

Report to Bureau/Council 2015

Chemistry and Human Health Division

I. Executive Summary

Division VII is composed of three different subcommittees, each with their own goals and objectives, accomplished through their project activities.

The **Drug Discovery and Development (DDD)** subcommittee is focused on providing information and tools that can be utilized by medicinal chemists in their research activities directed toward new disease treatments. The project outputs have been directed toward reference books for drug discovery, glossaries of terms used by medicinal chemists, and short courses on medicinal chemistry in venues outside the US and Europe.

The **Toxicology and Risk Assessment (TRA)** subcommittee has projects that are concerned with the possible risk of chemical agents on human health. To help in the understanding of these risks, it has produced glossaries of terms, explanatory dictionaries, and books on concepts in toxicology. As medical practice expands beyond the use of small organic molecules in the treatment of diseases, the subcommittee has produced papers describing immunochemistry and nanomaterials in human health applications. A project supported by WHO has produced learning material for teaching young schoolchildren about hazardous chemicals used in agricultural-based countries.

The mission of the subcommittee **Nomenclature for Properties and Units (NPU)** is to ensure that in clinical chemistry and laboratory medicine, there is a common understanding of what is being measured in a biological system, and how the results will be expressed. In collaboration with the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC), it is developing a terminology for properties and units in clinical laboratories of a number of countries, particularly in Scandinavia. Future goals are to harmonize the NPU terminology with that of other clinical chemistry organizations throughout the world.

II. Project Activities

Drug Discovery and Development

Successful projects conducted this past year have continued to provide courses on medicinal chemistry to universities in countries around the world.

Project 2014-022-1-700. Highlights in Medicinal Chemistry. In January 26-30, 2015, a weeklong course was conducted at the University of Rio de Janeiro in Brazil. This was part of a summer school program for post-graduate students conducted by Prof. Eliezer Barreiro and organized by Janos Fischer. The course was funded by a joint program between IUPAC and ACS Medicinal Chemistry Division, and utilized speakers from both organizations.

Project 2014-011-2-700. Medicinal Chemistry, India. In February 9-13, 2015, a weeklong course was conducted at Sri Ramachandra University in Chennai, India. The course was a joint project with the ACS Medicinal Chemistry Division, and received partial funding from the Indian local government. Attendees were from both academia and industry, and speakers included local faculty along with those from universities and pharmaceutical companies in the US. This was the second course conducted in Chennai, and plans are to move the next one to another location.

Project 2013-016-1-700. Following the successful series of books on Analog-based Drug Discovery, a new series was initiated on Successful Drug Discovery. The first volume was published in March, 2015 by Wiley, and included 25 authors from Germany, Hungary, Japan, UK and USA. A second volume is already in the planning stage.

Project 2014-019-1-700. Emerging Problem of Novel Psychoactive Substances. A new project was initiated to critically review the current status of novel psychoactive substances which are appearing on the illicit drug market. The hope is that the results will provide useful information to scientific, social and governmental bodies in dealing with the growing problem.

Project 2010-057-3-700. This project, which is an updated Glossary of Terms used in Computational Drug Design, has been completed and is in the final stage of editing before publication in PAC and other journals.

The 2014 IUPAC Richter Prize was awarded to Helmut Buschmann of Germany at the EFMC International Symposium for Medicinal Chemistry in Lisbon, Portugal, August 2014. He was recognized for his work that discovered and developed the novel analgesic drug, tapentadol.

At the same meeting, Robin Ganellin was presented a plaque for being named an Emeritus Fellow for his over 20 years of service to the Division. Besides being a participant on many projects, he was the first Chair of the Medicinal Chemistry and Drug Development subcommittee for over ten years.

Toxicology and Risk Assessment

Project 2010-51-1-700. This project on Advances in Immunochemistry and Application in Human Health led to a series of papers on the structural aspects and molecular recognition of the immune system, and the diagnostic and therapeutic applications of antibodies. These papers were published recently in an entire volume of Pure and Applied Chemistry, 2014, Volume 86, Issue 10.

Project 2013-001-2-700. This project involved developing a Glossary of Terms used in Neurotoxicology and Reproductive /Developmental Toxicology. It was subsequently divided into two glossaries, and the one for neurotoxicology is complete and will be published in a future issue of PAC. The second glossary, (Project 2014-041-1-700) focusing on reproductive/developmental toxicology is in final stages of development.

Project 2013-007-1-700. Recent Advances in Nanoparticles and Colloidal Systems and their Impact on Human Health. This is a joint project with Division V to develop a document critically discussing colloidal and nanoparticle systems used for human health applications, such as drug delivery, in vivo imaging, food technology and cosmetics. The manuscript is planned for publication in PAC later in 2015.

Project 2014-013-1-700. Nanomaterials and Human Health: The Trends and Future. This was a two day workshop in September 15-16, 2014 held at the University of Kent in the UK to discuss nanotechnology methods and concepts based on polymers, lipids, conjugates, etc. as delivery systems for human health applications. It was attended by participants from nine countries in Europe. The workshop provided financial support and an opportunity for young scientists to show their contributions in the field.

The previously successful project, Toxicology in the Classroom (Toxiclaro) is a multimedia resource to help teachers educate their students about the dangers of pesticides on human health in agriculture-based countries. It is available in a CD format, and a printed version to assist teaching in schools where access to computers and audio-visual equipment is limited. A description of this project appeared in Chemistry International, Volume 36, No. 5 18-19 (2014). A follow-up project, 2013-023-1-700, has begun, which will expand the student's understanding of chemical risks to human health and the environment.

In 2014, the Emeritus Fellow award was bestowed on Doug Templeton for his 25 years of contributions to IUPAC , including projects, technical reports and recommendations. He was President of Division VII, 2008-2011.

Nomenclature for Properties and Units

A major step was taken early in 2014 when an agreement was reached between IUPAC, IFCC and the Danish National eHealth Authority, the three organizations that have been collaborating on the development of terminology used in clinical chemistry and laboratory medicine. A Steering Committee was established with representatives from IUPAC, IFCC and the DeHA, in order to manage the governance, operation, development and promotion of the NPU terminology. With this agreement and Steering Committee in place, future projects can work toward the widespread adoption and application of the NPU, and to align it with other international healthcare terminology. It is currently being used in Denmark, Sweden and Norway.

Project 2009-005-1-700. Demonstration of NPU-SNOMED CT Mapping/Harmonization of Terms Used in Clinical Laboratory Sciences. This was a pilot project to demonstrate the feasibility of harmonizing the NPU terminology with the internationally owned and developed clinical reference terminology, SNOMED CT. It was started before the Steering Committee was established but showed that harmonization was achievable.

Project 2014-017-1-700. Piloting NPU-SNOMED CT Mapping. This project will continue the harmonization of NPU – SNOMED CT terminologies by selecting a subset of terms to be mapped, and to develop a practical method for meeting quality criteria which can be applied between terminology developers.

Project 2007-033-3-700. Silver Book Revision. This project was undertaken as an update of the Silver Book (Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences). The revision has now been completed, and a new chapter on terminology of nominal properties has been added. The Silver Book 2014 will be published this year as both printed and electronic versions.

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