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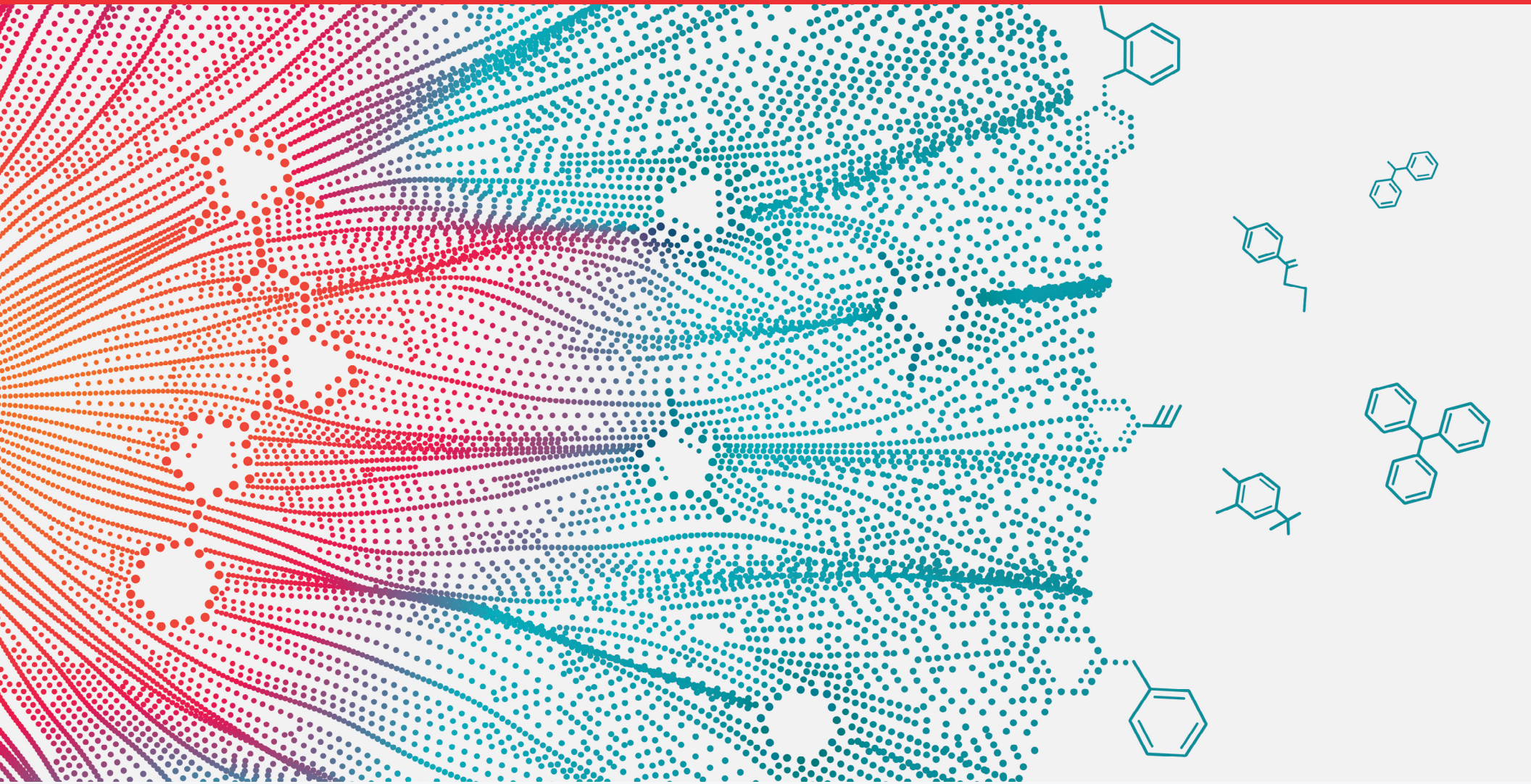


Powering confident insights

Explore your small-molecule data to its core

Thermo Scientific Mass Frontier Software

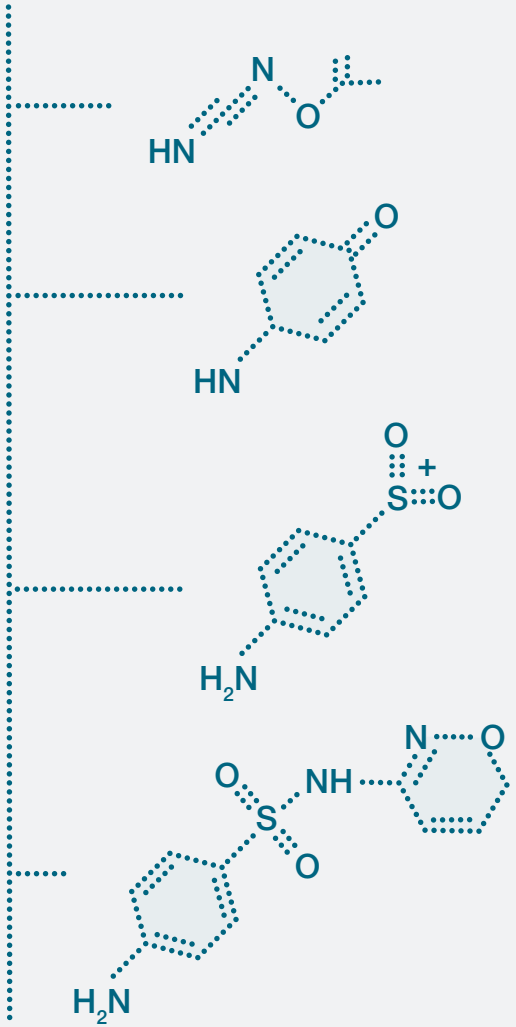
ThermoFisher SCIENTIFIC

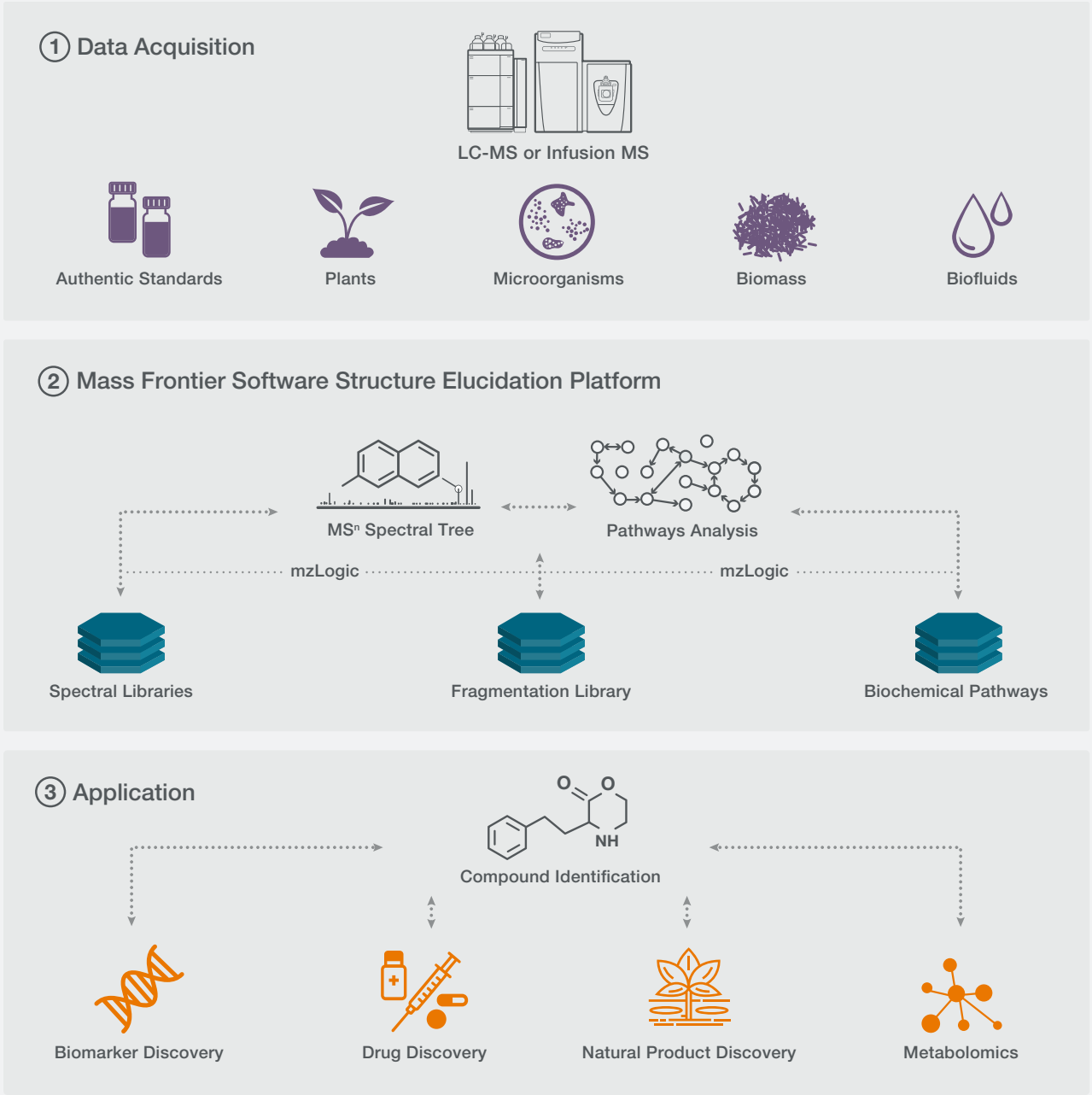
Simplify deep exploration of your small-molecule data and capture structural insights

Interpretation and characterization of mass-spectral data can be an enormous challenge due to extreme compound structural diversity and complex samples.

Thermo Scientific™ Mass Frontier™ software solves this challenge through powerful algorithms and fully-curated knowledge databases of spectral and fragmentation data, as well as the ability to confidently interrogate your fragmentation data through the use of fragmentation assignments which use more than 99% of all published fragmentation mechanisms.

Now you can rapidly deconvolute and search information-rich, complex data sets against mzCloud™, an extensively curated mass-spectral fragmentation library. Due to the high quality and chemical diversity of mzCloud's data, analysts are empowered to rapidly turn complex data into actionable, sharable insights with confidence.



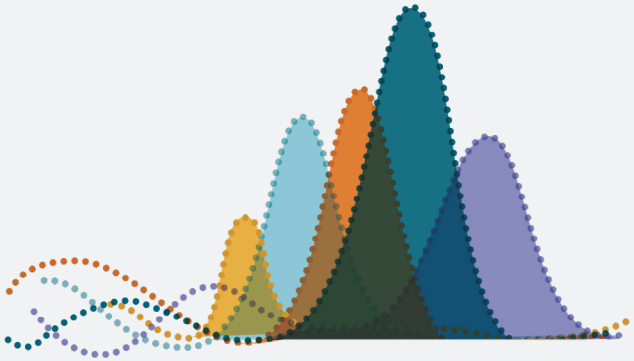


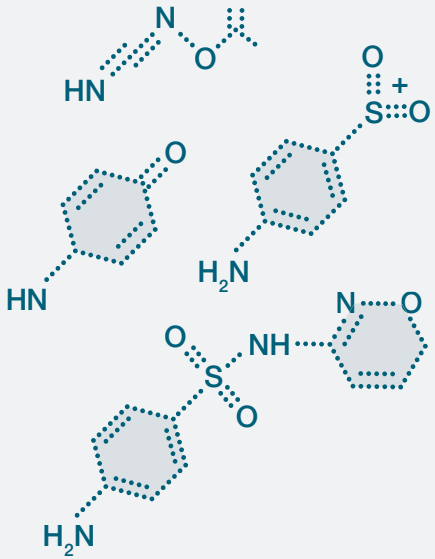
Use the comprehensive Mass Frontier software toolsets and explore your high-resolution or nominal-mass MSⁿ data to conquer your unknown identification challenges. By integrating access to spectral and fragmentation libraries and pathway databases, you can streamline your unknown identification workflow. From mzCloud to mzLogic, you can be confident about your structural insights, even for true unknowns.

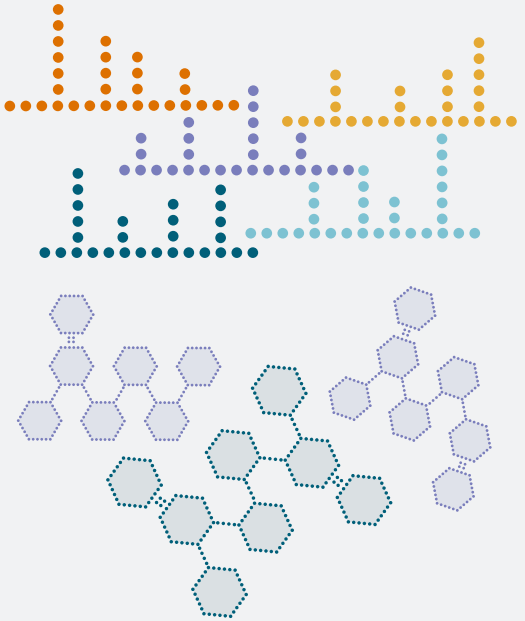
"I have been using Mass Frontier software for over 10 years and think every mass spectrometrist should have a copy. I like the functionality of mzCloud integration, and the look and design; everything is well organized and intuitive."

Dr. Tobias Kind
UC Davis Genome Center

Go from complex data to actionable, sharable insights







See what's there

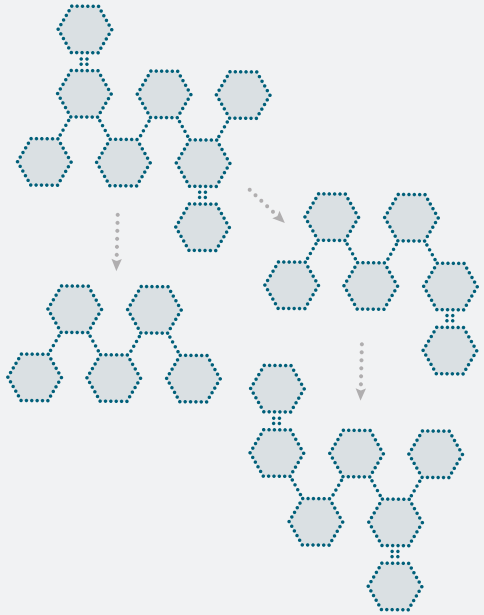
- Deconvolute high-resolution and nominal-mass LC-MS and infusion data
- Capture all relevant data, regardless of sample complexity
- Support for Thermo Scientific™ .raw and common file format mzML

Make your unknowns, known

- Search deconvoluted components against mzCloud, one of the world's most comprehensive mass-spectral database, or your own proprietary spectral libraries
- Match MS^n data for complete confidence in identifications
- Transform complex data into knowledge

Relate spectra to fragments and structures

- Perform similarity and sub-structure searching of MS^n data with ease to provide high-certainty putative identifications when there are no confident library assignments
- Automatically annotate MS^n spectral trees with predicted fragments for unknown structural elucidation



Build pathways

- Draw, edit, and confirm structures, generate elemental formulas, and visualize isotopic patterns
- Use confidently identified components to create and edit reaction pathways in a publication-quality display
- Access the more than 370 curated biochemical pathways included with the Pathway Explorer tool

Capture and share knowledge

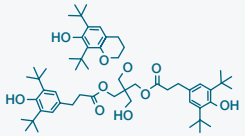
- Curate, manage, and share proprietary libraries to leverage your valuable knowledge across your organization and network
- Capture high-quality, annotated precursor and fragmentation information, including adducts, mass recalibration, and collision energy breakdowns for every spectral peak with the same curation tools as used with mzCloud

Bridge chemical diversity

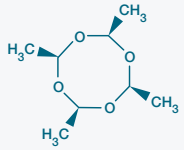
Small molecules span an amazing array of chemical diversity, which adds to the difficulties of confident compound identification.

Now it's easier than ever before to identify unknowns using comprehensive mass-spectral and fragmentation libraries, with fragmentation mechanisms and pathways that cover a diverse set of applications.

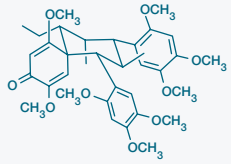
Impurities and Degradants



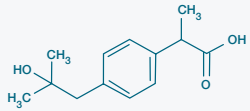
Environmental and Food Safety



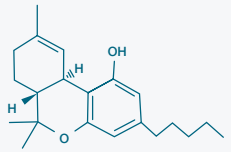
Natural Products and Traditional Chinese Medicine



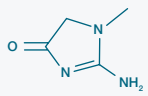
Metabolite Identification



Forensic Toxicology



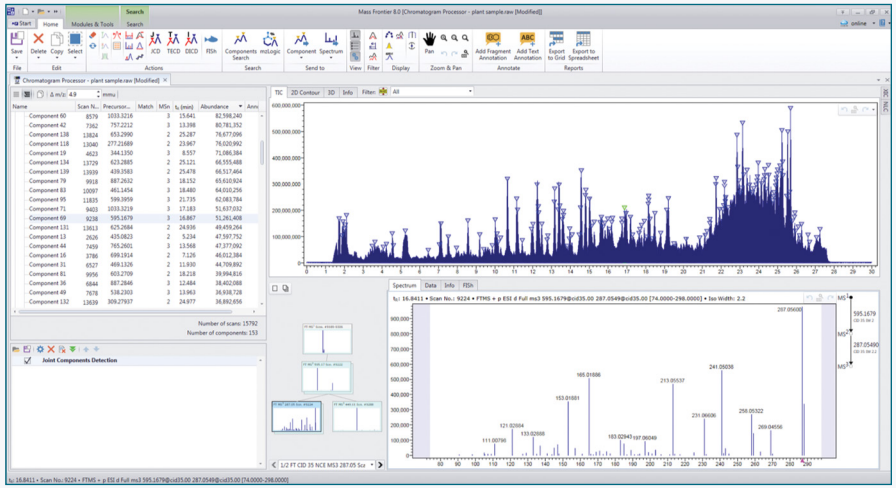
Metabolomics



See what's there

Maximize component detection

You can't afford to miss anything. With powerful deconvolution of high-resolution, nominal-mass LC-MS and infusion data, Mass Frontier software ensures that you maximize component detection regardless of sample complexity. This capability is extremely useful when there are many coeluting components buried in chromatographic peaks.



Mass Frontier software extracts the multiple components that can occur underneath chromatographic peaks. Each blue triangle is a detected component.

Simplify interrogation of detected components

Sample components and associated mass-spectral information can be automatically interrogated with a Mass Frontier software component search against the mzCloud mass-spectral library and/or your own custom spectral libraries. Mass Frontier software automatically applies the appropriate search parameters.

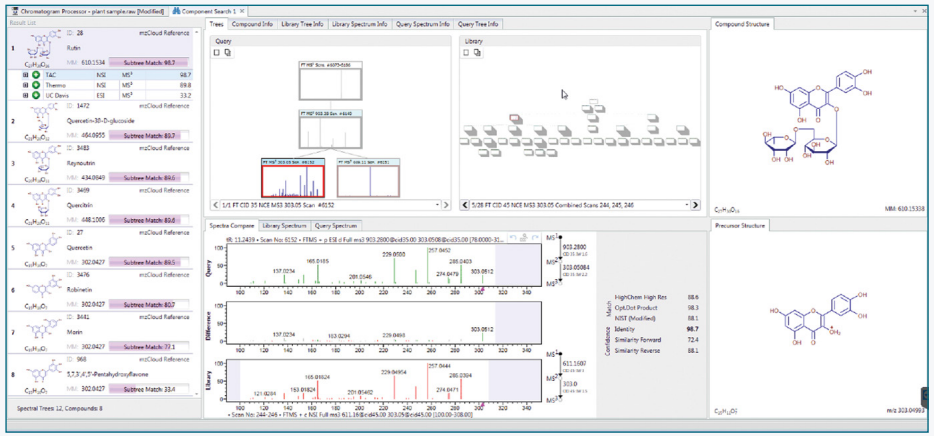
Make your unknowns, known

Access the extensive mass-spectral library

Mass Frontier software leverages mzCloud, one of the world's largest and most extensively curated mass-spectral fragmentation library available today. Experts evaluate all spectra and data added to the library, providing you with strong confidence in the quality of its contents.

Each record includes extensive metadata: name and synonyms, structure, computationally and manually annotated fragments, adducts and multiply charged ions, molecular formulas, experimental information, mass accuracies and resolution, and numerous other identifiers.

Utilize your MS^n data's deeper insights through the ability to compare spectral fingerprints of fragment ions against the comprehensive MS^n spectral tree fragmentation data contained within mzCloud through common sub-structure matching. Match fragmentation spectra from your own fragmentation 'query tree' to mzCloud's spectral trees, allowing you to confidently identify ion structures or sub-structures and reconstruct the molecular structure. Rapidly identify unknown compound classes which do not exist in reference libraries at the time of analysis.



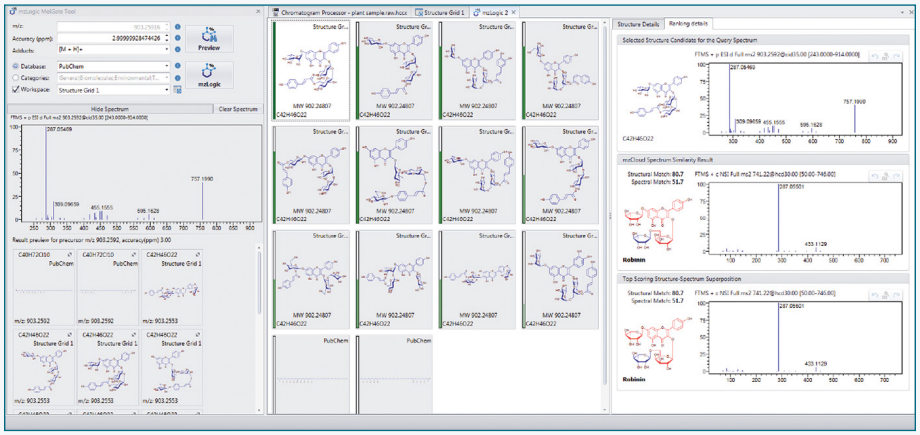
Capitalize on extensive library curation and content to obtain high-confidence matches using the comprehensive mzCloud mass-spectral library.

Relate spectra to fragments and structures

Propose identifications using mzLogic

Even when there isn't a mzCloud spectral library match, its extensive stepped collision energy fragmentation data from multi-stage MS^n spectra can be combined with the use of online structural libraries and databases.

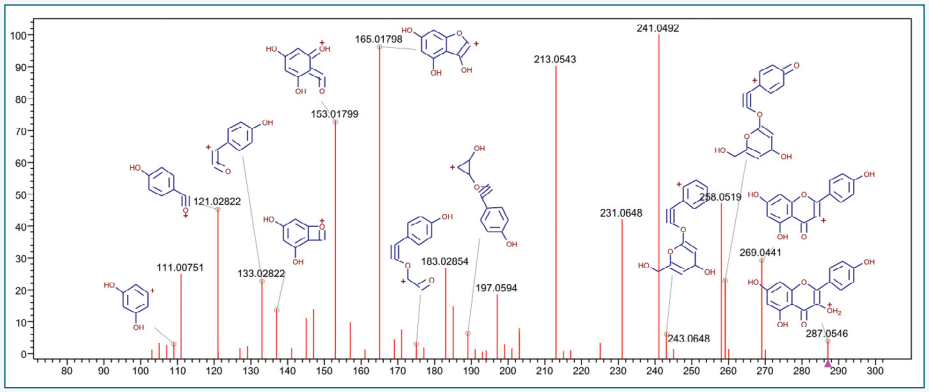
The novel mzLogic data analysis algorithm uses spectral similarity and common sub-structure information from mzCloud's real-world spectral data to rank the proposed candidates structures. Fast, automated logical analysis using the mzLogic algorithm eliminates thousands of candidates and hours of manual work by delivering high probability candidates based upon their maximum common sub-structure and spectral similarity.



With Mass Frontier software (version 8.0), you canmake high-certainty putative identifications and candidate proposals using mzLogic and fragment annotations to propose the best candidates.

Understand fragmentation

Understanding fragmentation pathways adds more insight and certainty to your analyses. The powerful HighChem Fragmentation Library™ and mzCloud precursor-ion fingerprinting speed structural elucidation of unknowns.



Fragmentation spectra can be manually or automatically annotated across the entire spectral tree, making visualizing results and reporting easier.

Mass Frontier software fragmentation pathway capabilities use proprietary interpretation algorithms with the HighChem Fragmentation Library of more than 52,000 fragmentation schemes, 217,000 individual reactions, 256,000 chemical structures, and 216,000 decoded mechanisms obtained from peer-reviewed publications.

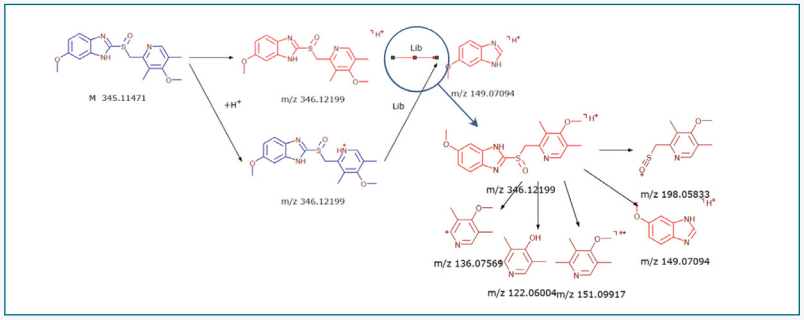
Build pathways

Create your knowledge pathway

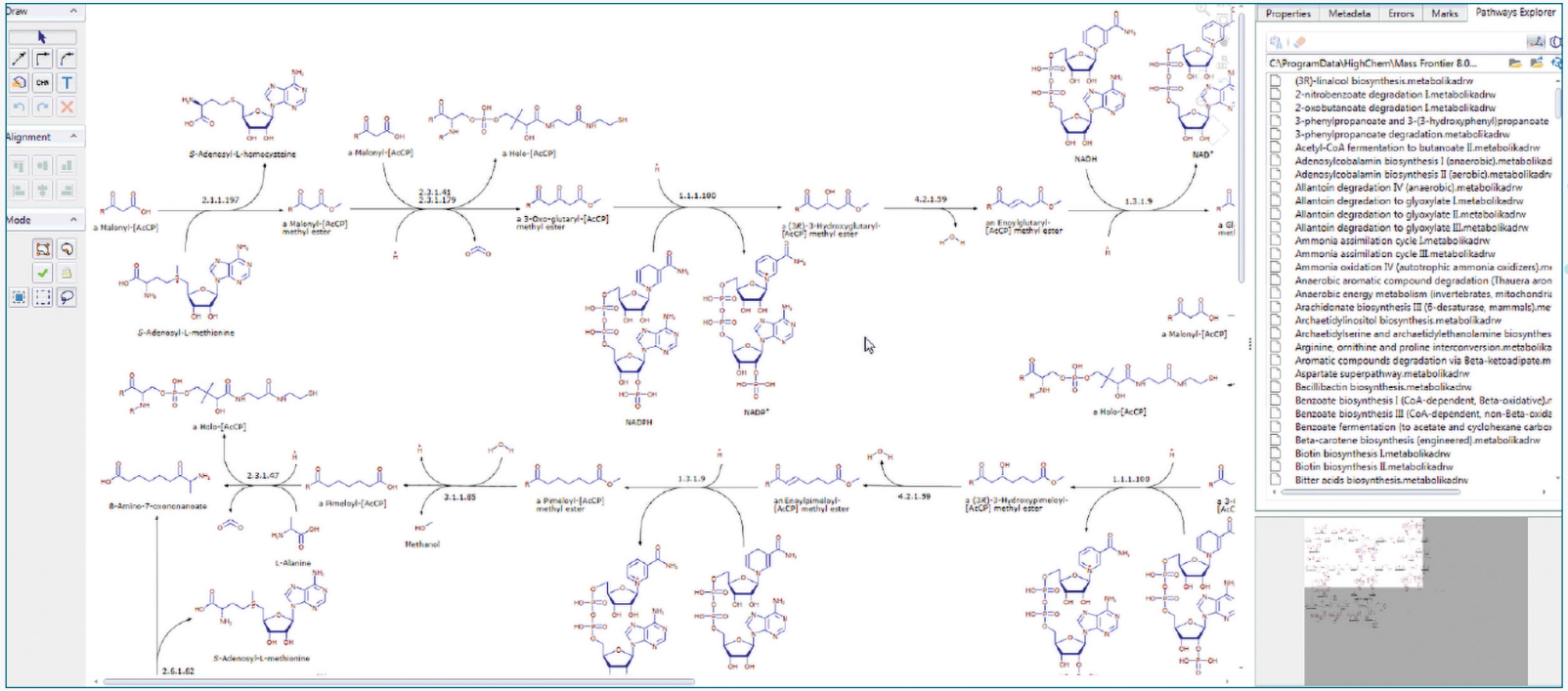
Use Mass Frontier software to search, create, and explore reaction pathways to add to your knowledge.

The Metabolika™ biological pathway module uses Microsoft® PowerPoint® software-like graphics to help users create and edit reaction pathways. In addition, the module can be used to search substructures and predict fragments in combination with mzLogic, further increasing your chances of identifying compounds.

The Pathway Explorer module includes more than 370 curated and annotated biochemical pathways for a range of organisms.



Compound structures and fragmentation schemes are easily accessed and visualized, to increase your understanding of your fragmentation data.



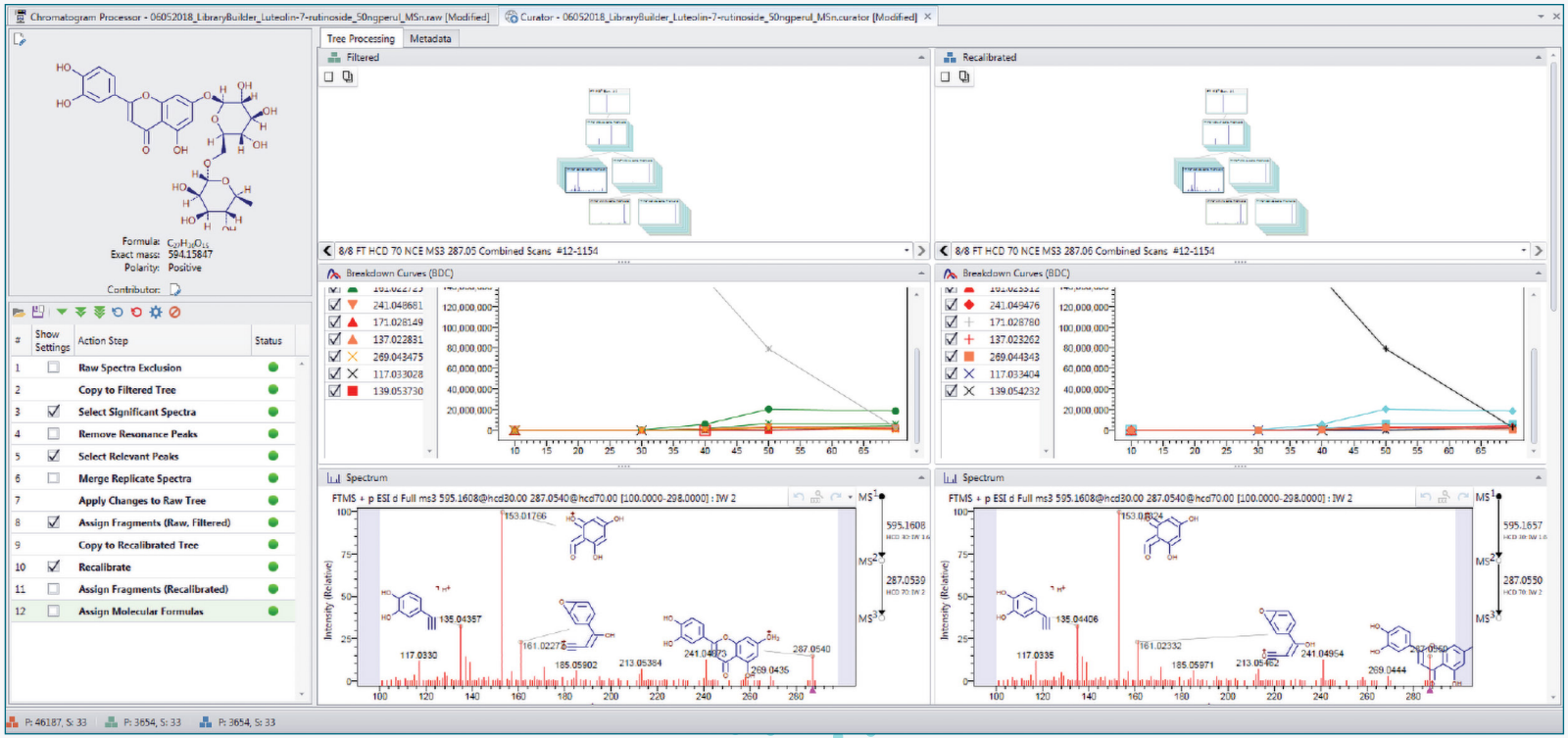
Create, edit, and search reaction pathways, using the Mass Frontier software Metabolika module.

Capture and share knowledge

Your data becomes your knowledge

With the ability to create, curate, and share spectral libraries, Mass Frontier software ensures you can capture and share insights across your workgroup and organization.

The Mass Frontier software Curator module provides the same tools used to curate entries in mzCloud, enabling you to create your own high-quality mass-spectral libraries. Using the Mass Frontier software and Server Manager, you can build and share mass-spectral library information across your organization's network.



From raw data and spectral trees, to filtered and recalibrated spectral trees, the Mass Frontier software Curator module simplifies spectral library curation, empowering you to create extensive proprietary MS^n spectral libraries.

Suite of small-molecule analysis solutions

For research and routine applications

For identification of compounds using high-resolution accurate-mass (HRAM) data, Thermo Scientific™ Compound Discoverer™ software (version 3.0 and later) provides users with the ability to batch analyze samples using streamlined, node-based workflows that reduce processing clicks.

For research applications requiring detailed understanding of compound identifications, fragmentation, and pathways, Mass Frontier software adds to the insights provided by Compound Discoverer software. In addition, Mass Frontier software is able to process nominal-mass data, and to create, curate, and share libraries.

mzCloud

mzCloud is a fully-searchable, extensively-curated database of high-resolution tandem mass spectra arranged into spectral trees. Its MS/MS and multi-stage MS^n spectra are acquired at various collision energies, precursor *m/z*, and isolation widths using collision-induced dissociation (CID) and higher-energy collisional dissociation (HCD). mzCloud allows searches of spectra, spectral trees, structures and substructures, monoisotopic masses, peaks *(m/z)*, precursors, and names.

www.mzCloud.org

mzLogic

The mzLogic data analysis algorithm enhances MS^n data processing. Using your experimental fragmentation data along with the highest-quality curated spectral library mzCloud, it combines spectral library similarity with chemical database searching to propose the best candidates for true unknowns.

www.thermofisher.com/mzLogic

Compound Discoverer Software

Identify small-molecule unknowns and find real differences in samples quickly and confidently using Compound Discoverer software. The software streamlines workflows and time-to-results with customizable node-based workflows, integrated compound identification capabilities, and statistical analysis tools.

www.thermofisher.com/CompoundDiscoverer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Whether you are a new user, or looking to upgrade, try the latest version of Mass Frontier software for 60 days, free of charge. Access the full functionality of Mass Frontier software and discover the insights you can obtain with your nominal-mass or HRAM Thermo Scientific™ Orbitrap™ mass spectrometer data.

Download it today: thermofisher.com/MassFrontier

The Connected Lab

- Monitor your system and access your data remotely and securely from anywhere in the world
- Leverage real-time monitoring of your instrument with automatic email notifications anytime, anywhere
- Store data in secure accounts and share with colleagues and collaborators around the world

www.thermofisher.com/connectedlab

System requirements

Windows® 7 Pro 64 bit or Windows® 10 64 bit

Testing configuration should include Microsoft Office 2010, 2013, or 2016.

Minimum computer requirements

Intel™ compatible processor with a minimum speed of 1 GHz

8 GB RAM

30 GB of disk space

DVD-ROM

Monitor resolution display of 1024×768 p

Recommended Data Processing PC

Intel™ compatible processor with a minimum speed of 2.5 GHz

32 GB or higher of RAM

100 GB of solid-state drive (SSD) disk space

DVD/R-ROM

Dual monitors with resolution display of 1920×1080 p

Find out more at **thermofisher.com/MassFrontier**

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