

Seminar

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1 Research background

2 Results

3 Discussion

4 Extra

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Research background

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Results

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Discussion

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END

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Research background

Introduction

- The trouble with analysis of untarget LC-MS/MS dataset
- Existing identification approaches
 - 1 Spectral library match
 - 2 Matching with fragmentation spectra of in silico simulation
 - 3 In silico prediction with matching learning
- State-of-the-art technology: SIRIUS 4 prediction through structural libraries
- From in silico, towards biological research: identification and biomarker
- Classified visualization boost biological analysis?

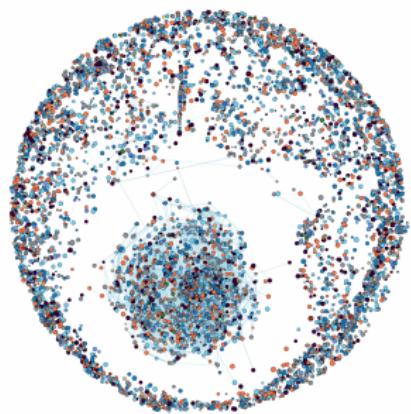
Introduction

- Chemical classification
 - 1 Taxonomy and Ontology
 - 2 key metabolites or drug in hierarchies
- MCnebula workflow
 - 1 Classified visualization
 - 2 Abundance-based classes selection
 - 3 Leveraging State-of-the-art technologies
 - 4 ...

Results

Overview of MCnebula

Parent-nebula

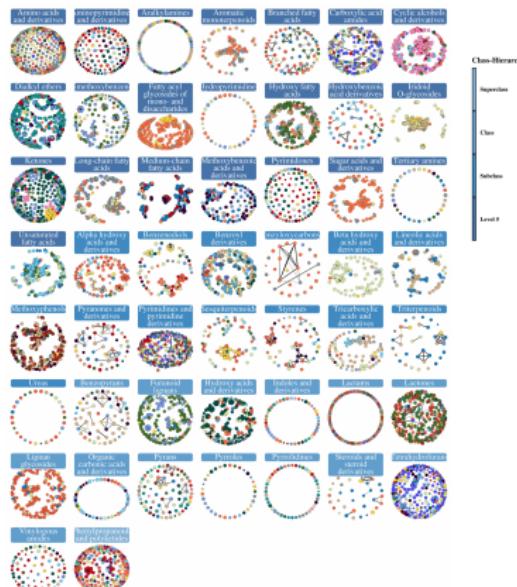

Class

- Alkaloids and derivatives
- Barbiturates
- Hydrocarbon derivatives
- Lipids, nitrogenous and related compounds
- Lipids and lipid-like molecules
- Nucleosides, nucleotides, and analogues
- Organic acids and derivatives
- Organic anions
- Organic nitrogen compounds
- Organic oxygen compounds
- Organoheterocyclic compounds
- Organonitrogen compounds
- Phenolic compounds
- Phenyl compounds and phenyl ethers

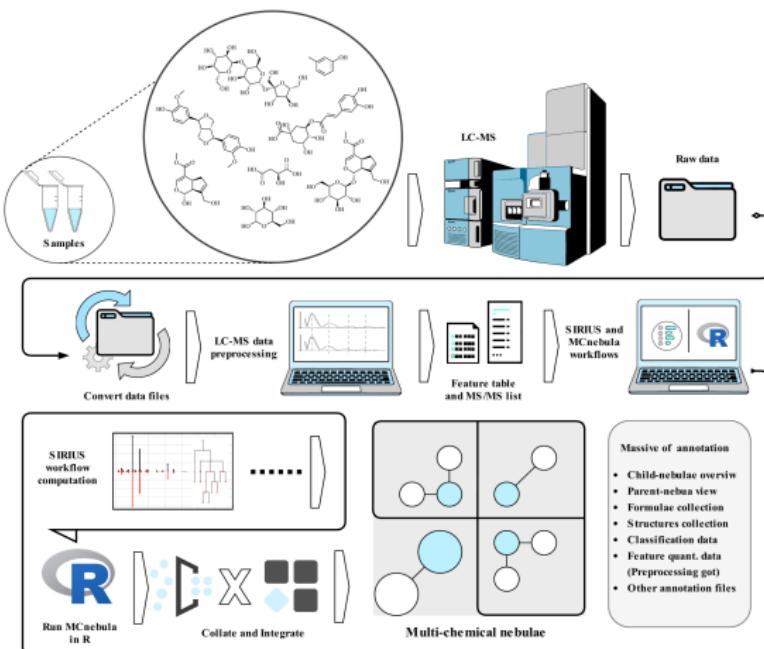
Tauclidean similarity

- 0.5
- 0.6
- 0.7
- 0.8

Child-nebula



Overview of MCnebula



Evaluation

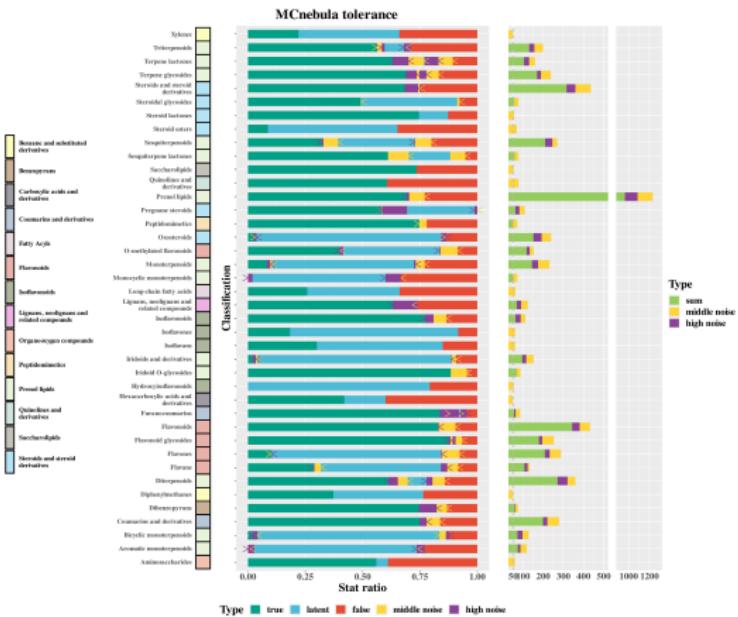


Figure 3: mc.tl.bar

Evaluation

Classification

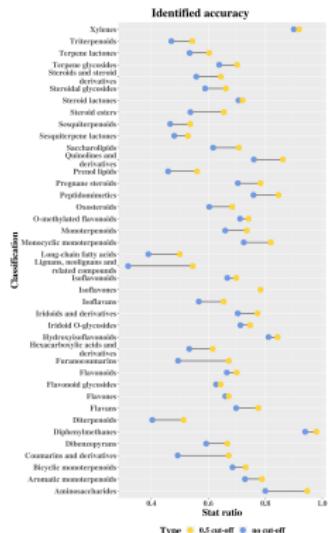
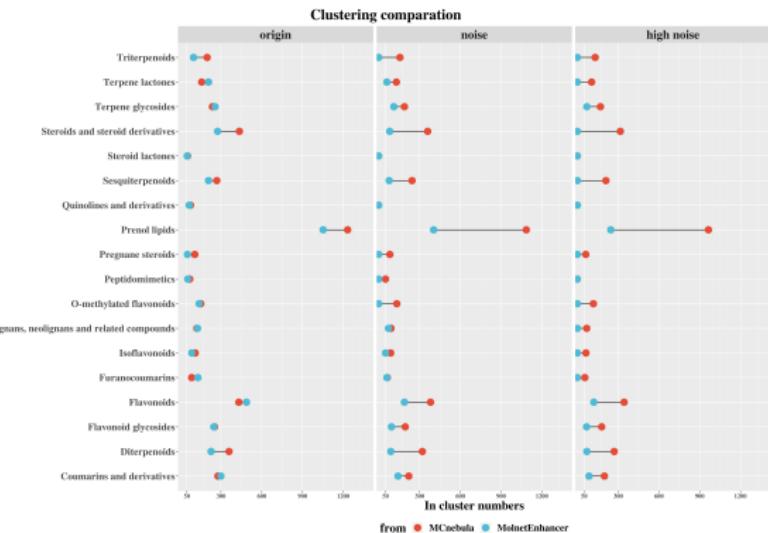
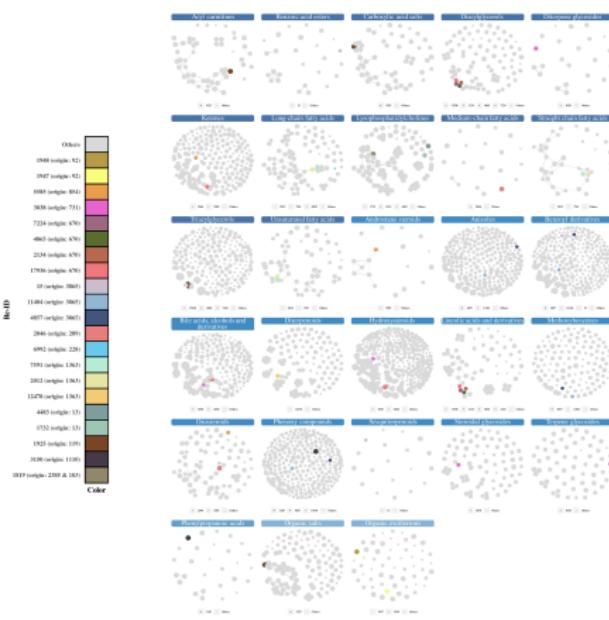


Figure 4: cp.id.accuracy

Serum dataset



Serum dataset

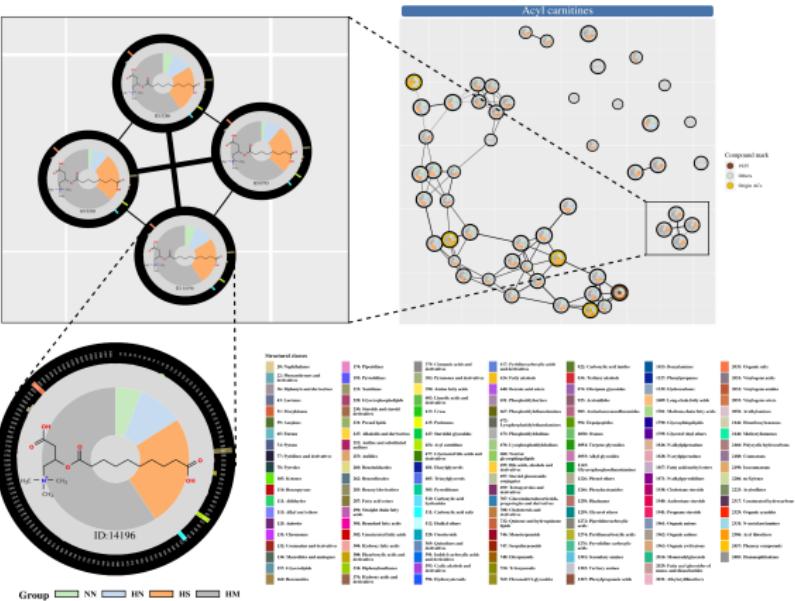
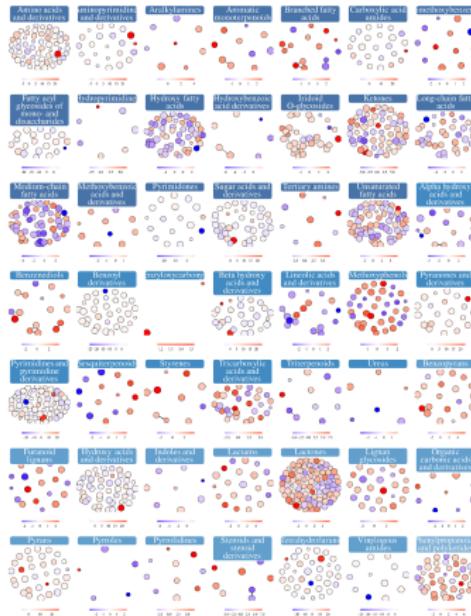
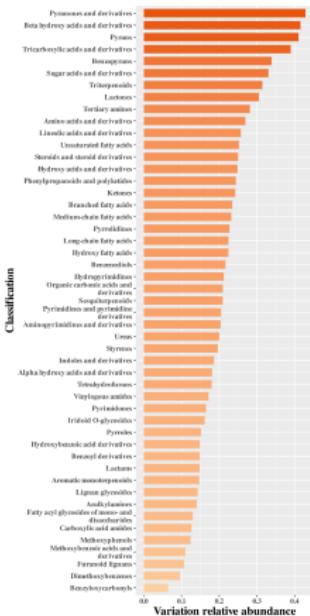


Figure 6: ac.zo.3rank

E. ulmoides dataset



Research background

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Results

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Discussion

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Extra

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Discussion

Discussion

- Limitation of molecular networking (MS/MS dependent classify)
- Biases of feature selection and settlement
 - structure
 - classification
- Discovery in serum dataset
- Botanical dataset analysis

Research background

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Results

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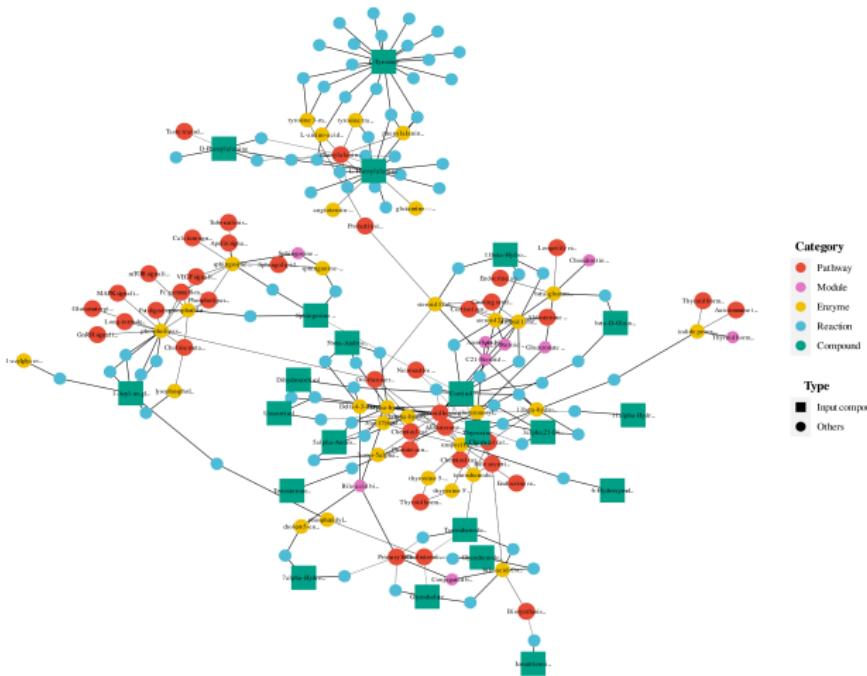
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Extra

Pathway



Chemical reference

- 1 Chemical synonyms
- 2 OCR for multiple PDF
- 3 String dist
- 4 Format

Research background

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Results

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