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In the news

Sándor Görög makes an outstanding contribution

With Professor Sándor Görög celebrating his 80th Birthday last December, it is a great pleasure to mark that milestone in ***Trends in Analytical Chemistry (TrAC)***, for which he has been a Contributing Editor for 28 years. He has also been Editor of ***Journal of Pharmaceutical and Biomedical Analysis*** since it was founded in 1983.

Sándor's main fields of interest are analytical chemistry (pharmaceutical analysis with emphasis on the use of spectroscopic, chromatographic and hyphenated techniques in the identification and determination of impurities and degradation products); and, pharmaceutical chemistry with emphasis on steroids.

His first article in ***TrAC*** was on steroid analysis in the pharmaceutical industry [1], on which topic he was also joint author of a book [2] and Editor of a series of volumes [3].

His list of publications shows that he was author or editor of 11 books, 14 chapters in books (see attached list) and some 175 scientific papers. Apart from playing an active role as a Contributing Editor on ***TrAC***, he has published some 20 contributions in the journal, including review articles, meetings reports, book reviews and editorials. Most recently, he was joint Guest Editor with Steven W. Baertschi of the Special Issue of ***TrAC*** on The Role of Analytical Chemistry in Drug-Stability Studies [4].

Following university, Sándor was based at Chemical Works Gedeon Richter Ltd, where, after 55 years with this leading pharmaceutical company in Hungary, he was Scientific Advisor when he retired last December.

Fig. 1. Sándor Görög celebrates his 80th Birthday.

In 1990, following the dramatic changes in Eastern Europe with the fall of the so-called Iron Curtain, Sándor was well placed to make a politically interesting comment on how these changes might affect analytical chemistry in the region.

In an Editorial [5], he sketched a picture of the situation of analytical chemistry in Eastern Europe at that time and then outlined the future prospects.

He foresaw that, with the Iron Curtain eliminated and travelling possibilities liberalized, a great wave of scientists, among them analytical chemists, would seek the opportunity to gain valuable experience in leading western laboratories.

Sándor also assessed that there could be rapid development in the cooperation between the local industrial companies in Eastern Europe manufacturing analytical instruments and leading western companies.

"In summary, although the present situation is rather difficult and further difficulties can be expected in the near future, I look to the future of analytical chemistry in Eastern Europe with 'cautious optimism'," he wrote.

Sándor is continuing as a Contributing Editor on ***TrAC***, and is currently joint Guest Editor with Boris Milan of a forthcoming Special Issue of ***TrAC*** on Qualitative Analysis.

We on ***TrAC*** are so grateful to have had, and to continue to have, the benefit of Sándor's knowledge, experience and wisdom in the field of analytical chemistry.

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[2] S. Görög, Gy. Szász, Analysis of Steroid Hormone Drugs, Akadémiai Kiadó,

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[3] S. Görög (Editor), Advances in Steroid Analysis, Akadémiai Kiadó, Budapest, Hungary – Elsevier, Amsterdam, The Netherlands, 1982; 1985; 1988; 1991; and, 1994.
[4] S. Görög, S.W. Baertschi, Special Issue on The Role of Analytical Chemistry in Drug-Stability Studies, Trends Anal. Chem. 49 (2013) 55–159.
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Electronic tongues measure ripeness of grapes

Electronic tongues can offer grape growers detailed information on the degree of grape maturity, according to a study carried out by researchers at the Universitat Politècnica de València (UPV), in collaboration with the Torre Oria winery in Valencia, Spain [1].

In the study, researchers Inma Campos and Román Bataller (Fig. 2) and colleagues applied electronic tongues developed in their laboratory to measure the maturity of eight different types of grapes (Macabeo, Chardonnay, Pinot Noir, Cabernet Sauvignon, Shyrah, Merlot and Bobal) in several locations of vineyards of Utiel and Requena, Valencia. They observed a good correlation between the response of the tongues and parameters analyzed in traditional tests – the acidity of the fruit and the amount of sugar in the grapes.

The results confirmed the usefulness of electronic tongues for controlling grape maturity and, therefore, evaluating the most appropriate time for harvesting. Among the main advantages, the tongues are cheap and portable.

"The portability is especially useful in assessing the degree of ripeness because, with current methods of analysis, further assessment in a laboratory is usually required," said Ramón Martínez-Máñez, researcher at the Centre for Molecular Recognition and Technological Development (IDM) – UPV.

Similarly, producers also highlight the potential usefulness of the tongue to perform analysis on the fruit at the premises where the produce is taken.

The researchers are currently working on new applications of electronic tongues in the sector. Specifically, they are evaluating their use to control the fermentation of grapes in vats.

"These devices allow continuous monitoring of the process, which would result in greater control over the product, and ultimately an increase in competitiveness," stated Campos.

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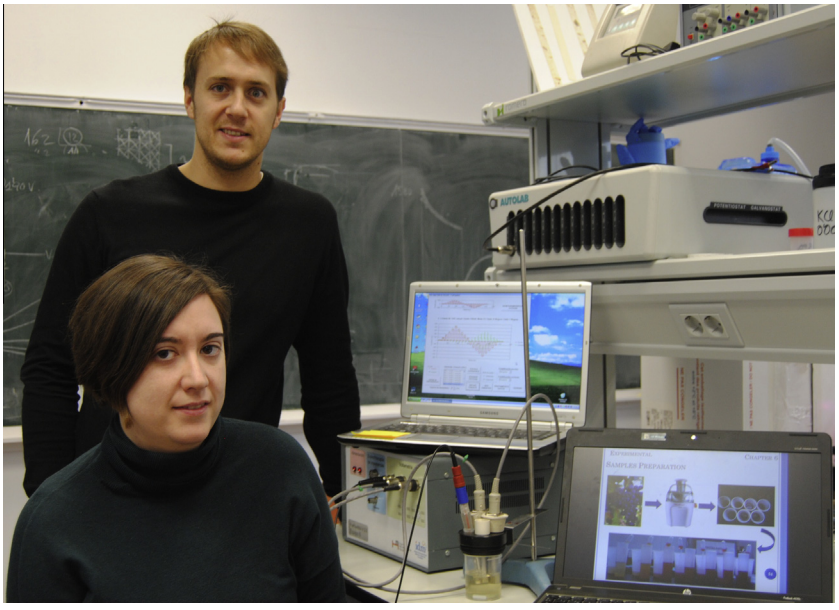

Fig. 2. Inma Campos and Román Bataller in their laboratory.

TrAC's Top 10 cited articles published since 2009*

1. **Liquid-phase microextraction**
   by A, Sarafraz-Yazdi and A. Amiri
   Trends Anal. Chem. 29 (2010) 1.
2. **Biomolecule-nanoparticle hybrids for electrochemical biosensors**
   by S. Guo and S. Dong
   Trends Anal. Chem. 28 (2009) 96.
3. **Bioactive paper provides a low-cost platform for diagnostics**
   by R. Pelton
   Trends Anal. Chem. 28 (2009) 925.
4. **Review of the most common pre-processing techniques for near-infrared spectra**
   by Å. Rinnan, F.v.d. Berg and S.B. Engelson
   Trends Anal. Chem. 28 (2009) 1201.
5. **Dispersive liquid-liquid microextraction for determination of organic analytes**
   by A.V. Herrera, M. Asensio-Ramos, J. Hernández-Borges and M.T. Rodríguez-Delgado
   Trends Anal. Chem. 29 (2010) 728.
6. **Coupling ultra-high-pressure liquid chromatography with mass spectrometry**
   by D. Guillarme, J. Schappler, S. Rudaz and J.-L. Veuthey
   Trends Anal. Chem. 29 (2010) 15.
7. **Electrochemical sensing based on carbon nanotubes**
   by P. Yáñez-Sedeño, J.M. Pingarrón, J. Riu and F.X. Rius
   Trends Anal. Chem. 29 (2010) 939.
8. **Liquid-phase microextraction techniques within the framework of green chemistry**
   by F. Pena-Pereira, I. Lavilla and C. Bendicho
   Trends Anal. Chem. 29 (2010) 617.
9. **The application of quantum dots, gold nanoparticles and molecular switches to optical nucleic-acid diagnostics**
   by W. Russ Algar, M. Massey and U.J. Krull
   Trends Anal. Chem. 28 (2009) 292.
10. **Carbon nanostructures for separation, preconcentration and speciation of metal ions**
    by K. Pyrzynska
    Trends Anal. Chem. 29 (2010) 718.

*Extracted from *SciVerse Scopus*, 8 January 2014

LGC acquires Dr. Ehrenstorfer GmbH

LGC has acquired Dr. Ehrenstorfer GmbH, the world's leading producer of pesticide and other organic reference materials, based in Augsburg, Germany.

Dr. Ehrenstorfer offers over 8000 products, including a number of very

specialized materials, to the residue-analysis and environmental-testing market. Reference materials are fundamental to the reliability of analytical results, upon which key decisions around the safety and quality of products and processes are made every day. Dr. Ehrenstorfer holds the "gold standard" for reference-material producers, with ISO 9001 certification and accreditation to ISO/IEC 17025 and ISO Guide 34.

This acquisition gives LGC an unparalleled breadth of ISO Guide 34 accredited facilities for reference-materials production, with four sites across the USA, UK and Germany. LGC has a long history in reference materials, as a producer within the UK National Measurement Institute (NMI) and as a distributor for many of the world's NMIs, pharmacopoeias and globally-recognized private producers.

"The reference-standards market has seen strong growth in all the industries in which LGC operates," stated LGC CEO Tim Robinson. "With the acquisition of Dr. Ehrenstorfer, we are able to offer our customers access to an extensive range of pesticide and environmental reference materials alongside our own certified reference materials and those of other world-leading suppliers. We also look forward to working with Dr. Ehrenstorfer's well-established network of distributors around the world."

"I am very proud of the contribution that Dr. Ehrenstorfer has made to the testing of pesticide residues and other organic contaminants over many years," said Dr. Ehrenstorfer Company Manager Eva Ehrenstorfer-Schäfers. "New contaminants of concern are continually emerging, and laboratory techniques advancing, and we are delighted that, under LGC's ownership, we will be able to respond to our customers' needs even more rapidly."

Prior to setting up Dr. Ehrenstorfer for the production of pesticide-reference materials, Siegmund Ehrenstorfer, had concentrated on pesticide-residue analysis as a food chemist in a German government institute in the 1960s. Later, the product range was expanded to include other organic materials, such as polychlorinated biphenyls (PCBs) and polyaromatic hydrocarbons (PAHs) used by laboratories in the food, environmental and healthcare industries, in both public and private sectors.

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Centrifuge decelerates polyatomic polar molecules

A centrifuge decelerator makes it possible for the first time to decelerate continuous beams of polyatomic polar molecules (Fig. 3) [1].

A natural way to decelerate a molecule is to make it climb a potential hill, thereby transforming its kinetic energy into potential energy. Such a hill can be provided through the interaction of a molecule with an external field, be it electric, magnetic or gravitational. For example, the application of electric fields makes use of the dipole moment that a large number of molecules possess because of an uneven charge distribution within the molecule. The dipole moment interacts with the external electric fields, and, by making the molecules move from a region with a weaker field to a region with a stronger field, they lose kinetic energy. In a similar fashion, magnetic molecules can be decelerated with external magnetic fields.

"The disadvantage of these two methods is that, for most molecules of interest, the typical height of electric or magnetic hills is of the order of 1 K, whereas molecules from our liquid-nitrogen-cooled source have initial kinetic energies of the order of 100 K," said Sotir Chervenkov, leader of the experiment at Max-Planck-Institute of Quantum Optics (MPQ), Garching, Germany. "Hence, the molecules have to climb a sequence of around 100 hills. This implies that one has to apply this process many times in succession, which leads to operation in the pulsed regime."

To circumvent this limitation, there had to be a sufficiently high potential (~100 K) in order to decelerate molecules in one stretch. Such a high potential is provided by the gravitational field of the Earth. Simple calculation showed that, for a molecule to be decelerated from around 200 m/s down to a trappable velocity of around 20 m/s, it had to fly upwards in the gravitational field of the Earth for 2 km, which renders such an experiment impossible or at least very demanding. The alternative was to create an analogue of a gravitational field in the laboratory.

"We are the first group worldwide which exploits this possibility," claimed Chervenkov. "Everyone who has been on a merry-go-round has experienced the outward force, which exists in a rotating frame. This force can be much larger than the gravitational force of the Earth, and is exploited in centrifuges for a multitude of biological, chemical, medical and industrial applications."

"Now, we employ a rotating frame for a conceptually different purpose, namely to decelerate a gas of neutral molecules from

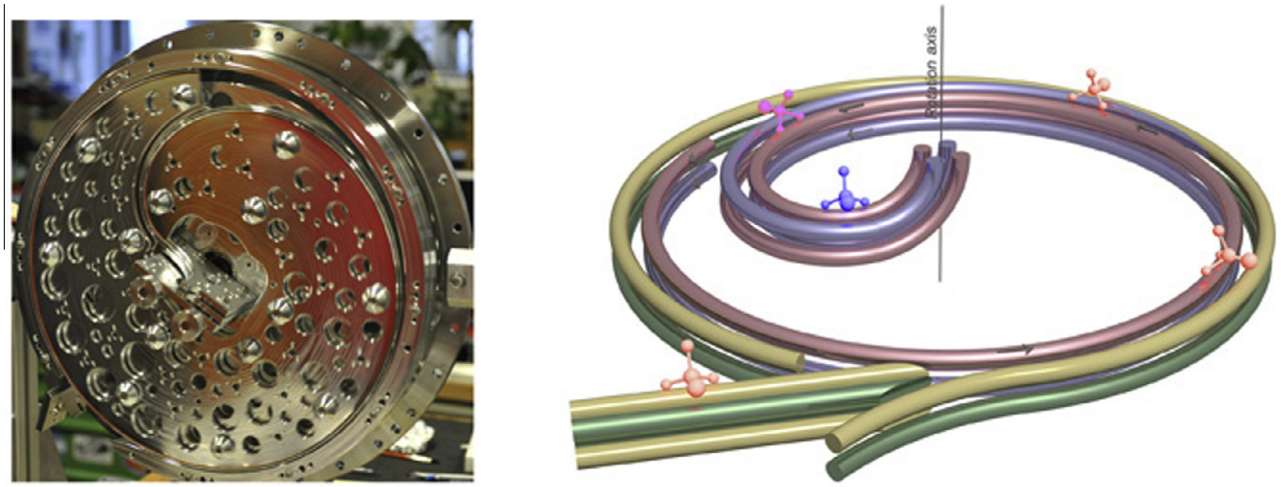

Fig. 3. Left: Centrifuge decelerator. Right: On a fast rotating disc, an electric quadrupole guide forces the molecules to move towards the rotation axis. As the molecules have to resist the centrifugal force, they lose kinetic energy and are slowed down to almost a complete halt. (Credit: MPQ, Quantum Dynamics Division).

about 200 meter per second to almost a standstill," said Xing Wu, a doctoral candidate who performed the first measurements.

"First, the molecules propagate around the periphery of the centrifuge in a stationary storage ring with a diameter of 40 cm composed of two static and two rotating electrodes," explained Martin Zeppenfeld, who initially proposed the idea. "Then, a rotating, spiral-shaped, electric quadrupole guide picks up the molecules at almost any point around the storage ring and whirls them to the rotation axis. Thus the centrifuge deceleration is a two-step process: the velocity of the molecules decreases first upon their transition from the laboratory into the rotating frame; and, further, while propagating in the rotating guide, as they are forced to climb a huge potential hill and are continuously slowed down, eventually reaching the rotation axis at close-to-zero velocity."

The MPQ team demonstrated the capabilities and the universality of the technique by decelerating three species with different masses and a dipole moment of the order of 1.5 Debye (i.e. CH_3F, CF_3H, and CF_3CCH). They varied both the rotation speed of the disc and the voltage at the quadrupole guide. For optimal conditions, they achieved continuous output beams with intensities of several billion molecules/m^2/s for molecules with kinetic energies below 1 K.

"Novel features of the centrifuge decelerator are its continuous operation, high beam intensity, applicability to a large set of molecules, and ease of operation," said Professor Gerhard Rempe. "It therefore has the potential to become an extremely valuable method in the cold-molecule research.

"The universality of the centrifugal force might also enable one to slow down atoms that cannot be laser-cooled, and possibly even cold neutrons."

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Ancient animals were mainly dark-skinned

Pigments preserved in fossilized skin have been analyzed to show that huge reptiles, such as mosasaurs and ichthyosaurs, which ruled the seas During the Age of the Dinosaurs, were mainly dark-skinned [1].

At SP Technical Research Institute of Sweden and MAX IV Laboratory, Lund University, Sweden, the unique soft tissue remains were obtained from a 55 million-year-old leatherback turtle, an 85 million-year-old mosasaur and a 196–190 million-year-old ichthyosaur (Fig. 4). This is the first time that the color schemes of any extinct marine animals have been revealed.

"This is fantastic!" said Johan Lindgren at Lund University, who leads the international research team that has studied the fossils. "When I started studying at Lund University in 1993, the film ***Jurassic Park*** had just been released, and that was one of the main reasons why I got interested in biology and paleontology. Then, 20 years ago, it was unthinkable that we would ever find biological remains from animals that have been extinct for many millions of years, but now we are there and I am proud to be a part of it."

With colleagues from Denmark, England and the USA, he found that the most sensational result of the investigation was that these ancient marine reptiles were, at least partially, dark-colored when alive, and that probably contributed to more efficient thermoregulation and provided camouflage and protection against harmful UV radiation.

The fossils analyzed comprised skeletal remains and dark skin patches containing masses of micrometer-sized, oblate bodies. These microbodies had been thought to be the fossilized remains of bacteria that had contributed to the decomposition and the degradation of the carcasses. However, by studying the chemical content of the soft tissues, Lindgren and his colleagues showed that they were remnants of the animals' own colors, and that the micrometer-sized bodies were fossilized melanosomes, or pigment-containing cellular organelles.

"Our results really are amazing," said study co-author Per Uvdal, who works at the MAX IV Laboratory. "The pigment melanin is almost unbelievably stable. Our discovery enables us to make a journey through time and to revisit these ancient reptiles using their own biomolecules. Now, we can finally use sophisticated molecular and imaging techniques to learn what these animals looked like and how they lived."

Mosasaurs (98–66 million years ago) are giant marine lizards that could reach 15 m in body length, whereas ichthyosaurs (250–94 million years ago) could become even larger. Both ichthyosaurs and mosasaurs died out during the Cretaceous Period, but leatherback turtles are still around today. A conspicuous feature of the living leatherback turtle, Dermochelys, is that its back is almost entirely black, which probably contributes to its worldwide distribution. The ability of leatherback turtles to survive in cold climates has mainly been attributed to their huge size, but it has also been shown that these animals bask at the sea surface during daylight hours. The black color

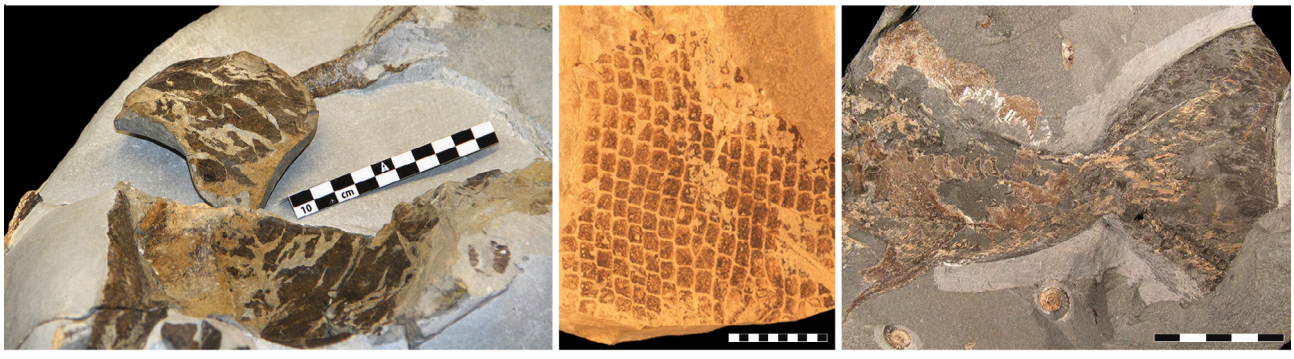

Fig. 4. Spectacular soft-tissue fossils: left, skin from a 55 million-year-old leatherback turtle (scale bar, 10 cm); center, scales from an 85 million-year-old mosasaur (scale bar, 10 mm); and right, a tail fin from a 196–190 million-year-old ichthyosaur (scale bar, 5 cm). (Photographs by Bo Pagh Schultz, Johan Lindgren and Johan A. Gren, respectively).

enables them to heat up faster and to reach higher body temperatures than if they had been lightly colored.

"The fossil leatherback turtle probably had a color scheme and similar lifestyle similar to Dermochelys. Similarly, mosasaurs and ichthyosaurs, which also had worldwide distributions, may have used their dark-colored skin to heat up quickly between dives," said Lindgren.

If these interpretations are correct, then at least some ichthyosaurs were uniformly dark-colored when alive, unlike most marine animals alive today. However, the modern deep-diving sperm whale has a similar color scheme, perhaps as camouflage in a world without light, or as UV protection, given that these animals spend extended periods of time at or near the sea surface in between dives. Lindgren also believes that the ichthyosaurs were deep-divers, and, if their colors were similar to those of the living sperm whale, then this would also suggest a similar lifestyle.

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High-pressure MS wins Innovation Award

M908, the world's first and only hand-held, high-pressure mass spectrometry (HPMS) system (Fig. 5), won first place in ***The Analytical Scientist*** Innovation Awards 2013.

The awards select a single winner and recognize a short-list of the top 15 advances from across the broad field of analytical sciences. Showcasing the wide range and level of progress across the industry, the awards included breakthroughs, such as 3D gas-chromatography systems, live-cell RNA detection and laboratory MS platforms.

In singling out 908 Devices's M908, the award demonstrated the impact that small, simple and robust MS analysis will have for first responders in safety and security and HAZMAT applications, and the future transformative impact that HPMS will have on a range of research and industrial applications.

The awards recognized products that enhanced sample preparation, separation, identification, qualification or analysis and contributed to making the world safer and the diagnosis of disease more effective. Nominations were submitted by the readers of ***The Analytical Scientist*** and the shortlist was selected by a panel of three independent experts and the publication's editorial team. As well as the HPMS system from 908 Devices, the short-list included advances from Thermo Fisher Scientific, Bruker Corporation and Waters Corporation.

Fig. 5. M908, the world's first and only hand-held, high-pressure mass spectrometry (HPMS) system.

M908 is a chemical-detection tool that is battery operated and 10 times smaller and lighter than any other commercial MS device. Its HPMS technology enables the M908 to operate much closer to atmospheric pressures than conventional MS systems using patented, micro-scale ion traps in a package designed for MilSpec ruggedness and reliability. HPMS technology, combined with M908's integrated algorithms, provides the selectivity to detect and identify hundreds of target threats with low false-alarm rates and single second sensitivity at low ppb levels. Weighing 1.7 kg, the M908 can detect and identify trace levels of chemical weapons, toxic industrial chemicals (TICs), explosives and drugs in safety and security applications. Currently going through field trials and third-party testing, M908 is scheduled to be generally available this year.

"We are delighted to have had our technology recognized in these awards," said 908 Devices CEO Kevin J. Knopp. "Our customers within the safety and security market need accurate, reliable and actionable intelligence in detection of chemical and explosive threats. Addressing that need, we have harnessed the powerful capabilities of mass spectrometry into a truly hand-held device that will dramatically change the way these threats are detected and identified. Beyond safety and security, our HPMS technology offers an analytical platform for life science research, food safety and a host of other applications that will benefit from small footprint analysis on the workbench or hand-held field operation."

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Pittcon 2014 honors scientists

The Pittcon 2014 Program Committee has announced the recipients of 10 prestigious awards honoring scientists who have made outstanding contributions to analytical chemistry and applied spectroscopy. Each award will be presented during a symposium at Pittcon 2014, Chicago, Illinois, USA in March.

Presentations will include topics in fields such as bioanalysis, nanotechnology, genomics and proteomics, fuels and energy, environment and materials. Methodologies include near-infrared spectroscopy, molecular and vibrational spectroscopy, mass spectrometry, capillary electrophoresis, electrochemistry, liquid chromatography and microfluidics or lab-on-a-chip.

The awards and the recipients are as follows:

Pittsburgh Spectroscopy Award

Geraldine L. Richmond, University of Oregon, USA

Pittsburgh Analytical Chemistry Award

Richard M. Crooks, The University of Texas at Austin, USA

Pittsburgh Conference Achievement Award

Benjamin Garcia, University of Pennsylvania, School of Medicine, USA

ACS Division of Analytical Chemistry Award for Young Investigators in Separation Science

Michael Roper, Florida State University, USA

Chromatography Forum of the Delaware Valley Dal Nogare Award

Mary J. Wirth, Purdue University, USA

SEAC – Charles N. Reilley Award

Joseph Hupp, Northwestern University, USA

SEAC – Young Investigator Award

Stephen Maldonado, University of Michigan, USA

Ralph N. Adams Award

Mark E. Meyerhoff, University of Michigan, USA

The Coblentz Society – Williams Wright Award

Walter M. (Mike) Doyle, Axiom Analytical, Inc, USA

The Coblentz Society – ABB–Bomen-Nicholson Award

Yukihiro Ozaki, Kwansei Gakuin University, Japan

Wallace H. Coulter Plenary Lecture

Professor Steven A. Carr, Director of Proteomics at the Broad Institute of MIT and Harvard, Cambridge, MA, USA, will open Pittcon 2014 with the Wallace H. Coulter Plenary Lecture on "Quantitative Proteomics in Biology, Chemistry and Medicine".

Fig. 6. Professor Steven A. Carr, Walter H. Coulter Plenary Lecturer at Pittcon 2014.

Prof. Carr (Fig. 6) will address the new era of quantitative biology enabled by mass spectrometry (MS)-based proteomic technologies. The content, the relative abundance, modification states and interaction partners of proteins can now be defined in a dynamic and temporal manner on a near-global basis in organelles, whole cells and clinical samples, so providing information of unprecedented detail.

At the Broad Institute, Prof. Carr and his team employ these technologies in studies including:

- delineating the genetic underpinnings of mitochondrial disorders;
- connecting cancer genotype to molecular phenotype;
- unraveling the basis of the innate-immune response;
- identifying the mechanism of action of drug-like molecules; and,
- discovering and verifying protein biomarkers of disease.

"Significant improvements in MS-based proteomic technologies over the past few years have greatly increased the value and the necessity of analyzing proteins and their modifications in biology and medicine," said Prof. Carr. "The number of proteins observed in cells and tissues now begins to approximate the expected expressed proteome.

"The ability to measure and to quantify globally changes in key protein modifications, such as phosphorylation, ubiquitinylation and acetylation, provides a window into function and pathogenesis not accessible by genomic methods. These capabilities have facilitated adoption of proteomics as a natural adjunct to genomic methods, yielding new knowledge and testable hypotheses in biology and medicine," he said.

Complete details and biographies of awardees:

www.pittcon.org.