Food and Environmental

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Suspect Screening Data Processing Utilizing SCIEX OS Software

Simplifying Suspect Screening using Non-Targeted Data and MS/MS Spectral Library

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What: Non-targeted, data independent acquisition for suspect screening is advantageous for collecting MS and MS/MS data on all compounds in a sample. Processing this type of data with a targeted list ensures that all MS/MS data for all peaks are collected during acquisition.

Processing: In SCIEX OS Software, the workflow for suspect screening with SWATH® Acquisition data is made simple and intuitive for identification and confirmation by the ability to import a suspect list from an MS/MS spectral library. This method of processing is particularly useful especially when there is no reference standard available, as the screening is performed based on the exact mass and isotope pattern calculated from the molecular formula, plus or minus the expected adduct(s) of the suspected substance.

Creating a processing method for hundreds of suspect compounds could be a tedious task. This task is made simpler by using the Import from Library feature. From the information in the selected MS/MS spectral library, users can easily import Compound ID, chemical formula, and up to 3 fragment ions of the highest intensity from the MS/MS spectrum, if the fragment ions are needed for analysis or ion ratio calculations.
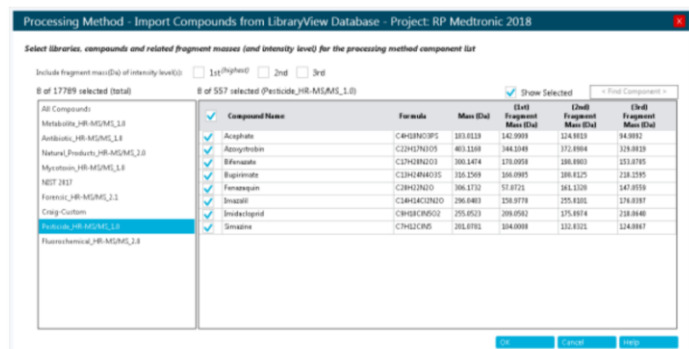
Once the suspect compounds are added to the Components list, the user can select an RT mode, if the RT is not known. A typical setting in this case is Find 5 Peaks.
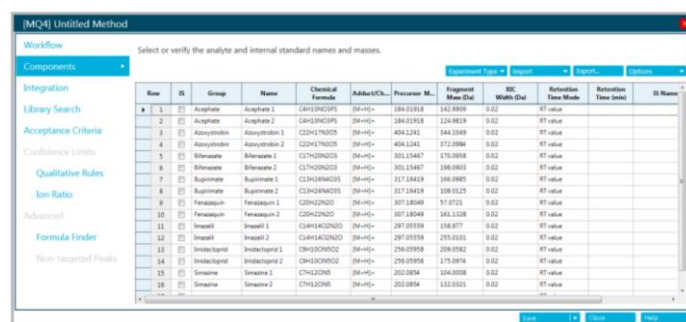
Next, MS/MS library searching is set up by choosing a library and a library search algorithm. Then the Qualitative Rules are set up which are used to identify positive hits.
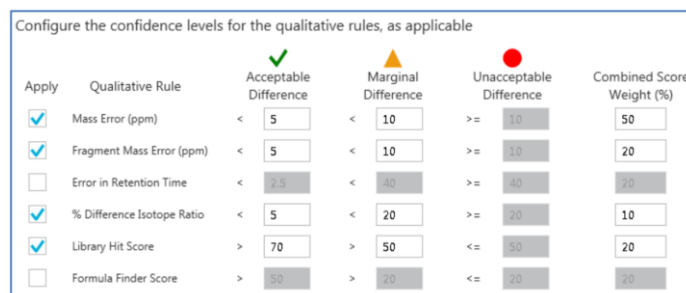
Once the processing has finished, filtering tools using visual cues easily calls out positive hits in the sample. These filtering tools can reduce data review time and increase confidence in results.

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