

Resource Summary Report

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Compound Discoverer

RRID:SCR_028693

Type: Tool

Proper Citation

Compound Discoverer (RRID:SCR_028693)

Resource Information

URL: <https://mycompounddiscoverer.com/>

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Description: Software platform by Thermo Fisher Scientific designed for identifying, comparing, and interpreting small molecules in complex biological, environmental, and forensic samples. It uses customizable workflow, known as nodes, to automate mass spectrometry data processing, spectral library searching, and statistical analysis. Compound Discoverer is integrated with SIRIUS (via a custom workflow node) to bridge the gap between high-resolution MS/MS data and confident molecular identification. While Thermo Scientific's Compound Discoverer excels at library searching and statistical analysis, SIRIUS provides powerful in silico tools to accurately predict molecular formulas, chemical classes, and de novo structures. High-resolution mass spectrometry (HRMS) data analysis software for untargeted metabolomics, lipidomics, and contaminant screening. Utilizes modular workflows to extract features, match spectra against libraries like mzCloud, and confidently identify complex organic compounds.

Synonyms: Thermo Scientific Compound Discoverer

Resource Type: software application, software resource

Defining Citation: [PMID:41919739](#)

Keywords: High-resolution mass spectrometry (HRMS) data analysis, small molecule data processing and metabolomics, identifying, comparing, interpreting, small molecules,

Availability: Restricted

Resource Name: Compound Discoverer

Resource ID: SCR_028693

Record Creation Time: 20260721T194536+0000

Record Last Update: 20260815T042945+0000

Ratings and Alerts

No rating or validation information has been found for Compound Discoverer.

No alerts have been found for Compound Discoverer.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We have not found any literature mentions for this resource.