

**DIVISION VII
Chemistry and Human Health**

**Minutes Division Committee Meeting
London, XII 12 -14th 2003**

Location and Schedule:

Novartis Foundation
41 Portland Place, London, W1B 1BN
Telephone: +44(0) 20 7636 9456
<http://www.novartisfound.org.uk>

beginning at 12:00 am, Saturday, December 13th, 2003

Distributed to

Division Committee :

Anders Kallner ((President, Division of Chemistry and Human Health)) anders.kallner@ks.se
Paul Ehrhardt (President elect) paul.erhardt@utoledo.edu **new email !**
Mukund Chorghade chorghade@prodigy.net; chorghade@comcast.net
Rita Cornelis rita.cornelis@ugent.ac.be **new email !**
Urban Forsum urban.forsum@imk.liu.se
Robin Ganellin c.r.ganellin@ucl.ac.uk; ; robin.ganellin@tesco.net **new email !**
Michael Liebman m.liebman@wriwindber.org **new email !**
Thomas Perun Tjperun@aol.com
John Duffus: j.h.duffus@blueyonder.co.uk
Janos Fischer: j.fischer@richter.hu
Pedro Soares de Araujo: psdarauj@usp.br
Henk Timmerman: timmermn@chem.vu.nl
Birger Heinzow (Secretary): bheinzow@lanu.landsh.de

cc.

National Representatives:

[Dr. Pierre-Etienne Bost](mailto:pebost@pasteur.fr) (2002-2003 France) E-MAIL: pebost@pasteur.fr
[Dr. Abraham J. Domb](mailto:adomb@md.huji.ac.il) (2002-2003) Israel E-MAIL: adomb@md.huji.ac.il
[Dr. Giovanni Gaviraghi](mailto:ggaviraghi@sienabiotech.it) (2002-2003) Italy E-MAIL: ggaviraghi@sienabiotech.it
[Prof. Masayuki Totani](mailto:mtotani@swu.ac.jp) (2002-2003) Japan, E-MAIL: mtotani@swu.ac.jp
[Prof. No-Sang Park](mailto:nspark@pado.krict.re.kr) (2002-2003) Korea E-MAIL: nspark@pado.krict.re.kr
[Prof. Nikolay E. Nifantiev](mailto:nen@ioc.ac.ru) (2002-2003) Russia E-MAIL: nen@ioc.ac.ru

1.-Opening, Welcome and Introduction of new Titular Members

Anders Kallner, Division President, chaired the meeting and welcomed the Division Committee members. By introducing themselves the newly elected TM Prof. Pedro Soares de Araujo from Brazil and the NR from Russia, Prof. Nikolay Nifantiev, who attended the DC for the first time, presented their main interests and activities in the field of chemistry and human health: Biochemistry, regulation of metabolism, molecular biology, and inhibition of angiogenesis, cancer research, drug development and trials in cancer treatment respectively.

2.-Approval of the Agenda and Minutes from the previous Division Committee Meeting, Ottawa, August 9th, 2003

The agenda was accepted and the Minutes from the Ottawa DC Meeting were approved. Minutes from the Subcommittee for Medicinal Chemistry and Drug Development (SCMCDD) and from the Subcommittee on Toxicology and Risk Assessment (SCTRA) from Ottawa have been received and circulated.

3.-Division VII Presidents Report

AK thanked the DC members and NR for their support and contributions and stated that the transition from the old to the new system has been successfully mastered by the Division. The structure of the subcommittees has been proven to be useful and necessary for continuation of the numerous activities. Special thanks were directed to the retiring members, Jytte Molin Christensen, Rita Cornelis and Tom Perun and expressed his hopes that the DC can relay on their expertise and ideas in the future.

The report received from YO (young observer) Philippe Barthelemy philippe.barthelemy@univ-avignon.fr was discussed and the IUPAC YO-programme considered a successful way to make young scientist acquainted with IUPAC. The application for sponsorship of a conference on "New directions in chemistry" as an outcome of this YO programme underlines this point. No report was received from YO Tania van den Ancker ancker@usq.edu.au. The DC is very much interested in an evaluation of the YO programme by the secretariat.

4. DC Nominations and Election procedure

Election of the Vice President of the Division will take place at the DC meeting in 2005, since PE is willing to stay on for a second term until 2007. For the forthcoming term 2006-2007 elections must be held in 2005, a Nomination Committee shall be installed, again consisting of members from inside and outside IUPAC. TP will chair the Nomination Committee together with RC and another 3 members from outside IUPAC shall be recruited before June 2004 to prepare the list of nominations in 2005. 4 positions on the DC have to be filled with 2 nominees for each position. The CV of the candidates should be limited to 5 pages, to avoid lengthy internet downloads. Suggestions shall be conveyed directly to TP. Candidates, willing to serve, should be approached later next year: members of projects, subcommittees and possible candidates from outside by individual contact.

5. - Report from Subcommittees

5.1 Subcommittee on Drug Discovery and Development (RG)

RG referred to the last subcommittee meetings in Ottawa and in London 10-XII-2003 with 10 and 12 attendees respectively. John Bremner from Australia joined the SC. Education on issues of patenting for scientists in general, as well as for medicinal chemists, was identified as a suitable new project. Per Lindberg and Paul Erhardt will submit a proposal, starting with a discussion group to identify major issues and to consider how to best address the variety of interdisciplinary scientists and decision makers engaged in this area.

A project Glossary on Chemical and Biological Biomarkers by ML is under consideration, addressing marks of genetic risk, early stages of disease and disease outcome (Theranostics).

John Proudfoot John Proudfoot will propose a project to prepare a compendium to be published as a monograph or book on sites of action/molecular targets of major drug families and related mechanistic aspects in continuation of JFs project on analogue-based drug discovery.

Other possible new projects under consideration are: i) glossary of terms used in biomolecular screening, ii) nutraceuticals derived from plant sources of South America (Antonio Monge), iii) nutraceuticals derived from marine sources (ML and NF), iv) prediction of storage stability of drugs and compound libraries. (MC and Richard Wife from Biospex)

5.2 Subcommittee on NPU (UF)

AK gave a report of the recent activities. The latest Subcommittee meeting was held 2003-10-24 – 2003-10-27 in Malmö, Sweden. 3 CNPU-database projects have been finished: transfusion medicine (UF), molecular biology a 1200 page electronic text file (PSA) and properties in toxicology (Wolf Külpmann).

The CNPU-database must be kept up-to date and needs financing. UF will explore possible opportunities and co-operation with LOINC, HL-7 and others. The project on transmission standards for report and request received funding from the EU and is currently seeking funding from the Microsoft-Foundation for continuation.

AK suggested that Nikolay Nifantiev (NN) shall explore the introduction of the NPU-database into the Russian system. To make him more acquainted with the CNPU database system AK and PSA will mail information to Prof. Nifantiev accordingly.

3 new project are under consideration: i) Revision of the Silver Book (Chris Rigg), ii) Extension of the CNPU-system to Imaging and iii) Problems of metrology dealing with uncertainty.

5.3 Subcommittee on Toxicology and Risk Assessment (John Duffus)

The SC had meetings in Ottawa and in London (October). Co-operation with the TOXNET website and the "World Library on Toxicology" (Phil Wechsler) is developing further. The subcommittee might become involved in the new ToxLearn site and will also provide a revised glossary of terms for this NLM project. ML suggested to have toxicogenomic aspects included. Discussion will continue at the next scheduled meeting of the SOT in Baltimore.

No formal relationship has been established with IUTOX, but will continue with individual contacts.

6. Review of Activities

It was recommended to provide summaries for the general public, since the condensed information on Natural and unnatural substances related to human health, prepared by TP, was well received. This should be pursued for applied projects being of public interest. PE circulated his article: A human drug metabolism database, published in Current Drug Metabolism 4: 411-422, 2003

6.1. Completed Projects

- 6.1.1 Natural and unnatural substances related to human health (John Topliss)
- 6.1.2 Exposure assessment and decision rules in compliance testing (JMC)
- 6.1.3 2000-014-1-700 - Recommendations for the use of nanotechnology in clinical laboratories (P.Wilding). An overview has been published and the document will be finalized this year.
- 6.1.4 2001-059-1-700 - Properties and units for transfusion medicine and immunohaematology (UF). The project has been completed.
- 6.1.5 2001-066-1-700 - Global use of the C-NPU concept system for properties in toxicology (Wolf K lpmann). The project has been completed.
- 6.1.6 2001-068-1-700 - Properties and units in Medical Molecular Biology (P. Soares de Araujo). The project has been completed.

6.2. Current Projects

- 6.2.1. 1999-047-1-700 - Immunochemistry of metal sensitization (D.Templeton). The project has been partly completed and two manuscripts will be published soon. The group (Doug Templeton, Mike Schwenk and Reinhild Klein) will continue with the project.
- 6.2.2. 2000-009-1-700 - Metabolism terms. (PE) The completed glossary can be passed on to external review soon.
- 6.2.3. 2000-010-1-700 - Human drug metabolism database(PE). The project has been delayed due to lack of financing. PE has approached industry for assistance and explored other possibilities. Since this project has a potential for commercial utilisation it is important to solve problems of copyright, that might arise from commercialisation. Three different aspects of use can be named: purely commercial, semi-commercial and scientific. Seeking financial support from outside, it must be without exclusivity. PE will further inquire into the copyright issue of such databases pointing out that an acknowledgement about IUPAC's initial support of this project will be one of the first things that anyone will read every time they go to the database's web site. Companies choosing to fund this project have already assumed that it will be copyrighted and they only want to be able to download it into their own informational systems without expecting that they might gain any kind of exclusivity for this type of access to the database.
- 6.2.4. 2000-034-2-700 - Glossary for Toxicokinetics of chemicals (M. Nordberg). The project has been completed and the glossary with approx. 300 terms has been forwarded to ICTNS. J. Lorimer has criticized that some definitions must be revised, because they are not consistent with definitions in the Gold Book. The DC recommends to follow ISO rules, however the matter of which criteria and format to be followed must be solved, before the project can be completed. ICTNS recommends: "In compiling a glossary, the current edition of the 'Gold Book' should be inspected in case a particular term has been defined previously within IUPAC. If it has, but there is a need to repeat the definition, then whenever possible the original wording should be retained. If it is considered essential to change the wording, e.g., if the original is too technical for a more general readership or if general terms need to be replaced by more specific ones for a narrower readership, then the changes made should be kept to a minimum and the justifying reasons given in a footnote, together with a reference to the original 'Gold Book' entry.
In certain areas, and particularly in metrology, it is important for IUPAC to retain consistency with definitions given by 'higher authorities' such as in the International Vocabulary of Basic and General Terms in Metrology [VIM] and the International Organization for Standardization [ISO].

As no specific advice for drafting a glossary is given by ICTNS, the revision might just require that deviation from 'Gold Book' entries and rewordings for different usage should be specified and justified. Since this problem relates to other glossary projects, ICTNS should be asked for comments and guidance. PE will convey this important issue and ask for a clear direction with an overall guideline and specific formatting "requirement.

- 6.2.5. 2001-048-2-700 - Research and training in medicinal chemistry in India, Pakistan and Sri Lanka (MC). The project has been successfully completed. A follow-up of the project will be to run workshops upon the recommended curriculum. Prof. Nifantiev expressed his interest and MC will provide the requested information. It was suggested to contact UNESCO for possible co-operation
- 6.2.6. 2001-049-2-700 - Glossary of terms used in process chemistry/manufacturing of active pharmaceutical ingredients, and pharmaceuticals (MC and E. Breuer). The draft has been completed and circulated and is ready for review by ICTNS. For the external review board members from the Internatl. J. Process Chemistry shall be approached. Updating every two years is planned.²
- 6.2.7. 001-050-2-700 - Chemical, pharmacological aspects of natural products with medicinal and nutritive value (MC). The final document is ready for the review process. It contains three main aspects: Indian Ayurvedic drugs, therapeutic products of Islamic medicine and Chinese medicine. It was recommended to make it a monograph including pictures of the plants. The secretariat shall be asked for support in finding a publisher or in publishing it as a pdf including coloured pictures.
- 6.2.8. 2001-053-2-700 – Fundamental Toxicology for Chemists (JD). John Duffus and Howard Worth will edit the second edition of the textbook within the next two years. The existing chapters will be updated and new chapters added. RSC is presently sending out the contracts to the co-authors.
- 6.2.9. 2001-058-1-700 - Concepts and structure for requests in clinical laboratories (UF). The project is moving ahead.
- 6.2.10. 2001-067-1-700 - Properties and units for function examinations (A.Jabor). The project is in the final stage and will be completed next year at the SC meeting in Prague.
- 6.2.11. 2001-070-1-700 - Properties and units for urinary calculi (A.Jabor). The project is in the final stage and will be completed next year at the SC meeting in Prague
- 6.2.12. 2001-077-1-700 – Best practice for workplace exposure: a critical review of methodology (JMC) This projects has been cancelled due to conflicts of interest with new retirement laws in Denmark. It had been budgeted for \$ 4,000.00 from the IUPAC Div. VII funds. PE will request that the remaining funds to be returned to the Div. VII budget to support new projects.
- 6.2.13. 2002-001-1-700 - IUPAC compendium of terms for chemists applied to drug development (RG). There is good progress and 6 glossaries have been finished in developing a single editorial format, new terms will be identified and included. The review process shall start with the glossary on Medicinal Chemistry.
- 6.2.14. 2002-051-1-700 - Analogue-based drug discovery (J.Fischer). Completion of the project is envisaged next year by end of June.

6.3. Interdivisional Activities

- 6.3.1. 2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy. (Prof. Davies, UK). Prof. Nifantiev has become involved in the project, which has been delayed.

6.4. Project Applications under review (Dec. 2003)

- 6.4.1. C-NPU concepts and traceability of measurements (Gunnar Nordin). Div. VII will take no further action.
- 6.4.2. 2003-044-1 Glossary of terms in combinatorial chemistry (Derek Maclean). Prof. Maclean has moved to San Francisco and the external reviews are still pending. FM is having problems in collecting outside reviewers. New names have just been suggested and will be approached.
- 6.4.3. 2003-001-2 Explanatory dictionary of concepts in toxicokinetics (Monica Nordberg). The external review process has been delayed because two of the reviewers did not respond (since mid October). BH will provide two names of experts in the field to the secretariat to continue with the review process. The DC has already approved the project with a budget of 5.500 USD.
- 6.4.4. 2003-028-1 Glossary for chemists of terms used in toxicology- revision and updating (JD). PE will write a brief, formal request to the Secretary General and ask for funding from the

reserve because our Division budget has now been drawn to a zero balance. It was noted that this project represents a very timely update for an IUPAC glossary that has previously been highly regarded amongst the research community. The present submission received praiseworthy comments during external review and was unanimously voted for approval subsequent to its discussion by Div. VII Committee (7500 USD).

7. - Discussion of future plans

7.1. New projects

- 7.1.1 Educational Material on Pesticide Toxicity (J Duffus and BH). A project should first collect already existing information in this field and review the material and provide a recommendation. A project application to develop educational material might be prepared later, when the ongoing toxicology projects reach completion. The developments with respect to ToxLearn will be taken into consideration.
- 7.1.2 Bioinformatics and data-mining. ML outlined his ideas on data mining in the field of cancer research and estrogenic compounds by use of information technology. CAS has agreed to give free access to their database. He will complete the project application within the next days. AK noted the utility of this project for other Divisions.
- 7.1.3 Educational Material for IUPAC Courses in the field of Medicinal Chemistry. (MC and A Monge) The project is still under serious consideration (see 5.1) and the involvement of UNESCO shall be pursued. A project application was again encouraged. As another project a book on practical aspects of education involving small scale experiments is under consideration and was also welcomed by the DC.
- 7.1.4 "Chemistry and Cooking" as a possible project idea has been explored further and RC agreed to become convener for this project now heading under "Molecular gastronomy" until a project proposal has been delivered. Prof. Erbersdobler (Germany) expressed his interest in co-operation.
- 7.1.5 Combination Effects in Pharmacology and Toxicology. An application was received from Joseph Lehar from Computational Biology in Boston/US to revive the abandoned project of Prof. Gerald Poech (Austria). The project was reviewed by the DC and approved. BH will forward the application to the secretariat to start the external review process asap.

7.2 Conferences

A conference on Biodiversity will be held in New Delhi in 2004. MC will attend the conference and present his projects on glossaries and curricula. He agreed to provide a summary report after the conference for publication in CI.

YO Philippe Barthelemey asked for sponsoring a conference under New Directions in Chemistry on "Supramolecular Assemblies". His application was supported by the DC and PE will inform Fabienne Meyers accordingly. He will convey to PB that he should consider a project application in this field depending upon the outcome and discussions on this emerging topic.

IUPAC conference, 2005 in Beijing. The Div was asked to present their work and PE and UF will provide a poster as requested. Additionally a ½ day symposium on Chemistry and human health (6 speakers) was proposed. MC will contact the organizers and AK will inform the secretariat. Proposals for lectures at the symposium should be directed to MC with a cc to PWE and BH asap

7.3 Division brochure

MC volunteered to write a Division VII brochure which will be ready for publication very soon.

8.-Cooperation within IUPAC

ICTNS: The ICTNS shall be approached and clarification of the way how to prepare a glossary entry be asked for.

9.-Cooperation with other Organizations

ICSU: 5 areas were defined by ICSU in which applications are invited until February. The DC considers this a too short notice to prepare a sound application and no project will be handed in accordingly. The next ICSU main focus will be science for health. AK will attend and keep the DC informed. As a possible topic the drug metabolism database was identified and will be conveyed by AK.

SOT: John Duffus participated in a telephone conference, co-operation might develop within the NIH/NLM project "World Library on Toxicology" and the "ToxLearn" concepts. He will be

attending the SOT Congress in Baltimore and the 2005 Symposium and offered to make some formal contribution to the Symposium.

NIH: Phil Wexler has expressed his interest in the IUPAC glossary of terms in Toxicology and intends to display an updated version on the NIH Toxnet website: <http://toxnet.nlm.nih.gov/> .

IFSTP: (International Federation of Societies of Toxicologic Pathology). BH will keep in contact with the IFSTP President Dr. Robert Ettlín (Basel, Switzerland)

10. Personalia

Addresses of the new members of the Subcommittees shall be provided to the secretariat (Fabienne Meyers).

11. Finances

The Division budget 2002/4 has been fully spent. For the next biennium 43.700 USD can be used for projects, enabling the Division to start 7 –10 new projects.

12. -Any other business

The next DC meeting will be held in Boston June 11-13.2004 and a second meeting is planned for February 2005. MC was asked to arrange for the venue and provide hotel suggestions in Boston.

Adjourned 18:30

prepared by:
B. Heinzow
Division Secretary