

From X!Tandempipeline

INPUTS

- peptide_counts.txt
- protein_list.txt
- metadata.csv
- metaHIT99_db.tsv

1) load_protspeps Loads peptides counts, proteins list and metadata. Creates: **metaproteome_object**

2) add_taxonomy Integrates the taxonomic DB into a **metaproteome_object**. Creates: **metaproteome_object**

ANALYSIS

19) inspect_sample_elements Displays the frequency of the entities (peptides, subgroups, groups) per sample. Creates: **PDF file**

20) plot_PCA Displays the PCA results from peptides, subgroups, groups or taxonomic levels. Creates: **PDF file** and **csv**

21) identify_differences Displays the most over and under represented taxonomic elements from an **spectral_count_object with taxonomy**. Creates: **PDF** and **csv files**

22) add_kegg Integrates the functional annotation to the taxonomic elements in **spectral_count_object with taxonomy**. Creates: **spectral_count_object with taxonomy and annotation**

5) remove_element Removes elements from a **spectral_count_object**. Creates: **spectral_count_object**

6) select_element Selects elements from a **spectral_count_object**. Creates: **spectral_count_object**

7) filter_unshared Keeps the non shared elements (peptides, subgroups or groups) from a **spectral_count_object** in function of a metadata feature (sample, condition, etc.). Creates: **spectral_count_object**

8) filter_shared Keeps the common elements (peptides, subgroups or groups) from a **spectral_count_object** in function of a metadata feature (sample, condition, etc.). Creates: **spectral_count_object**

9) filter_text Keeps or discards the elements (peptides, subgroups or groups) that matched a chunk of text in a variable of peptides_proteins dataframe from a **spectral_count_object**. Creates: **spectral_count_object**

10) crumble_taxonomy Express the the abundance of peptides, subgroups or groups from a **spectral_count_object** in function of a taxonomic level (specie, genus, family, order, class, phylum or superkingdom). Creates: **spectral_count_object with taxonomy**

3) getsc_specific
Obtains abundance of specific spectral counts by peptides, subgroups or groups. Creates **spectral_count_object**

VISUALIZATION

11) plot_dendocluster Plots a non-supervised clustering dendogram from a **spectral_count_object**. Creates: **PDF file**

12) plot_venn Creates a venn diagram of 2 or 3 conditions from a **spectral_count_object**. Creates: **PDF file** and a **venn_lists_object**

14) plot_intensities_ratio Creates a scatter plot of the abundance ratio of the elements (peptides, subgroups, groups) between 2 conditions/samples from a **spectral_count_object**. Creates: **PDF file**

15) plot_intensities Creates violin plots of the mean of abundances per sample/condition of the elements (peptides, subgroups, groups) from a **spectral_count_object**. Creates: **PDF file**

16) plot_fulltaxonomy Creates bar plots of the mean of abundances per sample of the elements (peptides, subgroups, groups) from a **spectral_count_object**. Creates: **PDF** and **csv file**

17) plot_stackeditaxo Creates stacked bar plots of samples or conditions with the spectral abundance as counts or as percentage, these values are formatted based on **spectral_count_object with taxonomy**. Creates: **PDF file**

18) plot_pietaxo Creates a pie chart of one sample or condition with the spectral abundance as counts, these values are formatted based on **spectral_count_object with taxonomy**. Creates: **PDF** and **csv file**

24) plot_biomarkers Creates boxplots of the spectral abundance as counts of all the taxonomic entities, these values are obtained from **spectral_count_object with taxonomy**. Creates: **PDF**

EXPORT

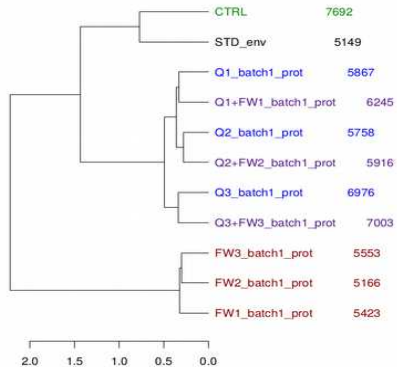
4) export_object Exports a metaproteome or a spectral count object. Creates: **RDATA / rds file**

13) export_vennlists Exports the lists from a **venn_lists_object**. Creates: **csv files**

23) export_ipath3 Exports the **spectral_count_object with taxonomy and annotation**. Creates: **csv file**

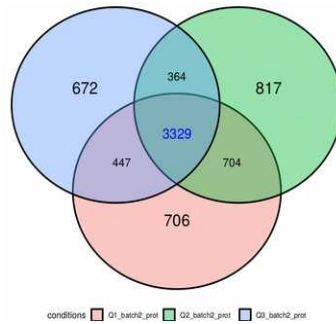
plot_dendocluster

Non-supervised clustering dendrogram of the experimental samples. Display the number of entities.



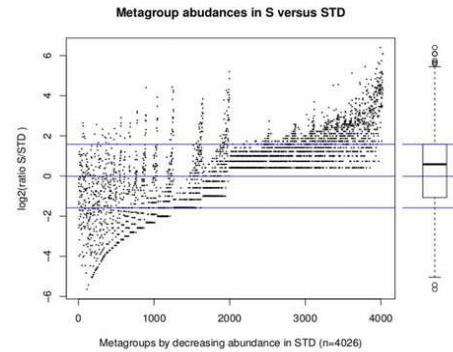
plot_venn

Venn diagram of the entities of 2 or 3 conditions.



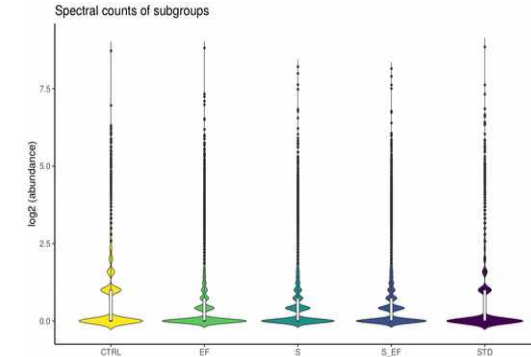
plot_intensities_ratio

Scatter plot of the abundance ratio of the entities between 2 conditions.



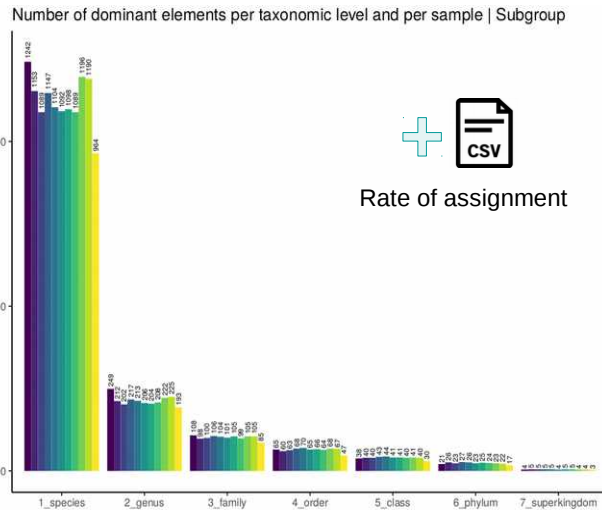
plot_intensities

Violin plots of the mean of abundances of the entities per condition.



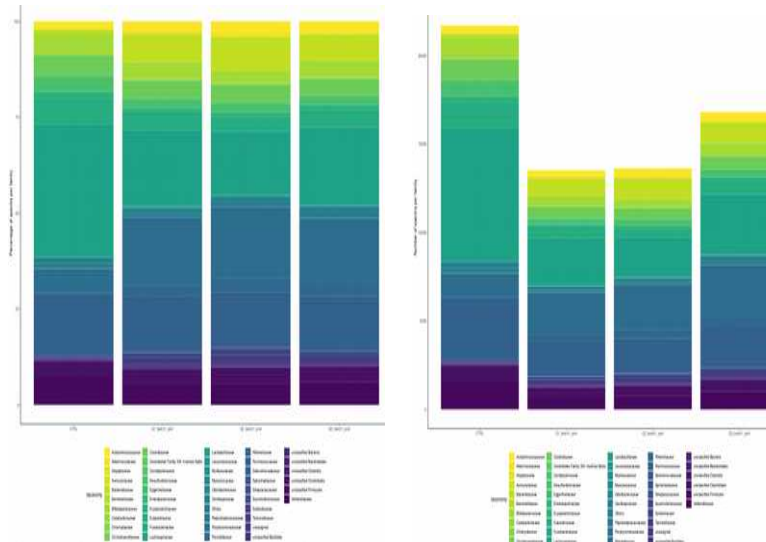
plot_full_taxonomy

Bar plots of the mean of abundances of the entities per sample. Seven taxonomic levels are displayed.



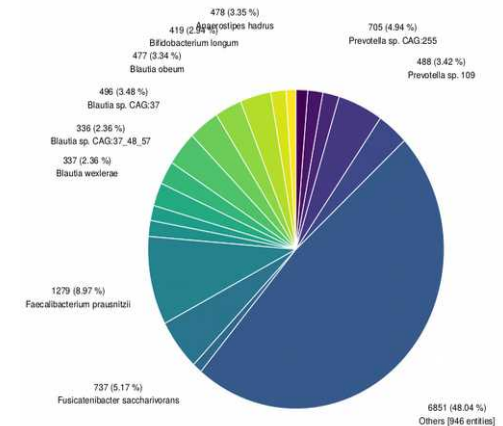
plot_stackedtaxo

Stacked bar plots of conditions with the spectral abundance of the taxonomic elements as counts or as percentage.



plot_pietaxo

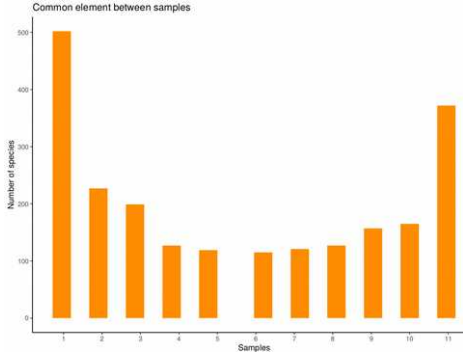
Pie chart of one condition with the spectral abundance as counts or as percentage.



Values of abundance for each taxonomic entity + CSV icon

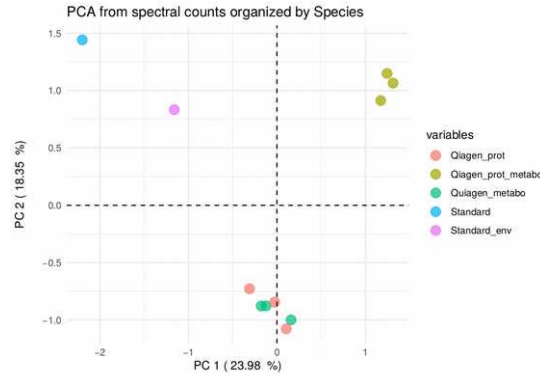
inspect_sample_elements

Barplots indicating the presence of entities per sample. Useful to observe the heterogeneity in the samples.



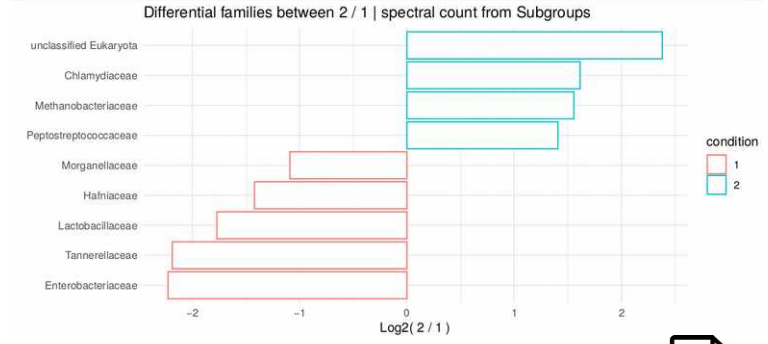
plot_PCA



Plot of two selectet axis after performing a Principal Component Analysis of the entities of a 'spectral_count_object'



identify_differences

Barplots of the most differential taxonomic entities between two conditions or samples.



List of the taxonomic entities with their ratios between conditions  

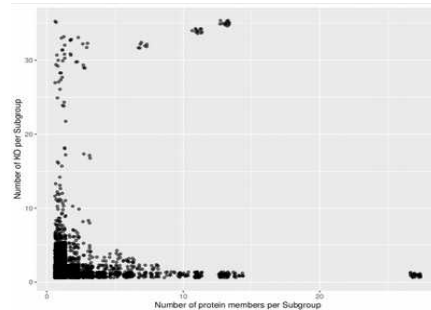
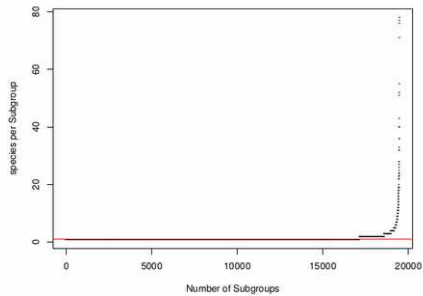
add_kegg

Adds the functional annotation from KEGG DB to the taxonomic entities.

KEGG DB



Quality Control plots



spectral_count_object with taxonomy and functional annotation

export_ipath3

Creates a CSV file with the suitable format to display metabolic pathways using the tool iPATH3

spectral_count_object with taxonomy and functional annotation



Paste in 

