B175 Solid State Nuclear Magnetic Resonance (NMR) of Street Drugs — The New Presumptive Drug Test

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After attending this presentation, attendees will understand the effectiveness of NMR analysis in relationship to preemptively identifying unknown street drugs.

This presentation will impact the forensic science community by offering a new method of preemptively determining the identity of an unknown compound.

Solid state NMR has proven itself to be an interesting new tool for obtaining quick, easy, and inexpensive NMR spectra for research and instructional purposes. It can also be used to attain spectral profiles on pure samples of drugs that produce "legal highs." This work attempts to create an NMR database of synthetic compounds known to be in use recreationally or analogs thereof. Such a library would be useful to those working in crime laboratories to identify unknown chemical compounds found at crime scenes. This test is more accurate than a color indicator and is easier to administer than a traditional mass spectrometric analysis. A single test requires only 20 minutes and is very cost effective.

Major classes of compounds tested include psychedelics, cathinones, and cannabinoids. Standard samples were provided by Cayman Chemical and street samples were provided by the Pennsylvania State Police. These street samples were mostly mixtures of compounds, most notably XLR-11, PB-22, and AB-Fubinaca. Compounds were dissolved in the appropriate deuterated solvent and centrifuged to insure the compounds completely dissolved. Any sample that crashes out of solution during injection could prove dangerous to the inner line of the instrument. The line was purged before and after each test with the corresponding solvent, then the instrument was shimmed with deionized water.

The standards' spectra are comparable to those of the samples. An interactive library will be compiled so a drug profile can be quickly compared against a library and a presumptive identity can be established. This method will not be meant to definitively identify an unknown compound but it can aid in rapid presumptive analysis so that follow-up analyses are more targeted.

Since NMR measures excitation in proton nuclei and not fragmentation patterns, a consistent result of a given compound is not always guaranteed; however, NMR will consistently give a general profile of a given compound. If there is no discrepancy in shimming and solvent choice, NMR can be used to compare spectral similarities among unknown compounds. A quick and easy presumptive test for drugs, provided by the solid-state NMR, can be useful to save time on a more in-depth instrument and accurately identify at least the class of compound of a known substance.

NMR, Cathinones, Presumptive Test