

**ANALYZE SMARTER.
DISCOVER FASTER.**



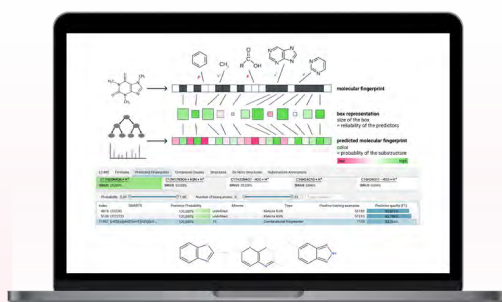
SIRIUS is the comprehensive software solution for high-throughput identification of small molecules from fragmentation mass spectrometry data.

SIRIUS is engineered to overcome the inherent limitations of library-dependent identification methods by not only accurately characterizing known compounds, but also reliably identifying “unknown unknowns” in complex biological samples.



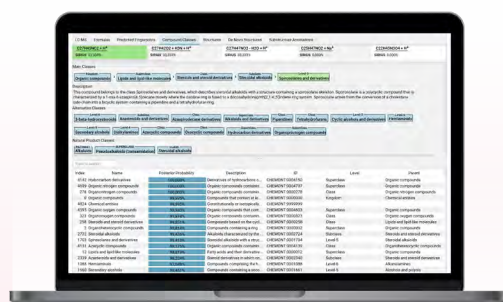
Molecular Formula Annotation

- dual approach that analyzes both isotope and fragmentation patterns
- no spectral library required
- distinct search strategies ranging from generic applications to the discovery of “unknown unknowns”
- network-enhanced annotation for complex biological datasets



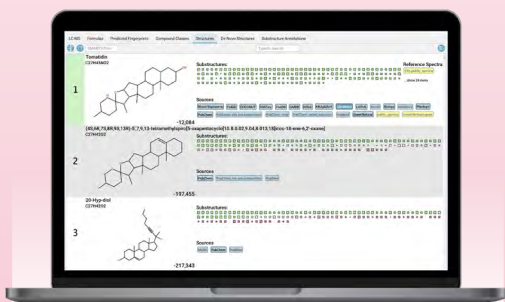
Molecular Fingerprint

- unique, machine-readable molecular fingerprint
= set of structural properties
- predicted from fragmentation pattern
- crucial, intermediary feature that powers highly accurate structure and class prediction



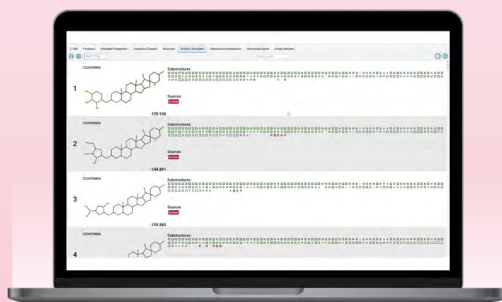
Chemical Classification

- complete chemical class hierarchy (ClassyFire compound classes)
- neither spectral nor structural reference data required
- contextual understanding even for novel or unannotated compounds



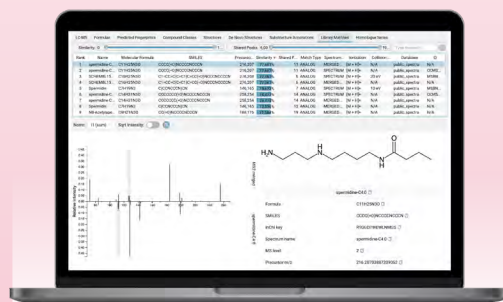
Molecular Structure Annotation

- efficient search in massive molecular structure databases
- identification of the most likely structure candidate
- wide range of built-in databases
- custom databases with own structures
- confidence score for every structure prediction result



De Novo Structure Generation

- overcoming the limitations of searching finite structure databases
- discovery of truly novel molecules
- structures generated from scratch based on the molecular formula and the predicted molecular fingerprint



Spectral Library Search

- rapid matching against spectral libraries
- analog search to identify related compounds with similar core structures
- spectral library hits as auxiliary annotations alongside the main structural results
- spectral matches as validation level for result verification



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SIRIUS

SIRIUS is the comprehensive software solution for high-throughput identification of small molecules from fragmentation mass spectrometry data.

Beyond the core algorithmic features, SIRIUS provides a comprehensive set of additional features streamlining the analysis workflow from feature detection to detailed result validation.



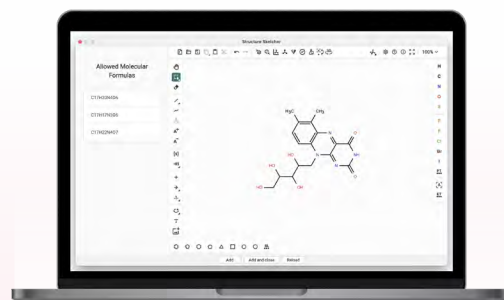
Full LC-MS Data Processing

- high-throughput processing
- extraction and alignment of chromatographic features across multiple samples
- robust feature and adduct detection
- quality metrics to effectively prioritize and filter results
- powerful job-scheduling enables parallelization across multiple cores



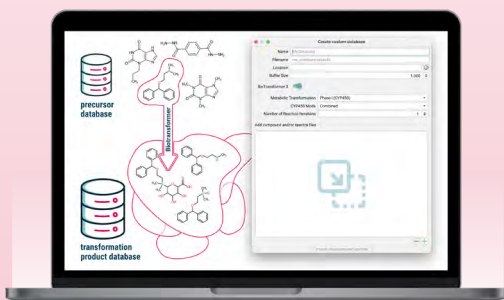
Substructure Validation

- powerful visualization tools for manual assessment of structural assignments
- substructure highlighting to display supported molecular features
- substructure annotations to link peaks to the proposed substructures
- highlighting of shared substructure explanations observed in analogs



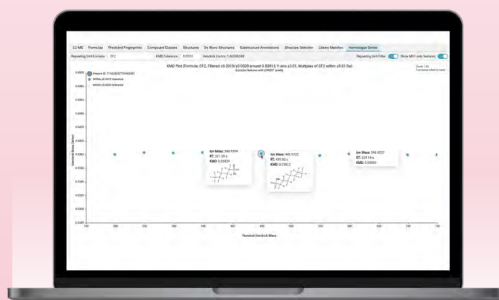
Structure Sketcher

- integrated chemistry workbench to quickly edit chemical structures directly within the software
- use your chemical knowledge
- manual modification of existing or submission of new candidate structures
- re-scoring of sketched structures against predicted fingerprints



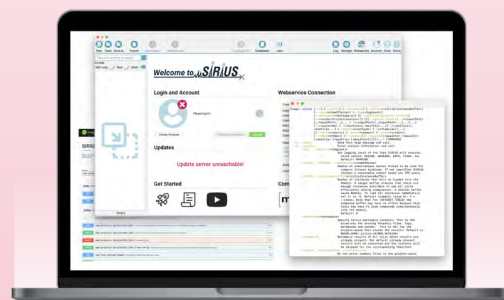
Biotransformer Integration

- seamlessly incorporation of biotransformation predictions
- custom, *in silico* databases of expected metabolic or degradation products generated on the fly
- simplified identification of drug metabolites or environmental breakdown products



Plots for Homologous Series

- Kendrick Mass Defect plots
- grouping of related molecules into homologous series
- grouping of compounds that share a common core structure but differ by specific, repeating chemical units
- easy-to-spot structural patterns across samples



Powerful Suite of Interfaces

- intuitive Graphical User Interface (GUI) for visual analysis
- Command Line Interface (CLI) to automate large analysis
- Application Programming Interface (API) for pipeline integration
- persistence layer between interfaces
- fast, reproducible results with streamlined workflows



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