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Congress Report

Analytica Conference 2016 – Joint Symposium with GTFCh and GDCh on "High-resolution mass spectrometry – Where do we stand today in clinical and forensic toxicology?" Munich, Germany, May 11, 2016

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The Analytica Conference took place in conjunction with the Analytica fair from May 10 to 12, 2016 in Munich. Since 45 years, the Analytica is a leading trade fair for analytical equipment and solutions, laboratory technology and life science applications.

Since many years, Hans H. Maurer has been regularly invited by the GDCh to organize one of the symposia during the Analytica Conference on behalf of the German speaking Society of Toxicological and Forensic Chemistry (GTFCh). He could welcome about 150 participants at this year's symposium to see well known international experts speaking on different aspects of high-resolution mass spectrometry, particularly on the pros and cons of Orbitrap and QTOF-based systems.

The first talk was held by Hans Maurer himself and was devoted to the question whether to use ion trap or Q-Orbitrap for a metabolite-based drug screening. As robust LC-MS instruments using TOF or Orbitrap mass analyzers are getting more and more affordable to laboratories, screening approach using such instruments and high resolution mass spectral libraries are frequently requested. However, also traditional low resolution screening solutions still have their benefits. Hans Maurer highlighted in his talk the pros and cons of both approaches also in the context with other screening approaches and concluded that HRMS strategies will be the future particularly when instruments will get even more cheaper and if software tools will be developed that help users to control the huge amount of HR data.

The presentation by Kara L. Lynch from the University of California (San Francisco, USA) was entitled "QTRAP or QTOF for comprehensive drug screening?". She developed a broad-spectrum drug screen on a QTOF and compared its performance to a quadrupole linear ion trap (QLIT). Kara found that using targeted data analysis, QLIT was slightly more sensitive than QTOF; however, this difference did not significantly affect compound identification in patient samples. Overall, QTOF performed similarly to QLIT and could serve as an alternative method for general unknown screening, when using targeted data collection.

Anders Helander from the Karolinska Institutet and Karolinska University Laboratory (Stockholm, Sweden) reported from his experience with the use of a Q Exactive for monitoring new psychoactive substances (NPS) in the Swedish STRIDA project. This project monitors the occurrence and health hazards of NPS, based on samples from acute intoxication cases presenting in emergency departments and intensive care units (>700 cases per year in 2014-2015). When new drugs appear and reference material is available, they are included in the HRMS method and searched for retrospectively without need to re-run samples. Currently, they are covering more than 250 substances and they analyzed more than 2000 samples since start of the project.

The first talk after the coffee break, which was full of interesting discussions and meeting old friends, was held by Ilkka Ojanperä from Helsinki, Finland. He summarized his experiences with the use of a QTOF for drug screening in postmortem toxicology. Ilkka highlighted the power of HRMS in targeted screening but also the option to perform untargeted screening, to identify unknowns, and to do retrospective data mining.

Fig. 1. Speakers from left to right: Anders Helander, Ilkka Ojanperä, Kara Lynch, Hans H. Maurer, and Felix Hernández (Lewis Couchman had to leave earlier).

Fig. 2. Part of the audience (at maximum 150 as reported by the Analytica conference organizer).

Lewis Couchman (King's College Hospital, London, UK) used his talk to provide a comprehensive introduction into the use of Q-Orbitrap for drug quantification. He critically mentioned pros and cons of the HRMS solution for quantification and found that designing accurate and robust quantitative experiments using HR requires different considerations to typically used triple-quadrupole mass analyzers. Lewis particularly mentioned strategies for maximizing the number of data points to ensure sufficient representation of chromatographic peaks, judicious choice of internal standards when using non-selective MS^2 data capture, and more recent approaches for multiplexed drug quantitation using parallel reaction monitoring.

Finally, Felix Hernández (Castellón, Spain) demonstrated the potential of HRMS (QTOF) in wastewater drug testing. He concluded that HRMS can provide valuable structural information for unknowns by obtaining accurate-mass product-ion spectra after performing MS/MS experiments. Also acquiring full scan data at different collision energies (all ion fragmentation) can be advantageous in tentative identifications without the use of standards.

After three hours of an exciting symposium, chairman Maurer thanked the speakers and the audience and closed the session inviting everybody to the next Analytica Conference in 2018. This and the next symposium was and will be accredited by the GTFCh with four credit points for members who are already certified Forensic Toxicologists GTFCh, Forensic Chemists GTFCh, Forensic-Clinical Chemists GTFCh, or Clinical Toxicologists GTFCh.