Package	Source	Version	Note		
	<u>-</u>	R ver	sion		
Base packages	CRAN	4.1.2	<u> </u>		
1 4 4 11	CDAN	Common			
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 randomizr	CRAN	0.4-02	-		
Tandonnizi	CKAN	Integr	etion		
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	_		
СРС	OII	Corre	ction		
pmp	BC	1.6.0	-		
StatTarget	BC	1.24.0	Use version 1.24.0 or higher before 1.29.4,		
~		1.2	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	-		
mgcv	CRAN	1.8-40	-		
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	_	
	CRAN	0.92	_	
corrplot CRAN 0.92 - Annotation				
CAMERA	BC	1.50.0		
RAMClustR	CRAN	1.2.2	-	
xMSannotator	GH	1.3.2	Use package yufree's package version	
AMSamotator	OII	1.3.2	(yufree/xMSannotator	
			or plyush1993/xMSannotator).	
mWISE	GH	0.1.0	-	
metid	GH	1.2.13	Databases from	
Incud	OII	1.2.13	(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	
		1.1.1	https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11-	
CompoundDb	BC	0.99.8	02	
CompoundDo] DC	Normal	ization	
affy	BC	1.72.0	-	
ABCstats	GH	1.0.0	-	
MAFFIN	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	-	
Immina BC 5.30.3 - Imputation				
MetProc	CRAN	1.0.1	-	
MAI	BC	1.0.1	-	
MsCoreUtils	BC	1.6.2		
impute	BC	1.68.0	-	
mice	CRAN	3.14.0	_	
missForest	CRAN	1.5	-	
HH22L-OLC2f	CNAIN	1.J	_	

Deamethods BC 1.86.0	StatTools	GL	0.0.915	-	
tWLSA	pcaMethods	BC	1.86.0	-	
ImputeR CRAN 2.2	imputeLCMD	CRAN	2.1	-	
vegan CRAN 2.6-2 - missMethods CRAN 0.3.0 - Grouping corr CRAN 0.4.3 - gplos CRAN 1.3.1 - tidyverse CRAN 1.3.1 - igraph CRAN 1.3.1 - oppropriations CRAN 2.0.5 - cobCompositions CRAN 2.0.4 - compositions CRAN 2.0.4 - gridExtra CRAN 2.3 - stringi CRAN 2.3 - stringi CRAN 2.3 - pand CRAN 2.3 - Statistics pademended pademended 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 - -	tWLSA	GH	1.0	-	
MissMethods	imputeR	CRAN	2.2	-	
CRAN 0.4.3 -				-	
corr CRAN 0.4.3 - gplots CRAN 3.1.3 - tidyverse CRAN 1.3.1 - igraph CRAN 2.0.5 - robCompositions CRAN 2.3.1 - compositions CRAN 2.3.1 - compositions CRAN 2.3 - 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 3.4.0 - caret CRAN 6.0-92 Other methods may require additional packages klaR CRAN 0.6-1	missMethods	CRAN	0.3.0	-	
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gplots	corrr	CDAN		1	
tidyverse CRAN 1.3.1		-			
igraph					
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 0.6-1 The shapiro.wilk.test function should be used if some error with norma		+			
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Description CRAN 0.2.1		CRAN	1.7.6	-	
Statistics	notame	GH	0.0.5	-	
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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 0.1.1 - ropls BC 1.26.4 - tdfdr CRAN 0.1 - MetabolomicsBasics CRAN 1.1-29 - Ime4 CRAN 3.1-3 -			Stati	stics	
ClassDiscovery ggforceCRAN CRAN3.4.0 3.4.0- Required packages (archive)")GaretCRAN CRAN1.1.0 4.0-92- Other methods may require additional packagesKlaRCRAN CRAN CRAN0.6-14 4.6-14 5.6-15 5.6-14 5.6-14 5.6-14 5.6-14 5.6-14 5.6-15 5.6-14	pcaMethods	BC	1.86.0	-	
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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 - Ime4 CRAN 3.1-3 -				"Required packages (archive)")	
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MetabolomicsBasics CRAN 1.2 - lme4 CRAN 1.1-29 - lmerTest CRAN 3.1-3 -				-	
Ime4 CRAN 1.1-29 - ImerTest CRAN 3.1-3 -				-	
ImerTest CRAN 3.1-3 -	MetabolomicsBasics	CRAN	1.2	-	
		CRAN		-	
mgcv CRAN 1.8-40 -	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	- Required packages (archive)
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	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	

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: 146				