

Expanding Suspect Screening and Non-Targeted Identification

High resolution mass spectrometry provide 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 in combination with the licensed NIST '17 MS/MS Library, provides spectra for over **17000 compounds** including pesticides, pharmaceuticals and personal care products (PPCPs), and natural products found in foods and traditional medicines.

This library is for use with for use with the X500R QTOF System powered by SCIEX OS Software and also compatible for use with SCIEX TripleTOF® and QTRAP® Systems with MasterView™ Software and LibraryView™ Software.

Furthermore, this library package enables searching across a breadth of compound classes to enhance the accuracy and efficacy of suspect and non-targeted screening.

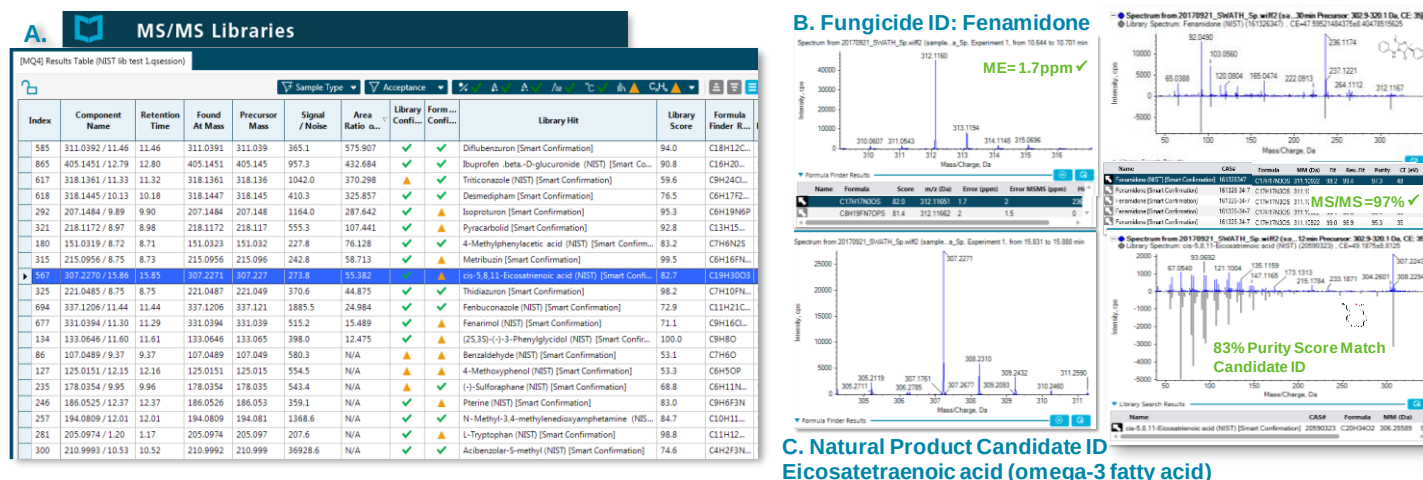


Figure 1. Gain further natural compound and pesticide identification through the addition of the licensed NIST '17 High Resolution MS/MS Spectral Library. (A) Control QUCheRS extract of an arugula sample was spiked with several pesticides of interest. The sample was analyzed using SWATH® Acquisition 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.

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Document number: RUO-MKT-02-7170-A