

Chemistry and Human Health Division (VII)

IUPAC General Assembly Report (August 2007)

Submitted by Paul Erhardt, President Div. VII

Executive Summary

This report provides an update about Division VII's (DVII's) activities since the last General Assembly in Beijing, 2005. A proactive approach taken by our Subcommittee on *Public Relations and Elections* (PRE) allowed DVII to have a very successful TM election process followed by finalization of our NRs, designation of our administrative officers, and selection of our AMs. The resulting membership of DVII is shown in Attachment 1 wherein it can be noted that nineteen (19) different nations are now represented among our twenty-four (24) active participants. The recent election of new TMs for 2008 has also gone very smoothly with the nominees again representing a high diversity in expertise, geography and gender. Two of the three winners are experts in the NPU discipline (see definitions below) and the other winner an expert in toxicology. On a different note is the problem created by Brazil's lapsed payment of its National Subscription because this will bar DVII's President Elect from assuming office in 2008. If this has not been resolved by the time of the GA, DVII will be forced to exercise a backup plan so as to prevent a gap from occurring in this key post. Backup plans are already being discussed among the administrative officers.

DVII's technical diversity is organized within three Subcommittees, namely *Medicinal Chemistry and Drug Development* (MC), *Nomenclature, Properties and Units in Laboratory Medicine* (NPU), and *Toxicology and Risk Assessment* (SOT). Together, these Subcommittees were involved in thirty (30) IUPAC Projects, six (6) of which were completed during this period while another six (6) were initiated [five (5) from DVII's 2006-7 allotted budget and one (1) from extramural funding]. Detailed reports from each of the technical and PRE Subcommittee's are appended as Attachments 2 to 5. Publication lists can be found therein. In total, three (3) books, fourteen (14) technical papers, six (6) news articles and one (1) Web database were released by DVII during this period.

DVII held two meetings since the Beijing GA, the first occurring in the U.S., and a more recent one in Belgium. Given that the first meeting drew ca. 25% of DVII's 2006-7 allotted budget, a decision was made to meet every nine (9) months rather than every six (6) months with one of our meetings to coincide with a GA. As a result, our meetings are now scheduled for one-and-a-half days rather than for one day. Due to budgetary constraints, however, it now appears that we will only be able to meet formally once between the GAs. Backup plans, such as adoption of a teleconference between each of our formal meetings, so as to allow DVII's healthy momentum to be maintained, will be discussed during the GA. It should be noted that DVII is heavily involved with organizing and participating in the GA's accompanying WCC. Six (6) of our members are either chairing the entire Session or specific Symposia, or delivering Keynote lectures within the overall program designated as *Chemistry Protecting Health* (Attachment 6). We are also assembling a portfolio of DVII posters which we hope to display as a block during one of the WCC Sessions, although these programmatic details have not been finalized. Major highlights for DVII during this reporting period are further conveyed within the following six (6) IUPAC Goals. Each of the latter is set-off as a bold-font header.

Leadership in Addressing Global Chemical Issues

The critical need for standardization of properties and units associated with human toxicology assessment was recently addressed by DVII's NPU and SOT Subcommittees' report entitled "*Properties and Units in the Clinical Laboratory Sciences: Part XX. Properties and Units in Clinical and Environmental Human Toxicology* [PAC, **79**, 87-152 (2007)].

Provision of Tools

The NPU's generic database, now published on the net under the URL: <<http://dior.imt.liu.se/cnpu/>>, represents an electronically available tool that can be used in a variety of clinical-related analytical settings. The SOT's "*Glossary for Chemists of Terms Used in Toxicology*," "*Glossary of Terms Relating to Pesticides*" and "*Explanatory Dictionary of Terms in Toxicology*" were published in PAC, as well as being made available electronically for review on the IUPAC website. Several MC-sponsored glossaries are likewise nearing completion: "*Combinatorial Chemistry Terms*;" "*Drug Metabolism Terms*;" "*Pharmaceutical Technology*;" "*Pharmaceutical Process Chemistry*;" "*Biomolecular Screening*;" and, an all-encompassing "*Compendium of Glossaries*."

Assist Chemical Industry in Sustainable Development, Wealth Creation and Improving Quality of Life

The MC Subcommittee, in particular, has strong ties with the industry. It's following projects demonstrate some of the ongoing activities that DVII is involved with in this area: "*Prototype Analysis of Molecular Biomarkers in Cancer*;" "*Natural Products with Medicinal and Nutritional Value*;" and, "*Latin American Plants as Sources for Nutraceuticals*." Leading additional efforts to connect IUPAC with industry, the PRE has become active in COCI. In this regard, the PRE's list of DVII activities (Attachment 7) is being used by COCI as a model for all of the other IUPAC Divisions.

Foster Communication

The following projects from the NPU Subcommittee pertain, in particular, to this IUPAC goal: "*Global Use of the SC-NPU Concept System for Properties in Toxicology*;" "*Internationally Agreed Terminology for Observations in Scientific Communication*;" and, "*Translation of the SC-NPU Database Elements and Properties Into French*." Similarly, the SOT project entitled "*Explanatory Dictionary of Concepts in Toxicokinetics*" and the MC project entitled "*Biological Context by Data Mining*" directly relate to enhancing communication among chemists within the specific context of using some of DVII's tools, as well as fostering communication in general.

Education

Two stellar efforts relevant to educational projects include the recently published text entitled "*Fundamental Toxicology, 2nd Edition*" by the SOT Subcommittee, and the recently published text entitled "*Analogue-based Drug Discovery*" by the MC Subcommittee. Specific training projects include: "*Training of School Children on Pesticides and Health*" (a SOT activity); "*Research and Training in Medicinal Chemistry in the Indian Subcontinent*;" and,

“*Practical Studies for Medicinal Chemistry Students*” (the latter two projects being MC activities).

Membership and Public Relations

In addition to DVII’s efforts to diversify its membership via the IUPAC election and selection process as already discussed in the Executive Summary, the PRE produced a DVII poster that was displayed at the last EFMC Meeting in Istanbul and at the last ACS meeting in San Francisco. This poster is being further upgraded and it, along with several DVII Subcommittee and specific project-related posters are being organized for possible presentation as a ‘block’ or ‘row’ at the upcoming GA in Torino.

Also of particular note in this category is that the first “*IUPAC-Richter Prize*” has been awarded to Professor Malcolm Stevens, Nottingham University, UK, for his work on heterocyclic anticancer drugs. This prize of US \$10,000 was presented at the EFMC-organized International Symposium on Medicinal Chemistry held in September at Istanbul, Turkey. Recognition of Dr. Stevens and this prestigious award will again be provided at the next GA (see [Attachment 6](#)).

List of Attachments

1. Division VII Members and Roles During 2006-2007 [**page 4**]
2. Subcommittee Report: Medicinal Chemistry and Drug Development (R. Ganellin) [**pages 5 to 8**]
3. Subcommittee Report: Nomenclature, Properties and Units in Laboratory Medicine (F. Pontet) [**pages 9 to 11**]
4. Subcommittee Report: Toxicology and Risk Assessment (J. Duffus) [**pages 12 to 15**]
5. Subcommittee Report: Public Relations and Elections (T. Perun) [**page 16**]
6. World Chemistry Congress Program for Session 2: *Chemistry Protecting Health* [**page 17**]
7. List of Division VII Activities for use by COSI’s Interactions with the Private Sector [**page 18**]

Attachment 1

**IUPAC Division of Chemistry and Human Health
2006-2007 Membership**

| <u>Name</u> | <u>Desig.</u> | <u>Role</u> | <u>Term</u> | <u>NAO</u> |
|------------------------|---------------|-----------------------------------|-------------|-------------|
| Ole Andersen | AM | SOT | 06-07 | Denmark |
| Sergey Bachurin | NR | MC | 06-07 | Russia |
| Georg Becher | NR | S TBD | 06-07 | Norway |
| Derek Buckle | AM | MC | 06-07 | UK |
| Mukund Chorghade | TM | Secretary; CCE Rep; MC | (Sec.) | US |
| Rita Cornelis | NR | SOT | 06-07 | Belgium |
| John Duffus | TM | Chair SOT; ICTNS & "SOT" Rep | 04-07 | UK |
| Paul Erhardt | TM | President; USNC & PAC Rep; MC | 04-07 | US |
| Janos Fischer | TM | IUPAC-Richter Prize Rep; MC | 04-07 | Hungary |
| Robin Ganellin | AFM | Chair MC | (Chair) | UK |
| So-Yeop Han | NR | "AFMC" Rep; MC | 06-07 | Korea |
| Javed Iqbal | NR | MC | 06-07 | India |
| Mike Liebman | TM | MC | 06-09 | US |
| Kari Mattila | NR | S TBD | 06-07 | Finland |
| Grzegorz Mlostn | NR | MC | 06-07 | Poland |
| Peter Nedekov | NR | MC | 06-07 | Bulgaria |
| Monica Nordberg | TM | SOT | 06-09 | Sweden |
| Tom Perun | AFM | Chair SOPRE; COCI & "ACS" Rep; MC | (Chair) | US |
| Francoise Pontet | AFM | Chair NPU; "IFCC" Rep | (Chair) | France |
| Ferran Sanz | TM | "EFMC" Rep; MC | 06-09 | Spain |
| Pedro Soares de Araujo | TM | Vice President; NPU | 04-07 | Brazil |
| Doug Templeton | TM | "Can. MRC" Rep; SOT | 06-09 | Canada |
| Henk Timmerman | TM | "IUPHAR" & "ISSX" Rep; MC | 04-07 | Netherlands |
| Mario Varasi | AM | MC | 06-07 | Italy |

Abbreviations

Desig. pertains to IUPAC membership designation wherein: **AFM** = Affiliate Member; **AM** = Associate Member; **NR** = National Representative; and, **TM** = Titular Member.

Role pertains to Division-related responsibilities and primary technical expertise wherein for the latter: **MC** = Subcommittee on Medicinal Chemistry and Drug Development; **NPU** = Subcommittee on Nomenclature, Properties, and Units in Laboratory Medicine; **SOT** = Subcommittee on Toxicology and Risk Assessment; and, **S TBD** = Subcommittee To Be Determined. For responsibilities, liaison relationships with non-IUPAC-associated organizations are indicated by placement of the latter's codes within quotation marks and: "**ACS**" = American Chemical Society; "**Can. MRC**" = Canadian Medical Research Council; **CCE** = Committee on Chemistry Education; **COCI** = Committee on Chemistry and Industry; "**EFMC**" = European Federation of Medicinal Chemistry; **ICTNS** = Interdivisional Committee on Terminology, Nomenclature and Symbols; "**IFCC**" = International Federation of Clinical Chemistry; "**ISSX**" = International Society for the Study of Xenobiotics; "**IUPHAR**" = International Union of Pharmacology; **PAC** = Journal of Pure & Applied Chemistry; **SOPRE** = Subcommittee for Public Relations and Elections; "**SOT**" = Society of Toxicology; and, **USNC** = U.S. National Committee for IUPAC.

IUPAC Bylaws On Division Composition

Maximum membership: 10 Titular Members (TMs); 6 Associate Members (AMs); 6 + 4 (by Bureau & Council Amendment) = 10 National Representatives (NRs); and, Unlimited Affiliate Members (AFMs).

Attachment 2**Report from the Subcommittee on Medicinal Chemistry and Drug Development for the period August 2005 to August 2007**

Meetings: Since the last IUPAC General Assembly (in Beijing, August 2005) the Subcommittee on Medicinal Chemistry and Drug Development has held three meetings (Modena, Italy, 11 September 2005, Atlanta, Georgia, USA, 26 March 2006 and London, U.K., 7 October 2006). They were attended respectively by 8, 10 and 14 members. The next meeting will be held in Turin, Italy, 3 August 2007.

Minutes have been posted on the IUPAC web-site for all of the above meetings.

Membership: Core membership continues as before. The National Representative (NR) for Russia has changed (from Nikolay Nifantiev to Sergey Bachurin). We have also picked up 10 new medicinal chemists either as new NR's, as new Division VII Committee Members, or as having been involved in the Division Committee election, or through personal contact (David Alker, Derek Buckle, A. Ganesan, So-Yeop Han, Javed Iqbal, Brigitte Lesur, Yvonne Martin, Grzegorz Mloston, Giorgio Tarzia and Mario Varasi).

Honorary Membership: The Subcommittee wishes to honour the IUPAC services of four past members of the Medicinal Chemistry Section with an "Honorary Fellowship" which is more than the usual "IUPAC Fellowship". This is being pursued by the Division President.

Projects: As previously, no new projects have arisen from proposals outside of the Subcommittee membership. One project has been completed, one project has been cancelled, and four new projects have been formally proposed and approved. Several projects involving glossaries were thought to be complete but have required additional work because ICTNS changed the format requirements so that the Gold Book is no longer the appropriate format to follow. They are very close to being completed.

Individual Projects:**Nomenclature and Terminology**

2003-044-1-700 Glossary of Combinatorial Chemistry Terms. The project leader has been changed because of his work commitments (from Derek Maclean to A. Ganesan). Derek stays on as a team member.

2000-009-1-700 Glossary of Drug Metabolism Terms. (Paul Erhardt)
Definitions are being adjusted to IUPAC format.

2002-001-1-700 Compendium of Glossaries. (Robin Ganellin)
Definitions are being adjusted to IUPAC format.

2001-049-2-700 Glossary of Terms in Pharmaceutical Technology. (Eli Breuer)
Definitions are being adjusted to IUPAC format.

2001-049-2-700 Glossary of Terms in Pharmaceutical Process Chemistry. (Mukund Chorghade)
Definitions are being adjusted to IUPAC format.

2005-050-1-700 Prototype Analysis of Molecular Biomarkers in Cancer. (Michael Liebman)
Molecular Biomarkers have become a major focus of disease management and drug development, particularly in oncology. This prototypic study will identify the existing biomarkers in breast cancer and

classify them in terms of disease progression and also as to their clinical vs. research use. The project is underway.

2004-025-1-700 Compendium of Molecular Targets for Drugs. (John Proudfoot)

The Project has been terminated because it was discovered that a substantial proportion of the anticipated material for this project was already available on the world-wide web. A short article was written by John Proudfoot for CI.

2004-019-3-700 Glossary of Terms for Biomolecular Screening. (John Proudfoot)

Glossary sections were prepared by three sub-teams and recompiled into one document. This is undergoing internal review by the team members and contains draft definitions of approximately 150 terms related to biomolecular screening. Reviewers for the final glossary have been identified.

Training and Development

2001-048-2-700 Research and Training in Medicinal Chemistry in the Indian Subcontinent. (Mukund Chorghade)

Medicinal chemistry and drug discovery are currently key growth areas in India. Mukund is in the late stages of organizing the first of two projected four day workshops on the basic aspects of Medicinal Chemistry to take place in India in late 2007. The workshops will be sponsored by the Indian government with additional funding and facilities provided by some of the leading Indian pharmaceutical companies and the ACS. Some of the subcommittee members will participate in the workshops as lecturers.

2004-028-1-700 Practical Studies for Medicinal Chemistry Students. (Antonio Monge)

The purpose of this project is to provide experimental studies for training medicinal chemistry students regardless of the academic level of the university. To this end, expensive chemical material and reagents, and the most highly sophisticated instrumentation have been avoided. The various experiments and studies have been combined into a book which provides developing countries with a practical text for studying medicinal chemistry. A draft printed version has been produced containing 41 experiments contributed by academic teachers from ten countries. All are written in English; most are also in Spanish or Portuguese. Considerable help was provided by Cheryl Wurzbacher (through the IUPAC Secretariat) to refine the English version and a final editing was carried out by Robin Ganellin. Since January 2007 an electronic version has been made freely available via IUPAC on the World-Wide Web, entitled "Practical Studies for Medicinal Chemistry" eds, A. Monge and C.R. Ganellin.

New Technologies and Special Tools

2000-010-1-700 Project on Human Drug Metabolism Database. (Paul Erhardt)

The project is on hold pending the procurement of additional funding.

2001-050-2-700 Natural Products with Medicinal and Nutritional Value. (Mukund Chorghade)

Document is being edited and adjusted to IUPAC format.

2005-031-2-700 Latin American Plants as Sources for Nutraceuticals. (Antonio Monge)

The objective is to provide possible commercial opportunities for local industry in Latin American countries. Contributors have been identified from most Central and South American countries and they have provided lists of locally used potential nutraceutical plants. The assessment of which are appropriate for inclusion in the project is in progress.

2002-051-1-700 Analogue-based Drug Discovery. (Janos Fischer)

This project metamorphosed into a book which was published by VCH-Wiley in January 2006. The book was edited by J. Fischer and C.R. Ganellin. It has been described in Chemistry International 2005, vol 27 (6), 26. It has received almost 40 positive reviews to date including one in J Med Chem 49 (15), 4799, 2006 where it was highly acclaimed. Sales are sufficiently robust that the publisher has contacted Janos

to propose a 2nd edition for 2009. It is now sold out and being reprinted. Janos proposed that a second volume would be more appropriate than a revised or updated edition. A project proposal will be submitted to support work on this next volume.

2005-032-1-700 Stand-Alone Drugs. (Janos Fischer)

The project will study drugs having no structural and pharmacological analogues with the intention of providing a perspective on situations where it has not proven possible to improve an existing drug with an analogue-based approach. There was a spirited debate among the members on the nature and scope of structural and pharmacological “analogy” and the ultimate scope of the project is still under discussion.

2005-049-1-700 Biological Context by Data Mining. (Michael Liebman)

To extend the usefulness and applicability of the glossaries, it would be worthwhile to explore methods for identifying the various contexts in which the terms appear in the scientific literature. In the ideal situation, this project can transcend the three Subcommittees of the Division to incorporate activities of each.

2005-042-1-300 Working Party on Chemistry for Biology. (Robin Ganellin representative)

An interdivision feasibility study jointly with the Organic and Biomolecular Chemistry and the Physical and Biophysical Chemistry Divisions. Progress unknown.

New Projects under discussion:

Update of Glossary of Terms in Medicinal Chemistry.

Research and Training in Medicinal Chemistry in Latin America.

Trends in Patenting Drug-Related Technologies.

Prize: The IUPAC-Richter Prize of US \$ 10,000 to be awarded 5 times over the next 10 years has been established by a generous gift from Gedeon Richter Ltd, Budapest, Hungary.

The Prize will recognise a prominent scientist for outstanding contributions in medicinal chemistry and drug discovery. The first Prize has been awarded to Professor Malcolm Stevens, Nottingham University, UK, for his work on heterocyclic anti-cancer drugs, and was presented to him at the time of his lecture at the EFMC International Symposium on Medicinal Chemistry, Istanbul, Turkey on 1st September 2006. The lecture is to be repeated at the IUPAC World Chemistry Congress in Turin, Italy, August 2007. The selection committee was chaired by Robin Ganellin and included Janos Fischer as a non-voting member and representative of Gedeon Richter.

41st IUPAC World Chemistry Congress (Turin,Italy)

Janos Fischer and Robin Ganellin helped set up and will chair two symposia on Analogue-based Drug Discovery and Cancer Chemotherapy respectively for Session 2 “Chemistry Protecting Health.”

External Contacts: Continue with the European Federation for Medicinal Chemistry (EFMC) and the Asian Federation for Medicinal Chemistry (AFMC).

Bibliography:

Books

Analogue-based Drug Discovery, Eds. J. Fischer and C.R. Ganellin, Wiley-VCH, Weinheim, 2006.

Practical Studies for Medicinal Chemistry, Eds A. Monge and C.R. Ganellin
IUPAC, 2007, as a web edition
(http://www.iupac.org/publications/cd/medicinal_chemistry/index.html)

Chemistry International articles

Antonio Monge. "Natural Products, a Possibility for the R&D of Drugs for Developing Countries."
C.I. 2005, 27 (6), 21-22.

Chemistry International News Items

"Practical Studies for Medicinal Chemistry".
C.I. 2007, 29 (2).

The 6th International Medicinal Chemistry Symposium (AIMECS 07) will be in Istanbul, Turkey, 8-11
July 2007.
C.I. 2007, (1).

Malcolm F.G. Stevens is Awarded the First IUPAC-Richter Prize.
C.I. 2006, 28 (6).

IUPAC-Richter Prize in Medicinal Chemistry.
C.I. 2005, 27 (6).

Analogue-Based Drug Discovery.
C.I. 2005, 27 (6).

Subcommittee Members Teach Short Course on Medicinal Chemistry.
C.I. 2005, 27 (3).

C. Robin Ganellin
Subcommittee Chair
26 May 2007

Attachment 3**SC-NPU, IFCC-IUPAC,
Activity report for the period August 2005 - August 2007****Membership:**

Urban Forsum, Chair, (2005)
 Francoise Pontet, Chair (starting 2006-01-01)
 Pedro Soares de Araujo, Secretary (2005)
 Gunnar Nordin, Secretary (starting 2006-01-01)
 René Dybkær (proposed Distinguished Fellow)
 Ivan Bruunshuus
 Jarkko Ihalainen
 Daniel Karlsson
 Xavier Fuentes-Arderiu
 Gunther Schadow
 Ulla Magdal Petersen
 Wolf Külpmann
 Henrik Olesen (proposed Distinguished Fellow)
 Antonin Jabor

Meetings:SC-NPU

Rome Italy 2005-10-07 – 10-09

Paris, France 2006-04-08 – 04-10

Brussels, Belgium 2006-12-03 – 12-05

Meeting with the Estonian Society for Laboratory Medicine (U. Forsum)

Taagepera Estonia 2005-09-26

Meeting with representatives (John Zlockie and co-workers) of the CLSI on the future of the C-NPU data base. (U. Forsum, I Bruunshuus)

Wayne Pa USA 2005-11-14

C-NPU active participation at the Workshop on “Quantities, numbers and parts” IFOMIS University of Saarbrücken (U. Forsum, D. Karlsson)

Saarbrücken Germany 2005-12-01 – 02

CEN TC 251 wg 2 meeting (ENV 1614 standard) (D. Karlsson)

Rome Italy 2005-10-08

Symposium “Aktuelles zu medizinische Klassifikationen und Terminologien. GMDS- project group “Standardisierte Terminologien in der Medizin”. (W. Külpmann)

Freiburg Germany 2005-09-15

SC-NPU generic database

The SC-NPU generic database is, as of 2002-04-25, published on the net under the URL: <<http://dior.imt.liu.se/cnpu/>>. The database is published on the IFCC homepage (Scientific division) and IUPAC (Division of Chemistry and Human Health.) homepage with a link to the server Dior, and to the Danish National Board of Health server. During the meeting in Wayne Pa USA with representatives of the CLSI (former NCCLS) it was agreed that the C-NPU and CLSI should seek a permanent hosting of the database probably as part of the CLSI website and server. Unfortunately, this collaborative project of hosting this database on the CLSI website had to be dropped because of CLSI board decision of declining IFCC offer, the support of C-NPU database not being aligned with CLSI mission.

The IFCC SD has thus proposed that the database be hosted on the IFCC website. The cost of such a management has been communicated to IFCC officers, so that IFCC SD could finalize its decision. A meeting in Amsterdam, at Euromedlab IFCC-FESCC congress is scheduled on June 6th, 2007.

Ongoing projects

1. Properties and units for function examinations (IUPAC: 2001-067-1-700). An updating has been undertaken.
2. Properties and units for urinary calculi (IUPAC: 2001-070-1-700). A full reformatting of the manuscript is being done.
3. Global use of the SC-NPU concept system for properties in toxicology (IUPAC:2001-066-1-700). Published in Pure and Applied Chemistry, in January 2007.
4. Internationally agreed terminology for observations in scientific communication. (IUPAC 2004-023-1-700) Chair : Françoise Pontet. Two drafts have been circulated and discussed during the last Sub-Committee meetings.
5. Mapping of IFCC-IUPAC laboratory coding system to SNOMED CT (IUPAC 2006-008-1-700) Chair : Ulla Magdal. Has just started on 2006-07-01. Abstract is on IUPAC website.
6. Securing and structural updating of information in the NPU coding system and its environment (IUPAC 2006-012-1-700) Chair : Ulla Magdal. Has just started on 2006-07-01. Abstract is on IUPAC website.
7. Recent advances in Nomenclature, Properties and Units : strategy for promoting SC-NPU achievements (2006-048-1-700) Chair : Françoise Pontet. Has just been accepted, budget pending.
8. Translation of SC-NPU database elements and properties into French (F. Pontet). Is being updated in 2007.
9. German translation of the SC-NPU data base (W Külpmann) done during 2005-2006 and is under review in the SC-NPU.
10. The Portuguese translation of the SC-NPU data base has been updated in 2005.
11. Paper on IFCC WG-HbA1c name and units (G. Nordin). This manuscript on the impact of systematic nomenclature on the naming of this particular important property has been agreed on by a ballot in IFCC. It is now submitted to Clinical Chemistry and Laboratory Medicine.
12. Revision of ENV 1614 has been done in collaboration with CENT C 251. It is now published.
13. The final draft of the 3rd edition of VIM is under editorial revision and will be sent to ISO in early June for final publication, due in the 2nd half of 2007.

Future projects

Silver Book revision. Georges Férard has accepted to chair this project and will present his proposal soon.

The SC-NPU is currently working on a number of other projects to become work items during 2006. One proposal is under discussion as draft, and two are in preparation.

Representation in other committees.

IFCC Scientific Division : Françoise Pontet

ICTNS of the IUPAC : Urban Forsum (2005)

JCGM of the BIPM (WG2-VIM), IFCC : René Dybkær, Françoise Pontet

JCGM of the BIPM (WG1-GUM), IFCC, ILAC, CCQM : René Dybkær

CEN TC 251 wg2 : Daniel Karlsson

Publications 2005-2006 :

1. Nordin G, Klinteberg B, Persson B, Forsum U. Får en laboratorieundersökning kallas vad som helst? "NPU-systemet" reder upp i begreppsöran och ger systematisk stringens. Läkartidningen, 2005, 102: 1308 – 1315 (in Swedish).
2. Forsum U, Hallander HO, Kallner A, Karlsson D. Impact of qualitative analysis in laboratory medicine. TrAC-Trends in Analytical Chemistry, 2005, 24: 546 -555.
3. Forsum U, Karlsson D. Terminology, categories and representation of examinations in laboratory medicine. Clin. Chem. Lab. Med. 2005;43:344-345.
4. Külpmann. W Das NPU-System (IFCC, IUPAC) de Messgrößen und Einheiten in der Laboratoriumsmedizin. J Lab Med 2005, 29:2-5 (in German).

5. D'Orazio P, Burnett RW, Fogh-Andersen N, Jacobs E, Kuwa K, Külpmann W, Larsson L, Lewenstam A, Maas AHJ, Mager G, Naskalski J, Okorodudu AO; the IFCC SD WG on Selective Electrodes and Point of Care Testing. *Clin Chem* 2005, 51,9:1573-1576.
6. Fuentes-Arderiu X. Description of examinations and their results and the standard ISO 15189. *Clin Chem Lab Med* 2006;44: (to be published in september 2006).
7. Fuentes-Arderiu X. Vocabulary of terms in protometry. *Accred Qual Assur* 2006; 11:640–643.
8. Magdal U, IFCC-IUPAC Committee of Nomenclature, Properties and Units. Mapping laboratory codes. Semantic mining conference on SNOMED CT 2006. Poster presentation.
9. Duffus J. , Bruunshuus I., Cornelis R., Dybkær R., Nordberg M., and Kuelpmann W. Properties and Units in the Clinical Laboratory Sciences, Part XX. Properties and Units in Clinical and environmental human toxicology. *Pure and Applied Chemistry*. **79** (2007) 87-152

Françoise Pontet
SC-NPU Chair

**Subcommittee on Toxicology and Risk Assessment
Report, May 2007**

1. Projects completed or in progress - August 2005 to May 2007

1.1 2001-053-2-700C - Fundamental Toxicology, 2nd Edition

This project was completed with the publication of the textbook by the Royal Society of Chemistry in January 2006.

Reference:

J.H.Duffus and H.G.J.Worth Eds.
Fundamental Toxicology - 2nd Edition.
Royal Society of Chemistry, 2006.

1.1 2001-066-1-700 - Global use of the C-NPU concept system for properties in toxicology

This project has been completed with the report, "Properties and Units in the Clinical Laboratory Sciences: Part XX. Properties and Units in Clinical and Environmental Human Toxicology. Technical Report (IFCC-IUPAC 2006)". The report was revised to satisfy PAC requirements and subsequent reviewers' comments and was published in PAC.

Reference:

J.H. Duffus, I. Bruunshuus, R. Cornelis, R. Dybkær, M. Nordberg, and W. Kuelpmann
Properties and units in the clinical laboratory sciences Part XX. Properties and units in clinical and environmental human toxicology (IUPAC Technical Report) *Pure Appl. Chem.* 79(1), 87-152, 2007.

1.2 2003-001-2-700 - Explanatory dictionary of concepts in toxicokinetics

This project has been completed and revised to satisfy PAC requirements and should be published in PAC shortly. The Royal Society of Chemistry has reviewed the PAC paper in draft and has decided that it could be the basis for a successful book. A contract has been signed between the authors of the PAC paper, IUPAC and the RSC to prepare this book. It is thought by the working group and the RSC that it should have twice as many entries to be eligible for publication as a book of a reasonable length. Monica Nordberg has submitted to IUPAC a second project, "Explanatory Dictionary, part 2", to cover the the expanded definitions of about 20 more terms. Together with the completed project, this should provide the basis required for a book to be entitled "Concepts in Toxicology".

Reference;

M. Nordberg, J.H. Duffus, D.M.Templeton
IUPAC Explanatory Dictionary of Key Terms in toxicology (IUPAC Recommendations 2006)
Pure Appl.Chem., Vol.79, *in press*, 2007.

1.3 1999-047-1-700 - Immunochemistry of metal sensitization

Two papers resulting from this project have already been published. During the period which this report covers, a further paper (see below) has been published in PAC. Two additional manuscripts on "Lymphocyte Subpopulations" and "Immunological Effects of Mercury" are currently in draft form and were discussed by the authors at the recent meeting in Edinburgh. Doug Templeton, the project leader, is considering further activities within the scope of this project which may be carried out with the remaining part of the budget.

References:

R. Klein, M. Schwenk, D. M. Templeton

Cytokine profiles in human exposure to metals (IUPAC Technical Report)

Pure Appl. Chem. 78(11), 2155-2168, 2006

1.4 2004-045-1-711 - Training of school children on pesticides and health

The working group for this project met in Prague in April, 2006 and in Athens in May 2007. The dose response experiment teaching module has been successfully tested in Malawi. The project should be finalized by the end of this year. It is proposed to discuss the draft material with the Committee on the Teaching of Chemistry in Torino. The project will be presented By Dr Besbelli at the 4th International Conference on Children's Environmental Health. www.inchesnetwork.net in Vienna: 10th of June – 12th of June 2007.

1.5 2003-028-1-700 - Glossary for chemists of terms used in toxicology – revision and updating

Every term was considered and possible changes were assessed at the Subcommittee Meeting in March 2006. This took up most of the time allotted to the meeting of the Subcommittee. Consensus was reached on the terms discussed and the text has been revised accordingly. The resultant draft, version 12, was submitted to Pure and Applied Chemistry for publication as an IUPAC Recommendation, superseding the existing glossary of 1993. Following the review period on the IUPAC website, the Glossary was amended to take into account all the comments received. In this form, the Glossary was accepted for Publication.

Reference:

J.H. Duffus, M. Nordberg, D.M. Templeton

Glossary of Terms Used in Toxicology, 2nd Edition (IUPAC Recommendations 2007)

Pure Appl. Chem., Vol.79(7), pp.1153- *in press*, 2007

The revised glossary has been incorporated with acknowledgment to IUPAC in the U.S. National Library of Medicine TOXNET portal to the toxicology literature. This portal incorporates toxicology tutorials under the title ToxLearn. ToxLearn is a series of presentations designed for self study and these are being hyperlinked to the IUPAC glossary on the TOXNET site.

1.6 2004-002-1-600 - Glossary of Terms Relating to Pesticides

Monica Nordberg contributed to the 'Glossary of Terms Relating to Pesticides' which has been published in PAC.

Reference:

G.R. Stephenson, I.G. Ferris, P.T. Holland, and M. Nordberg
Glossary of terms relating to pesticides (IUPAC Recommendations 2006)
Pure Appl. Chem. 78(11), 2075-2154, 2006

1.7 2005-047-1-700 - Glossary of Terms Used in Ecotoxicology

A list of appropriate terms was compiled and current definitions collected and compared. New definitions were prepared as appropriate. The draft glossary was reviewed at a meeting of the working group in Edinburgh. Professor Mike Schwenck attended this meeting and helped with this revision. Following the meeting a new draft has been prepared and is currently being circulated among the working group. Some problematic terms have been identified and are being given special attention.

2. New projects

2.1 Explanatory dictionary - part 2

A project proposal has been submitted and is currently still under consideration for funding. A contract for a subsequent book has been signed with the RSC (see above under 1.2 **2003-001-2-700**).

2.2 Supplementary modules on Essential Toxicology

Howard Worth and John Duffus are planning to submit a project with the aim of producing presentations of educational material in clinical chemistry to supplement those already available on the IUPAC website with the title "Essential Toxicology".

3. Other Activities

The activity related to human biomonitoring, initiated from contacts with Rick Becker, Senior Director - Public Health Team, American Chemistry Council (ACC), has led to a Workshop on "Human Biomonitoring". John Duffus was involved in planning this Workshop and Monica Nordberg is attending it as an active participant. The Workshop will consider a draft proposal for methodology to establish appropriate reference values for human biomonitoring. Four important environmental toxicants will be considered as case studies and the methods examined critically. Assuming the Workshop is successful, the methodology will be published and further meetings may be held which may justify IUPAC support of relevant projects.

PUBLICATIONS CITED ABOVE

J.H.Duffus and H.G.J.Worth Eds., *Fundamental Toxicology - 2nd Edition*. Pub. Royal Society of Chemistry, 2006.

G.R. Stephenson, I.G. Ferris, P.T. Holland, and M. Nordberg. Glossary of terms relating to pesticides (IUPAC Recommendations 2006). *Pure Appl. Chem.* 78(11), 2075-2154, 2006

J.H. Duffus, I. Bruunshuus, R. Cornelis, R. Dybkær, M. Nordberg, and W. Kuelpmann. Properties and units in the clinical laboratory sciences Part XX. Properties and units in clinical and environmental human toxicology (IUPAC Technical Report). *Pure Appl. Chem.* 79(1), 87-152, 2007.
R. Klein, M. Schwenk, D. M. Templeton. Cytokine profiles in human exposure to metals (IUPAC Technical Report). *Pure Appl. Chem.* 78(11), 2155-2168, 2006

J.H. Duffus, M. Nordberg, D.M.Templeton. Glossary of Terms Used in Toxicology, 2nd Edition (IUPAC Recommendations 2007). *Pure Appl.Chem.*, Vol.79(7), pp.1153- *in press*, 2007

M. Nordberg, J.H. Duffus, D.M.Templeton. IUPAC Explanatory Dictionary of Terms in Toxicology (IUPAC Recommendations 2006). *Pure Appl.Chem.*, Vol.79, *in press*, 2007.

PRESENTATION AT SOCIETY OF TOXICOLOGY ANNUAL CONGRESS, SAN DIEGO, MARCH 2006

Workshop at U.S. Society of Toxicology Annual Congress, San Diego, U.S.A., March 6, 2006. "Distance learning in toxicology." J. H. Duffus

PRESENTATIONS TO BE GIVEN IN TURIN, AUGUST 2007

Third IUPAC-UNESCO-Unido Safety Training Program, 2007. "Distance learning in toxicology: the IUPAC contribution". J. H. Duffus

IUPAC General Assembly World Chemistry Leadership Meeting, "Regulatory Toxicology - A Need For Better Science,". J. H. Duffus

Attachment 5**Report of the Public Relations and Elections Subcommittee**Public Relations

Following the Beijing meeting, the material in the poster for the Chemistry and Human Health Division displayed at the meeting, was updated and modified. A draft version was presented to the Division Committee in Atlanta, and members of the DC made suggestions on the content and organization. The final version contained sections on Mission, Organization, Membership, Publications and Selected Current Projects. The Publications were divided into Books, Glossaries and Others. The Selected Current Projects were categorized into the three subcommittees sponsoring them. Also added was a section on submitting a project proposal, and a description of the IUPAC Richter Prize in Medicinal Chemistry. This revised material was presented at the COCI Annual Meeting in July. It was well received, and generated a healthy discussion on the merits of collaborating on joint projects. Some of the goals and activities of COCI are similar to those of Division VII, so there is the possibility of sharing resources where appropriate. It was recognized that the interaction between the two organizations should be two-way, and a representative of COCI (Alex Pokrovsky) was identified to attend the next Division Committee meeting. This will complement my representation of Division VII with COCI. The organization and presentation of the Recent Activities of Division VII was selected as a model for presentations by other IUPAC Divisions that were not represented in person at the COCI meeting. The poster material was sent to the Secretariat who developed a new poster for Division VII. This was presented for the first time at the International Symposium on Medicinal Chemistry (ISMC) held in Istanbul, August 29- September 2, 2006. A Power Point version of the material was also prepared, and it can be made available to any members of the Division Committee who have an opportunity to use it as a PR vehicle at meetings they attend. Likewise, the poster has also been prepared in both portrait and landscape formats for use in appropriate settings by DC members.

Elections

The election of new Titular Members (TMs) for the Division Committee in 2008 went smoothly. The nominees represented a diversity in expertise, geography and gender. Two of the three winners are experts in the NPU discipline (one being the current Chairperson of this Subcommittee), and the other winner an expert in toxicology. Two years ago, two of the new members were toxicology experts and one involved medicinal chemistry. Four years ago, two new members were medicinal chemists, one a toxicologist, and one was involved in NPU activities. These results demonstrate the healthy technical-diversity of the Division as it continues to evolve from the former merger of these three distinct but inter-related disciplines. The candidates who did not receive enough votes to become TMs have agreed to become Associate Members (AMs) of the Division, and one candidate is a National Representative. These additional new members will further increase Division VII's overall geographical representation, as well as contributing new expertise.

Tom Perun
Subcommittee Chair

Attachment 6**IUPAC General Assembly and World Chemistry Congress
Torino, Italy August 5-11, 2007****Scientific Program Session 2: *Chemistry Protecting Health***

**Co-Chairs: Giuseppe Ronsisvalle (Universita di Catania)
Paul Erhardt (University of Toledo, USA)**

Symposia

1. *Analog-Based Drug Design*
Chair: Janos Fischer
Keynote: Joerg Senn-Bilfinger
2. *Multi-Target Drugs*
Chair: Giuseppe Ronsisvalle
Keynote: Albert Gasco
3. *Cancer Chemotherapeutic Agents*
Chair: Robin Ganellin
Keynote: Malcolm Stevens (IUPAC-Richter Prize recognition event)
4. *Prodrugs and Soft Drugs*
Chair: Howard Ando
Keynote: Nicholas Bodor
5. *Clinical Laboratory Nomenclature, Properties and Units*
Chair: Francoise Pontet
Keynote: Rene Dybkaer

Attachment 7**RECENT ACTIVITIES OF DIVISION VII — CHEMISTRY AND HUMAN HEALTH****BOOKS**

Medicinal Chemistry for the 21st Century (1992) (1994)
 Fundamental Toxicology for Chemists (1996)
 Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development (1999)
 Handbook of Pharmaceutical Salts: Properties, Selection and Use (2002)
 Analogue-based Drug Discovery (2005)
 Fundamental Toxicology, 2nd Edition (2006)

GLOSSARIES

Glossary of Terms in Quantities and Units in Clinical Chemistry (1996)
 Glossary of Terms Used in Computational Drug Design (1997)
 Glossary of Terms Used in Medicinal Chemistry (1998)
 Glossary of Terms Used in Combinatorial Chemistry (1999)
 Glossary of Terms Used in Toxicokinetics (2004)
 Glossary of Terms Used in Pharmaceutical Technology
 Glossary of Terms Used in Pharmaceutical Process Chemistry
 Glossary of Drug Metabolism Terms
 Glossary of Terms Used in Toxicology

OTHER RECENT PUBLICATIONS

Essential Toxicology — Educational Modules in PDF Format on IUPAC Website
 Natural and Synthetic Substances Related to Human Health (2002-2003)
 Mechanisms of Immunosenescence to Metals (2004)
 Properties and Units in the Clinical Laboratory Sciences (2004)
 Impact of Qualitative Analysis in Laboratory Medicine (2005)
 Postgenomic Chemistry (2005)
 Guidelines for Terminology for Microtechnology in Clinical Laboratories (2006)
 Surveys of Research and Training in Medicinal Chemistry
 United States
 Europe
 Japan
 India, Pakistan and Sri Lanka
 Explanatory Dictionary of Concepts in Toxicology

SELECTED CURRENT PROJECTS**Medicinal Chemistry and Drug Development**

Human Drug Metabolism Database
 Chemical and Pharmacological Aspects of Natural Products with Medicinal and Nutritive Value
 Compendium of Terms Associated with Drug Discovery and Development
 Glossary of Terms Used in Biomolecular Screening
 Practical Studies in Medicinal Chemistry — An Integrating Approach for Developing Countries
 Plants as Sources for Nutraceuticals in Latin America
 Prototype Analysis of Molecular Biomarkers in Cancer

Toxicology and Risk Assessment

Quantifying the Effects of Compound Combinations
 Educational Material for Teaching Toxicology
 Training of School Children on Pesticides and Health
 Distance Learning in Toxicology; Effective Teaching through Technology

NPU/Clinical Chemistry

Recommendations for the Use of Nanotechnology in Clinical Laboratories
 Concepts and Structure for Requests in Clinical Laboratories
 Global Use of the C-NPU Concept System for Properties in Toxicology
 Internationally Agreed Terminology for Observations in Scientific Communication
 Immunochemistry of Metal Sensitization

THE IUPAC RICHTER PRIZE IN MEDICINAL CHEMISTRY

Acknowledges the key role that medicinal chemistry plays toward improving human health. Awarded every two years to an internationally recognized scientist whose accomplishments demonstrate an outstanding level of contribution to the practice of medicinal chemistry or drug discovery.