B71 The Dealkylation of Secondary Amines in the Presence of Botanical Materials

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Learning Overview: After attending this presentation, attendees will understand the risk of false positive results associated with analytes containing secondary amines in the presence of certain botanical materials when using an acid/base extraction and gas chromatography/mass spectrometry (GC/MS) analysis.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by identifying a conversion of secondary amine containing compounds into possible controlled substances that could generate false positive results in forensic drug chemistry testing of botanical materials.

Botanical materials, such as marijuana and damiana, present complicated matrices to a forensic drug chemistry lab. The use of n-propylamphetamine as an internal standard for analysis through an acid/base extraction followed by Gas Chromatography/Mass Spectrometry (GC/MS), exhibited the dealkylation of the amine in the presence of certain botanical materials yielding amphetamine. Studies into the reaction parameters impacting the conversion suggest the potential for other n-substituted amphetamines and structurally similar secondary amines to dealkylate under similar conditions. This conversion may result in the production of compounds regulated by either state or federal law. Terefore, their presence in such samples can result in legal penalties despite the ambiguity of the source.

Botanical materials of a variety of species and families common in drug lab cases or everyday uses including Marijuana (*Cannabis L. sativa*), Damiana (*Turnera diffusa*), Marshmallow Leaf (*Althaea officinalis*), Kratom (*Mitragyna speciosa*) and numerous herbs from the *Lamiaceae* (mint) family were tested to determine with which materials this dealkylation may occur. Reference standards of common plant compounds such as chlorophyll A and B were also prepared as 1 mg/mL solutions in methanol. In addition to n-propylamphetamine, various other substituted amphetamine compounds were also tested including, methamphetamine, n-ethylamphetamine, n-butylamphetamine, ephedrine, mephedrone, and methcathinone.

An acid/base extraction was performed on the different botanical materials in water spiked with the various secondary amine compounds and tested by Gas Chromatography/Mass Spectrometry (GC/MS). An Agilent® DB-1 Capillary Column, 12 m X 200µm X 0.33 µm was used. Injection volume of 1 µL, splitless injection mode with constant pressure at an inlet temperature of 265°C and detection temperature of 300°C was used for all analyses.

First, all botanical materials were tested in the presence of n-propylamphetamine. Conversion to amphetamine was observed with Damiana leaf and leaf powder, Marshmallow leaf, chlorophyll A and chlorophyll B. The dealkylation of methamphetamine, n-ethylamphetamine, n-butylamphetamine, ephedrine and mephedrone was tested only with Damiana and Marshmallow leaves and was observed with both botanical materials for all secondary amine compounds in this study.

Mechanistic investigations indicate the potential for an oxidative n-dealkylation pathway catalyzed by a metal centered porphyrin ring. The difference in catalysis by different botanical materials can be explained by the degradation of this porphyrin structure as the plant ages after being harvested.

The dealkylation of secondary amine containing drugs in the presence of certain botanical materials raises legal questions regarding the source of the resulting primary amine-controlled substances identified during analysis. Identifying the factors and causes of this reaction are important for quality control in forensic drug chemistry labs.

False Positive, Botanical Materials, GC/MS