

Project Title: Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)	
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NIJ Forensic Science R&D Symposium Presentation Title (please note this title will be used for future marketing materials): Developing an Approach to Standardize the Naming of Novel Psychoactive Substances (NPS)	
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<p>Developing an Approach to Standardize the Naming of Novel Psychoactive Substances (NPS)</p> <p>Alex J. Krotulski*, Sara E. Walton, Max Denn, Brianna Stang, Barry K. Logan</p> <p>Center for Forensic Science Research and Education, Fredric Rieders Family Foundation, Willow Grove, PA</p> <p>Novel psychoactive substances (NPS) continue to appear in forensic casework with increasing regularity as they are mixed with or substituted for traditional drugs or purchased online as legal or alternative “highs”. When NPS are detected by forensic laboratories, their name (and associated identity) is reported on the final forensic report. This information is utilized downstream by various local, state, and federal agencies, including medical examiner and coroner offices certifying deaths and the CDC consolidating information on drug morbidity and mortality. The accurate reporting and tracking of NPS are contingent on the proper use of nomenclature and consistency between laboratories. Mismatches in NPS naming (e.g., <i>N,N</i>-dimethylpentylone vs. dipentylone) can cause unnecessary confusion and mistakes in communication, interpretation, and reporting. A central authority on NPS naming is needed; however, the framework for naming must first be established.</p> <p>NPS nomenclature is complex and not all substances under the NPS classification are necessarily “new”. Some are derived from previous pharmaceutical drug discovery patents but repurposed for illicit use, while others are “old” drugs that have resurfaced and/or are being used in a new or</p>	

different way. Some drugs are named based on initials of the inventor and numbers based on the series in which they are discovered (e.g., JWH-018 and John W Huffman). Some drugs are named based on abbreviations of their structure features with numbers (e.g., AP-237 and aryl piperazine). Some drugs are given fabricated names that become common language (e.g., fentanyl, etonitazene, alprazolam).

The Center for Forensic Science Research and Education (CFSRE), through its NPS Discovery program and in collaboration with Cayman Chemical, has launched an initiative to help standardize the manner in which NPS are named. The goal is to develop tools and techniques with enhanced workflows to name new and old drugs more accurately and comprehensively. This will allow storage and consolidation of information in a database that is easily accessible and searchable, and rapid dissemination of information about the existence of drugs, literature, trends, effects, etc. to the forensic science community.

Currently, the CFSRE and Cayman Chemical are developing naming resource documents for synthetic cannabinoids and NPS opioids, specifically the nitazene analogues. Synthetic cannabinoid naming is the most structured under the NPS umbrella, using a semi-systematic alpha-numeric scheme that correlates back to the structure. However, with the constant emergence of new synthetic cannabinoids, this process needs to be documented yet flexible to include evolving chemistries. Recent emergence of the synthetic cannabinoids BZO-HEXOXIZID (formerly MDA-19) and CHO-4'Me-5'Br-FUBOXPYRA (formerly CH-FUBBMPDORA) are examples of our naming efforts and ways it has helped standardize the language across the forensic science community. For the nitazene analogues, all names are based on the prototypical drug in the series, etonitazene. Modifications to etonitazene are reflected within the name and/or as prefixes. *N*-Pyrrolidino etonitazene is an example of our naming efforts within this group.

The primary outcome of this initiative will allow the forensic science community to become more standardized with drug naming and will avoid unnecessary communication issues between forensic laboratories, reporting entities, and other stakeholders.