

Division VII Report to Bureau 2016

I. Highlights and Executive Summary

The projects and activities conducted in Division VII have been overseen by three separate subcommittees: Drug Discovery and Development (DDD) , Toxicology and Risk Assessment (TRA), and Nomenclature for Properties and Units in Clinical Chemistry (NPU). Major thrusts have been to provide documents and recommendations that convey the importance of areas of chemistry that involve global issues that impact human health.

A major multidisciplinary effort has involved a joint project with Division IV on nanotechnology and its applications in medicine and other human usage including food technology and cosmetics. The potential toxicology of these applications will be examined. Two scientific reports will be issued this year, and an article for readers in the general public is in the planning stage.

The emergence of novel psychoactive compounds in the illicit drug market is being examined in another project, which will provide information useful to scientific, societal and governmental organizations involved with the growing problem.

The potential risk of low levels of chemicals in the environment will continue to be a problem as the global population increases. A project addressing the potential risks of the increased levels of cadmium in the ecosystem is near completion.

The importance of IUPAC as a major organization has been given impetus by the worldwide recognition of the IUPAC-Richter Prize as an award for meritorious research in medicinal chemistry leading to important new drug entities. This has been given to five previous winners, all from different countries, and will be continued on a biannual basis for ten more years.

Another important achievement has been the establishment of a steering committee, in concert with the International Federation of Clinical Chemistry,

which will oversee the development and promotion of NPU terminology for clinical chemistry and laboratory medicine throughout the world.

In the area of chemical education, two successful short courses in medicinal chemistry were conducted in 2015, one in Brazil and one in India. Plans are already being made to continue these courses in 2017. A series of books on drug discovery has been published over the last ten years, and the fourth one, "Successful Drug Discovery" was published in 2015. The next one in the series is already being compiled.

A project on advances in immunochemistry 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 were published in single issue of PAC in late 2014.

A number of glossaries were completed during the last biennium. The "Glossary of terms used in Neurotoxicology" was published in PAC and the Glossary of Terms used in Reproductive and Developmental Toxicology" is complete and submitted to PAC. Similarly, the "Glossary of Terms used in Computational Chemistry" has been finished and submitted to PAC.

One of the goals of the Division has been to partner with other IUPAC Divisions and outside organizations in order to share costs and maximize the importance of the outcomes achieved. This has largely been successful as demonstrated in the discussions of activities in the following sections of the report.

Another goal has been to make the outcomes more accessible to the scientific and lay public where appropriate, in order to show how IUPAC activities can affect human health in a general sense. The new IUPAC website should enable members to present such material with the proper controls.

II.

Brand IUPAC in the Minds of Stakeholders

One of the major activities of the DDD subcommittee has been the sponsorship and implementation of the IUPAC-Richter Prize for excellence in medicinal chemistry. This \$10,000 award was funded by the Gedeon Richter company of Budapest for ten years, and five prize winners were selected over this period. The winners came from five different countries showing the diversity of medicinal chemistry. This award has led to an increased recognition of the role of IUPAC in pharmaceutical research and development.

The NPU subcommittee has been working closely with the International Federation of Clinical Chemistry (IFCC) to improve patient safety in medical settings through the harmonization of the terminology used in measuring properties and units in clinical laboratories. In 2014, a major step was achieved by establishing a steering committee with members from IUPAC, IFCC and the Danish National eHealth Authority. The purpose is to manage the governance, operation, development and promotion of the NPU terminology, and to broaden its usage throughout the world. IUPAC has been a major player in this effort.

Emphasize Multidisciplinary Projects Addressing Critical Global Issues

The field of nanotechnology has grown exponentially over the last decade, and the TRA subcommittee has recognized the need to develop and produce documentation describing the use of nanomaterials in human health applications, such as drug delivery, imaging, food technology and cosmetics. This is a joint project with Division IV which will examine the preparative and analytical methods as well as the possible effects on occupational and environmental safety. The outcome will be to produce reports for the scientific community as well as the lay public.

An emerging problem is the increase in usage of novel psychoactive compounds in the illicit drug market. These compounds are chemically related to known drugs but are designed to be undetected by current analytical methods. A project in the DDD subcommittee will critically review the current status with the goal of providing useful information to scientific, societal and governmental bodies dealing with the growing problem.

The DDD subcommittee has produced a number of widely used books describing the discovery of new drug molecules which have found their place in the armamentarium of agents used to treat human diseases. Many of the drugs described have been developed to resolve global health problems such as tuberculosis and hepatitis C. The chapters describe the details of the research involved in the development of these agents to help medicinal chemists throughout the world in their own research.

A project in the TRA subcommittee is addressing the risk assessment of the increased presence of low levels of cadmium in the ecosystem. Cadmium exposure can occur from multiple sources, and has a long half-life in human tissues. A report from the project will focus on health issues related to low level exposure from sources throughout the world.

Support Chemistry Education, Particularly in Developing Countries

Two weeklong courses in medicinal chemistry were given by the DDD subcommittee in 2015, one in Brazil and one in India. Both courses were jointly sponsored and funded by the ACS Division of Medicinal Chemistry. The course in Brazil was conducted at the University of Rio de Janeiro as part of a summer school program for post graduate students with partial funding by the university. The course in India was conducted at Sri Ramachandra University in Chennai, with partial funding by the Indian local government. The success of these courses was demonstrated by requests to conduct similar courses in other locations.

A number of glossaries were completed during this biennium. The Glossary of Terms used in Neurotoxicology was completed by the TRA subcommittee and

published in PAC. It will also be published in the Journal of Neurotoxicology. A companion glossary of Terms Used in Reproductive and Developmental Toxicology is also ready for publication by the TRA subcommittee. A Glossary of Terms used in Computational Chemistry has been completed from the DDD subcommittee, and will be published shortly in PAC.

III.

Brand IUPAC in the Minds of Stakeholders

The IUPAC-Richter Prize has achieved worldwide recognition among medicinal chemists as a top award for meritorious advances in the discovery of new drugs for human diseases. A new contract with the Gedeon Richter Company has been agreed to, which will provide the funding for another ten years. The first prize winner in this new agreement has just been chosen, the chemist who is the inventor of sofosbuvir, the major component of the recently introduced treatment for hepatitis C. A total of 15 candidates were received, all of whom had exceptional qualifications for winning the prize. This was the best group of candidates since the prize was begun, and shows the growing significance of the award.

Now that the NPU Steering Committee has been established, a major goal is to encourage the use of the NPU terminology in other countries beside those in Scandinavia. The newest project is to determine the feasibility of mapping and harmonizing the NPU Clinical Laboratory Sciences terminology with the SNOMED CT terminology used in many other parts of the world. The beginning of this effort is underway, but will require additional major funding to perform full-scale mapping. This support will need to come from IUPAC and IFCC as well as other sources. Partial funding is being sought from the Swedish government.

In 1995, the first issue of the "Silver Book" was published. After 20 years, this Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences will be reissued as the second edition, and will include:

1. Updated recommendations and technical reports.
2. An enlargement of the subject field by several disciplines.
3. A development of concepts for properties that have no quantity dimensions.
4. Explain and illustrate the recommendations by examples.

The book has been completed and is in the final stages of publication this year.

Emphasize Multidisciplinary Projects Addressing Critical Global Issues

The joint project between Division VII and Division IV, “Recent Advances in Nanoparticles and Colloidal Systems and their Impact on Human Health”, has grown in significance, and two documents will be issued. One will be entitled “Nanomaterials and their impact on human health: preparation and analytical characterization.” The second will be “Nanomaterials in body care and medical applications: their impact on human health.” In addition to these documents which should be published in PAC this year, a specially written report for the general public will be submitted to science magazines and newspapers with science sections.

Support Chemistry Education, Particularly in Developing Countries

The success of the previous short courses in medicinal chemistry have provided impetus for continuing these courses in the current biennium. The medicinal chemistry course in India and Southeast Asia is already in the planning stage for 2017. The site will move to Bangalore which is closer to relevant industrial and academic organizations and will increase the accessibility of participants. The course material will also be expanded from the fundamentals of medicinal chemistry to include translational medicine and proof of concept studies in the clinic. With the emergence of biologics in the development of new drugs, this topic will be included in the new material. This again will be a joint course with the ACS Medicinal Chemistry Division, and partial funding will be sought from the government of India, global pharmaceutical companies, and Indian contract research organizations.

IV. Publications

Immunochemical Regulation and Applications. D. Templeton and M. Schwenk, PAC 2014; 86 1433-1434.

Structural Aspects of Molecular Recognition in the Immune System. Part I: Acquired Immunity. D. Templeton and K. Moehle, PAC 2014; 86 1435-1481.

Structural Aspects of Molecular Recognition in the Immune System. Part II: Pattern Recognition Receptors. J. Robinson and K. Moehle, PAC 2014; 86 1483-1538.

Immunodiagnostics and Immunosensor Design. V. Gubala, R. Klein, D. Templeton and M. Schwenk, PAC 2014; 86 1539-1571.

Applications of Immunochemistry in Human Health: Advances in Vaccinology and Antibody Design. R. Klein, D. Templeton and M. Schwenk, PAC 2014; 86 1573-1617.

The NPU Format for Clinical Laboratory Science Reports Regarding Properties, Units, and Symbols (IUPAC Technical Report). G. Ferard and R. Dybkaer, PAC 2014; 86 1923-1930.

Nanomaterials and Human Health: The Trends and Future Workshop. V. Gubala, University of Kent, September 15-16, 2014.

Glossary of Terms Used in Neurotoxicology. D. Templeton, M. Schwenk and J. Duffus, PAC 2015; 87 841-927.

Successful Drug Discovery. J. Fischer and D. Rotella, Wiley-VCH March 2015.

Highlights in Medicinal Chemistry. Short course conducted at the University of Rio de Janeiro, January 25-31, 2015.

Medicinal Chemistry II. Short course conducted at Sri Ramachandra University, February 8-12, 2015.

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