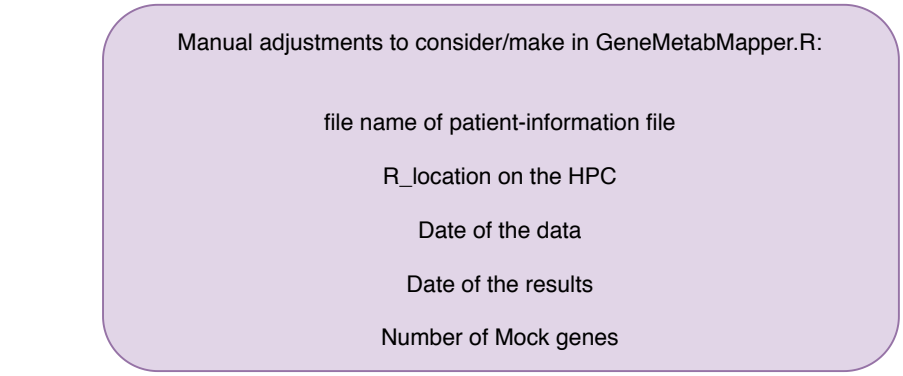
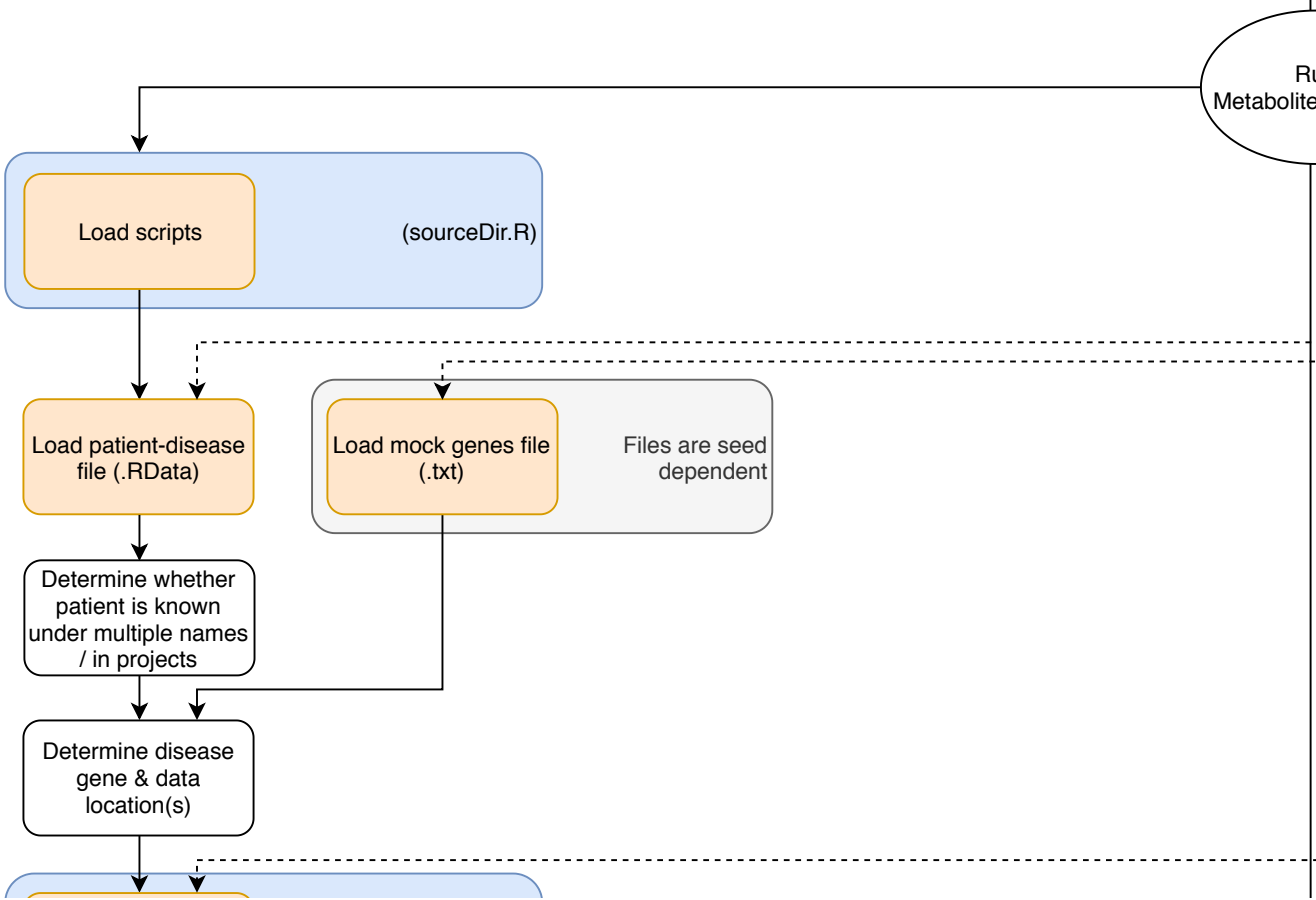
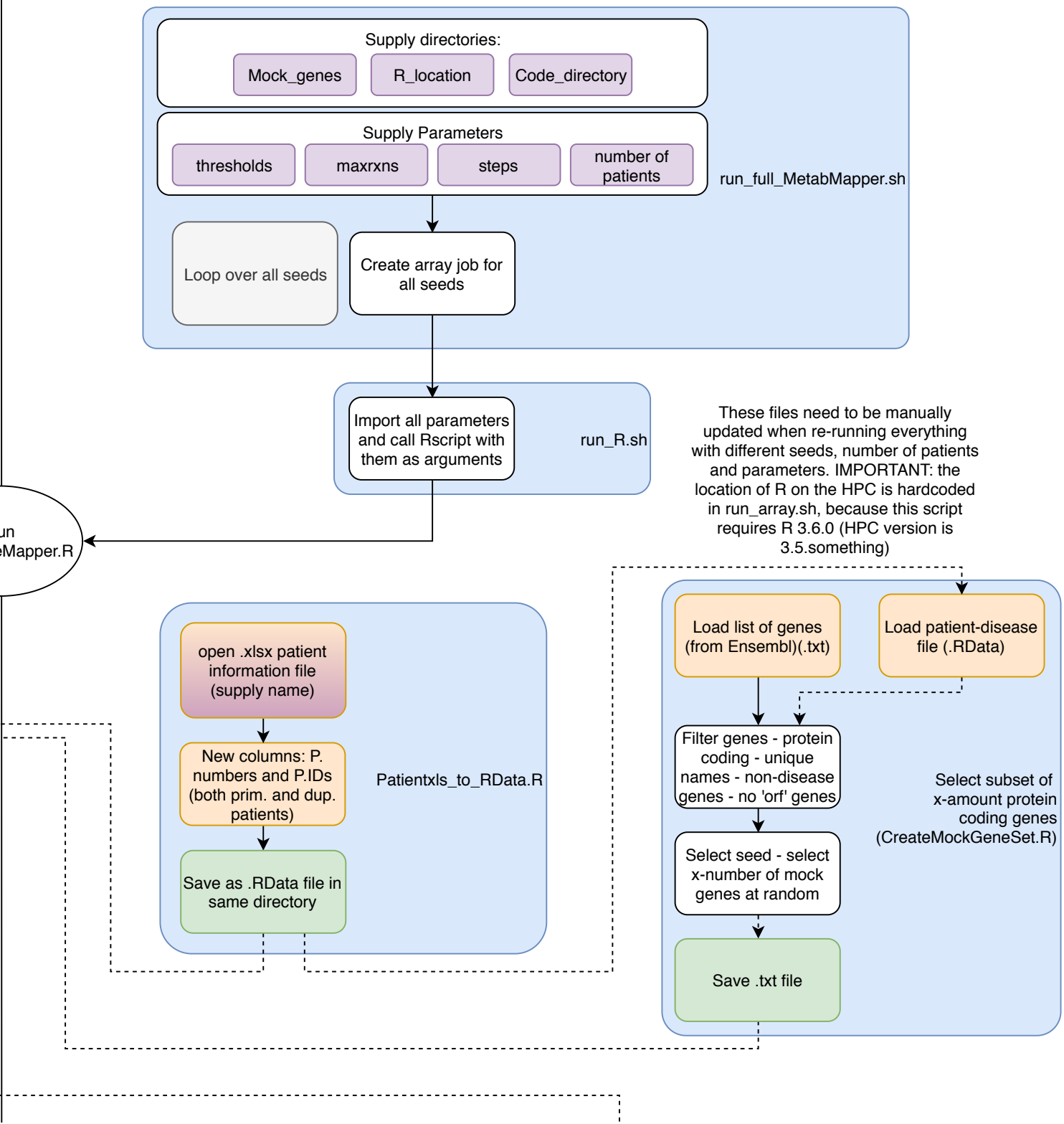
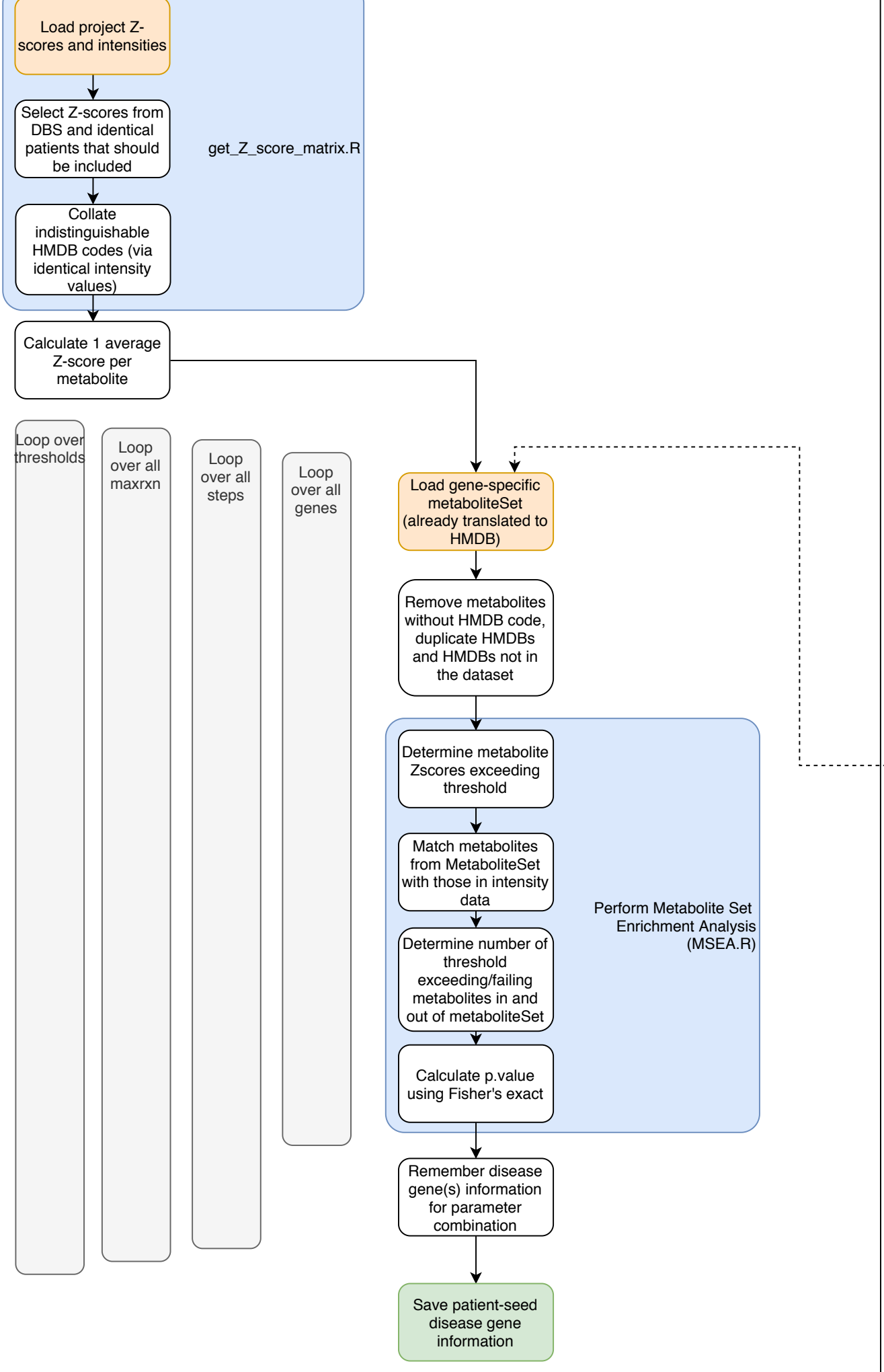
Running Metabolite Mapper script on the HPC (GeneMetabMapper.R)

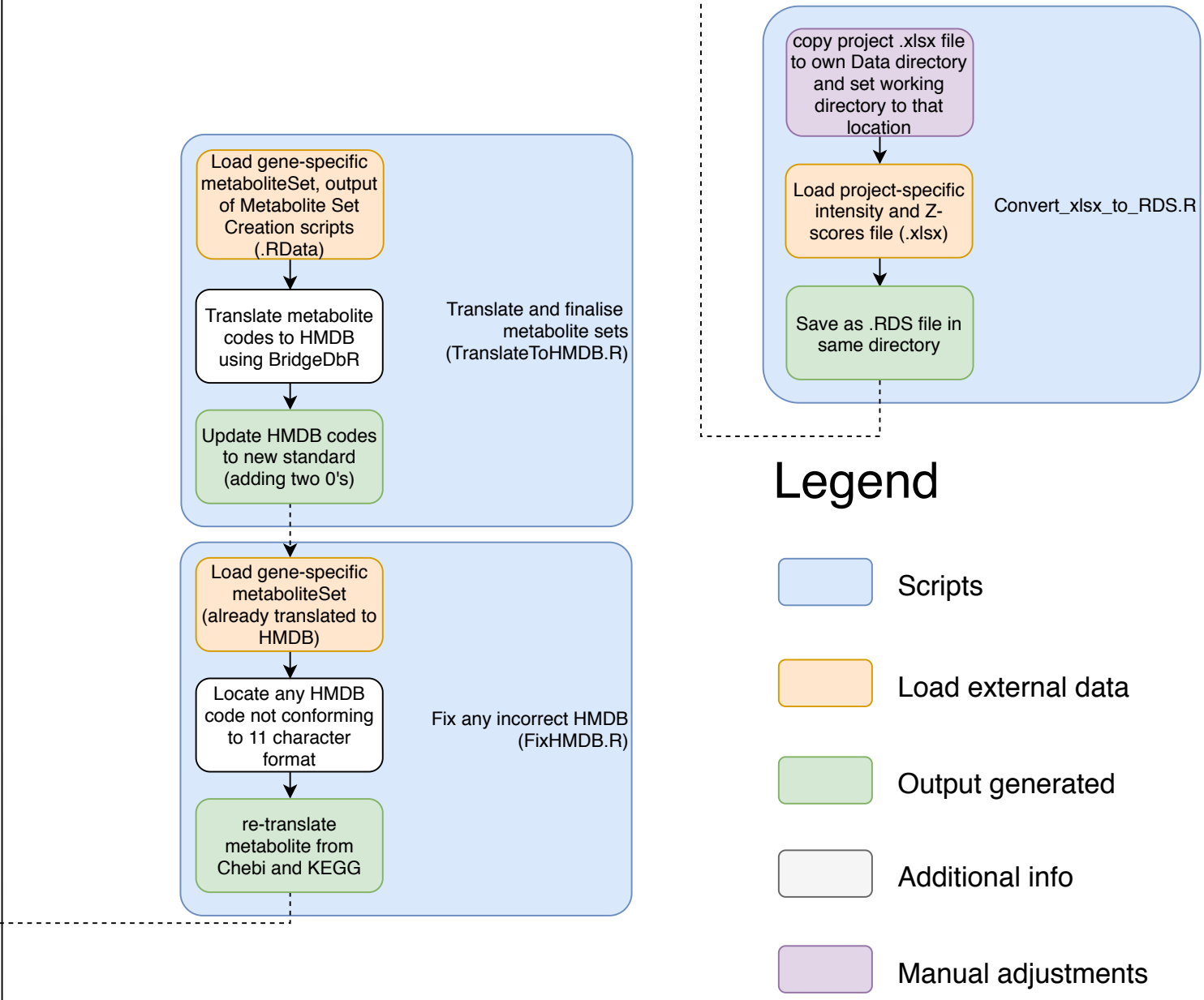




Externally executed scripts, their output necessary for correct functioning of Metabolite Mapper scripts




Load project Z-scores and intensities
Select Z-scores from DBS and identical patients that should be included
Collate indistinguishable HMDB codes (via identical intensity values)
get_Z_score_matrix.R
Calculate 1 average Z-score per metabolite
Loop over thresholds
Loop over all maxrxn
Loop over all steps
Loop over all genes
Load gene-specific metaboliteSet (already translated to HMDB)
Remove metabolites without HMDB code, duplicate HMDBs and HMDBs not in the dataset
Determine metabolite Zscores exceeding threshold
Match metabolites from MetaboliteSet with those in intensity data
Determine number of threshold exceeding/failing metabolites in and out of metaboliteSet
Calculate p.value using Fisher's exact
Perform Metabolite Set Enrichment Analysis (MSEA.R)
Remember disease gene(s) information for parameter combination
Save patient-seed disease gene information



Scripts used

HPC set for calling MetaboliteMapper

- run_full_MetabMapper.sh
- run_R.sh

Core set

- MetaboliteMapper.R
- sourceDir.R
- MSEA.R

- get_Z_score_matrix.R

External
- CreateMockGeneSet.R
- TranslateToHMDB.R
- FixHMDB.R
- Convert_xlsx_to_RDS.R
- Patientxls_to_RData.R