B161 Low-Field Nuclear Magnetic Resonance (NMR) Applications in Forensic Drug Analysis

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After attending this presentation, attendees will understand the potential utility of low-field NMR spectroscopy in the qualitative and quantitative analysis of drugs. This presentation will focus on the use of low-field NMR as a substitute for high-field NMR for differentiating structural isomers of New Psychoactive Substances (NPS) that can be difficult to distinguish with other methods. The use of low-field NMR to provide accurate quantitation will also be discussed.

This presentation will impact the forensic science community by suggesting an alternative to current methods employed by forensic laboratories that have limitations for confirming specific positional isomers. This presentation will demonstrate that low-field NMR can be a suitable technique by using examples from several drug classes. Limitations of the technique will also be discussed.

Forensic laboratories commonly receive new synthetic cannabinoids, cathinones, and opioids that are difficult to report. Slight changes to chemical structures (e.g., shifting the position of functional groups, such as methyl groups or halogens, around an aromatic ring) can cause problems with identification using traditional methods. Classic gas chromatography/mass spectrometry cannot easily distinguish between certain positional isomers.

NMR is a powerful tool used to elucidate the structure of these isomers using 1D and 2D spectra from ^{1}H, ^{13}C, ^{19}F, and ^{15}N nuclei probes to assign elements to their specific position on the molecule. High-field NMR is typically used for these determinations but is not practical in many forensic laboratories due to the cost of the instrumentation as well as cryogen, facility, and staff requirements. In contrast, low-field NMR is less costly, has a smaller footprint, does not need cryogens, and requires little maintenance; however, this comes at the cost of spectral resolution and sensitivity.

This study evaluated the use of ^{1}H NMR on low-field benchtop NMR (60 MHz) and 600 MHz systems to differentiate positional isomers of several classes of NPS. The positional isomers were readily differentiated on both instruments, as expected. The use of quantum mechanic spin system modeling of ^{1}H spectra on the high-field system for portability of experimentally observed spectra to other magnet field strengths was also investigated and successfully demonstrated by transforming 600 MHz spectra to 60 MHz. This capability suggests that the generation of field-strength independent spectral libraries may be feasible and would facilitate data dissemination across instruments without the need to acquire a large collection of reference spectra.

Quantitation based on NMR is unique in that it can be performed relative to a distinct reference compound without requiring a calibration curve derived from the analyte of interest as utilized commonly in chromatographic methods. Purity determination for certain drugs (e.g., methamphetamine) can affect sentencing guidelines and can also be used by law enforcement for intelligence purposes. This study also explored the use of low-field NMR for quantifying methamphetamine in commonly encountered sample mixtures to mimic casework.

Low-Field NMR, New Psychoactive Substances, Methamphetamine

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