



浙江中醫藥大學  
ZHEJIANG CHINESE MEDICAL UNIVERSITY

# Seminar

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# Articale

# Title

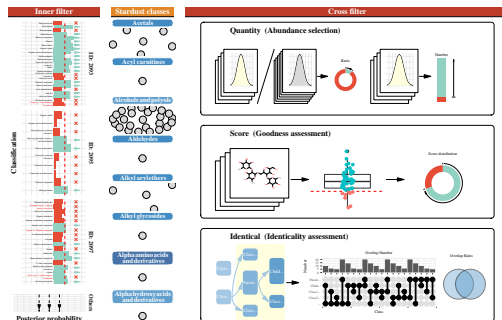
MCnebula: Critical chemical classes to classify and boost identification by visualization for untargeted LC-MS/MS dataset analysis

# Introduction

- LC-MS/MS processing
- Identification: library match, machine prediction ...
- Method for analysis:
  - Classification
  - Statistics
  - Visualizaiton
- Taken together: MCnebula
  - ABC selection
  - ...
  - packages: MCnebula2 exMCnebula2

# Method

- Chemical structure and formula
- Chemical classification
- ABC selection
  - Inner filter
  - Cross filter
    - abundance selection
    - goodness assessment
    - identity assessment



# Method

- Add ‘noise’ into spectra
  - Global mass shift
  - Individual mass shift
  - Global intensity shift
  - Individual intensity shift
- ‘Identify’ structure via InChIKey Planar
- Tools for data collating and visualization
  - S4 programming
  - Package ggplot and grid ...
  - ...
- Statistics
- ...

# Results

## ■ Overview

**Table 1:** Function evaluation

Group	Item	MCnebula	SIRIUS	GNPS	MZmine	XCMS	MetaboAnalyst	MS.DIAL
Identificaiton	MS1	**	**	**	-	**	**	**
	Library match	***	***	***	-	**	-	**
	Machine prediction	***	***	-	-	-	-	-
Classifying	Structure based	**	-	***	-	-	-	-
	MS/MS based	***	***	-	-	-	-	-
	Select classes	***	-	-	-	-	-	-
Visualize dataset	Spectral based	**	-	***	-	-	-	*
	Classes based	***	-	-	-	-	-	-
	Indepth annotation	***	-	***	-	-	-	-
Others	Preprocessing	*	*	**	***	***	*	***
	Statistics	**	-	-	**	**	***	**
	Path enrichment	*	-	-	-	-	***	-
Usage	Report	***	-	-	-	-	**	-
	Availability	***	***	***	***	***	***	***
	Difficulty	**	*	**	***	***	*	*

# Results

## ■ Method evaluation

### ■ Dataset

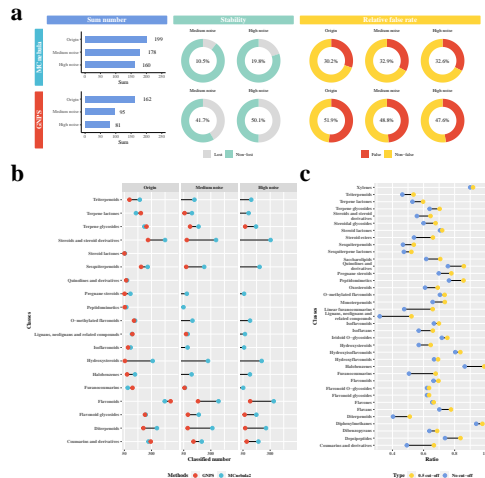
- Original dataset of reference library
- Medium noise
- High noise

### ■ Methods

- MCnebula
- GNPS

### ■ Dimension

- Classified accuracy
- Identified accuracy





# Results

- 
- a** Acyl carnitines
- b** Acyl carnitines
- Taxonomic similarity
- Spectral similarity
- c** Acyl carnitines
- Spectral similarity
- d**
- Classes / Groups
- Ring group N0N
  - Ring group B0V
  - Ring group B0B
  - Ring group B0E
  - Ring 100: Ketones
  - Ring 101: Glyceroaldehydes
  - Ring 102: Sugar acids and derivatives
  - Ring 120: Glyoxal-oxalaldehydes
  - Ring 125: Steroids and steroid derivatives
  - Ring 220: Fused Spiols
  - Ring 003: Lipoic acids and derivatives
  - Ring 004: Acyl carnitines
  - Ring 005: Monoglycerols
  - Ring 013: Carboxylic acid salts
  - Ring 070: Epoxycarboxylic acids
  - Ring 090: Sulfon acids, alcohols and derivatives
  - Ring 093: Tertiary alcohols
  - Ring 1000: Glycerol glycerolates
  - Ring 1040: Glyoxal-glyoxalaldehydes
  - Ring 1041: Vinylglyoxal acids

# Discussion

- About MCnebula and ABC selection
- About evaluation
- About analysis of serum dataset
- About analysis of herbal dataset
- End

# Schedule

- Finish writing the thesis
- ...