New psychoactive substances in forensic drug cases: Strategies to tackle the drug isomer challenge

Ruben F. Kranenburg[1,2], Arian C. van Asten[2,3]

[1] Dutch National Police, unit Amsterdam, Forensic Laboratory

[2] Van 't Hoff Institute for Molecular Sciences, University of Amsterdam (UvA)

[3] Co van Ledden Hulsebosch Center, Amsterdam Center for Forensic Science and Medicine, UvA

The illicit-drug market is facing the rise of many synthetic substances closely related to traditional drugs such as amphetamine and MDMA. These so-called Novel Psychoactive Substances (NPS) often comprise of isomeric compounds with legal control varying per individual isomer. Drug isomer differentiation has therefore become a relevant problem in forensic drug analysis laboratories.

Established methods, such as Gas Chromatography–Mass Spectrometry (GC–MS), fall short in terms of selectivity, as isomeric NPS have identical masses, very similar fragmentation spectra and can co-elute in fast screening methods. In forensic laboratories, a need has arisen for efficient analytical methods capable of distinguishing NPS isomers in drug mixtures or tablet formulations.

Three new strategies were investigated to overcome the isomeric NPS dilemma:
1) Vacuum ultraviolet (VUV) spectroscopy provides distinctive spectra for ring-isomers. Also, GC-VUV is complementary to GC–MS for certain NPS classes consisting of both ring- and aliphatic chain isomers.
2) Low-energy electron ionization (EI) produces less fragmented, more information-rich, mass spectra for NPS isomers allowing for ring-isomeric differentiation.
3) Multivariate statistics were applied to discriminate among ring-isomers. Principal Component Analysis – Linear Discriminant Analysis (PCA–LDA) models reveal intrinsic ring-isomer selectivity in visibly similar 70 eV mass spectra.