

# National Institute of Justice

**Award Title:** Characterization of Designer Drugs: Chemical Stability, Exposure, and Metabolite Identification

**Award Description:**

Designer drugs such as synthetic cannabinoids and cathinones have become increasingly prevalent in recent years, as have their interrelated health and societal consequences. The objective of this research proposal is to gain a more thorough understanding of designer drugs with respect to their chemical exposure profile and biological elimination pathways. This will be accomplished through two main research goals: 1) determining the stability of currently popular designer drugs and identifying major degradation products, including pyrolysis products; and 2) identifying their major metabolites. The study will initially focus on compounds from the JWH and AM series of synthetic cannabinoids and progress to synthetic cathinones, followed by emerging designer drugs as they become prevalent. Emerging designer drugs will be chosen and prioritized by their relevance to forensic practitioners, with guidance from partnership with the Virginia Department of Forensic Science and other forensic laboratories identified over the course of the proposed project. Compounds selected for analysis will undergo identity confirmation and be analyzed for purity using chromatographic techniques followed by forced degradation studies from which major degradation products will be identified. The designer drugs will then undergo pyrolysis studies, and major pyrolysis products of each sample will be identified. For compounds with reported routes of use that include smoking, RTI International will prepare samples in a manner representative of how users report preparing doses, and smoke them using a cigarette smoking machine. Major components of both mainstream and side-stream smoke will be determined, as well as dosage yields from mainstream smoke. Parent compounds and select degradation and/or pyrolysis products will be incubated with lung microsomes and liver hepatocytes for in vitro metabolite identification. Data analysis will be accomplished using sophisticated data interrogation techniques, such as mass defect filtering of high-resolution mass spectrometry (MS) data. Most forensic laboratories are not equipped with the research capabilities required to keep up with the rapid turnover of designer drugs being marketed for recreational use. As a non-profit research institute, RTI has access to equipment and facilities, such as high-resolution mass spectrometers and nuclear magnetic resonance (NMR) imaging instruments not typically found in forensic laboratories. Identification of metabolites; degradation products, including pyrolysis products; and components of smoke from herbal formulations will aid in understanding the effects these compounds and routes of exposures have on the human body. By performing a thorough and systematic study, we may be able to predict markers of use for broad classes of compounds and help practitioners keep up with designer drug manufacturers. In addition to submitting quarterly financial reports, semi-annual progress reports, and a final report to the National Institute of Justice (NIJ), RTI plans to publish study results in prominent journals and present the results at annual meetings of leading forensics organizations. Photographs of each designer drug characterized and their mass spectra, including electron impact-mass spectrometry (EI-MS) spectra and liquid chromatography-mass spectrometry LCMS) fragmentation spectra indicating optimal transitions to monitor for identification of compounds, will be made available to forensic laboratories through an NIJ-funded Web-accessible database, [www.forensicdb.org](http://www.forensicdb.org). All analytical data, along with quarterly financial, semi-annual progress, and final reports, will be made available for archiving by the NIJ Data Resource Program. ca/ncf

<b>Awardee Name:</b> Research Triangle Institute	<b>Award Number:</b> 2012-R2-CX-K001
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