K42 General Unknown Screening of Drugs and Toxic Compounds in Human Samples Using a Hybrid Triple Quadrupole/Linear Ion Trap LC/MS/MS System

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After attending this presentation, attendees will learn about using LC/MS/MS for a general toxicology screen. Sample preparation is simplified versus other screening techniques. This general screening technique also has the capability to detect unexpected drugs and metabolites, as well as targeted analytes.

This presentation will impact the forensic community and/or humanity by demonstrating a relatively new and novel screening technique that is, in general, simple and faster compared to most techniques. It allows faster and more specific detection and identification of analytes in a screening assay.

General unknown screening (GUS) procedures in clinical or forensic toxicology are used to detect and identify the exogenous compounds present in human samples, whether expected or not. A comprehensive LC/MS/MS GUS method has been developed for drugs, toxic compounds and their respective metabolites in biological fluids

A simple, non-selective solid-phase extraction sample preparation was used. The mass spectrometer is operated in the Information Dependent Acquisition (IDA) mode, where ions are selected from a single MS ion-trap survey scan and the two most intense ions are submitted for MS/MS acquisition. The complete cycle time lasts approximately 1.36 s. A library of MS/MS spectra of parent compounds and metabolites has been built up and the MS/MS spectra acquired can be searched against the library for analyte identification and confirmation.

This method proved to be very efficient to identify unexpected compounds in biological samples (as far as they corresponded to library entries), as well as to give clues about the presence of metabolites owing to MS similarities with their respective parent compound. More than 1000 MS/MS spectra in the positive mode and 250 in the negative mode were entered in the library, together with compound name, developed chemical structure, CAS number, retention time, relative retention time and UV spectrum. Clinical cases will be presented where compounds not found by other screening or target techniques could be identified unambiguously.

A unique combination of the innovative operating modes offered by hybrid triple-quadrupole linear ion-trap mass spectrometers and new software features rendered it possible to develop a comprehensive and efficient method for the General Unknown Screening of drugs, toxic compounds, and metabolites in blood or urine.

Toxicology, LC/MS/MS, Drug Screening

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