Chemistry and Human Health (Division VII)
IUPAC Bureau Report, Warsaw, April 2011

Prepared March 21, 2011

Submitted by Doug Templeton, President Division VII

Executive Summary

This report presents an update of activities in Division VII (DVII) since the last Bureau meeting in Sofia (April, 2010). The Division has met twice in the past year, graciously hosted by the European Environmental Agency in Copenhagen (March 2010) and at the Academy of Medical Sciences in London (Nov. 2010). Here I address business arising from these meetings and highlight initiatives being targeted in this Biennium and during IYC. This Executive Summary deals with Division initiatives and structure, membership, budget, projects, highlights of Subcommittee activities, adherence to IUPAC goals, and current and future initiatives. Annexes provide details of membership, projects, and activities of our individual Subcommittees. DVII will meet next in Puerto Rico during the General Assembly.

1. Structure of the Division

DVII is organized into four Subcommittees (SCs), three of which deal with technical aspects of our mission. These are the SCs on Medicinal Chemistry and Drug Development (MCDD); Nomenclature for Properties and Units (NPU); and Toxicology and Risk Assessment (TRA). The fourth SC manages our Public Relations and Elections (PRE). The SCs are chaired by Robin Ganellin (MCDD), Françoise Pontet (NPU), John Duffus (TRA), and Tom Perun (PRE). Detailed reports from the technical SCs are appended (Annexes 1-3). NPU was formerly called Nomenclature, Properties and Units in Laboratory Medicine. The name change was unanimously approved at the last GA and has now been adopted.

Our executive positions consist of a President, Past President or President-elect, and Secretary. Our operating procedures mandate a four-year term for the Division President with the role, effectively of Vice President, being served for the first two years of that term by the Past President and in the last two years, as currently, by the President-elect (Françoise Pontet, who will assume the Presidency in 2012).

2. Operating procedures and rules of DVII

DVII filed rules and operating procedures with the Secretariat, which approved by the GA in Glasgow. Two initiatives specific to DVII were presented in that document; they are rules for declaring DVII Emeritus Fellowship, and for granting IUPAC Sponsorship on a limited Divisional basis. Both have now been implemented successfully. A link has now been added to our Divisional web site with biographies of
our Emeritus Fellows and highlighting contributions to IUPAC. The operating procedures have also helped clarify to our membership and Division Executive, streamlined procedures for reviewing Project Applications, Technical Reports, and Recommendations.

3. Membership

We have had a significant rejuvenation of the Division Committee, notably with five new TMs beginning terms in Jan. 2010. In addition, our Division operating procedures, approved by Council in Glasgow 2009, permit us to remove non-performing TMs, and we exercised this procedure for one TM in 2010, subsequently “promoting” one of our AMs to a 6th new TM spot and adding a NR to our AM roster. Three of the new TMs are already actively involved as Task Group chairs, and one has begun serving as Division Secretary. Our current membership (2011) is reported in Annex 4. Our membership represents diversity of gender, geography, and expertise with respect to our technical SCs.

4. Budget

In the previous Biennium (2008/2009), DVII complied strictly with budgetary guidelines (expenses 70.6% Commitments, 29.5% Operations, Total 100.1%). In this biennium, we have so far exceeded our Operations guideline significantly (39%) for the following reasons: Two Division meetings were held in 2010 in order to engage effectively our large roster of 6 new TMs and capitalize on their early enthusiasm. IYC planning was a focus of the second meeting. There was an admirably strong, but nevertheless costly, turnout at both meetings, and we continue our policy of bringing our active SC chairs to the meetings. We have funded four new projects (Total Commitments 78%).

5. Projects

All together, the three technical SCs are currently involved in 34 projects reported upon monthly by the Secretariat. These are listed in Annex 5. These, together with projects submitted or under discussion, are described in the individual SC reports (Annexes 1 - 3). A classification of our current projects shows the following balance (number of projects in parentheses):

- Education and Training (4)
- Properties and Units (8)
- Glossaries (8)
- Data Bases (4)
- Drug Discovery (6)
- Clinical Chemistry and Toxicology (4)

6. Highlights of SC activities  (details are in the appended SC reports)
6.1. MCDD - This SC remains very active, meeting approximately four times in each Biennium, in addition to regular DVII meetings. They currently manage 17 projects, all of which have arisen within the SC. The IUPAC-Richter prize is awarded by this SC every two years, and was awarded again in 2010 to Arun Ghosh (see point 7.6). An IYC initiative is to make videotapes of lectures in lay terminology available to the public online. For a pilot from Prof. Ghosh, see http://vimeo.com/19567220. The successful book “Analogue-based Drug Discovery” which went to a second printing in 2008, was followed by a second volume at the request of the publisher, and was published in summer 2010. A third volume is planned. Meetings in Rajkot and Nagpur, India, were held in Feb. 2011, organized by DVII Committee member M. Chorghade and attended by Prof. Nicole Moreau (IUPAC President) and Dr. Francoise Pontet (Division VII President-elect). They highlighted biotechnology and drug development, and are promising to forge strong links between India and the Division that have not existed up to now.

6.2. NPU - The SC has close contacts with the International Federation of Clinical Chemistry (IFCC) in maintaining a web-based generic database (NPU), of which they share ownership. They are collaborating on mapping of the database to the Systematized Nomenclature of Medicine - Clinical Terms (SNOMED-CT) through contact with the International Health Terminology Standards Development Organization (IHTSDO) in Copenhagen, and with the Logical Observation Identifiers Names and Codes (LOINC) at Indiana University. Legal arrangements continue to be negotiated for joint ownership of the harmonized database. These initiatives were first presented to the Bureau in Bratislava, and are progressing both on the legal and project sides. A major initiative with IFCC to update the IUPAC Silver Book (Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences) is underway. NPU maintains representation on both Joint Committee for Guides in Metrology (JCGM) working groups WG1 (GUM – Guidelines for Uncertainty in Measurement) and WG2 (VIM - International Vocabulary of Metrology). René Dybkaer’s book “An Ontology on Property” has been published on the IUPAC website.

6.3. TRA - Projects on childhood education, and several glossaries are underway. Contacts with the WHO and its International Program in Chemical Safety (IPCS) are being established in collaboration with COCI. Participation in a Biomonitoring Equivalents Workshop established contacts with the US Environmental Protection Agency, Health Canada, and the American Petroleum Institute, among others. I met with Herman Autrup, President-elect of IUTOX, in Washington DC in early March 2011 to discuss closer links between IUPAC and IUTOX, through ongoing collaboration as well as in the contexts of ICSU and IYC. The first phase of the Toxicology in the Classroom (Toxiclaro) project has been completed with the construction of a successful interactive website for children (see Chem. Int., Vol. 31 No. 6, November-December 2009). The current website is http://www.prn.usm.my/toxicology_2010/. The Toxiclaro initiative originated from the IUPAC Chemistry and Human Health Division and the IUPAC Committee on Chemistry Education (CCE), which formally met to plan the project in May 2005 at the Federal Agency for Risk Assessment, Berlin, Germany. The project is managed by a task group of professionals from the World Health Organization (WHO), IUPAC, and the National Poison Centre of Malaysia.
6.4. PRE - This SC has been helpful in providing IUPAC material for public dissemination and branding. Five Divisional posters have been updated for Puerto Rico and travel with the DP and SC Chairs to various meetings throughout the year.

7. Advancing IUPAC Goals

7.1 Leadership in global chemical issues - Recent highlights include ongoing revision of the *Glossary of terms used in toxicology*, whose predecessor was adopted by a number of legislative bodies. As this expands and incorporates more terminology (e.g. from the glossaries in Ecotoxicology (2009) and Immunotoxicology (under review, Jan. 2011)), plans are underway to make an inclusive glossary available on-line with frequent updates by the authors. The NPU database and ongoing revision of the Silver Book are also noteworthy. Harmonization of terminology with the Danish IHSTDO/SNOMED-CT and the American LOINC is a major undertaking described in more detail in the NPU-LM report. The book *Concepts in Toxicology* published by the Royal Society of Chemistry (UK) is intended to clarify a number of issues relevant to risk assessment for legislators, and to the basic science of toxicology for chemists. The involvement of our SC-NPU-LM representing IUPAC as one of eight international bodies in the production of the 3rd revision of the Vocabulaire Internationale de Metrologie (VIM3) is a highlight.

7.2 Provision of tools - As noted above, about a dozen glossaries of terminology have recently been published or are currently under construction, including three new projects for a glossary in immunotoxicology, revision of terms in clinical chemistry, and terms in computational drug design, which are underway.

7.3 Assistance to the chemical industry in sustainable development, wealth creation, and improving quality of life - The PRE SC is active in COCI and the TRA is forging links with external bodies in collaboration with COCI. The MCDD has a long-standing association with industry, and its projects on natural products with medicinal value, nutraceuticals in Latin American Plants, and the volume 2 of the very successful book “Analogue-based Drug Discovery” are examples of current projects with immediate value to the chemical industry.

7.4 Fostering communication - Examples of particular relevance to this goal are the NPU-LM projects *Internationally agreed terminology for observations in scientific communication*, *Mapping of IFCC-IUPAC laboratory coding system to SNOMED-CT*, and *Translation of NPU database elements and properties into French*; and the TRA publication *Concepts in Toxicology*, and recent glossaries bridging chemical toxicology with ecology and the environment (Ecotoxicology) and chemistry with the field of immunology (Immunotoxicology, now under review).

7.5 Education – Of significant note is the completion of the first phase of Toxiclaro described in section 6.3 above. Other examples are the recently published *Fundamental Toxicology, 2nd Edition, Analogue-based Drug Discovery*, and *Concepts in Toxicology*. Ongoing projects include *Training of School Children on Pesticides and Health* (TRA), *Research and Training in Medicinal Chemistry in the Indian Subcontinent* (MCDD), and *Practical Studies for Medicinal Chemistry Students* (MCDD). TRA Chair John Duffus
has close links with CCE and participates globally in designing and delivering toxicology curricula. He is a major contributor to the US Society of Toxicology (SOT) initiative for on-line chemical toxicology curricula (ToxNet).

7.6 Public relations - The PRE SC is active in improving the visibility of DVII and of IUPAC. “Limited DVII sponsorship” is used to distribute IUPAC material and make an oral presentation on DVII activities. An example was the “Advances in Chemical Sciences Symposium” held in Boston, which was heavily attended by members of the pharmaceutical industry, who heard a presentation by the DVII Secretary. Details of this process for limited sponsorship are now formalized in the DVII operating procedures, and have been implemented successfully on two occasions. Two DVII posters have been produced to complement the individual SC posters, and these are presented by presentation at international meetings by the DP and SC Chairs. The IUPAC-Richter Prize adjudicated through the MCDD SC is gaining prestige, and provides an international forum for scientific presentation by the winner, with IUPAC’s name associated. The winner for 2010 was Arun Ghosh, the inventor of Darunavir (already approved as a first line defense against drug-resistant AIDS) and new β-secretase inhibitors for Alzheimer disease are under development, using protein backbone-based structural design. A video of high school students touring his lab and a subsequent Q & A session on how new drugs are “built” is posted on the Web as part of our IYC activity. It is available at http://vimeo.com/19567220.
## List of Attachments

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Annex 1 - Details from MCDD

A highlight in 2010 was the awarding of the Richter Prize to Prof. A. Ghosh for his outstanding achievements in the development of new drugs for the treatment of drug-resistant HIV. Prof. Ghosh gave a lecture at the Brussels International Symposium on Medicinal Chemistry this September. There, R. Ganellin introduced him, chaired his session, and presented the award to Prof. Ghosh. Moreover, Prof. Ghosh gave a talk at the US Medicinal Chemistry Symposium in Minnesota, and former Division VII president P. Erhardt honored him with an impressive introduction.


Ongoing projects:

2003-044-1-700 “Glossary of terms used in combinatorial chemistry”. Only USD500 have been spent. The project is to be continued, but the name “combinatorial chemistry” will be amended to suit the more up to date situation.

2000-010-1-700 “Human drug metabolism database” and 2000-009-1-700 “Glossary of Drug Metabolism Terms”: The budget of both projects is empty. The projects stopped, because there was not sufficient funding. The chairman of both projects, P. Erhardt, needs to get additional funds. T. Perun will contact P. Erhardt to learn how far the work has progressed, whether it will be continued, and if so, whether he will write a new project application to Division VII. If the projects cannot be finished, e.g., because the progress in this field is too rapid, they should be dropped from the list.

2001-049-2-700 “Glossary of terms in pharmaceutical process chemistry”. According to our present knowledge, this project is close to being finished.

2001-048-2-700 “Research and training in medicinal chemistry in India, Pakistan and Sri Lanka” is still running. A University training course in India was planned for February 2011. The travel financing seems to be still open.

2004-028-1-700 “Practical studies for medicinal chemistry students - an integrating approach for developing countries” is on the IUPAC web and is going to be published as a book in Spanish/Portuguese/English languages. According to the project chair A. Monge, the project will be completed upon realization of this publication.

2005-050-1-700 “Prototype analysis of molecular biomarkers in cancer” and 2005-049-1-700 “Prototype analysis of glossary terms to establish biological context by text data mining” are apparently both nearing completion to the point of review for PAC. The project chair (Liebman) is being encouraged.

2008-010-1-700 “Update of glossary of terms used in medicinal chemistry”. The project
chair D. Buckle reports that the project is on track and the manuscript is soon ready to enter the review process for publication. The formatting will be made in accordance with that of the draft of the Glossary of Immunotoxicology. The procedure for submitting, and the reviewing process were discussed with Dr. Buckle in London.
Annex 2 - Details from NPU-LM

G. Schadow will leave project 2004-023-1-700 on nominal properties. Jens Gleditsch from Norway joined as a member in the new project 2010-035-3-700, and attended the plenary subcommittee meeting in Linköping, Sweden, in October 2010. There was also a meeting in Corfu in April 2010. In addition there were project meetings of the Silver Book group and of the nominal properties group. A number of publications arose from the subcommittee members. The most important was a book by René Dybkaer, “An Ontology on Property”, published on the IUPAC website and available at (http://ontology.iupac.org/ontology.pdf).

The management of the NPU terminology by IFCC (International Federation of Clinical Chemistry and Laboratory Medicine) is presently the most important and time-consuming matter of SC-NPU. The NPU terminology is presently available in eight languages. So far the Danish Release Center has managed the English version. But, it announced some 4 years ago, that due to the financial situation, it cannot provide this work for international use anymore, but will restrict to keep the database for Denmark. Without the continuation of this work, the NPU system may be endangered in the future. The work consists of daily new definitions, which must be skillfully entered in the database, answering phone calls and giving advice to appliers. At present neither NPU nor IFCC see a way to give the required financial support. This is now a question of survival for the subcommittee. Complicated constructions between scientific institutions and countries are ongoing to find a solution, where different partners participate in financing the system. It is acknowledged by the partners that IUPAC will make its contribution in form of the usual projects structure.

Ongoing projects:

A second ongoing work is the 2006-008-1-700 “Mapping of IFCC-IUPAC laboratory coding system to SNOMED CT (SNOMED CT - Systematized Nomenclature of Medicine Clinical Terms)” and the 2009-005-1-700 project: “Demonstration of NPU-SNOMED CT mapping/harmonization of terms used in clinical laboratory sciences.” The International Health Terminology Standards Development Organization (IHTSDO) wants to integrate NPU and Logical Observation Identifier Names and Codes (LOINC), into the SNOMED-CT coding system. LOINC, which equips many machines with its nomenclature, is already to a great extent integrated, but there seems to be a delay with NPU.

Taken all together, due to the ever expanding flood of data and the restricted resources of NPU, there is a danger that this very well founded system, which integrates chemical terminology into medical practice, will not be adequately continued in the future.

2010-035-3-700 “Establishing definitions for non-referenced terms in the NPU terminology”. The project has just started. There are about 3000 terms. The work consists in searching authorized sources, giving sound definitions for these terms, and including the source references in the NPU terminology.
2004-023-1-700 “Internationally agreed terminology for observations in scientific communication” is close to being finished. The subcommittee has worked much on this topic because it was asked to write an article about the work in the IFCC Journal: Clinical Chemistry and Laboratory Medicine (CCLM). The work was just published in November 2010 under the title “An outline for a vocabulary of nominal properties and examinations - basic and general concepts and associated terms” (Nordin G, Dybkaer R, Forsum U, Fuentes-Arderiu X, Schadow G, Pontet F.; Clin Chem Lab Med. 2010 Nov;48(11):1553-66), as a milestone of the project (http://www.ncbi.nlm.nih.gov/pubmed/21062227).

Now it will also be submitted to PAC and to CCLM for mirror publications to become an IFCC-IUPAC-recommendation. Since the budget is empty this upcoming work will be done by mail. The Joint Committee for Guides in Metrology Working Group 2 (JCGM-WG2), working with VIM4 (Vocabulary of Basic and General Terms in Metrology), raised the question to include the new terminology in VIM4, which is to be issued in about 10 years from now. The intention is to incorporate VIM and the so-called VIN (Vocabulaire International pour les Propriétés Nominales), along with their superordinates in a single document. IFCC has agreed.

2007-033-3-700: “Revision of the Silver Book” Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences”. This project is quite advanced and should be finished by the end of 2011. There will be a new heading “Nominal properties” and there will be more practical examples in all chapters, while theoretical parts will be shortened. The place of the NPU terminology regarding other coding systems will be mentioned through a short paragraph made of several examples driven from other systems.

2006-012-1-700 “Securing and structural updating of information in the NPU coding system and its environment”. The text is available for users in Danish, has been translated into English and is about ready to be submitted to PAC and CCLM. The publication will be part of the series on NPU terminology in PAC and CCLM, and will be part No XXIII, a recommendation. It will soon be ready for submission.

2006-048-2-700: “Recent advances in Nomenclature, Properties and Units”. Money is almost used up.

2001-070-1-700: “Properties and units for urinary calculi”. The manuscript is almost finished, but has to be updated. The project will probably be finished soon.

2001-067-1-700 “Properties and units for function examinations”. The former chairman and members left the project. The budget is used up. So the project will be abandoned and F. Pontet will inform F. Meyers accordingly. There was a discussion about finding more support for NPU because of its importance. The advantages of the NPU system, with its unique features and advantages over related systems, were discussed.
Annex 3 - Details from TRA

The subcommittee is in an interphase, where various projects are either completed or have not yet been initiated:

2004-045-1-700 “Training of school children on pesticides and health” which is part of Toxiclaro “Toxicology in the classroom”, with W. Temple as chair, is a remarkably successful project in Asia. A prototype for animation has been produced in Universiti Sains, Malaysia. The program is now available as CD and accessible via the internet (http://www.prn.usm.my/toxicology_2010/). W. Temple is presently organizing a follow-up project as part of IYC activity, seeking funding from various institutions, including IUPAC, WHO, UNEP, Universiti Sains Malaysia, University of Otago New Zealand, and ISDE/AAMMA. Testing of the current product is underway, and initiatives for translation to platforms for other developing countries are underway.

2006-020-1-700 “Explanatory Dictionary of Terms used in Toxicology” has been published. The book “Concepts in Toxicology” is based on this material and has recently been published by the Royal Society. It has received considerable attention and has been favourably reviewed in several publications.

2007-053-1-700: “Glossary of terms in Immunotoxicology”. It required about 3 years to produce the final manuscript that is now under external review to become an IUPAC recommendation.

2009-034-2-700 “Risk Assessment of Effects of Cadmium on Human Health” (G. Nordberg) has just begun as on late 2010.

2010-051-1-700 “Advances in Immunochemistry and Applications to Human Health” (Michael Schwenck) - funding has just been announced.
Annex 4 – DVII Membership

Membership 2011

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10 TM, 6 AM, 10 NR

AM = Associate Member
NR = National Representative
TM = Titular Member
Annex 5 – Current DVII Projects

1999-047-1-700 Immunochemistry of Metal Sensitization (Doug Templeton)

2000-009-1-700 Glossary of Drug Metabolism Terms (Paul Erhardt)

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

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

2001-049-2-700 Glossary of Terms in Pharmaceutical Technology (Eli Breuer)

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

2001-067-1-700 Properties and Units for Function Examinations (Antonin Jabor)

2001-070-1-700 Properties and Units for Urinary Calculi (Antonin Jabor)

2002-001-1-700 Compendium of Glossaries (Robin Ganellin)

2003-044-1-700 Glossary of Combinatorial Chemistry Terms (A. Ganesan)

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

2004-023-1-700 Internationally Agreed Terminology for Observations in Scientific Communication (Françoise Pontet)

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

2004-045-1-711 Training of School Children on Pesticides and Health - "Toxiclaro" (Wayne Temple)

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

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

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

2005-050-1-700 Prototype Analysis of Molecular Biomarkers in Cancer (Michael Liebman)

2006-008-1-700 Mapping of IFCC-IUPAC Laboratory Coding System to SNOMED CT (Ulla Magdal)
2006-012-1-700  Securing and Structural Updating of Information in the NPU Coding System and its Environment (Ulla Magdal)

2006-020-1-700  Explanatory Dictionary of Terms in Toxicology - Part 2 (Monica Nordberg)

2006-048-1-700  Recent Advances in Nomenclature, Properties and Units : strategy for promoting SC-NPU achievements (Françoise Pontet)

2007-033-3-700  Revision of the "Silver Book" : Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences (Georges Férard)

2007-053-1-700  Glossary of Terms Used In Immunotoxicology (Doug Templeton)

2008-010-1-700  Glossary of Terms in Medicinal Chemistry Updated (Derek Buckle)

2008-013-1-700  Analogue-Based Drug Discovery (Janos Fisher)

2008-033-3-700  Silver Book (Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences) revision (Joint project with IFCC) (Françoise Pontet, Georges Férard)

2009-005-1-700  Demonstration of NPU – SNOMED CT mapping/harmonization of terms used in Clinical Laboratory Sciences (Urban Forsum)

2009-033-1-700  A Survey of Research into New Drugs for Neglected Diseases in Latin America (Antonio Monge)

2009-034-2-700  Risk Assessment of Effects of Cadmium on Human Health (Gunnar Nordberg)

2010-035-3-700  Establishing definitions for non-referenced terms in the NPU terminology (Helle Møller Johannessen)

2010-057-3-700  Update of Glossary Terms used in Computational Drug Design (Yvonne Martin)

2010-051-1-700  Advances in Immunochemistry and Applications to Human Health (Michael Schwenck)

2011-002-1-700  Extension of Revision of the Silver Book (Georges Férard)