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Liquid-chromatography high-resolution mass spectrometry for untargeted toxicology analysis

Alan H B Wu

University of California, USA

Testing for drugs abuse in blood and urine for clinical and forensic toxicology occurs in two steps: immunoassay screening followed by mass spectrometry (MS). While immunoassays are rapid and inexpensive, some assays suffer from poor sensitivity and specificity. Gas chromatography coupled with mass spectrometry is used for confirmatory analysis, but results are usually not available for real-time patient management. The implementation of liquid chromatography (LC)-tandem MS has reduced the pre-analytical steps needed for confirmatory analysis. However, matches to pre-existing MS libraries are required for general unknown screening. LC-high-resolution (HR) MS, such as with time-of-flight and Orbitrap MS technologies and use of soft ionization enable detection of unknown compounds based on precise molecular formula. These technologies are more powerful for general unknown screens because library spectra may not be available for many compounds, especially novel designer drugs, and because the toxicology laboratory does not have standards and controls for the hundreds of thousands of low molecular weight compounds that can cause poisonings. Although results are not definitive without standards, and cannot be used alone for forensic purposes, presumptive results can be reported for clinical toxicology cases. Confirmation analysis performed retrospectively with acquisition of the appropriate standards. In this manner, results can be reported quickly enabling medical decisions that can have an impact on patient outcomes. This lecture will describe LC-HR-MS techniques with examples of clinical cases solved.

Alan.Wu@ucsf.edu

Development and validation of analytical methodologies applied to strategic nutritional research in health sciences

Angela Santos-Fandila

Abbott Laboratories, Spain

The aim of this talk is to promote the use of Ultra-High Performance Liquid Chromatography coupled to Mass Spectrometry in tandem (UHPLC-MS/MS) in different areas and fields of science to cope with analytical problems of diverse nature. The high value and interest of this technique resides in the potential and versatility that it has, covering a wide range of possibilities from analytical support for research groups to production and quality control in the oil and food industries, or to hospitals and the healthcare sector, forensic and toxic laboratories, etc. The selectivity, specificity and high sensitivity have made that the fields of application of this technique are experiencing a rapid growth in recent years. In particular, in this talk, several applications in health sciences are presented to determine specifically important biomarkers modified by nutritional intervention. The difficulty with this type of application is mainly the validation of analytical methodology to obtain results of high confidence. The analytical methodology applied to biological systems has difficulties to provide a typical validation. The analytical methods presented in this summary have been validated under recommendations of the international guidelines for bioanalytical methods such as "Guidance for Industry, Bioanalytical Method Validation, US (2001) of FDA. This guide admits some difficulties such as lack of certified standards, reference materials or the inability to perform interlaboratory comparative determinations, being less demanding and strict than other international regulations aimed at routine laboratories in industrial systems such as the ISO 17025. Several examples of analytical methods to determine biomolecules of important roles in human biochemistry will be presented in this speech. These analyzed biomolecules by UHPLC-MS/MS are interesting in the nutritional industry to be candidates as innovative products focused on cognitive functions, improvements and development in muscle-bone system, neuroimmunology reinforcement, etc. In sum, UHPLC-MS/MS is a powerful tool for a research group focused on discovering new ingredients or technologies that could be applied to new nutritional products or improve those existing already in the market, to avoid or mitigate disease and ailments that affect today's society.

angela.santos@abbott.com