## B65 Identification of an Ultraviolet (UV) -Induced Promethazine Dimer

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**Learning Overview:** After attending this presentation, attendees will understand UV-induced degradation of promethazine in casework, which results in two chromatographic peaks with indistinguishable promethazine-like Electron Ionization (EI) mass spectra. Attendees will also learn about the application of tandem mass spectrometry for the structural characterization of the UV-induced product ion, a covalently linked promethazine dimer.

**Impact on the Forensic Science Community:** This presentation will impact the forensic science community by providing information on the structure, mechanism and rate of formation of a UV-induced dimer of promethazine.

**Hypothesis:** The central hypothesis is that the dimerization of the promethazine salt occurs through a process of UV exposure in the presence of chloroform. Additionally, the authors hypothesize that using a soft ionization technique such as electrospray ionization with collision-induced dissociation (ESI-CID-MS) will make it easier to detect the presence of the promethazine dimer that can be difficult to detect using traditional EI-MS. Finally, they hypothesize that with the use of tandem mass spectrometry (MS), they will be able to structurally characterize the promethazine dimer and identify structural modifications that occur due to UV exposure.

**Methods/Results:** Analyses involved dimerization of promethazine when exposed to intense short-wave UV light which was produced by the optimal crosslink setting of an XL-1500 Spectrolinker. A comparison of different UV exposure times shows that the concentration of promethazine dimer in solution increases as a function of the length of time the promethazine monomer is exposed to UV light. The process involves a 50 ppm promethazine solution poured into a covered glass petri dish, elevated by an adjustable lab stand inside the UV crosslinker and exposed to short-wave UV light. The resulting promethazine monomer and dimer were analyzed using an Agilent Technologies 7890B GC/5977A MS and a Thermo Scientific LTQ Velos Pro with HESI ionization source.

Preliminary results indicate that two different promethazine dimers are observed when using ESI: 1) a weakly associated dimer produced by clustering within the ESI source, and 2) a covalently bound dimer induced by UV exposure. These conclusions are based on the isolation and fragmentation parameters required for tandem MS. The tandem MS results indicate the weakly associated dimer fragments into monomer only, whereas the UV-induced dimer fragments into a series of ions corresponding to substituted promethazine monomer. Additionally, two chromatographic peaks are observed under traditional EI conditions. On-going reaction kinetics are focused on identifying the rate order of the conversion of promethazine monomer to dimer.

**Drug Chemistry, Dimerization, Tandem Mass Spectrometry**