


SIRIUS 5 Prediction settings for

This software is used for identifying the molecular formula, constructing fragmentation trees, and predicting the fingerprint.

SIRIUS

SIRIUS - Molecular Formula Identification

General
Instrument: Orbitrap
Filter by isotope pattern: ☒
MS2 mass accuracy (ppm): 5
MS/MS isotope scorer: IGNORE
Candidates stored: 10
Min candidates per ion stored: 1

Use DB formulas only
☒ Bio Database
☒ Biocyc
☒ ChEBI
☒ COCONUT
☒ EcoCyc Mine
☒ GNPS
all none

Possible ionizations
☒ [M + H]⁺
☒ [M + K]⁺
☒ [M + Na]⁺
all none


ILP
Tree timeout: 0
Compound timeout: 0
Use heuristic above m/z: 300
Use heuristic only above m/z: 650

Elements allowed in Molecular Formula

H	0	inf	C	0	inf	N	0	inf	O	0	inf
P	0	inf	B	0	auto	Si	0	0	S	0	auto
Cl	0	auto	Se	0	auto	Br	0	auto	F	0	0
I	0	0									

Select elements

ZODIAC - Network-based improvement of SIRIUS molecular formula ranking

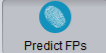
ZODIAC

General
Considered candidates 300m/z: 10
Considered candidates 800m/z: 50
Use 2-step approach: ☒

Edge Filters
Edge Threshold: 0.95
Min Local Connections: 10

Gibbs Sampling
Iterations: 20,000
Burn-In: 2,000
Separate Runs: 10


CSt:FingerID - Fingerprint Prediction

Predict FPs

Fallback Adducts
☒ [M + H]⁺
☐ [M]⁺
☒ [M - H2O + H]⁺
☒ [M + H3N + H]⁺
☐ [M + H2O + H]⁺
☐ [M + CH4O + H]⁺
all none enforce

General
Score threshold: ☒

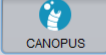
CSt:FingerID - Structure Database Search

Search DBs

Search DBs
☒ Bio Database
☒ Biocyc
☒ ChEBI
☒ COCONUT
☒ EcoCyc Mine
☒ GNPS
all none non in silico

General
Tag Lipids: ☒

CANOPUS - Compound Class Prediction

CANOPUS

Parameter-Free! Nothing to set up here. =)

☐ Recompute already computed tasks?

Show Command Compute Cancel