



浙江中醫藥大學
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Seminar

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1 MCnebulas development

2 MCnebulas2

3 Next Schedule

MCnebulas development

Reviewer comments

- Algorithmic innovation.
 - 1 Lack of innovative descriptions in algorithm.
 - 2 Lack of scientific evaluation.
- Software Engineering Implications.
 - 1 Immature and uncritical development.
 - 2 The methods lack independence.

Development: Algorithm or Software?

Algorithm

- Classified visualization.
 - 1 Novel but algorithmically underpowered.
 - 2 Fail to evaluate scientifically.
- Re-rank identifications.
 - 1 Technical and theoretical deficiencies.
 - 2 Periodic Uncertainty.

Software engineering

- Compatibility and ease-of-use.
 - 1 Adaptation of sirius version.
 - 2 Complexity of parameters.
- Functional expansion.
 - 1 Data processing.
 - 2 Workflow.
- Exhibition format.
 - 1 Documentation.
 - 2 Website.

MCnebulas2

Object-oriented programming: MCnebula2

- Advantages
 - 1 Clarity of code structure
 - 2 Easy expansion
 - 3 Easy maintenance
- Example R packages
 - 1 MetaboAnalystR
 - 2 TidyMass



Figure 1: MCnebula2

Code refactoring

- 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
 - 5 ...
- Visualization
 - 1 Re-write in S4 object.
 - 2 Flexibility.
- Statistic analysis
 - 1 Linear regression.
 - 2 Feature selection.
 - 3 PCA etc.
- Report
 - 1 Flexibility.

Next Schedule

Code refactoring

- Data filtering and arranging system.
- Visualization system.
- Statistic system.
- Report.
- Documentation.
- Website.
- Figures for article.
- Rerite article.