

## **Workshop Report, 2018 ASMS Conference, San Diego, CA**

### **Forensic ID: Qualitative Identification in Forensic Mass Spectrometry**

#### **Organized by the Forensics and Homeland Security Interest Group**

Kenyon M. Evans-Nguyen and Christopher Mulligan

Panel: Dr. Sandra Rodriguez-Cruz (DEA, Secretariat of SWGDRUG), Dr. Glen Jackson (West Virginia University), Dr. Travis Falconer (FDA Forensics Laboratory), and Dr. Brittany Casey (Dallas County Crime Investigation Laboratory)

Tuesday June 6<sup>th</sup> 2018, 5:45 – 7:00 pm

Initial attendance 83, final attendance 101

Audience composition (via a show of hands): 40% academia, 30% industry, 30% practitioner

#### **Preliminary Remarks (30 minutes)**

- Kenyon Evans-Nguyen introduced the session and discussed the motivation for the topic
- Sandra Rodriguez-Cruz briefly presented on the role of SWGRDUG and their guidelines for identification
- Travis Falconer presented the criteria for compound identification used at the FDA forensic laboratory
- Glen Jackson presented on some research using a new statistical approach to improving database identifications with GC-MS data

#### **Panel discussion – Audience Questions and Responses (45 minutes)**

Audience question: How smart are defense attorneys? Are they technical questions? Do they inquire about things like calibration and tuning?

- Sandra responded – It's a spectrum, and can range quite a bit. Generally – the science behind GC-MS is unquestioned.
- Glen responded – Typically, there is very little rigor or defense questioning for petty crimes and civil cases. While there is always some chance, it typically comes at more high profile cases

Audience question: When analyzing trace samples (e.g. pipe residue scrapings), what is done in the case that the full sample is consumed, but the evidence may be called into question?

- Sandra responded – For these scenarios, usually high performance instrumentation is used, some little is consumed. Further, we usually save the vial (extract) for further study, if needed.

Audience question: In our work, we used the “3 ion rule” for explosives identification. Are similar strategies used/seen in other sectors?

- All responded – while some have/do, its lab/sector specific, overall.

Audience question: How many people have seen the articles employing “confidence” level for chemical identification in literature, and are implementing them in some way?

- Audience rebuttal – there has to be a way/strategy of using all of the data we collect during an MS analysis, such as precursor/product ion, deuterated labeling, RT, tailing match, etc.) to get to a better “Confidence” level that can be used to assist qualitative identification.
- Travis responded – Perhaps an alternative strategy is reporting a confidence of misidentification instead.
- Audience rebuttal – The role of orthogonal methods is to be used for enhancing confidence.

Audience question: What is the proper strategy for handling isomeric analytes when attempting to test and categorize new analytical techniques via SWGDRUG recommendations.

- Sandra responded – Some of this is jurisdictionally regulated. For instance, federal guidelines are more rigorous towards isomers. This includes purchases, analyzing, and comparing known isomeric materials for cross-checking.

Respectfully Submitted,

Kenyon M. Evans-Nguyen (Chair 2018) and Christopher Mulligan (Chair 2019)