

Congress Report

Analytica Conference 2020 - Virtual Joint Symposium with GTFCh and GDCh on “Emerging Topics in Analytical Toxicology, Forensics, and Doping Control” October 20 and 23, 2020

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The Analytica is a leading trade fair for laboratory technology, analysis, and biotechnology that has been held at Munich every second year since 1968. The exhibition sector is traditionally accompanied by the Analytica Conference and Professor Hans H. Maurer has been regularly invited by the German Chemical Society (Gesellschaft Deutscher Chemiker, GDCh) to organize one of the Analytica Conference symposia on behalf of the Society of Toxicological and Forensic Chemistry (Gesellschaft für Toxikologische und Forensische Chemie, GTFCh). Due to the COVID 19 pandemic, the trade fair, which was planned for spring, was postponed to autumn 2020. In September, the organizers decided that the fair, as well as Analytica Conference, will be held purely virtually for the first time. Nevertheless, Professor Maurer was able to compile an international panel of speakers addressing various emerging topics in analytical toxicology, forensics, as well as doping control. The GDCh/GTFCh joint symposium was planned for Tuesday, October 20, but was replayed three days later to allow even more interested attendees to participate as all presentations needed to be prerecorded. The audience required to register for the virtual trade fair for free and to book the selected presentations of the Analytica Conference program afterwards. Ten presentations were included in the symposium, which was divided into three sessions leading to a whole day of exciting science.

The first session was dedicated to “Isotope Ratio Mass Spectrometry (IRMS) in Analytical Toxicology”. The first talk was entitled “Role of IRMS in Live Sciences with Focus on Forensic Sciences” and given by Dr. Andreas Rossmann (isolab GmbH, Schweitenkirchen, Germany). Dr. Rossmann gave an introduction and examples for the application of IRMS in our daily life such as authenticity control of foodstuff, but also underlined the potential of IRMS analyses of different human tissues for forensic investigations. In this context, he presented a case of an unknown, dead female found in Austria in the 1990s. Due to the results of the stable isotope analysis, the origin of the female was predicted to be from the Northern Caribbean and the woman could be identified as a missing person from the Dominican Republic two weeks later.

The second talk dealing with the “Profiling of New Psychoactive Substances by IRMS” was given by Dr. Michael Pütz from the Federal Criminal Police Office Wiesbaden, Germany. He described the significance of drug profiling for the comparative characterization of the physical and chemical properties of illicit drugs helping police authorities to establish links between samples of different seizures, to obtain information on trafficking routes, and to gather background information on the origin of samples. Drug profiling was described to be especially important for the new psychoactive substances (NPS) acting as synthetic cannabinoid receptor agonists (SCRA). In a large field study, the prevalent and hazardous SRCA MDMB-CHMICA was assessed via a flash-chromatography/UHPLC-MSⁿ impurity profiling workflow combined with IRMS analysis in numerous pure samples and Spice products of various brands from test purchases and police seizures. The stable isotope ratios and impurity signatures for the herbal

blends led to the conclusion that most samples contained MDMB-CHMICA from one source but individual synthesis batches.

The final talk of the first session, entitled “Power of IRMS in Doping Control”, was given by Dr. Corinne Buisson (French Anti-Doping Laboratory, Châtenay-Malabry, France). Dr. Buisson stated that anabolic androgenic steroids remain the most reported substances in doping controls and that the presence of exogenous steroids can be easily detected by conventional mass spectrometry methods. However, the determination whether endogenous steroids such as testosterone have been misused or not is more challenging. IRMS can prove the exogenous administration of endogenous steroids by establishing the isotopic signature of a target compound and is therefore routinely applied by anti-doping laboratories to investigate suspicious steroid profiles determined from each athlete. Most cases are analyzed due to suspected testosterone misuse, but analytical procedures for other substances such as 19-norandrosterone or boldenone have also been developed and even more applications of IRMS in doping control are in the pipeline.

The second session of the symposium focused on “Omics and MALDI Applications in Analytical Toxicology and Antidoping”. The first talk was given by Professor Markus R. Meyer from the Department of Experimental & Clinical Toxicology of the Saarland University in Homburg, Germany. His talk gave an excellent survey of the “Current Role of Omics in Analytical Toxicology”. While the application of OMICS or OMICS-like techniques is gaining more and more interest, most studies in clinical and forensic toxicology were dedicated to understanding the acute or chronic effects of drug intake, drug addiction, and/or finding markers to verify their (chronic) consumption. Nevertheless, only few studies are available to date performed with rather small sample sizes and poor comparability due to use of different species, experimental conditions, and other factors. Therefore, Professor Meyer concluded that more studies are needed to elucidate the benefit of OMICS or OMICS-like techniques in clinical and forensic toxicology particularly in contrast to already established techniques.

The following presentation was given by Dr. Luca Narduzzi (Laboratory for the Study of Residues and Contaminants in Food, Nantes, France). He focused on the „Role of Metabolomics in the Antidoping Toolbox” and described the gap between the detectability of doping substances right after administration and their effect represented by modifications of the athletes’ metabolism and illicit advantage over fair competitors as one of the main limitations in anti-doping. The signature of prohibited substances, such as the substance itself and its metabolites (referred to as markers-of-exposure), disappears from athletes’ bio-fluids within hours or few days, while their effects on the metabolism (so-called markers-of-effect) remain longer (sometimes over weeks). Anti-doping strategies are now moving towards the detection of markers-of-effect using metabolomics technologies, but current limitations must be considered.

The next talk was entitled „Fingerprint Development Methods for Touch Chemistry of Drugs and Explosives Using MALDI-TOF MS” and was given by Dr. Marc A. LeBeau (Laboratory of the Federal Bureau of Investigation in Quantico, USA). As chemical analysis of latent fingerprints, also known as “touch chemistry”, may provide leads or other forensically-relevant information in criminal investigations, the potential for touch chemistry using matrix-assisted laser desorption ionization/time-of-flight mass spectrometry (MALDI/TOF MS) to obtain molecular spatial distribution of target drugs and explosives across fingerprint residues was evaluated. Drug (procaine and pseudoephedrine) and explosive (TNT and RDX) powders and residues were identified in fingerprints under laboratory conditions using conventional fingerprint development methods and MALDI matrix. The results suggested that continued development of touch chemistry applications could prove useful for intelligence and investigations.

The last talk of the second session was given by Professor Eva Cuypers (Multimodal Molecular Imaging Institute of the University of Maastricht, The Netherlands) and dealt with “Mass Spec-

trometry Imaging in Forensic Research and Practice”. The interest in molecular mass spectrometric imaging (MSI) has grown over the past few years in the field of forensic sciences because it allows the conservation of sample spatial resolution. The techniques are label-free and rely on the desorption of molecules present on the surface of a solid flat sample. The newest generation of MSI techniques provide several opportunities on alternative forensic matrices such as hair and bone, but specific sample preparation as well as advantages and drawbacks of different techniques must be considered.

The final session of the symposium was entitled “Protein Analysis and Alternative Tools for Drug Metabolism Studies and Sampling in Bioanalysis” and was opened by the talk of Dr. Roland Staack from the Roche Innovation Center Munich, Germany. Dr. Staack asked the question “Bioanalysis of therapeutic proteins – What is the “correct” result and what is the right technology?”. Bioanalysis of therapeutic proteins is challenged by the potential presence of binding partners such as soluble targets, shredded receptors, or the presence of anti-drug antibodies. As a result, the drug could be present in a sample in a complexed and thus neutralized form and dependent on the required information, a bioanalytical strategy clearly discriminating between the different drug forms might be required. The presentation also covered the bioanalytical challenges of correct free/active and total drug quantification as well as concepts to identify potential method limitations for appropriate method development and validation.

My own presentation followed dealing with “Alternative Tools for Metabolism Studies of Drugs of Abuse”. The continuously increasing number of NPS available on the drugs of abuse market poses a challenge for clinical and forensic toxicologists as the inclusion of metabolites in mass spectral libraries is crucial, especially for urine screening purposes. Authentic human samples may represent the gold standard for identification of metabolites but are often not available and clinical studies cannot be performed due to ethical concerns. However, numerous alternative *in vitro* and *in vivo* models are available, such as human liver cell preparations, intact human liver cells, zebrafish larvae, rodents, or pigs, each showing individual advantages and disadvantages.

The final talk was given by Professor Olof Beck from the Department of Clinical Neuroscience of the Karolinska Institute in Stockholm, Sweden. He talked about “Novel Strategies for Microsampling – Dried Matrix Spots and Exhaled Breath”. The development of bioanalytical technologies has resulted in the possibility of using alternative sampling procedures to venous blood and urine for toxicological investigations. While the use of dried blood spots (DBS) for bioanalytical investigations is well established, the challenge has been to develop a solution for the need of the specimen with a known and exact volume of the dried blood and the production of dried plasma spots by filtering the blood as alternative to DBS. Exhaled breath carries aerosol particles from the lung that are formed from the airway lining fluid during the normal breathing maneuver. Exhaled breath has been demonstrated to be useful for the detection of an intake of a large number of misused and therapeutic drugs and an improved device for collecting exhaled aerosol particles has been developed. The easiness of collecting this specimen may provide a possibility of sampling at roadside or studying drug use in the society in the future.

Even if this year’s GDCh/GTFCh joint symposium was a special one due to the virtual nature and the lack of interaction between speakers and audience, the exciting and diversified agenda inspired and united scientists from clinical and forensic toxicology. Each session of the symposium was accredited by the GTFCh with two credit points for members who are already certified Forensic Toxicologists GTFCh, Forensic Chemists GTFCh, Forensic-Clinical Chemists GTFCh, and/or Clinical Toxicologists GTFCh.