

Confirmed Minutes
IUPAC Division of Chemistry and Human Health
Subcommittee for Medicinal Chemistry and Drug Development

March 22, 2003
New Orleans, USA.

Meeting Attendees: Eli Breuer, Mukund Chorgade, Paul Erhardt, Janos Fischer, Robin Ganellin, Nao Koga, Antonio Monge, Tom Perun, John Proudfoot, Camille Wermuth.

1. Robin welcomed the members attending – noting that recent events had made travel difficult for some members. Pierre Bost, Edmond Differding, Giovanni Gaviraghi, Stefan Jaroch, Osama Kebir, Toshi Kobayashi, Per Lindberg, Chris Lipinski, Derek Maclean, Joerg Senn-Bilfinger, Henk Timmerman, and John Topliss conveyed apologies at being unable to attend.

Robin thanked Tom Perun for coordinating with the ACS in making arrangements for the meeting venue.

Following on the lively discussions at the last subcommittee meeting regarding the elimination of the words “Medicinal Chemistry” from the subcommittee title, Robin was pleased to note that we are now the Subcommittee for Medicinal Chemistry and Drug Development.

2. **Minutes** of the previous Subcommittee meeting held in Barcelona (31 August 2002) were approved without change.
- 3.1 **Nomination.** The medicinal chemistry section of the German Chemical Society has nominated Stefan Jaroch (Schering AG) for membership of the subcommittee. Robin had written to Stefan inviting him to attend this meeting. Stefan had indicated he would attend but as a result of Company obligations he had been unable to and sent his apologies.
- 4.1.1 **Legal implications of Patenting Virtual Libraries** (Paul Erhardt, Per Lindberg).
Following discussions at the Barcelona meeting on Paul Erhardt’s article ["On the Reality of Virtual Libraries"](#) (Chemistry International 2002, 24, N°4, p16) there was interest in reconstituting a working party on this topic to elaborate and extend Paul’s letter and disseminate it to a wider audience. A position statement on this topic could be useful to organizations such as Chemical Abstracts and patenting agencies worldwide. At the Barcelona meeting Per Lindberg expressed an interest in following up but to date there has been no contact with Paul.

Robin distributed copies of a past letter from Professor Bernard Pullman (Anti-Cancer Drug Design 1989, 4, 172) which vigorously complained about "Guidelines for Publications in Molecular Modelling related to Medicinal Chemistry" (J. Med. Chem. 1988, 2230-2234) because it suggested that authors should refrain from publishing activities of specific unknown structures since this may compromise future patentability...etc. As a theoretical chemist making predictions about possible active structures Pullman found this attitude to be "shocking, unacceptable and disgraceful".

4.1.2 Glossary of Combinatorial Chemistry Terms (Derek Maclean).

Derek could not attend and Robin presented Derek's update in this area. A new project submission has been prepared with the aims of revising the [1999 technical report](#) and "bringing it up to IUPAC recommendation status and of providing a curated, authoritative on-line resource for combinatorial chemistry nomenclature". Task group members, in addition to Derek, include Eric Gordon, Arun Ganesan, Eric Martin and Mario Geysen. Additional participants are being sought to balance geographical, technical and professional expertise and opinion.

4.1.3 Generic Structures (Derek Maclean).

Derek and co-author Eric Gordon are working on a draft document titled "On the representation of Combinatorial Libraries". The objective is to facilitate a standardized representation of structures arising from combinatorial based approaches. A recently updated version (26 pages) is available from Robin. It was again suggested that this effort be formalized as a project.

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

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

Paul noted that, of the fifteen working party members, all but three had completed their assignments. He has undertaken to complete these assignments himself and expects the review process to be complete before the next meeting in August. The completed glossary will be sent to 15 external reviewers and also distributed to the Subcommittee members. Paul is exploring the idea of publication Pure and Applied Chemistry in a thematic issue devoted to metabolism.

4.1.5 Compendium of Glossaries. (Robin Ganellin).

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

The planned inclusion of glossaries currently in progress (Drug Metabolism, Pharmaceutical Technology and Pharmaceutical Process Chemistry) will likely delay the target publication date to 2004.

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

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

Eli had distributed a draft of the glossary to committee members after the Barcelona meeting, however there was little useful feedback. Robin, John and Nao agreed to review the glossary. However, it was viewed as important to have an extensive international representation during the refereeing process given the small number of task group members on this part of the project.

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

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

This glossary now contains definitions for more than 800 terms. Incorporation of suggestions from referees is in progress. It is expected that the final draft will be submitted to John Jost by April 1, and also circulated to subcommittee members. This draft will be posted on the IUPAC website as part of a new review process. Some clarification will be sought in regard to the length of this web-based review process. It was suggested that the regular updating of this glossary could constitute the basis for a project.

4.1.8 Glossary of Chemical Biomarkers for Therapeutic and Diagnostic Use.

Robin to write to Giovanni with regard to his position paper. Janos will contact Schering A.G. for somebody to assist Giovanni.

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

A course on Cancer was held in la Antigua, Guatemala (Sept 16-21 2002). Courses on "Project Management in R+D+i of Medicaments" (i = innovation) were held at Piura University, Peru (October 21-22), Catholic University of Peru, Lima (October 24-26), and University of San Andres, La Paz, Bolivia (November 27-30).

Additional courses are planned for 2003 in Peru and Bolivia (Benchmarking in R+D+i in medicaments, the creative imitation), and Columbia (Project Management in R+D+i in Cancer).

CYTED has published a book about patents in Spanish and English for distribution in South America.

4.2.2 Research and Training in Medicinal Chemistry in the Indian Subcontinent. (M. Chorgade).

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

Some 150 academics in India and Pakistan responded to the survey. No input was received from Pakistan. In general the conclusion is that there is little formal training in medicinal chemistry. Primary training is in the area of synthetic chemistry and medicinal chemistry training is "on the job". It is planned to publish the final report in Chemistry International.

There was some discussion on the extent of review necessary, since the report may propose specific recommendations for training.

4.2.3 Medicinal Chemistry in the Development of Societies. Biodiversity and Natural Products. (A. Monge).

Antonio outlined a proposed new project relating to nutraceuticals and functional foods derived from plants. Appropriate books or articles would provide relevant definitions and discuss the importance of nutraceuticals and functional foods to health care in developing countries. It was suggested that the working group should include representative(s) with expertise in nutrition and agricultural chemistry.

4.2.5 Practical Studies for Medicinal Chemistry Students. (A. Monge).

This book has been prepared in Spanish and Portuguese versions. There is interest in preparing an English language version for dissemination via the IUPAC website. The structure of the book is such that it could be of general benefit to novice medicinal chemists everywhere and it was suggested that a project proposal be prepared.

Additional comments related to the need for a review process to assess the safety aspects of proposed experiments

4.3.1 Natural and Synthetic Substances Related to Human Health (Tom Perun).

The manuscript was published in [Pure and Applied Chemistry \(2002\) 74 1957-1985](#). Tom has prepared a condensed version for dissemination to magazines, newspapers etc., and this document was circulated at the meeting. Tom has been in touch with John Jost to identify opportunities to publicize and use the condensed document.

It was noted that a commentary on the article appeared in [Chemistry International, March-April, 2003, 21-22](#).

Post meeting note: An official IUPAC report by Tom Perun, Paul Erhardt and Jim McAlpine has now been displayed as a public release (18 April 2003) through the EurekaAlert service on http://www.eurekaalert.org/pub_releases/2003-04/iuop-irn041803.php. This was effected through the help of Laura Abernathy of the IUPAC Secretariat.

4.3.2 Project on Human Drug Metabolism Database (P. Erhardt). IUPAC project [2000-010-1-700](#)

A commitment for funding from Pfizer, at a level sufficient to hire a database expert, has been obtained. The financial support does not compromise the nonproprietary, nonprofit nature of the database. Copyright for the database is in place.

4.3.3 Natural Products with Medicinal and Nutritional Value (M. Chorgade).
IUPAC project [2001-050-2-700](#)

Mukund updated on the current status of the project. Since the natural products discussed originate mostly from India and China, it was suggested that the title be modified to reflect the fact that the survey is not globally comprehensive. There was concern within the subcommittee that the absence of toxicity information could lead to misuse in a promotional setting. The absence of this information would also be an obstacle in the review process. It was agreed that a draft of the document would be circulated to the committee for evaluation and that there would be further discussion at the next subcommittee meeting.

4.3.5 Analogue-based Drug Discovery (Janos Fischer).

This has now been officially approved as a project.

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

Progress to date includes the classification of the top 300 selling drugs and the identification of seven authors to contribute case-history chapters on the discovery of a variety of analog-based drugs. There was some discussion on the tasks relating to specific chapters and Janos will update the outline in the near future.

One critical point of discussion related to the need for Janos to clarify whether certain IMS data could be used in the book.

4.3.7 Bioinformatics.

No discussion.

5 European Federation for Medicinal Chemistry (EFMC).

Robin noted that Gerhard Ecker is secretary to the executive committee and will invite him to attend the subcommittee meetings as the EFMC representative.

Next EFMC meeting: [18th International Medicinal Chemistry Symposium, Copenhagen and Malmo, August 15-19 2004.](#)

6 Asian Federation for Medicinal Chemistry (AFMC).

Next AFMC meeting: [5th AFMC International Medicinal Chemistry Symposium](#), AIMECS 03, October 14-17 2003, Kyoto Park Hotel, Kyoto, Japan

7 Links with other bodies.

Based on the observation that the AFMC AIMECS 03 meeting above noted IUPAC sponsorship in the absence of seeking such sponsorship, Paul Erhardt suggested that the process for seeking IUPAC sponsorship should be re-evaluated.

9 Next Meeting.

The next Subcommittee meeting will be in Ottawa, during the General Assembly, on Sunday August 10th. The room assignment will be available at the registration desk on the University of Ottawa campus.