

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

Istanbul Convention Centre, Istanbul, Turkey
11 August 2013

Members present: Tom Perun (Chair), Sergey Bachurin, Derek Buckle, Janos Fischer, Yvonne Martin Izabela Tworowska (young observer)

Apologies from: Edmund Differding, Paul Erhardt, Robin Ganellin, John Proudfoot, Dave Rotella, Johan Ulander, Georg Senn-Bilfinger.

Minutes of the last meeting: Approved without change.

Matters arising from the Minutes:

IUPAC-Richter Prize: Information concerning the 2012 recipient, Stephen Hanessian, is now available on the IUPAC web site.

Robin Ganellin has agreed to oversee the jury and select its members for the 2014 prize selection and is to advertise the prize on the web site in September. It is agreed that the 2014 awardee will receive their prize and present a lecture at the European Federation of Medicinal Chemistry, EFMC-ISMIC meeting in Lisbon. He/she will also give a lecture at the 2014 ACS Med Chem Symposium in Charleston. Richter will provide travel funds for the awardee to attend the EFMC-ISMIC meeting. Negotiations are in progress in the hope that Richter will continue to support the IUPAC-Richter prize beyond 2014.

Emeritus Fellows: TP is to add the name of Naofumi Koga, the most recent Emeritus Fellow, to the list of awardees on the IUPAC web site.

It was noted that the Sub-committee is permitted to propose one additional Emeritus Fellow every two years, with another opportunity to do so starting in 2014. Robin Ganellin, who chaired the Sub-committee between 2000 and 2012, was proposed and DB agreed to prepare an appropriate citation in support.

Membership:

Following the election of TP as Divisional President there is an urgent need for a replacement to chair the Sub-committee. While an overall chairman was required, it was suggested that someone based in Europe might chair European-based meetings while a US candidate might chair those based in the USA. Discussions will be held with possible candidates before a decision is made.

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 Francoise 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 at the end of this year.

With the loss of these three funded Titular Members TP emphasized the need to identify replacement medicinal chemists for the Division Committee to augment JF and CH (and himself). Unfortunately CH had failed to attend recent Division and Sub-committee meetings and TP would establish his continued commitment.

It was noted that Antonio Monge had now retired and would no longer participate in the Subcommittee.

Projects:

Divisional concern was expressed over the number of long-term uncompleted projects, many of which had no residual funds and for which no report was available. It was proposed that the current status of moribund projects should be ascertained prior to either closure or reassignment of responsibility if future progress was not expected. Following closure those with residual budget would have this reallocated to other projects.

Glossary of Combinatorial Chemistry Terms. Project 2003-044-1 (A. Ganesan). Although there is still money left in the budget there has been no activity on this project for several years. A request will be made for a copy of the existing document either from AG himself (action DB) or through a project team member. TP would request a list of team members from the Secretariat before a final decision is made concerning its viability.

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. It is understood that the issue is simply one of appropriate formatting and if this were so DB volunteered to assist with doing this. TP would request a copy of the existing document from Paul.

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. Current status unknown.

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 and accepted. No further information is available yet.

Glossary of Terms in Medicinal Chemistry. Project 2008-010-1-700 (D. Buckle). This project is now complete following publication in *Pure and Applied Chemistry* (**85**, 1725-1758, 2013). It will also be published this year in *Annual Reports in Medicinal Chemistry* for which the proofs have been received and reviewed. Post meeting note: Now published: *Ann. Rep. Med. Chem.*, **48**, 387-418, 2013.

Glossary of Terms in Computational Drug Design. Project 2010-057-3-700 (Y. Martin). The glossary is completed and will be sent out for review.

Compendium of Glossaries. Project 2002-001-1-700 (R. Ganellin). No new information received but it seems likely that this project will be terminated.

Training and Development Projects:

Research and Training in Medicinal Chemistry in Latin America. (A Monge). This project is now completed, and a much used e-book is available on the IUPAC website, with a link from the ACS Med Chem website.

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 R. Ganellin has just appeared as the featured article in the May-June 2013 issue of Chemistry International. It is recommended that opportunities for a wider exposure of the information gathered should be explored, particularly with respect to organizations with such interest and other tropical areas where these and related diseases persist. DB will contact RG to see whether he would be prepared to undertake this.

Medicinal Chemistry in India. Project 2012-032-2-700 (B. Balasubramanian). This project resulted in a five-day medicinal chemistry course in February 2013. It was attended by 113 scientists, 90 from industry. There are plans to repeat the course 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 course 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. Current status not known.

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. The Publisher, in agreement with JF, will continue the book project under a new title "Successful Drug Discoveries".

New Projects:

Successful Drug Discoveries. The new project proposal was submitted by JF in March 2013 and is an extension of the completed project "Analogue-based Drug Discovery". The plan of the new project is to present novel drugs that have been approved for use. It will include both pioneer drugs and drug analogues and preserve the structure of the completed book series. 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 by authors that are mainly key inventors. It will be edited by J. Fischer and D. Rotella with an anticipated publication date towards the end of 2014 or the beginning of 2015.

Physicochemical properties and SAR Analysis. A proposal is in preparation by J. Ulander and P. Lindberg but no further information is currently available.

Rare Diseases and Orphan Drugs – Challenges and Opportunities in India. A proposal has been submitted by R. Muthyala. After reviews were conducted, the project was not funded.

Other Business:

With the increasing diversification of medicinal chemistry, TP questioned the continued use of this term for the Sub-committee, suggesting that Drug Discovery and Development might be more appropriate. This would broaden the scope of activities and encourage projects with new technologies. It would also

align it more with the recent proposal made for the Medicinal Chemistry Division of the ACS. TP would canvas opinions from other members of the Sub-committee.

The first Russian Conference on Medicinal Chemistry will be held between 9-12 September 2013 in Moscow, Russia (www.medchem2013.com).

The Ninth Asian Federation of Medicinal Chemistry meeting, AIMECS 13, will meet on 15-18 October 2013 in Taipei, Taiwan. (www.aimecs13.tw).

The XXIIIrd EFMC-ISMC meeting will be held between 7-11 September 2014 in Lisbon, Portugal.

Date of next meeting: It was proposed that the next meeting would coincide with the Divisional meeting in Brussels May 2014. A second meeting will coincide with the EFMC-ISMC symposium in Lisbon in September 2014. It was appreciated that funding issues made it difficult for US members to attend European meetings and *vice versa*. TP would therefore ascertain the likely numbers attending the Dallas ACS meeting to assess the possibility of holding a US-based sub-committee meeting next year in March.