Confident Identification For Comprehensive Screening

Using the Wiley Registry of Tandem Mass Spectral Data: MSforID

Pierre Negri[1], Adrian M. Taylor[2]
[1]SCIEX, US; [2]SCIEX, CA

High resolution mass spectrometry (HRMS) using the SCIEX TripleTOF® or X500R QTOF systems provides forensic investigators a powerful tool for the detection and identification of toxic compounds or novel drugs of abuse. High MS and MS/MS acquisition rates ensure the acquisition of accurate mass spectral data on large numbers of analytes, even at low analyte concentrations. The comprehensive analyte-specific MS/MS fragment spectra in the compound identification workflow increases the selectivity, specificity and confidence in the results.

Combining this data with the Wiley Registry of Tandem Mass Spectral Data: MSforID enables accurate compound detection and identification through library spectral matching. Automated processing matches the MS data to the analyte mass and the MS/MS is matched to the analyte fragmentation pattern in the library, providing a "fit score" for assessment of confidence of compound identification. As shown in the example below, multiple points of high-quality data are used to detect and identify codeine and its main metabolite, norcodeine, from a postmortem case sample with excellent fit scores of 100% for both analytes.

Key Advantages of the Wiley High Mass-Accuracy LC-MS/MS Spectral Library

- The Wiley Registry of Tandem Mass Spectral Data: MSforID spectral library includes a variety of compounds including pesticides, pharmaceutical compounds, illicit drugs and other small bioorganic molecules, useful for researchers in metabolomics, pharmaceutical research, forensics and toxicology
- Includes a collection of 10,000 positive and negative mode high resolution MS/MS spectra for over 1,200 compounds, all carefully measured in a series of controlled conditions to enable accurate, reliable, and reproducible search results in a variety of settings
- Library is compatible with SCIEX OS Software to process data from the TripleTOF®, X-Series QTOF and QTRAP® Systems with SCIEX OS Software
- Provides the ability to create customized libraries specific to workflows by simply selecting the analytes of interest in LibraryView™ Software

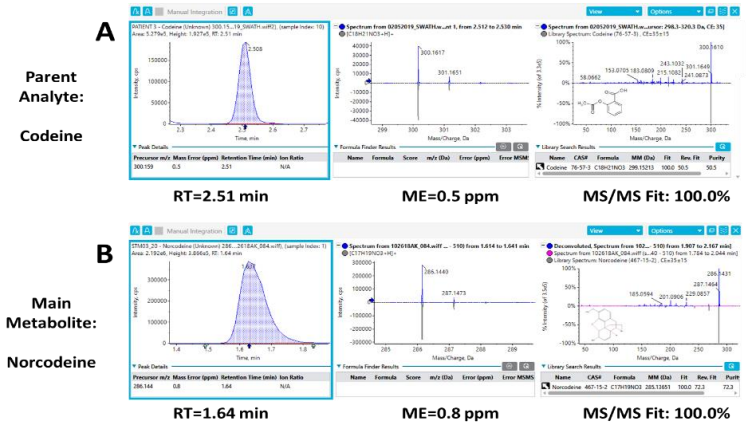

Figure 1: Achieve Wide Analyte Coverage and Confident Compound Identification Using the Wiley Registry of Tandem Mass Spectral Data: MSforID. XIC, TOF MS and MS/MS spectra obtained showing confident and accurate identification of (A) codeine and (B) its main metabolite, norcodeine, from a postmortem case sample. The sample was analyzed using IDA on the SCIEX X500R QTOF System and the acquired data was searched against the Wiley High Mass-Accuracy LC-MS/MS Spectral Library.

Headquarters
500 Old Connecticut Path | Framingham, MA 01701 USA
Phone 508-383-7700
sciex.com

International Sales
For our office locations please call the division headquarters or refer to our website at
sciex.com/offices