

**Confirmed Minutes.**  
**IUPAC Division of Chemistry and Human Health**  
**Subcommittee on Medicinal Chemistry and Drug Development**

September 11<sup>th</sup>, 2005  
Modena, Italy

**Meeting Attendees:** Janos Fischer, Robin Ganellin, Giovanni Garivaghi, Stefan Jaroch, Per Lindberg, Antonio Monge, Jörg Senn-Bilfinger, Georgio Tarzia.

Apologies for being unable to attend were received from: John Bremner, Eli Breuer, Mukund Chorghade, Gerhard Ecker, Paul Erhardt, Toshi Kobayashi, Derek Maclean, Tom Perun, John Proudfoot, Henk Timmerman.

A very big thank you to Prof. Livio Brasili (Modena) for negotiating the provision of the meeting room in Hotel Raffaello.

**1. Minutes of the last meeting**, which was held in Rio de Janeiro (13 February 2005) were accepted without further amendment. 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**

The agreement between IUPAC and Richter has been signed by Richter's CEO. The prize will recognise a scientist's outstanding contributions in medicinal chemistry and drug discovery. The first scientist will be honored at the medicinal chemistry symposium in Istanbul (8-29 through 9-2). Over the next 10 years the prize will be granted 5 times. The awardee will obtain \$10,000 including travel expenses (when with academic background) and is expected to give at least one lecture at a medchem symposium. The call for nominations will be announced on the IUPAC website and the IUPAC journal "Chemistry International". RG will explore further journals for the announcement, such as ChemMedChem and J. Med. Chem. and provide a draft announcement. The committee to evaluate the nominations and award the prize was discussed. The selection committee shall consist of: (i) The Subcommittee Chairperson; (ii) Four additional Subcommittee members. (iii) An outside IUPAC, established scientist who is affiliated with the ACS National medicinal chemistry Symposium; and (iv) An outside IUPAC, established scientist who is affiliated with the European Medicinal Chemistry Symposium and (v) An outside IUPAC established scientist who is affiliated with the Asian AIMECS Meeting.

## 2.2 Honorary membership

The Subcommittee would like to honor the IUPAC services of Mitscher, Topliss, Koga and Wermuth with an honorary fellowship, which is more than the usual "IUPAC fellowship" awarded to retired IUPAC members. This is being pursued by the Division President.

## 3.1 Report from the Beijing General Assembly Meeting

JF reported on the Division Committee meeting. Our Subcommittee's projects and project plans make nearly 50% of the whole Division's activities (10 projects out of a total of 23; 6 planned projects from a total of 12 Division-wide). There were 40 posters presented at the General Assembly without opportunity for discussion; 5 of the posters were from Division VII. They were not shown at the Technical Science IUPAC meeting. The next Division meeting will take place next March linked to the ACS meeting in Atlanta (26 March 2006). The next General Assembly will be in Torino, 2007.

## 3.2 Membership.

|                                       |   |
|---------------------------------------|---|
| <a href="#">Bremner, John</a>         | University of Wollongong, Australia   |
| <a href="#">Breuer, Eli</a>           | Hebrew University of Jerusalem, Israel  |
| <a href="#">Chorghade, Mukund</a>     | Chorghade Enterprises, USA  |
| <a href="#">Ecker, Gerhard</a>        | University of Vienna, Austria   |
| <a href="#">Erhardt, Paul</a>         | University of Toledo, USA   |
| <a href="#">Fischer, Janos</a>        | Gedeon Richter, Hungary   |
| <a href="#">Ganellin, Robin</a>       | University College London, United Kingdom   |
| <a href="#">Gaviraghi, Giovanni</a>   | Sienabiotech, Italy   |
| <a href="#">Jaroch, Stefan</a>        | Schering AG,<br>Germany <a href="mailto:stefan.jaroch@schering.de">mailto:stefan.jaroch@schering.de</a> |
| <a href="#">Kobayashi, Toshi</a>      | Pharmaceutical Manufacturers Association<br>(Japan) Technical Committee                                 |
| <a href="#">Liebman, Michael</a>      | Windber Research Institute, USA   |
| <a href="#">Lindberg, Per</a>         | AstraZeneca, Sweden   |
| <a href="#">Maclean, Derek</a>        | Kai Pharmaceuticals, USA  |
| <a href="#">Monge, Antonio</a>        | Universidad de Navarra, Spain   |
| <a href="#">Nifantiev, Nikolay</a>    | Zelinsky Institute of Organic Chemistry, Russia   |
| <a href="#">Perun, Tom</a>            | Abbott Labs, USA (retired)  |
| <a href="#">Proudfoot, John</a>       | Boehringer Ingelheim Pharmaceuticals, USA   |
| <a href="#">Sanz, Ferran</a>          | IMIM/Universitat Pompeu Fabra, Spain  |
| <a href="#">Senn-Bilfinger, Joerg</a> | Altana Pharma, Germany  |
| <a href="#">Tarzia, Giorgio</a>       | University of Urbino, Italy   |
| <a href="#">Timmerman, Henk</a>       | Universiteit Amsterdam, The Netherlands   |
| <a href="#">Topliss, John</a>         | University of Michigan, USA   |
| <a href="#">Wermuth, Camille</a>      | Prestwick Chemical, France  |

New National Representatives to IUPAC with obvious medicinal chemistry interests will be invited to attend our meetings. RG and TP have already written to invite the following:

Sergey O. Bachurin, Russia  
So-Yeop Han, South Korea,  
Javed Iqbal, India  
Grzegorz Mloston, Poland

Furthermore, RG also wrote to invite three of the candidates who stood for election to the Division Committee because they are medicinal chemists, namely: Derek Buckle, Ferran Sanz, and Mario Varasi. They all expressed interest in being involved with our Subcommittee. RG also invited Georgio Tarzia who had been on the Division Nominating Committee.

## 4. Projects

### **4.1 Nomenclature and Terminology**

#### **4.1.2 Glossary of Combinatorial Chemistry Terms** (Derek Maclean).

IUPAC Project [2003-044-1-700](#).

A new draft will be presented after a literature survey. As combinatorial chemistry has matured the glossary of the current technologies, which should be revised into a IUPAC recommendation, might be relevant for a longer period. PL suggested to discuss the project name, because high-throughput chemistry, array chemistry or parallel chemistry are terms which are more often used today than combinatorial chemistry. He will address DM in this respect.

#### **4.1.3 Generic Structures** (Derek Maclean).

No new information.

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

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

No new information.

#### **4.1.5 Compendium of Glossaries.** (Robin Ganellin).

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

No new information. Still need to identify the accepted format since this appears to have changed.

#### **4.1.6 Glossary of Terms in Pharmaceutical Technology.** (Eli Breuer).

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

ICTNS chairmen J. Lorrimer identified serious editorial issues with this glossary, such as IUPAC incompatible format (cf. Gold book), lack of references, and possible overlap with other IUPAC definitions and therefore requested substantial revision to the document. RG to contact EP and inform him about appropriate format.

**4.1.7 Glossary of Terms in Pharmaceutical Process Chemistry.** (Mukund Chorghade).

IUPAC Project [2001-049-2-700](#) (shares the project number of 4.1.6 above).

Same objections as to the glossary before. Further, a modification of the title is recommended, e.g. "Terms for Process Chemistry Pertaining to the Pharmaceutical Industry".

**4.1.8 Prototype Analysis of Molecular Biomarkers in Cancer.** (Michael Liebman).

No additional information. Robin has written several times to M asking him to submit the project for IUPAC recognition and to extend the time for completion to two years.

**4.1.9 Compendium of Molecular Targets for Drugs.** (John Proudfoot).

IUPAC Project [2004-025-1-700](#)

Slow progress in this project so far as studying data on knockouts, X-ray data, mechanism of action is time consuming. GT proposed to focus on therapeutic application as the ordering principle instead of best-selling drugs. The question arises as to how to limit and clarify the scope of this project. PL to ask David Keeling from AstraZeneca to join the project.

**4.1.10 Glossary of Terms for Biomolecular Screening** (John Proudfoot).

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

Slow but steady progress reported by JP. Several members of the project team will be meeting on September 14<sup>th</sup> in Geneva at the Society for Biomolecular Screening meeting.

**4.1.11 Glossary of Terms in Medicinal Chemistry.** (Mukund Chorghade).

MC was due to write a project proposal. RG to contact him about present status.

**4.2 Training and Development.**

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

Antonio identified three forthcoming courses at which he will lecture:

|                    |   |
|--------------------|---|
| Oct 24-29, 2005    | Benchmarking in Medicinal Chemistry at Universidad San Marcos, Lima, Peru.                    |
| Nov 9-12, 2005     | Research in Forgotten Diseases at Universitaria San Martin, Bogota, Columbia                  |
| Nov 30-Dec 2, 2005 | Project Management in Medicinal Chemistry at Universidad de la Republica, Montevideo, Uruguay |

AM has also written two short articles on natural products and forgotten diseases for CI.

#### **4.2.2 Research and Training in Medicinal Chemistry in the Indian Subcontinent.** (Mukund Chorghade).

IUPAC project [2001-048-2-700](#).

No new information.

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

IUPAC project [2004-028-1-700](#).

AM introduced this internet supported course in medicinal chemistry (posted on the IUPAC homepage) which was released in July 2005 and covers topics such as physicochemical properties of drugs, QSAR, molecular modelling, toxicology, synthetic drugs, natural products. RG pointed out that information on safety hazards is missing and has to be incorporated. A draft printed version has been produced and was provided at the meeting. Complimentary reviews by C. Wermuth and H. Stark have been received.

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

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

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

A poster was presented at the General Assembly in Beijing. The project is otherwise on hold pending additional funding.

#### **4.3.3 Natural Products with Medicinal and Nutritional Value** (Mukund Chorghade).

IUPAC project [2001-050-2-700](#).

The draft manuscript was strongly criticised by J. Lorrimer, regarding publication in Pure and Applied Chemistry. PE and RG have made suggestions for improvements to MC.

#### **4.3.4 Plants as Sources for Nutraceuticals in Latin America** (Antonio Monge)

A project submission form has been completed and submitted to the IUPAC Secretariat. The Subcommittee recommended the following as referees: L. Mitscher, C. Wermuth, P. Matyus.

*Post-meeting note: the project proposal has been submitted and has the reference number 2005-031-1-700.*

#### **4.3.5 Analogue-based Drug Discovery** (Janos Fischer).

IUPAC project [2002-051-1-700](#)

The book will be published by VCH-Wiley approximately at the beginning of 2006. Galley proofs have been sent to the authors in September. A reference to the book can be found on the IUPAC homepage. Furthermore, flyers were distributed at the Italian Swiss medicinal

chemistry symposium in Modena (following this Subcommittee meeting) to raise the awareness.

A poster on this project was presented by JF at the General Assembly Meeting in Beijing.

#### **4.3.7 Biological Context by Data Mining** (Michael Liebman).

No new information. Robin has written to Michael to ask him to submit the project for IUPAC approval and to extend the proposed project duration to two years.

#### **4.3.8 Trends in Patenting Drug-Related Technologies** (Paul Erhardt, Per Lindberg).

A project proposal had been prepared but has not been submitted.

Broad unsubstantiated patent claims, particularly from virtual screening efforts, create a "prior art" which might jeopardize discoveries in the future (cf. PE in CI 2002), as no IP position might be securable. It is intended to strengthen the patent knowledge of medicinal chemists to deal responsibly with patent application. Thus, a patent session should be set up during the EFMC meeting in Istanbul next year (PL, PE).

### **4.4 New Projects.**

#### **4.4.1** JF proposed a project on a Review of Isolated Drugs and drafted a Project Submission Form. The aim being to identify important drugs where it has not proved possible to make superior analogues, eg, aspirin, raloxifene, diltiazem, levodopa. The product will be a review article.

Post-meeting note: the project proposal has been submitted and assigned the number 2005-032-1-700.

#### **4.4.2** Nikolay Nifantiev proposed the project "Nutraceuticals from Marine Sources (Hawai and New Zealand), however, no action has been taken yet.

### **5 Division Committee**

New members elected to the DC are Doug Templeton, Monika Nordberg and Ferran Sanz.

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

The next Symposia will take place in Istanbul (August 29 to September 2, 2006) and Vienna (2008).

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

No new information.

### **8 Other Business**

**9 Next Meeting**

In conjunction with the ACS meeting (which starts on 26 March 2006) in Atlanta and the Division Committee (DC) meeting. We shall try to have our Subcommittee on Saturday 25 March 2006; confirmation of the date will follow in due course.