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Optimization of metabolome extraction procedures and implementation of a PeakForest database for the identification of microorganisms compounds by LC-HRMS



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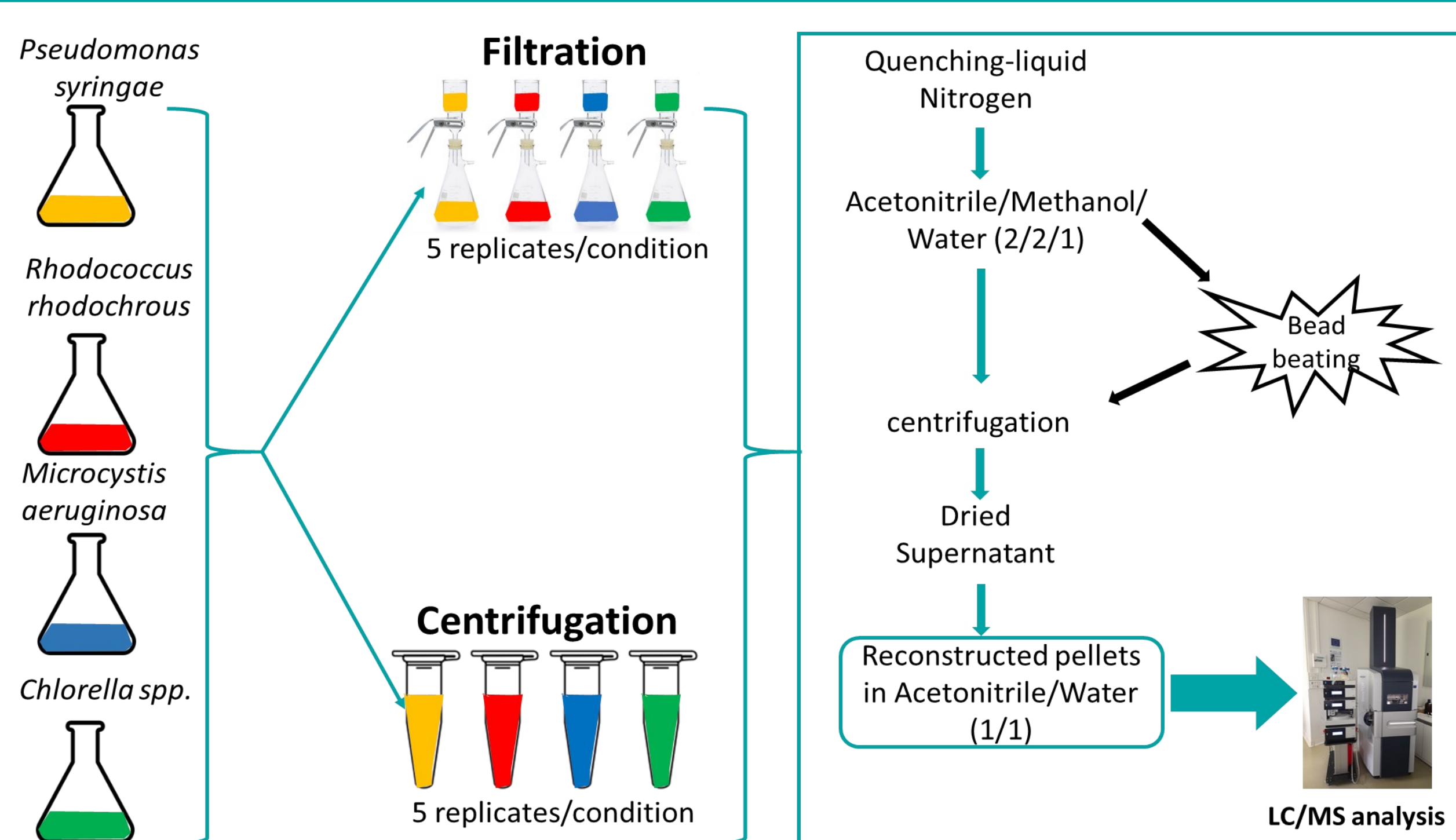


Background

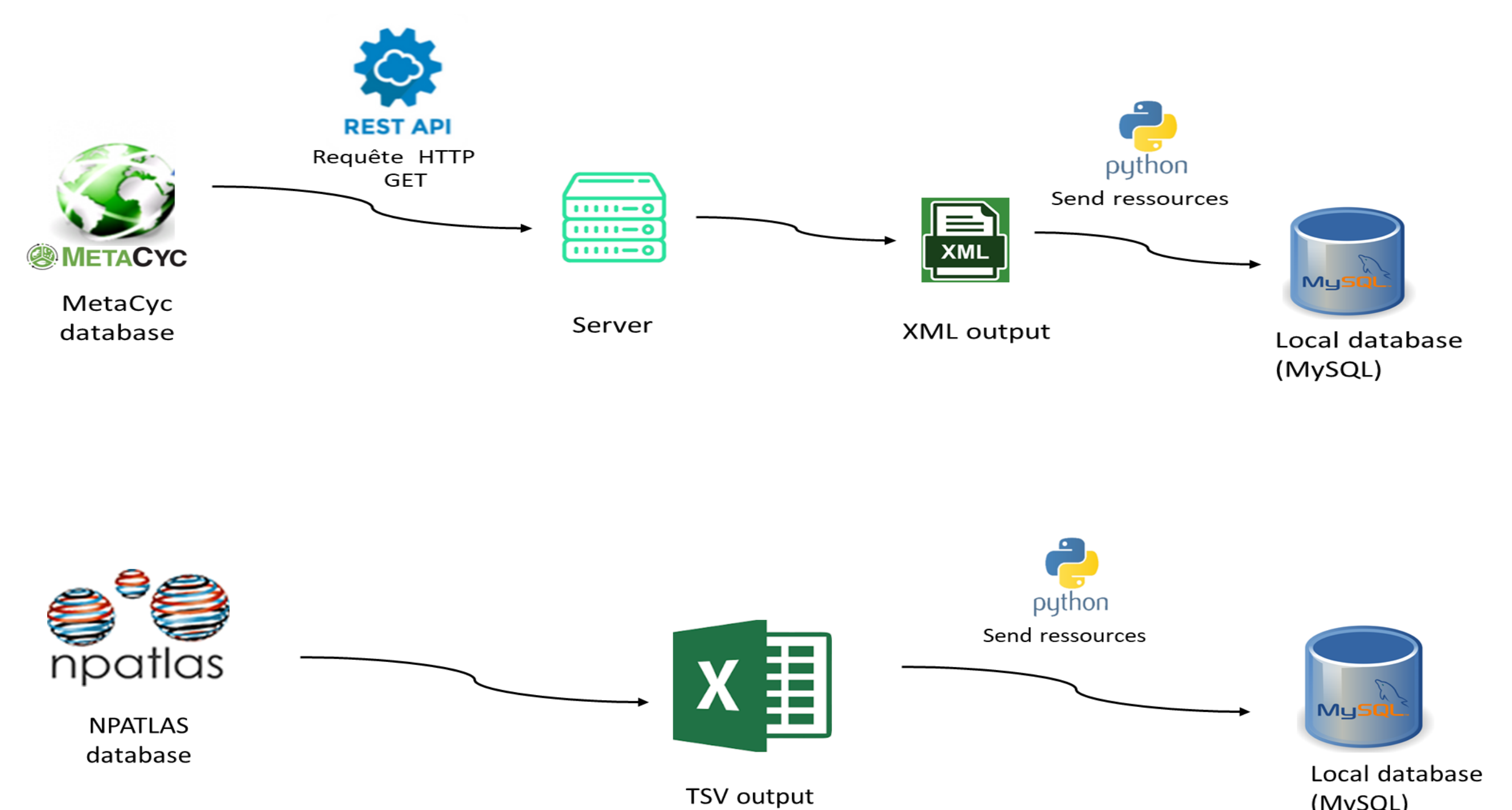
The investigation of microbial communities and their interactions with their environments is a field of research that engaged the scientific community for several decades. We study in the laboratory microorganisms isolated from freshwater and atmospheric ecosystems in different conditions. The aim of this internship was to optimize the metabolomic workflows of four microorganisms (*Pseudomonas syringae*, *Rhodococcus rhodochrous*, *Microcystis aeruginosa*, *Chlorella spp.*) from extraction to annotation of compounds.

Objectives: i) Optimize metabolome extraction protocol for each microorganism, ii) Implementation of a PeakForest database with MetaCyc and NPATLAS databases, iii) Annotation of microorganism's metabolomes.

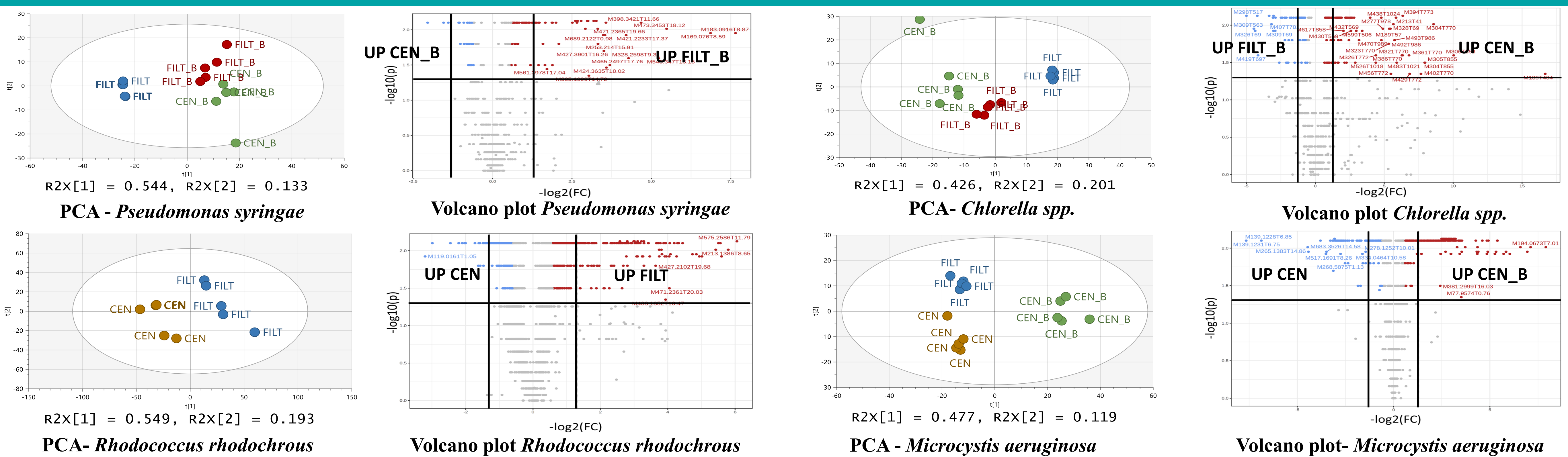
Protocols of extraction of compounds



Get Data from MetaCyc and NPAtlas databases

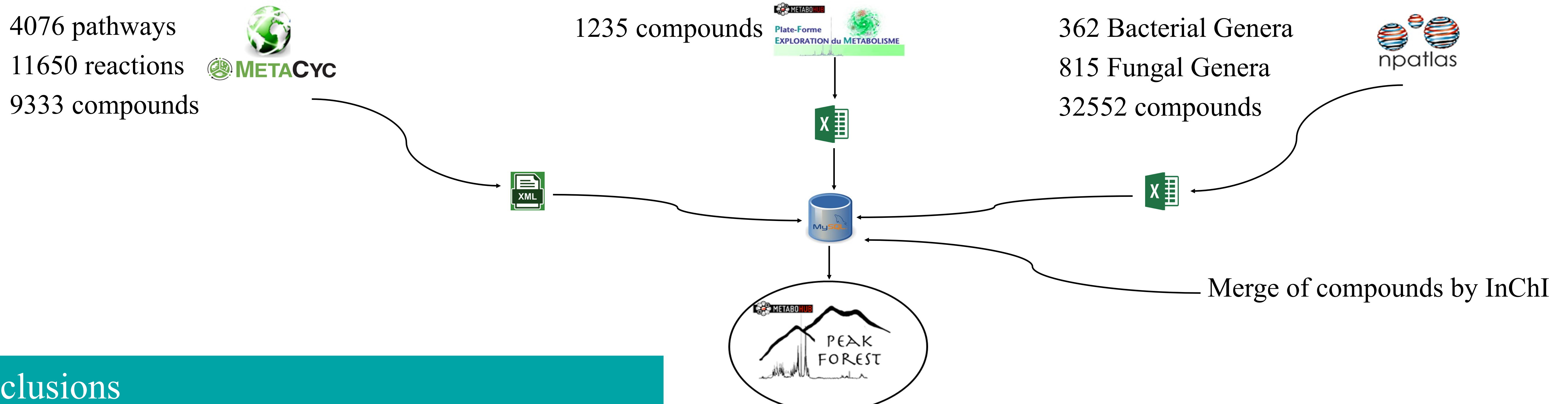


Comparison between protocols of extractions (positive ionization mode)



Principal Component Analyses (PCA) highlighted good repeatability between protocols (FILT= filtration, CEN= centrifugation, FILT_B= filtration + bead beating, CEN_B= centrifugation + bead beating). Volcano plot (Fold change >1.5 and pvalue < 0.05 compares the 2 best protocols). The addition of beads increased the amount of extracted metabolites for (*Pseudomonas aeruginosa*, *Microcystis aeruginosa* and *Chlorella spp.*)

Download of MetaCyc and NPAtlas databases and implementation of a PeakForest database



Conclusions

The first step of this internship allowed to optimize the extraction protocols of four microorganisms in order to annotate the compounds. For this purpose, a PeakForest database will soon be implemented with information from MetaCyc and NPATLAS. The aim was to set up a database more dedicated on microbial compounds. This database will be available to the community for curation or supplement information on compounds (spectral data, origins, pathways etc.).