MetabolitePilot™ Software 2.0

Advanced Metabolite Identification and Quantitation for Small Molecule Metabolism and Biotherapeutic Catabolism

MetabolitePilot Software offers an integrated and easy to use workspace for high throughput processing and interrogration of your advanced drug metabolism and biologics catabolism data. Powerful data processing algorithms accelerate metabolite and catabolite identifications, enables effective time-point and cross species comparisons, and simplifies reporting so you can drive your drug development program more efficiently.

Key Challenges in Advanced Drug Metabolism

- Missing low level and toxic metabolites/catabolites
- Repeat analysis to understand complete metabolite profile and structure due to missing, or poor quality, MS/MS spectra
- Complicated processing to understand metabolite profile across multiple time points and species
- Complex data processing for biotherapeutic catabolism analysis (peptides, proteins, ADCs)
- Manual interpretation of biotherapeutic catabolite structures and profile

NEW Capabilities in MetabolitePilot Software 2.0

Automated and Powerful Catabolism Data Processing for Therapeutic Peptides

- Catabolism analysis for therapeutic peptides, including non-linear, cross-linked and cyclic structures
- Support of non-natural amino acids and modifications
- Targeted searching of predicted hydrolytic cleavages
- Calculation and assignment of a-, b-, y- and internal fragments for linear and non-linear peptides

Advanced Catabolism Data Processing for Antibody Drug Conjugates

- Dedicated biologic protein processing templates to simplify analysis of cytotoxic drugs, linker, antibody, and antibody drug conjugation chemistry
- Prediction and targeted searching of catabolite structures for payload cleavages and biotransformations on drug linkers
- Targeted searching of predicted hydrolytic cleavages along antibody backbone, including ADC conjugation sites and specified amino acid modifications
- MS/MS annotations for ADCs with combined assignment of small molecule fragments and peptide fragments
- Interactive interpretation tool for MS/MS annotation and assignment

Process SWATH® Acquisition Data for Small Molecules and Large Molecule Biotherapeutics

- Ensure important metabolite or catabolite information is not missed by acquiring high-resolution MS/MS data on all sample components in a single run using SWATH Acquisition
- Improved identification of drug-related material based on characteristic fragment ions, neutral losses, and fragment isotope patterns
- Multiple filters for processing SWATH MS/MS spectra. The filters allow you flexibility to interpret your MS/MS data regardless of the number of points across the peak.

High Throughput Processing

- Expanded the number of samples that can be processed in a single batch to 200 from 30
- Import a batch file from Excel to populate the batch workspace quickly and easily, no more manually selecting sample files and processing parameters through menus
- Don't waste time creating a separate processing method for each new compound in a batch with the new ability to create methods on the fly

Enhanced UV data processing and viewing

- Correlate between species, time points, and with orthogonal UV data to be truly confident in your metabolite ID
- Ability to manually integrate analog peaks
- Ability to align and background subtract analog peaks, resulting in improved confirmation of metabolites

MetabolitePilot Software Features and Benefits

Intuitive Processing Setup

- Getting started is easy with intuitive main window
- Select from Phase I and II biotransformation sets plus new biologics, metabolism biotransformation set
- Easily add custom modifications, proprietary linkers and drug conjugates, or non-natural amino acids
- Create your own custom biotransformations
- Processing parameters for multiply charged species up to +10
- Processes LC-MS, UV-LC-MS, or SelexION LC-MS acquired data

Accelerated Processing for Faster Analysis

- High throughput processing of up to 200 samples in a single batch
- Simplify biotherapeutic catabolite processing with creation of drug-specific processing methods
- Save time with an option for automatic selection, reporting, and review of most relevant metabolites as defined in a batch processing method
- Automatic proposal of structure/sequence in batch setup with options for assigning structures based on area intensity or MS/MS quality.

Simplified Conversion of Data to Answers

- Quickly identify metabolite at catabolic hotspots with automated structure generation
- Minimize data review with the ranking of proposed structures/sequences based on accurate mass MS/MS
- Simplified correlation workspace to view metabolite/catabolite time course profiles

Comprehensive Reporting

- Choose different report outputs for different audiences: choose from detailed or summary reports from either the results or interpretation workspace.
- Four different report templates to choose from

MetabolitePilot Software 2.0 Compatibility Matrix

Operating System	Windows 7 64-bit, SP1
Supported Mass Spectrometers	X500R QTOF System X500B QTOF System TripleTOF® 5600 system TripleTOF 5600+ system TripleTOF 6600 system
Compatible Data Acquisition Software	SCIEX OS 1.2 software SCIEX OS 1.3 software Analyst® TF 1.5.1 software Analyst TF 1.6 software Analyst TF 1.7 software Analyst TF 1.7.1 software
Free Trial Download Link	http://sciex.com/licensing

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