IUPAC Chemistry and Health Division (Div VII) Report to Council 02-01-01/03-06-30 Anders Kallner, President

Highlights and Executive summary

The Division successfully finished the amalgamation between the previous Division of Clinical chemistry and the Section of Medicinal Chemistry by the end of the previous biennium and simultaneously changed to the new project driven organisation. Most of the projects from the previous Division and Section have been terminated or redirected to meet the strategic goals of the Union.

The activities of the Division are thus directed into three major areas in the interaction between chemistry and human health, i.e. discovery and design of drugs, toxicology and risk assessment and measurement of properties in laboratory medicine. This is reflected in the organisational structure of the Division that has formed three subcommittees:

Subcommittee for Medicinal Chemistry and Drug Development, (Chair Prof Robert Ganellin), Subcommittee for Nomenclature, Properties and Units (Chair Prof Urban Forsum) and Subcommittee for Toxicology and Risk Assessment (Chair Prof John Duffus).

These Subcommittees coordinate projects within the respective area. The Division also has a stand alone project, Glossary and classification of nanotechnology in laboratories.

The Division continues its collaboration with

International Federation of Clinical Chemistry and Laboratory Medicine (IFCC), particularly in nomenclature,

American Chemical Society, Division of Medicinal Chemistry

European Federation of Medicinal Chemistry

World Health Organisation, WHO, by supplying experts to educational programs in toxicology and laboratory management

and with ICSU by participating in projects on Gene Modified Organisms (GMO) and Health and Well-being.

The Division is representing IUPAC in ISO TC 212 "Clinical laboratory testing and in vitro diagnostic test systems" and in CEN (European Committee for Standardization) TC 140 "In vitro diagnostic medical devices" and has contributed to several new standards regarding reference laboratories, - methods and –materials, accreditation of medical laboratories and traceability of calibrators.

The main trust of the Division has been to develop glossaries in pertinent fields. A number of glossaries have been almost completed during the period by the three Subcommittees. I would particularly highlight the Glossary of Terms in Pharmaceutical Process Industry that comprises more than 800 terms and the multifaceted Project on Human Drug Metabolism Database. The Subcommittee on Medicinal Chemistry and Drug Development has also carried out education programs in Latin America and the Indian Subcontinent and completed a text book in Spanish and Portuguese on Medicinal chemistry. The Subcommittee on Nomenclature, Properties and Units has continued its work on nomenclature in laboratory medicine and incorporated additional areas e.g. immunochemistry, blood banking and microbiology. This list is available as a relation database on the Internet (see IUPAC homepage) and comprises more than 22000 entries. The nomenclature has

been translated into several languages and is in regular use in patient records and laboratory information systems. The Subcommittee for Toxicology and Risk Assessment has published several documents shown in the table (Section IV). A special new approach is the 'Glossary on toxicokinetic terms' now completed and will form the basis for a more extensive publication that not only defines but explains the terms and concepts.

II Overall report

The present projects of the Division are truly international in their character. The Division has launched educational projects in different parts of the world on its own and in collaboration with WHO. The efforts in bringing experience and expertise in medicinal chemistry and toxicology to universities in developing countries in South America, India and South East Asia have been of special importance and impact. The publications of the Division are of general importance as reference literature but will also give practical guidance in applied and basic science. Particularly the huge database on nomenclature, properties and units has been accepted as the standard in many countries. This database is a good example of a successful marriage between theory and practice.

The importance of a common and understandable nomenclature in laboratory medicine cannot be overemphasised. Mobility of patients and physicians and the continuous accumulation of knowledge and experience require that an equal heath care can be offered globally. Laboratory medicine plays an important role in providing objective information to physicians.

The European Union has published a Directive for In Vitro Medical Devices that will apply fully in Europe from December 2003. This Directive has major implications on the production and use of instruments and reagent sets. It has prompted writing of several standards that admittedly will have their largest importance in Europe but considering the huge instrument and reagent market in Europe all industries will be interested to comply. The collaboration between the CEN and ISO has made it possible to incorporate aspects and views from all participating countries including the US and Japan that both contribute substantially to production of instruments and reagents. The CEN standards are mandatory whereas the ISO standards are principally voluntary. It has been a great advantage that IUPAC has been represented in the Technical Committees to ascertain that the standards are based on scientific resolutions. The Union can only be accepted in these organisations as an observer without voting rights but as usual the important influence is during the initial phases of the creation of a standard.

Much interest has been devoted to Drug Metabolism and the Division has two major projects in the field, one addressing the terminology that should be used in the field and the other to produce a database on the metabolism of drugs. The importance of systematic nomenclature and readily available information on drug metabolism will increase as the medical profession and pharmacology will be able to individualize drug prescription and use. These projects will both contribute to developments in rational therapy.

Nanotechnology is a concept that is known from mechanics as well as chemistry. Laboratory medicine that deals with small and limited amounts of sample, rare and expensive reagents and an increasing demand for small – even implantable – accurate, easy-to-use and quick analytical instruments early got involved in developing such devises. The Division has developed – together with physicists – a systematic nomenclature to describe the devises, their function and performance.

Many laymen and the tabloid press in general believe that natural products that are being used in therapy by definition are harmless. This problem has been studied during several years in the Division and resulted in publications for the professionals as well as for laymen. Different means to disseminate information about safe and harmful natural products have been sought in collaboration with the IUPAC Secretariat.

III Other information and comments

The Division is pleased with the opportunity to bring together similar projects into subcommittees. This serves the double purpose of promoting and critically reviewing ideas and projects and recruiting new participants.

We believe that the Division plays a specific role in bridging the gap between basic and applied chemistry and will encourage and pursue projects that fulfil these ambitions. We would welcome an increased interdivisional collaboration regarding all effects – in the chemical industry and environment that has potential effect on human and animal health. A risk analysis using the IUPAC recommendations concerning the use of pesticides in agriculture could be mentioned.

IV Publications

- 1. Biological monitoring for exposure to volatile organic compounds (VOCs) (IUPAC Recommendations 2000)
- 2. R. Heinrich-Ramm, M. Jakubowski, B. Heinzow, J. Molin Christensen, E. Olsen, and O. Hertel. *Pure Appl. Chem.*, Vol. 72, No. 3, pp. 385-436 (2000).
- 3. Guidelines for terms related to chemical speciation and fractionation of elements. Definitions, structural aspects, and methodological approaches (IUPAC Recommendations 2000)
- 4. Douglas M. Templeton, Freek Ariese, Rita Cornelis, Lars-Göran Danielsson, Herbert Muntau, Herman P. van Leeuwen, and Ryszard Lobinski. *Pure Appl. Chem.*, Vol. 72, No. 8, pp. 1453-1470 (2000).
- 5. The Science of Chemical Safety Essential Toxicology An Educational Resource
- 6. John Duffus and Howard Worth (2001), http://www.iupac.org/publications/cd/essential_toxicology/index.html
- 7. Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report)
- 8. Robert F. M. Herber, John H. Duffus, Jytte Molin Christensen, Erik Olsen, and Milton V. Park, *Pure Appl. Chem.* Vol. 73, No. 6, pp. 993-1031 (2001)
- 9. "Heavy metals" a meaningless term? (IUPAC Technical Report)
- 10. John H. Duffus, *Pure Appl. Chem.* Vol. 74, No. 5, pp. 793-807 (2002)
- 11. Rules for stating when a limiting value is exceeded
- 12. J.M. Christensen, R.F.M. Herber, E. Olsen and E. Holst, *J. Accreditation and Quality Assurance* 7: 28-35 (2002).
- 13. IUPAC-IFCC (International Union of Pure and Applied Chemistry & International Federation of Clinical Chemistry, Commission on Clinical Chemistry), 1967. Quantities and units in clinical chemistry.
- 14. Recommendation 1966. Prepared for publication by Dybkær R, Jørgensen K. 45Copenhagen: Munksgaard.
- 15. J.C.Riggs, S.S.Brown, R.Dybkær, and H.Olesen,: Compendium of terminology and nomenclature of properties in clinical laboratory sciences ('The Silver Book'). IUPAC: Oxford: Blackwell Science, 1995, 290 pp.

- 16. H.Olesen, Properties and Units in the Clinical Laboratory Sciences I. Syntax and Semantic Rules, Eur J Clin Chem Clin Biochem 1995:33,627-636.
- 17. D.Kenny and H.Olesen, Properties and Units in the Clinical Laboratory Sciences II. Kinds-of-property, Eur J Clin Chem Clin Biochem 1997:35,317-344.
- I.Bruunshuus, W.Frederiksen, H.Olesen and I.Ibsen, Properties and Units in the Clinical Laboratory Sciences III. Elements (of properties) and their code values, Pure and Applied Chemistry, 1997:69,2577-258
- 19. H.Olesen, D.Kenny, I.Bruunshuus, I.Ibsen, K.Jørgensen, R.Dybkær, X.Fuentes-Arderiu, G.Hill, P.Soares de Araujo and C.McDonald, Properties and Units in the Clinical Laboratory Sciences IV. Properties and their code values, Pure and Applied Chemistry,1997:69, 2583-2591.
- 20. M.Blombäck, R.Dybkær, K.Jørgensen, H. Olesen and S.Thorsen, Properties and Units in the Clinical Laboratory Sciences V. Properties and Units in Thrombosis and Haemostasis, Eur J Clin Chem Clin Biochem 1995:33,637 -660.
- 21. H.Olesen, D.Cowan, I.Bruunshuus, K.Klempel and G.Hill, Properties and Units in the Clinical Laboratory Sciences VI. Properties and Units in IOC prohibited Drugs, Eur J Clin Chem Clin Biochem 1997:35,805 –831.
- 22. U.Forsum, H.Olesen, W.Frederiksen and B.Persson, Properties and Units in the Clinical Laboratory Sciences VIII. Properties and Units in Clinical Microbiology, Pure and Applied Chemistry, 2000:72, 555-745.
- 23. R.Cornelis, X.Fuentes-Arderiu, I.Bruunshuus and D.Templeton, Properties and Units in the Clinical Laboratory Sciences IX. Properties and Units in Trace Elements, Eur J Clin Chem Clin Biochem 1997:35,833 -843.
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