

DIVISION VII  
Chemistry and Human Health

**Minutes: Division Committee Meeting  
held at the University Club, Brussels, 30-XI - 2-XII-2001**

**Location: Club van de Universitaire Stichting**

**Division Committee Participants:**

Dr. Anders Kallner (President, Division of Chemistry and Human Health)

[anders.kallner@ks.se](mailto:anders.kallner@ks.se)

Prof. Robin Ganellin [c.r.ganellin@ucl.ac.uk](mailto:c.r.ganellin@ucl.ac.uk)

Dr. Thomas Perun [Tjperun@aol.com](mailto:Tjperun@aol.com)

Dr. Rita Cornelis [rita.cornelis@rug.ac.be](mailto:rita.cornelis@rug.ac.be)

Paul Ehrhardt (President elect) [perhard@utnet.utoledo.edu](mailto:perhard@utnet.utoledo.edu)

Urban Forsum [urban.forsum@ihm.liu.se](mailto:urban.forsum@ihm.liu.se)

Jytte Molin Christensen [jytte.molin@hotmail.com](mailto:jytte.molin@hotmail.com)

Mukund Chorghade [chorghade@prodigy.net](mailto:chorghade@prodigy.net)

Michael Liebman [liebmanm@mail.med.upenn.edu](mailto:liebmanm@mail.med.upenn.edu)

Birger Heinzow (secretary) [bheinzow@lanu.landsh.de](mailto:bheinzow@lanu.landsh.de)

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

The Division President AK chaired the meeting and welcomed the Division Committee members and thanked RC especially for organising the meeting. The new members of the Division Committee introduced themselves and their specific field of interest. New aspects in the field of chemistry and human health and personal expertise were introduced by PE on new drug design development and by ML on Bioinformatics

**2.-Approval of the Agenda and Minutes from the previous Division Committee Meeting, Brisbane, 29 June-4 July 2001**

The agenda was accepted and the Minutes from the Brisbane Meeting were discussed and approved with amendments. The approved Minutes will be circulated again within the DC and then sent to the Bureau by BH.

In light of erratic email distribution (some messages and attachments over the internet disappeared), it was decided that important documents and messages should be mailed with a request for confirmation of receipt and that a home page archive for confidential material or unconfirmed Minutes, Executive Reports, etc. shall be arranged.

The minutes from the Section of Medicinal Chemistry were tentatively approved.

The minutes from the CNPU and ComTox have been approved and are present on the IUPAC homepage.

**3.-Division VII Presidents Report**

The President discussed the dissolution of the Sections within the Division and the new structure. He expressed the need to expand the activities of the Division to new areas of Chemistry and Human Health. AK emphasised the role of the DC in generating and steering new projects under the general umbrella of Human Health. A detailed account of the activities and plans of Div. VII was given in his report to the Bureau dated July 2001. According to the strategic plan, all commissions will be dissolved at the end of 2001.

Two subcommittees: i) Drug Discovery and Development (chair Robin Ganellin) and ii) Nomenclature and Properties and Units (Urban Forsum) shall be established. Terms of reference (TOR) for the Subcommittee on new drug development have been presented by RG and were discussed. RG will

circulate the amended TORs and UF was asked to prepare terms of reference for his subcommittee on nomenclature and properties and units. The chairmen of the subcommittees shall invite the members of the subcommittee (including the NR) to the meetings. Rules and TORs for the Division Committee will be drafted by AK.

The new project driven system is now fully in operation and the budget of the Division VII will enable funding of 8 - 10 projects. Single project funding should normally not exceed ~ USD 5000.

#### **4. -Results from the GA in Brisbane and related Meetings**

The Interdivisional Committee on Nomenclature and Symbols (IDCNS) has been restructured into the Interdivisional Committee on Terminology and Symbols (IDCTS). Concern was expressed that this very important harmonising body that delivered highly valued services within the Divisions will disappear. AK will approach Prof. McNaught and ask for clarification.

The Medicinal Chemistry Section presented a symposium on "Drug Discoveries in the 21<sup>st</sup> Century" at the IUPAC Congress in Brisbane and had a joint meeting with the Asian Federation of Medicinal Chemistry.

#### **5. -Discussion of future plans and how the Division Committee could contribute**

AK emphasised the function of the Division Committee as generator of projects and recruiter of new people for projects in new areas of Chemistry and Human Health. ML pointed out that in the emerging field of bioinformatics, standard setting is not co-ordinated. He sees a major opportunity for IUPAC to establish formats for nomenclature and standardisation in the field of gene expression and micro array techniques and to promote the transfer and co-ordination of information. Terms of diagnostic tools and diagnosis have not evolved with hence the need for a Glossary of Bioinformatics

ML was asked by the Division Committee to contact knowledgeable people in this field and explore the feasibility of initiating a project in the field of molecular biology similar to the work of the former CNPU. To focus the ideas, topics of bioinformatics and drug development might be most suitable. As a pilot project ML will organise a 2-day conference for users on a high profile area. Another day should be added for prioritisation and if possible a consensus report should be prepared. A possible date would be late September 2002 and a more suitable venue is the Washington / DC area to get the involvement of the NIH. Funding from outside should be sought.

To make IUPAC more visible in the scientific community and to attract others to co-operate with the Division VII and advertise that scientists might submit new and personal projects, RG has drafted a document about the contributions of the Medicinal Chemistry Section and its relationship to industry as a source for letters to industry which he will circulate.

MC will distribute his article "IUPAC: A Glorious Past, Productive Present and Bright Future" which might be used as revised and condensed information for the same purpose. Both should be merged so as to form a one-page total document that has three paragraphs: An opening description of the IUPAC & DCHH based upon MC original, a second paragraph summarizing some of the (former) Med Chem Section's activities based upon RG's original, and a final paragraph (MC) indicating how anyone can send in ideas for new projects. Then, someone from the (former) Clinical Chem Section shall provide a second paragraph describing some of its former activities so that one or the other versions of this letter could finally go out, as appropriate, to various journals associated with either of the two fields.

#### **6. Review of the Projects of the Division VII**

##### **6.1 Completed and Current Projects( previous system) from Sections and Commissions and their Progress**

###### **VII.C Clinical Chemistry Section**

###### **VII.C.1 CNPU**

6.1.1 Recommendation for the Use of Nanotechnology in Clinical Laboratories [2000-014-1-700] (Peter Wilding) the status of this project will be inquired by ML. The option to abandon the project was issued.

6.1.2 Properties and Units in the Clinical Laboratory Sciences [710 /8/87]. This ongoing activity has been started by H. Olesen and finished in 2001. Seven new projects will ensure continuation in this field.

UF gave an update on the current situation of the database which has been kept and been continuously updated on an internet server in Copenhagen/DK. With the retirement of H. Olesen, the custody was transferred to UF in Linköping/Se who will upgrade and maintain the generic database. The generic database will be published by IFCC and made available on their web-server. The maintenance of the generic database requires at least one person/year. Due to limited financial resources in Sweden this is not feasible at present and the deterioration of the generic data might occur within one year. It would be logical and valuable to attach the database to WHO/ICD, however WHO did not accept to host and maintain the database. The in some sences competing system by LOINC, which has gained acceptance in the USA, has the problem of logical inconsistencies and will obviously run into problems. Suggestions to keep the database alive include contacts with the NLM and a commercial provider (IBM).

6.1.3 Nomenclature, Properties and Units in Clinical Molecular Biology[710/25/95] (Pedro Soares de Araujo) For two decades, the C-NPU has authored recommendations on how to express and code examination results in various specialities of Laboratory Medicine as published in PAC and the Silver Book. This project extended the principles to Medical Molecular Biology furnishing a basis for unambiguous international communication. The project has been resubmitted.

## **VII.C.2 ComTox**

6.1.4 Exposure Assessment and Decision Rules in Compliance Testing for Implementation of Exposure Limits [720/4/93] ( JMC) This project has been finalized on 12-2001.]

6.1.5 Exposure Assessment using the Logbook Method [720/7/95](E. Olsen), comments have been received and will be included, the document will be published in January 2002.

6.1.6 Immunochemistry of Metal Sensitization [# 1999-047-1-700] (D Templeton) the project is in excellent progress and nearly completed.

## **VII.M Medicinal Chemistry Section**

### **VII.M.1 CNPU**

6.1.7 Nomenclature Guidelines for Combinatorial Chemistry in the Synthesis and Screening of Compound Libraries [753/1/95] (Derek MacLean) the project has been finished with a glossary of terms in 1997 (PAC 71 (1999), 2349-65) and should be continued, however the contact with D. MacLean was lost due to a change of address. IUPAC Glossary of Combinatorial Terms. Derek MacLean is to make a project submission for updating the existing Glossary of Combinatorial Chemistry Terms, which shall be included in the Compendium of Glossaries (RG).

6.1.8 Legal implications of patenting virtual libraries. A position paper pertaining to patenting in the form of a one page statement has been finalized by PE. He will circulate his position statement letter to the DC for approval before the year ends. AK will clear the publication process with the Bureau.

### **VII.M.2 CTD**

6.1.9 Training and Research in Medicinal Chemistry in Developing Countries [# 763/1/95] (Antonio Monge Vega)The project has been completed.

### **VII.M.3 CNTST**

6.1.10 Natural and Unnatural Substances Related to Human Health (700/2/98).

Prof. Topliss (chairman) will have the final article ready for publication at the end of the year 2001 and RG will contact him to have the text published as an IUPAC publication.

6.1.11 Pharmaceutically Acceptable Salts of Drug Substances [772/1/94] (Camille Wermuth) has been completed and is due to be published by Wiley.

6.1.12 Technologies in Combinatorial Chemistry [773/1/95] (D. Mclean) has been superseded by [753/1/95] s a.) and as such been concluded.

6.1.13 Glossary of Drug Metabolism Terms [2000-009-1-700] (PE) The glossary is in progress.

6.1.14 Human Drug Metabolism Database [2000-010-700] (PE) The joint project (ICSU/IUPHAR/IUPAC) is in progress.

## **6.2. New Project System**

An updated list of the current ( see also: <[http://www.iupac.org/projects/p\\_review/](http://www.iupac.org/projects/p_review/)> )and planned projects and their status will be shortly circulated by AK. The listed projects Immunochemistry of Metals (D. Templeton); Glossary of Drug Metabolism Terms ( PE); Database of Human Drug Metabolism ( PE/IUPHAR); Recommendations for use of Nanotechnology (P. Wilding) were discussed above (6.1).

### **6.2.1. Project applications approved by the Division Committee and submitted to IUPAC review**

6.2.1.1 Glossary of Toxicokinetics [# 00-34](M. Nordberg) This project has been submitted and is now under review and has reached stage 4.

TP mentioned that Prof. J. Seydel from Borstel had the intention to produce educational material on pharmacokinetics which could be combined with the one on toxicokinetics, however, the status of his proposal is unknown. BH will contact J. Seydel and inquire, if a contact between Monica Nordberg and J. Seydel has been established.

6.2.1.2 Research and Training in Medicinal Chemistry in India, Pakistan and Sri Lanka [# 01-48] (M. Chorghade) and a similar project is planned for Egypt (O. Kebir). Of the listed reviewers only the top three should be considered for the external review process.

6.2.1.3 IUPAC Glossary on Pharmaceutical Process Chemistry [# 01-49]

M. Chorghade has written a first draft and plans to have a group meeting in November 2002.

6.2.1.4 Natural Products with Medicinal and Nutritional Value ; "Nutraceuticals" [# 01-50]

The name of the project [# 50] has been changed to: Aspects of Natural Compounds with Medicinal and Nutritional Value (MC). The project will be resubmitted by M. Chorghade.

6.2.1.5 Fundamental Toxicology for Chemists.[# 01-53] (John Duffus) It is planned to publish a revised second edition of this successful textbook and the former authors have agreed to contribute to its updating. The requested funding is for distribution of the text, i.e., to make it affordable to developing countries and to implement electronic distribution.

6.2.1.6 Concepts for Request in Clinical Laboratories [# 01-58] (UF)

6.2.1.7 Properties and Units for Transfusion Medicine and Tissue Typing[# 01-59] (UF)

6.2.1.8 Global use of the C-NPU Concept System for Properties in Toxicology[# 01-66 ] (Wolf Kulpmann). It is the aim to work out properties and units for Global use of the C-NPU concept system for properties in toxicology based on the former C-NPU commission's concepts and syntactic rules.

The CNPU projects 2001-48, -49, -50 and -58, -59 have been reviewed and endorsed by the Division Committee and are thus ready for external review.

### **6.2.2 New Project Ideas to be followed and submitted in the field of NPU**

The main task of a new **Subcommittee on Nomenclature and Properties and Units** will be to promote new projects in the field of Nomenclature, Properties and Units in the Clinical Laboratory Sciences and maintain scientifically and conceptually sound ways of expressing the outcome of measurements and other examinations in laboratory medicine. The NPU coding scheme and vocabulary is based on the SI system and of global use. The following projects shall be added to the database:

6.2.2.1 Properties and Units for Function Examinations [# 01-67] Dr. Antonin Jabor shall resubmit a project on properties and units for function examinations based on the former C-NPU commission's concepts and syntactic rules

6.2.2.2 Properties and Units in Molecular Biology[# 01-68] Pedro Soares de Araujo

6.2.2.3 Properties and Units for Urinary Calculi [#01-31] (Dr. Antonin Jabor) It is the aim to work out properties and units for Urinary Calculi based on the former C-NPU commission's concepts and syntactic rules

6.2.2.4 C-NPU Concepts and Traceability of Measurements[# 01-69] (Gunnar Nordin [gunnar.nordin@equalis.se](mailto:gunnar.nordin@equalis.se) ) The traceability project needs to emphasise the definition of the measurand, and the NPU structure could serve for this purpose. Furthermore, the traceability project has to outline various types of calibration hierarchies, which is especially important in the various types of measurements encountered in Laboratory Medicine. Finally, the extensive use of external quality assessment (proficiency testing) and increasing reliance on accreditation in this discipline should contribute valuable experience in further ensuring comparability of results.

6.2.2.5 Properties and Units in Flow Cytometry

### **6.2.3 Projects in the field of Drug Development**

New project of a **Subcommittee on Drug Discovery and Development** might include:

6.2.3.1 Evolution of Drug Discovery J. Fisher has been encouraged to submit an application. There is, however, a need for a budget adjustment before re-submission.

6.2.3.2 Bioinformatics A project concerning Bioinformatics (genome, micro array technique) will be initiated by M. Liebman as discussed above (see 5.).

6.2.3.3 Compendium of Glossaries (RG). RG asked for support to help with the index of the msc. PE has offered assistance with this task.

Other possible topics in the field of Medicinal Chemistry might be the following project ideas

6.2.3.4 Biomarkers for therapeutic and diagnostic effectiveness (B.K. Trivedi)

6.2.3.5 Educational material for IUPAC courses in the field of Medicinal Chemistry (MC and A. Monge Vega)

6.2.3.6 Pharmacokinetics for Chemists, (J. Seydel) BH will contact J. Seydel.

### **6.2.4. Project from other areas**

6.2.4.1 Educational Material for Pesticide Handling in Developing Countries with Warm Climates. BH will further explore the feasibility of this project together with John Duffus. MC offered his input.

6.2.4.2 Estrogen Substitution Therapy -a previously suggested topic from RC- was discussed. The Division Committee concluded that a therapeutic/pharmacological focus is not within the scope of Division VII. Hence dealing with the health aspects and pros and cons of substitution therapy would not be appropriate, but the evaluation of estrogen-like activity of natural compounds should be explored further. ML offered to follow this topic by means of a feasibility project with one expert meeting to be organised.

6.2.4.3 Data base on chemical disasters. BH will contact Dr. Nagymajtenyi from Hungary for clarification about the status of this project idea.

6.2.4.4 Determination of the concentration component of air exposures to volatile compounds. E. Olsen will submit this project in the near future.

6.2.4.5 Neurochemically Active Metals: Manganese. This project will not be submitted instead a new project on Exposure Assessment will be submitted: Educational materials for the IUPAC homepage,

which can be downloaded free of charge. E. Olsen, Jytte Molin Christensen, John Duffus, Stephen M. Rappaport and Chai Zifang.

6.2.4.6 Risk Assessment in the Workplace E.Olsen is presently seeking funding for translation of an existing Danish document and preparing a document with a global perspective of this important issue.

6.2.4.7 A project on particulate matter (R. Nolan, John Duffus) will not be supported, unless a suitable document from the previous project is presented by R. Nolan.

### **6.3 Interdivisional Projects**

6.3.1 Molecular Basis of Biodiversity, Conservation and Sustained Innovative Utilization [1999-003-1-300]. The cooperation with Div. III is represented by A. Monge".

6.3.2 The project Medicinal Chemistry in the Development of Societies and Biodiversities of Natural Compounds should be resubmitted by A. Monge to the Inter-Divisional Committee.

It was emphasized that the initiation of new projects and their presentation on the internet is somewhat unclear due to parallel lists. AK and BH will contact the bureau to inquire on the updating of the existing information on the IUPAC homepage. The title is erroneous: Div VII is Chemistry and Human Health, not Environment.

### **7.-Cooperation within IUPAC**

Prof. A. Monge Vega has been named as the representative of Div VII to the Organic Chemistry Inter-Divisional Committee on Biotechnology.

Peter Atkins will chair the restructured Committee on Chemistry Education [CCE]. MC has been nominated to the CCE as representative of the Div VII. His project proposals on "Research and Training in Medicinal Chemistry in South Asia" and "Glossary of terms" would fit well with the themes of general education and "public appreciation of chemistry and with chemistry education in developing countries, including exchange of information among countries on curricula and innovative ways of teaching chemistry" as have been outlined by Dr. Becker.

The Project on Traceability (De Bièevre) will involve Gunnar Nordin.

AK addressed several projects submitted from other Divisions which include issues of Human Health and which might be of interest for active co-operation or where additional input (review) could be offered:

Isotope MS (Div II)

Glossary of Terms of photodynamic therapy (Div. III)

Post Genomic Chemistry

Endocrine Active Substances Effectiveness of QSA and Endocrine Disruptors (Div. VI)

Projects relating to Kinetic Issues have been submitted from different areas. A need for harmonisation of these projects concerning nomenclature was expressed. AK will forward a letter to express interest and to underline specific aspects.

BH will establish contact with the project leader and seek further information on the projects:

Pest Management for crops: (Nr.: 39/20-22)

Agricultural Spray drift (Nr.: 39/23, 26) The goal of this project is harmonisation of the use of agrochemical spray drift studies for risk assessment and development of mitigation measures

### **National Representatives**

The Division Committee is entitled to nominate 6 NR, they should come from countries not represented in the Division. It was unanimously decided to nominate for a global representation of the Division:

Prof. Zhongliang Chen (China)

Dr. Pierre-Etienne Bost (France)

Dr. Giovanni Gaviraghi (Italy)

Dr. No-Sang Park (Korea)

Dr. Totani (Japan)  
Dr. Petedov (Russia)

The NR will be informed about the activities of the Division and be invited to the Division Committee and Subcommittee Meetings. They are encouraged to become involved in the projects of the Division and make their own proposals for new projects.

RG criticised that former NR which have been actively involved and contributed to the work of the Section of Medicinal Chemistry are not among the listed recent nominations. It was agreed that these former NR should remain associated with projects and/or the Subcommittee activities.

## **8.-Co-operation with other organisations**

**8.1 IFCC:** The links between IFCC and IUPAC Section on Clinical Chemistry will be kept by continuing with active collaboration, although formal links have been deleted.

**8.2 ICSU and IUPHAR** Co-operation is related to the Drug Metabolism Database and has been proven to be very successful. Application for funding through ICSU should be given consideration. AK will circulate the necessary information. The home page can be found under: [www.ICSU.org](http://www.ICSU.org)

**8.3 WHO:** The location of the Compendium remains in Sweden till the end of 2001. WHO has been approached to assume responsibility for the updating and maintenance of the database as from 2002, but the outcome is not yet certain.

## **9. Finances and Allocations**

In Brisbane the new project system has been discussed at an interdivisional meeting.

The Division can expect allocation for 2002-2003 of about 70.000 USD. The priorities will be set by the Division Committee. 75% should be used for projects and 25% may be spent for operational expenses. The funds, once awarded to a project, are committed for the lifetime of the project, even if it extends beyond, e.g., the proposed two years.

In a recent communication, the Treasurer (Dr. Buxtorf) has given the following ground rules:

The Division budgets are based on past expenses of the Division (98-99).

Each division will receive an additional 10,000 USD.

GA funds will only be allocated to the Division Committees.

## **10. Any other business**

The next GA 2003 will be held in Ottawa/Canada. It was suggested that the Division be present at the IUPAC Congress with a symposium on Recent Advances in Chemistry and Human Health. Possible topics are Risk Assessment, Nickel, and Bioinformatics in Medicinal Chemistry.

### **Next meeting**

The next meeting of the Division Committee might be held in Riga/LATVIA, 30-05-2002 (tentative or S.Diego -June 2002). AK will make the necessary inquiries and provide information concerning travel and accommodation. Members who are interested in participation of the 5<sup>th</sup> Conference of the Baltic Association on Laboratory Medicine are asked to suggest topics for plenary lectures.

Adjourned 18:00

prepared by:  
B. Heinzow  
Division Secretary