B211 New Psychoactive Substances in Forensic Drug Cases: Crossing the Borders of Gas Chromatography/Mass Spectrometry (GC/MS) Selectivity

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Learning Overview: After attending this presentation, attendees will understand the limitations of traditional techniques for drug identification in the current market comprised of many isomeric substances; gain insight into novel tools to add complementary selectivity to GC/MS, such as Gas Chromatography-Vacuum Ultraviolet (GC-VUV); learn about strategies of "crossing borders" of traditional GC/MS selectivity; and get more out of current available data using chemometric tools and Likelihood Ratio (LR) calculations.

Impact on the Forensic Science Community: This presentation will impact the forensic science community, specifically drug experts, by enabling them to identify and overcome possible isomeric challenges in drug isomer analysis, reducing the risks for false positive or false negative results in case reports.

The global drugs-of-abuse market is facing major changes over the past decade. New Psychoactive Substances (NPS) form an emerging group of more than 700 synthetic drugs and are comprised of many closely related and isomeric classes of compounds. Most of these compounds are not legally controlled and are sold as "legal highs," while others are banned substances in various countries. When a "legal high" is put under judicial control, other closely related yet uncontrolled compounds often increase in popularity and occurrence. This fuels a perpetual cycle in which increasingly diverse NPSs are continuously being developed.

This transformation of the drugs-of-abuse market changes the needs of forensic drug analysis laboratories. Established methods, such as GC/MS, fall short in terms of selectivity, as isomeric NPS have identical masses, very similar fragmentation spectra, and can co-elute in fast screening methods. Traditional spectroscopic measurements using Fourier Transform Infrared (FTIR) or Raman find limitations in multicomponent mixtures, as is often the case in adulterated samples or tablet formulations. Thus, in forensic laboratories, a need has arisen for analytical methods capable of distinguishing known, as well as identifying yet unknown, NPS isomers.

Three new strategies have been investigated in the Dutch National Police and University of Amsterdam groups to tackle the isomeric NPS dilemma: (1) VUV spectroscopy provides distinctive and very reproducible spectra for various ring-isomers. Selectivity-wise, GC-VUV is complementary to GC/MS for certain NPS classes consisting of both ring- and aliphatic chain isomers; (2) low-energy Electron Ionization (EI) on a Gas Chromatography/quadrupole Time-Of-Flight (GC/qTOF) system produces less fragmented, more information-rich, mass spectra for NPS isomers. Multivariate statistics were applied to discriminate among ring-isomers; and (3) Infrared Ion Spectroscopy (IRIS) at the FELIX laboratory successfully differentiated ring-isomeric forms of NPSs and correctly identified an NPS directly from a complex case sample. Finally, IRIS presents a promising approach for the identification of unknown NPSs for which reference standard compounds are not available when combined with quantum chemical prediction of IR spectra for candidate molecular structures.

GC-VUV, NPS, Isomers

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