

Conference Call

Tanner, New South Wales, Australia; Christopher Collett, St. Andrews, UK; Matthew Pringle, Sheffield, UK; Piotr Nowak, Groningen, the Netherlands. The RSC Books Poster Prize was awarded to Nandhini Ponnuswamy, Cambridge, UK. The RSC Chemical Science Poster Prize went to Tomohiro Higashino, Kyoto, Japan, and the RSC Organic and Biomolecular Chemistry award went to Michael Rawling, Strathclyde, UK.



The ICPOC21 banquet.

Overall, ICPOC21 probably counted at least as many memorable moments as there were participants. Many of these were happy occasions (see below), but ICPOC also included a special tribute in honor of Rory More O'Ferrall, who passed away on 15 June 2012. Rory was one of the most well-respected practitioners in the field. He was an active participant and frequent contributor at previous IUPAC conferences on physical organic chemistry. He was also a member of the International Scientific Advisory Board for ICPOC21, and the committee was very grateful for his advice and support during the organization. Rory will be fondly remembered by all who knew him and sadly missed by his family and many friends.

The many happy moments included award winners receiving their prizes, young chemists giving their first presentation at an international conference, and older chemists meeting friends or future collaborators. In addition to such pleasant events, highlights of ICPOC21 included the demonstration of the applicability of physical organic chemistry to a wide diversity of research, providing delegates with surprising new insights. In addition, the inclusion of a symposium honoring Jeremy Sanders, a series of sessions on new approaches to aromaticity, a series of sessions focused on systems chemistry, and several talks on reactions in non-traditional solvents as well as chemistry beyond the transition state provided the audience with a taste

of physical organic chemistry beyond the more traditional, though no less interesting, topics covered at ICPOC21. The flash poster presentations allowed representatives of the next generation of physical organic chemists to give their (first) presentations on an international stage. Overall, possibly the highlight of the conference was the realization that the international physical organic community is as vital and vibrant as it has ever been, promising exciting times ahead for physical organic chemistry.

While on the topic of exciting times ahead, the next ICPOC will be held in Ottawa, Canada, from 10–15 August 2014. Preparations for ICPOC22 are already being made by the Scientific Committee chaired by Heidi Muchall. Further information can be found at <http://events.science.uottawa.ca/icpoc22/welcome.html>.

Niklaas Buurma <Buurma@Cardiff.ac.uk> has been a lecturer in physical organic chemistry at Cardiff since 2006. He is a member of the Royal Society of Chemistry and of the RSC Physical Organic Chemistry Group committee. He was a member of the ICPOC21 scientific committee.

Human Errors and Out-of-Specification Test Results

by Ilya Kuselman and Ales Fajgelj

Out-of-specification (OOS) test results of chemical composition are results that fall outside the specifications of acceptance criteria established in the pharmaceutical industry, or do not comply with regulatory, legislative, or specification limits in other industries and fields, such as environmental and food analysis. Investigation of OOS test results is described in the U.S. FDA (Food and Drug Administration) Guidance 2006.¹ The guidance established an empirical organizational approach to investigation and decisions, which can be utilized at the different stages of investigation. When an OOS test result is identified, it is important to determine the root causes of the event and to avoid reoccurrence of such results. An investigation of the causes based on metrological concepts is proposed in the corresponding IUPAC/CITAC (Cooperation on International Traceability in Analytical Chemistry) Guide 2012.² This approach allows distinguishing between OOS test results, which indicate an actual change in chemical composition of an analyzed object, and OOS test results, which are metrologically related with a certain confidence probability (i.e., caused by measurement uncertainty and other metrological problems).

Conference Call

However, it is known that human activity is never free from errors: about 70 percent of incidents and accidents are caused by human errors. There is extensive literature on investigation and quantification of human error in aviation, engineering, medicine, accident analysis, and other fields. In analytical chemistry there are only some detached publications on the topic. Even those publications point to human error as the dominant cause of OOS test results.³ Reducing error probability starts with study and classification of the errors, education, and training. Therefore, IUPAC has recently approved a new project titled "Classification and Modeling Human Errors Contributing to Measurement Uncertainty of Chemical Analytical Test Results" (No. 2012-021-1-50). As part of this project, a workshop was organized in conjunction with the ISRANALYTICA 2013 Conference and Exhibition, on 29 January 2013 in Tel Aviv, Israel, <www.bioforumconf.com/workshop-on-human-errors>. The Israel Analytical Chemistry Society and CITAC took part in organizing the workshop. The event was sponsored by IUPAC, Israel Laboratory Accreditation Authority, and SIGMA-ALDRICH Corporation, and arranged by Bioforum Ltd.

Opening remarks were given by the chair of the Organizing Committee, Ilya Kuselman of the National Physical laboratory of Israel. Kuselman explained the missions of IUPAC and CITAC and delivered the first lecture "Introduction to Investigating OOS Test Results and Human Errors in Analytical Chemistry." Then, Zigmund Bluvband, ALD Group Ltd., Israel, winner of the prestigious Elmer Sperry Award 2012, gave a talk on "Human Errors in Aviation," which included a short

film on the topic. Karen Ginsbury, Pharmaceutical Consulting Israel Ltd., delivered a lecture on unmasking the causes of analyst errors, reducing mistakes in the laboratory, and investigating OOS test results. Producer's and consumer's risks of OOS test results were the subject of the lecture by Francesca Pennechi, National Institute of Metrological Research, Italy.

Yoel Donchin, Hadassah Hebrew University Medical Center, Israel, impressed the workshop participants with his lecture "Avoiding Medical Error in the Hospital: Mission Possible?" The lecture included short films on the topic and humor, as in the presentation by Zigmund Bluvband. Causes of errors in analytical chemistry, detected using a web-based survey of proficiency testing, were classified in the lecture by Stephen L.R. Ellison, Laboratory of Government Chemist Ltd., UK. A practitioner report by Ales Fajgelj, International Atomic Energy Agency, Austria, et al., on the use of corrective actions in management of human errors in analytical laboratories, and the report by Paulina Goldschlag, Laboratory for Pesticide Residue Analysis, Plant Protection and Inspection Services, Israel, on spurious errors in pesticide residue analysis practice, were also of great interest.

Finally, a round-table discussion moderated by Ales Fajgelj allowed everybody to receive answers to their questions, and to learn from the experiences accumulated in other laboratories, and even in other fields (e.g., aviation and medicine). It was a diverse, fruitful, and informative meeting, the first such one in analytical chemistry, but certainly not the last. Development of the methods for quantification and reduction of human errors in analytical laboratories, which will increase the reliability of chemical analytical test results, will certainly attract greater attention from the analytical, quality, and metrological communities in the near future.

References

1. U.S. FDA (2006) Guidance for Industry. Investigating Out-of-Specification Test Results for Pharmaceutical Production.
2. Kuselman I, Pennechi F, Burns C, Fajgelj A, de Zorzi P (2012) IUPAC/CITAC Guide: Investigating Out-of-Specification Test Results of Chemical Composition Based on Metrological Concepts (IUPAC technical report). *Pure Appl. Chem.* Vol 84, No 9, pp. 1939-1971.
3. Kuselman I, Pennechi F, Fajgelj A, Karpov Yu (2013) Human Errors and Reliability of Test Results in Analytical Chemistry. *Accred. Qual. Assur.* Vol 18, No 1, pp. 3-9.



Ilya Kuselman (left) and Ales Fajgelj at the ISRANALYTICA 2013 Conference and Exhibition.