

FORENSIC LITERATURE THESIS

LITERATURE THESIS

Title	: <i>Positional Isomer Differentiation for NPS Analysis</i>
Keywords	: Illicit drugs, New Psychoactive Substances, Isomers
Forensic Expertise Area	: <i>Forensic Chemistry, Instrumental Analysis</i>
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SHORT DESCRIPTION

As of August 2020, 125 countries and territories have reported the appearance of over 1000 individual New Psychoactive Substances (NPS) since monitoring began in 2008.¹ This ever-changing NPS landscape has resulted in many analytical challenges for forensic drug chemists. Frequently, NPS are introduced to the scene whose chemical structures only differ from existing drugs of abuse by the addition, subtraction, or relocation, of a single chemical moiety. Substances that share the same molecular formula and core structural backbone but only differ in the precise placement of a single atom or functional group are considered positional isomers², and they can be difficult to differentiate using a typical forensic analytical scheme.³ Depending on the jurisdiction, positional isomers of controlled substances are not always covered under existing legislation,⁴⁻⁷ making the ability to distinguish them of utmost importance.

To combat this problem, a substantial amount of research has been conducted in recent years to identify new and improved methods of positional isomer differentiation. Some methods suggested include statistical analysis of data generated from typical forensic instrumentation,⁸⁻⁹ alternative sample preparation by derivatization,¹⁰ as well as the application of instrumentation that is not currently commonly used by the typical forensic drug laboratory.¹¹⁻¹³ The aim of this literature thesis is to explore the research that has been conducted to address the challenge of positional isomer differentiation in order to summarize the options currently available for forensic drug laboratories.

REFERENCES

1. United Nations Office on Drugs and Crime, Global Synthetic Drugs Assessment 2020. Vienna, 2020.
2. Title 21 Code of Federal Regulations §1300.01 Definitions relating to controlled substances. <https://www.law.cornell.edu/cfr/text/21/1300.01> (accessed 1 April 2021).

3. S.D. Brandt, P.V. Kavanagh, Addressing the challenges in forensic drug chemistry. *Drug. Test. Anal.* 9(2017) 342-346.
4. 21 U.S. Code § 812 – Schedules of controlled substances <https://www.law.cornell.edu/uscode/text/21/812>, 1970 (accessed 1 April 2021).
5. Title 21 Code of Federal Regulations §1308.11 – Schedule I. <https://www.law.cornell.edu/cfr/text/21/1308.11> (accessed 1 April 2021).
6. Code of Virginia, § 54.1-3446. Schedule I. <https://law.lis.virginia.gov/vacode/title54.1/chapter34/section54.1-3446/> (accessed 1 January 2021).
7. Netherlands Opium Act 2020, <https://wetten.overheid.nl/BWBR0001941/2020-11-17> (accessed 1 April 2021, translated from Dutch)
8. E.L. Stuhmer, V.L. McGuffin, R.W. Smith, Discrimination of seized drug positional isomers based on statistical comparison of electron-ionization mass spectra. *Forensic. Chem.* 20(2020) 100261.
9. J. Bonetti, Mass spectral differentiation of positional isomers using multivariate statistics. *Forensic Chem* 9(2018) 50-61.
10. R.F. Kranenburg, J. Verduin, L.I. Stuyver, R. de Ridder, A. van Beek, E. Colmsee, A.C. van Asten, Benefits of derivatization in GC–MS-based identification of new psychoactive substances. *Forensic. Che.* 20(2020) 100273.
11. R.F. Kranenburg, F.A.M.G. van Geenen, G. Berden, J. Oomens, J. Martens, A.C. van Asten. Mass-Spectrometry-Based Identification of Synthetic Drug Isomers Using Infrared Ion Spectroscopy. *Anal. Chem.* 92(2020) 7282-7288.
12. W., Cheng, W., Wong, Forensic drug analysis of chloro-N,N-dimethylcathinone (CDC) and chloroethcathinone (CEC): Identification of 4-CDC and 4-CEC in drug seizures and differentiation from their ring-substituted positional isomers. *Forensic. Sci. Int.* 298(2019) 268-277.
13. R.F. Kranenburg, A.R. Garcia-Cicourel, C. Kukurin, H., Janssen, P.J. Schoenmakers, A.C. van Asten. Distinguishing drug isomers in the forensic laboratory: GC–VUV in addition to GC–MS for orthogonal selectivity and the use of library match scores as a new source of information. *Forensic. Sci. Int.* 302(2019) 109900.

REQUIRED/RECOMMENDED EXPERTISE

- Basic understanding in forensic chemistry. Familiarity with analytical instrumentation and data analysis is recommended.

