Package	Source	Version	Note
R version			
Base packages	CRAN	4.1.2	-
Common purpose			
data.table	CRAN	1.14.2	-
dplyr	CRAN	1.0.9	-
stringr	CRAN	1.4.0	-
doParallel	CRAN	1.0.17	-
BiocParallel	BC	1.28.3	-
ggplot2	CRAN	3.3.6	-
Randomization			
tuple	CRAN	0.4-02	-
randomizr	CRAN	0.22.0	-
Integration			
ipo	BC	1.20.0	-
Autotuner	BC	1.7.0	-
MetaboAnalystR	GH	3.0.2	-
xcms	BC	3.17.3	-
MSnbase	BC	2.20.1	-
MsFeatures	GH	1.2.0	-
warpgroup	GH	0.1.0.9001	-
ncGTW	BC	1.8.0	-
cpc	GH	0.1.0	-
Correction			
pmp	BC	1.6.0	-
StatTarget	BC	1.24.0	Use version 1.24.0 or higher before 1.29.4, because QC-LOESS is deleted (see also in folder "Required packages (archive)")
MetNormalizer	GH	1.3.02	-
batchCorr	GL	0.2.5	-
BatchCorrMetabolomics	GH	0.1.14	-
TIGERr	CRAN	1.0.0	-
notame	GH	0.0.5	-
openxlsx	CRAN	4.2.5	-
pbapply	CRAN	1.5-0	-
caret	CRAN	6.0-92	-
rpart	CRAN	4.1.16	-
ipred	CRAN	0.9-13	-
catboost	GH	0.20	-
xgboost	CRAN	1.6.0.1	-
dbnorm	GH	0.2.2	-
ProteoMM	BC	1.12.0	-
WaveICA	GH	0.1.0	-
WaveICA2.0	GH	0.1.0	-
NormalizeMets	CRAN	0.25	-
RUVSeq	BC	1.28.0	-
tibble	CRAN	3.1.7	-
fpc	CRAN	2.2-9	-
FactoMineR	CRAN	2.4	-
cluster	CRAN	2.1.3	-

proBatch	BC	1.10.0	-
gPCA	CRAN	1.0	-
pcpr2	GH	0.0.0.1	-
MetabolomicsBasics	CRAN	1.2	-
factoextra	CRAN	1.0.7	-
rafalib	CRAN	1.0.0	-
RSEIS	CRAN	4.1-1	-
ggsci	CRAN	2.9	-
corrplot	CRAN	0.92	-
Annotation			
CAMERA	BC	1.50.0	-
RAMClustR	CRAN	1.2.2	-
xMSannotator	GH	1.3.2	From kuppal2 repo (https://github.com/kuppal2/xMSannotator). Fix for R 4.0 fun string 95 to `n2<-as.data.frame(n1, stringsAsFactors = T)`. According to yufree repo (https://github.com/yufree/xMSannotator). Install manually (tar.gz), type = "source". Also see instruction from GH and SF.
mWISE	GH	0.1.0	-
metid	GH	1.2.13	Databases from (https://github.com/jaspershen/demoData/tree/master/inst/ms2_databada) should be copied in "ms2_database" folder in metID library folder.
tidyverse	CRAN	1.3.1	-
batchCorr	GL	0.2.5	-
curl	CRAN	4.3.2	-
piggyback	CRAN	0.1.3	-
MetaboAnnotation	BC	1.1.1	Database from *OUKS* release 1.10.1 or https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11-02
CompoundDb	BC	0.99.8	-
Normalization			
affy	BC	1.72.0	-
ABCstats	GH	1.0.0	-
clusterSim	CRAN	0.50-1	-
DiffCorr	CRAN	0.4.2	-
lmm2met	GH	1.0	-
MetabolomicsBasics	CRAN	1.2	-
lme4	CRAN	1.1-29	-
lmerTest	CRAN	3.1-3	-
mgcv	CRAN	1.8-40	-
gamm4	CRAN	0.2-6	-
NormalizeMets	CRAN	0.25	-
RColorBrewer	CRAN	1.1-3	-
limma	BC	3.50.3	-
Imputation			
MetProc	CRAN	1.0.1	-
MAI	BC	1.0.0	-
impute	BC	1.68.0	-
mice	CRAN	3.14.0	-

missForest	CRAN	1.5	-
StatTools	GL	0.0.915	-
pcaMethods	BC	1.86.0	-
imputeLCMD	CRAN	2.1	-
tWLSA	GH	1.0	-
imputeR	CRAN	2.2	-
vegan	CRAN	2.6-2	-
missMethods	CRAN	0.3.0	-
Grouping			
corrr	CRAN	0.4.3	-
gplots	CRAN	3.1.3	-
tidyverse	CRAN	1.3.1	-
igraph	CRAN	1.3.1	-
ggraph	CRAN	2.0.5	-
robCompositions	CRAN	2.3.1	-
compositions	CRAN	2.0-4	-
gridExtra	CRAN	2.3	-
stringi	CRAN	1.7.6	-
notame	GH	0.0.5	-
pmd	CRAN	0.2.1	-
Statistics			
pcaMethods	BC	1.86.0	-
OutlierDetection	GH	0.1.1	Should be installed from "rubak/spatstat.revdep" (see also in folder "Required packages (archive)")
ClassDiscovery	CRAN	3.4.0	-
ggforce	CRAN	0.3.3	-
HotellingEllipse	CRAN	1.1.0	-
caret	CRAN	6.0-92	Other methods may require additional packages
klaR	CRAN	0.6-14	The klaR package should be exactly version 0.6-14 for RFS (see also in folder "Required packages (archive)")
cwhmisc	CRAN	6.6	The shapiro.wilk.test function should be used if some error with normality test in UVF.
tuple	CRAN	0.4-02	-
pamr	CRAN	1.56.1	For ML model in caret
pls	CRAN	2.8-0	For ML model in caret
kernlab	CRAN	0.9-31	For ML model in caret
randomForest	CRAN	4.7-1.1	For ML model in caret
rsample	CRAN	0.1.1	-
ropls	BC	1.26.4	-
tdfdr	CRAN	0.1	-
MetabolomicsBasics	CRAN	1.2	-
lme4	CRAN	1.1-29	-
lmerTest	CRAN	3.1-3	-
mgcv	CRAN	1.8-40	-

gamm4	CRAN	0.2-6	-
drc	CRAN	3.0-1	-
limma	BC	3.50.3	-
NormalizeMets	CRAN	0.25	-
Boruta	CRAN	7.0.0	-
permimp	CRAN	1.0-2	-
party	CRAN	1.3-10	-
glmnet	CRAN	4.1-4	-
MASS	CRAN	7.3-57	-
pROC	CRAN	1.18.0	-
reshape2	CRAN	1.4.4	-
leaps	CRAN	3.1	-
gWQS	CRAN	3.0.4	-
vegan	CRAN	2.6-2	-
pairwiseAdonis	GH	0.0.1	-
multcomp	CRAN	1.4-19	-
MWASTools	BC	1.18.0	-
glmmsr	CRAN	0.2.3	-
MetStaT	CRAN	1.0	-
mixOmics	BC	6.18.1	-
DRomics	CRAN	2.4-0	-
TOXcms	GH	1.0.3	Require dr4pl and hashmap packages
timecourse	BC	1.66.0	-
timeOmics	BC	1.6.0	-
lmms	CRAN	1.3.3	-
polyPK	CRAN	3.1.0	Use version from "plyush1993/polyPK" (see also in folder "Required packages (archive)")
openxlsx	CRAN	4.2.5	-
tidyverse	CRAN	1.3.1	-
factoextra	CRAN	1.0.7	-
FactoMineR	CRAN	2.4	-
dendextend	CRAN	1.15.2	-
rafalib	CRAN	1.0.0	-
cluster	CRAN	2.1.3	-
dbscan	CRAN	1.1-10	-
umap	CRAN	0.2.8.0	-
NMF	CRAN	0.24.0	-
Rdimtools	CRAN	1.0.9	-
dimRed	CRAN	0.2.5	-
RSEIS	CRAN	4.1-1	-
ggsci	CRAN	2.9	-
pheatmap	CRAN	1.0.12	-

Rtsne	CRAN	0.16	-
NbClust	CRAN	3.0.1	-
clustertend	CRAN	1.6	-
mclust	CRAN	5.4.10	-
clValid	CRAN	0.7	-
pvclust	CRAN	2.2-0	-
fpc	CRAN	2.2-9	-
Hmisc	CRAN	4.7-0	-
corrplot	CRAN	0.92	-
psych	CRAN	2.2.5	-
pwr	CRAN	1.3-0	-
effectsize	CRAN	0.7.0	-
Directly used packages:		144	