



Seminar

Lichuang Huang

Supervisor: Cao Gang

Zhejiang Chinese Medical University

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1 Background

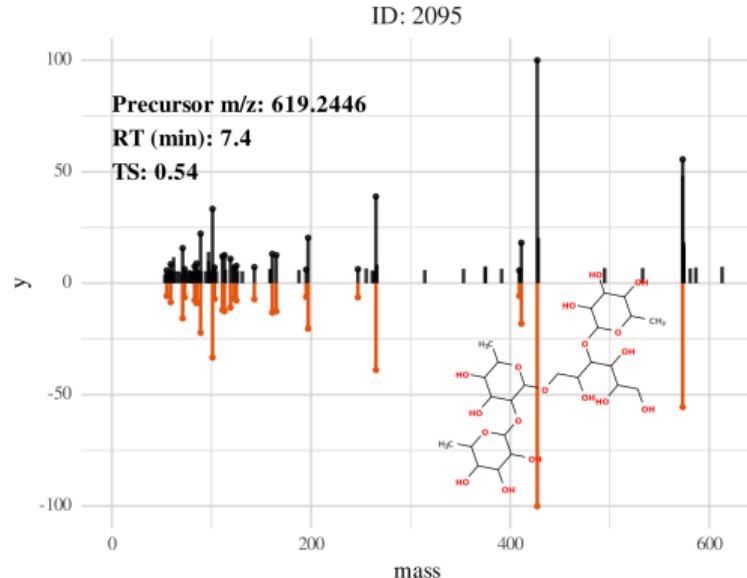
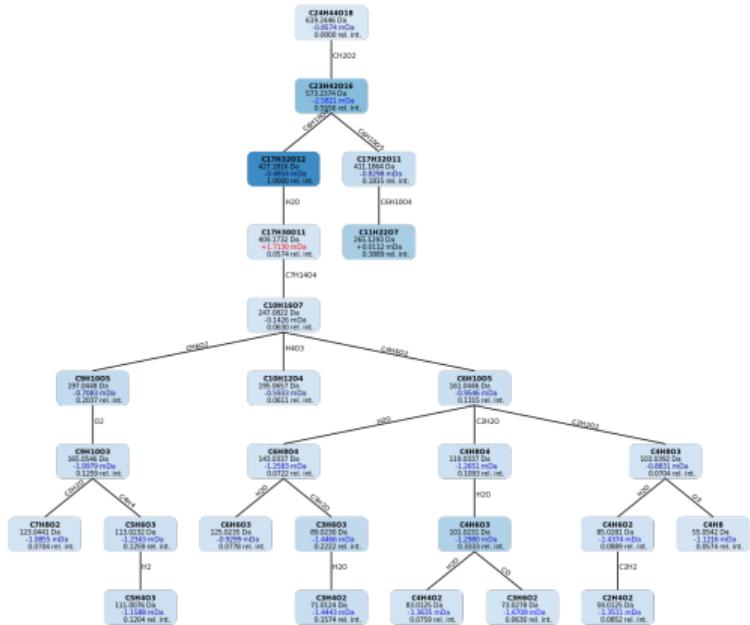
2 MCnebula workflow

3 Structure of article

Background

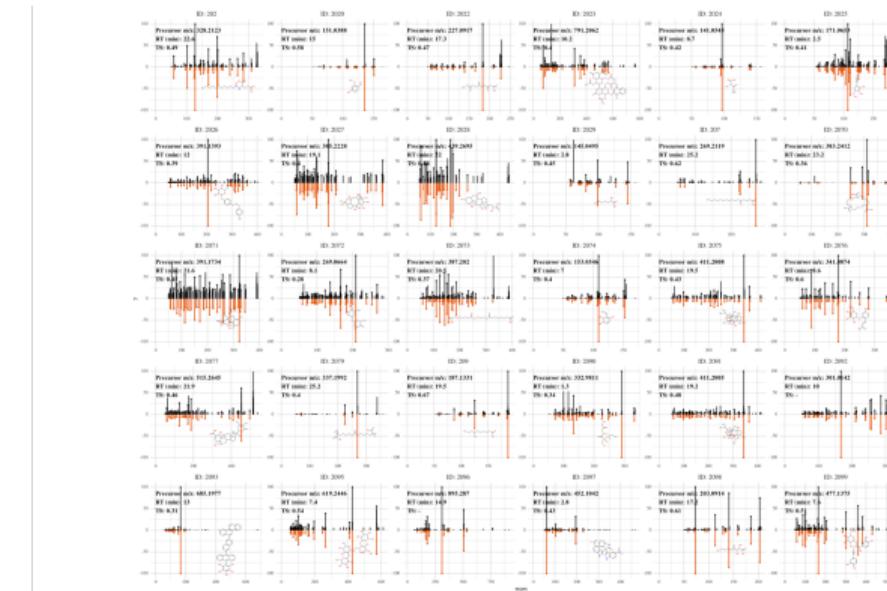
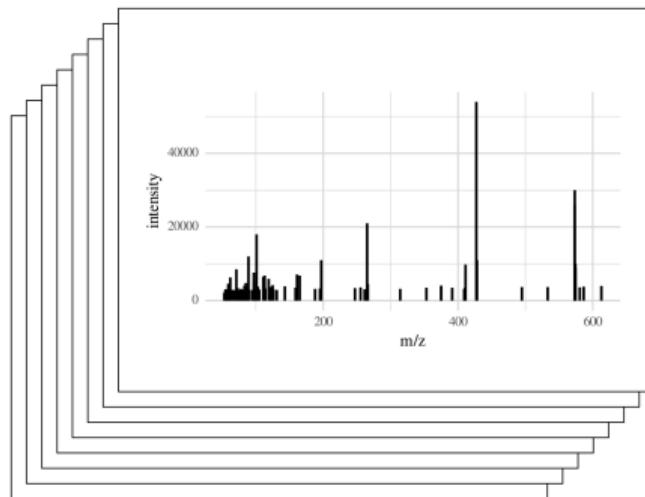
From MS/MS spectrum to compound

Compounds smashed by energy



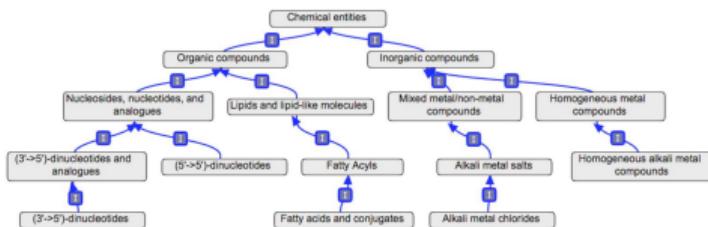
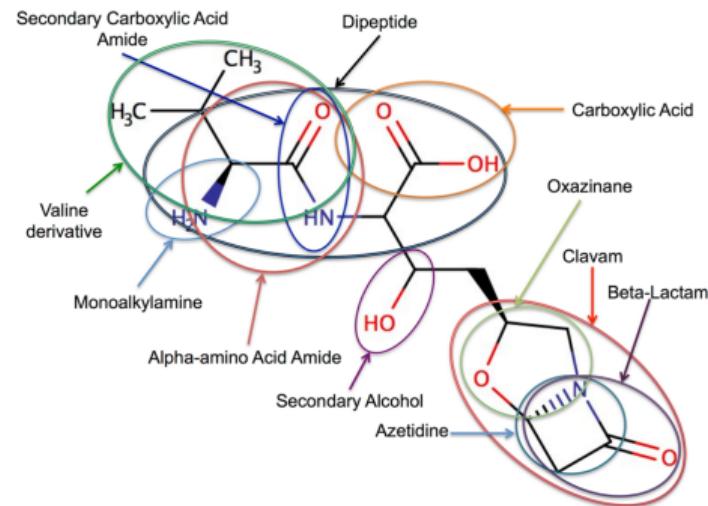
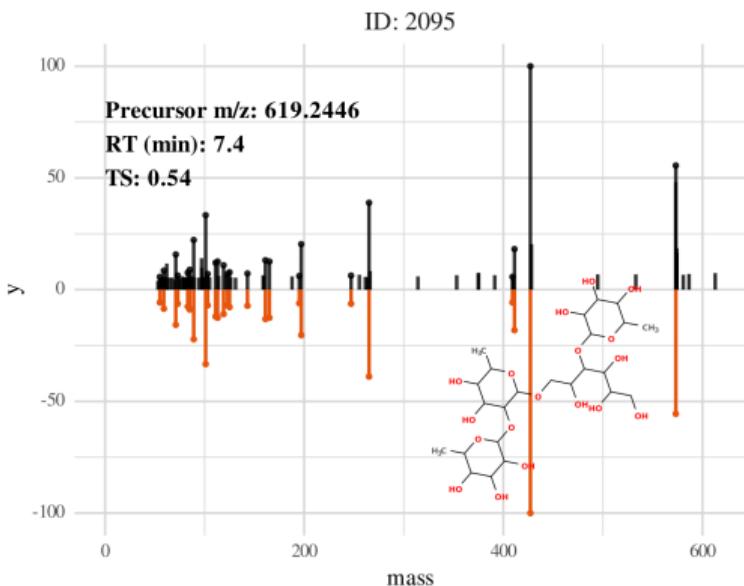
Massive MS/MS spectra

A metabolitic research need lots of identification.

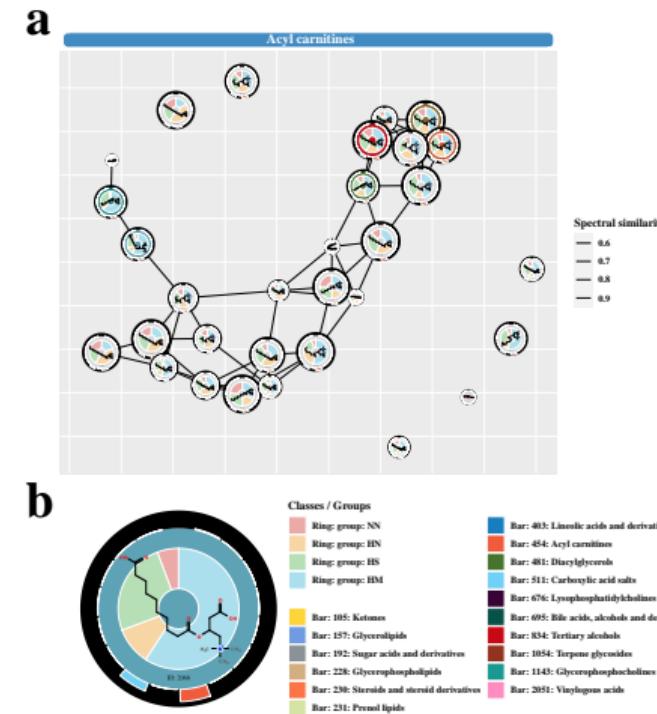
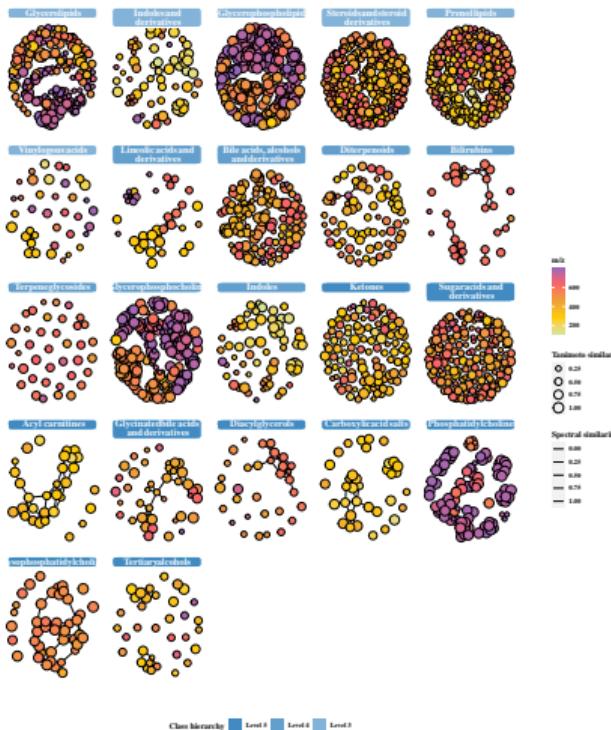


Classification in MS/MS spectra view

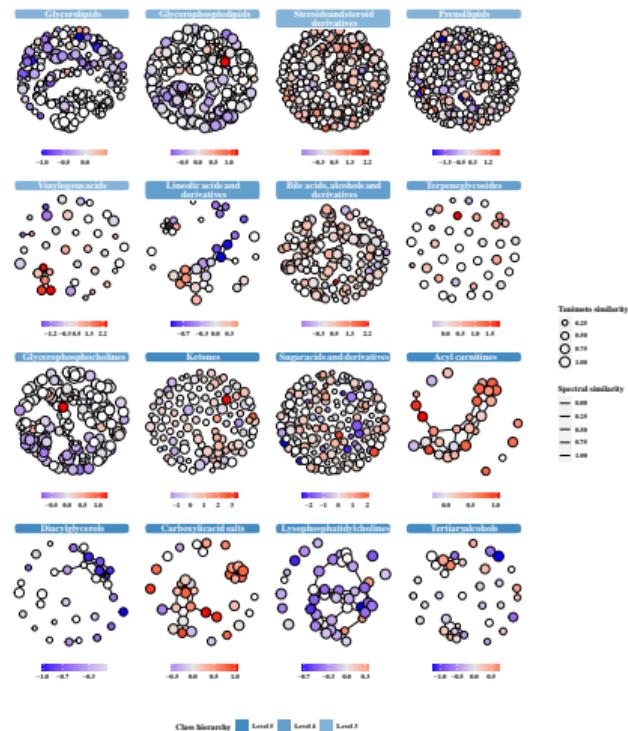
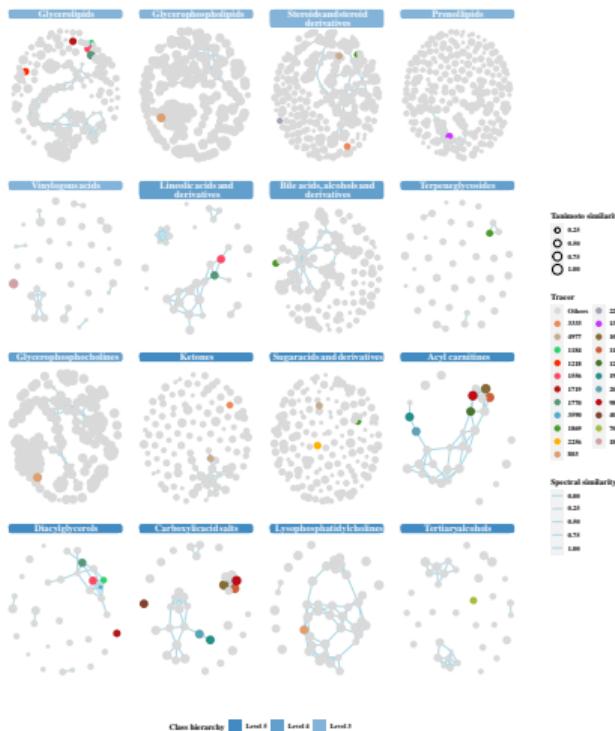
- classes for sub- or dominant structure
- Hierarchy



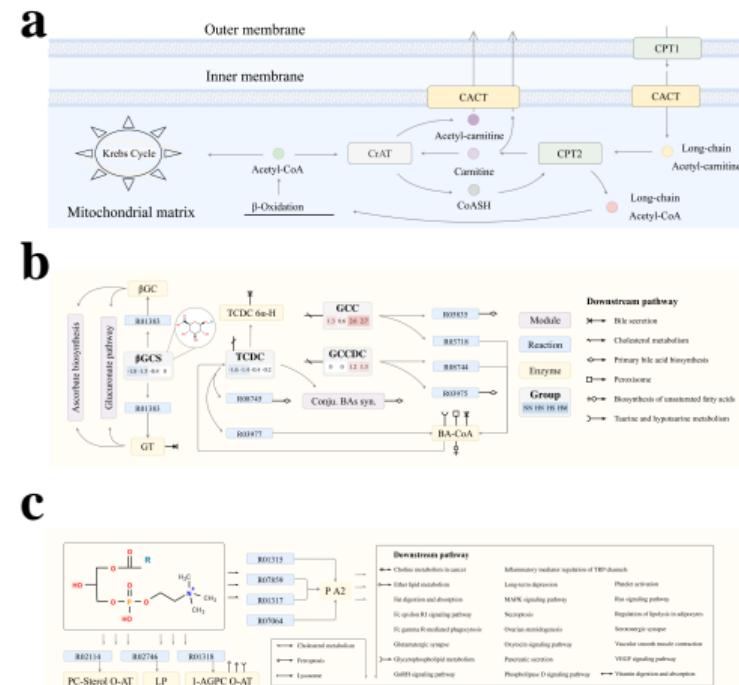
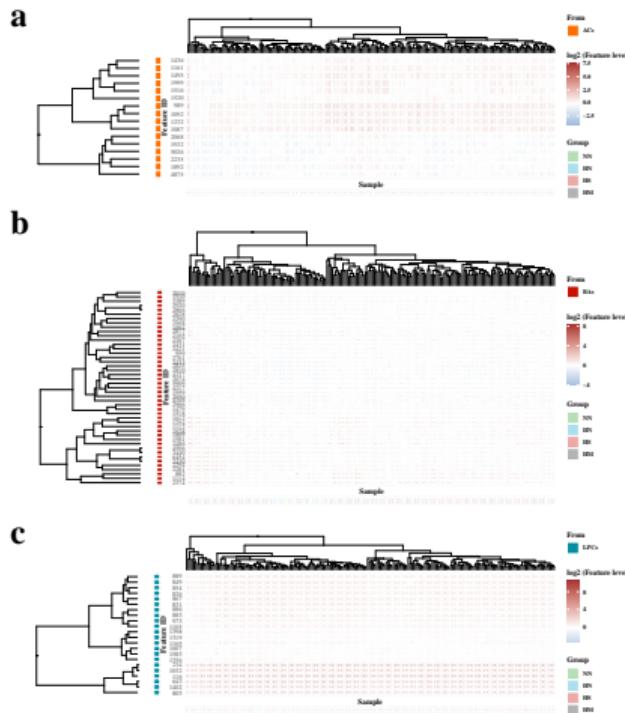
MCnebula proposed visualization



MCnebula expansion



MCnebula expansion

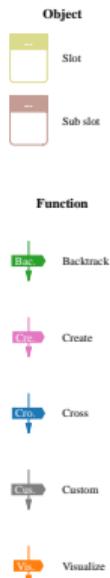
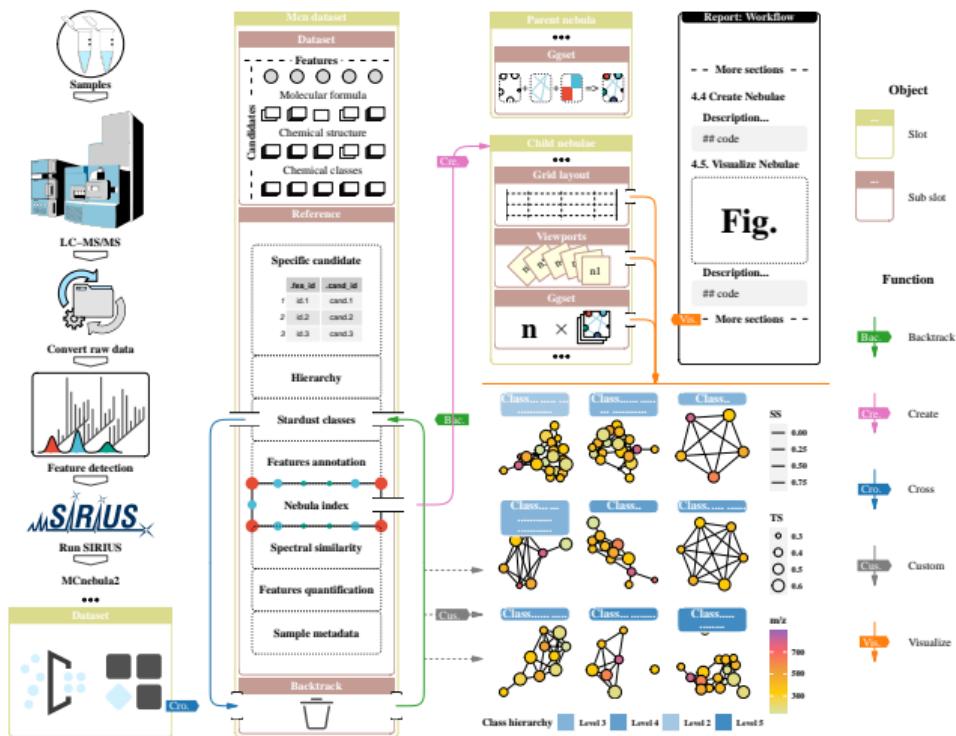


MCnebula expansion

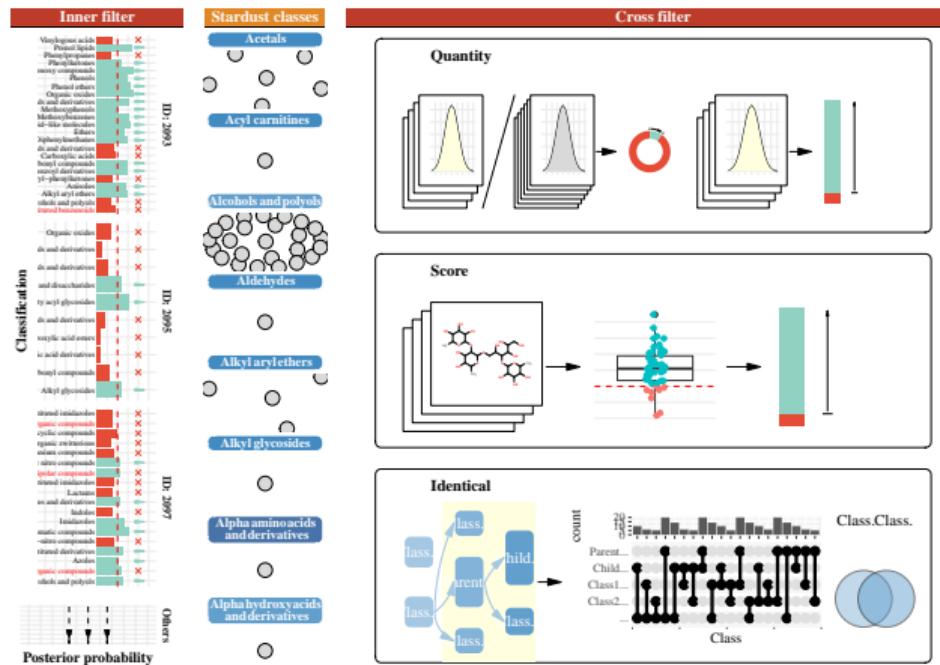


MCnebula workflow

Data stream of MCnebula



Principle of filtering of Chemical classes



Package exMCnebula2

- Pathway enrichment
- Heat map analysis
- Query compounds
- Format identification
- Demo analysis
- ...

Structure of article

Structure

- introduction
 - challenge
 - identification
 - library match
 - *in silico*
 - ...
 - chemical classes
 - MCnebula
- results
 - serum dataset
 - herbal dataset
- methods (algorithm)
 - chemical formula and structure
 - top candidate
 - chemical classes
 - **ABC selection**
 - **details of cross filter**
 - network presentation
 - visualization
 - data structure
 - report system
 - ...
- discussion