B138 Seized-Drug Mass Spectral Libraries: Data Quality Control Measures

William E. Wallace, PhD, National Institute of Standards and Technology, 100 Bureau Drive, #8362, Gaithersburg, MD 20899-8362; Weihua Ji, NIST, 100 Bureau Drive, Gaithersburg, MD 20899; Karen W. Phinney, National Institute of Standards and Technology, 100 Bureau Drive, #8314, Gaithersburg, MD 20899; and Stephen Stein, National Institute of Standards and Technology, 100 Bureau Drive, Stp 8362, Gaithersburg, MD*

After attending this presentation, attendees will better understand spectrum self-consistency as well as consensus comparison among several spectral library entries as a means for mass spectral library quality control.

This presentation will impact the forensic science community by providing greater understanding, and thus greater confidence, as to how curated mass spectral libraries are created and maintained.

Spectrum quality control measures suitable for forensic drug analysis have been developed. The mass spectral library maintained by the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) currently includes close to 2,300 spectra (version 04-01-2015). The National Institute of Standards and Technology (NIST) Mass Spectrometry Data Center has reviewed each SWGDRUG spectrum and brought the level of curation up to the standards of the NIST library. Having high-quality, controlled-substance libraries is critical to the criminal justice system.

Each spectrum in the SWGDRUG library was compared via standard library search methods to spectra of the same compound found in any of five mass spectral libraries. These libraries were: the NIST/Environmental Protection Agency (EPA)/National Institutes of Health (NIH) library (240,000 compounds), the Wiley Designer Drug® library (16,343 compounds), the Wiley Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants and Their Metabolites® (8,650 compounds), the Cayman Chemical Company library (748 compounds), and the Adams Essential Oil Components library (2,200 compounds). Confirmation of a good-quality SWGDRUG spectrum was contingent primarily on matching with a match factor of 750 or better (out of 999) any and all spectra in the five reference libraries. Outlier spectra in any library were flagged for further scrutiny using NIST's Mass Spectral (MS) Interpreter program.

Although the number of SWGDRUG spectra that were found to contain errors is small (on the order of fewer than 1%), the variety of errors found was wide. In essence, each error found was unique to that entry. Systematic, library-wide errors were not found.

Spectral errors are generally of three types: (1) missing peaks; (2) spurious peaks not attributable to the compound structure; and, (3) incorrect mass assignments (often from incorrect rounding of mass values). In addition, there are a variety of compound identification errors. These include: (1) incorrect chemical structure; (2) incorrect chemical name; (3) incorrect Chemical Abstracts Service (CAS) number or other identifier; and, (4) incorrect isomer identification. In a few cases, a compound exists only in the SWGDRUG library, so comparison was not possible. These were flagged for measurement by NIST for addition to the NIST library.

The use of NIST's MS Interpreter program was instrumental for adjudicating cases in which only a few measurements were available. MS Interpreter assigns peaks to plausible molecular substructures based on a set of rules for estimation of fragmentation energetics using a chemical structure (connection table) type analysis. MS Interpreter is freely available at chemdata.nist.gov/mass-spc/interpreter/.

Of the 2283 SWGDRUG spectra examined, 605 were not in the NIST library, 89 had only one measurement on record in any library, 10 had only poor quality spectra available, and 12 had incompatible spectra in two or more libraries. Additionally, 173 NIST/EPA/NIH entries required CAS number updates, 14 had incorrect chemical structures, and 4 had incorrect compound names.

The compounds not in the NIST library or of poor quality will be measured and added, if certified samples can be found. This should be completed in time for next year's library release, NIST17, available Spring 2017.

Mass Spectral Database, Consensus Comparison, Quality Control