A143 Chiral Separation of Amphetamine Type Substances Using Ion Mobility Spectroscopy- Mass Spectrometry

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After attending this presentation, attendees will be introduced to a novel technique, Chiral Ion Mobility Spectrometry (CIMS), which may be used for the separation of controlled and non-controlled enantiomers found in amphetamine type substances (ATS). The presentation will highlight both the degree of separation of enantiomers found in amphetamine type substances utilizing inexpensive achiral modifiers and the mechanism by which these separations take place and coupled to a mass spectrometer for unambiguous identification of the ATS compounds of interest.

This presentation will impact the forensic science community by describing a novel method for chiral separations offering advantages over the more time consuming and expensive methods currently in use. The high cost of chiral separation chromatography columns, the time needed, and the complexity is somewhat problematic for routine use. CIMS is a possible solution to these challenges by providing a high speed and low cost analytical technique not only for chiral separations but also as potential high throughput general drug analysis technique.

Chiral Separations have been a challenging aspect of analytical chemistry. There currently exists thousands of chiral separation phases predominantly used in liquid chromatography, gas chromatography and some capillary electrophoretic assays. The chiral phases themselves are expensive, while the time and resources required in selecting an appropriate phase for a particular enantiomer adds complexity. This presentation highlights a proposed separation mechanism when using achiral modifiers in the gas phase to separate enantiomers found in Amphetamine Type Substances (ATS). The presentation will show, for the first time, the use of straight chain achiral alcohols as drift gas modifiers and propose a mechanism for the gas phase chiral interactions responsible for the separations. Experimental results suggest that the interaction between the modifier and the analyte is ion-neutral based, with numerous modifiers adducting to a single analyte molecule. This interaction has been exploited to produce the desired separation of enantiomers of forensic interest using inexpensive achiral modifiers as opposed to the more expensive enantiomerically pure chiral modifiers such as S-2-Butanol. Common precursors used to make methamphetamine are ephedrine and pseudoephedrine, both chiral in nature. The ability to detect and separate these enantiomers as impurities in seized drugs has proven valuable as a forensic tool in many criminal investigations and has also been used for drug provenance studies. Achiral modifiers are used to separate RS and SR Ephedrine from SS and RR Pseudoephedrine. The resulting ion clusters formed have been characterized utilizing electrospray ionization to feed an ion mobility spectrometer coupled to a quadrupole mass spectrometer. The experimental data suggests that gas-phase chiral separations are possible and outlines a new, fast, and effective tool that may ultimately identify synthetic pathways and provide fast analysis and identification of seized amphetamine type substances.

This presentation will describe the capabilities of gas-phase chiral separations using commercially available electrospray ionization (ESI) ion mobility mass spectrometry (IMS-MS), to quickly separate and identify enantiomers introducing achiral modifiers into the drift gas. This approach provides an alternative technique to the more commonly used gas, liquid and capillary electrophoretic assays that are currently slower and more costly to perform. The proposed mechanisms of the separation will also
be discussed.

Ion-Mobility, Chiral, Mechanism

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