the ACS Med Chem website along with a link to the electronic version of the book. Prof. Monge is retiring from his university and will no longer be participating in committee activities.

Research and Training in Medicinal Chemistry in the Indian Subcontinent. Project 2001-048-2-700 (M. Chorghade). This project resulted in a symposium that was well-received and well-attended.

A Survey of Research into New Drugs for Neglected Diseases in Latin America. Project 2009-033-1-700 (A. Monge). This project is complete and a publication co-authored by Robin Ganellin has just appeared as the featured article in the May-June 2013 issue of Chemistry International. It is hoped that an associate of Antonio in Latin America will continue activities in this area after his retirement.

Medicinal Chemistry India. Project 2012-032-2-700 (B. Balasubramanian). This project resulted in a five-day symposium in February 2013. It was attended by 113 scientists, 90 from industry. There are plans to repeat the symposium in two years. Discussion involved the possibility of either holding it in another Asian country (such as Singapore, Philippines, Malaysia, or China) or spinning off a similar symposium in one of these countries. This would depend on identification of a local organizer.

Projects for New Technologies and Special Topics:

Human Drug Metabolism Database. Project 2011-018-1-700 (P. Erhardt). The investigator has submitted a grant proposal to request additional funds for this effort.

Natural Products with Medicinal and Nutritional Value. Project 2001-050-2-700 (M. Chorghade). No report is available on the status of this project.

Biological Context by Text Datamining. Project 2005-049-1-700. (M. Liebman). No report is available on the status of this project.

Analogue-based Drug Discovery III. Project 2011-011-1-700. (J. Fischer). This project is completed with the publication of the book in January of 2013. 40 experts from nine countries have been participating in the book project. Discussion about a possible Volume IV centered on the issue of declining sales of the books in the series, and the publisher's interest in changing the title. Based on the recent information from the Publisher (Wiley-VCH) about 300 books have been sold in about three months. Janos Fischer reported on the book project in *Chemistry International* (2013), 35(1), 24-25. The book's 15 chapters bring important, successful drug discoveries. The major part of the chapters are written by key inventors. The Publisher in agreement with Janos will continue the book project under a new title "Successful Drug Discoveries". The project "Analogue-based Drug Discovery III" was completed in two years according to the schedule.

New Projects:

Successful Drug Discoveries.

The new project proposal has been submitted by Janos Fischer on March 28, 2013. This new project is an extension of the completed project "Analogue-based Drug Discovery" affording three books published in 2006, 2010 and 2013 by Wiley-VCH. The last project focused on drug analogues. The plan of the new project is to present novel drugs that have been approved for use. This will include both pioneer drugs and drug analogues. The new project has a broader scope, nevertheless, the structure of the completed book series will be preserved. The new book will consist of three parts : I. General Aspects of Drug Discoveries, II. Drug Class Studies and III. Case Studies. At least 15 new chapters are planned in the new book. The book authors are mainly key inventors from Europe, Japan and USA. The book will be edited by Janos Fischer and David Rotella. The new book will be published at the end of 2014 or at the beginning of 2015.

Physicochemical properties and SAR Analysis. Proposal is in preparation by J. Ulander and P. Lindberg.

Rare Diseases and Orphan Drugs – Challenges and Opportunities in India. A proposal has been submitted by R. Muthyala.

Other Business:

The next EFMC-ISMC meeting will be held in Lisbon in 2014.

The Asian Federation of Medicinal Chemistry meeting, AIMECS 13, will meet October 15-18 in Taiwan.