

## CONFIRMED MINUTES

IUPAC Division of Chemistry and Human Health  
Subcommittee on Medicinal Chemistry and Drug Development  
31<sup>st</sup> March-1<sup>st</sup> April 2011, Anaheim, USA

**Meeting Attendees:** Derek Buckle (taking Minutes), Mukund Chorghade, Paul Erhardt, Robin Ganellin (Chair), Yvonne Martin, Tom Perun, John Proudfoot, Johan Ulander and guest David Black

**Apologies:** David Alker, Sergey Bachurin, John Bremner, Janos Fischer, A. Ganesan, Javed Iqbal, Toshi Kobayashi, Michael Liebman, Per Lindberg, Derek Maclean, Peter Matyus, Antonio Monge, Ferran Sanz, Joerg Senn-Bilfinger, Giorgio Tarzia, Henk Timmerman, Zhu JunYao.

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

The minutes of the last meeting held in Brussels (3-4<sup>th</sup> September 2010) were accepted without revision. They will be sent to the secretariat for posting on the IUPAC home page.

### 2. Matters arising from the Minutes

#### 2.1 IUPAC-Richter Prize for 2012

Nominations for the 2012 IUPAC-Richter Prize are required by the end of 2011. In the light of confusion over recipient claims for attending meetings at which they were asked to lecture it should be made clear to both recipients and conference organisers what would and would not be covered. Specifically it was suggested that expenses would be provided solely for the speaker and would cover economy class air travel only. In addition, conference organisers would be asked to waive registration fees. All other expenses were to be reimbursed by the award itself. There will be further discussion at the next meeting in Puerto Rico in July 2011.

It was noted that 2010 IUPAC-Richter Prize recipient, Professor Arun K Ghosh (Purdue University, USA), had presented a well-received lecture on 7<sup>th</sup> September at the Brussels ISMC Symposium at which RG presented him with his plaque. As he had already presented one lecture at the 31<sup>st</sup> National Medicinal Chemistry meeting in Minnesota in 2010 this represented an excellent overall coverage for IUPAC.

#### 2.2 IUPAC Emeritus Fellows

Both the toxicology and our own subcommittee have had plaques made for Emeritus Fellows and the first of these was presented to Camille Wermuth by RG at the Brussels ISMC meeting. It was noted that John Topliss was no longer able to travel to receive his award and that he had asked for it to be received on his behalf. Dr. Stephen Munk had agreed to do this at the Denver, Colorado, ACS meeting at the end of August 2011 as part of the ACS Division of

Medicinal Chemistry Hall of Fame reception, Les Mitscher would also attend; RG agreed to get the plaques for John Topliss and Les Mitscher sent to TP so that he could present them.

RG observed that the plaques do not actually indicate that they acknowledge the recipient as an Emeritus Fellow and it is hoped that this can be rectified in the future. It was suggested that a medal might be an alternative to plaques since once struck these would require only the recipient's name to be engraved, however, the plaques also contain a citation stating the recipient's major contributions to IUPAC.

### 3. Membership

Funding to attend Subcommittee meetings remains an ongoing issue such that European member attendance at US meetings is poor and *vice versa*. Currently the Project system is the only means of funding, even for the Subcommittee Chair. In order to increase the attendance/participation of NRs there were two suggestions. One was to encourage them to chair Projects and the other that more use could be made of electronic communications e.g. teleconferencing, Skype etc.

For potential new members who have accepted invitations to join the Subcommittee, see item 5 below.

JP indicated that his wish to relinquish the position of Secretary was not reflected on the IUPAC web site, from which the issue of succession planning developed. Also, RG, indicated that he has been acting as a Chair since 2000 (initially as President of the Medicinal Chemistry Section) and that he therefore ought to stand down. To facilitate this RG agreed to write job descriptions for both the Chairperson and Secretary that could be given to interested candidates or to those targeted directly by the current incumbents. When produced these would be appended to the Minutes; *see Addendum*. In the interim, DB agreed to undertake the role of Secretary and JP agreed to organise the change on the IUPAC web site. It was suggested that a generic email address such as [SMCDD-secretary@IUPAC.com](mailto:SMCDD-secretary@IUPAC.com) might be more appropriate than that of the specific incumbent.

### 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](#)

It is still unclear what the new terminology for this Project will be. As Ganesan has just taken over the Chair at the University of East Anglia, UK it is likely that progress will be put on hold while he sorts out his new department.

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

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

PE noted that he was requested to update the finalisation date for this Project to 2012 although he still hopes that it will complete by the end 2011.

**4.1.5 Compendium of Glossaries** (Robin Ganellin)  
IUPAC Project [2002-001-1-700](#)

This Project remains on hold awaiting the completion of ongoing Glossaries.

**4.1.7 Glossary of Terms in Pharmaceutical Process Chemistry**  
(Mukund Chorghade) IUPAC Project [2001-049-2-700](#)

This Project will be completed so that it can be officially closed with a target date of December 2011. MC has been encouraged to apply for additional funding to maintain and update this glossary and others.

**4.1.8 Prototype Analysis of Molecular Markers of Cancer** (Michael Liebman)  
IUPAC Project [2005-050-1-700](#)

No further information is available but there is a need to close this Project. PE agreed to contact ML.

**4.1.10 Glossary of Terms for Biomolecular Screening** (John Proudfoot)  
IUPAC Project [2004-019-3-700](#)

The Glossary has been submitted and is expected to be published soon. The Project is now completed.

**4.1.11 Glossary of Terms in Medicinal Chemistry** (Derek Buckle)  
IUPAC Project [2008-010-1-700](#)

This Glossary is now formatted and was circulated to Task Group members for comments in February 2011. A final review of all the included terms was made during the meeting. It will be sent to Jack Lorimer for comment before proceeding to peer view.

**4.1.12 Glossary of Terms in Computational Drug Design** (Yvonne Martin)  
IUPAC Project [2010-057-3-700](#)

Seven Task Group members are in place and a list of some 370 old and new terms has been established. The list is in the process of refinement.

**4.2 Training and Development**

**4.2.1 Research and Training in Medicinal Chemistry in Latin America**  
(Antonio Monge)

A course on “The what, when and the how of Chemical Innovation” had been held in Lima, Peru in October 2010, and also Antonio lectured on “Creative

imitation in the discovery of new compounds with medicinal activity” at the National Chemical Congress.

#### **4.2.2 Research and Training in Medicinal Chemistry in the Indian Sub-continent** (Mukund Chorghade)

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

The two symposia in Rajkot and Nagpur, India, February 2011 respectively were very successful. Subcommittee members who lectured were Mukund Chorghade, Paul Erhardt, Michael Liebman, Joerg Senn-Bilfinger and Henk Timmerman plus Dr. B. K. Trivedi (a former Secretary of the Med. Chem. Section). MC, PE and JS-B were also awarded a special medal, and MC received a special award from the Governor of Gujarat. MC would like to hold further similar symposia in India. He would like to host the 2017 General Assembly there also. Financial support for attendees remains an unresolved issue.

MC put forward the suggestion of a Project on Neglected Diseases in the Indian Sub-continent which was generally favoured. RG envisaged three such Projects; the existing one on Latin America by AM, that on India by MC, and a third on Africa possibly overseen by Dr. Ramaiah Muthyala who will be contacted by PE.

*Post meeting note: Dr. Muthyala's interest is with rare diseases rather than with neglected diseases.*

#### **4.2.5 Practical Studies for Medicinal Chemistry Students** (Antonio Monge)

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

The web based version of the book has been quite successful with a hit rate spread over the various published experiments of between 200-600 per month over the last year. One hundred copies of a paper version are scheduled for publication in Argentina, 40 of which will be printed in Madrid for distribution.

#### **4.2.6 A Survey of Research into New Drugs for Neglected Diseases in Latin America** (Antonio Monge)

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

A network of 42 researchers from 30 institutions in 10 different Latin American countries has been established which identifies people, diseases and universities in which they are working. Unfortunately, precisely what each is actually doing is not known.

RG noted that he had recorded two relevant recent symposia; a 2-day RSC meeting on Anti-malarial Drugs in London in March 2011 and another from Cambridge Health Institute on Encouraging Development of Therapies for Neglected Diseases in Philadelphia in April 2011. They could provide useful contacts for the Project when more detail was known.

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

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

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

PE reported that he intended to request \$2,500 of additional funding in order to progress this Project to an intermediary endpoint. In the meantime he agreed to circulate the Project to the Subcommittee.

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

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

The existing paper will be submitted for publication and the further aim is to extend the project to update it to provide information on Reverse Pharmacology and Hybrid molecules.

#### 4.3.4 Latin American Plants as Sources for Functional Foods (Antonio Monge)

IUPAC Project [2005-031-2-700](#)

Project completed following publication.

#### 4.3.5 Analogue-based Drug Discovery II (Janos Fischer)

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

Project completed following publication of the book in July. See also Minute 4.4b. Both JF and RG (editors) attended the Wiley-VCH desk in Brussels ISMC meeting and were available to sign copies of the book.

#### 4.3.6 Standalone Drugs (Janos Fischer)

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

RG reported that in an attempt to make this chapter of ABDD II more visible he had had discussions with Wiley regarding making it available on the IUPAC web site. From these discussions it emerged that Wiley were prepared to make it electronically available *via* a link to Wiley from the IUPAC web site <http://www.iupac.org/web/ins/2005-032-2-700> namely to <http://onlinelibrary.wiley.com/book/10.1002/9783527630035> ; but it is not free! *Post meeting note: RG has informed Fabienne about this and she has taken it up with Frank Weinreich, Wiley, who has promised to remedy the problem and make the chapter freely available.*

#### 4.3.7 Biological Context by Text Datamining (Michael Liebman)

IUPAC Project [2005-049-1-700](#)

No new information available. PE will contact ML about this too (cf. 4.1.8).

#### 4.3.8 Trends in Patenting Drug-related Technologies (Paul Erhardt, Per Lindberg)

Understandably, PE stated that he did not wish to proceed with this initiative until his outstanding Projects were completed. He would, however, draft a Project application so that it could be speedily submitted when required.

#### 4.4 New Projects

##### 4.4a Physicochemical Properties and SAR-analysis (Johan Ulander & Per Lindberg)

JU reported that he has made a number of contacts and identified a co-author for a review/monograph as an endpoint to this Project. Targeting to a web publication was also considered possible. YM agreed to become a Task Group member.

##### 4.4b Analogue-based Drug Discovery III (Janos Fischer)

A third volume of the successful Analogue-based Drug Discovery series was in hand with over 21 chapters in place and a further 12 awaiting confirmation. The current status was considered adequate to support a further Project proposal.

##### 4.4c Neglected Diseases (Pat Woster)

No new information available but it was noted that PW has recently taken up a new post at the Medical University of South Carolina, USA.

#### 5. Division Committee

TP reported that new TMs would now serve for a two year term rather than the current four and that Janos Fischer, Paul Illing and Chris Hill were appointed as new TMs. Their terms would extend from the beginning of 2012 till the end of 2013. With the new tenure periods this meant that all TMs would complete their tenure at the end of 2013, although new incumbents could have their period extended by a further 2 years.

TM also recorded that new NRs had been identified from countries such as Bangladesh, Brazil, France, India, Netherlands, Pakistan, Tanzania and Thailand. The final list awaited approval, but without funding to assist their participation it was likely that few NRs would be able to attend Subcommittee meetings.

*Post meeting note: RG has written to Prof. Anjali Rahatgaonkar (NR, India), Prof. Rob Leurs (NR, the Netherlands), Dr Chris Hill ( TM 2012, UK) and Dr. Serge Mignani (NR, France) to invite them to attend our Subcommittee meetings. Hill and Magnani have accepted and will be present in Puerto Rico.*

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

Nothing to report.

#### 7. Asian Federation for Medicinal Chemistry (AFMC) (Toshi Kobayashi)

Despite the ongoing catastrophe in Japan following the recent earthquake and tsunami the AIMECS 11 meeting in Tokyo between November 29<sup>th</sup> to

December 2<sup>nd</sup> 2011 is still scheduled to take place ([www.aimecs11.org](http://www.aimecs11.org)) at the Keio Plaza Hotel.

## 8. IYC 2011 and IUPAC World Chemistry Congress

Following our request, Arun Ghosh had provided a video of a discussion he had with some students but no others were, as yet, forthcoming. It was suggested that as Prous provided web cams of all EFMC ISMC symposia RG would check their web site to see whether videos of earlier Prize recipients were available. *Post meeting note: Jan Heeres has submitted an interesting series of slides relating to the many discoveries of Paul Janssen.*

MC informed the committee that a one day division conference had been arranged for Wednesday 3<sup>rd</sup> August 2011 under the title 'Chemistry of Life'. A sum of \$1,000 was available to start the initiative but since additional funding was unlikely MC suggested that speakers should come from the subcommittee itself rather than by soliciting speakers from elsewhere. PE, RG, YM, TP and the future Divisional Chairperson, Francoise Pontet, were confirmed speakers. Talks were tentatively scheduled to last up to 40 minutes and MC requested abstracts before the deadline of 30<sup>th</sup> April. Additional speakers might include Antonio Monge and MC himself. MC would send a letter of invitation to all the committee to solicit other speakers, but it is possible that short talks might be selected from the posters that are being presented. It was anticipated that the cost to speakers would be the \$250 registration fee and an additional three nights' accommodation; this is not insubstantial!

## 9. Any Other Business

None to report

## 10. Date of Next Meeting

The next meeting will be part of the General Assembly and will coincide with the World Chemistry Congress in Puerto Rico and will be held between 9.00-5.30 in the Luna Boardroom of the Sheraton Puerto Rico Hotel on Sunday 31<sup>st</sup> July 2011.

## Addendum:

### **Job description for the Honorary Secretary of the Subcommittee on Medicinal Chemistry and Drug Development**

In recent years the Chair has been doing many of the functions which might have been carried out by the Hon Secretary, e.g. making arrangements for meetings and contacting people. The major function of the Secretary has therefore become one of recorder. This can of course be reconsidered depending on the functions which are ultimately taken by the new Chair, when appointed.

Meanwhile, the minimum requirement of the Hon Secretary is to take and issue minutes of the proceedings of the Subcommittee meetings. This can be done in association with the Chair to check complete accuracy.

One problem for the Hon Secretary is the difficulty of obtaining travel funds to attend all the meetings. To alleviate this, it is possible to split the function between two people who might divide the job geographically between North America and Europe. It would also be less onerous for the Hon Secretary to have to attend one meeting per year instead of two.

The potential for increasing electronic communication, especially oral by, for example, Skype phone-in and teleconferencing, means that the Hon Secretary should be electronically adept.

### **Job description for the Chair of the Subcommittee on Medicinal Chemistry and Drug Development as practiced by Robin Ganellin (CRG) ca 2002-2011**

1. To arrange (biannual) two Subcommittee meetings each year (generally one in North America and one in Europe). This involves confirmation of the date, selecting the place and possibly arranging beverage and food refreshment. It also requires one to inform members in good time and to find out who will attend. In the past CRG has been very fortunate in having the help of Tom Perun in making the arrangements for the meetings associated (in time) with the ACS meetings. Originally this whole process was carried out by the Hon. Secretary.
2. To arrange the agenda in consultation with the Subcommittee members.
3. To request progress reports from Project Leaders/Chairs if they are not attending the Subcommittee Meeting.
4. To actively chair the Subcommittee meetings.
5. To assist the Hon Secretary to complete the minutes by providing additional information as required. To get the draft minutes confirmed by the membership and then displayed on the IUPAC web site.
6. To stimulate the formation of new Projects and assist the putative Project Chairs with the completion of new Project Submission Forms.
7. To monitor the progress of Projects and provide advice to help bring them to completion.
8.
  - a. To participate in the projects where appropriate.
  - b. In the past CRG has also assisted by providing the cover sheet for project reports.
9. To report on activities to the Division President as required but especially to help him/her make the biennial report to the Bureau.
10. To attend meetings of the Division Committee and report on activities of the Subcommittee.



11. The Chair may make arrangements for the award of the IUPAC-Richter Prize in Medicinal Chemistry and Chair the Selection Committee.
12. To send invitations to join the Subcommittee to potential new Subcommittee Members e.g. invite attendance from National Representatives and newly elected members of the Division Committee who have a professional interest in Medicinal Chemistry.
13. The Chair, together with the Subcommittee, should submit names for consideration to be elected Emeritus Fellows and should provide appropriate CV information and wording for the certificate/plaque/medal.
14. To offer advice to Subcommittee members, e.g. how to claim for reimbursement of travel expenses for attending our meetings.
15. The Chair does not receive special funding for attending Subcommittee meetings or for administration costs (e.g. hire of room and refreshments) and, if reimbursement of administration costs, travel and hotel expenses are required, then he/she will have to recover these from current projects-preferably, (but not necessarily) those projects discussed at the Subcommittee Meeting. The process requires the Chair to seek permission from the respective project Chairs and then to request the appropriate expense claim form from the Secretariat. The Chair typically does not have to cover the travel expenses to attend the Division Committee meetings since these have in the past been provided from the Division budget.