MetaboConverter: A Python Software for Analyzing Metabolomic Data

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Background

Chlorpyrifos (CPF): A widely used organophosphate pesticide.

CPF may link to increase autism (ASD) risk.

We screened gut metabolites in zebrafish

Challenge: significant changes in the concentrations of over 1,200 metabolites was a challenging and time-consuming task.

1554	Ximaosteroid E	C27 H40 O2	397.309
1555	YMK	C20 H32 N4 O5 S	423.208
1556	YUA001	C13 H19 N O2	254.174
1557	Zaleplon	C17 H15 N5 O	342.078
1558	Zooxanthellactone	C22 H30 O2	327.231
1559	β-Alanyl-L-arginine	C9 H19 N5 O3	246.155
1560	β-D-Fructose 6-phosphate	C6 H13 O9 P	259.022
1561	γ-Glu-gln	C10 H17 N3 O6	276.118
1562	γ-Glu-gln	C10 H17 N3 O6	276.118
1563	γ-Glutamyl-3-(sulfosulfanyl)alanyl	C10 H17 N3 O9 S2	386.03
1564	γ-L-glutamyl-L-leucine	C11 H20 N2 O5	259.12
1565	Δ17-6-keto prostaglandin F1α	C20 H32 O6	367.212
1566	Y-L-Glutamyl-L-glutamic acid	C10 H16 N2 O7	277.102
1567			

MetaboConverter

A python package for organizing, sorting, and analyzing metabolomic data

User Cases

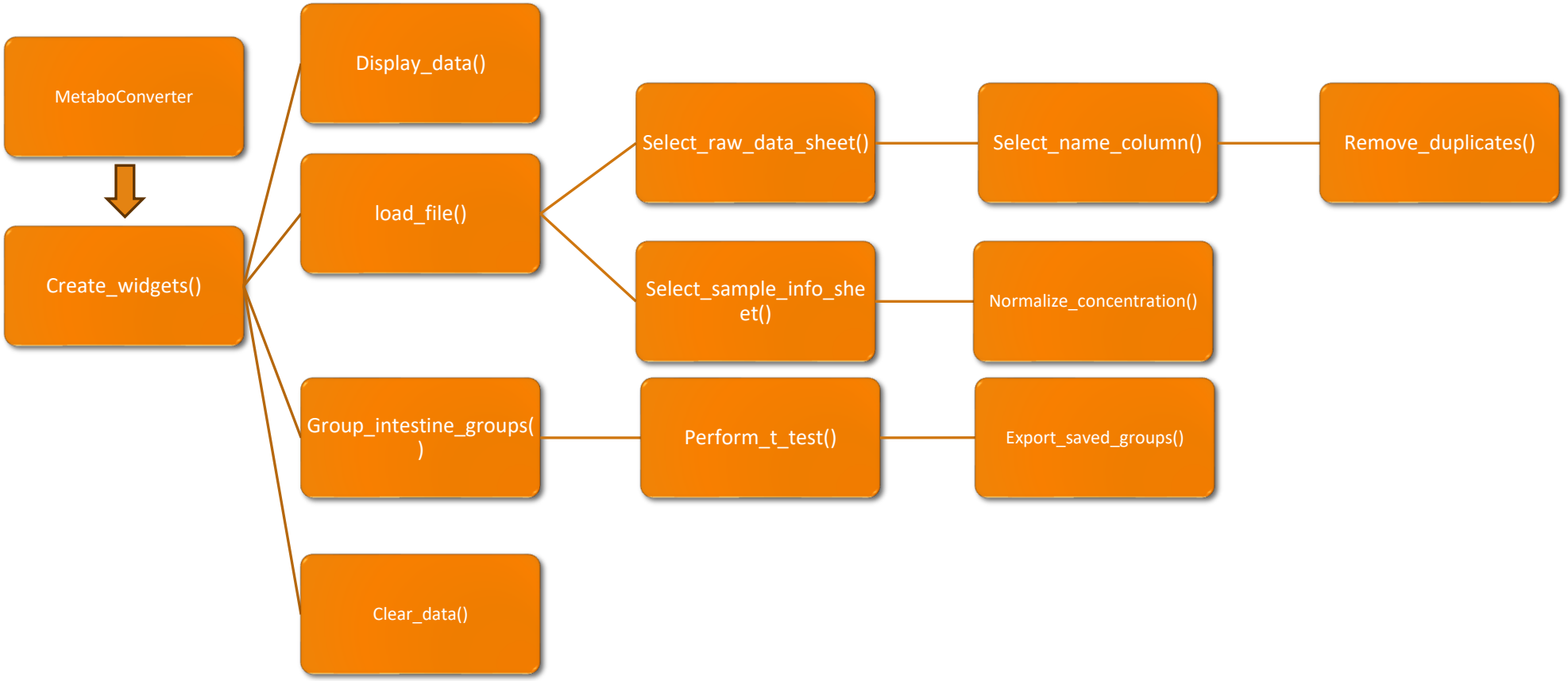
1. A researcher want to identify specific Metabolites for further study

2. A researcher want to find up-regulators and down-regulators within their metabolomic data

Demo

JaydenMao102/MetaboConverter

Design


MetaboConverter
Create_widgets()
Display_data()
load_file()
Group_intestine_groups()
Clear_data()
Select_raw_data_sheet()
Select_sample_info_sheet()
Perform_t_test()
Select_name_column()
Normalize_concentration()
Export_saved_groups()
Remove_duplicates()

Project Structure

```
MetaboConverter/
  |- README.md
  |- MetaboConverter/
     |- __init__.py
     |- MetaboConverter.py
     |- sample_data.xlxs
  |- src
     |- test.py
  |- doc/
     |- FunctionalSpec
     |- ComponentSpec
     |- Final presentation
  |- pyproject.toml
  |- LICENSE
  |- setup.py
  |- requirement.txt
```

Future Works

Update GUI, make it more user-friendly

Update code for better logic (e.g. allow user to select control group)

Update tests

Lesson learned:

Limit scope for projects

(…)

Thank you!