B73 An Evaluation of the Repeatability, Reproducibility, and Uncertainty of Retention Indices and Electron Impact Spectra of Selected Novel Psychoactive Substances (NPS)

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After attending this presentation, attendees will be familiar with ongoing work related to the characterization and identification of NPS.

This presentation will impact the forensic science community by disseminating current results related to forensic identification of NPS and uncertainties associated with retention indices and Electron Ionization (EI) ion abundances.

The analytical challenges presented by synthetic cannabinoids and cathinones (NPS) include the lack of reference materials and the rapid appearance of new synthetic variants. Consequently, the traditional forensic identification tools cannot keep pace with the flow of new structures and compounds appearing in physical and toxicological evidence. The structural similarity among families of NPS may afford tentative identifications or classifications, but laboratories often must report inconclusive results and new variants may go unrecognized for some time. This can have implications in law enforcement as well as public health, given the range of toxic effects being associated with ingestion of many of these drugs.

A long-term goal of this project is to develop algorithms capable of classifying novel synthetics based on structure and to create similarity measurements that can characterize new NPS as compared to existing and known structures; however, before this goal can be achieved, verified and validated data and figures of merit must be established for the necessary measurands: retention time/retention index and mass spectra; specifically, relative ion abundances. There is no point in attempting to build a quantitative predictive model for mass spectral identification without knowing how much relative ion abundances vary across time and instruments. Reported here are results to date of a selected group of NPS compounds (JWHs, UR-144, and cathinones, as well as methamphetamine and amphetamine) analyzed using three different GC/MS systems over time. All instruments are models commonly used in forensic science laboratories. Variables recorded included tuning conditions, elapsed time since tuning, time since inlet change, time since column maintenance, and all relevant instrumental settings. Retention indices were calculated relative to a C7-C30 alkane ladder. Three levels of sample concentrations were examined: near the detection limit, mid-range, and near the upper end of the linear dynamic range of the instrument. DB-1 and DB-5 columns of different lengths were used. Sample concentrations were at low (close to the method detection limit), mid-range, and high concentrations. Ion repeatability and reproducibility were determined based on the ratios of the ten most abundant ions in the spectrum. In cases in which ions were critical for identification but not one of the top ten abundant, these ions were included and characterized. Figures of merit to date for all instruments will be presented and initial estimates of uncertainty will be presented.

Novel Psychoactive Substances, Uncertainty Estimation, GC/MS