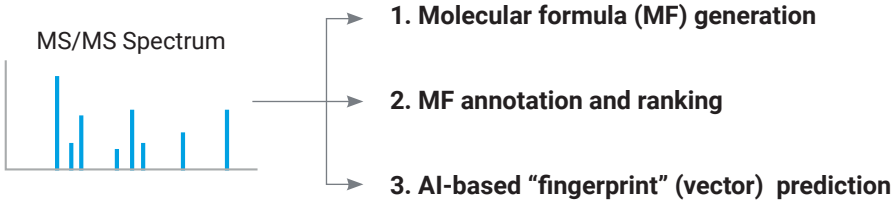
Enhancing Unknown Identification with MH Explorer and Complimentary SIRIUS with CSI:FingerID

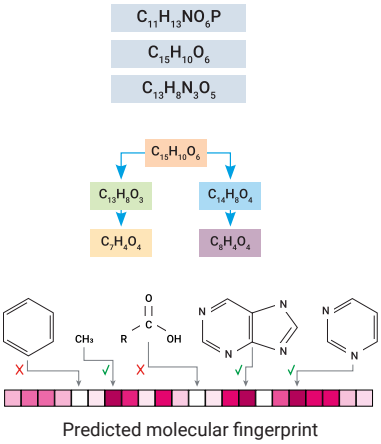
Identification without reference to spectrum or RT information

Expand your identification workflows using SIRIUS with CSI:FingerID, an advanced AI-based tool designed to unlock the full potential of your mass spectrometry data. CSI:FingerID leverages deep kernel learning and supervised learning models to predict structural features (molecular fingerprints) of unknowns from high-resolution tandem mass spectra. This enables a direct correlation between spectra and molecular structures. Unlike traditional spectral library searches that are limited, CSI:FingerID expands unknown identification by leveraging extensive structural databases. Agilent has contributed more than 10,000 spectra to train the AI models behind CSI:FingerID.

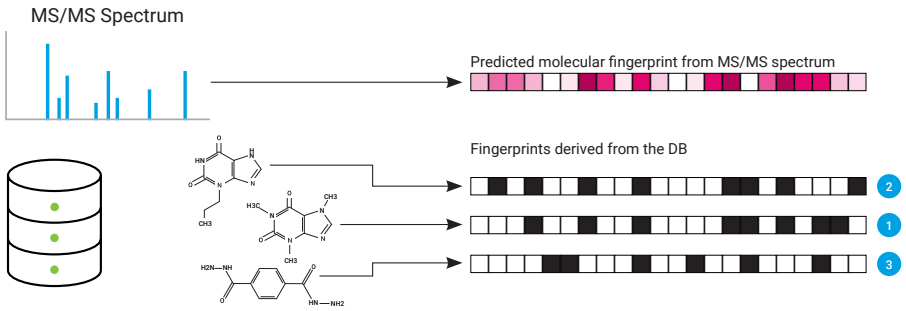
Predicting the molecular fingerprint



Molecular formulas are generated from high-resolution unknown MS/MS spectrum using either de novo, database-restricted (e.g., PubChem), or bottom-up strategies. A molecular “fingerprint” (vector) is predicted for each candidate structure using advanced AI algorithms.



Identification without reference spectra



The predicted molecular fingerprint of the unknown is compared to the molecular fingerprints of structures derived from the structural DB, ranking candidates to identify the unknown.

CSI:FingerID is consistently among top performers in the prestigious annual Critical Assessment of Small Molecule Identification (CASMI) contest delivering automatic, fast, and superior identification of true unknowns.

SIRIUS, hosted by Bright Giant, also includes CANOPUS which predicts compound classes from the molecular fingerprint predicted by CSI:FingerID without any database search involved.

Agilent

Trusted Answers

Capture the Power of SIRIUS CSI:FingerID with complimentary, direct access from MassHunter Explorer

Agilent MassHunter Explorer software with CSI:FingerID offers significant technical benefits for true unknown identification.

It also delivers substantial financial benefits by offering up to 100,000 complimentary CSI:FingerID queries per year for Explorer users, including commercial entities.

MassHunter Explorer
Direct Access to SIRIUS

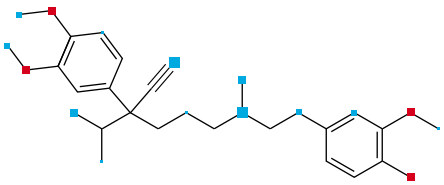
Identification of true unknows with SIRIUS CSI:FingerID via database search

Compound class prediction with CANAPUS without database reference

100,000 complimentary queries per year, even for commercial organizations saving thousands every year.

A drug metabolite identification—from verapamil incubated with liver microsomes-, shows the value of CSI:FingerID for unknown identification. While this metabolite does not have corresponding MS/MS spectra in NIST23, MassBank or HMBD, CSI:FingerID predicted the compound to be p-O-Desmethyl Verapamil through molecular fingerprinting and a database structure search as the top hit over a second compound with a similar structure.

p-O-Desmethyl Verapamil



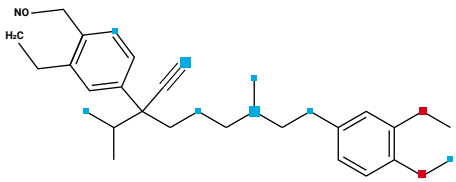
Substructures:

Sources:
Blood Exposome, DSSTex, HMOB, MeSH, NORMAN, PubChem, PubChem bio and metabolites
PubChem drug, PubMed, SuperNatural

$C_{26}H_{36}N_2O_4$ -25.464

Benzeneacetonitrile, alpha-(3-(2-(3,4-dimethoxyphenyl)ethyl)methylamino)propyi)-4-hydroxy-3-methoxy-alpha-(1-methylethyl)-, (R)-

Substructures:



Sources:
Blood Exposome, CHEBI, DSSTex, HMOB, MeSH, NORMAN, PubChem, PubChem bio and metabolites
PubChem drug, PubMed

-38.790

Dührkop, K., Fleischauer, M., Ludwig, M. et al. SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. Nat Methods 16, 299–302 (2019). https://doi.org/10.1038/s41592-019-0344-8

www.agilent.com/chem/masshunter-explorer

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