Auxiliary files (RData) folder:

"fix for R 4.0 get_peak_blocks_modulesvhclust.R" – for implementation xMSannotator in R ≥ 4.0.0.

"all params IPO CDF 7QC.RData", "funs params IPO CDF 7QC.RData", "IPO_optimiz_ret_align_CDF_7QC.RData", "IPO_optimiz_xcms_CDF_7QC.RData" – files with optimized parameters by IPO.

"CROP.RData", "mltpl_depict.RData", "mltpl_detect.RData", "mltpl_remove.RData" – for CROP algorithm implementation.

"Paramounter_part1 (V2).R", "Paramounter_part2 (V2).R" – for Paramounter algorithm implementation.

"core_SERRF_only_reduced.R", "evaluationMethods.R", "utils.R", "normalizations.R" – for SERRF algorithm implementation.

Datasets (csv) folder:

- 8 peaks.csv – dataset with selected features after entire processing steps.
- annotated 8 peaks.csv – as 8 peaks.csv but with metabolites name.
- metadata.csv – dataset with sample metadata (Age, Sex, Creatinine level, etc.).
- xcms after IPO MVI filter repeats annot.csv – dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation and averaging by technical repeats with annotation information.
- xcms after IPO MVI QC-XGB filter repeats annot.csv - dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation, QC-XGB correction, filtration by QC RSD and averaging by technical repeats with annotation information.
- xcms after IPO MVI QC-XGB filter repeats annot+filtr LMM adj KEGG.csv - dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation, QC-XGB correction, filtration by QC RSD, averaging by technical repeats with annotation information, annotation-based filtration and adjusting by LMM algorithm. This dataset is data table after entire processing scheme.
- xcms after IPO MVI QC-XGB filter repeats annot+filtr.csv - dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation, QC-XGB correction, filtration by QC RSD, averaging by technical repeats with annotation information and annotation-based filtration.

- xcms after IPO MVI QC-XGB filter repeats.csv - dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation, QC-XGB correction, filtration by QC RSD and averaging by technical repeats.

- xcms after IPO MVI QC-XGB filter.csv - dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation, QC-XGB correction and filtration by QC RSD.

- xcms after IPO MVI QC-XGB.csv - dataset after xcms integration and alignment (with IPO optimized parameters), missing value imputation and QC-XGB correction.

- xcms after IPO MVI.csv - dataset after xcms integration and alignment (with IPO optimized parameters) and missing value imputation.

- xcms after IPO.csv - dataset after xcms integration and alignment (with IPO optimized parameters).

- xcms CAMERA.csv – peaks annotation by CAMERA.

- xcms RAMClust.csv – peaks annotation by RAMClust.

- xcms xMSannotator KEGG.csv – peaks annotation by xMSannotator (KEGG database).

- xcms xMSannotator.csv – peaks annotation by xMSannotator (HMDB database).

- xcms mWISE.csv - peaks annotation by mWISE (KEGG database).