

**DIVISION VII**  
**Chemistry and Human Health**

**Minutes: Division Committee Meeting**  
**Ottawa, 9 -VIII-2003**

**Location: IUPAC General Assembly, Ottawa University Campus, LMX 360**

**Beginning at 9:00 am, Saturday , August 9<sup>th</sup> , 2003**

**Division Committee :**

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**attending for discussion:** Dr. Ted Becker ,Dr. Fabienne Meyers, Laura Abernathy, Prof. James Bull (editor PAC), Prof. Peter Atkins (chair CCE) and members of the Subcommittee on Toxicology and Risk Assessment (John Duffus [j.h.duffus@blueyonder.co.uk](mailto:j.h.duffus@blueyonder.co.uk) , Monica Nordberg, Doug Templeton)

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

The Division President AK chaired the meeting and welcomed the Division Committee members, Prof. Totani from Japan, task group leader Dr. J. Fischer, and the young observers Dr. Tanja van den Ancker from Australia and Prof. Barthelemy from France. By introducing themselves Dr. van den Ancker mentioned her main interest in green chemistry, whereas Prof. Barthelemy has his interests in surfactant chemistry and drug development.

**2.-Approval of the Agenda and Minutes from the previous Division Committee Meeting, Brussels 6 – 8 XII 2002**

The agenda was accepted and the Minutes from the Brussels DC Meeting were approved. Draft minutes from the Subcommittee for Medicinal Chemistry and Drug Development (SCMCDD, New Orleans 2003-03-22) and from the Subcommittee on Toxicology and Risk Assessment (SCTRA, Brussels 2003-4-23) have been circulated and will be approved at their SC meetings during the GA.

**3.-Division VII Presidents Report**

AK gave a brief report of the Bureau meeting, where he delivered his report of the Division activities. The three Division VII subcommittees have been approved.

The existence and the function of the Bureau has been challenged and a new organizational structure has been proposed.

The problem of providing continuity for maintaining electronic glossaries and data bases under the new project system was again discussed. Deliberations with WHO and LOINC in the past revealed a lack of interest to collaborate in developing and maintaining. the NPU-database . In the past the update has been provided by the committees, it was concluded that the Division should support future project applications for updating of existing databases.

#### 4. DC Nominations and Election procedure

For the forthcoming service term 2004-2005 an Election Committee had been installed consisting of members from inside and outside IUPAC and six candidates were nominated for the 4 open positions. TP reported on the results of the ballot procedure which included 32 possible ballots of which 19 were received. According to the votes cast Henk Timmerman, John Duffus, Janos Fischer and Pedro Soares de Araujo will be nominated to fill in the available positions within the DC.

It was recommended to the Secretary General that the voting procedure should be reviewed to become more practical and that the CV of the candidates should be limited to 5 pages, to avoid lengthy internet downloads.

#### 5. - Report from Subcommittees

##### 5.1 Subcommittee on Drug Discovery and Development (RG)

RG referred to the last subcommittee meeting in New Orleans with 10 attendees and the circulated minutes. The subcommittee will hold a well attended meeting at the GA. RG emphasized that the recent change in name including Medicinal Chemistry made it clear again that IUPAC is a stakeholder in this important field of Chemistry and Human Health and thus the interest in the subcommittee from outside IUPAC and industry is very positive. The medicinal chemistry section of the German Chemical Society has nominated Stefan Jaroch (Schering AG), who became a member of SCMCD and will attend the meeting in Ottawa.

The link of websites of the European Federation of Medicinal Chemistry and the ACS with the IUPAC site have been established.

The short version of the document "Natural and Synthetic Substances" has just been made available to media sources through the efforts of a new person at the Secretariat, Laura Abernathy. It has gone through many changes and includes now statements about vitamins and toxic substances. The excellent collaboration with Laura on the press release, which has been made available through the EurekaAlert service, was very much appreciated. The "IUPAC report- Natural and synthetic substances" can be viewed at [http://www.eurekaalert.org/pub\\_releases/2003-04/iuop-irn041803.php](http://www.eurekaalert.org/pub_releases/2003-04/iuop-irn041803.php)

After discussion of MC with John Jost a contact list has been established and 5000 copies of the Division brochure shall be printed with the help of the secretariat. MC has finalized the letter addressing Chemical Industry asking for support, which will include the Division brochure and shall be distributed by the end of the year with a focus on the biotechnology industry.

Per Lindberg expressed an interest in following up on Paul Erhardt's paper: "[On the Reality of Virtual Libraries](#)" (Chemistry International 2002, 24, N°4, p16) to elaborate and extend the letter and disseminate it to a wider audience. A position statement on this topic has been distributed previously to organizations such as *Chemical Abstracts* and patenting agencies worldwide.

The paper on Generic Structures (D. McLean) has been published and accepted by the Journal of Combinatorial Chemistry and could form the basis for a project with the IUPAC chemical identifier registry. Derek McLean and co-author Eric Gordon had prepared the document "On the representation of Combinatorial Libraries", with the aim to facilitate a standardized representation of structures arising from combinatorial based approaches. D. MacLean has been asked to submit this as a project and it is likely that he will soon do so, although he has left his position with PETNet Pharmaceuticals, LA. A new project submission has been prepared with the aims of revising the 1999 technical report and of bringing it up to IUPAC recommendation status and of providing on-line resource for combinatorial chemistry nomenclature.

G Gaviraghi has developed a proposal for a Glossary on Chemical Biomarkers focussing on radioligand and radiotracers. In the discussion the broad application of biomarkers was emphasized and suggested to recruit someone to take up the task. In the context of biomarkers ML reported on a network of the Universities of Pennsylvania cancer research centers, which lists markers for cancer and aims at validating their use and possible potential in diagnosing and treating cancer. ML will find out if someone from this network might be interested in this project. It was also suggested to explore if this could become an ICSU project. The topic will be further deliberated in the forthcoming subcommittee meeting.

The plan to establish training courses in medicinal chemistry in India beginning with the University at Poona was presented by MC.

As possible new projects i) nutraceuticals and functional food and ii) a book on training in medicinal chemistry were named. Such a book has been prepared in Spanish and Portuguese versions. There is interest in preparing an English language version for dissemination via the IUPAC website.

## 5.2 Subcommittee on NPU (UF)

UF gave a report of the recent activities. The next Subcommittee meeting is scheduled for 2003-10-24 – 2003-10-27 in Lund, Sweden.

Following up on the question of a permanent location of the C-NPU data base and the question of what international organizations are the stake-holders in maintenance and use of the database UF circulated a letter 2003-01-12 (Appendix 1) to the top level of 6 possible stakeholder organizations (IFCC, IUPAC, HL-7, LOINC, CEN TC 251 and NCCLS) with the view of obtaining a consensus and possibly a meeting of the stake-holders during the Ottawa GA LOINC responded (appendix 2), however did not find the time for negotiating a common strategy ripe and suggested further exploration of common ground. The IFCC president suggested merger with LOINC. Considering the weak response, co-operation with CEN at the top level was considered necessary and AK will request an approach by IUPAC for official relationship with CEN. The database is at present hosted by the University of Linköping on its Dior server reachable via links from the IUPAC and IFCC homepages.

The project on transfusion medicine and immunohaematology is finished and in press in PAC, (K Varming, U. Forsum, I. Bruunshuus, H. Olesen. Properties and Units for Transfusion Medicine and Immunohaematology Properties and Units in the Clinical Laboratory Sciences)  
The document on clinical molecular biology has been finished and is anticipated to be accepted by the C-NPU at its next meeting. The question of transmission standards for report and request is still pending mainly due to the anticipated finalization of the VIM revision. Dr. Françoise Pontet, Hôpital Lariboisière, Paris, France has accepted to become a new member of the C-NPU sub-committee.

## 5.3 Subcommittee on Toxicology and Risk Assessment (John Duffus)

The SC had a meeting in Brussels and minutes have been circulated. Some new members have been included for the SC (B. Heinzow, Wayne Temple /NZ) and a new members list will be forwarded to the Division President by John Duffus. Minutes shall be sent to the IUPAC secretariat after approval for publication on the IUPAC homepage.

## 6. Review of Activities

### 6.1. Completed Projects

The excellent co-operation of the secretariat, Fabienne Meyers and Laura Abernathy, on publication issues and dissemination of information concerning completed projects was expressed.

### 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 have been submitted. He will continue with the project and has included Prof. Mike Schwenk (Stuttgart) and Dr. Reinhild Klein (Tübingen) from Germany in the task group.
- 6.2.2. 2000-009-1-700 - Metabolism terms. (PE) The project work is nearly completed and the list of entries for the glossary contains approx. 150 terms of which 30 need revision. It is anticipated that the glossary can be passed on to external review in early 2004.
- 6.2.3. 2000-010-1-700 - Human drug metabolism database (PE). The project has been delayed due to lack of resources, PE will approach industry for assistance and will explore other possibilities to move on. ML suggested CAS as a possible partner and will provide the appropriate contact, RG will also suggest possible contacts.
- 6.2.4. 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.
- 6.2.5. 2000-034-2-700 - Glossary for Toxicokinetics of chemicals (M. Nordberg). The project has been completed and the glossary with approx. 300 terms is now under external review.
- 6.2.6. 2001-048-2-700 - Research and training in medicinal chemistry in India, Pakistan and Sri Lanka (MC). The project has been successfully completed. MC has received responses from some 150 academics in India. In conclusion 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.
- 6.2.7. 2001-049-2-700 - Glossary of terms used in process chemistry/manufacturing of active pharmaceutical ingredients, and pharmaceuticals (MC and E. Breuer). There are two separate glossaries in this project. They will be published separately. The one by E. Breuer (Trends in Pharmaceutical Technology) has 800 terms and is due for review and will then be submitted for publication in PAC. The one by M. Chorgade (Terms in Pharmaceutical Process Chemistry) has also been completed and after it has been reviewed it will be submitted for

- publication in PAC and Organic Process Research and Development. Updating every two years is planned.
- 6.2.8. 2001-050-2-700 - 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.
  - 6.2.9. 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 on Toxicogenomics, Toxicology of Pharmaceuticals and Aspects of Clinical Chemistry will be included. A contact with DIV VI, Chemistry and the Environment, produced the valuable suggestion to include a chapter on behavior and pathways of chemical in the environment with Dr. Monika Herrchen from Germany ( e-mail: [herrchen@ime.fraunhofer.de](mailto:herrchen@ime.fraunhofer.de)) as possible author.
  - 6.2.10. 2001-058-1-700 - Concepts and structure for requests in clinical laboratories (UF). The project has been delayed.
  - 6.2.11. 2001-059-1-700 - Properties and units for transfusion medicine and immunohaematology (UF). The project has been completed.
  - 6.2.12. 2001-066-1-700 - Global use of the C-NPU concept system for properties in toxicology (Wolf Kùlpmann). The task group met at the GA in Ottawa and plans to finalize the project by the end of 2003.
  - 6.2.13. 6.2.7. 2001-067-1-700 - Properties and units for function examinations (A.Jabor). UF will contact Antonio to inquire about the projects status, which should be in the final stage.
  - 6.2.14. 2001-068-1-700 - Properties and units in Medical Molecular Biology (P. Soares de Araujo). The project is near completion scheduled for October. It was discussed to create a new project on proteomics, to deal with this subject separately.
  - 6.2.15. 2001-070-1-700 - Properties and units for urinary calculi (A.Jabor). UF will send a reminder to Antonio. It is anticipated that the project is near completion.
  - 6.2.16. 2001-077-1-700 – Best practice for workplace exposure: a critical review of methodology (JMC).Abandoned ( see also TOP 10).
  - 6.2.17. 2002-001-1-700 - IUPAC compendium of terms for chemists applied to drug development (RG). There is good progress in developing a single editorial format for the different glossaries. As part of the compilation new terms will be identified and redundancies shall be deleted. John Duffus was requested to provide the revised working document of his Glossary on Toxicology. The Toxicokinetic Glossary shall be included and the review version provided until the end of this year.
  - 6.2.18. 2002-051-1-700 - Analogue -based drug discovery (J.Fischer). The work started in January 2003 and is progressing. It was pointed out that nearly every second drug on the market is an analogue. Most of the work will be completed by the end of this year. The official deadline is June 30, 2004.

### 6.3. Interdivisional Activities

The interdivisional discussion on biomolecular chemistry (T. Norin) will be attended by AK.

- 6.3.1. 1999-003-1-300 - Molecular basis of biodiversity, conservation and sustained innovative utilization (Div VII member: A. Monge). A status report prepared by U.K.Pandit was received.
- 6.3.2. 2002-005-1-300 Post Genomic Chemistry ( S. Varfolomeyev). No information was available
- 6.3.3. 2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy. (Div. VII NR: N Nifantiev) BH contacted Prof. Davies (UK), the task group leader, who reported that Prof. Nifantiev has become involved in the project.

### 6.4. Project Applications in review (Nov. 2002)

- 6.4.1. Revision of the Gold Book (A.Jenkins). AK contacted A Jenkins and agreed on support with the review process.
- 6.4.2. NPU concepts and traceability of measurements (G.Nordin). AK will attend a joint meeting during the GA in Ottawa.
- 6.4.3. Integrating environmental exposure pathways for medicinal products (M Herrchen). The DC has reviewed the Proposal on Integrating Environmental Exposure Pathways for Medicinal Products (#2003-016) and pointed out that the term "medicinal" compounds covers agents with many different biological activities (antibiotics, anticancer agents, cardiovascular agents, CNS compounds, etc.) and that it would be difficult to include all of these drugs in a single scheme. It was agreed that the primary sponsor of the project should be Division VI, with

collaboration by Division VII where appropriate and John Duffus was named as liaison and will offer his co-operation to Monica Herrchen.

## 6.5. Conferences

Prof. Kononowicz has received funding for the Joint Meeting on Medicinal Chemistry, Krakow, 15-17. October 2003 to make participation of eminent invited lecturers possible.

## 7. - Discussion of future plans

### 7.1. New projects

- 7.1.1 Concepts in Toxicokinetics (M Nordberg and J Duffus). The project on applied toxicokinetics was discussed and received approval. A project application shall be prepared at the earliest convenience and not exceed 6000 USD. BH will contact Prof. Albrecht Ziegler ([AZiegler@pharmakologie.uni-kiel.de](mailto:AZiegler@pharmakologie.uni-kiel.de)) from Germany to become involved in the project. MN will contact Prof. Ziegler immediately upon her return to Sweden in order to finalize the project application.
- 7.1.2 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 further educational material will be prepared later. In a recent issue of the Lancet 'Pesticide poisoning in the developing world - a minimum pesticides list', was published highlighting the importance of this topic. BH will contact Dr. K. Racke (Vice President Div VI) and Prof. Peter Atkins (CCE) during the GA to discuss possible co-operation of the groups. Dr. Racke expressed his sincere interest for co-operation and the CCE welcomed the project. Prof. Elisa Pestana (Portugal) and Prof. Ram S. Lamba (Puerto Rico) expressed their interest in direct co-operation
- 7.1.3 Bioinformatics. ML outlined ideas for possible projects in this field. His inquiries into the subject of a glossary on bioinformatics suggest that there is no opportunity for standardization because of different interests of industry and academia. As a possible engagement in this field he presented recent developments in genome sequence analysis, and systems biology as the bottom up view from genomics and proteomics and the top down look from disease ( especially cancer) to find the information related to it. Two possible projects are:
- a) Expansion of concepts of biomarkers in risk assessment, diagnosis, therapeutic targets and development of diagnostics related to cancer. He will provide information from the University of Pennsylvania website and identify partners for a project.
- b) Data mining in the field of cancer research by use of information technology has been approached in a pilot project with breast cancer and environmental influences. So far only abstracts have been screened, but knowledge extraction will continue with full articles. The use of the glossaries as combined filter to extract literature shall be explored further. A possible partner might be CAS.
- ML announced that he will write up a project proposal by the end of August.
- 7.1.4 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 two Profs from Germany have expressed their interest in co-operation to produce a book in English with internet availability to support education in medicinal chemistry in less fortunate countries. A project application was encouraged.
- 7.1.5 Traceability and Uncertainty of Measurements. AK outlined the European Commissions directives on in vitro diagnostics, which require traceability and uncertainty statements. No conclusion was reached whether this topic shall become a new project or an issue for collaboration.
- 7.1.6 AK suggested the topic of "Chemistry and Cooking" as a possible project idea. The discussion added up to two aspects: to educating lay-people that cooking is chemistry and thus everybody becomes a chemist in the kitchen and to include information on cooking procedures and human health. Recent discussions on acrylamide and polycyclic nitroaromatic compounds in food occurring by "natural" chemistry were pointed out. The aim of the project is to produce information-similar to the former project on natural compounds-for the public to become more familiar with chemistry. RC will approach a Belgian colleague who writes regularly on this topic and BH will contact Prof. Ebersdobler (Germany) if he might be interested in co-operation.
- 7.1.7 Combination Effects in Pharmacology and Toxicology. Recent correspondence between BH and Joseph Lehar from Computational Biology in Boston/US might revive the abandoned project of Prof. Gerald Poech (Austria). The draft recommendations will be provided to by BH and MC will contact him upon his return to Boston. Prof. em. Poech agreed to participate as

member of the task group. The DC would welcome if Joseph Lehar applies for a project accordingly.

- 7.1.8 Glossary in Combinatorial Chemistry. Derek McLean was encouraged to provide the project application as soon as possible.

## 7.2 Conferences

A conference on Biodiversity will be held in New Delhi in 2004. MC will contact the organizers and provide information concerning IUPAC sponsorship. MC will attend the conference and was asked to provide a summary report after conference for publication in CI.

The DC was informed that three conferences to be held in India, Hungary, and Yugoslavia in 2004 will receive modest IUPAC financial support. During his visit the Secretary General Ted Becker emphasized that IUPAC sponsorship of a conference attests to its quality but does not carry financial support. However financial support via two programs is possible:

i) New Directions in Chemistry and

ii) Conferences in Developing and Economically Disadvantaged Countries.

Such conferences may be held in any country that is a Member (NAO) or Associate Member (ANAO) of the Union.

Alternatively, this program can also be used to support an "IUPAC Lecturer" to give talks at conferences otherwise not supported by IUPAC in developing and economically disadvantaged countries. Divisions may identify eminent scientists who are willing to participate in conferences and perhaps also present talks (as "IUPAC Lecturer") at universities in the host country.

## 7.3 Division brochure

MC volunteered to write a Division VII brochure which is now ready for publication and will be printed with the help of the IUPAC secretariat.

## 8.-Cooperation within IUPAC

**CCE:** The chairman Prof. Peter Atkins joined the meeting and explained ways of co-operation. The CCE task is to co-ordinate educational activities within IUPAC and to facilitate public understanding of chemistry. He introduced CCE as a generally interested party in future project proposals, which might be circulated before formal submission. CCE has many valuable contacts which might help in the progress of projects. MC was nominated as DC VII liaison to CCE and will present at their meeting two projects for deliberation: "Drug discovery/ Development process from conception to commercialization" and "Research and training in medicinal chemistry in India, Pakistan and Sri Lanka".

**Secretariat:** During his visit of the DC Ted Becker asked for advance notice of interesting forthcoming results and their value to non-specialists. Fabienne and Laura will prepare articles for CI, and news releases accordingly. The Division members complimented the secretariat on their excellent work and on the handling of media information.

**PAC:** Prof. James Bull - editor of PAC - introduced the peer review process of PAC for IUPAC sponsored events and made clear that the responsibility for the technical quality of the contents of publications arising from projects is with the DC, nomenclature aspects will be handled by the secretariat through ICTNS.

**ICTNS:** The ICTNS meeting will be attended by UF.

## 9.-Cooperation with other Organizations

**ICSU:** A recent request from T Rosswall, the ICSU Executive Director, for nominations for their Policy Committee on Developing Countries has led to the nomination of John Duffus by the DC VII for further consideration to the Bureau.

AK attended a meeting of representatives of several ICSU Unions and bodies in Paris February 2003. The general topic "Science for Health and Well-being" was recommended as primary focus for funding in 2005. An executive summary was circulated.

As a possible ICSU project, the ideas outlined by ML (see 5.1) might be suitable and shall be further explored.

**IFCC:** The excellent cooperation with IFCC and DIV VII in the field of NPU is continuing and CNPU might become a standing committee within IFCC.

**WHO:** Dr. Antero Aiño from IPCS takes part in the review of the Toxicokinetic project. No other joint activities are visible at present.

**EFMC:** The exchange of links on websites has been arranged.

**SOT:** John Duffus attended the SOT meeting in Salt Lake City and contacted Dr. Sue Ford, Director of the undergraduate toxicology program at St. John's University. So far no tangible co-operation has evolved.

**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/>. John Duffus is in close contact to develop interactive educational tools and provide input for the planned "world library of toxicology". Prototypes can be seen under : <http://www.sis.nlm.nih.gov/Tox/ToxTutor.html>

**IFSTP:** (International Federation of Societies of Toxicologic Pathology). BH contacted the IFSTP President Dr. Robert Ettlin (Basel, Switzerland) who expressed interest in cooperation and will bring the proposal for collaboration up at their next EC meeting in September in Hamburg.

## 10. Personalia

*Post Meeting:* JMC informed the DC on her decision to withdraw from all IUPAC activities and projects together with Eric Olson due to legal requirements of their retirement and suggested to close the project (2001-077-1-700).

Tom Perun shall provide the addresses of the newly elected members of the Division Committee and SCMCD.

## 11. Finances

The Division budget has been allocated and no remaining funds are available, since money not spent has to be returned to the treasurer. However there are still funds available from the IUPAC pool and project applications supported by the DC are welcomed and in favor to receiving support outside of the Division budget.

## 12. -Any other business

**Next** meeting of Division Committee VII will be held in London December 13/14. 2003.

Robin Ganellin was asked to arrange for the venue.

Adjourned 18:00

prepared by:

B. Heinzow

Division Secretary

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New Division Committee members (2004)

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