

DIVISION VII
Chemistry and Human health

1. Draft
Minutes of Division Committee Meeting
held in London, April 28, 2001

Location: Novartis Foundation

Prepared by Birger Heinzow (Division Secretary- email: bheinzow@lanu.landsh.de).
8th May 2001

Participants:

Dr. Anders Kallner ((President, Division of Chemistry and Human Health)) anders.kallner@lab.ks.se
Prof. Robin Ganellin (President, Medicinal Chemistry Section) c.r.ganellin@ucl.ac.uk
Dr. Thomas Perun (Secretary) Tjperun@aol.com
Dr. Rita Cornelis (President, Clinical Chemistry Section) rita.cornelis@rug.ac.be
Dr. Birger Heinzow (Secretary) bheinzow@lanu.landsh.de

Saturday 12:00 am – 18:30

TOP

1.-Opening remarks

Division President Dr. Kallner chaired the meeting and welcomed the participants, special thanks were addressed towards Prof. Ganellin for organising the local most suitable venue and accomodation.

2.-Approval of the Agenda

The Agenda and the Minutes from Brussels were approved.

3.-Division VII Presidents Report

Dr. Kallner summarised the recent information received from the Secretary General. The restructuring of IUPAC is developing as planned and the new structures will definitely implemented without any exemptions (no Commissions!).

The allocated funds to the Division VII have been almost spent.

For meetings in conjunction with Conferences (e.g. ACS) the chair should inquire about possible room and service charges and optimise the meeting places in order to avoid post-billing.

ICSU has initiated a project on GM Food and 80.000 \$US have been allocated to IUTOX for leading the project: Questions and definitions of benefits and risks of genetically modified food (GMF). Dr. J. Cardellina will be asked to be involved. The options of i) a IUPAC project or ii) representation of IUPAC by liaison were discussed, decisions will be made after deliberation in Brisbane, when the requested input has been specified.

Inquiries will be made to the Bureau how such a liaison can be funded.

4. -Report Medicinal Chemistry Section - VII.M

Dr. Ganellin gave a report on the Section meeting, March 31, 2001, San Diego in conjunction with the ACS meeting, the minutes will follow very soon.

The MCS homepage, currently linked to the ACS Medicinal Chemistry site will be transferred to IUPAC.

Suitable links at ACS, IFCC shall be installed. Dr. Kallner will suggest to Fabienne Myers that the Terms Clinical Chemistry and Medicinal Chemistry are included in the titles respectively, to increase visibility and access in internet search routines(hits).

Commission on Nomenclature and Terminology - CNT, VII.M.1

WP on Nomenclature and Publication Guidelines for Combinatorial Chemistry in the Synthesis and Screening of Compound Libraries (chair: Dr. Derek McLean)

Patenting of Virtual libraries. It is intended to make this a project since the problems of patenting virtual libraries could have serious impact for drug development

IUPAC Glossary of Combinatorial Terms has been published as a technical report in PAC in December and co-published in the Journal of Combinatorial Chemistry. A review and update at 3-5 year intervals was recommended.

There are two separate projects on Drug Metabolism both headed by Paul Erhardt.

(a) WP on a glossary of drug metabolism terms. The project on a database of human metabolism, under the IUPAC leadership of Paul Erhardt was held up for 9 months. There are currently 15 members on this WP and they plan to review approx. 150 terms.

(b) A joint project with IUPHAR on a database of human drug metabolism which has received a grant from ICSU.

WP Compendium of Glossaries which will merge the different glossaries in one compendium in sections with cross references (co-ordinators: Prof. Ganellin) was debated and Dr. Kallner suggested that it should be based on an Access Database with easy internet access rather than a hard copy Compendium only.

WP IUPAC Glossary on Pharmaceutical Technology (Eli Breuer, Janos Fischer) status is unknown

IUPAC Glossary on Pharmaceutical Process Chemistry (Giovanni Gaviraghi, Mukund Chorghade, Janos Fisher), project application is in progress. M Chorghade and E. Breuer should consider merging their projects, still with two documents to be produced.

Commission on Training and Development – CTD, VII.M.2

WP Research and Training in Medicinal Chemistry in South America and Middle America (chair: Prof. Monge Vega). Prof. Monge Vega will organise a training course coming August in Rio de Janeiro. In order to keep this as an output oriented project it is necessary to publish the material. It was decided that this project together with the Training Course on the Indian subcontinent (M. Chorghade) should be merged and submitted as: Educational material for IUPAC courses in Medicinal Chemistry.

The project Medicinal Chemistry in the Development of Societies and Biodiversities of Natural Compounds has been finished and two position papers have been published.

The activities: Research and Development in MC in Developing Countries With Respect to Patents and Contracts, was considered not suitable as an IUPAC project and should be handled explicitly as personal opinion and not be related to IUPAC. Prof. Ganellin must inform Prof. Monge Vega accordingly.

Commission on New Technologies and Special Topics – C-NTST, VII.M.3

WP on Pharmaceutically Acceptable Salts of Drug Substances (chair: Prof. Wermuth) has completed the textbook to be published by Wiley.

Task Group on Natural and Unnatural Substances Related to Human Health (700/2/98). Prof. Topliss (chairman) has produced a draft for circulation containing information for scientific writers. It is recommended to continue with this project to produce a popular material and a glossary.

Compendium of Guidelines from Regulatory Agencies. The preparation of a compendium should be postponed since the 5th International Conference on Harmonisation (ICH) will already deal with the issue. Prof. Ganellin will invite Dr. Kobayashi to attend the meeting in Brisbane and provide guidance for formulating a project.

Human Drug Metabolism Database (P. Erhardt). The project has been approved by ICSU, IUPHAR is also involved.

Natural Products with Medicinal and Nutritional Value; "Nutraceuticals" (M. Chorghade). This could become a future project.

Probes for Therapeutic and Diagnostic Effectiveness. (Giovanni Gaviraghi). It was suggested to write a position paper outlining the scope of the topic, which was considered very suitable for future project application. Dr. Ganellin will write to Dr. Gaviraghi accordingly.

Timing of Analogue Research (J. Fisher, B.K. Trivedi). A proposal shall be presented in Brisbane

Dr T. Kobayashi has summarised topics for possible collaboration with WHO, a 4 pages summary was distributed. No projects are visible at present.

Prof. Seydel (representative of the GDCh / jseydel@fz-borstel.de) had the intention to produce a glossary on pharmacokinetics, however the topic could not be discussed since he did not attend the meeting. The status is unknown, collaboration with Prof. Monica Nordberg was recommended

The co-operation within the project on postgenomic chemistry is unclear, this topic shall be explored further in Brisbane.

5.-Report Section of Clinical Chemistry – VII.C

Dr. Cornelis, President of the Section on Clinical Chemistry presented the status of projects:

Recommendation on Nanotechnology in the Clinical Laboratory (Prof. Wilding) the project application has been accepted.

The Interdivisional Project: IUPAC-Recommendation: Terms and Definitions in speciation and fractionation of elements has been co-published in PAC (Vol. 72: /8 1453 - 1470, 2000 and the Analyst.

Commission on Nomenclature, Properties and Units - C-NPU, VII.C.1 :

Compendium-Database: Properties and Units in Clinical Laboratory Sciences, main project of the Commission will remain updated until 2001. It was previously agreed that the maintenance of the database shall be taken over by WHO, however since the change in directorship no response has been received

The compilations of codes for. NPU in transfusion medicine and tissue typing (18/87), NPU for urinary calculi, NPU for dynamic function tests (32/97), Properties and units in flow cytometry(26/95) and NPU in Clinical Molecular Biology(26/95) are proceeding and status is according to plan.

Dr. Kallner has informed Dr. Forsum that new activities must be formulated and submitted as projects.

Commission on Toxicology – ComTox, VII.C.2 :

The Commission met in Szeged 9-29-2000, the minutes prepared by Prof. Templeton and a report from John Duffus on which the following report is based are available.

The project : IUPAC-Recommendation on Biological Monitoring for exposure to Volatile organic compounds (VOC) (co-ordinator Dr. Heinrich-Ramm) has PAC been published in PAC and received very favourable reviews in several Internat. Journals.

Risk assessment for occupational exposure to chemicals: an IUPAC Commission on Toxicology Review (co-ordinator: Dr. Duffus) is being submitted to PAC for publication as a Technical Report.

720/11/97 (JD) - Fundamentals of toxicology. After the success of the RSC book "Toxicology for Chemists" (Duffus and Worth), it was suggested there was a need for something more elementary. A computerised (Power Point) presentation has been adopted, with the aim of producing a series of slides, though a textbook format is also under consideration.

The content was presented to the International Congress on Chemical Education (Budapest, Aug. 2000) and was very well received. As a result, JD is preparing a CD version. UNESCO will support the development of the CD with the aim of circulating a pilot of about 300 copies, especially in developing countries. JD is adding a "Read Me" file and Bibliography, which he undertakes to circulate to the Commission before Brisbane. Bob Andrews the head of RSC Publishing is interested in publishing a second edition of "Fundamental Toxicology for Chemists" if the authors wish to proceed with it. JD will put this to ComTox and CTC in Brisbane.

Copyright issues, if displaying the material in the web, shall be cleared with RSC by J. Duffus.

720/12/97 (RN) - Risk assessment with a focus on particulate matter. Progress on this project has been rather disappointing. Dr. Nolan had promised to producing a draft by the year end 2000, with the aim of having a product for evaluation before Brisbane. No paper has yet been received and serious

concerns were expressed. Dr. Cornelis will inform Dr. Duffus in order to urge Dr. Nolan to proceed with the task.

720/4/93 (JMC) - Exposure assessment and decision rules. A final draft of the manuscript gone to Prof. Metanomsky and has been reviewed by the IUPAC interdivisional Committee on Nomenclature and Symbols (IDCNS). The problem is now that Prof. Lorimer's, suggested that the title should be change and the content to cover "Rules for stating when a limiting value is exceeded in results of clinical chemical analysis." This would require rewriting the paper, which is unacceptable to the members of the working party.

720/8/95 (JD) - Risk assessment: Educational material. The manuscript has been put into the IUPAC review process with the aim of publishing a technical paper in PAC.

720/7/95 (EO) - Exposure assessment using the logbook method. This is ready for publication, with Dr. Patricia Stewart doing some final polishing of the language. External reviewers have been identified.

720/9/97 (Dr. Ole Hertel, and EO from COMTOX) Modelling outdoor exposure.- The paper has been sent to reviewers for targeted completion in 2001.

Immunochemistry of sensitisation to metals. This project has been approved and is under preparation. (DT Project Director, with JMC and RHR).

Determination of the concentration component of air exposures to Volatile compounds. EO will submit a project on this based on his recent studies. The project will include both modelling and measurement and final discussion will be in Brisbane.

Data base on chemical disasters. A first draft will be prepared by LN before next year's Szeged meeting on chemical disasters. It will be distributed to participants of that meeting for comment. Prof. Nagymajtenyi will shortly submit a Project Application for "Chemical Disasters: Consensus Document and Review", and will apply for IUPAC sponsorship for the meeting as part of the project.

Module-based uncertainty evaluation system. The MODUS initiative will form the basis of a Project Application from JMC.

"Textbook". The Commission has produced a number of manuscripts in recent years on the topics of Biomonitoring and risk assessment. The idea was formulated to put these together into a textbook, with additional material and editing to fill any gaps. A tentative title is "Application of Chemistry and Biomonitoring -- Importance for Human Health". JD will attempt to get a list of all past COMTOX publications and suggest a more precise theme at, or before, the Brisbane meeting, with a view to a "Book Project".

Neurochemically active metals: Manganese. EO will submit a Project with Drs. Roels and Rappaport.

"The physicochemical characterisation of asbestos fibres" as a possible future project by Dr. Nolan arising from the current 720/12/97. Such a project application will depend upon successful completion of the ongoing project on particulate matter.

The project applied for by Prof. Monica Nordberg on Toxicokinetics of Chemicals has been approved. In the review process it was suggested to involve a statistician. Prof. Seydel (jseydel@fz-borstel.de) should be contacted in order to harmonise the projects..

Dr. Heinzow reported on integrated pest management and sustainable development in Thailand. It is recommended that educational materials tailored for the level of education at the grass-root level, retailers/distributors, extension workers and health personnel are prepared.

In the light of the recent ESDC report "Strategy for educational policy" a toxicological curriculum into the education on the secondary school level (e.g. within chemistry or ecological sciences) could be introduced to broaden the awareness in rural and industrial areas on toxicological risks of hazardous substances.

>From the discussions both at Thailand ATSD/DOA (Agricultural Toxic Substances Division/Division of Agriculture) and at the Chulalongkorn University the impression surfaced that a training

course/educational material similar to the material prepared by IUPAC (Duffus and Worth) might be very useful.

The idea is to produce educational material (level to be specified e.g. school level, university, regulators) with a focus on pesticides (another on environmental/industry sites problems) and their practical problems in developing countries with warm climate. This material should be tailored to a more sustainable use of brocades and chemicals and should extend beyond Thailand

It is recommended that ATSD explore their specific needs and possible co-operation partners and approach the President of the Chemical Society of Thailand (Dr. Surapol Patharakorn) to seek support from IUPAC.

Dr. Heinzow will inform on the progress and feasibility of a project application.

6. Structure of the Division, Nomination and forthcoming Election

According to the strategic plan all commissions must be dissolved in 2001. The Nomination Committee

chaired by Prof. McQueen has proposed a slate of 10 candidates of who the electorate have to select the 6 Members of the Division Committee. It is assumed that all candidates have agreed to serve.

It is not clear if time limits will apply for previous service.

Dr. Kallner will make inquiries and will contact the Secretary General if all positions are mandatory.

Prof. Ganellin will not serve as the president-elect, it is not clear if Prof. Rich is willing to serve. Prof.

Erhardt and Prof. Duffus might otherwise be approached.

For the ballot it was recommended to distribute information on the candidates

7.-New IUPAC-Project procedure and new projects

At Brisbane the new project system will be discussed at an interdivisional meeting (29th June at 16:00 h), Dr. Kallner will raise the need of faster decision-making upon submitted project applications.

The Division can expect allocation for 2002-2003: ~ 70.000 USD, it seems that the decision (priorities) will be with the Division Committee. 75% should be used for projects and 25% for operational expenses to be kept separate. 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

8.-Cooperation within IUPAC

The MCS meeting scheduled for the 29th was rescheduled to Monday the 2nd of July. Prof. Upendra Pradit will be informed by Dr. Kallner and Prof. Monge Vega be named as representative of Div VII to the Organic Chemistry interdivisional project on biomolecular chemistry.

Possible co-operation might be established in the field of Post Genomic Chemistry, and on Endocrine Active Substances, input has been offered for the latter project. The Solubility Data project was considered useful, no input from Div. VII can be offered.

Before advice on a Conference on Natural Products can be given to M. Chorghade, more information is necessary. The comments about the Conference on Natural Products will be given to the Secretariat. For the project Electrical properties of polymers no co-operation can be offered.

9.-Cooperation with other organisations

IFCC : The links between IFCC and IUPAC Section on Clinical Chemistry will be kept by continuing with active collaboration.

ISO. Dr. Kallner is represented on ISO 212: in vitro diagnostics

ICSU and IUPHAR Co-operation is related to the Drug Metabolism Database

WHO: The location of the compendium will be in Sweden until 2001. WHO is to be approached to assume responsibility for the updating and maintenance of the data base. The change of guard for the compendium by WHO is under consideration, other collaboration has failed.

10.-New Directive on Risk Assessment of Chemicals

Discussion postponed until Brisbane

11.-General Assembly in Brisbane

The Division meetings will resume on Friday, participation in the Project Approval Process (29th June at 16:00 h) is important. The need to speed up the project approval process was clearly expressed and concerns were raised that with a slow procedure the Division Committee will loose initiative and possible project applicators will loose their interest. The possibility to transfer the responsibility to the Division Committee would require a change in bylaws, this shall be further discussed in Brisbane. The Interdivisional meeting in biomolecular chemistry (2nd July at 16:00 h) will be attended by Prof. Monge Vega and other members of the Division.

The Medicinal Chemistry Section has scheduled its meeting from 29th to 2nd of July. Prof. Ganellin will inform the members of the Section Committee.

The implications of the ESDC report and co-operation with CCE (former CTC) shall be discussed at the Section meetings.

Dr. Heinzow informed that he will be unable to attend the GA, due to other commitments. Dr. Cornelis volunteered to act as Secretary in lieu.

Dr. Anders Kallner
(President)

minutes prepared by Dr. Birger Heinzow (secretary of the Division)