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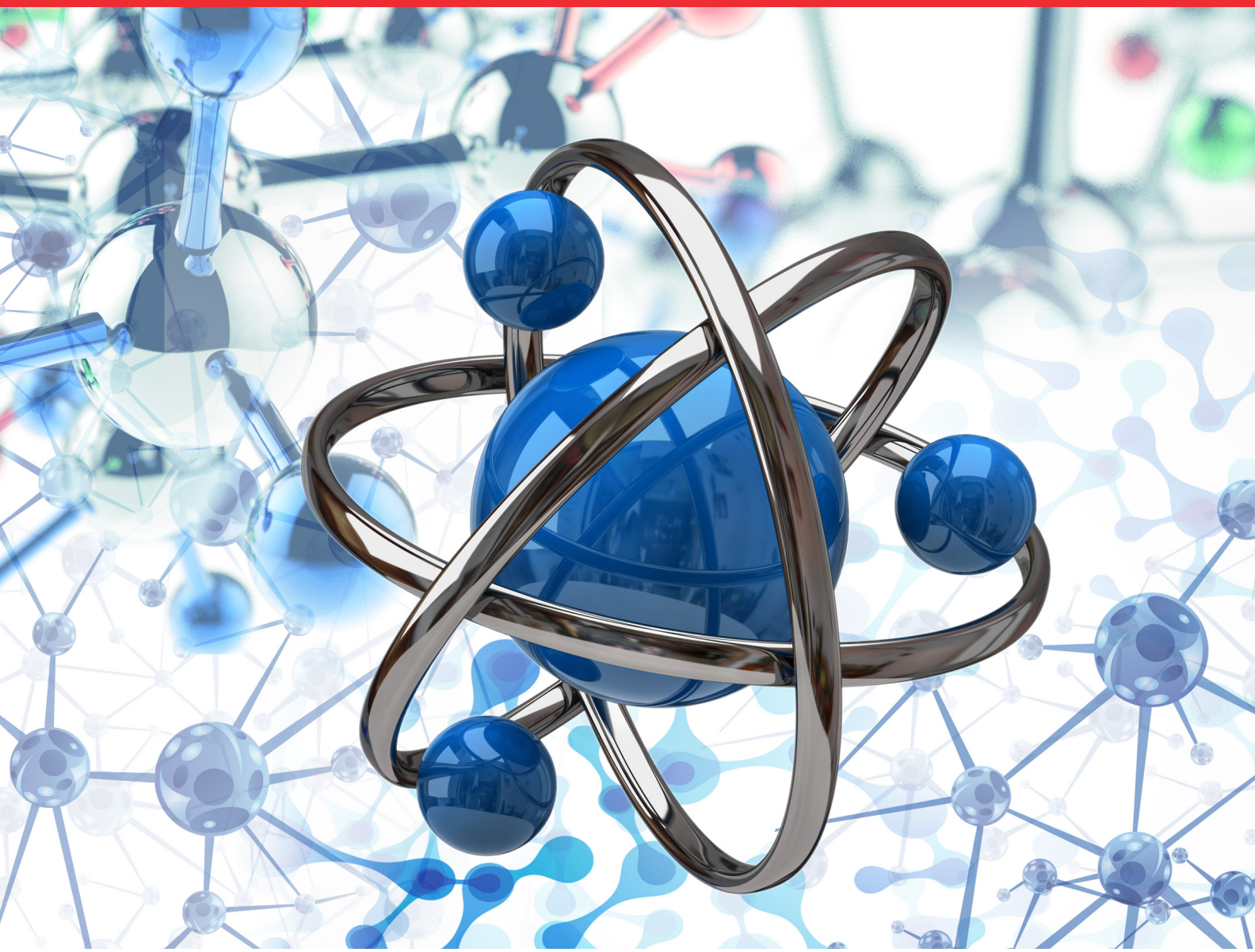


# Integrated solutions

## for small molecule research

Thermo Scientific Compound Discoverer Software

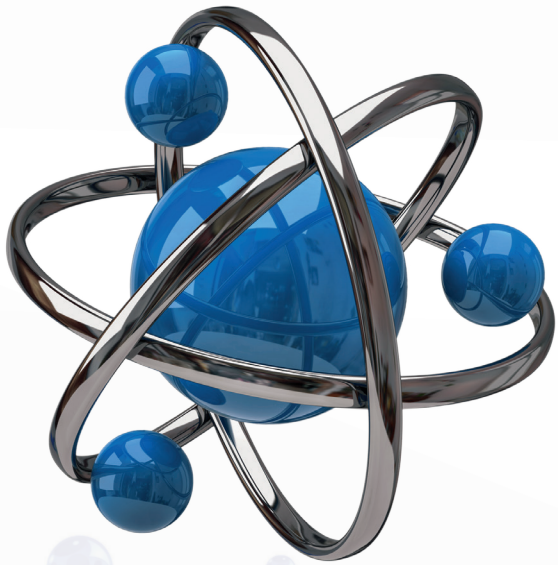
ThermoFisher SCIENTIFIC

# Compound Discoverer Software

## The complete small molecule identification and characterization solution

Thermo Scientific™ Compound Discoverer™ software is a flexible solution that offers a full suite of powerful tools to address mass spectrometry-based (MS) small molecule differential analysis, identification, and pathway mapping. Compound Discoverer software is the only small molecule analysis solution able to make full use of the high-resolution accurate-mass (HRAM) data provided by powerful Thermo Scientific™ Orbitrap™ mass spectrometer instruments.

Learn more!
www.thermofisher.com/compounddiscoverer

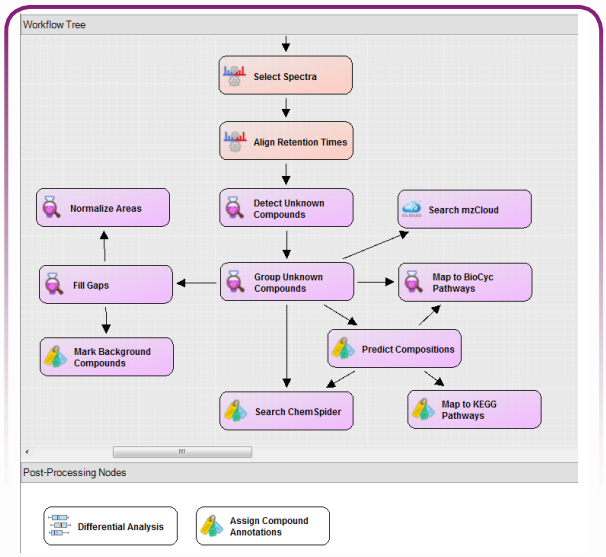


# Designed for Science

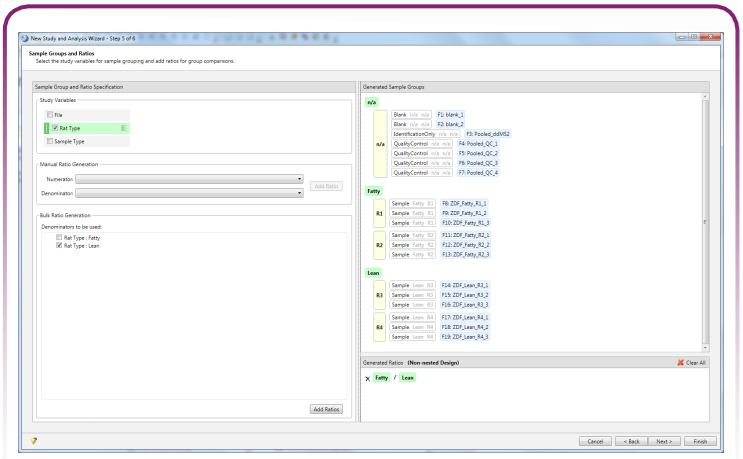
## Logical Study and Analysis Setup

### Node-Based Workflow Templates Tailored to Small Molecule Applications

With the ability to customize your workflows with a unique node-based processing design, and the capacity to handle results from thousands of injections, Compound Discoverer software can meet the needs of your most challenging research.




Untargeted metabolomics workflow template allows powerful differential analysis with identifications, statistics and QC - based area normalization in a single workflow.



Automatic sample grouping and ratios in the study and analysis wizard, along with biological replicate and QC normalization support, gives you more confident differential analysis results.

# Find Real Differences

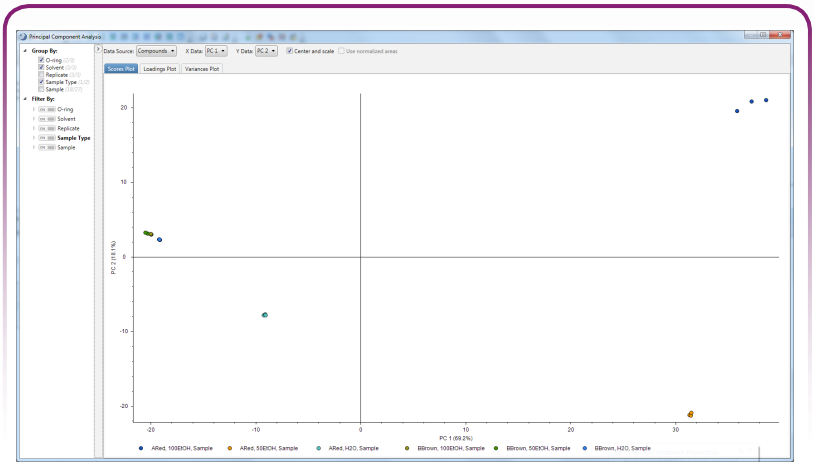
## Solve your most difficult research challenges

### Flexible visualization tools

Whether you are performing metabolomics research or looking for new emerging environmental contaminants, the powerful visualization tools within Compound Discoverer software enable you to quickly find the differences that matter.

Quickly see trends in compounds across the study or identify the key compounds of interest between multiple sample groupings with interactive linked displays. Move quickly from high-level PCA visualizations to individual compounds with a simple click.

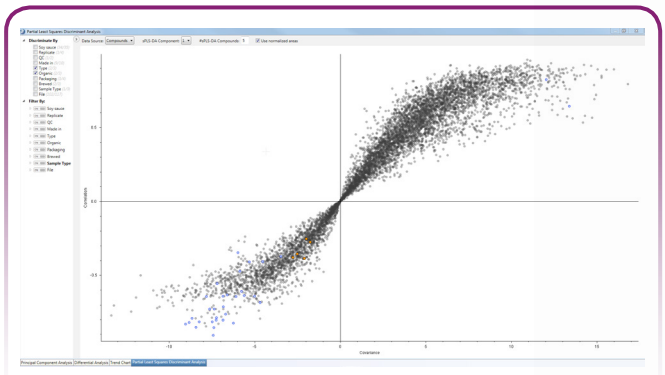
A



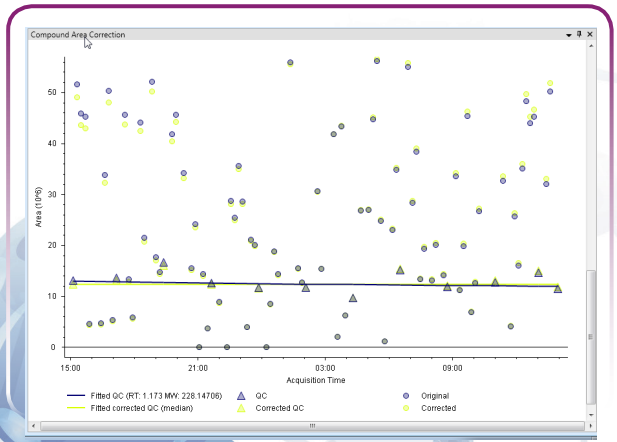
Options for interactive visualization include:
A. principal component analysis (PCA) scores, loadings, and trend plots
B. differential analysis "volcano" plots
C. partial least squares discriminant analysis (PLS-DA) - S-plot

B

C



Pooled QC-based area corrections for each unknown compound helps to correct various systematic biases for large scale metabolomics studies.

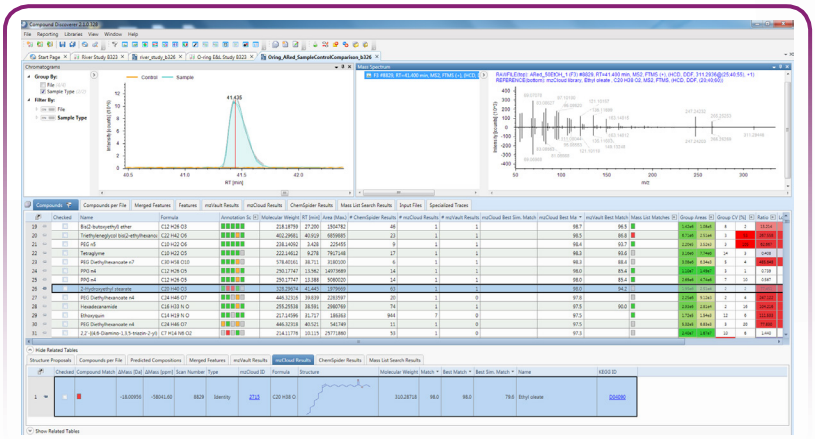


# Identify More Unknowns

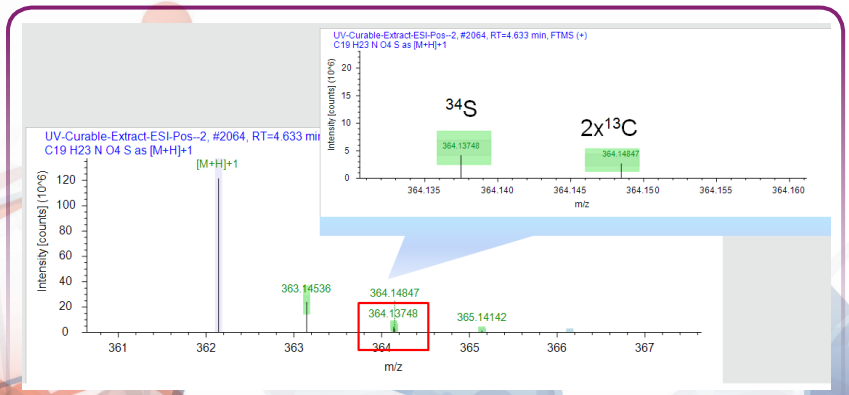
## Powerful compound identification

### Turn data into knowledge

Determining the compounds of interest in a complex analysis is only a part of the problem. Compound identification remains one of the toughest challenges in many research applications. Compound Discoverer software includes the most confident elemental composition prediction for unknowns utilizing fine isotopic structures from high resolution Orbitrap full MS, as well as MS/MS information to improve predictions. Combined with parallel library searching such as the unique high quality mzCloud™ online fragmentation library (mzCloud.org) and molecular weight or formula based searches of ChemSpider™, user-created mzVault spectral library or other custom databases, Compound Discoverer software gives you the power to turn unknowns into knowledge.



Automatically identify sample compounds using the mzCloud™ curated HRAM $MS^n$ library — directly within Compound Discoverer. mzCloud search returns not only precursor ion accurate mass matches, but also similarity matches without precursor ion mass match which provides valuable sub-structure information for the unknown compound of interest.



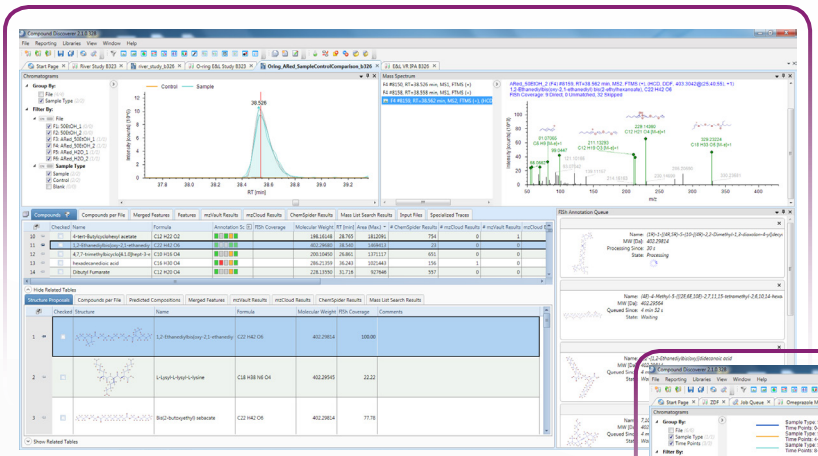

Confident elemental composition utilizing fine isotopic information from HRAM Orbitrap mass analyzer full MS and MS/MS.

# Turn Spectra into Structures

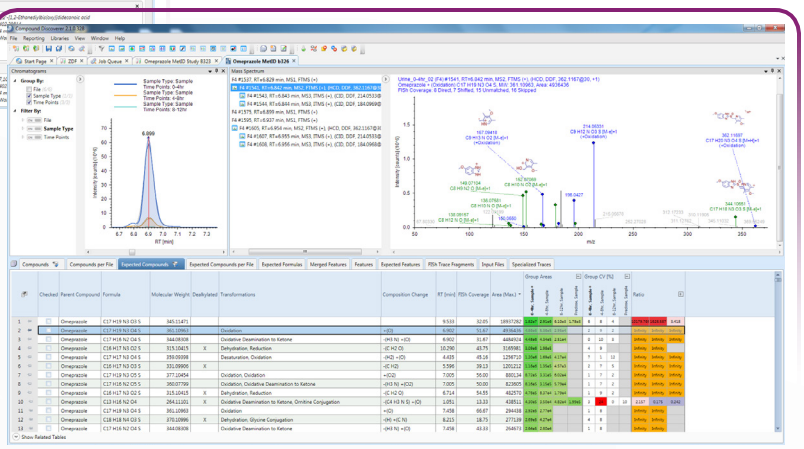
## Maximum usability

### From spectra to structure

Detecting the compounds of interest in a sample is only the beginning. The determination of the structure of metabolites, impurities, degradants, and other related compounds is simplified with automatic batch FISh (Fragment Ion Search) annotations. Matching fragments are automatically annotated on the spectra of $MS^2$ and $MS^n$ data.

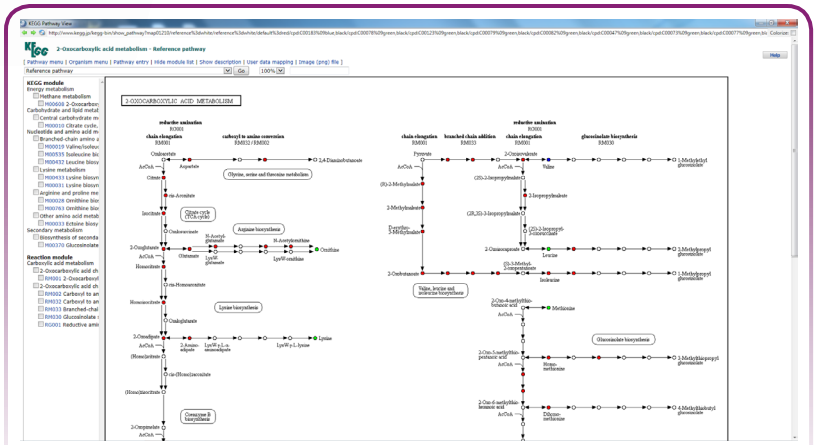


FISh calculation on a batch of ChemSpider proposals to aid in structural confirmation of the unknown compounds. Matching fragment structures are automatically annotated on the spectra.

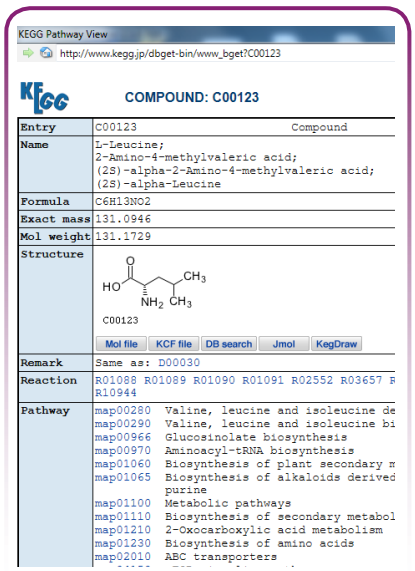


Automatic annotation of metabolites in human urine. Color-coded transformation fragments quickly localize the site of modification.

# Large Data Sets to Pathways
## No Problem

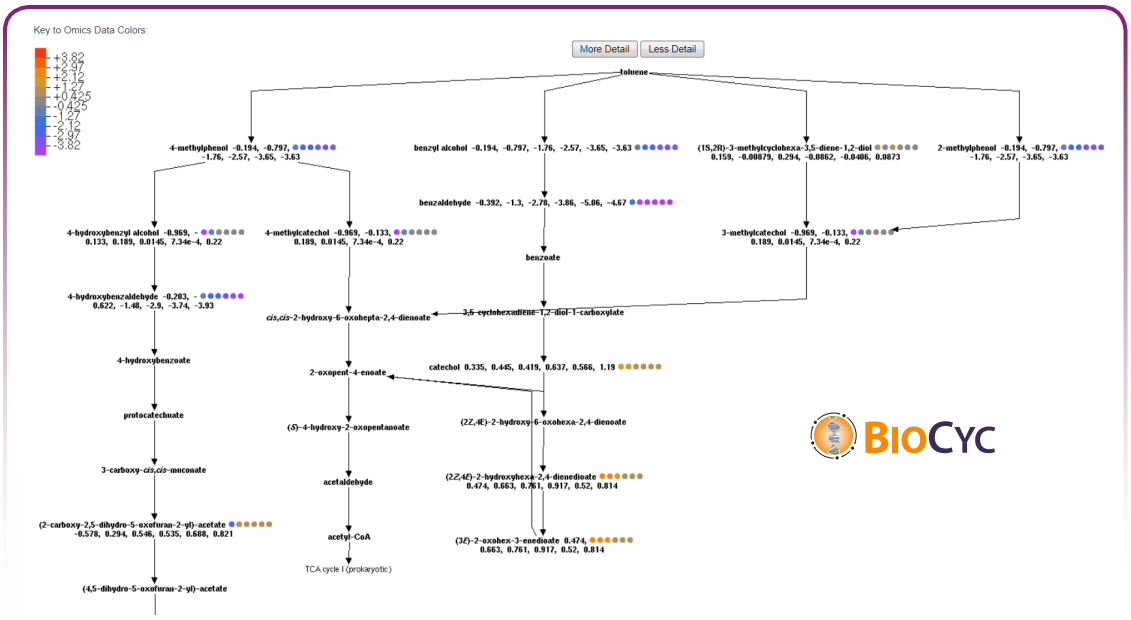


Map detected metabolites to KEGG pathways




## Map, display compounds to biological pathways

Move from data to biological interpretation: Compound Discoverer software allows automatic search against KEGG™ and BioCyc™ databases. Powerful identifications and statistical tools, complemented with visualization of metabolic pathways all within one software package.




Map compounds to BioCyc pathways

# Small Molecule Software Tools

## Solve big challenges in many applications

### Metabolomics

By combining the tools necessary for the determination of compounds of interest in large complex biological datasets, Compound Discoverer software offers a unique solution for quickly finding and identifying important statistical differences between sample sets.

### Extractables and Leachables

E&L testing is part of product safety testing for many industries. Compound Discoverer software's tools and powerful workflows help customers quickly and confidently identify E&L compounds with increased throughput.

### Impurities and degradents

Identification of impurities and degradation products in drugs and food is a critical aspect of product safety testing. Compound Discoverer software's tools and customizable approaches enable confident detection of related components in complex samples.

### Environmental and food safety

Food and environmental fate studies, and the analysis of contaminants in soil and water, present data processing challenges similar to those of related or unknown compound identification. Thus, Compound Discoverer software is also ideally applicable to the analysis of metabolic fate and unknown compound identification of food and environmental degradents and contaminants.

### Pharma MetID

The detection of related compounds in biological samples and determination of their structures is a key aspect of pharmaceutical research. Compound Discoverer software allows you to find and identify your metabolites while its reporting tools give you greater flexibility.

### Forensic toxicology

Targeted screening applications can only confidently find what they are looking for. Compound Discoverer software enables forensic toxicology researchers to look for and find metabolites of drugs of abuse or structurally related designer drugs. This information can then be transferred back to screening applications to help you keep up with an ever-expanding list of drugs and drug metabolites.

### Required operating system

Windows® 7 SP1 or Windows 10 64-bit.

### Recommended computer specifications

- CPU: i7 3930 × 3.3 GHz or equivalent
- Memory: 32 GB RAM
- HDD: 2 drives, 1 TB SSD and 1 TB HDD

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