


## SIRIUS 5 Prediction settings

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]<sup>+</sup>  
☒ [M + K]<sup>+</sup>  
☒ [M + Na]<sup>+</sup>  
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**

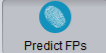
ZODIAC

**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]<sup>+</sup>  
☐ [M]<sup>+</sup>  
☒ [M - H2O + H]<sup>+</sup>  
☒ [M + H3N + H]<sup>+</sup>  
☐ [M + H2O + H]<sup>+</sup>  
☐ [M + CH4O + H]<sup>+</sup>  
all none enforce

**General**  
Score threshold: ☒

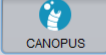
**CSt:FingerID - Structure Database Search**

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