active audience. The topics focused on and detailed the challenges pointed out by Dr. Choudhary. Problems related to a steady, reliable, and sustainable supply of raw materials were many, and experiences from India were very useful to know when productive measures have to be taken. In this context, traditional medicinal knowledge and other ethnopharmacological aspects are very important, as made very clear in several presentations. Another important issue, covered in detail by several lecturers, was safety. A variety of topics were discussed, including documentation by chemical analysis, new approaches to toxicological testing, adulteration, and risk assessment. A less scientific safety concern is the inaccurate and even misleading information available on the Web, which can contribute to destroying the reputation of proven, high-quality, and reliable herbal medicines.

Naturally, a part of the lecture program was devoted to recent developments in chemical isolation, chemical analysis, testing of bioactivity, and development of new *in vivo* and *in vitro* screening. A proposal to establish focal-point laboratories for chemical and biochemical analyses caught significant attention and will apparently be followed up. When properly equipped and run, and adequately engaged by the industry, such facilities could greatly contribute to the scientification of the herbal-medicine industry as a whole and certainly contribute to make safe and approved herbal medicines much more accessible.

### Follow-up and Future Actions

As some of the readers will know, the CHEMRAWN committee has introduced a tool termed FAC as a precautionary instrument at all its conferences. FAC stands for Future Action Committee, which is an integrated part of any CHEMRAWN conference. Such a committee is appointed before the conference and is in session during the conference to pick up and further digest good, interesting, new, brave ideas that are put forward during the lectures, discussions, and special FAC sessions. Such a committee, with six members from six countries, was working at this conference as well, and the last session of the conference discussed a conceptual report presented by the committee. A lot of valuable feedback was received, which hopefully will become clear when papers and reports from the conference are published in due course.

A tangible outcome of the conference and all the hard work leading up to it can in fact already be noted. The fact that the preparation of CHEMRAWN XX was so successful generated a lot of support for a project, pushed forward in parallel by Professor Mosihuzzaman, to establish an International Centre for Natural Product

*Conference Chair, Professor M. Mosihuzzaman, and Conference Secretary, Vice Chancellor Liaquat Ali (Bangladesh University of Health Sciences, BUHS). (Photo: Leiv K. Sydnes)*

During the closing of the conference all the hard work done by the Conference Chair, Professor M. Mosihuzzaman, Conference Secretary, Vice Chancellor (BUHS) Liaquat Ali, and the Local Organizing Committee was acknowledged with gratitude and enthusiasm, well deserved after a splendid event.

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## Chemistry and Human Health

### *by Thomas Perun, Division VII President*

The IUPAC Chemistry and Human Health Division ( Division VII) met during the General Assembly last August in Busan, Korea. The annual meeting of the Division is an opportunity for the committee to review the progress of existing projects and to discuss possible new initiatives. Projects will usually result either in IUPAC recommendations or in technical reports and books. Division VII recognizes members for meritorious service to IUPAC and to the health sciences in general through its Emeritus Fellows Program. Up to three Emeritus Fellows are appointed each Biennium. Professor Doug Templeton and Professor Robin Ganellin were the most recently recognized. A brief review of the Division mission and organization follows.

### Mission

The mission of Division VII is to promote pure and applied chemistry in the service of human health and well-being. Major aspects are the development of therapeutic drugs, the standardization of clinical laboratory methods, and the protection of humans from potential

harmful substances. All three sectors have seen many new developments in the past 20 years, and Division VII helps IUPAC and the chemical community to keep up with the rapid changes in health-related areas.

## Organization

Division VII is composed of three different subcommittees, each with their own objectives accomplished through 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 Toxicology and Risk Assessment (TRA) subcommittee has projects that are concerned with identifying the possible risk of chemical agents on human health. The Nomenclature for Properties and Units (NPU) subcommittee's objective 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.

### Subcommittee on Drug Discovery and Development (DDD)

One of the goals of this subcommittee is to provide information to medicinal chemists that shows how to be successful in their discovery of new agents for the treatment of common and neglected diseases. A series of three books on Analog-based Drug Discovery has been very popular and a new series on Successful Drug Discovery is underway. Successful courses on medicinal chemistry techniques have been given in parts of the world where research activities are less developed—surveys of research activities in such laboratories have provided information to a broader group of scientists, with the hope of enabling synergistic interactions. Many glossaries of terms have been published which have been utilized extensively by workers in these fields.

The IUPAC Richter Prize was established in 2006 to honor individuals who have made outstanding contributions to the practice of medicinal chemistry or to the discovery and development of new drugs. To date, five scientists from different countries have received this prodigious award. The next award will be presented in 2016 (see announcement p. 27).

### Subcommittee on Toxicology and Risk Assessment (TRA)

The ever increasing use of chemical materials in the workplace and in daily life is accompanied by the possibility of unwanted health effects due to accidental or intentional chemical exposures and emissions. Today's problems make it necessary to reevaluate older chemicals according to present day test standards, including the evaluation of novel in vitro methods, the quantification of risks of chemical emissions, and the study of the interaction of these chemicals with biologically relevant molecules. Projects dealing with these issues have been carried out by the subcommittee. Toxicology is an interdisciplinary science, and a common terminology is essential. To help in this understanding, the subcommittee has produced a number of glossaries, explanatory dictionaries, and books on concepts in toxicology. It has also developed course material for teaching schoolchildren about hazardous chemicals in their environment. A joint project with the Chemistry and the Environment Division (Div IV) is developing a document critically discussing the use of nanoparticles in human health applications, such as drug delivery, in vivo imaging, food technology, and cosmetics.

*Division VII meeting in Korea (Busan) August 2015, showing members and guests.*

**Subcommittee on Nomenclature for Properties and Units (NPU)**

In laboratory medicine one of the most basic challenges is to ensure that there is a common understanding of what is being measured in a biological system, as well as how the results will be expressed and in what units. To address this issue, the subcommittee has partnered with the International Federation of Clinical Chemistry (IFCC) and the Danish National e-Health Authority (DeHA) to develop, test, and refine an intuitive and comprehensive NPU terminology. This is essential to providing quality assurance and to unequivocally interpreting the results of clinical laboratory analysis. In 2014, a formal agreement between the three partners was developed to provide a template for greater international promotion of the NPU terminology as an aid to harmonized practice and better patient safety.

**Scientists interested in participating in activities related to Chemistry and Human Health are invited to contact the Division President, Tom Perun <tjperun@aol.com>.**
**www.iupac.org/body/700**

# From Big Data to Chemical Information

*by Colin L. Bird and Jeremy G. Frey*
*Chemistry, University of Southampton*

A meeting on Big Data [1] was jointly organized by the RSC Special Interest group on Chemical Information and Computer applications (CICAG) [2] and the UK Engineering and Physical Sciences Research Council Grand Challenge of Dial a Molecule (DaM) [3] and held 22 April 2015 at the Royal Society of Chemistry, Burlington House, London, UK.

"Big data" is very much a current term, for chemistry no less than for other disciplines. While there is an understandable tendency to interpret "big" as "voluminous", scope is an equally important yardstick for chemical data. Meeuwis van Arkel summed up the situation in a letter to *Chemistry & Engineering News*, [4] "Chemists need information from a multitude of different sources, each with its own origins. But there's a huge gap between volume and relevance that needs to be bridged. ... Big data must be focused on breaking huge blocks of information down to the smallest particles. Only when we can ensure that our tools enable confident decision making at every stage of chemical research will we realize big data's value rather than feel as if we are drowning in the chaos of too much."

In April 2015, the RSC Chemical Information and Computer Applications Group (CICAG) and the EPSRC-funded Dial-a-Molecule Grand Challenge Network co-sponsored a meeting: "From Big Data to Chemical Information" (programme available from the RSC web site). [5] The morning session addressed the "Rise and Impact of Big Data"; the afternoon session considered "Approaches to Managing Big Data and Maximizing Opportunities", then concluded with a keynote by Tony Williams, "Activities at the Royal Society of Chemistry to gather, extract and analyze big datasets in chemistry". While it was to be expected that the speakers would offer different perspectives on "big data", it was perhaps less obvious that several of them would suggest that chemical data is not necessarily "big" data. Nevertheless, consistent aspects were the heterogeneity, high dimensionality, and complexity of chemical data, the utilisation of which is often complicated by uncertainty.

## Challenges

Richard Whitby (University of Southampton) began by presenting the Dial-a-Molecule challenges associated with making novel molecules quickly, the main issue for the synthetic organic chemist being in deciding how to plan a synthesis such that we know it will work. Consequently, organic synthesis will have to change to being a data-driven discipline. At present, we do not know enough about reaction outcomes, and so need to capture data at the source, especially for reactions that we deem to have failed. The reaction space is huge, so it is difficult to say where we are, as the amount of information is still restricted. Current computer-aided synthesis design programs are essentially idea generators. Richard contended that it should be possible to use data more effectively, particularly by getting more information into reaction databases rather than in publications.

Jeremy Frey (University of Southampton) introduced issues that can arise from the diversity and heterogeneity of chemical data, noting that it comes from a lot of sources of different sizes, so some data might not be what we think it is. The use of social networking has increased the amount of user-generated content, but in a form that is potentially not processable. Such content might even include information about failed reactions, albeit emerging by unconventional routes. Echoing Richard's message, Jeremy advanced the need to automate data capture, emphasising the importance of metadata, which researchers are known to be reluctant to assign. Metadata has to be captured at the source; there are real risks with adding it later. Semantic Web technologies offer hope, with the caveat that human understanding of machine-machine interactions is