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Conference Report

*CH*analysis 2023 – Artificial Intelligence meets Analytical Excellence

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In the usual venue of Beatenberg, the Division of Analytical Sciences (DAS) of the Swiss Chemical Society hosted its annual event, this time as a two-day conference. As many as 82 participants (an increase of 14% from 2022) attended *CH*analysis on March 30-31, 2023. Sponsorship by Agilent, Brechbühler, Chemistry Europe, GMP, Helvetica/Wiley, LTB Berlin, Novartis, NuInstruments/Ametek, PerkinElmer, Roche, SCNAT, Shimadzu, Specetek, Springer Nature, Syngenta, Tofwerk, Waters was extremely important to the success of the event: enabling two days of analytical science and food at a modest fee. Indeed, twice as many participating representatives from industry engaged in the event as before. As described below, an evening opening with a plenary talk, followed by six thematic sessions, a poster session, and a panel discussion kept the Swiss analytical community together.

The plenary talk by ***Yury Tsybin*** (SpectroSwiss) reviewed the field of Fourier Transform Mass Spectrometry (FT-MS), especially its advances in achieving super resolution, thanks to last generation FPGA modules and digital techniques. Tsybin explained how the method for FT processing, *i.e.* magnitude or absorption mode, is crucial to determine the figures of merit of the MS. Nowadays, compact instrumentation competes with or even excels over that of larger traditional facilities in both resolution and sensitivity.

The first of the thematic sessions was on *instrumentation*. Prof. ***Marc Pfeifer*** (HESSO) showed that the pandemic has accelerated the rollout of telemedicine and the decentralization of diagnostic testing that was already occurring owing to progress being made in information and communications technology (ICT), device miniaturization and integration as well as in molecular science and engineering biology. Indeed, *in vitro* medical diagnostics is founded on the analytical sciences, *e.g.* chromatography, capillary electrophoresis, mass spectrometry. Still, there is further potential for data aggregation and data science. ***Yaotian Wu*** showed impressive progress on self-powered sensors based on electrical-optical conversion, such as LCD, E-paper and distance-based readouts. ***Ankit Jain*** discussed a microfluidic screening device for enzyme engineering as sustainable functionalized biocatalysts. ***Tara Forrest*** highlighted the advantage of 'Click' chemistry for increased stability in potentiometric sensing of environmental or biomedical samples, by suppressing unwanted ion transport, as compared to state-of-the-art solid contact electrodes.

The second thematic session was on *micro/nano-analytics*. ***Andreas Riedo*** (University of Bern) explained the protocols for MS exploration during space missions in the search for signatures of life. Amino acids, lipids, and hydrocarbons are the most promising organic molecules for this purpose, which under favorable conditions, *e.g.* when protected from the harsh conditions at the surface, may survive for billions of years. ***Naresh Kumar*** shared his insights on tip-enhanced Raman for surface molecular analysis at the Nanoscale. ***Chan Cao*** discussed mechanisms and applications of biological nanopore (aerolysin) methodologies for single-molecule sensing and sequencing. As applications she highlighted protein post-translational modification including deep learning algorithms and molecule-based digital data storage. ***Pascal Becker*** reported on ICP-MS methods for forensic analysis using reduced amounts of material.

The third thematic session was on analytical *methods*. ***Simon Lobsinger*** (METAS) reviewed the challenges of food contaminant analysis and key role of certified reference materials. Contaminants can enter the food or form inside it during production, processing, storage or transportation, through contact with packaging materials and manufacturing devices, as well as through contamination from the environment. In addition, they can also have their origin from natural sources (natural toxins) or can even be added intentionally (food fraud). ***Monique Kuonen*** proposed an alternative method to traditional argon-based inductively coupled plasma (ICP) ionization. She used a nitrogen (atmospheric air) microwave source, which is clearly cheaper to operate, coupled to inorganic MS. Finally, ***Oscar Mendo-Diaz*** presented a 'fingerprint method' to spot persistent organic pollutants (chlorinated paraffins) and determine their fractional occurrence in a complex mixture. The use of a rapid digital technique known as RASER was crucial to analyze big data volumes. ***Alissa Agerova*** discussed the identification of cyanotoxin oligopeptides with an aerolysin nanopore (see Cao's talk).

In the fourth session industrial and chemical *processes* were addressed. ***Dorina Kotoni*** (Novartis) reviewed forced degradation studies for regulatory practices of pharmaceutical products. Showing results of a benchmarking study with nine pharma companies, her work aimed to determine whether solution phase stress testing of solid drug products produced degradation products that were both unique when compared to other stress conditions and relevant to the formal drug product stability data. ***Milos Selakovic*** reported from the project Exalomics, which attempts to screen VOCs in human breath and achieve a rapid diagnosis at the point-of-care. ***Selim Kazaz*** addressed the question "*why hydrogen dissociation catalysts do not work for hydrogenation of p-metals?*". ***Alessia Cesarini*** discussed the analysis of alkane uptake over commercial C1-C4 coupling catalysts by combinatorial neutron imaging.

The fifth thematic session (on Friday morning) focused on *data*. Advanced digital techniques had been appearing throughout the event in almost all presentations. ***Luc Patiny*** (Zakodium, Fig. 1), inspired the audience when he reviewed the many public browser-based codes available for chemistry, *e.g.* www.c6h6.org. ***Yousuf Hemani*** presented an effective data collection and processing method based on so-called compressed sensing to speed-up the collection of an X-ray absorption spectrum, also in the home lab. ***Claudia Masucci*** combined the use of a microplasma as a flexible atomic and molecular data generation source, to super-resolution instrumentation, as discussed by Tsybin in the opening plenary. The session was crowned with the METAS award 2023 by the prize winner ***Michele Stravs*** (Eawag, Fig. 2), for his work on digital techniques for filed-portable high resolution MS.

The sixth and last session on '*Omics*' was opened by ***Paolo Nanni*** (Functional Genomics Center of the UZH and ETH) who delivered a complete review of MS in proteomics. Many life science studies involve MS at some step, either to check the

Fig. 1. Digital transformation affected also analytical science, as highlighted in the keynote by Luc Patiny, as well as many other presentations. © Claudia Auinger

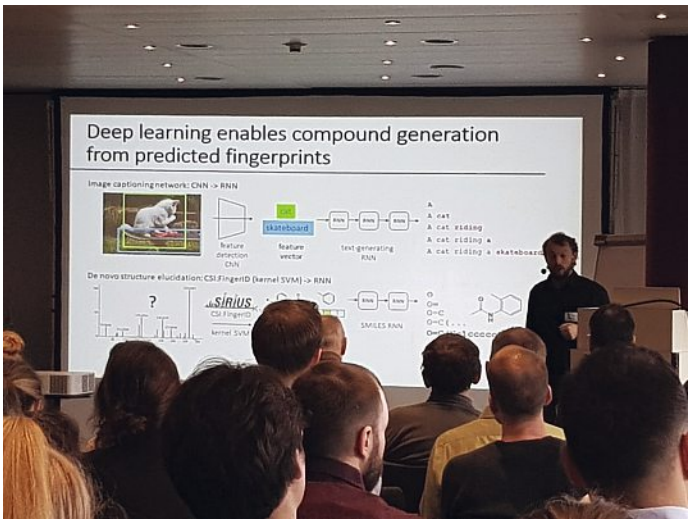

Fig. 2. METAS Award 2023 was presented to Michele Stravs (Eawag), who introduced a number of deep learning procedures for environmental analysis. © Claudia Auinger

quality of molecules (*i.e.* identity of a protein), to characterize them in detail (*i.e.* glycan profiling of an antibody), to discover new markers for biological processes (*i.e.* metabolites involved in a specific disease), or to validate findings obtained by other analytical means (*i.e.* increased level of specific protein post-translational modifications). Mass spectrometry is increasingly relevant also in the biopharmaceutical sector, where the filing of new biotechnological products follows detailed characterization procedures. ***Salome Püntener*** reported on Single-Molecule Peptide Identification using Fluorescence Blinking Fingerprints, also using deep learning. ***Arya Agarwal*** discussed the alternatives to ELISA (to overcome cross-reactivity) to detect oxytocin and vasopressin, which are both peptides that play pivotal roles in various physiological processes. Finally ***Bastiaan Duivelshof*** (Fig. 3), who received the best oral presentation award of this conference, reported on using protein-specific retention behavior to improve the characterization of therapeutic antibodies.

The poster session was lively and interesting and gave an excellent opportunity for all researchers to engage in academic and industry-related discussions before the gala dinner. The best poster award was attributed by the DAS board to ***Aori Qileng***.

Fig. 3. Best oral presentation was awarded by the DAS board to the final *CH*analysis speaker, Bastiaan Duivelshof (LHS, Geneva), pictured here with DAS VP Davide Bleiner (RHS). © Eric Bakker

Both awards were sponsored by Springer Nature's *Journal of Analytical and Bioanalytical Chemistry*. Finally, the DAS and the *CH*analysis participants (Fig. 4) discussed the changing of didactics in analytical science between academia and apprentices, also inspired by an impromptu talk by ***Gunnar Schwarz***. The next analytical event is during Euroanalysis, on 31 August in Geneva, to celebrate the DAS Simon-Widmer awardee 2023. *CH*analysis will come back to Beatenberg on 11–12 April 2024.

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Fig. 4. The 82 *CH*analysis participants in Beatenberg. © Eric Bakker