Thermo Scientific Compound Discoverer Software

A New Generation

of integrated solutions for small molecule structure ID

Thermo SCIENTIFIC

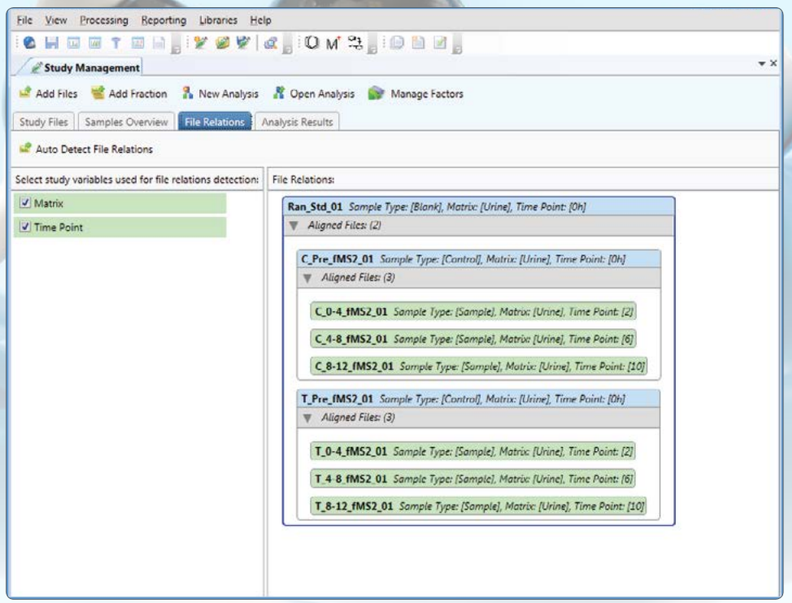
Transforming
Small Molecule Research

Solutions for Small Molecule Structural ID

Thermo Scientific™ Compound Discoverer™ software provides a new direction for small molecule structural identification in diverse research fields. A common set of tools in a single software package enables confident detection and identification of small molecules.

Whether your research focus is metabolite identification, impurities analysis, environmental research, or forensic toxicology, the tools available within Compound Discoverer software can help accomplish the most complex related detection and identification.

From sample management and study design, to robust processing options and reporting, Compound Discoverer software brings together all of the features and capabilities needed to support research applications in a wide range of fields.



Sample definition begins with the creation of a study in an easy-to-use, drag-and-drop interface to associate samples based on user-defined variables.

Design for Science
Logical Study and Analysis Setup

Sample Management with Science in Mind

The samples we analyze come from the experiments we plan. With this simple fact in mind, Compound Discoverer software enables robust data handling by allowing the creation of studies that assemble data from one or more experiments, thus facilitating analyses and comparisons not previously possible.

An intelligent sequence and analysis design speeds up the association of samples and the design of the experiment for batch processing.

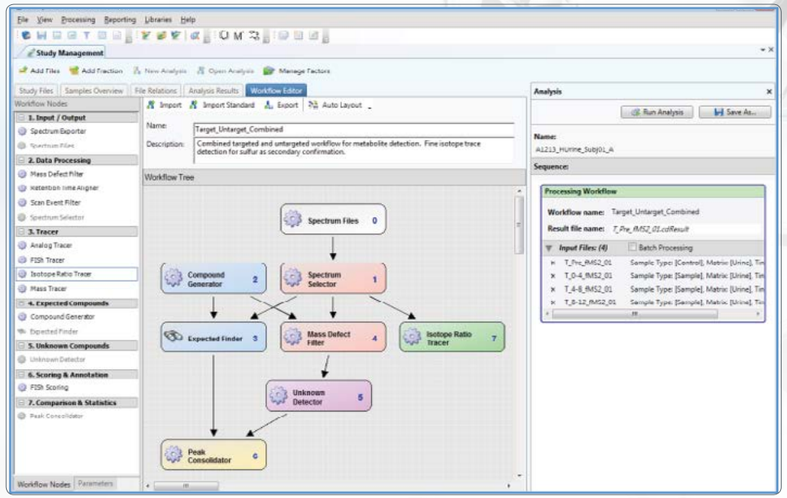
Flexible yet Powerful

Customizable Workflows

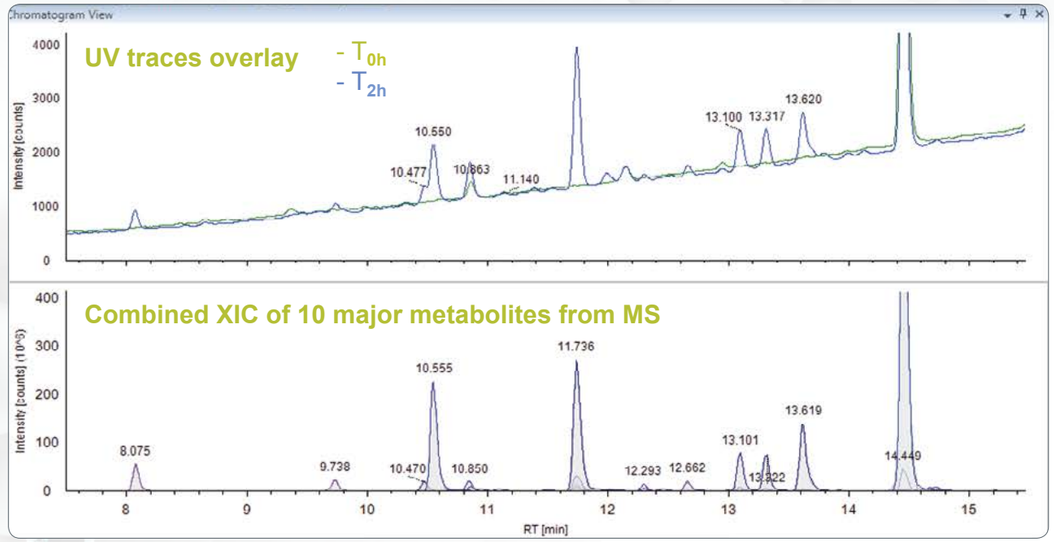
Customization means Greater Control

Modular processing workflows assembled from a suite of advanced algorithms (nodes) provide the power to adapt your data analysis to the questions at hand. The drag-and-drop workflow editor gives you increased control over how your data will be analyzed.

Powerful workflow options allow you to analyze analog and mass spectrometer data, detect components with targeted and untargeted mechanisms, and utilize very high resolution to quickly perform fine isotope searches.



The workflow editor provides complete control of your data processing.



Combining multiple analyses increases the confidence that all components in a study are found. Here data from different time points measured by PDA and HRAM mass spectrometry are combined from a metabolism study of darunavir in human microsomes.

Finally See Everything

Powerful Review

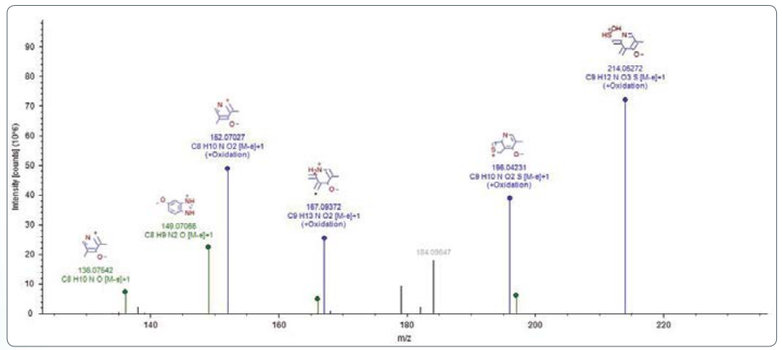
Decide with Confidence - Customizable Views

Accurate identification requires the ability to review many pieces of experimental information simultaneously. With customizable layouts and multiple monitor support, Compound Discoverer software enables a level of visibility previously unavailable. Stack and overlay multiple types orthogonal data to give you confidence in your analysis and assignment.

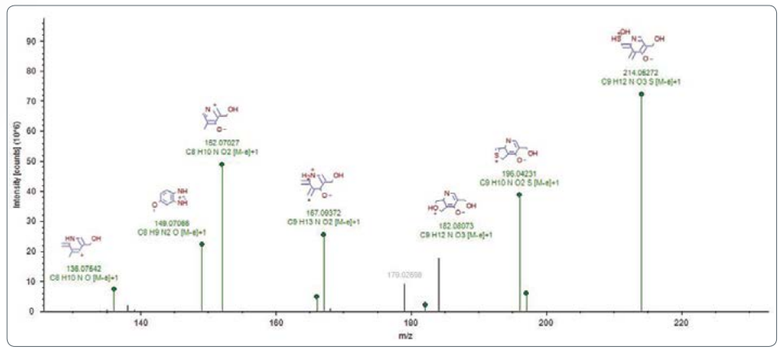
It's your data
Maximum Usability

From Spectra to Structure

Detecting the components of interest in a sample is only the beginning. The determination of the structures of metabolites, impurities, degradants, and other related components is simplified with automatic annotations. Transformations are quickly localized with color-coded fragmentation of MS^2 and MS^n data.



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



Automatic re-annotation using a putative structure confirms the assignment.

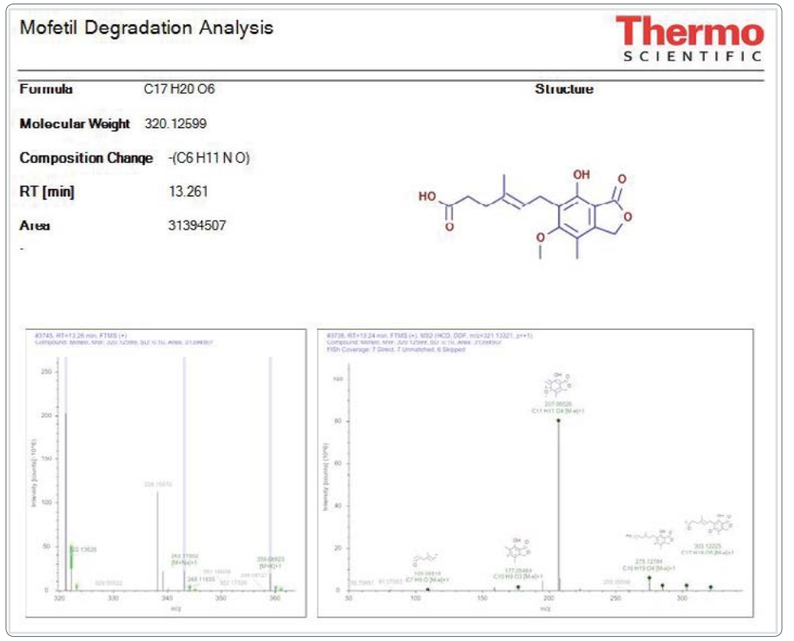
Small Molecule Research
More than Metabolite ID

Making Real Use of Results

Powerful tools for processing data quickly create valuable results; however, there is still the need to transfer that knowledge and supporting information.

With a full suite of options, Compound Discoverer software allows for customized reporting to assure that results can be transferred to those who need it.

With multiple available formats for output, data can be transferred into informatics solutions, while extensive graphical options support the creation of detailed structure identification reports.



Transmitting information with a structural identification report for the degradation products of mofetil.

Small Molecule ID Tools

for diverse applications

Pharma MetID – The detection of related components 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 keep up with an ever expanding list of drugs and drug metabolites.

Minimum Computer Requirements(Recommended):

OS: Windows 7 SP1 64 bit

CPU: 3.4 GHz dual-core (i7 3930x 3.3 GHz or equivalent)

Memory: 8 GB RAM (32 GB RAM)

HDD: 500 GB hard drive (2 Drives, 1 TB SSD + 1 TB HDD)

Impurities and Degradents – Identification of impurities or products of degradation in drug products or foods is a critical aspect of safety testing. Customizable approaches using the tools within Compound Discoverer software allows you to confidently detect related components.

Environmental Research – Environmental fate studies as well as soil and water research share common needs with metabolite identification applications. The tools in Compound Discoverer software apply here for determining metabolic fate and the structures of environmental metabolites and degradents in complex samples.

For Research Use Only. Not for use in diagnostic procedures.

www.thermoscientific.com/en/product/compound-discoverer-software.html

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ISO 9001

Africa +43 1 333 50 34 0
Australia +61 3 9757 4300
Austria +43 810 282 206
Belgium +32 53 73 42 41
Canada +1 800 530 8447
China 800 810 5118 (free call domestic)
400 650 5118
Denmark +45 70 23 62 60
Europe-Other +43 1 333 50 34 0
Finland +358 9 3291 0200
France +33 1 60 92 48 00
Germany +49 6103 408 1014
India +91 22 6742 9494
Italy +39 02 950 591
Japan +81 45 453 9100
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New Zealand +64 9 980 6700
Norway +46 8 556 468 00
Russia/CIS +43 1 333 50 34 0
Singapore +65 6289 1190
Spain +34 914 845 965
Sweden +46 8 556 468 00
Switzerland +41 61 716 77 00
UK +44 1442 233555
USA +1 800 532 4752

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