Package	Source	Version	Note
		R ver	sion
Base packages	CRAN	4.1.2	-
	an	Common	
data.table	CRAN	1.14.2	-
dplyr	CRAN	1.0.7	-
stringr	CRAN	1.4.0	-
doParallel	CRAN	1.0.16	-
BiocParallel	BC	1.22.0	-
ggplot2	CRAN	3.3.5	-
. 1	GD AN	Random	nization
tuple	CRAN	0.4-02	-
randomizr	CRAN	0.22.0	-
	D.C.	Integr	
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	-
	D.C.	Corre	
pmp	BC	1.6.0	-
StatTarget	BC	1.24.0	-
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	6.0-90	-
rpart	CRAN	4.1-16	-
ipred	CRAN	0.9-12	-
catboost	GH	0.20	-
xgboost	CRAN	1.5.0.2	-
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	3.1.6	-
fpc FactoMinaP	CRAN	2.2-9	-
FactoMineR	CRAN	2.4	-
cluster	CRAN	2.1.2	-
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	4.0-3	-				
ggsci	CRAN	2.9	-				
88**-	Annotation						
CAMERA	BC	1.50.0	-				
RamClustR	GH	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	1.1.0	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	1.3.1	-				
batchCorr	GL	0.2.5	_				
	•	Normal	lization				
affy	BC	1.72.0	-				
clusterSim	CRAN	0.49-2	-				
DiffCorr	CRAN	0.4.1	-				
lmm2met	GH	1.0	-				
MetabolomicsBasics	CRAN	1.2	-				
lme4	CRAN	1.1-28	-				
lmerTest	CRAN	3.1-3	-				
mgcv	CRAN	1.8-38	-				
gamm4	CRAN	0.2-6	-				
gpboost	CRAN	0.7.1	-				
NormalizeMets	CRAN	0.25	-				
RColorBrewer	CRAN	1.1-2	-				
limma	BC	3.50.0	<u> </u> -				
16.5	T ~- :	Imput	tation				
MetProc	CRAN	1.0.1	-				
impute	BC	1.68.0	-				
mice	CRAN	3.14.0	-				
missForest	CRAN	1.4	-				
StatTools	GL	0.0.915	-				
pcaMethods	BC	1.86.0	-				
imputeLCMD	CRAN	2.0	-				
tWLSA	GH	1.0	-				
imputeR	CRAN	2.2	-				
vegan	CRAN	2.5-7	-				
missMethods	CRAN	0.2.0	-				

		Grou	ning
corrr	CRAN	0.4.3	- -
gplots	CRAN	3.1.1	_
tidyverse	CRAN	1.3.1	-
igraph	CRAN	1.2.11	-
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	-
	T = =	Statis	stics
pcaMethods	BC	1.86.0	-
OutlierDetection	GH	0.1.1	Should be installed from "rubak/spatstat.revdep"
ClassDiscovery	CRAN	3.4.0	-
caret	CRAN	6.0-90	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	2.8-0	For ML model in caret
kernlab	CRAN	0.9-29	For ML model in caret
randomForest	CRAN	4.7-1	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	1.1-28	-
ImerTest	CRAN	3.1-3	-
mgcv	CRAN	1.8-38	-
gamm4	CRAN	0.2-6	-
drc	CRAN	3.0-1	-
limma	BC	3.50.0	-
NormalizeMets	CRAN	0.25	-
Boruta	CRAN	7.0.0	-
permimp	CRAN	1.0-2	-
party	CRAN	1.3-9	-
glmnet	CRAN	4.1-3	-
MASS	CRAN	7.3-55	-
pROC	CRAN	1.18.0	-
reshape2	CRAN	1.4.4	-

leaps	CRAN	3.1	-	
gWQS	CRAN	3.0.4	-	
vegan	CRAN	2.5-7	-	
pairwiseAdonis	GH	0.0.1	-	
multcomp	CRAN	1.4-18	-	
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	-	
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	2.1.2	-	
dbscan	CRAN	1.1-10	-	
umap	CRAN	0.2.7.0	-	
NMF	CRAN	0.23.0	-	
Rdimtools	CRAN	1.0.9	-	
dimRed	CRAN	0.2.4	-	
RSEIS	CRAN	4.0-3	-	
ggsci	CRAN	2.9	-	
pheatmap	CRAN	1.0.12	-	
Rtsne	CRAN	0.15	-	
NbClust	CRAN	3.0	-	
clustertend	CRAN	1.6	-	
mclust	CRAN	5.4.9	-	
clValid	CRAN	0.7	-	
pvclust	CRAN	2.2-0	-	
fpc	CRAN	2.2-9	-	
Hmisc	CRAN	4.6-0	-	
corrplot	CRAN	0.92	-	
psych	CRAN	2.1.9	-	
pwr	CRAN	1.3-0	-	
effectsize	CRAN	0.6.0.1	-	
Directly used packages: 136				