Expanded Suspect Screening with SCIEX All-in-One MS/MS and NIST'17 MS/MS Libraries

KC Hyland[1], Oscar Cabrices[1], Paul Winkler[1], Adrian Taylor[2], Craig Butt[3]
[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON; [3]SCIEX, Framingham, MA

ABSTRACT

High resolution mass spectrometry gives scientists powerful tools to detect and identify contaminants, residues, and endogenous constituents in complex food and environmental samples. The SCIEX All in One High Resolution MS/MS Spectral Library enables accurate compound identification through MS/MS spectral matching. This comprehensive library, bundled with the NIST '17 MS/MS Library, provides spectra for over 17,000 compounds including pesticides, pharmaceuticals and personal care products (PPCPs), and natural products found in foods and traditional medicines.

The libraries are compatible with SCIEX software solutions allowing spectral data acquired on SCIEX QTOF and QTRAP® systems to be searched. This library package allows searching across a breadth of compound classes to enhance the accuracy and efficacy of suspect and nontargeted screening.

INTRODUCTION

To identify unknown compounds in a complex sample, a typical workflow might start with performing a Suspect Screening to search against a spectral library or database of characterized compounds. When the screen fails to provide a candidate ID, additional processing features and functionality can be employed to determine potential candidate formulae and structures, even beyond the scope of the suspect library. However, the additional processing involved in doing a true structural elucidation can be daunting, and the confidence in the compound identification is limited without matching data to a previously published resource.

In combination with the licensed National Institute of Technology (NIST) MS/MS Spectral Library, SCIEX has assembled a comprehensive MS/MS spectral library bundle containing 17,708 compound entries. The libraries are compatible with SCIEX software solutions and all SCIEX hardware platforms, allowing spectral data acquired on SCIEX QTOF and QTRAP® systems to be searched. This library package allows searching across a breadth of compound classes to enhance the accuracy and efficacy of suspect and nontargeted screening.

Several datasets were collected for screening against the SCIEX All-in-One with NIST'17 MS/MS library, as well as other compound- class specific spectral libraries built and verified by SCIEX. Data were collected on multiple SCIEX MS platforms, as indicated. All data were processed using the latest SCIEX OS software, and the MSMS data searched against the library were collected in a variety of acquisition techniques, including IDA (Information Dependent Acquisition) and SWATH® Acquisition (Data Independent Acquisition).

Figure 1. The SCIEX OS software 1.4 platform allows processing of data collected on any SCIEX mass spectrometer platform- hig resolution QTOFs like TripleTOF® or X500R systems, as well as triple quadriupole nominal mass platforms such as the QTRAP® 6500+ System. QTOF and QTRAP instruments can collect MSMS spectral data, which can be searched against a library for compound screening, identification, or confirmation.

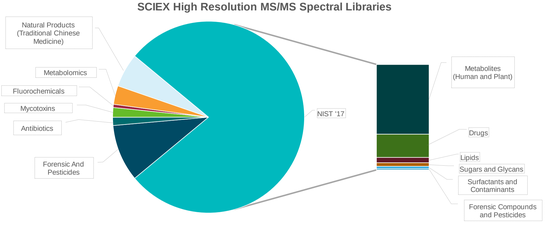


Figure 2. The inclusion of the NIST '17 MS/MS library license increases compound coverage all the way from human and plant Metabolites, to additional Forensic Compounds and Pesticides contained in the proprietary SCIEX MS/MS Spectral Libraries for use on TripleTOF® and X-Series QTOF Systems.

RESULTS

Figure 3. Obtain further synthetic drug identification through the addition of the licensed NIST '17 High Resolution MS/MS Spectral Library. A control urine sample was spiked with several forensic compounds of interest. The sample was analyzed using SWATH® Acquisition on the SCIEX X500R QTOF System and the acquired data searched against the All-in-One High Resolution MS/MS Spectral Library and NIST '17 MS/MS Spectral Library. All analytes were confidently identified using SCIEX OS Software data processing. In this example, the syntethic opioid hydrocodone (Isobaric Compound with Codeine), provided 99.8% fit against the NIST reference MS/MS spectrum using the smart confirmation algorithm and using the formula finder feature with mass error of 0.7 ppm

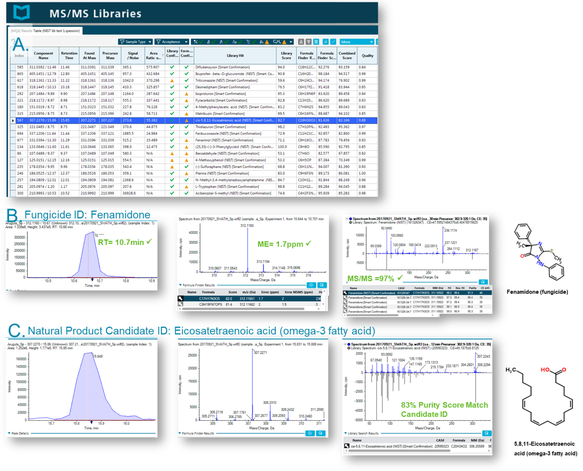
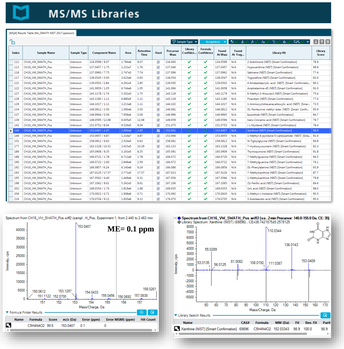


Figure 4. Gain further natural compound and pesticide identification through the addition of the licensed NIST '17 High Resolution MS/MS Spectral Library. (A) Control QuEChERS extract of an arugula sample was spiked with several pesticides of interest. The sample was analyzed using SWATH® Acquisition on the SCIEX X500R QTOF System and the acquired data searched against the All-in-One High Resolution MS/MS Spectral Library and NIST '17 MS/MS Spectral Library. All analytes were confidently identified using SCIEX OS Software data processing. (B) In this example, one of the target pesticides (Fenamidone) is shown as a positive identification, with matches for RT, precursor match, and MS/MS library hit. (C) A naturally occurring plant compound has been tentatively identified in this sample. An omega-3 fatty acid was suggested from a positive match in the library. Omega-3 fatty acids are known to be found in arugula and represent one of the health benefits of this food. It is demonstrated that true nontargeted approaches are effective and that screening against this library provides cross- compound class coverage applicable to complex matrices.

Figure 5. The library also allows detection and identification of hundreds of metabolite products. In this instance, Xanthine (a human metabolite of caffeine, theobromine) was identified in data acquired using SWATH® Acquisition for Data Independent MSMS spectral collection.



CONCLUSIONS

Gain comprehensive compound coverage using the SCIEX All-In-One High Resolution MS/MS Spectral Library bundle containing spectral information for over 17000 compounds across a multitude of compound classes and properties. The inclusion of the NIST '17 MS/MS library license increases compound coverage all the way from human and plant Metabolites, to additional Forensic Compounds and Pesticides contained in the proprietary SCIEX MS/MS Spectral Libraries for use on TripleTOF® and X-Series QTOF Systems.

Advantages of the SCIEX All-in-One High Resolution MS/MS Spectral Library

- Includes a SCIEX proprietary 3900 analyte library created using certified reference materials, including compounds commonly tested for in forensics, food, environmental and metabolomics samples.
- The NIST '17 MS/MS Library license adds a comprehensive range of different compounds (13,808 small molecules) for enhanced coverage.
- Contains MS and MS/MS spectral data for both positive and negative ionization for library matching.
- Use the integrated MS and MS/MS information to build methods without the need to infuse standards and optimize conditions for a given compound.
- Easily create processing methods for a TOF-MS-IDAMS/MS workflow or SWATH® Acquisition for use on TripleTOF® and X-Series QTOF Systems.
- Quickly setup XIC tables for quantitation and identification with SCIEX OS Software or MasterView™ software. Build customized libraries by simply selecting only the compounds of interest using the LibraryView™ Software.

TRADEMARKS/LICENSING

Document number: RUO-MKT-10-7860-A