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Rapid Distinction and Assignment of Positional Isomers of New Psychoactive Drugs in Mixtures by Trapped Ion Mobility Mass Spectrometry

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Summary

New psychoactive substances (NPS) are structural derivatives of conventional illicit drugs, designed to circumvent the law. Some NPS are positional isomers of the original drug and pose a challenge to identify confidently in forensic casework, often requiring laborious and time-consuming approaches. Here we present a new trapped ion mobility mass spectrometry (TIMS-MS) method for the fast and highly selective analysis of NPS isomers found in real cases. Solutions of (mixtures of) cathinones were directly infused into a TIMS-time-of-flight mass spectrometer via electrospray ionization (positive mode) requiring no or only little sample preparation. The study focused on cathinones, a popular class of NPS comprising a large number of positional isomers. The suitability of the new method for the highly accurate identification of cathinone isomers in challenging mixtures will be demonstrated.

Applying TIMS-MS, each individual cathinone exhibited a bimodal mobility distribution due to the presence of protomers, leading to a complex profile of convoluted peaks when isomer mixtures were analyzed. However, addition of a neutral crown ether to the sample prior to TIMS analysis, resulted in a single peak for each cathinone isomer, which greatly reduced the complexity of the obtained mobilograms and facilitated the analysis of mixtures. Recorded mass spectra and extracted-ion-mobilograms were processed with an in-house developed script. Based on TIMS-MS data acquired for pure standards, a model was created that allowed accurate deconvolution of mobilograms of isomer mixtures. This way, the NPS composition of unknown samples could be established, revealing the relative contribution of individual isomers to the total MS signal. Relative amounts down to 10% could assigned reliably. The developed workflow was successfully used for the unambiguous identification of NPS isomers in confiscated forensic case samples in less than 5 min per sample.