E85 Nuclear Magnetic Resonance (NMR) Spectroscopy as a Screening Agent for Designer Opioids

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After attending this presentation, attendees will understand the utility of NMR spectroscopy as a screening agent for designer opioids.

This presentation will impact the forensic science community by revealing a new, non-destructive approach to qualitatively and semi-quantitatively analyze pure opioid standards and mock street sample mixtures after minimal sample preparation.

The formulations of synthetic opioids are constantly changing to maintain their legal statuses. These new drugs, often with equivalent or higher potency compared to traditional opioids, are typically derivatives or analogues of controlled substances such as heroin and fentanyl. The lack of analytical standards and the evolving formulation make it increasingly difficult for forensic scientists to identify these new designer drugs.

In this preliminary proof-of-principle study, 16 designer opioids were analyzed with proton NMR, proton-proton Correlation Spectroscopy (COSY), and Total Correlation Spectroscopy (TOCSY). For each sample, 1mg of the drug in solid powder form was dissolved in 0.75ml of either $CDCl_3$ or D_2O, depending on its solubility prior to NMR scans. Then, 1,024 1H-NMR scans were run, lasting two hours. There were 16 COSY and TOCSY scans run per sample, lasting two hours per sample. After the standards were analyzed, mock street samples were prepared by adding caffeine, acetaminophen, and glucose to one of the standards and running proton and COSY scans. A similar method was used in previous studies to rapidly scan for synthetic cannabinoids.[1]

The preliminary results proved that several signature signals in the proton NMR spectra of designer opioids can be used for rapid screening and identification. The three potential signature signal ranges include 6.52ppm–8.28ppm, 4.59ppm–4.76ppm, and 3.02ppm–3.53ppm. Due to structural differences, some designer opioids did not produce a signature signal, which was expected and can be used to exclude certain compounds. For example, most fentanyl derivatives produced a signal in the range 4.59ppm–4.76ppm; however, opioids that are not fentanyl derivatives do not have this signature signal in their spectra. Of the 16 designer opioids analyzed, 15 produced at least one signal within the range 3.02ppm–3.53ppm. The COSY spectra and TOCSY spectra confirm the interactions between the protons on the benzene rings and alkane regions. In the COSY spectra of fentanyl derivatives, there is an interaction between the protons that produced the signals in the range 3.02ppm–3.20ppm. The opioid signature signals could still be isolated and identified from a mixture profile even in the presence of minimal interference (peaks move <.05ppm) or overlap contributed by the cutting agents. The NMR method also enhances the identification of additional isomers in a mixture.[2] Additionally, the proton NMR peaks were integrated and peak areas were utilized to provide semi-quantitative compositions of the opioids and cutting agents within each mixture.

Non-destructive NMR investigation on designer opioids will allow rapid screening of opioids, while also providing semi-quantitative analysis of the substances in mixed street samples. Subsequent GC/MS analysis can still be performed to confirm the identification. The NMR methods will potentially assist investigators in the prediction of the next designer opioid and help law enforcement keep up with new formulations of designer opioids.

Reference(s):

1. Fowler et al. Screening and quantification of synthetic cannabinoids in herbal products with NMR spectroscopic methods. *Anal. Methods.* 7.18 (2015): 7907-916.

2. Marino et al. Rapid Identification of Synthetic Cannabinoids in Herbal Incenses with DART-MS and NMR. *Journal of Forensic Science.s* 61 (2015): S82-S91.

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