

DIVISION VII
Chemistry and Human Health

Minutes: Division Committee Meeting
Brussels, 6-XII - 8-XII-2002

Location: Club de la Fondation Universitaire, Egmontstraat 11, B-1000 Brussels

Beginning at 9:00 am, Saturday 7-XII

Division Committee :

Anders Kallner ((President, Division of Chemistry and Human Health)) anders.kallner@ks.se

Mukund Chorghade chorghade@prodigy.net

Jytte Molin Christensen New E-mail: Q-International@wanadoo.fr

Rita Cornelis rita.cornelis@rug.ac.be

Urban Forsum urban.forsum@imk.liu.se

Robin Ganellin c.r.ganellin@ucl.ac.uk

Thomas Perun Tjperun@aol.com

Birger Heinzow (Secretary): bheinzow@lanu.landsh.de

National Representative:

Masayuki Totani (Japan) mtotani@swu.ac.jp

Task Group leader:

Eric Olsen

excused:

Paul Ehrhardt perhard@utnet.utoledo.edu

Michael Liebman liebmanm@mail.med.upenn.edu

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 and Eric Olsen (EO) from DK/France and thanked RC especially for organising the meeting.

2.-Approval of the Agenda and Minutes from the previous Division Committee Meeting, Boston, 14-16 June 2002

The agenda was accepted with amendments and the Minutes from the Boston Meeting were discussed and approved.

The draft minutes from the SCDDD (Subcommittee on Drug Discovery and Development) (Barcelona 2002-08-31) have been circulated and will be approved at the next SC meeting.

Minutes from the SCNPU (Subcommittee on NPU) and SCTRA (Subcommittee on Toxicology and Risk Assessment) will be prepared and circulated.

3.-Division VII Presidents Report

AK gave a brief report of the Bureau meeting in Paris. The structure of Division VII with subcommittees has been approved. The existence and the function of the Bureau has been challenged and will be reviewed.

The minutes of the Project Committee Meeting (Paris 2002-09-13) have been distributed. It was remarked that the questions brought up with the textbook: Fundamental Toxicology, are obviously due to misinterpretation of the role of the RSC.

The continuation of the project 2001-029 (H. Klich) is unclear since Prof. Klich died in September. AK will inquire about the status.

The problem of providing continuity for maintaining electronic glossaries and data bases under the new project system was discussed. This problem arises mainly because of limited lifetime of projects and the lack of funding for continuation. In the past this update has been provided by the committees.

4. DC Nominations and Election procedure

4.1. Nominations Committee

For the forthcoming election (term 2004-2005) an Election Committee will be installed consisting of members from inside and outside IUPAC. Tom Perun (Chair) and Rita Cornelis were nominated and

Henk Timmerman from NL is a possible candidate from outside. Further nominations shall be proposed to TP by the DC members directly at their earliest convenience. TP will finalise a list of members who accepted to become the EC and circulate the list within the DC. AK will inquire whether EC members are electable or not to the next DC. Subcommittees are not part of the electorate for the Titular Members of the Division Committee.

5. - Report from Subcommittees

5.1 Subcommittee on Drug Discovery and Development (RG)

Minutes of the previous subcommittee meeting (Orlando 4-3.02) have been approved and are displayed on the IUPAC website. In the 5-2002 issue of Chemistry International two articles by Paul and Robin concerning Medicinal Chemistry have been published.

RG gave a report on the meeting of the SCDDD (Barcelona 8-31.02), the minutes have been circulated within the DC. RG has successfully raised interest of several new colleagues in IUPAC activities and becoming members of the Subcommittee. 12 scientists attended the meeting. John Proudfoot, distinguished scientist at Boehringer Ingelheim Inc., Ridgefield, Connecticut, USA, has been nominated as secretary of the subcommittee, this and his Associate Membership was approved by the DC.

Following serious criticism by several world figures in Medicinal Chemistry at the last International Conference on Medicinal Chemistry that the name "Medicinal Chemistry" has been unfavourably abandoned in the IUPAC structure of Divisions and Commissions, the DC discussed this apparent loss of visibility and in response suggested appropriately to rename the Subcommittee into: Subcommittee on Medicinal Chemistry and Drug Development. AK will convey this to the Bureau and request that the name is changed to Medicinal Chemistry and Drug Development.

It was suggested to link the websites of the European and Asian Federations of Medicinal Chemistry with the IUPAC site. Again the name Medicinal Chemistry would make it clear that IUPAC is a stakeholder in this important field of Chemistry and Human Health.

The information for Fabienne Meyers on the installation of links with AFMC and EFMC and ACS will be provided by RG.

After discussion with Ted Becker and John Jost, MC will finalise a letter addressing Chemical Industry asking for support in 2003.

5.2 Subcommittee on NPU (UF)

The NPU database link <http://dior.imt.liu.se/cnpu/> has been established on the IUPAC homepage. U Forsum will contact Fabienne about the long term host for the database, at present EQUALIS (the Swedish non-profit external quality assessment organisation) will host the database. The issue of long-term maintenance of the database has to be solved. IFCC will continue with an annual support of 5000 SF. Contacts with a French group have been established, who might be interested in adopting the NPU-scheme. IUPAC and IFCC are the proprietors of the coding scheme. UF will bring the issue of copyright and financial issues up with the IFCC scientific division and the IUPAC division of chemistry and human health in case that the database is used in a commercial context.

The problems of different transmission standards of report and request were discussed and at present the US standard is taking the lead. The C-NPU will discuss this in a forthcoming meeting to look into the feasibility of merging the different approaches.

CEN ENV 1614 is still not upgraded to an EN. The VIM Committee is presently revising VIM and it is advisable to incorporate any change in the VIM before. UF will prepare a draft to underline the necessity of continuation and to make these activities more visible to possible stakeholders (IFCC, IUPAC, ISO, CEN TC 251, HL-7, LOINC, Names-Labs, NCCLS and possibly other).

5.3 Subcommittee on Toxicology and Risk Assessment (John Duffus)

Terms of reference for the Subcommittee have been accepted at the DC meeting in Boston and are attached to the Boston minutes(2002), a Committee Member list has not been formally accepted yet, however an informal meeting was held recently. John Duffus will convey a list of members to AK at his earliest convenience.

5.3.1. Exposure Assessment using the Logbook Method [720/7/95](E. Olsen) The final draft has been externally reviewed and will be put on the IUPAC homepage for public review soon.

6. - Review of Activities

6.1. Completed Projects

6.1.1. 720/4/93 - Exposure assessment and decision rules in compliance testing for implementation of exposure limits (JMC) The paper in Accreditation Quality Assurance 7: 28-35 (2002),

(authors JM Christensen, E Holst, E Olsen, PT Wilrich) has gained much attention in DK. A course on compliance testing run by the Danish authorities is based on the project. Formulas for the calculation of the power function and the probability of obtaining an inconclusive result, is available at the website <http://www.ami.dk/research/conformity/>. At the same website a freeware computer program, conform1e.exe, is available for the calculations. JMC will provide a summary of the publication for the Secretariat (Fabienne Myers) to be published in CI.

- 6.1.2. 700/2/98 - Natural and Synthetic Substances Related to Human Health. RG reported that J Topliss has finalized a 60 page document which will be published in the October issue of PAC. The next step is drafting and distribution of a short version for the media and laymen, to raise interest in people writing articles for the general public regarding the misconception about natural versus synthetic medicines. PE and Jim McAlpine will assist TP, who has condensed the paper to 1 1/2 pages. MC, who has recently attended a seminar on PR by the ACS, suggested to use the instrument press release to distribute the information about this project. He will provide a list of contacts for TP. The best approach would be through the IUPAC secretariat. RG remembered the need for an IUPAC Press Officer to handle these issues professionally.

6.2. Current Projects

- 6.2.1. 1999-047-1-700 - Immunochemistry of metal sensitization (D.Templeton). The project has been completed and is ready for review.
- 6.2.2. 2000-009-1-700 - Metabolism terms. (PE) A list of entries for the glossary will be provided by the end of the year by PE.
- 6.2.3. 2000-010-1-700 - Human drug metabolism database(PE). The project is running according to schedule, currently a JAVA programme is developed for this Oracle database mounted on a dual server system interfaced to the internet.
- 6.2.4. 2000-014-1-700 - Recommendations for the use of nanotechnology in clinical laboratories (P.Wilding). A final document will be ready by the end of the year.
- 6.2.5. 2000-034-2-700 - Glossary for toxicokinetics of chemicals (M. Nordberg). The project is making good progress and a list of 287 terms for the glossary has been selected and is now under revision. The task group will meet next April to finalise definitions. M Nordberg is asked to send a copy of the draft glossary to RG:
- 6.2.6. 2001-066-1-700 - Global use of the C-NPU concept system for properties in toxicology (Wolf K lpmann) The task group met in Hannover (2002-08-03/04) and has been changed to R. Cornelis, J. Duffus, R. Dybkaer, M. Nordberg, advisers: D. Templeton, J. Christensen. The project is making good progress.
- 6.2.7. 2001-067-1-700 - Properties and units for function examinations (A.Jabor) The project has nearly been completed.
- 6.2.8. 2001-068-1-700 - Properties and units in Medical Molecular Biology (P. Soares de Araujo). The project will be finished next year, some topics need further in depth disussion. It was discussed to create a new project on proteomics, to deal with this subject separately.
- 6.2.9. 2001-070-1-700 - Properties and units for urinary calculi (A:Jabor) The project is close to finalisation.
- 6.2.10. 2001-048-2-700 - Research and training in medicinal chemistry in India, Pakistan and Sri Lanka (MC). The project will be completed January next year, MC will present results in India by the end of the year.
- 6.2.11. 2001-049-2-700 - Glossary of terms used in process chemistry/manufacturing of active pharmaceutical ingredients, and pharmaceuticals (MC and E. Breuer) The project is nearly completed and can go into the review process on the IUPAC website next year. Results will be distributed by lectures and will be published in Organic Process Research & Development. Updating every two years is planned.
- 6.2.12. 2001-050-2-700 - Chemical, pharmacological aspects of natural products with medicinal and nutritive value (MC) J. Cardelina has not been reached, the progress is rather slow.
- 6.2.13. 2001-058-1-700 - Concepts and structure for requests in clinical laboratories (UF) A first draft will be circulated next year.
- 6.2.14. 2001-059-1-700 - Properties and units for transfusion medicine and immunohaematology (UF) The project has been almost finished.
- 6.2.15. 2002-001-1-700 - IUPAC compendium of terms for chemists applied to drug development (GD). An electronic version has been prepared by PE, the editorial work will start now.

To enhance attention and to invite more comments on actual projects under review MC will inquire if information can be included in the ACS actual website presentation alerting on projects under review. The question came up about the copyright status of draft manuscripts displayed on the internet for review.

6.3. Interdivisional Activities

- 6.3.1. 1999-003-1-300 - Molecular basis of biodiversity, conservation and sustained innovative utilization. A. Monge is representing the Division and MC was named as liaison. No information on the progress of the project could be provided.
- 6.3.2. 2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy. N Nifantiev has become involved and A Kallner corresponded with him, but has not yet received information from Prof. Nifantiev on the status of the project..
- 6.3.3. 2002-005-1-300 Post Genomic Chemistry. A request for a budget was made. The DC approved allocation of 1500 \$.
- 6.3.4. 2002-030 Fighting bacterial resistance. The opinion within the DC was mixed, it was noted that the project has a main focus on drug development and is not including the genetic aspect of the issue of bacterial resistance. 1000 \$ will be offered from the Division VII budget because of some vested interest in this area.

6.4. Project Applications in review (Nov. 2002)

- 6.4.1. Revision of the Gold Book (A.Jenkins). AK will write to A Jenkins and inquire about possible input on nomenclature by DIV VII:
- 6.4.2. Fundamental Toxicology for Chemists. (John Duffus) The project has reached level 5 and should be accepted soon. The DC supports this projects with priority, since the previous textbook has gained much approval and made the activities of IUPAC Division VII visible to the outside. JD was asked to correspond with the PC concerning questions of RSC support and will provide an updated budget. Due to the long review process he has to inquire whether the previous task group members are still willing to cooperate or not. 5000 \$ could be allocated to this task.
- 6.4.3. NPU concepts and traceability of measurements (G.Nordin). A new project application will be submitted. Funding with 2200 \$ can be allocated.
- 6.4.4. Analogue-based drug discovery (J.Fischer). J. Fisher has revised his project proposal and favourable comments have been received. The application was approved by the DC. The budget should be reduced to 3000 \$.
- 6.4.5. Best practice for workplace exposure assessment, critical review of methodology (E.Olsen). A revised application has been circulated The task could be supported with 4000 \$.

6.5. Conferences

The DC was informed that 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). A new project on applications of Toxicokinetics was discussed and received positive support. A project application will be prepared.
- 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 will be prepared later in 2003. 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.
- 7.1.3 Bioinformatics. TP will contact ML to inquire if he is still interested in a project and ask him to provide a project or ideas.
- 7.1.4 Clinical trials. Because of absence the opinion PE conveyed in a recent letter is cited : "Recently approved drugs and protocols associated with approved drugs for a variety of therapeutic classes can be obtained from the FDA for use as models by individual request. The notion to have more of a globalized standard (perhaps at least representing a minimal level of protocol) strikes me as being a good idea that seemingly should already be the subject of discussion among more of our biologically oriented counter-parts, e.g. IUPHAR. However, I am not directly aware of such an activity anywhere so perhaps we could indeed explore such a possibility". This issue might hence be suitable for ICSU funding in cooperation with IUPHAR and IUTOX. Possible contact in IUPHAR are F. Sjöquist (Clinical

- Pharmacology Section) and E Dybing (Norway) President of IUTOX. Tom will contact PE and ML and draft a sketch for a possible project. AK will contact Ted Becker.
- 7.1.5 Glossary of terms on Biomarkers . (G Gaviraghi) No information was available.
 - 7.1.6 Biomarkers for therapeutic and diagnostic effectiveness. RG has received no response from BK Trivedi. IFCC is not interested in this project. The idea might be brought up again in 2004.
 - 7.1.7 Educational material for IUPAC courses in the field of medicinal Chemistry. (MC and A Monge) The project is still under consideration.
 - 7.1.8 Database on Chemical Disasters. BH contacted Prof. Nagatigayemi/Szeged but has received no response.
 - 7.1.9 White book on susceptibility of children to chemicals and pharmaceuticals. No project has been formulated. The topic is however considered of high impact and might also be suitable for a larger ICSU funded interdisciplinary project.

7.2 Conferences

A conference on Biodiversity will be held in New Delhi in 2004. MC will contact the organisers and provide information concerning IUPAC sponsorship.

7.3 Division brochure

MC volunteered to write a Division VII brochure and will circulate a first draft by the end of January 2003.

8.-Cooperation within IUPAC

A joint meeting with CCE shall be scheduled during the GA in Ottawa. AK will make the request. JD was nominated as liaison to CCE. He has been granted travel subsistence (coming from revenues of the Toxicology Textbook) to meet with CCE in Ottawa.

9.-Cooperation with other Organisations

ICSU: Recent ICSU Grant information has been distributed within the DC. IUPAC may submit two applications for the small grant program [up to \$50,000] and up to two for the large grant program [\$50,000 to \$100,000].

IFCC: Good cooperation with IFCC and DIV VII in the field of NPU is continuing.

WHO: IPCS circulated a letter to the GEENET network and asked for assistance in surveillance and support in response to chemical incidents, including those of deliberate origin. This activity might be of interest to IUPAC especially with respect to capacity-building resources and activities. Contact person at WHO/IPCS are Dr. Olowokure (olowokureb@who.int) and Dr. Gutschmidt (gutschmidt@who.int) in Geneva. BH will inform Ted Becker.

EFMC and AFMC: Exchange of links on websites will be arranged for. RG will contact Fabienne.

NIH: Phil Wechsler has expressed his interest in the IUPAC glossary of terms in Toxicology and intends to display an updated version on the NIH Toxnet website. Further cooperation in developing interactive educational tools (ToxTutor) is under consideration.

10. Personalia

For the vacant NR position Abraham J. Domb was nominated.

For Associate Membership Wayne Temple (NZ), Henrik Timmerman (NL), Reuben Jih-Ru Hwu (Taiwan), Wjciech J Stec (PL), Nesrin Emekli (Turkey) and K. Gurjar (India) were nominated.

MC will arrange for providing a CV of Dr. Gurjar to the Division President and Secretary. AK will inform the Bureau.

The mailing list shall include TM, NR, AM, SC chairs and secretaries and project leaders.

10. Finances

Of the total budget 41,000 USD have been allocated to accepted projects and the last balance amounted to + 11.300 USD remaining for projects. The requests for funding by the current project applications under review amount to a total of 20500 USD (1000 + 1500 + 3000 + 4000 ; + 3000 + 5000 + 3000). The balance of DC allocation will be inquired by BH. AK will inquire whether money not spent in single projects (after completion) will be relocated to the Division budget.

support the project on Bacterial Resistance with	USD 1 000
support the project on Post Genomics with	USD 1 500
accept the project on Analogue Drugs 02-051 (J Fisher)	USD 3 000
accept the project on Workplace Assessment (Eric Olsen)	USD 4 000
reserve for a project on Toxicokinetic Concepts (Nordberg)	USD 3 000
reserve for the Textbook project 01-53 (J. Duffus)	USD 5 000
<u>reserve for project on Traceability (G Nordin)</u>	<u>USD 3 000</u>

11. -Any other business

The next meeting of Division Committee VII will be held at the GA 2003 in Ottawa, 9. - 10. August. A meeting will CCE and COCI on the 11th will be requested. UF will attend the ICTNS meeting 12th of August.

Adjourned 18:00

prepared by:
B. Heinzow
Division Secretary