

| <i>Package</i> | <i>Source</i> | <i>Version</i> | <i>Note</i> |
|-----------------------|---------------|----------------|--|
| R version | | | |
| Base packages | CRAN | 4.1.2 | - |
| 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 | - |
| Randomization | | | |
| 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 | - |
| cpc | GH | 0.1.0 | - |
| Correction | | | |
| 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 | - |
| mgcv | CRAN | 1.8-40 | - |
| MetCorR | GH | 0.1.0 | - |
| 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 | - |

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| 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 | - |
| 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 (yufree/xMSannotator or plyush1993/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 | | | |
| 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 | - |
| Imputation | | | |
| MetProc | CRAN | 1.0.1 | - |
| MAI | BC | 1.0.0 | - |
| MsCoreUtils | BC | 1.6.2 | - |
| impute | BC | 1.68.0 | - |
| mice | CRAN | 3.14.0 | - |

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| 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 | - |
| Grouping | | | |
| corr | CRAN | 0.4.3 | - |
| 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 | - |
| 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 | 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 | - |
| lme4 | CRAN | 1.1-29 | - |
| lmerTest | CRAN | 3.1-3 | - |
| mgcv | CRAN | 1.8-40 | - |

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| 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 | - |

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| Rtsne | CRAN | 0.16 | - |
| NbClust | CRAN | 3.0.1 | - |
| clustertend | CRAN | 1.6 | - |
| mclust | CRAN | 5.4.10 | - |
| clValid | CRAN | 0.7 | - |
| pvcust | 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 | - |