K38 A Metabolic Profile Determination of 2F-Viminol, A Novel Synthetic Opioid (NSO) Identified in Forensic Investigations

Aracelis A. Velez, BS, Wyncote, PA 19095; Alex J. Krotulski, PhD, Center for Forensic Science Research & Education, Willow Grove, PA 19090; Donna M. Papsun, MS, NMS Labs, Horsham, PA 19044; Karen S. Scott, PhD, Arcadia University, Glenside, PA 19038*

Learning Overview: After attending this presentation, attendees will know about the proposed metabolites of 2F-viminol through the visualization of elucidated metabolite structures and metabolic pathways that were determined from Liquid Chromatography/quadrupole Time-Of-Flight/Mass Spectrometry (LC/qTOF/MS) data obtained through analysis of human liver microsome incubations of the drug.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing information about an NSO with limited pharmacological characterization. The findings will also provide laboratories with biomarker information for the identification of this drug in toxicological samples, such as blood or urine.

Although minor progress has been made in the opioid epidemic, opioid-related deaths in many parts of the United States continue to rise or remain high as synthetic opioids become more prevalent. NSOs, including various fentanyl analogs as well as emerging non-fentanyl-derived compounds, have been identified in products for stand-alone use, as constituents of counterfeit preparations, and as adulterants in other common opioid products such as heroin. A particular new NSO, 2F-viminol, has been identified in casework at the Center for Forensic Science Research and Education through their Novel Psychoactive Substances (NPS) Discovery Program. Thus far, little information and published literature are available for this new opioid. Viminol, a previously developed opioid, is structurally similar and is chlorinated at the 2-position. Despite how structurally different viminol is from other subclasses of opioids, studies have shown it to display significant analgesic and pharmacological properties, comparable to those of morphine. The replacement of chlorine with fluorine on the molecule could make 2F-viminol a more potent drug than viminol, with considerable toxicity due to the prolonged half-lives and increased lipophilicity of fluorinated drugs; however, studies will need to be conducted to confirm this information.

Studying the metabolism of NSOs is crucial to identifying the products of biotransformation that a drug undergoes in the body after ingestion. Currently, there is no literature available with information regarding the metabolism of 2F-viminol. To address this, Human Liver Microsomes (HLM) were used to perform *in vitro* metabolism studies using a drug standard. The goal was to predict and confirm its *in vivo* metabolism. Experimental samples prepared using HLMs and 2F-viminol were analyzed via a SCIEX™ TripleTOF® 5600+ LC/qTOF/MS. The generated metabolic structures were elucidated using SCIEX™ MetabolitePilot™ software (version 2.0). Data features evaluated included formula, accurate mass and mass error, retention time, fragment data, and a proposed structure. After final data review, the primary metabolite(s) of 2F-viminol can then be confirmed in authentic samples and added to screening protocols, helping to extend the window of detection for the parent drug in toxicological samples. Overall, at least three metabolites of 2F-viminol were discovered, including N-dealkylated species.

Novel Synthetic Opioid, Metatbolism, Toxicology

*Presenting Author