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 3.3.6	-
ggplot2	CRAN	3.3.0 Random	- igation
tuplo	CRAN	0.4-02	lization
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	-

ProBatch BC 1.10.0	cluster	CRAN	2.1.3	_	
PCA			-	-	
Depth 2	-1	-	•	_	
MetabolomicsBasics		+		_	
Factoextra CRAN 1.0.7 -	• •	+		_	
Rafalib				_	
RSEIS		_		-	
Second		+	-	-	
Corplot		+			
Annotation CAMERA BC 1.50.0 -		-		-	
RAMClustR				ation	
xMSannotator GH 1.3.2 Use package yufree's package version (yufree/xMSannotator or plyush1993/xMSannotator). mWISE GH 0.1.0 - metid GH 1.2.13 Databases from ophyush1993/xMSannotator phinosphen/demoData/tree/master/inst/ms2_databasle phould 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://delabo.AnnotationTutorials/releases/tag/2021-11-02 CompoundDb BC 0.99.8 - Normalization affy BC 1.72.0 - ABCstats GH 1.0.0 - AMAFFIN GH 1.0.0 - clusterSim CRAN 0.50-1 - DiffCorr CRAN 1.2 - Imm2met GH 1.0 - Metabol	CAMERA	BC	1.50.0	-	
MWISE	RAMClustR	CRAN	1.2.2	-	
MWISE	xMSannotator	GH	1.3.2	Use package yufree's package version	
mWISE GH 0.1.0 - metid GH 1.2.13 Databases (https://github.com/jaspershen/demoData/tree/masser/instrins2_databada/s) 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/jorianer/MetaboAnnotation/Tutorials/releases/tag/2021-11-02 CompoundDb BC 0.99.8 - Normalization affy BC 1.72.0 - ABCstats GH 1.0.0 - dusterSim CRAN 0.50-1 - DiffCorr CRAN 0.4.2 - Imm2met GH 1.0 - MetabolomicsBasics CRAN 1.1-29 - ImerTest CRAN 0.2-6 - NormalizeMets CRAN 0.					
MetabolanicsBasics GRAN 1.2.13 Databases from (https://github.com/jaspershen/demoData/tree/master/inst/ms2_database) should be copied in "ms2_database" folder in metID library folder.				or plyush1993/xMSannotator).	
CRAN 1.3.1	mWISE	GH	0.1.0		
Should be copied in "ms2_database" folder in metID library folder.	metid	GH	1.2.13	Databases from	
metID library folder.				(https://github.com/jaspershen/demoData/tree/master/inst/ms2_databada)	
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 - ABCstats GH 1.0.0 - clusterSim CRAN 0.50-1 - DiffCorr CRAN 0.50-1 - Imm2met GH 1.0 - MetabolomicsBasics CRAN 1.1-29 - Ime4 CRAN 1.1-29 - Ime7Test CRAN 3.1-3 - mgcv CRAN 1.8-40 - gamm4 CRAN 0.2-5 - <td< td=""><td></td><td></td><td></td><td>should be copied in "ms2_database" folder in</td></td<>				should be copied in "ms2_database" folder in	
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/2021-11-02-02-02-01-02-02-02-01-02-02-02-01-02-02-02-01-02-02-02-02-01-02-02-02-02-02-01-02-02-02-02-02-02-02-02-02-02-02-02-02-				metID library folder.	
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Diggyback	batchCorr	GL		-	
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 - MAFFIN GH 1.0.0 - clusterSim CRAN 0.50-1 - DiffCorr CRAN 0.4.2 - Imm2met GH 1.0 - MetabolomicsBasics CRAN 1.2 - ImerTest CRAN 3.1-3 - mgcv CRAN 1.8-40 - gamm4 CRAN 0.25 - RColorBrewer CRAN 1.1-3 - limma BC 3.50.3 - Imputation BC 1.68.0 - mice CRAN 3.14.0 - missForest CRAN 1.5 -	curl	CRAN	4.3.2	-	
https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11- CompoundDb	piggyback	CRAN	0.1.3	-	
Normalization	MetaboAnnotation	BC	1.1.1	https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11-	
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clusterSim CRAN 0.50-1 - DiffCorr CRAN 0.4.2 - Imm2met GH 1.0 - MetabolomicsBasics CRAN 1.2 - Ime4 CRAN 1.1-29 - ImerTest 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 - MetProc CRAN 1.0.1 - MAI BC 1.0.0 - impute BC 1.68.0 - mice CRAN 3.14.0 - missForest CRAN 1.5 -	ABCstats	GH	1.0.0	-	
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ImerTest 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 -	MetabolomicsBasics	CRAN	1.2	-	
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 -	lme4	CRAN	1.1-29	-	
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 -	lmerTest	CRAN	3.1-3	-	
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 -	mgcv	CRAN	1.8-40	-	
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 -		CRAN	0.2-6	-	
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 -	NormalizeMets	CRAN	0.25	-	
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 -	RColorBrewer	CRAN	1.1-3	-	
MetProc CRAN 1.0.1 - MAI BC 1.0.0 - impute BC 1.68.0 - mice CRAN 3.14.0 - missForest CRAN 1.5 -	limma	BC	3.50.3	-	
MAI BC 1.0.0 - impute BC 1.68.0 - mice CRAN 3.14.0 - missForest CRAN 1.5 -					
impute BC 1.68.0 - mice CRAN 3.14.0 - missForest CRAN 1.5 -	MetProc	CRAN	1.0.1	-	
mice CRAN 3.14.0 - missForest CRAN 1.5 -	MAI	BC	1.0.0	-	
missForest CRAN 1.5 -	impute	BC	1.68.0	-	
	mice	CRAN	3.14.0	-	
StatTools GL 0.0.915 -	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	-		
corrr	CRAN	Grou 0.4.3	ping -		
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	-		
26.1.1	D.C.	Statis			
pcaMethods	BC	1.86.0	-		
OutlierDetection	GH	0.1.1	Should be installed from		
			"rubak/spatstat.revdep" (see also in folder		
ClassDisasysamy	CRAN	3.4.0	"Required packages (archive)")		
ClassDiscovery			-		
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		
	65.131		0.6-14 for RFS (see also in folder "Required		
			packages (archive)")		
cwhmisc	CRAN	6.6	The shapiro.wilk.test function should be used		
tuple	CRAN	0.4-02	if some error with normality test in UVF.		
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	- For ML moder in caret		
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:				145