Package	Source	Version	Note			
	1	R ver	rsion			
Base packages	CRAN	4.1.2	-			
	ı	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	-			
	T	Random	nization			
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	-			
срс	GH	0.1.0	-			
		Corre	ction			
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	1.10.0			
	GH	0.0.0.1	-		
pcpr2 MetabolomicsBasics	CRAN	1.2	-		
	CRAN	1.0.7	-		
factoextra rafalib	CRAN	1.0.7	-		
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	1.2.2	II.a madraga vyyfyga's madraga vygwian		
XIVISamiotator	GH	1.5.2	Use package yufree's package version (https://github.com/yufree/xMSannotator).		
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 <i>OUKS</i> release 1.10.1 or https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11-02		
CompoundDb	BC	0.99.8	_		
Normalization Normalization					
- I	BC		lization		
affy	BC		ization -		
•		Norma	lization - -		
affy	BC	Norma 1.72.0	-		
affy ABCstats	BC GH	Norma 1.72.0 1.0.0	-		
affy ABCstats clusterSim	BC GH CRAN	Norma 1.72.0 1.0.0 0.50-1	- - -		
affy ABCstats clusterSim DiffCorr	BC GH CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2	- - -		
affy ABCstats clusterSim DiffCorr Imm2met	BC GH CRAN CRAN GH	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0	- - - -		
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics	BC GH CRAN CRAN GH CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2	- - - - -		
affy ABCstats clusterSim DiffCorr lmm2met MetabolomicsBasics lme4 lmerTest	BC GH CRAN CRAN GH CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29	- - - - - -		
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4	BC GH CRAN CRAN GH CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv	BC GH CRAN CRAN GH CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4	BC GH CRAN CRAN GH CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets	BC GH CRAN CRAN GH CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer	BC GH CRAN CRAN GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer Iimma MetProc	BC GH CRAN CRAN GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer Iimma	BC GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1 1.0.0			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer Iimma MetProc	BC GH CRAN CRAN GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer limma MetProc MAI	BC GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1 1.0.0			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer Iimma  MetProc MAI impute	BC GH CRAN CRAN GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1 1.0.0 1.68.0			
affy ABCstats clusterSim DiffCorr lmm2met MetabolomicsBasics lme4 lmerTest mgcv gamm4 NormalizeMets RColorBrewer limma MetProc MAI impute mice	BC GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1 1.0.0 1.68.0 3.14.0			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer limma  MetProc MAI impute mice missForest	BC GH CRAN CRAN GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1 1.0.0 1.68.0 3.14.0 1.5			
affy ABCstats clusterSim DiffCorr Imm2met MetabolomicsBasics Ime4 ImerTest mgcv gamm4 NormalizeMets RColorBrewer Iimma  MetProc MAI impute mice missForest StatTools	BC GH CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	Norma 1.72.0 1.0.0 0.50-1 0.4.2 1.0 1.2 1.1-29 3.1-3 1.8-40 0.2-6 0.25 1.1-3 3.50.3 Impu 1.0.1 1.0.0 1.68.0 3.14.0 1.5 0.0.915			

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 CRAN	1.3.1	-		
ggraph robCompositions	CRAN	2.3.1	-		
compositions	CRAN	2.0-4	-		
gridExtra	CRAN	2.3	<del>  -</del>		
stringi	CRAN	1.7.6	-		
notame	GH	0.0.5	-		
pmd	CRAN	0.2.1	-		
		Stati	stics		
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		
1 '	CDAN		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	- If some error with normality test in OVF.		
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  For ML model in caret		
randomForest	CRAN	4.7-1.1	For ML model in caret		
		0.1.1			
rsample	CRAN	1.26.4	-		
ropls	BC		-		
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	-		
	1	1			

	1	1			
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	-		
openxlsx tidyverse	CRAN CRAN	4.2.5 1.3.1	-		
-			- - -		
tidyverse	CRAN	1.3.1			
tidyverse factoextra	CRAN CRAN	1.3.1 1.0.7			
tidyverse factoextra FactoMineR	CRAN CRAN CRAN	1.3.1 1.0.7 2.4	-		
tidyverse factoextra FactoMineR dendextend	CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2	- -		
tidyverse factoextra FactoMineR dendextend rafalib	CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0	- - -		
tidyverse factoextra FactoMineR dendextend rafalib cluster	CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3	- - - -		
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan	CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10	- - - - -		
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0	- - - - - -		
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0	- - - - - -		
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9			
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools dimRed	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9 0.2.5			
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools dimRed RSEIS	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9 0.2.5 4.1-1			
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools dimRed RSEIS ggsci	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9 0.2.5 4.1-1 2.9			
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools dimRed RSEIS ggsci pheatmap	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9 0.2.5 4.1-1 2.9 1.0.12			
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools dimRed RSEIS ggsci pheatmap Rtsne	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9 0.2.5 4.1-1 2.9 1.0.12 0.16			
tidyverse factoextra FactoMineR dendextend rafalib cluster dbscan umap NMF Rdimtools dimRed RSEIS ggsci pheatmap Rtsne NbClust	CRAN CRAN CRAN CRAN CRAN CRAN CRAN CRAN	1.3.1 1.0.7 2.4 1.15.2 1.0.0 2.1.3 1.1-10 0.2.8.0 0.24.0 1.0.9 0.2.5 4.1-1 2.9 1.0.12 0.16 3.0.1			

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				