

CONFIRMED MINUTES

IUPAC Division of Chemistry and Human Health
Subcommittee on Medicinal Chemistry and Drug Development
March 20 – 21, 2010, San Francisco, USA

Meeting Attendees: Derek Buckle, Paul Erhardt, Janos Fischer, Robin Ganellin, Tom Perun, Joerg Senn-Bilfinger, Toshi Kobayashi, Yao Zhu-Jun, Mukund Chorghade (in part). By teleconference: John Proudfoot.

Apologies: Sergey Bachurin, Eli Breuer, J. Bremner, Mukund Chorghade, G. Gaviraghi, Michael Liebman, Per Lindberg, Yvonne Martin, Peter Matyus, Antonio Monge, Henk Timmerman

1. Introductions and Minutes of the last Meeting.

RG welcomed our new member Zhu-Jun Yao and, following a brief introduction of those present, the minutes of the last meeting held in Glasgow (2-3rd August 2009) were accepted without revision. They will be sent to the secretariat for posting on the IUPAC home page. It was noted that the Salt Lake City minutes are now on the web site.

2. Matters arising from the Minutes

2.1 IUPAC Richter Prize for 2010

It was reported that advertising for the 2010 Richter Prize was slow to get into J. Med Chem., but it received timely circulation in the Med. Chem. Newsletter and elsewhere. As a result, nominations for 10 candidates were received, six of which were from the 2008 applicants. The panel, consisting of 2 members from the US, 3 from Europe and 2 from Australasia, proposed that Professor Arun K Ghosh (Purdue University, USA) should receive the award for his outstanding use of structure-based design for the identification of novel HIV protease and β -secretase inhibitors. It was noted that the HIV protease inhibitor, Darunavir, resulting from this work was now approved by the FDA. RG summarised the very impressive career of Arun Ghosh which started with 6 years at Merck, West Point, PA, followed by a rapid progression in academia leading to his present position as Ian P. Rothwell Distinguished Professor of Chemistry and of Medicinal Chemistry at Purdue University.

It was proposed that the award lecture, entitled '*Behind the Design of Darunavir for AIDs and β -secretase Inhibitors for Alzheimer's Disease*' would be presented on June 9 at the 32nd National Medicinal Chemistry meeting at the University of Minnesota, Minneapolis and repeated on September 7 at the Brussels ISMC 21st Symposium. In order to alternate the presentation, between Europe and the USA, the prize itself would be awarded in Brussels. It was anticipated that the expenses associated with these two lectures would be met by the two Symposia respectively.

RG has contacted all 2010 nominators to inform them that the award has been made. Three (or possibly 5) runners up would be invited to submit for the 2012 award.

RG reported that Terry Renner, the new IUPAC Executive Director, had requested information on the Richter Prize for PR purposes. This was subsequently provided.

2.2 IUPAC Emeritus Fellows

The term Emeritus Fellows rather than Distinguished Fellows is now the preferred Divisional designation but urgent finalisation is required (hopefully in Copenhagen on 29th March) if plaques are to be available for presentations at Minneapolis (for US recipients) and Brussels (European recipients) this year. The three nominations from the Subcommittee on Medicinal Chemistry and Drug Development are Les Mitcher, John Topliss and Camille Wermuth. RG read out a short citation for each. It was proposed that an announcement of these awards should be made in Chemistry International by RG.

3. Membership

The Subcommittee is keen to recruit people that have made an impact on their national committees and suggestions for new members are always welcome. A particular problem was noted for those who are also members of the Division Committee when time and financial constraints can result in a conflict of interest. This is particularly so with Titular Members who receive funding to attend Division Committee meetings whereas only project leaders receive funding to attend Subcommittee meetings. This was apparent at this Subcommittee meeting when two members attended the following Division Committee meeting in Copenhagen but could not come to San Francisco.

TP reported that nominations for Titular Membership starting in 2012 were now solicited. There is a need to take into consideration both disciplinary interest and geographic representation. It was noted that the Subcommittee is well represented on the Divisional Committee and that four Titular Members were due to retire at the end of 2011 (Ole Andersen, Xavier Fuentes-Arderiu, Françoise Pontet, Giorgio Tarzia)

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. RG to request a short report.

4.1.4 Glossary of Drug Metabolism Terms (Paul Erhardt)

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

Undergoing conversion to the requisite format with the hope that it will be complete by the year end.

4.1.5 Compendium of Glossaries (Robin Ganellin)

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

This Project is awaiting the completion of one new glossary.

4.1.7 Glossary of Terms in Pharmaceutical Process Chemistry

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

Almost complete.

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

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

No new information available.

4.1.10 Glossary of Terms for Biomolecular Screening (John Proudfoot)

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

The final version has been sent to Doug Templeton and is awaiting last comments prior to submission to Pure and Applied Chemistry at the end of March. Publication will also be on the Society for Biomolecular Sciences' web site and possibly in their journal.

Post meeting note: *The revised glossary was submitted to PAC on March 28th.*

4.1.11 Glossary of Terms in Medicinal Chemistry (Derek Buckle)

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

A large proportion of the new terms have now been reviewed at both the Glasgow and San Francisco Subcommittee meetings. After consideration of the remaining terms the document will be formatted for finalisation as an adjunct to the earlier Glossary.

Post Meeting Note: *The possibility of combining the old and new Glossaries was discussed at the Division Committee, however this might become too large to be accepted for publication in Annual Reports of Medicinal Chemistry. Would need to explore this.*

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

YM has agreed to update the existing Glossary (1997) but the submission proposal lacks a full analysis of the statistics for its use. Available data indicate that the Glossary is still being used so RG will reformulate the submission based on the existing statistics.

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)

Strong support continues for this initiative and a one-day medicinal chemistry workshop was held in New Delhi in January 2010. Although successful, this event came at a busy time. Many international speakers withdrew and even some local people were unable to attend. There is a remit for a future joint meeting with the RSC, IUPAC and the ACS in Rajkot in January/February 2011. No funding for travel is presently available. If we are to participate then 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)

The experiments published on the IUPAC web site continue to attract considerable interest, particularly in South America. A book version with parallel texts in Spanish or Portuguese and English that is ready for publication is being pursued by Prof. Rosa Cattana, Universidad Nacional de Rio Cuarto, Cordoba, Argentina, subject to clarification of contracts. Contention exists over the use of the term 'editors' rather than 'compiladores'.

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

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

This project was accepted in December 2009 and a sum of \$6,000 was assigned. AM has contacted key organisations in eight countries and received 19 surveys from four of these to date. RG will ask for clarification on the questions asked and the organisations to which the surveys were sent.

It was noted that as part of their Drug Discovery Series the RSC have a book in preparation on Neglected Diseases in Drug Discovery. It is edited by M.J. Palmer and T.N.C. Wells and is due for publication in October 2011. It was also noted that there is a session here at the ACS Meeting on Sunday morning (March 21) on Medicinal Chemistry in Rare Orphan and Neglected Diseases.

TP indicated that Pat Woster is very active in this area and may be interested in taking part in the initiative. Opportunities to expand the initiative beyond Latin America would also be sought.

Post Meeting Note: *RG to send TP a copy of the original Project Submission Form.*

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 but it should be maintained regardless.

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 from Mexico has been accepted for publication and will appear later this year.

4.3.5 Analogue-based Drug Discovery II (Janos Fischer)

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

This 21 chapter book (520 pages) is now complete. It comprises 4 general chapters, 9 chapters on drug classes and 8 chapters of case studies, and is due for publication in July. JF already has an outline plan for Analogue-based Drug Discovery III which has yet to be submitted as a project. MC suggested that recent Indian research in which unexpected pharmacology was observed when metformin was used as a coupling agent for two pharmacologically distinct agents (e.g. daunamycin linked to artemesin) might provide an interesting future chapter. The results of such combinations are rather unpredictable and have been termed 'cassette molecules' or 'composite molecules'.

4.3.6 Standalone Drugs (Janos Fischer)

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

JF and RG remarked that it is difficult to gather suitable data for this project on account of the dearth of negative data available in the published literature.

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 Erdhardt, Per Lindberg)

PE stated that he was happy to remain associated with this project but not in a major capacity. It was suggested that Steve Smith (ex-GSK and now in Brussels) might be asked to contribute.

4.3.9 Working Party on Chemistry for Biology (Robin Ganellin)

IUPAC Project [2005-042-1-300](#)

It was agreed that this should be excluded from future agendas as no known progress was being made.

4.4 New Projects

No new information available.

5 Division Committee

It was noted that Françoise Pontet would be the next Divisional President and that Michael Schwenk is the new Divisional Secretary. The next meeting is in Copenhagen, Denmark, March 28-30, 2010.

6 European Federation for Medicinal Chemistry (EFMC)

The next EFMC ISMC Symposium would be held in Brussels on the 6-9th September 2010 (www.ismc2010.org). The IUPAC Richter Prize and lecture would be presented on 7th September.

7 Asian Federation for Medicinal Chemistry (AFMC)

It was noted that there is a joint ACS-AFMC Session here in San Francisco on March 22.

The next AIMECS 11 meeting is due to be held in Tokyo on November 29th to December 2nd 2011 (www.aimecs11.org). Toshi requested IUPAC Sponsorship. RG to send him a form.

8 Any Other Business

It was noted that 2011 would be the International Year of Chemistry and that RG is attending the joint Second IUPAC-ACS Collaboration Summit on March 21 in San Francisco to discuss this, among other things.

Post Meeting Note: *RG has arranged with Prof. Kathy A. Kantardjieff (Professor of Physical Chemistry, California State University, Fullerton, and Chair of the International Union of Crystallography) to plan for a day's Symposium on Structure-based Drug Design to be held at the IUPAC World Chemistry Congress 2011 in Puerto Rico. She will apply for an ACS Challenge Grant (up to USD 35,000). The idea is to mix crystal structures with medicinal chemistry. The details have to be worked out. RG will write to her.*

9 Date of Next Meeting

The next meeting will be held in Brussels on Saturday 4th September 2010, just prior to the XXIst EFMC Symposium on 5 - 9th September.

