

Report to IUPAC Bureau, April 2012

IUPAC Division VII (Chemistry and Human Health)

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Part I - Summary of Division Activities

This report presents an update of activities in Division VII (DVII) since the last Bureau meeting in Warsaw (April, 2011). The Division has met once in the interim, during the General Assembly in Puerto Rico (Aug. 2011). Here I address DVII business in the past year highlight initiatives being targeted in the new Biennium. This report presents Division initiatives and structure, membership, budget, projects, highlights of Subcommittee activities, adherence to IUPAC goals, and current and future initiatives.

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 Discovery* (MCDD); *Nomenclature for Properties and Units* (NPU) (formerly *Nomenclature, Properties and Units in Laboratory Medicine*); 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 presented in Part III of this report.

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 by the President-elect. Doug Templeton completed his term as DP Dec. 31, 2011, and Françoise Pontet, became President. However, as she has been unable to assume duties for personal reasons, Templeton is serving as Acting DP until June 30, 2012, at which time Pontet is expected to begin.

2. Operating procedures and rules of DVII

DVII earlier filed rules and operating procedures with the Secretariat, which have now been in effect for the past Biennium. 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. We regret to report the death of Emeritus Fellow Prof. F. William Sunderman in April 2011. Bill was a founding member of the IUPAC Division of Clinical Chemistry in 1972 served as Division President from 1981-1985. Prof. Rita Cornelis, formerly Chair of the IUPAC Commission on Toxicology, was appointed a Fellow at the time of the IYC closing ceremony in Brussels, Dec. 2011.

The operating procedures have also helped clarify to our membership and Division Executive, streamlined procedures for reviewing Project Applications, Technical Reports, and Recommendations. We have a process in place for removing

inactive TM's, e.g., those who do not attend Division meetings or answer correspondence requesting reviews, or submit Projects. We have exercised this prerogative twice (most recently after the Puerto Rico GA) and replaced their TM slots by promotion of AM's who are active and placed well in the previous TM elections.

3. Membership

We have had a significant rejuvenation of the Division Committee, notably with three new TMs and two new AMs beginning terms in Jan. 2012, each of whom is either serving on one or more Task Groups or preparing a project proposal. Our current membership (2012) is reported in the Annex. It represents diversity of gender, geography, and expertise with respect to our technical SCs.

4. Budget

We completed 2011 on budget (actually \$20 over) for the Biennium. Four new projects were approved in 2011, and one so far in 2012.

5. Projects

Together the three technical SCs are currently involved in 26 ongoing projects (see Part IV). These, together with projects submitted or under discussion, are described in the individual SC reports. A classification of our current projects shows the following balance (number of projects in parentheses):

Terms and Glossaries (8)
Data Bases (4)
Drug Discovery (5)
Clinical Chemistry (6)
Toxicology and Health (3)

Ten projects were completed in the 2010/2011 Biennium.

6. Highlights of the Technical SCs' activities (See Part III for detailed 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 was to make videotapes of lectures in lay terminology available to the public on-line. 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 ready for publication in 2012. Meetings in Rhajkot 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. Françoise 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 website is now in use and projects are planned to address monitoring of effectiveness, expansion, and translations from the English. 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.

Part II - Meeting IUPAC's Goals

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 (2012), 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. We are working closely with IFCC towards joint management of the NPU database. 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. Volume III of the successful series “Analog-based Drug Design”, requested by the publisher, is due out this year. The involvement of our SC-NPU 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.

2. Provision of tools

As noted above, about a dozen glossaries of terminology have recently been published or are currently under construction, including the recent glossaries in Biomolecular Screening (PAC 2011), Immunotoxicology (PAC, In Press), Medicinal Chemistry (under review), and revision of terms in clinical chemistry, and terms in computational drug design, which are underway.

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 series “Analogue-based Drug Discovery” are examples of current projects with immediate value to the chemical industry.

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).

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), the latter published in a trilingual (English/Spanish/Portuguese) edition. 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) and has won the 2012 SOT's Education Award.

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" was posted on the Web as part of our IYC activity. It is available at <http://vimeo.com/19567220>. The 2012 Prize is under adjudication.

Part III - Detailed Subcommittee Summaries

1. Medicinal Chemistry and Drug Discovery (MCDD)

Meetings and membership

The Subcommittee has continued to meet biannually alongside suitable ACS meetings, or International Symposia on Medicinal Chemistry (ISMC) in Europe. Thus, meetings were held in Brussels (September 2010, ISMC, 12 attendees), Anaheim (March 2011, ACS National Meeting, 8 attendees), and Puerto Rico (July 2011, IUPAC General Assembly, 9 attendees). These meetings are important for group discussions in developing ideas for the various projects. The Minutes of meetings are posted on the IUPAC web site. Funding to attend the Subcommittee meetings remains an ongoing issue. Meetings held at ACS National Meetings have been useful because the ACS picks up much of the expense of room reservations.

R. Ganellin has signalled that, after being in the Chair for more than a decade, (since 2000, initially as President of the Medicinal Chemistry Section) it is time to seek a

replacement. Also, since J. Proudfoot has resigned as Secretary, a new Honorary Secretary is required. To facilitate replacements, Ganellin has written job descriptions for the two positions which have been circulated to the Subcommittee members.

IUPAC-Richter Prize in Medicinal Chemistry

The prize is awarded biennially in even years. The 2010 Prize recipient was Prof. Arun K. Ghosh (Purdue University, USA) from a list of 10 outstanding candidates, for his structure-based design of novel HIV protease and β -secretase inhibitors, and for the drug, Darunavir. IUPAC was given very good publicity among medicinal chemists by his lectures at the ACS 32nd National Medicinal Chemistry meeting in Minneapolis and the 21st ISMC meeting in Brussels. Nominations have been received for the 2012 Prize, and a selection committee is evaluating the candidates. The winner will deliver his award address at the ACS National Medicinal Chemistry Symposium to be held in Tucson, Arizona, May 2012.

Emeritus Fellows

A plaque was presented to Camille Wermuth at the Brussels ISMC meeting in front of 1000 medicinal chemists (September 2010). John Topliss and Les Mitscher received their plaques in August 2011 during the ACS Division of Medicinal Chemistry Hall of Fame reception in Denver, Colorado. This gives IUPAC and the Emeritus Fellows very good publicity.

IYC 2011

As a contribution to the International Year of Chemistry we asked the three past IUPAC-Richter-Prize winners to provide a video suitable for non-expert audiences. Arun Ghosh (2010 Prize) provided a video of a discussion with some students (<http://vimeo.com/19567220>). Jan Heeres (2008 Prize) submitted a series of slides relating to the many discoveries of Paul Janssen but, unfortunately, it is not yet up to web standard. Malcolm Stevens (2006 Prize) did not reply.

IUPAC World Chemistry Congress (Puerto Rico, 2011)

The Subcommittee provided 5-7 speakers for the Division's one day conference at this meeting, under the umbrella title of "Chemistry of Life".

Selected Project updates

- As part of project 2001-048-2-700, Research and Training in Medicinal Chemistry in the Indian Sub-continent (Mukund Chorghade), a five-day Medicinal Chemistry Workshop was held in New Delhi during January 2010. Two Medicinal Chemistry workshops were held in February in Rajkot and Nagpur (India); five SC members lectured and IUPAC President Nicole Moreau attended.

- Practical Studies for Medicinal Chemistry Students, 2004-028-1-700 (Antonio Monge) produced an e-book (Eds. C.R. Ganellin and A. Monge) which is on the IUPAC home page and has had 83,000 successful hits during the first 6 months. All of the described experiments had been accessed. A printed version (539 pages) in Spanish/Portuguese/English languages, generated directly from the web version was produced in April 2011 by Dr. Rosa Cattana, Universidad Nacional de Rio Cuarto, Cordoba, Argentina. A copy was sent to the IUPAC Secretariat for their archives.
- A Survey of Research into New Drugs for Neglected Diseases in Latin America , 2009-033-1-700 (Antonio Monge) has established a network of 42 researchers from 30 institutions in 10 different Latin American countries, which identifies people, diseases and universities in which they are working. The next stage was to identify their facilities and what they are doing. A draft publication has been prepared for submission to scientific journals throughout the region. The ACS Division of Computational Chemistry has proposed holding a workshop on the subject, and is interested in a collaboration with IUPAC.
- The third volume in the successful series, Analogue-based Drug Discovery (Project 2011-011-1-700) is well underway with a projected publication in 2012. The book has 20 chapters and 53 authors.
- The Glossary of Terms in Medicinal Chemistry (2008-010-1-700) has been completed and is being sent to outside reviewers. It will be published in Pure and Applied Chemistry and in Annual Reports in Medicinal Chemistry.

2. Nomenclature for Properties and Units (NPU)

Meetings

The SC met in Berlin, Germany, May 2011 and Paris, France, November 2011.

Project updates

Ongoing projects in 2011 include:

- Mapping of the IFCC-IUPAC laboratory coding system to SNOMED CT (IUPAC 2006-008-1-700) Chair: Ulla Magdal, Work on this has been suspended due to lack of resources and ongoing negotiations with SNOMED CT. When the present draft model for SNOMED CT Observable Entities is finalized, the project will have to be reevaluated, as the SNOMED CT model will be more complex than the one first planned for. The mapping will demand more resources than originally assumed, and the functionality that was implemented in the LabTerm database in 2008 will not suffice.
- Establishing definitions for non-referenced terms in the NPU terminology (IUPAC 2010-035-3-700) Chair: Helle Johannessen. Most of the basic terms and concepts

of the NPU terminology are defined by references to other terminologies, but about 3000 basic concepts have no formal reference or definition. The project aims at creating formal definitions for the undefined concepts. This will support managers of the terminology in precise and consistent use of these concepts, and will be an aid in translation of the terminology into other languages.

- International vocabulary for nominal examinations in scientific communication. (2008-019-1-700) Chair: Françoise Pontet. Milestones were presented as a document published in the IFCC journal (CCLM) and as a poster at the IFCC joint World and European Congress. A final manuscript for an IFCC-IUPAC recommendation was to be submitted by 30 June 2011.
- Silver Book (Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences) revision (joint IUPAC 2008-033-3-700 + IFCC CPD project) Co-Chairs: Françoise Pontet, Georges Férard. An extension of the deadline and budget were accepted by IUPAC and IFCC, including support for a new chapter on nominal properties and providing a summary leaflet.
- Recent advances in Nomenclature, Properties and Units: strategy for promoting SC-NPU achievements (IUPAC 2006-048-1-700) Chair: Françoise Pontet. Several communications are listed above and a folder for wide distribution has been issued.
- Translation of the NPU coding system into French (F. Pontet). A second version is intended to be posted on the SFBC (French Society of Clinical Biology) website as an Excel format, with instructions for use in French.
- Securing and structural updating of information in the NPU coding system and its environment (IUPAC 2006-012-1-700) Chair: Ulla Magdal. Part XXIII “The NPU terminology, principles, and implementation – a user’s guide” of the series “Properties and units in the clinical laboratory sciences” was accepted for publication by PAC and CCLM. (Published January 2012, which finalized the project.)
- The NPU terminology in its English version is published on the website: <http://www.sst.dk/EnglishNPU>. Searchable publication of basic NPU data is under development for the new IFCC website.
- HbA1c: Continuous education for health professionals is ongoing.

Invited lectures

A number of invited lectures at international meetings, e-publications, and articles have been presented by members.

These include:

- Pontet F. Health informatics: the NPU coding system. Indian Society of Chemists and Biologists 15th International Conference on “Bridging gaps in discovery and

- development: Chemical & Biological Sciences for affordable health, wellness & sustainability“(ISCB 2011). Rajkot, India, 4-7 Feb. 2011 (invited lecture).
- Pontet F. The NPU coding system: a recommended terminology. International Conference on Chemistry for Mankind: innovative ideas in life (ICCM-2011). Nagpur, India, 09-11 Feb. 2011 (invited plenary lecture).
 - Pontet F, Nordin G, Dybkaer R, Forsum U, Fuentes-Arderiu X, on behalf of the IFCC-IUPAC Joint Committee-Subcommittee on Nomenclature for Properties and Units (C-SC-NPU). What are nominal properties and examinations? IFCC--WorldLab--EuroMedLab Berlin.15-19 May 2011 (poster)
 - Candás Estébanez B, Valero Politi J, Fuentes Arderiu X. Nomenclatura y unidades de las propiedades biológicas. Rincón Iberoamericano; 2011. <http://www.ifcc.org/newRia/pdf/books/Nomenclatura-y-unidades-de-las-propiedades-biologicas.pdf> [Spanish]
 - Candás Estébanez B, Valero Politi J, Huguet Ballester J, Fuentes Arderiu X. Nomenclatura i unitats de les propietats biològiques. *In vitro veritas* 2011; 12:15-78. <http://www.acclc.cat/continguts/ivv125.pdf> [Catalan]
 - Fuentes-Arderiu X. Measuring with zero measurement uncertainty a primitive quantity. *Accred Qual Assur* 2011;16:103.
 - Fuentes-Arderiu X. Scalar and ordinal quantities. *Accred Qual Assur* 2011;16:273.
 - Fuentes-Arderiu X. About measuring systems and measurement procedures. *Accred Qual Assur* 2011;16:329.
 - Fuentes-Arderiu X, Porras-Caicedo A. About ‘measurement result’ and ‘measured value’. *Accred Qual Assur* 2011;16:387-8.
 - Sánchez-Álvarez J, Cano-Corres R, Fuentes-Arderiu X. Heteroscedasticity and homoscedasticity, and precision profiles in clinical laboratory sciences. *Clin Chim Acta* 2011;412:2351-2.
 - Fuentes-Arderiu X, Miró Balagué J. Naturalesa de les propietats biològiques examinades al laboratori clínic. *In vitro veritas* 2011;12:150-9. <http://www.acclc.cat/continguts/ivv135.pdf> [Catalan]
 - Fuentes-Arderiu X. Taxonality: a useful neologism. *eJIFCC* 2011;22: <http://www.ifcc.org>.
 - Fuentes Arderiu X. Propiedades biológicas en las ciencias de laboratorio clínico: una aproximación ontológica. *NOTICONAQUIC* 2011;56:9-16. [Spanish]
 - Férard, G., Férard, J.F., 2012. Quality Assurance in ecotoxicology: the why’s and how’s, in: Férard, J.F., Blaise, C. (Eds.), *Encyclopedia of Aquatic Ecotoxicology*, Springer, Dordrecht (in press).

Ownership of the NPU database

A draft agreement that addresses ownership, intellectual property rights and future maintenance and development of the NPU terminology and NPU database, is under discussion with IUPAC, IFCC, C-SC-NPU and Danish Board of Health.

Links with VIM

A large part of the work in the clinical laboratories consists in providing examination results for the properties of persons, and the relevant special language in this field must build on the general language of metrology. It is therefore useful that scientists from the IFCC/IUPAC C-SC NPU are sitting on the WG 2, VIM, of the Joint Committee for Guides in Metrology, charged with explaining and updating the third edition 2012 of the International vocabulary of metrology - Basic and general concepts and associated terms (VIM). IFCC was formerly represented by Francoise Pontet (IUPAC DVII TM) and now Xavier Fuentes-Arderiu (IUPAC DVII AM), and IUPAC by René Dybkaer.

These links should continue to ensure that this fundamental vocabulary is being properly utilized in the NPU work, and also that the special needs of the clinical laboratory sciences will be considered in the development of the 4th edition of the VIM.

3. Toxicology and Risk Assessment (TRA)

Project 2004-045-1-700, "Training of school children on pesticides and health" which is part of the larger project, Toxiclaro "Toxicology in the classroom", with Wayne Temple as chair, has reached its final stage (see Chem. Int., Vol. 31 No. 6, November-December 2009). An interactive website for schoolchildren with animations based on the original text 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/). The website works best with MS Windows but can be viewed with Apple Macintosh computers with occasional problems which may be browser related. Wayne 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 product is continuing, and there are initiatives for translation to platforms for other developing countries. This project has been managed by a task group of professionals from the World Health Organization (WHO), UNEP Chemicals, IUPAC, and the National Poison Centre of Malaysia.

Several projects have been completed or are nearing completion. In particular, the Glossary of Terms Used in Immunotoxicology has received its final editing following the "Pure and Applied Chemistry" refereeing process and has been published online (February 16, 2012) as an ASAP article before formal publication in "Pure and Applied Chemistry" as an IUPAC Recommendation.

Groundwork has been done for two new projects. The first, which has now been approved for IUPAC funding is being led by Dr Jane Huggins and has the objective of converting key concepts from the IUPAC-sponsored book "Concepts in Toxicology" into web-based self-teaching presentations using Adobe Captivate software which is designed to encourage learning by the use of questions with associated feedback.

The second is a logical continuation of the development glossaries of terms used in toxicology. The existing glossaries need to be integrated into one database and gaps identified relating to reproductive toxicology and neurotoxicology must be addressed. An application for IUPAC support of this as an IUPAC Project is being prepared.

Gunnar Nordberg is preparing a request for extension of the IUPAC Cd Risk Assessment project. It seems there will be only limited interaction with the SCTM/PHIME group which is preparing a rather short report to be submitted to a non-PAC journal. Gunnar will contact Alfred Bernard to make sure that he would remain in IUPAC group.

A characteristic of toxicology is that there is overlap with most other scientific disciplines. Thus, there is scope for projects at the interfaces and collaboration is an essential part of such projects. Participation in the Biomonitoring Equivalents Workshop in 2008 established contacts with the US Environmental Protection Agency, Health Canada, and the American Petroleum Institute, among others. These links have been maintained and could lead to further developments. The Chair of TRA and the Division President met with Professor 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. It was identified that there were mutual interests in education in toxicology and possible involvement in an international conference were discussed. Since TRA Chair, John Duffus, is a member of CCE and participates in the U.S. Society of Toxicology (SOT) initiative for on-line chemical toxicology curricula (ToxNet), it may be possible to build further on this connection. In addition, there is a continuing effort in collaboration with COCI to establish a working relationship with SAICM (Strategic Action in International Chemical Management) managed by UNEP Chemicals in collaboration with WHO and the International Programme on Chemical Safety.

4. Public Relations and Elections (PRE)

The election of new titular members of the Chemistry and Human Health Division began in 2010 with the selection of a Nominating Committee comprised of Thomas Perun, (Chair), Derek Buckle, John Duffus, Xavier Fuentes-Arderiu, and Birger Heinzow. Five candidates were chosen to represent a diversity of disciplines and geographic locations. All of the candidates had contributed to IUPAC projects or had expressed interest in participating in IUPAC activities. Three new TMs were elected to take office in the 2012-2013 term. The terms for TMs have been changed from four years to two years, so all current and new TMs will end their terms in 2013. Those with years of eligibility remaining will have the possibility of being re-elected. Following the

election, a vacancy occurred among TMs and was replaced by one of the original candidates based on the number of votes.

The current summary of Division VII activities has been updated, and has been used by Division members in talks given to other organizations. A poster depicting the organizational structure of the Division, its major accomplishments, and current projects has been prepared and was exhibited in Puerto Rico. The poster has also been exhibited at the ACS National Meeting 2011 in Denver, and at the AIMECS 2011 meeting in Tokyo. A talk about the Division and activities of its subcommittees was also presented as part of a symposium on “Chemistry of Life” at the World Chemistry Congress in Puerto Rico.

Part IV - Projects and Publications

1. List of current projects

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

2001-049-2-700 Glossary of terms used in process chemistry/manufacturing of active pharmaceutical ingredients, and pharmaceuticals (Mukund Chorghade)

2001-070-1-700 Properties and Units for Urinary Calculi (Gunnar Nordin)

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

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

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

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)

2008-033-3-700 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)

2011-011-1-700 Analogue-based Drug Discovery - Vol. III (Janos Fisher)

2011-018-1-700 Human Drug Metabolism Database (Paul Erhardt)

2011-032-1-700 ‘Concepts in Toxicology’ Instructional Materials (Jane Huggins)

2. Projects completed in the current Biennium

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

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)
- 2004-019-3-700 Glossary of Terms for Biomolecular Screening (John Proudfoot)
- 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)
- 2008-013-1-700 Analogue-Based Drug Discovery (Janos Fisher)

3. Publications 2010-2012 (partial)

Monge, A., Traditional foods as a source of functional foods, *Cyta*, 8: 159-167 (2010).

Nordin G., Dybkaer R., Forsum U., Fuentes-Arderiu X., Schadow G. & Pontet F., on behalf of the IFCC-IUPAC Committee on Nomenclature, Properties and Units (C-NPU). An outline for a vocabulary of nominal properties and examinations – basic and general concepts and associated terms. *Clin. Chem. Lab. Med.* 48: 1553-66 (2010).

Dybkaer R. ISO terminological analysis of the VIM3 concepts 'quantity' and 'kind-of-quantity'. *Metrologia* 47:127-34 (2010).

Fuentes-Arderiu X. Remembering the "Stockholm consensus". *Accred. Qual. Assur.* 15: 581-584 (2010).

Nordberg, M., Duffus, J.H. & Templeton, D.M., Explanatory dictionary of key terms in toxicology: Part II, *Pure Appl. Chem.* 82: 679-751 (2010).

Proudfoot, J. et al., Glossary of Terms Used in Biomolecular Screening. *Pure Appl. Chem.* 83: 1129-1158 (2011).

Fischer, J. & Ganellin, C.R. (Eds.) *Analogue-based Drug Discovery*, Vol II, Wiley-VCH, 2011. 560 pp.

Templeton, D.M., Schwenk, M., Klein, R. & Duffus, J.H., Glossary of Terms Used in Immunotoxicology, *Pure Appl. Chem.* (In Press 2012; <http://dx.doi.org/10.1351/PAC-REC-11-06-03>).

Annex - Current membership of the Division (2011)

Name	Status	Term	NAO
Dr. Françoise Pontet	TM-President	2012-2013	France
Prof. Michael Schwenk	TM-Secretary	2010-2013	Germany
Prof. Douglas M. Templeton	TM-Past President (Acting President 2012)	2012-2013	Canada
Prof. Sergey O. Bachurin	TM	2010-2013	Russia
Dr. Derek R. Buckle	TM	2010-2013	United Kingdom
Dr. János Fischer	TM	2012-2013	Hungary
Dr. Christopher Hill	TM	2012-2013	United Kingdom
Dr. Paul A. Illing	TM	2010-2013	United Kingdom
Dr. Yvonne C. Martin	TM	2010-2013	USA
Prof. Wayne Temple	TM	2012-2013	New Zealand
Dr. Xavier Fuentes-Arderiu	AM	2012-2013	Spain
Dr. Mirja Kiilunen	AM	2010-2013	Finland
Dr. Serge Mignani	AM	2012-2013	France
Dr. Helle Møller Johannessen	AM	2012-2013	Denmark
Prof. Monica Nordberg	AM	2010-2013	Sweden
Dr. Aimin Wang	AM	2012-2013	USA
Dr. Sulejman Alihodžić	NR	2012-2013	Norway
Prof. Eliezer Jesus Barreiro	NR	2012-2013	Brazil
Prof. Pavlina Dolashka	NR	2012-2013	Bulgaria
Dr. Matityahu Fridkin	NR	2012-2013	Israel
Prof. Rob Leurs	NR	2012-2013	Netherlands
Prof. Nilufar Nahar	NR	2012-2013	Bangladesh
Dr. Shahnaz Perveen	NR	2012-2013	Pakistan
Dr. Poonsakdi Ploypradith	NR	2012-2013	Thailand
Prof. Anjali M. Rahatgaonkar	NR	2012-2013	India
Prof. Mei Xiang Wang	NR	2012-2013	China/Beijung
	10 TM, 6 AM, 10 NR		

AM = Associate Member
 NR = National Representative
 TM = Titular Member