

<i>Package</i>	<i>Source</i>	<i>Version</i>	<i>Note</i>
R version			
Base packages	CRAN	4.0.0	-
Common purpose			
data.table	CRAN	1.13.0	-
dplyr	CRAN	1.0.6	-
stringr	CRAN	1.4.0	-
doParallel	CRAN	1.0.15	-
BiocParallel	BC	1.22.0	-
ggplot2	CRAN	3.3.2	-
Randomization			
tuple	CRAN	0.4-02	-
randomizr	CRAN	0.20.0	-
Integration			
ipo	BC	1.14.0	-
Autotuner	BC	1.2.0	-
MetaboAnalystR	GH	3.0.2	-
xcms	BC	3.9.1	-
warpgroup	GH	0.1.0.9001	-
ncGTW	BC	1.2.0	-
Correction			
pmp	BC	1.0.0	-
StatTarget	BC	1.20.0	This version allows to set high value in the CV cutoff
MetNormalizer	GH	1.3.02	-
batchCorr	GL	0.2.5	-
BatchCorrMetabolomics	GH	0.1.14	-
notame	GH	0.0.5	-
openxlsx	CRAN	4.1.5	-
pbapply	CRAN	1.4-3	-
caret	CRAN	6.0-86	-
rpart	CRAN	4.1-15	-
ipred	CRAN	0.9-9	-
catboost	GH	0.20	-
xgboost	CRAN	1.2.0.1	-
dbnorm	GH	0.2.2	-
ProteoMM	BC	1.6.0	-
WaveICA	GH	0.1.0	-
NormalizeMets	CRAN	0.25	-
RUVSeq	BC	1.22.0	-
edgeR	BC	3.12.1	This version allows to load RUVSeq package
tibble	CRAN	3.0.3	-
fpc	CRAN	2.2-7	-
FactoMineR	CRAN	2.3	-
cluster	CRAN	2.1.0	-
proBatch	BC	1.4.0	-
gPCA	CRAN	1.0	-
pcpr2	GH	0.0.0.1	-
MetabolomicsBasics	CRAN	1.1	-

factoextra	CRAN	1.0.7	-
rafalib	CRAN	1.0.0	-
RSEIS	CRAN	3.9-0	-
ggsci	CRAN	2.9	-
Annotation			
CAMERA	BC	1.44.0	-
RamClustR	GH	1.1.0	-
xMSannotator	GH	1.3.2	From kuppal2 repo (https://github.com/kuppal2/xMSannotator). Fix for R 4.0 fun string 95 to <code>n2<-as.data.frame(n1, stringsAsFactors = T)</code> . 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	Forked from b2slab/mWISE to plyush1993/mWISE and depends were manually changed to R (>= 4.0).
metID	GH	1.1.0	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	1.3.0	-
batchCorr	GL	0.2.5	-
Normalization			
affy	BC	1.66.0	-
clusterSim	CRAN	0.49-1	-
DiffCorr	CRAN	0.4.1	-
lmm2met	GH	1.0	-
MetabolomicsBasics	CRAN	1.1	-
lme4	CRAN	1.1-23	-
lmerTest	CRAN	3.1-2	-
mgcv	CRAN	1.8-32	-
gamm4	CRAN	0.2-6	-
gpboost	CRAN	0.6.7	-
NormalizeMets	CRAN	0.25	-
RColorBrewer	CRAN	1.1-2	-
limma	BC	3.38.3	-
Imputation			
MetProc	CRAN	1.0.1	-
impute	BC	1.62.0	-
mice	CRAN	3.11.0	-
missForest	CRAN	1.4	-
StatTools	GL	0.0.915	-
pcaMethods	BC	1.80.0	-
imputeLCMD	CRAN	2.0	-
imputeR	CRAN	2.2	-
vegan	CRAN	2.5-6	-
missMethods	CRAN	0.2.0	-
Grouping			
corr	CRAN	0.4.3.9000	-

gplots	CRAN	3.0.4	-
tidyverse	CRAN	1.3.0	-
igraph	CRAN	1.2.6	-
ggraph	CRAN	2.0.3	-
robCompositions	CRAN	2.3.0	-
compositions	CRAN	2.0-1	-
gridExtra	CRAN	2.3	-
stringi	CRAN	1.5.3	-
notame	GH	0.0.5	-
pmd	CRAN	0.1.9	-
Statistics			
pcaMethods	BC	1.80.0	-
OutlierDetection	CRAN	0.1.1	Require spatstat package version 1.64-1 (CRAN)
ClassDiscovery	CRAN	3.3.13	-
caret	CRAN	6.0-86	Other methods may require additional packages
klaR	CRAN	0.6-14	The klaR package should be exactly version 0.6-14 for RFS
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	2.7-3	For ML model in caret
kernlab	CRAN	0.9-29	For ML model in caret
randomForest	CRAN	4.6-14	For ML model in caret
ropls	BC	1.20.0	-
tdfdr	CRAN	0.1	-
MetabolomicsBasics	CRAN	1.1	-
lme4	CRAN	1.1-23	-
lmerTest	CRAN	3.1-2	-
mgcv	CRAN	1.8-32	-
gamm4	CRAN	0.2-6	-
drc	CRAN	3.0-1	-
DRomics	CRAN	2.2-0	-
limma	BC	3.38.3	-
NormalizeMets	CRAN	0.25	-
permimp	CRAN	1.0-0	-
party	CRAN	1.3-5	-
glmnet	CRAN	4.0-2	-
MASS	CRAN	7.3-52	-
pROC	CRAN	1.16.2	-
reshape2	CRAN	1.4.4	-
leaps	CRAN	3.1	-

gWQS	CRAN	3.0.3	-
vegan	CRAN	2.5-6	-
pairwiseAdonis	GH	0.0.1	-
multcomp	CRAN	1.4-13	-
MetStaT	CRAN	1.0	-
mixOmics	BC	6.12.1	-
timecourse	BC	1.60.0	-
factoextra	CRAN	1.0.7	-
FactoMineR	CRAN	2.3	-
dendextend	CRAN	1.13.4	-
rafalib	CRAN	1.0.0	-
RSEIS	CRAN	3.9-0	-
ggsci	CRAN	2.9	-
pheatmap	CRAN	1.0.12	-
Rtsne	CRAN	0.15	-
NbClust	CRAN	3.0	-
clustertend	CRAN	1.4	-
mclust	CRAN	5.4.6	-
clValid	CRAN	0.6-9	-
pvclust	CRAN	2.2-0	-
fpc	CRAN	2.2-7	-
Hmisc	CRAN	4.4-1	-
corrplot	CRAN	0.84	-
psych	CRAN	2.0.7	-
pwr	CRAN	1.3-0	-
effectsize	CRAN	0.3.2	-
Directly used packages:			118