# Report to Council, Brisbane 2001-07-07/08 Anders Kallner

#### **Executive Summary**

This biennium is the third after it was decided to merge the Division VII, 'Clinical Chemistry' and the section 'Medicinal Chemistry' into a new Division VII, 'Chemistry and Human Health'. The merger – as usual – means amalgamating different cultures and attitudes. It also means that the previous narrow interests of clinical chemistry and medicinal chemistry should be widened without jeopardizing the ongoing and planned projects in the existing main fields.

The new Division was organized in two Sections, Medicinal Chemistry (MC) and Clinical Chemistry (CC) with a view to finish ongoing projects and establish new with wider scopes. The formal dissolution of the sections is proposed to the 41<sup>st</sup> Council meeting.

The Sections have met separately during the biennium and furthered their projects within the existing commissions. The MC has three Commissions that usually meet together whereas the CC has two Commissions that work independently. Major items for the MC has been nomenclature and glossaries (combinatorial chemistry, drug metabolism and process chemistry), long standing work on curricula for medicinal chemistry in developing and developed countries and monographs related to the above topics. The CC has continued a giant all inclusive terminology and nomenclature work that covers all properties investigated in laboratory medicine in one Commission. The other Commission deals with aspects on toxicology and has contributed to risk and exposure assessments in work situations and everyday life.

The division participates in an ICSU project on producing a monograph on gene modified food.

A number of areas have been identified which are discussed as parts of a widened scope for the Division, e.g. nutrition, biodiversity, patents, DNA technology, bioinformatics, industrial waste, screening of drugs. Many of these topics will be addressed in collaboration with other groups within IUPAC and with other professional organisation. A slate of candidates for the next Division Committee has been established and the election will be carried out by mail after the General Assembly.

#### Report

### **Organisation**

A Division Committee of the President, vice President, Secretary, the Section Presidents and Secretaries has led the Division. The elected President resigned mid 2000 and was succeeded by the vice President. The Division Committee has met twice during the biennium and business has been performed by E-mail.

By the end of 2000 the half-century long mutual representation of the Division Committee and the Executive Board of the IFCC (International Federation of Clinical Chemistry and Laboratory Medicine) on each other's meetings was terminated. This was a logical step in restructuring the Division. A close collaboration will continue on the project level.

## Clinical Chemistry Section

The Commissions work independently in a project-oriented fashion have met on several occasions during the period.

### VII C1. Commission on Nomenclature, Properties and Units

The C-NPU:s main project 'Properties and Units in Clinical Laboratory Sciences' will continue during 2001. The Commission has searched support for a sustainable organisation and maintenance of the database in external organisations, particularly the WHO. The work is presently maintained with grants from the Swedish Government Agencies and continued in collaboration with the IFCC.

The following projects are presently developed and will be added to the database when completed:

- NPU in transfusion medicine and tissue typing
- NPU for urinary calculi
- NPU for dynamic function tests
- NPU in flow cytometry
- NPU in clinical, molecular biology.

Previous parts of the work of the Commission has been published in PAC and is available on the IUPAC homepage by a link to the server that the Commission presently employs. The systematic syntax and nomenclature has been successfully introduced to laboratories in Denmark and Sweden and facilitates the exchange of laboratory results.

### VII C2. Commission on Toxicology

The Commission successfully completed the following projects, resulting in publication of the work in PAC:

- Guidelines for terms related to chemical speciation and fractionation of elements, definitions, structural aspects, and methodological approaches
- IUPAC-recommendations on biological monitoring to exposure to volatile organic compounds
- The project
- Risk assessment for occupational exposure to chemicals.
- is in the final stage of reviewing and acceptance by PAC is imminent
- The following registered projects are still in the pipeline:
- Fundamentals of toxicology
- Risk assessment with a focus on particulate matter
- Exposure assessment and decision rules
- Risk assessment Educational material
- Exposure assessment using the logbook method
- Modelling outdoor exposure

The projects have made substantial progress during the past biennium. The final manuscripts, ready for external review, are expected to be delivered by the time of the GA in Brisbane.

Approved new project:

- Immunochemistry of sensitisation to metals
- Newly submitted project, waiting for approval by the IUPAC bodies:

- Glossary of toxicokinetics of chemicals
- New proposals, waiting for approval by the Commission Members in Brisbane:
- Determination of the concentration of air exposures to volatile compounds
- Data base on chemical disasters
- Module-based uncertainty evaluation system
- Textbook: Application of chemistry and biomonitoring Importance for human health
- Neurochemically active metals
- The physicochemical characterisation of asbestos fibres
- Determination of the concentration component of air exposure to volatile compounds

### Medicinal Chemistry Section

The Section has met twice yearly at locations in association with International Symposia on Medicinal Chemistry, except in Berlin, which was the last IUPAC General Assembly. Attendance ranged from 10 to 16. Many of the attendees work in industry and their travel expenses were paid for by their companies.

#### VII. M.I Commission on Nomenclature and Terminology

A Working Party on Nomenclature and Publication Guidelines for Combinatorial Chemistry in the Synthesis and Screening of Compound Libraries has led to the publication of a Glossary of Combinatorial Chemistry Terms as a Technical Report in PAC and J Combinatorial Chem. This will ensure its use within the ACS (American Chemical Society) as a standard glossary of terms. Further work is focussed on producing an opinion document on the legal implications of patenting virtual libraries. This is a very important issue which has profound implications for R&D in the pharmaceutical industry. A Working Party on a Glossary of Drug Metabolism. There are 15 project members and they plan to review approximately 150 terms.

Working Parties have been initiated on Glossaries of Terms in Pharmaceutical Process Chemistry and on Terms in Pharmaceutical Technology. A project proposal to IUPAC is imminent. The Organic Process Chemistry journal has agreed to publish the final version.

### VII. M.2 Commission on Training and Development

A Working Party on a Medicinal Chemistry Curriculum initiated two major surveys from the pharmaceutical industry and academia, respectively, on what training was preferred for medicinal chemists entering research in the pharma industry. The results have given rise to nine publications.

With regard to training medicinal chemists in Latin American countries, medicinal chemistry courses have been organised in Montevideo, Uruguay (Sept 99), and Rio de Janeiro, Brazil (August 01). A Society of Medicinal Chemistry for the Spanish speaking Latin American countries has been established, and a Research Symposium organised in Cuba, April 2001.

Training in medicinal chemistry in the Indian subcontinent has been pursued and the Indian CSIR has been stimulated to run courses in four different cities in India.

A Working Party on "Medicinal Chemistry in the Development of Societies: Biodiversity and Natural Products" has given rise to several publications.

### VII. M.3 Commission on New Technologies and Special Topics

A project proposal on a human drug metabolism database has been accepted for a joint venture with IUPHAR, supported with funding of \$50,000 from ICSU.

A Working Party on "Natural and Non-natural Substances Related to Human Health", has produced a draft manuscript to provide an information source for helping to answer the lay misconception about synthetic versus natural drugs.

A Working Party has recently been established on the "Evolution of Drug Discovery and the Timing of Analogue Research". The output could be a book on the productivity of me-too drug research.

#### Miscellaneous

#### ICSU

The Section has contributed to an ICSU initiated project on Gene Modified Food for development, health and human nutrition; The scientific basis for benefit and risk assessment. through participation of Prof Åke Bruce at a planning meeting in Manchester, UK. The outcome of this study will be a monograph and the meeting resulted in a list of contents and assignment of suitable authors of selected chapters. He considers this an important field and will continue to be involved.

#### WHO

The Division has participated in a meeting of consultants to the Committee on Biological Standard with a view to improve the characterization and traceablity of WHO Biological standards.

Discussions are continued with the WHO to collaborate on the development and maintenance of the 'Compendium of Nomenclature'

#### **Publications**

#### Clinical Chemistry Section

Guidelines for terms related to chemical speciation and fractionation of elements. Definition, structural aspects, and methodological approaches. PAC 2000;72:1453-1470. IUPAC recommendations on biological monitoring to exposure to volatile organic compounds PAC 2000;72:

Risk assessment for occupational exposure to chemicals, PAC, Accepted for publication Properties and Units in the Clinical Laboratory Sciences. Parts VIII, X, XII and XVI. PAC 2000;72(3,4,5and 6):

### **Medicinal Chemsitry Section**

'Glossary of Combinatorial Chemistry Terms' as a Technical Report in PAC, 1999;71:2349-2365 and Journal. J.Combinatorial Chem., 2000;2:562-578. Surveys of curricula (nine parts) are published in Chemistry International (1995;17: 212; 1999;21:138; 2001;23:43). Surveys from US and Japan were published in 1998. The survey from Europe was published in Eur.J.Med.Chem. 2000;35:163-174.

"Medicinal Chemistry in the Development of Societies: Biodiversity and Natural Products" Eur. J. Med. Chem. 2000;35: 1121-1125 and several national journals in Latin America.

## Monographs

Drug Metabolism: Databases and High-Throughput Testing During Drug Design and Development ed. by P.W. Erhardt was published by Blackwell, 1999. IUPAC Handbook of Pharmaceutically Acceptable Salts, ed. by C.G. Wermuth is due to be published by Wiley & Sons in 2001