step3
select MVs induced
metabolites (< 3-fold)

step4
exclude background
metabolites

xxx_overlap.csv
OVERLAPPED MASS FILE

xxx_ratio.csv
>3 OVERLAPPED
MASS FILE

xxx_ratio_delback.csv
INDUCED
METABOLITE FILE

metabolites
lists
+MVs

vs

-MVs

step1
categorize metabolites into
unique and common metabolites

step 1-4 are done for
individual screened bacterium.

step5
count duplicate for
each taxonomic class

step8
visualize hit metabolites
into a 3D plot

step7
extract metabolites meet
with the requirement

HIT FILE

ALL SELECTED
METABOLITE FILE

step5
combine all data

HIT CANDIDATE FILE

MS intensity ×10⁵

RT

m/z

step2
exclude background
metabolites

xxx_plusonly.csv
UNIQUE MASS FILE

xxx_delback.csv
HIT FILE

step1-4
differentialMSanalysis
.ipynb

step5-6
preprocess_for3Dplot
.ipynb

step7-8
3Dplot_generation
.ipynb