A182 Identification and Quantification of Synthetic Cannabinoids in Herbal Products With NMR

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After attending this presentation, attendees will understand the fundamental principles of Nuclear Magnetic Resonance (NMR) spectroscopy, specifically their applications for rapid detection of synthetic cannabinoids in herbal incenses. The attendee will also appreciate the power of combining proton NMR with 2D NMR techniques to promptly elucidate the accurate structures of cannabinoids with no ambiguity and quantify cannabinoids in herbal incenses through the use of proton NMR.

This presentation will impact the forensic science community by introducing a simplified NMR spectroscopic approach to quickly identify and quantify synthetic cannabinoids and isomers found in herbal incenses.

In addition to the five classes of cannabinoids scheduled in S. 3187, three new compounds were temporarily added to the Schedule I controlled substance list in 2013. Newer compounds are being synthesized promptly and relentlessly to circumvent the ban, which exacerbates the analytical difficulties for forensic labs, some of which are still experiencing backlogs.

This hypothesis implements the use of proton-NMR and proton-proton correlation NMR spectroscopy (COSY) to positively identify and quantify synthetic cannabinoids in herbal products with minimal sample preparation, all of which can be completed within two hours with eight-minute or shorter NMR scans.

Prior to the NMR study, a simple extraction was employed in 1-mL NMR solvent such as deuterated chloroform ($CDCl_3$) or d6-acetone to remove synthetic cannabinoids from 50mg of solid herbs. After a one-minute proton-NMR scan in $CDCl_3$, synthetic components were detected and processed. Subsequently, signature chemical shift values were retrieved and used to identify the synthetic cannabinoids. Most signature peaks from indole cannabinoids were found to be in the 6.5-8.5ppm or 3.8-4.5ppm chemical shift ranges, which do not overlap with the herbal background signals from blank herbal extracts. An eight-minute COSY scan in $CDCl_3$ on the same sample further confirmed the identities of the cannabinoids, particularly in the 2-D “fingerprint” regions. After four-minute proton-NMR scans, as many as three cannabinoids in herbal products can be quantified with the presence of maleic acid as an internal standard and d6-acetone as the NMR solvent.

With the combination of proton- and COSY NMR, 38 herbal samples were rapidly screened for synthetic cannabinoids. Synthetic cannabinoids were found in all but three herbal incenses. Among the herbal samples investigated, AM-2201, JWH-122, JWH-210, RCS-4, XLR-11, and UR-144 were found to be the predominant ingredients. The quantitative NMR results are comparable to chromatographic quantification results, both yielding 0.5-40mg of cannabinoids per gram of herbal product. The standard deviation varies due to the uneven spreading of synthetic components on herbs during the manufacturing process.

In conclusion, accurate identification and quantification of synthetic cannabinoids in powder and herbal samples can be rapidly achieved with proton and COSY NMR. This simple NMR method can differentiate isomers such as JWH-019, JWH-180, and JWH-122. As an alternative to conventional GC/MS methods, this NMR method can help forensic chemists achieve accurate identification and quantification within two hours which increases the analytical throughput and could potentially help to decrease sample backlogs.

Cannabinoids, NMR, COSY

 ** Presenting Author*