

| <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        | -  |
| 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          | -  |

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| 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 ( <a href="https://github.com/yufree/xMSannotator">https://github.com/yufree/xMSannotator</a> ).   |
| mWISE              | GH   | 0.1.0   | -   |
| metid              | GH   | 1.2.13  | Databases from ( <a href="https://github.com/jaspershen/demoData/tree/master/inst/ms2_databada">https://github.com/jaspershen/demoData/tree/master/inst/ms2_databada</a> ) 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 <a href="https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11-02">https://github.com/jorainer/MetaboAnnotationTutorials/releases/tag/2021-11-02</a>                         |
| CompoundDb         | BC   | 0.99.8  | -   |
| Normalization      |      |         |   |
| affy               | BC   | 1.72.0  | -   |
| ABCstats           | 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   | -   |
| impute             | BC   | 1.68.0  | -   |
| mice               | CRAN | 3.14.0  | -   |
| missForest         | CRAN | 1.5     | -   |
| StatTools          | GL   | 0.0.915 | -   |
| pcaMethods         | BC   | 1.86.0  | -   |
| imputeLCMD         | CRAN | 2.1     | -   |
| tWLSA              | GH   | 1.0     | -   |

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| 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  | -  |
| gamm4              | CRAN | 0.2-6   | -  |
| drc                | CRAN | 3.0-1   | -  |
| limma              | BC   | 3.50.3  | -  |
| NormalizeMets      | CRAN | 0.25    | -  |

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| 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  | -   |

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|-------------------------|------|-------|-----|
| 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: |      |       | 144 |