B17 Rapid Identification of Designer Drugs With Nuclear Magnetic Resonance (NMR) Spectroscopy

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After attending this presentation, attendees will understand the principles of Nuclear Magnetic Resonance (NMR) spectroscopy and how it can be applied to the rapid characterization and identification of designer drugs. Attendees will also learn about the power of combining multiple NMR techniques, such as proton spectroscopy, Correlation Spectroscopy (COSY), Total Correlation Spectroscopy (TOCSY), and Diffusion Ordered Spectroscopy (DOSY) in the analysis of designer drug samples. TOCSY can provide information about long-range proton-proton interactions, allowing for accurate identification with extra 2D molecular "fingerprints" beyond COSY. DOSY has the potential to separate the components of a mixture based on their diffusion coefficients. Consequently, signals from solvents and other materials can be separated from synthetic cannabinoid signals without chromatographic separations.

This presentation will impact the forensic science community by introducing a simple but highly discriminatory NMR procedure that can be used to quickly identify a wide variety of designer drugs such as "Spice" (synthetic cannabinoids), "Molly" (phenethylamines), and "Bath Salts" (cathinones).

Designer drugs are a persistent problem for forensic laboratories. As the government bans synthetic cannabinoids, phenethylamines, and cathinones, those who produce these substances create new substances to maintain the legality of their business. The ever-changing nature of this market can be a burden to forensic laboratories that receive large amounts of seized materials containing unfamiliar substances.

The proposed methodology expands upon the laboratory's previous work in which proton and COSY NMR methods were developed to quickly identify and quantify synthetic cannabinoids in herbal samples. The whole analytical process took less than one hour after cannabinoids were extracted from 50mg of herbal incense with an NMR solvent such as $CDCl_3$. The same simple pre-NMR sample preparation technique is preserved to rapidly obtain NMR results. The current expansion includes incorporating more NMR techniques such as TOCSY and DOSY. TOCSY experiments were performed on herbal samples with previously known synthetic cannabinoids. These experiments revealed that signals coming from the alkyl region of the cannabinoid molecules can be elucidated further, as this is a region where signals tend to overlap or may be hard to assign with proton NMR and COSY. DOSY experiments with herbal samples successfully separated solvent and other materials from cannabinoid signals in samples that contain only one cannabinoid. Due to signal overlap, separation based on diffusion coefficient is extremely difficult in samples containing multiple cannabinoids. As of now, signals from two different cannabinoids cannot be separated efficiently using DOSY.

The original methodology is further expanded to include additional designer drugs typically found in "Molly" and "Bath Salt" mixtures. Eleven phenethylamine and cathinone standards were characterized using proton-NMR and COSY with similar parameters compared to the synthetic cannabinoid experiments, with the exception of D_2O as the NMR solvent. Potential signature peaks were identified that could be utilized to quickly identify the components of a street sample. Compared to the results from liquid chromatographic separation with Diode Array Detection (DAD) on the same standards, NMR proves to be a more reliable process at the identification because many of the substances are fairly similar, often isomers of each other, and therefore elute at similar times.

In conclusion, the addition of TOCSY and DOSY NMR methods can improve the discriminatory power of NMR for the identification of synthetic cannabinoids in herbal incense blends. The NMR parameters can also be successfully applied to other designer drugs. These methodologies could be valuable screening tools for backlog reduction, allowing analysts to quickly obtain "fingerprints" of the substance while preserving the original sample for further testing.

Designer Drugs, NMR, TOCSY