K79 The Development and Validation of an Analytical Method for the Identification of New Psychoactive Substances (NPS) Using the Retention Index and Gas Chromatography/Mass Spectrometry (GC/MS)

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Learning Overview: After attending this presentation, attendees will understand NPS and the application of some principles of GC and retention indices to identify controlled substances.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by proposing a validated GC/MS analytical method that could eliminate or minimize the need for NPS analytical standards to perform systematic illicit drug identification. This method is suitable for laboratorial forensic routine after a simple validation protocol.

The United Nations Office on Drugs and Crime (UNODC) defines NPS as "substances of abuse, either in a pure form or a preparation, that are not controlled by the 1961 Single Convention on Narcotic Drugs or the 1971 Convention on Psychotropic Substances, but which may pose a public health threat."[1] The rate at which these substances are introduced into the market poses a challenge to both regulatory and law enforcement institutions.

In 2016, Brazil adopted a generic classification for the synthetic cannabinoid group, the most widespread NPS class worldwide, to anticipate controls upon the arrival of new substances in the country. After that, a generic classification for synthetic cathinones was also included as a controlled group.

Additionally, forensic science institutes in Brazil have faced analytical challenges when dealing with the unequivocal identification of these new seized substances. Some of these challenges are related to the unavailability of analytical chemical standards due to changes to the functional groups in the molecule during synthesis, the slow rate of commercial production in comparison with drug market changes, high costs, etc.

To work around this problem, the present work benefits from Kovátz Retention Indices, which make use of a homologous n-alkane series to both reference and normalize retention times. This type of retention index has been used for high accuracy chemical compound identification with relative standard deviations smaller than 0.35% in the case of illicit drugs.[2,3] It allows for inter-laboratory applicability and verification, and it is robust under different gas flow conditions.[4]

The proposed GC/MS method has been validated with resolution, robustness, and precision measures as figures of merit. A mixture of 21 drugs have been tested to cover as much of the elution time window as possible. The mix was composed of three synthetic cannabinoids (AM-2201, MAM-2201, JWH-081), one cathinone (N-ethylpentylone), three phenylethylamines (5-MAPB, 2-FA, 25C-NBOMe), two piperazines (o-CPP, p-CPP), one opioid (U-47700), one tryptamine (5-MeO-MiPT), one aminoindane (5-IAI), one of vegetal origin (*Salvia divinorium*), methiopropamine, and seven traditional drugs (THC, heroin, amphetamine, methamphetamine, MDMA, cocaine, ephedrine). The GC/MS method has shown to present enough resolution to separate the majority of compounds. One coelution occurred between methiopropamine and methamphetamine. In such cases, mass spectra interpretation may be used in compound disambiguation. The lowest resolution (1.09) was obtained for N-ethylpentylone. The smallest Kováts index difference (4.9) occurred between amphetamine and 2-FA.

These preliminary results seem to indicate the association of Kováts indices with GC/MS as an efficient, low-cost, easy-to-adapt alternative to forensic labs in both the identification and categorization of NPS.

Reference(s):

1. https://www.unodc.org/LSS/Page/NPS.
2. Imhoi Koo, Xue Shi, Seongho Kim, Xiang Zhanga. Compound Identification Using Retention Index for Analysis of Gas Chromatography–Mass Spectrometry Data. *Journal of Chromatography A*. 2014; 1337: 202-210.
3. Kelly K, Bell S. Evaluation of the Reproducibility and Repeatability of GCMS Retention Indices and Mass Spectra of Novel Psychoactive Substances. *Forensic Chemistry*. 2018; 7: 10–18.
4. V.I. Babushok, P.J. Linstrom, J.J. Reed, I.G. Zenkevich, R.L. Brown, W.G. Mallard, S.E. Stein. Development of a Database of Gas Chromatographic Retention Properties of Organic Compounds. *Journal of Chromatography A*. 2007; 1157:414-421.

New Psychoactive Substances, Gas Chromatography/Mass Spectometry, Kovátz Retention Indices