



浙江中醫藥大學  
ZHEJIANG CHINESE MEDICAL UNIVERSITY

# Seminar

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2022-10-27

**1** Update of visualization system

**2** Progress

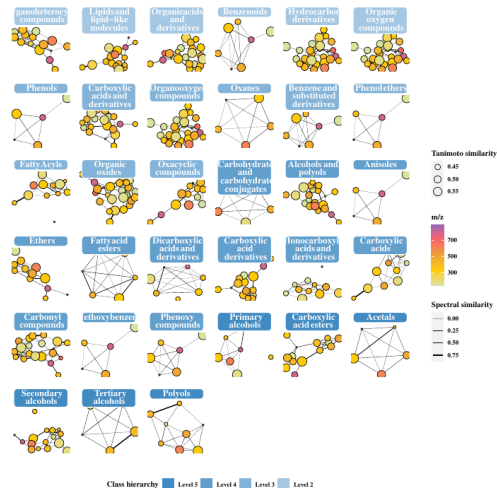
**3** Next Schedule

# Update of visualization system

# Child nebulae: Unify scale limits

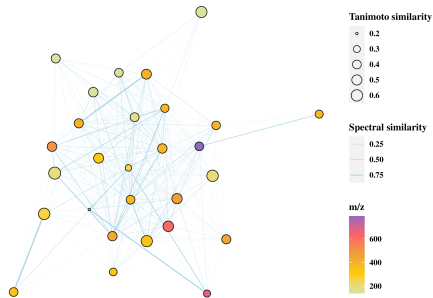
1 visualize\_all(x)

- nodes fill
  - mz
  - ...
- nodes size
  - tani.score
  - ...
- edge width
  - similarity

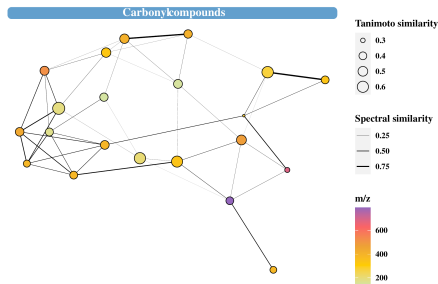


# Parent- and child-nebula

1 visualize(x, “parent”)

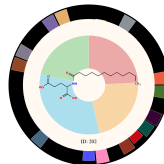
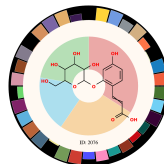
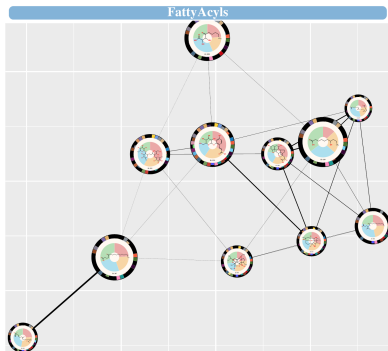


2 visualize(x, item)



# Annotate child nebula

- 1 visualize(x, name)
- 2 show\_node(x, id)



## Classes / Groups

- Bar: 487: Monocarboxylic acids and derivatives
- Bar: 555: Carboxylic acids
- Bar: 598: Carboxylic acid esters
- Bar: 821: Acetals
- Bar: 826: Secondary alcohols

- Bar: 2: Organoheterocyclic compounds
- Bar: 4: Carbohydrates and carbohydrate conjugates
- Bar: 9: Lipids and lipid-like molecules
- Bar: 116: Alcohols and polyols
- Bar: 121: Phenols
- Bar: 125: Anilines
- Bar: 227: Ethers
- Bar: 235: Organic acids and derivatives
- Bar: 236: Carboxylic acids and derivatives
- Bar: 254: Primary alcohols
- Bar: 286: Organosulfon compounds
- Bar: 287: Fatty acid esters
- Bar: 308: Dicarboxylic acids and derivatives
- Bar: 452: Carboxylic acid derivatives

- Bar: 834: Tertiary alcohols
- Bar: 918: Carbonyl compounds
- Bar: 1036: Oxanes
- Bar: 1188: Benzene and substituted derivatives
- Bar: 1191: Polyols
- Bar: 1226: Phenol ethers
- Bar: 1298: Benzoxazoles
- Bar: 2064: Fatty Acyls
- Bar: 2078: Organic oxides
- Bar: 2146: Methoxybenzenes
- Bar: 2158: Oxacyclic compounds
- Bar: 2167: Hydrocarbon derivatives
- Bar: 2378: Organic oxygen compounds
- Bar: 2457: Phenacyl compounds

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# Progress

# Code refactoring: data processing

Formerly finished:

- S4 data structure ✓
- Extract data ✓
  - 1 project\_conformation ✓
  - 2 project\_metadata ✓
  - 3 project\_api ✓
  - 4 project\_dataset ✓
- Filter data
  - 0 collate\_data ✓
  - 1 filter\_formula ✓
  - 2 filter\_structure ✓
  - 3 filter\_ppcp ✓
  - 4 create\_reference ✓

- organize data
  - 1 create\_features\_annotation ✓
  - 2 create\_stardust\_classes ✓
  - 3 cross\_filter\_stardust ✓
    - quantity ✓
    - score ✓
    - identical ✓
  - 4 create\_nebula\_index ✓
  - 5 compute\_spectral\_similarity ✓
  - 6 create\_parent\_nebula ✓
  - 7 create\_child\_nebulae ✓



# Code refactoring: visualization

This time finished:

- for organizing visualization

- 1 command ✓

- new\_command ✓

- call\_command ✓

- 2 ggset ✓

- new\_ggset ✓

- mutate\_layer ✓

- add\_layer ✓

- delete\_layer ✓

- modify\_set\_labs ✓

- modify\_unify\_scale\_limits ✓

- modify\_rm\_legend ✓

- modify\_... ✓

- call\_command ✓

- ...

- visualization

- 1 create\_child\_layout ✓

- 2 activate\_nebulae ✓

- 3 quantification ✓

- features\_quantification ✓

- sample\_metadata ✓

- 4 annotate\_nebula ✓

- draw\_structures ✓

- draw\_nodes ✓

- 5 visualize ✓

- visualize ✓

- visualize\_all ✓

- show\_node ✓

- show\_structure ✓

## Next Schedule

# Overall

- Data filtering and arranging system. ✓
- Visualization system. ✓
- LC-MS runing in XCMS.
- Statistic system.
- Report.
- Documentation.
- Website.
- Figures for article.
- Rerite article.