

| <i>Package</i> | <i>Source</i> | <i>Version</i> | <i>Note</i> |
|-----------------------|---------------|----------------|--|
| R version | | | |
| Base packages | CRAN | 4.0.0 | - |
| Common purpose | | | |
| data.table | CRAN | 1.13.0 | - |
| dplyr | CRAN | 1.0.6 | - |
| stringr | CRAN | 1.4.0 | - |
| doParallel | CRAN | 1.0.15 | - |
| BiocParallel | BC | 1.22.0 | - |
| ggplot2 | CRAN | 3.3.2 | - |
| Randomization | | | |
| tuple | CRAN | 0.4-02 | - |
| randomizr | CRAN | 0.20.0 | - |
| Integration | | | |
| ipo | BC | 1.14.0 | - |
| Autotuner | BC | 1.2.0 | - |
| MetaboAnalystR | GH | 3.0.2 | - |
| xcms | BC | 3.9.1 | - |
| warpgroup | GH | 0.1.0.9001 | - |
| ncGTW | BC | 1.2.0 | - |
| Correction | | | |
| pmp | BC | 1.0.0 | - |
| StatTarget | BC | 1.20.0 | This version allows to set high value in the CV cutoff |
| MetNormalizer | GH | 1.3.02 | - |
| batchCorr | GL | 0.2.5 | - |
| BatchCorrMetabolomics | GH | 0.1.14 | - |
| notame | GH | 0.0.5 | - |
| openxlsx | CRAN | 4.1.5 | - |
| pbapply | CRAN | 1.4-3 | - |
| caret | CRAN | 6.0-86 | - |
| rpart | CRAN | 4.1-15 | - |
| ipred | CRAN | 0.9-9 | - |
| catboost | GH | 0.20 | - |
| xgboost | CRAN | 1.2.0.1 | - |
| dbnorm | GH | 0.2.2 | - |
| ProteoMM | BC | 1.6.0 | - |
| WaveICA | GH | 0.1.0 | - |
| NormalizeMets | CRAN | 0.25 | - |
| RUVSeq | BC | 1.22.0 | - |
| edgeR | BC | 3.12.1 | This version allows to load RUVSeq package |
| tibble | CRAN | 3.0.3 | - |
| fpc | CRAN | 2.2-7 | - |
| FactoMineR | CRAN | 2.3 | - |
| cluster | CRAN | 2.1.0 | - |
| proBatch | BC | 1.4.0 | - |
| gPCA | CRAN | 1.0 | - |
| pcpr2 | GH | 0.0.0.1 | - |
| MetabolomicsBasics | CRAN | 1.1 | - |

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| factoextra | CRAN | 1.0.7 | - |
| rafalib | CRAN | 1.0.0 | - |
| RSEIS | CRAN | 3.9-0 | - |
| ggsci | CRAN | 2.9 | - |
| Annotation | | | |
| CAMERA | BC | 1.44.0 | - |
| RamClustR | GH | 1.1.0 | - |
| 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 | Forked from b2slab/mWISE to plyush1993/mWISE and depends were manually changed to R (>= 4.0). |
| 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 | 1.3.0 | - |
| batchCorr | GL | 0.2.5 | - |
| Normalization | | | |
| affy | BC | 1.66.0 | - |
| clusterSim | CRAN | 0.49-1 | - |
| DiffCorr | CRAN | 0.4.1 | - |
| lmm2met | GH | 1.0 | - |
| MetabolomicsBasics | CRAN | 1.1 | - |
| lme4 | CRAN | 1.1-23 | - |
| lmerTest | CRAN | 3.1-2 | - |
| mgcv | CRAN | 1.8-32 | - |
| gamm4 | CRAN | 0.2-6 | - |
| gpboost | CRAN | 0.6.7 | - |
| NormalizeMets | CRAN | 0.25 | - |
| RColorBrewer | CRAN | 1.1-2 | - |
| limma | BC | 3.38.3 | - |
| Imputation | | | |
| MetProc | CRAN | 1.0.1 | - |
| impute | BC | 1.62.0 | - |
| mice | CRAN | 3.11.0 | - |
| missForest | CRAN | 1.4 | - |
| StatTools | GL | 0.0.915 | - |
| pcaMethods | BC | 1.80.0 | - |
| imputeLCMD | CRAN | 2.0 | - |
| imputeR | CRAN | 2.2 | - |
| vegan | CRAN | 2.5-6 | - |
| missMethods | CRAN | 0.2.0 | - |
| Grouping | | | |
| corr | CRAN | 0.4.3.9000 | - |

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| gplots | CRAN | 3.0.4 | - |
| tidyverse | CRAN | 1.3.0 | - |
| igraph | CRAN | 1.2.6 | - |
| ggraph | CRAN | 2.0.3 | - |
| robCompositions | CRAN | 2.3.0 | - |
| compositions | CRAN | 2.0-1 | - |
| gridExtra | CRAN | 2.3 | - |
| stringi | CRAN | 1.5.3 | - |
| notame | GH | 0.0.5 | - |
| pmd | CRAN | 0.1.9 | - |
| Statistics | | | |
| pcaMethods | BC | 1.80.0 | - |
| OutlierDetection | CRAN | 0.1.1 | Require spatstat package version 1.64-1 (CRAN) |
| ClassDiscovery | CRAN | 3.3.13 | - |
| caret | CRAN | 6.0-86 | 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 | 2.7-3 | For ML model in caret |
| kernlab | CRAN | 0.9-29 | For ML model in caret |
| randomForest | CRAN | 4.6-14 | For ML model in caret |
| ropls | BC | 1.20.0 | - |
| tdfdr | CRAN | 0.1 | - |
| MetabolomicsBasics | CRAN | 1.1 | - |
| lme4 | CRAN | 1.1-23 | - |
| lmerTest | CRAN | 3.1-2 | - |
| mgcv | CRAN | 1.8-32 | - |
| gamm4 | CRAN | 0.2-6 | - |
| drc | CRAN | 3.0-1 | - |
| limma | BC | 3.38.3 | - |
| NormalizeMets | CRAN | 0.25 | - |
| permimp | CRAN | 1.0-0 | - |
| party | CRAN | 1.3-5 | - |
| glmnet | CRAN | 4.0-2 | - |
| MASS | CRAN | 7.3-52 | - |
| pROC | CRAN | 1.16.2 | - |
| reshape2 | CRAN | 1.4.4 | - |
| leaps | CRAN | 3.1 | - |
| gWQS | CRAN | 3.0.3 | - |

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| vegan | CRAN | 2.5-6 | - |
| pairwiseAdonis | GH | 0.0.1 | - |
| multcomp | CRAN | 1.4-13 | - |
| MetStaT | CRAN | 1.0 | - |
| mixOmics | BC | 6.12.1 | - |
| DRomics | CRAN | 2.2-0 | - |
| TOXcms | GH | 1.0.3 | Require dr4pl and hashmap packages |
| timecourse | BC | 1.60.0 | - |
| timeOmics | BC | 1.0.1 | - |
| lmms | CRAN | 1.3.3 | - |
| tidyverse | CRAN | 1.3.0 | - |
| factoextra | CRAN | 1.0.7 | - |
| FactoMineR | CRAN | 2.3 | - |
| dendextend | CRAN | 1.13.4 | - |
| rafalib | CRAN | 1.0.0 | - |
| RSEIS | CRAN | 3.9-0 | - |
| ggsci | CRAN | 2.9 | - |
| pheatmap | CRAN | 1.0.12 | - |
| Rtsne | CRAN | 0.15 | - |
| NbClust | CRAN | 3.0 | - |
| clustertend | CRAN | 1.4 | - |
| mclust | CRAN | 5.4.6 | - |
| clValid | CRAN | 0.6-9 | - |
| pvclust | CRAN | 2.2-0 | - |
| fpc | CRAN | 2.2-7 | - |
| Hmisc | CRAN | 4.4-1 | - |
| corrplot | CRAN | 0.84 | - |
| psych | CRAN | 2.0.7 | - |
| pwr | CRAN | 1.3-0 | - |
| effectsize | CRAN | 0.3.2 | - |
| Directly used packages: | | | 121 |