

B129 Capillary Electrophoresis/Mass Spectrometry (CE/MS) as an Effective Tool for Identification of Illicit Drugs and Their Optical Isomers

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After attending this presentation, attendees will better understand the application of CE/MS for the separation of chiral compounds of forensic importance.

This presentation will impact the forensic science community by suggesting a rapid and highly sensitive method to separate and identify drugs and their optical isomers.

Many pharmaceutical and illicit drugs have structural and optical isomers. For some illicit drugs, identification of these is essential since scheduling and sentencing could vary based on which isomer of a compound is present in a sample. For example, amphetamine and Lyric[®] (S-pregabalin) are drugs which may be legally available as a single optical isomer. Also, information about the route of synthesis and country of production can be gained from isomer analysis. Amphetamines and cathinones can be synthesized through several routes which may result in different isomer quantities in the final drug. While Gas Chromatography/Mass Spectrometry (GC/MS), High-Performance Liquid Chromatography (HPLC), and Ultra High-Performance Liquid Chromatography/Mass Spectrometry (UHPLC/MS) are capable of separating some structural isomers, they require chiral derivatization or chiral columns for separation of optical isomers; however, these procedures are time-consuming and/or expensive. Capillary Electrophoresis/Ultraviolet (CE/UV) and High-Performance Liquid Chromatography/Ultraviolet (HPLC/UV) are also used for structural and optical isomer identification, but they lack confirmatory compound identification capability. Therefore, the forensic community will benefit from a confirmatory technique that can provide structural and optical isomer identification with ease. This presentation introduces a simple CE/MS technique for identification of structural and optical isomers of illicit drugs using (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid (18-C-6-TCA) and Cyclodextrin (CD) derivatives as an effective background electrolyte that can provide optimum separation and high sensitivity detection of chiral compounds.

Analyses were performed using narrow (<20µm inner diameter), underivatized fused silica capillaries utilizing a porous tip for CE/MS interface. Various chiral selectors such as 18-C-6-TCA and CD derivatives were used as background electrolytes for CE/MS analyses. Samples were injected hydrodynamically and separations occurred at 25kV.

The separation of R- and S-pregabalin was achieved using only 18-C-6-TCA in approximately ten minutes. Quantitative studies showed a linear trend across three orders of magnitude between $1\mu g/mL$ and $1,000\mu g/mL$. Furthermore, analysis of a Lyrica[®] tablet resulted in only one electrophoretic peak confirming the compound optical purity. In addition to pregabalin, the optical isomers of cathinone and nor-mephedrone (metabolite of mephedrone) formed complexes with 18-C-6-TCA, which allowed for their separation. The optical isomers of amphetamine and methamphetamine were separated using highly sulfated γ -CD. Future work includes analyzing more drugs whose chirality is important either due to scheduling or for intelligence purposes.

Using a background electrolyte containing 18-C-6-TCA or CD, CE/MS allows for the separation and high sensitivity detection of isomers.

Illicit Drugs, Optical Isomers, CE/MS