A144 Differentiation of Synthetic Cathinone and Synthetic Cannabinoid Regioisomers by GC-QQQ-MS/MS

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After attending this presentation, attendees will learn the use of Gas Chromatography Tandem Mass Spectrometry (GC/MS/MS) for the mass spectrometric differentiation of synthetic cathinone and synthetic cannabinoid regioisomers with both electron and chemical ionization modes.

This presentation will impact the forensic science community by providing the product ion scan mass spectra for the unequivocal identification of synthetic cathinone and synthetic cannabinoid regioisomers.

The abuse of designer drugs, especially for synthetic cathinones and synthetic cannabinoids, has proliferated worldwide with the ease of acquisition through the internet or head shops. Despite the efforts to regulate these psychoactive substances, new designer drugs, including isomers and derivatives, continue to emerge, replacing the controlled substances.[1] Gas Chromatography/Mass Spectrometry (GC/MS) is the gold standard analytical technique in many forensic laboratories as this technique enables the unambiguous identification of unknown compounds with the use of an Electron Ionization (EI) mass spectral library; however, the identification of designer drugs is often challenged due to their similar structures (derivatives) and the presence of positional isomers (regioisomers) resulting in very similar mass spectral profiles in EI mass spectra and insufficient information for identification.[2] There have been many efforts to characterize regioisomers of amphetamine derivatives by mass spectrometric differentiation as well as chromatographic separation by GC/MS and Liquid Chromatography Mass Spectrometry (LC/MS).[3] In this study, the mass spectrometric differentiation of several synthetic cathinone and synthetic cannabinoid regioisomers is performed by Gas Chromatography Triple Quadrupole Tandem Mass Spectrometry (GC-QQQ-MS/MS) with EI and Chemical Ionization (CI) modes. The discrimination of regioisomers is achieved by obtaining the product ion scan mass spectra at different collision energies, 10, 20, and 30eV. As a result of collision-induced dissociation of precursor ions, with nitrogen as a collision gas, the peaks for product ions are presented with different relative abundances in their mass spectra depending on the regioisomers. The advantage of using GC-QQQ-MS/MS as an alternative method for regiosiomer differentiation over Nuclear Magnetic Resonance (NMR) spectroscopy is the ability to analyze trace amounts of sample. In addition, the obtained product ion scan mass spectra can be used as a supplemental library along with an EI full scan mass spectral database that is currently used in the library search for an unknown compound.

This approach will be presented for the analysis of regioisomers of 20 different synthetic cathinones and synthetic cannabinoids. For example, the regioisomers of AM694 were successfully discriminated with the characteristic product ion scan mass spectra at different collision energies.

References:

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2. Zaitsu, K.; Miyagawa, H.; Sakamoto, Y.; Matsuta, S.; Tsuboi, K.; Nishioka, H.; Katagi, M.; Sato, T.; Tatsuno, M.; Tsuchihashi, H.; Suzuki, K.; Ishii, A., Mass spectrometric differentiation of the isomers of mono-methoxyethylamphetamines and mono-methoxydimethylamphetamines by GC–EI–MS/MS. Forensic Toxicol 2013, 31 (2), 292-300.

Synthetic Cathinones, Synthetic Cannabinoids, GC-QQQ-MS/MS

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