

# MAPPING OMICS DATASETS ON KEGG METABOLIC PATHWAYS

MASTER'S PROJECT IN BIOINFORMATICS

**DUARTE ALVES VELHO**

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Under the guidance of:

Andreia Salvador;

João Sequeira

- STATE OF THE ART

- OMICS AND META-OMICS TECHNOLOGIES ARE POWERFUL APPROACHES FOR EXPLORING THE FUNCTIONS OF MICROORGANISMS;
- SOFTWARE DEVELOPED FOR OMICS AND META-OMICS ANALYSIS IS A VALUABLE RESOURCE FOR ANALYSIS;
- VISUALIZING THE RESULTS IN PATHWAYS ALLOWS FOR A GREATER UNDERSTANDING OF BIOLOGICAL PROCESSES, PARTICULARLY IN MT EXPERIMENTS WHERE DIFFERENT GENES/PROTEINS AND PATHWAYS ARE DIFFERENTIALLY EXPRESSED, BUT THERE ARE NOT MANY RESOURCES TO DO SO;
- THERE ARE SEVERAL BIOINFORMATICS RESOURCES FOR META-OMICS ANALYSIS, BUT MANY OF THEM REQUIRE SIGNIFICANT COMPUTATIONAL EXPERTISE.

Tools	What tools do	Advantages	Disadvantages	Languages	Type of Identifiers	Interactivity	Number of Samples	Taxonomy	Differential Expression	Input	Output
DAVID	Integrates functional genomic annotations with intuitive graphical	Provides exploratory visualization tools for functional classification	Requirement for internet access	Perl and Java	Gene IDs, protein IDs	Yes	Not specified	Yes	Yes	Txt	HTML
Reactome	It provides an intuitive web-based user interface	Integration with various data analysis tools for ID mapping	Limited by the breadth of its curated data	JavaScript, Perl	UniProt IDs, GenBank/EMBL/DBJ IDs, RefSeq IDs, EntrezGene IDs	Yes	Not specified	Human and 20 other species	Yes	Txt	SVG, PNG, EPS, PDF, MySQL, BioPAX, SBML, PSI-MI-TAB
CellDesigner	Modeling tool that allows users to visualize, model, and simulate biochemical networks	Offers a comprehensive graphical representation of networks	Requires understanding of SBML	Java	Not specified	Yes	Not applicable	No	Yes	SBML	SBML, PNG, SVG
GenMAPP	Allows users to visualize and analyze genome-scale data	Offers new visualization modes for complex data analysis	Limited primarily to the species and gene ids within its database	Visual Basic 6.0	Ensembl gene IDs, UniProt IDs, Entrez Gene IDs, Affymetrix probe set IDs	Yes	Not specified	Yes	Yes	Microsoft Jet format for (.gex), (.gdb), (.mapp)	HTML, PNG, SVG

Fig. 1 - Example of tools that map metabolic pathways.

- KEGG (KYOTO ENCYCLOPEDIA OF GENES AND GENOMES)

- COMPREHENSIVE DATABASE INTEGRATING GENOMIC, CHEMICAL AND SYSTEMIC FUNCTIONAL INFORMATION;
- ALLOWS TO VIEW THE RESULTS IN PATHWAYS.

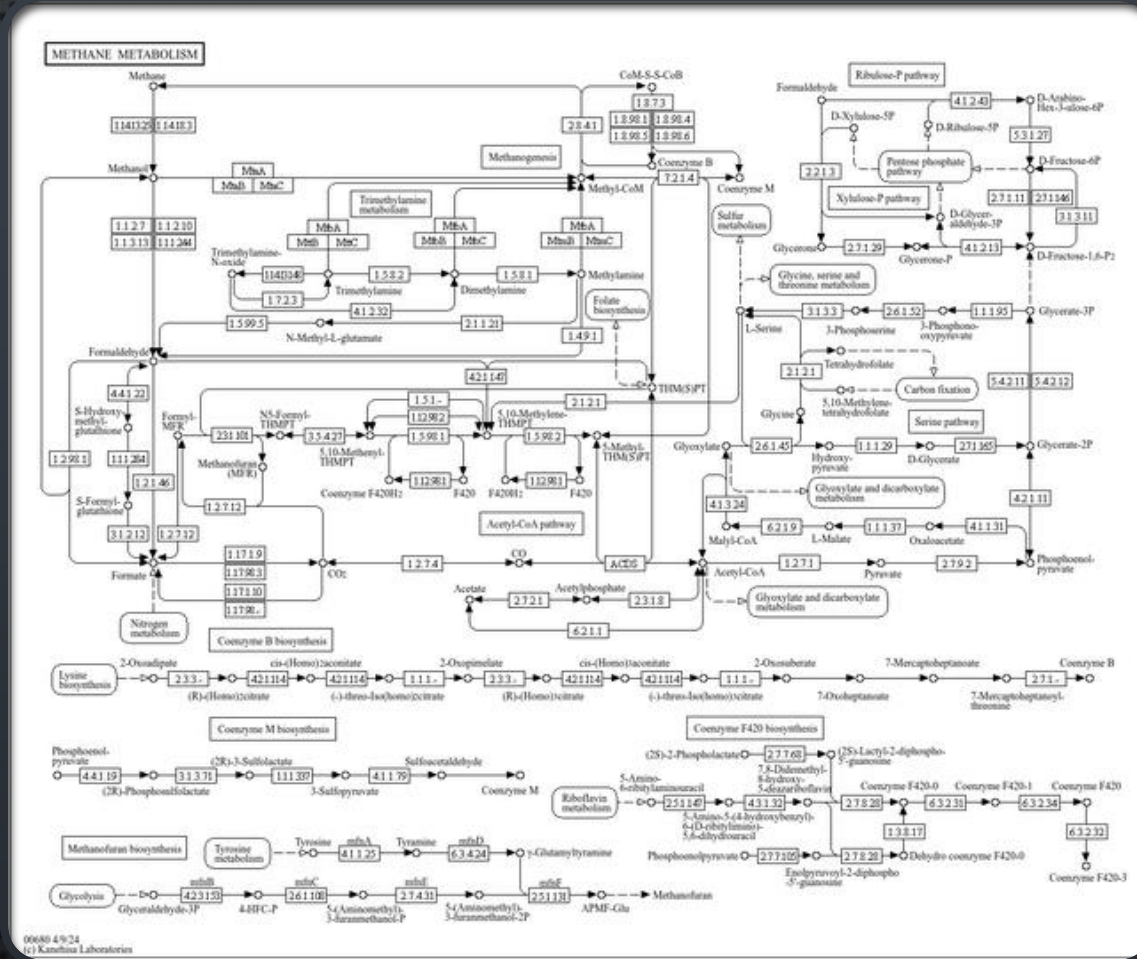


Fig. 2 - Representation of MAP00680 in KEGG.

- KEGGCHARTER

- COMMAND LINE INTERFACE;
- EASY TO USE;
- TOOL DESIGNED TO OVERLAY THE DIFFERENTIAL GENE EXPRESSION AND TAXONOMIC INFORMATION OF ENZYMES ON KEGG METABOLIC MAPS;
- BASED ON BIOPYTHON.



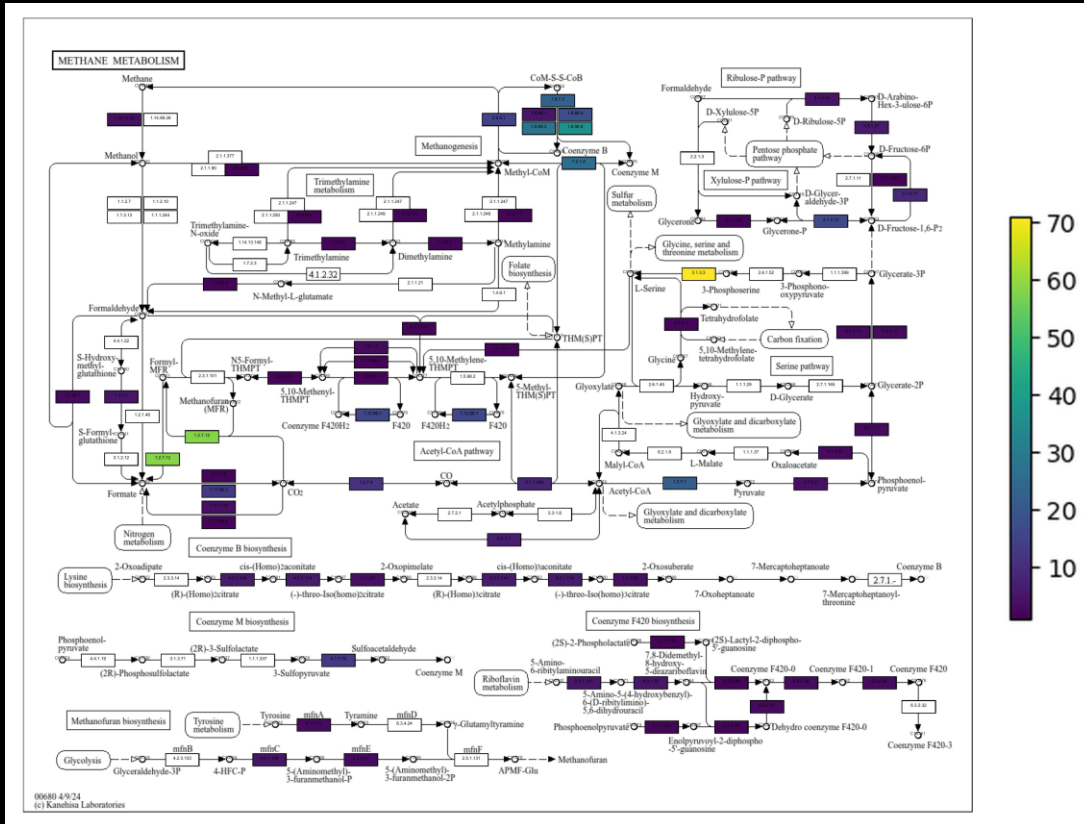


Fig. 3 - KEGG metabolic map of methane metabolism, with differential analysis of quantified expression for each function from a simulated dataset.

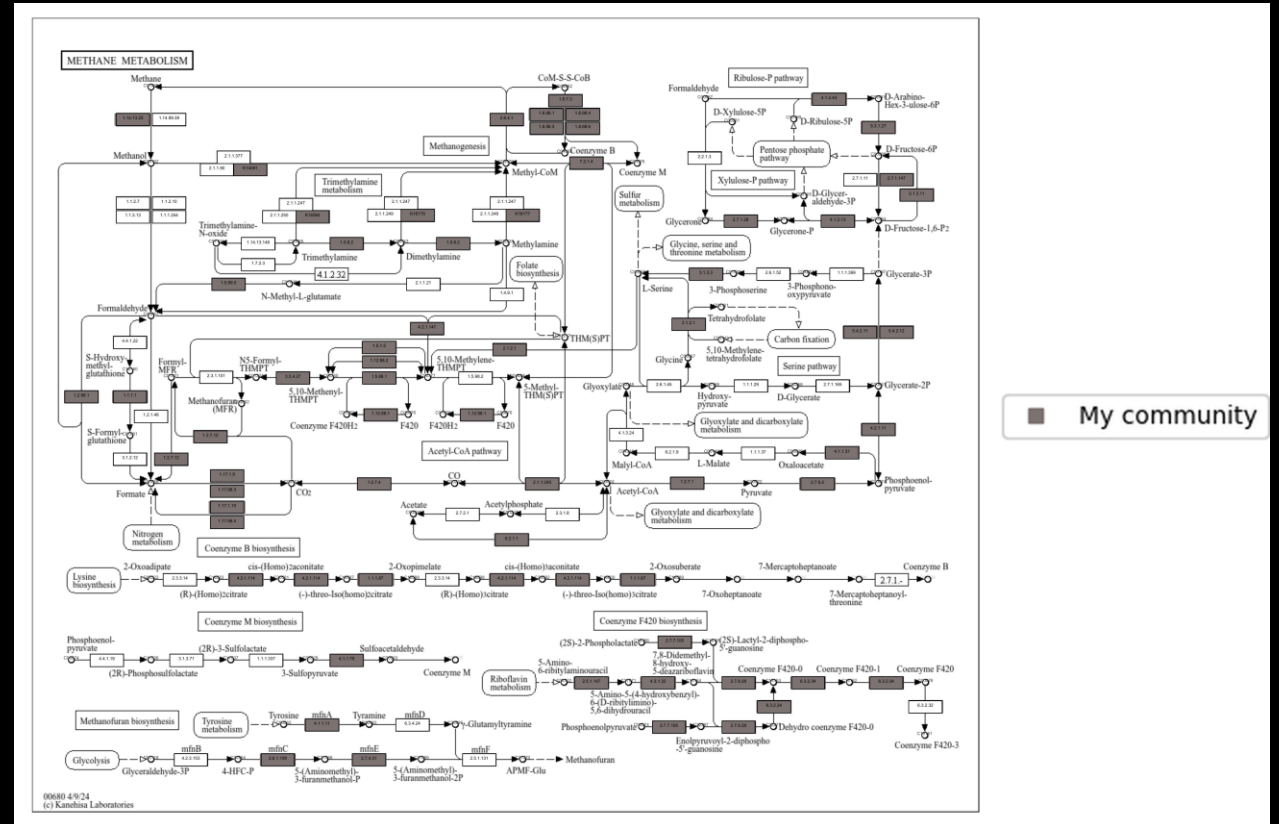
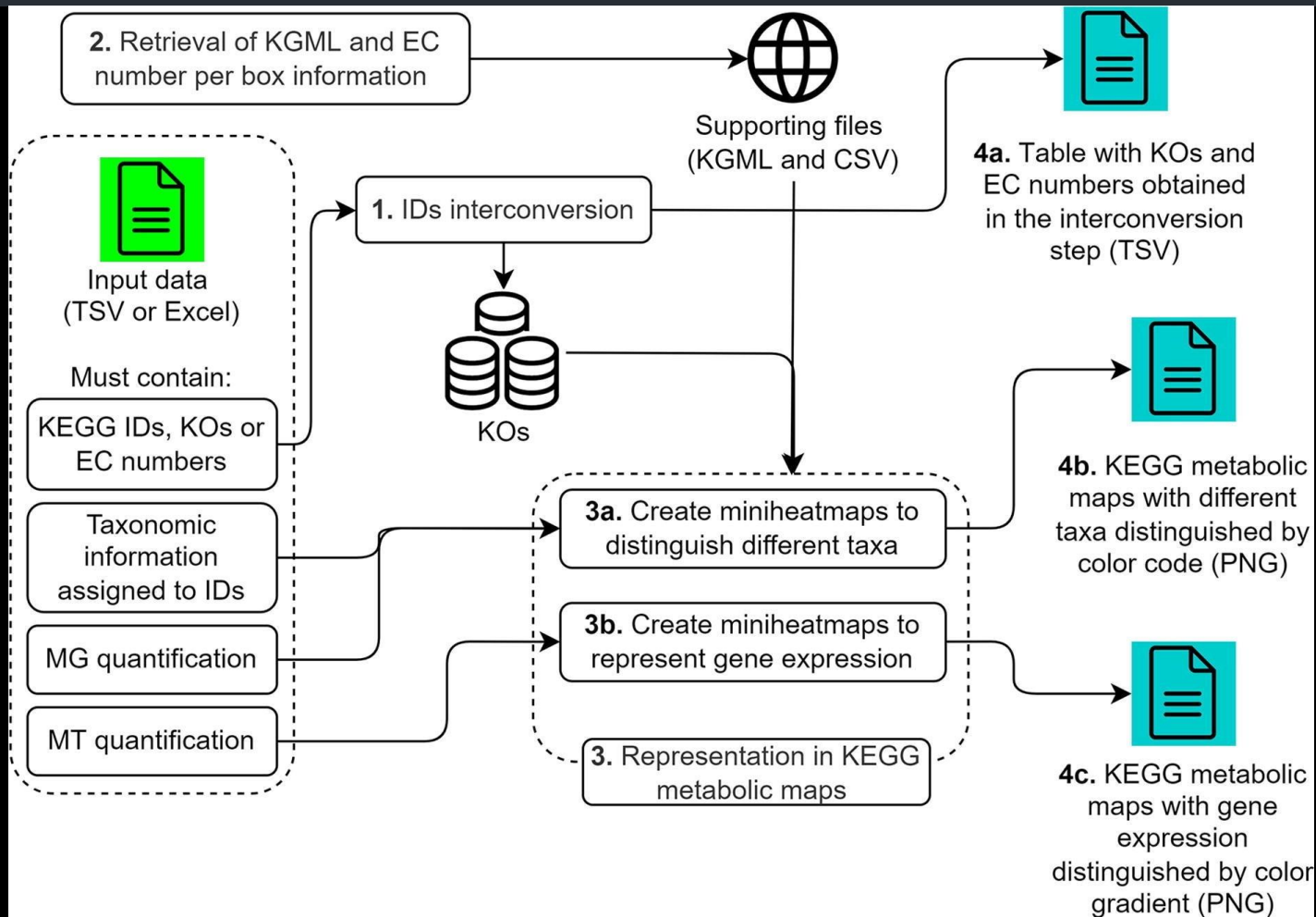


Fig. 4 - KEGG metabolic map of methane metabolism, with identified taxa for each function from a simulated dataset.

- OBJECTIVE OF THIS PROJECT

- EXPAND THE KEGGCHARTER GRAPHS TO INCLUDE MULTI-LEVEL REPRESENTATION OF GENE EXPRESSION INFORMATION;
- DEVELOPMENT OF NEW INTERACTIVE REPRESENTATIONS ON TOP OF THE GRAPHS CURRENTLY PRODUCED, TO ALLOW MORE INFORMATION TO BE INCLUDED IN METABOLIC MAPS, COMBINING TAXONOMY AND EXPRESSION LEVELS IN THE SAME GRAPH.

# • KEGGCHARTER'S WORKFLOW



Source: [1] UPIMAPI, reCOGnizer and KEGGCharter: Bioinformatics tools for functional annotation and visualization of (meta)-omics datasets.



# PROJECT MANAGEMENT TO DATE

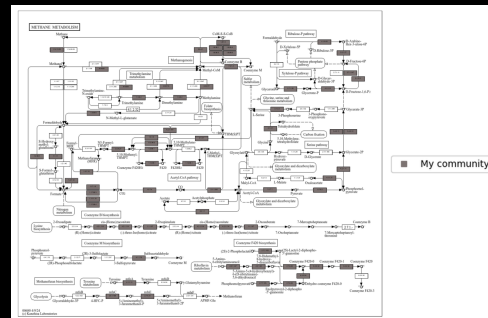
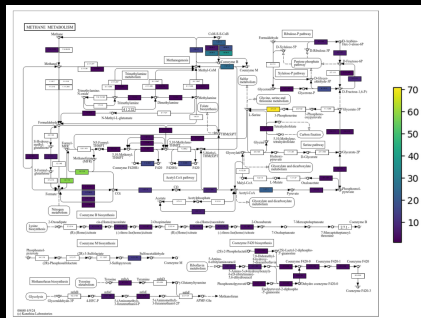
# STEP 1: RUN KEGGCHARTER TO SEE THE OUTPUTS;

```
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s_directory -keggc 'KEGG' -koc 'KO' -ecc 'EC number' -cogc 'COG ID' -iq -it "My community" -mm 00680 -o firs  
t_time_running_KC
```

resources\_directory  
first\_time\_running\_KC

KGML

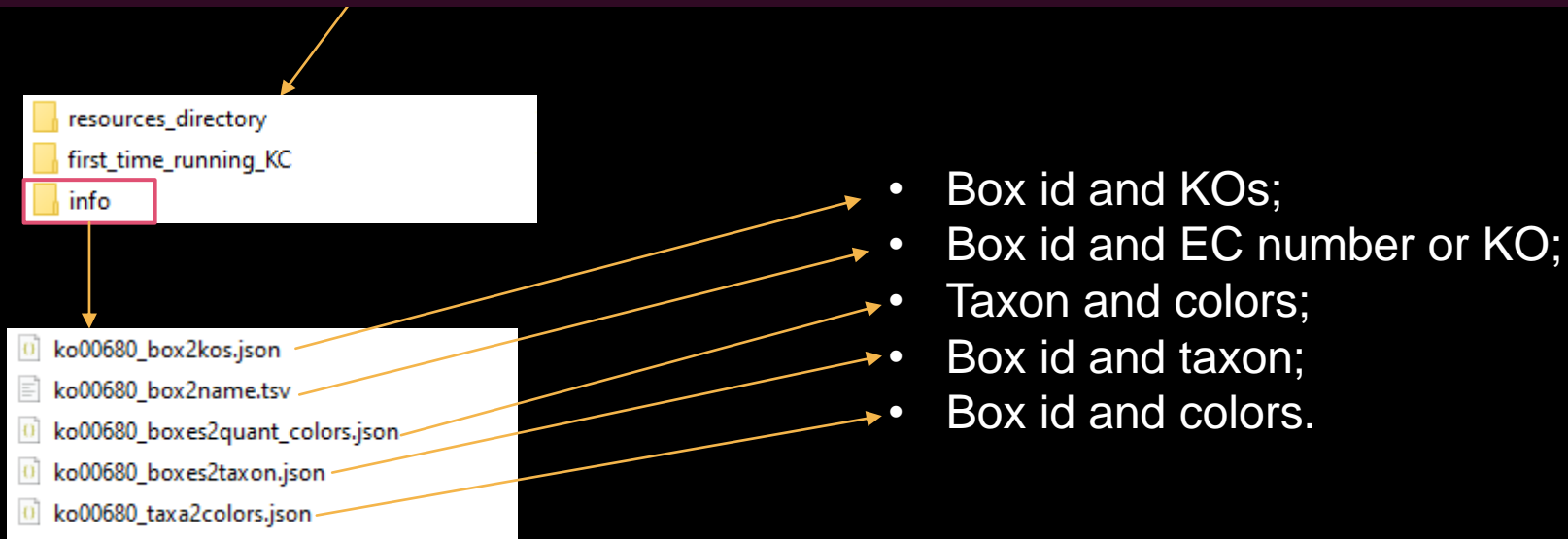
Two PNG Maps (differential; potential)



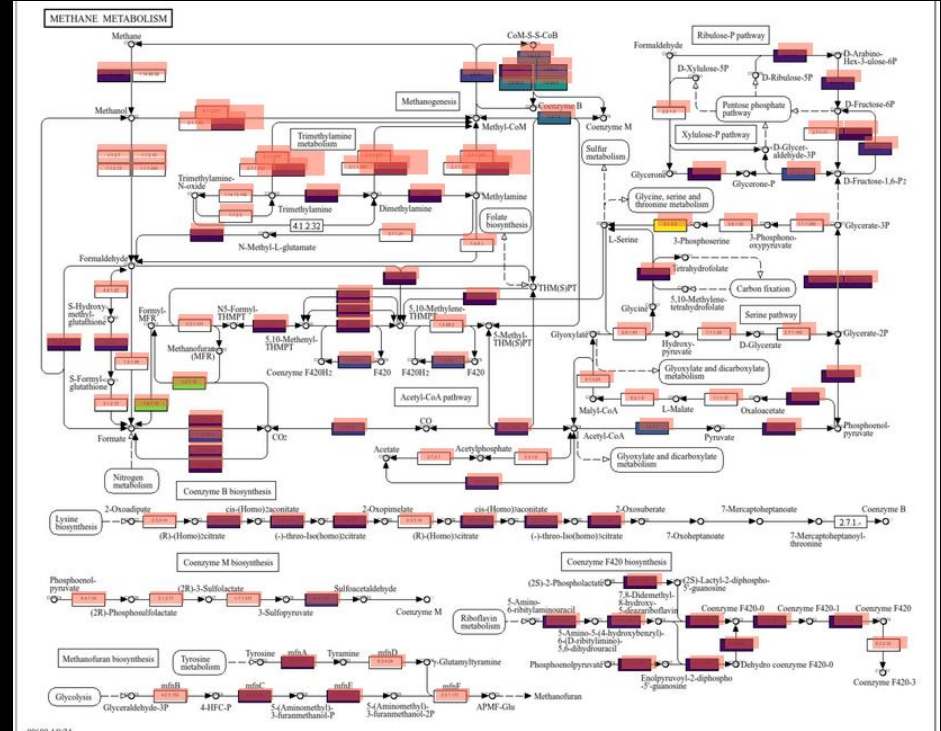
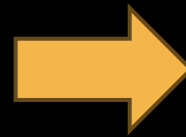
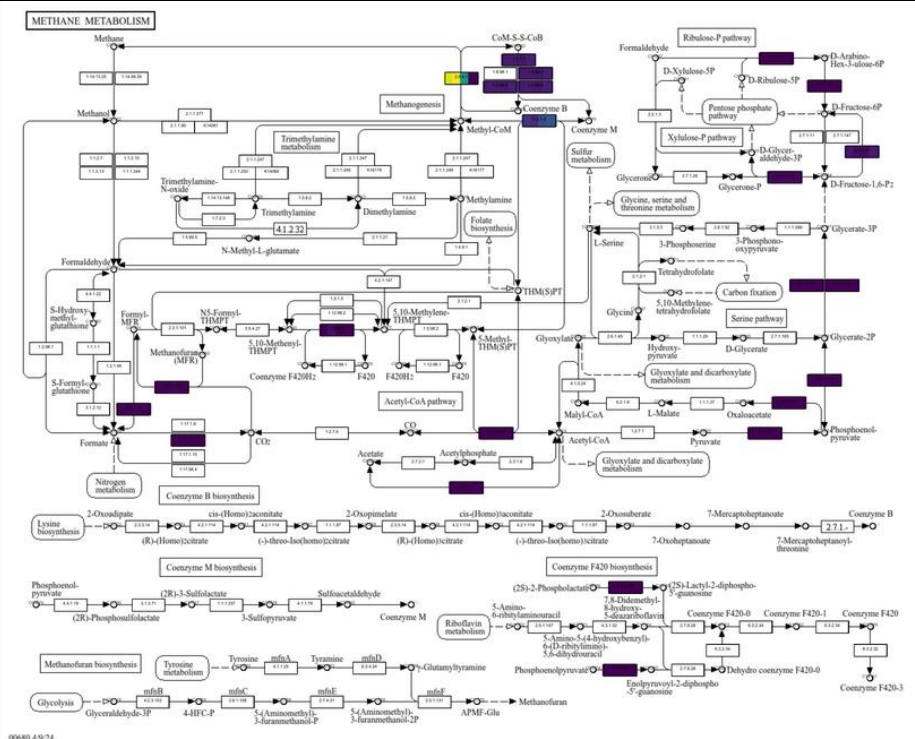
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```

STEP 2: THROUGH MODIFICATIONS TO THE TOOL,  
GENERATE NEW RESULTS;

```
(base) duartevelho1@DESKTOP-ROLJJ8V:~/Projeto/KEGGCharter$ python keggcharter.py -f keggcharter_input.tsv -r
d resources_directory -keggc 'KEGG' -o KC_additions -mm 00680 --map-all --taxa-column 'Taxonomic lineage (GE
NUS)' -qcol MP1,MP2,MP3,MP4
```

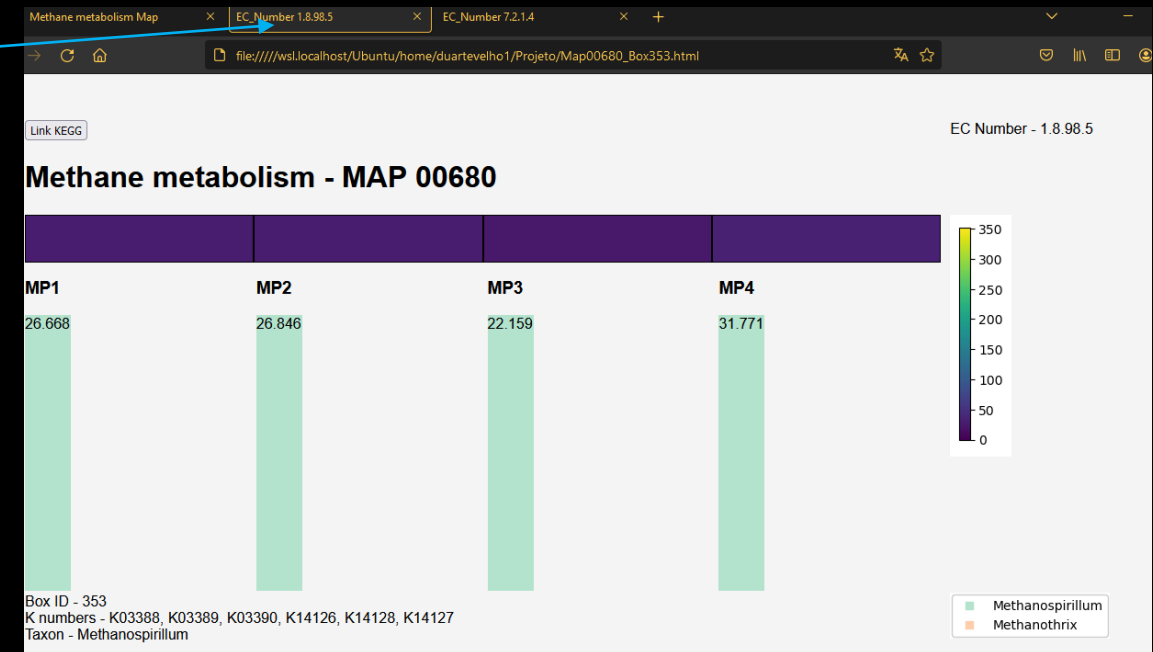
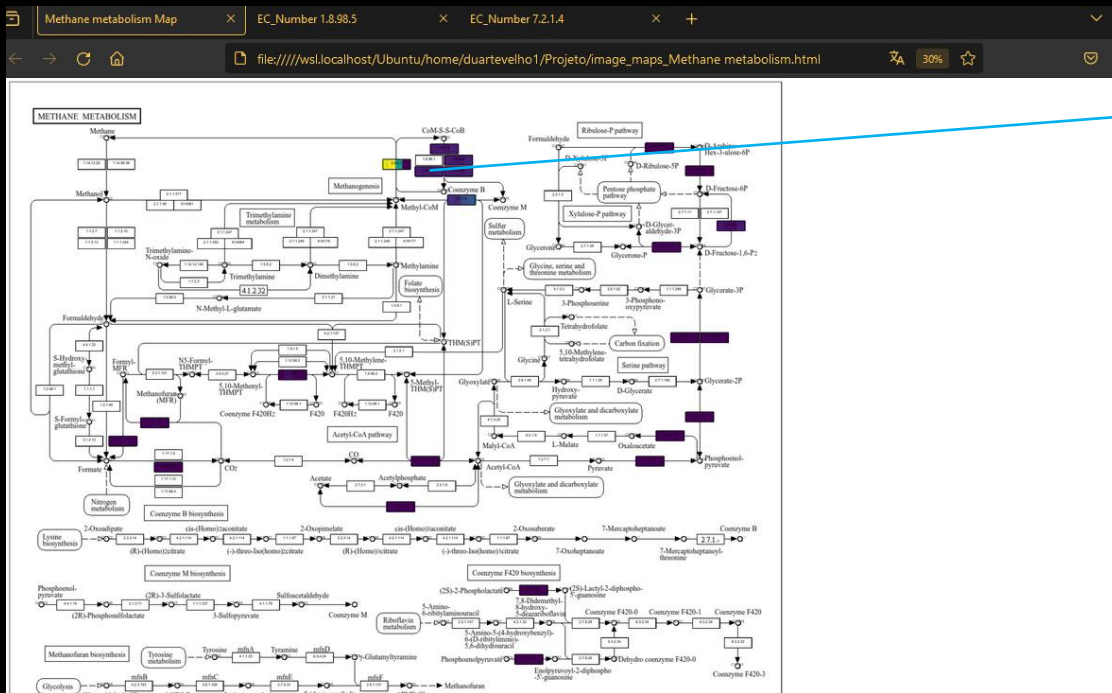


# STEP 3: MAKE THE PNG IMAGES CLICKABLE/INTERACTIVE;





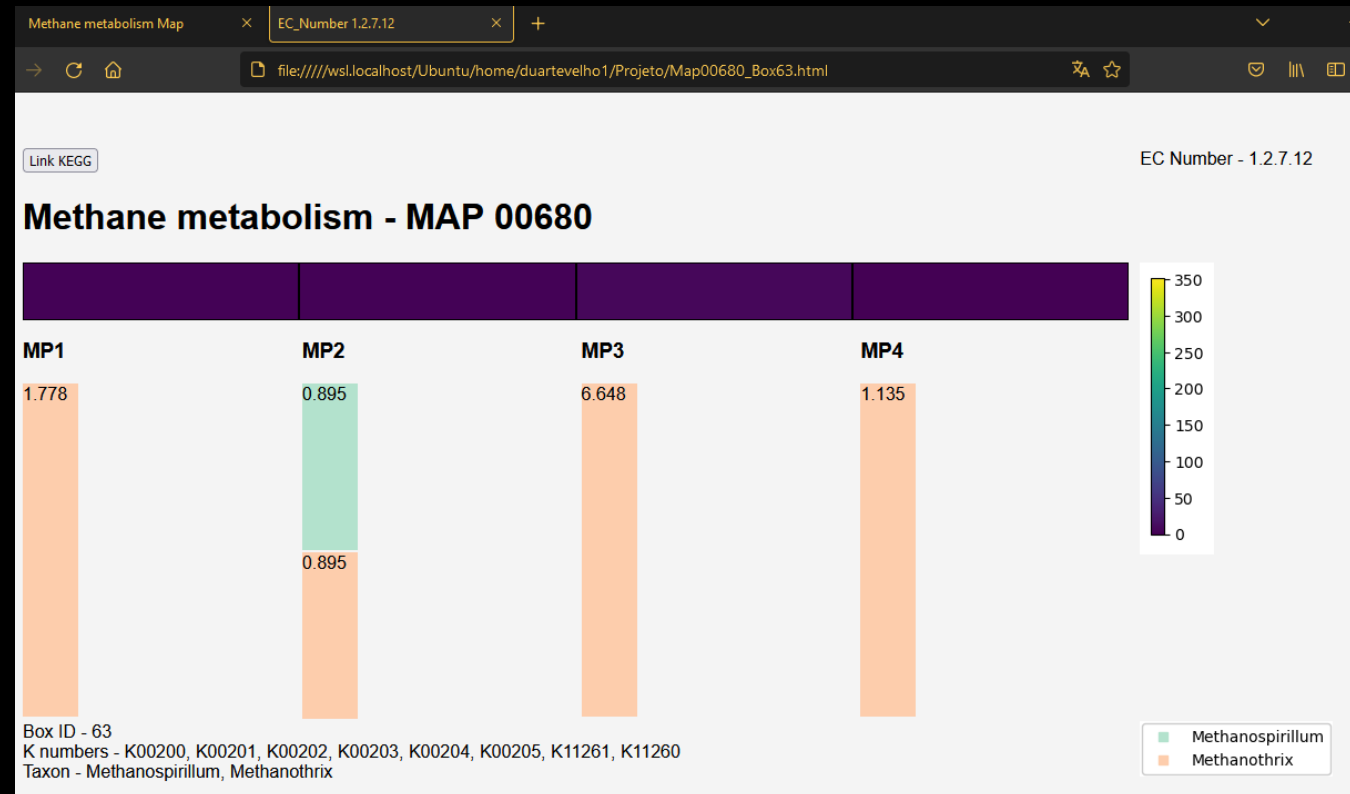
# STEP 4: CREATE DYNAMIC HTML PAGES FOR EACH MAP BOX;





# STEP 5: ENRICH THE HTML PAGES WITH RELEVANT INFORMATION.

- What's new: We were able to represent a new quantification, associated with taxonomy (until now it didn't exist)



- SUMMARY

- STEP 1: RUN KEGGCHARTER TO SEE THE OUTPUTS;
- STEP 2: THROUGH MODIFICATIONS TO THE TOOL, GENERATE NEW RESULTS;
- STEP 3: MAKE THE PNG IMAGES CLICABLE/INTERACTIVE;
- STEP 4: CREATE DYNAMIC HTML PAGES FOR EACH MAP BOX;
- STEP 5: ENRICH THE HTML PAGES WITH RELEVANT INFORMATION.



University of Minho  
School of Engineering



**Thanks!**

# • BIBLIOGRAPHY

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- SALOMONIS, N., HANSPERS, K., ZAMBON, A.C., VRANIZAN, K., LAWLOR, S.C., DAHLQUIST, K.D., DONIGER, S.W., STUART, J., CONKLIN, B.R., PICO, A.R.: GENMAPP 2: NEW FEATURES AND RESOURCES FOR PATHWAY ANALYSIS. BMC BIOINFORMATICS 8, 217 (2007).