

# Wide Compound Coverage for Confident Analyte Identification Using SWATH® Acquisition on the SCIEX TripleTOF® and X-Series QTOF Systems

## Using the Wiley MMHW LC-MS/MS Spectral Library

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The ability to develop comprehensive screening procedures for the detection of toxic compounds, drugs of abuse and their metabolites is critical for forensic laboratories to accurately identify and quantify substances with a high level of confidence. SWATH® Acquisition on the SCIEX TripleTOF® and X-Series QTOF Systems provides a fast, comprehensive analysis of forensics samples and allow detection and identification of drugs, metabolites and other emerging compounds present in complex biological matrices.

The Wiley MMHW LC-HR-MS/MS spectral library enables accurate detection and identification of novel psychoactive substances (NPS), toxic compounds and drugs of abuse through library spectral matching. The flexibility of SCIEX accurate mass instruments and supporting software allows the acquisition of high resolution MS/MS spectra, enabling library searching using the Wiley MMHW LC-HR-MS/MS library for increased confidence in compound identification.

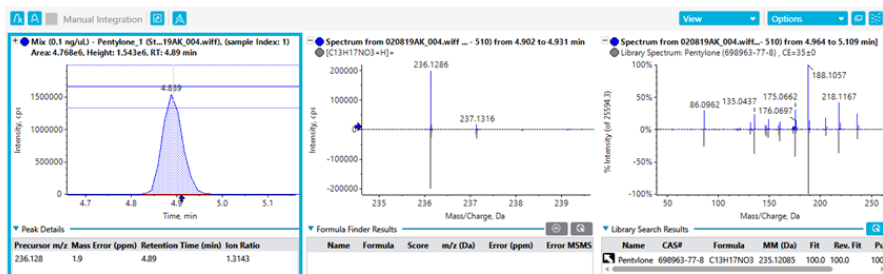
In the example below, a processing method was built in SCIEX OS Software by adding the precursor and fragment ions of various drugs of abuse in the components table. The "Library Search" function was enabled and the Wiley MMHW LC-MS/MS Spectral Library was selected. As shown in Figure 1, pentylone, fentanyl, 24I-NBOMe and ADB-FUBINACA were detected from a urine sample spiked with multiple compounds of interest. Multiple points of high-quality data such as analyte retention time and exact fragment masses are used to detect and identify these drugs of abuse. The exact fragment masses ( $m/z$  236.128, 337.227, 428.072, and 383.188 Da) were extracted and the experiment fragment mass errors were found to be 1.9, 0.3, 1.7 and -0.5 ppm for pentylone, fentanyl, 24I-NBOMe and ADB-FUBINACA, respectively. These mass errors indicate excellent mass accuracy across the compounds detected. Further, the MS/MS spectra match those of the library with a fit score above 99% for all the analytes detected.



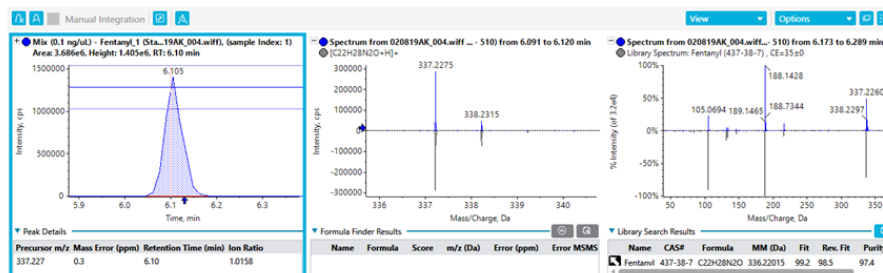
## Key Advantages of SWATH Acquisition with the Wiley MMHW LC-MS/MS Library

- High speed acquisition of the TripleTOF® and X-Series QTOF Systems enables the use of SWATH Acquisition, even at fastest gradient speeds
- Comprehensive MS and MS/MS data collected on every sample for wide compound coverage
- Compatible with the Wiley MMHW LC-HR-MS/MS spectral library which includes over 5,000 drugs and metabolites, for drugs commonly tested in forensic samples, including blood and urine
- Library is compatible with SWATH® Acquisition workflows on the TripleTOF®, X-Series QTOF and QTRAP® Systems with SCIEX OS Software
- Accurate screening of drug metabolites increases selectivity, allows confirmation of the body passage and minimizes the risk of false negative results, hence enhancing the screening accuracy of illicit substances and other drugs of abuse

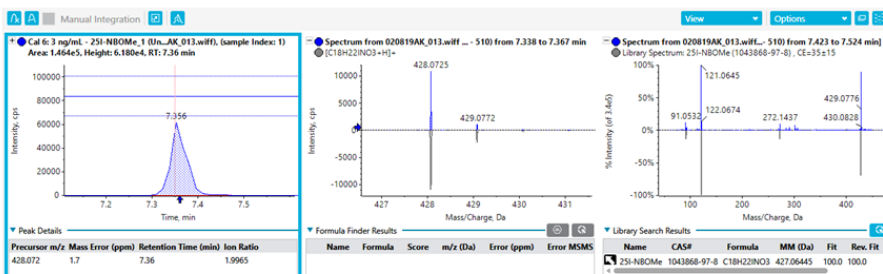
**Analyte:** Pentylone  
**RT:** 4.89 min  
**Precursor m/z:** 236.128 Da  
**Mass error:** 1.9 ppm  
**MS/MS Fit:** 100%



**Analyte:** Fentanyl  
**RT:** 6.10 min  
**Precursor m/z:** 337.227 Da  
**Mass error:** 0.3 ppm  
**MS/MS Fit:** 99.2%



**Analyte:** 25I-NBOME  
**RT:** 7.36 min  
**Precursor m/z:** 428.072 Da  
**Mass error:** 1.7 ppm  
**MS/MS Fit:** 100%



**Analyte:** ADB-FUBINACA  
**RT:** 8.49 min  
**Precursor m/z:** 383.188 Da  
**Mass error:** -0.5 ppm  
**MS/MS Fit:** 100%

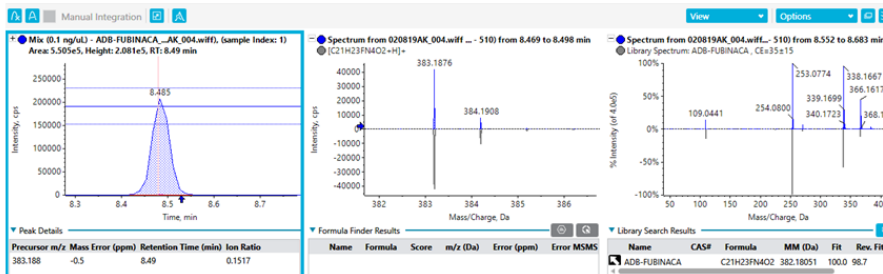


Figure 1: Gain Comprehensive Analyte Coverage and Increase Confidence in Analyte Identification Using the Wiley MMHW LC-HR-MS/MS Library. XIC, TOF MS and MS/MS spectra obtained showing confident and accurate identification of pentylone, fentanyl, 24I-NBOME and ADB-FUBINACA from a urine sample spiked with several forensic compounds of interest. The sample was analyzed using SWATH® Acquisition on the SCIEX X500R QTOF System and the acquired data was searched against the Wiley MMHW LC-HR-MS/MS Library.

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