

Ease the burden of managing metabolite identification

As a leader responsible for metabolite identification in your organization, what keeps you awake at night? SCIEX can give you peace of mind by helping you ...



Manage product safety

Help ensure product safety with complete structural elucidation—even for challenging analytes such as phase II metabolites—with electron activated dissociation (EAD). The ZenoTOF 7600 system can collect both EAD and collision-induced dissociation (CID) MS/MS spectra in a single LC-MS/MS experiment.



Meet deadlines

Robust and reliable instruments allow for predictable scheduling and on-time project completion. When needed, our systems are supported by highly respected services and backed by the SCIEX Now support network to ensure that service calls are quickly reported and tracked.



Efficiently recruit and train staff

Streamline new-hire training with knowledge base articles available on demand from the SCIEX Now Learning Hub. SCIEX OS software is designed to be easy to learn and use for data collection, processing and reporting within a single platform.



Meet regulatory requirements

SCIEX OS software is compliant-ready to help ease the burden of regulatory activities, including managing user access levels, and to reduce the potential for human error.



Manage capital expenses

Invest only in what you need, so you don't have to spend money on features and system performance that are unnecessary for your samples.



Why use EAD for metabolite identification?

EAD is a fragmentation method available on the ZenoTOF 7600 system that causes ions in an LC-MS/MS experiment to fragment in locations that are different from where they fragment with CID, providing

additional information to scientists in a single experiment. For metabolite identification, this could mean confident identification of a single site of metabolism instead of 2 or 3 sites using CID only, removing the need for additional safety testing.



 $\operatorname{MS/MS}$ spectra obtained using CID and EAD fragmentation.

CID predicted 4 possible sites of metabolism. EAD enabled the identification of a single metabolite.

Recommended systems

Confidently complete your metabolite identification studies during your development process with dependable instruments that run on intuitive, compliant-ready software. Our LC-MS systems offer fit-for-purpose sensitivity and robustness.

Complex metabolite identification

ExionLC AE system and ZenoTOF 7600 system on SCIEX OS software with Molecule Profiler software



Why choose this option:

The ZenoTOF 7600 system provides comprehensive characterization and confident identification. For example, in the figure to the right, CID identifies 2 possible sites of glucuronide metabolites while EAD identifies a single site, eliminating the need for secondary testing for safety purposes.

When to choose this option:

- If you need a secondary analytical technique, such as NMR, to confidently identify the location of metabolism
- If you need method sensitivity for low-abundant metabolites



EAD enables the confident identification of glucuronide conjugation using diagnostic fragments. While CID generated 2 possible sites of glucuronide conjugation, the power of EAD provides site-specific characterization that narrows it down to a single metabolite candidate. Here, the glucuronide conjugation was localized.



Recommended systems

Confidently complete your metabolite identification studies during your development process with dependable instruments that run on intuitive, compliant-ready software. Our LC-MS systems offer fit-for-purpose sensitivity and robustness.

Routine metabolite identification

ExionLC AE system and X500R QTOF system on SCIEX OS software with Molecule Profiler software





Why choose this option:

SWATH data acquisition combined with Molecule Profiler software allows for streamlined method development and data processing. As a result, automatic structure proposals of metabolites are generated and presented with relative evidence for quick, easy review and confirmation. This is achieved through advanced peak-finding algorithms optimized for SCIEX high-resolution mass spectrometry platforms and integrated MS/MS fragment interpretation and structural assignment tools. These capabilities deliver high-throughput batch processing (up to 200 rows) plus the ability to import batches from a spreadsheet and create processing methods on the fly.

When to choose this option:

- If you are running larger batches of samples
- If more established LC-MS methods with cthat use CID fragmentation work well
- If ease of use and the increased uptime of a robust system are priorities





Rich MS/MS information with SWATH Acquisition. An example of the isotope pattern information collected in the product ion spectrum using SWATH Acquisition versus information dependant acquisition (IDA).

Why choose SCIEX?

Imagine the advantages of unambiguous metabolite identification using LC-MS, even for challenging analytes such as phase II conformation of glucuronide metabolites.

Learn how you can reduce the need for additional safety testing in your organization by implementing EAD functionality available exclusively from SCIEX.





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