openNCA Computation Engine Demonstration Installation and Test Cases

These instructions provide brief installation and testcase execution guidance.

There are two approaches presented:

Installation using the pre-built package

Open R or RStudio

openNCA Computation Engine v3.0 (commit c3d3f48) has been qualified with R-3.5.1. So, at the moment, consider R-3.5.1 as a minimum installation requirement. openNCA CE is being used in a Production Qualified Environment with R-4.0.3.

Set your default folder for installation in the R session

In the next step you will download a zip file from GitHub and extract to this folder. The default folder will then have a child "demo" folder containing the sources for installation and testcase files for demonstration use.

Download Testcase scripts, data, and installation files to a folder of your choice

https://github.com/tensfeldt/openNCA/raw/master/demo/demo.zip

Execute the installation script to install openNCA Computation Engine package library from source

Source or load and execute all of the lines for the ./demo/install/openNCA_install_package.R script. This script will install the openNCA library package from source.

If you do have the package **curl** installed, the following illustrates downloading demo.zip and unzipping to your Downloads folder using an R script:

```
home <- Sys.getenv("HOMEPATH")
setwd(file.path(home, "Downloads/demonstration"))
zipfile <- "demo.zip"
curl::curl_download("https://github.com/tensfeldt/openNCA/raw/master/demo/demo
unzip(zipfile, exdir=getwd())
list.files(recursive=TRUE)
source("./install/openNCA_install_package.R")
library(openNCA)
```

```
R version 3.5.1 Patched (2018-11-18 r75627) -- "Feather Spray"
Copyright (C) 2018 The R Foundation for Statistical Computing
Platform: x86_64-w64-mingw32/x64 (64-bit)

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'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> home <- Sys.getenv("HOMEPATH")
> setwd(file.path(home, "Downloads/demonstration"))
```

```
> zipfile <- "demo.zip"
> curl::curl_download("https://github.com/tensfeldt/openNCA/raw/master/de
> unzip(zipfile, exdir=getwd())
> list.files(recursive=TRUE)
 [1] "demo.zip"
 [2] "install/openNCA_build_package.R"
 [3] "install/openNCA_download_demo.R"
 [4] "install/openNCA_install_package.R"
 [5] "openNCA Computation Engine Demonstration Installation and Test Case
 [6] "README.html"
 [7] "README.md"
 [8] "release_files/openNCA_c3d3f48_3.0.0.tar.gz"
 [9] "tc2001_M1SD.R"
[10] "tc2002_M1SD.R"
[11] "tc2003_M1SS.R"
[12] "tc2004_M2SD.R"
[13] "tc2005_M2SS.R"
[14] "tc2006_M3SD.R"
[15] "tc2008_M4SD.R"
[16] "tc2009_M4SS.R"
[17] "testcases/DEMO1001_M1SD/DEMO1001-CEST.csv"
[18] "testcases/DEMO1001_M1SD/DEMO1001-DT.csv"
[19] "testcases/DEMO1001_M1SD/DEMO1001-KEL.csv"
[20] "testcases/DEMO1001_M1SD/DEMO1001-MCT.csv"
[21] "testcases/DEMO1001_M1SD/DEMO1001-PPRM.csv"
[22] "testcases/DEMO1002_M1SS/DEMO1002-CEST.csv"
[23] "testcases/DEMO1002_M1SS/DEMO1002-DT.csv"
[24] "testcases/DEMO1002_M1SS/DEMO1002-KEL.csv"
[25] "testcases/DEMO1002_M1SS/DEMO1002-MCT.csv"
[26] "testcases/DEMO1002_M1SS/DEMO1002-PPRM.csv"
[27] "testcases/DEMO1003_M2SD/DEMO1003-CEST.csv"
[28] "testcases/DEMO1003_M2SD/DEMO1003-DT.csv"
[29] "testcases/DEMO1003_M2SD/DEMO1003-KEL.csv"
[30] "testcases/DEMO1003_M2SD/DEMO1003-MCT.csv"
[31] "testcases/DEMO1003_M2SD/DEMO1003-PPRM.csv"
[32] "testcases/DEMO1004_M2SS/DEMO1004-DT.csv"
[33] "testcases/DEMO1004_M2SS/DEMO1004-KEL.csv"
[34] "testcases/DEMO1004_M2SS/DEMO1004-MCT.csv"
[35] "testcases/DEMO1004_M2SS/DEMO1004-REF.csv"
[36] "testcases/DEMO1005_M3SD/DEMO1005-DT.csv"
[37] "testcases/DEMO1005_M3SD/DEMO1005-KEL.csv"
[38] "testcases/DEMO1005_M3SD/DEMO1005-MCT.csv"
[39] "testcases/DEMO1005_M3SD/DEMO1005-REF.csv"
[40] "testcases/DEMO1007_M4SD/DEMO1007-DT.csv"
[41] "testcases/DEMO1007_M4SD/DEMO1007-KEL.csv"
[42] "testcases/DEMO1007_M4SD/DEMO1007-MCT.csv"
[43] "testcases/DEMO1007_M4SD/DEMO1007-REF.csv"
[44] "testcases/DEMO1008_M4SS/DEMO1008-DT.csv"
```

```
[45] "testcases/DEMO1008_M4SS/DEMO1008-KEL.csv"
[46] "testcases/DEMO1008_M4SS/DEMO1008-MCT.csv"
[47] "testcases/DEMO1008_M4SS/DEMO1008-REF.csv"
> source("./install/openNCA_install_package.R")
  converting help for package 'openNCA'
    ae                                    html
    aepct                                 html
    aet                                   html
    aetau                                 html
    aetpct                                html
    at                                    html
    auc_XbpctO                            html
    auc_XbpctP                            html
    auc_XpctO                             html
    auc_XpctP                             html
    auc_all                               html
    auc_dn                                html
    auc_inf_o                             html
    auc_inf_oc                            html
    auc_inf_p                             html
    auc_inf_pc                            html
    auc_last                              html
    auc_lastc                             html
    auc_lin                               html
    auc_lin_log                           html
    auc_lin_up_log_down                   html
    auc_log                               html
    auc_t                                 html
    auc_t1_t2                             html
    auc_tau                               html
    aumc_XpctO                            html
    aumc_XpctP                            html
    aumc_inf_o                            html
    aumc_inf_p                            html
    aumc_last                             html
    aumc_lin                              html
    aumc_lin_log                          html
    aumc_lin_up_log_down                  html
    aumc_log                              html
    aumc_tau                              html
    aurc_all                              html
    c0                                    html
    cav                                   html
    cendinf                               html
    cendinf_dn                            html
    cest                                  html
    clast                                 html
    clfo                                  html
```

clfow	html
clfp	html
clfpw	html
clftau	html
clftauw	html
clo	html
clow	html
clp	html
clpw	html
clr	html
clrt	html
clrtau	html
cltau	html
cltauw	html
cmax	html
cmax_dn	html
cmaxc	html
cmin	html
cmin_dn	html
create_dependency_list	html
create_dosing_intervals	html
ctrough	html
ctroughend	html
dependent_parameters	html
dof	html
dosec	html
est_c0	html
estimate_concentration	html
estimate_missing_concentration	html
estimate_told_concentration	html
get_told_concentration	html
interpolate_lin	html
interpolate_log	html
kel	html
kel_r	html
lasttime	html
makenumeric	html
maxrate	html
midptlast	html
model_display_parameters	html
model_parameters	html
model_spec	html
mr_auc_inf_o	html
mr_auc_inf_p	html
mr_auc_last	html
mr_auc_tau	html
mr_cmax	html
mrt_evif_o	html

mrt_evif_p	html
mrt_ivif_o	html
mrt_ivif_p	html
mrt_last	html
openncа_version	html
parameter_indices	html
parameter_regex	html
parameter_required	html
parameters_by_class	html
parse.reg	html
ptf	html
ptr	html
ptroughr	html
ptroughrend	html
rate	html
ratelast	html
rmempty	html
run_M1_SD_computation	html
run_M1_SS_computation	html
run_M2_SD_computation	html
run_M2_SS_computation	html
run_M3_SD_computation	html
run_M3_SS_computation	html
run_M4_SD_computation	html
run_M4_SS_computation	html
run_computation	html
specific_gravity_adjustment	html
tendinf	html
tlag	html
tlast	html
tmax	html
tmaxrate	html
tmin	html
unit_conversion	html
unitclass_parameters	html
update_mct_data	html
v0	html
valid_models	html
validate_timeconc_data	html
vol_sum	html
vsso	html
vssow	html
vssp	html
vsspw	html
vzfo	html
vzfow	html
vzfp	html
vzfpw	html

```
    vzftau                                  html
    vzftauw                                 html
    vzo                                     html
    vzow                                    html
    vzp                                     html
    vzpw                                    html
>
```

Installation and building package from source using devtools

Dependencies for installation and building from source

devtools: Tools to Make Developing R Packages Easier

curl: A Modern and Flexible Web Client for R

Open R or RStudio

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Create/Set up a folder for installation in the R session

In the next steps you will download files from GitHub and extract to the installation folder. Once complete, this folder will have a child "demo" folder containing the sources for installation and R and testcase dataset files for demonstration use.

Download Testcase scripts, data, and installation files to the install folder

https://github.com/tensfeldt/openNCA/raw/master/demo/demo.zip

Download the build package script from Github

Download from
https://github.com/tensfeldt/openNCA/blob/master/demo/install/openNCA_build_
and store in your installation folder

Execute the installation script to build the openNCA Computation Engine package library

Source or load and execute all of the lines for the ./demo/install/openNCA_build_package.R script. This script will build the openNCA library package from source.

The following illustrates downloading demo.zip, extracting all the files, and executing the openNCA_build_package.R script within in the installation **Downloads/demonstration** folder using an R script:

```
library(curl)
home <- Sys.getenv("HOMEPATH")
setwd(file.path(home, "Downloads/demonstration"))
curl_download("https://github.com/tensfeldt/openNCA/raw/master/demo/install/op
source("openNCA_download_demo.R")
unlink("openNCA_download_demo.R")
curl_download("https://github.com/tensfeldt/openNCA/raw/master/demo/install/op
source("openNCA_build_package.R")
unlink("openNCA_build_package.R")
library(openNCA)
```

```
R version 3.5.1 Patched (2018-11-18 r75627) -- "Feather Spray"
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Platform: x86_64-w64-mingw32/x64 (64-bit)

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```

```
R is a collaborative project with many contributors.
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'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> library(curl)
> home <- Sys.getenv("HOMEPATH")
> setwd(file.path(home, "Downloads/demonstration"))
> curl_download("https://github.com/tensfeldt/openNCA/raw/master/demo/ins
> source("openNCA_download_demo.R")
  converting help for package 'openNCA'
    ae                                  html
    aepct                               html
    aet                                 html
    aetau                               html
    aetpct                              html
    at                                  html
    auc_XbpctO                          html
    auc_XbpctP                          html
    auc_XpctO                           html

    auc_XpctP                           html
    auc_all                             html
    auc_dn                              html
    auc_inf_o                           html
    auc_inf_oc                          html
    auc_inf_p                           html
    auc_inf_pc                          html
    auc_last                            html
    auc_lastc                           html
    auc_lin                             html
    auc_lin_log                         html
    auc_lin_up_log_down                 html
    auc_log                             html
    auc_t                               html
    auc_t1_t2                           html
    auc_tau                             html
    aumc_XpctO                          html
    aumc_XpctP                          html
    aumc_inf_o                          html
    aumc_inf_p                          html
    aumc_last                           html
    aumc_lin                            html
    aumc_lin_log                        html
    aumc_lin_up_log_down                html
```

aumc_log	html
aumc_tau	html
aurc_all	html
c0	html
cav	html
cendinf	html
cendinf_dn	html
cest	html
clast	html
clfo	html
clfow	html
clfp	html
clfpw	html
clftau	html
clftauw	html
clo	html
clow	html
clp	html
clpw	html
clr	html
clrt	html
clrtau	html
cltau	html
cltauw	html
cmax	html
cmax_dn	html
cmaxc	html
cmin	html
cmin_dn	html
create_dependency_list	html
create_dosing_intervals	html
ctrough	html
ctroughend	html
dependent_parameters	html
dof	html
dosec	html
est_c0	html
estimate_concentration	html
estimate_missing_concentration	html
estimate_told_concentration	html
get_told_concentration	html
interpolate_lin	html
interpolate_log	html
kel	html
kel_r	html
lasttime	html
makenumeric	html
maxrate	html
[illegible]	[illegible]

mrgptlast	html
model_display_parameters	html
model_parameters	html
model_spec	html
mr_auc_inf_o	html
mr_auc_inf_p	html
mr_auc_last	html
mr_auc_tau	html
mr_cmax	html
mrt_evif_o	html
mrt_evif_p	html
mrt_ivif_o	html
mrt_ivif_p	html
mrt_last	html
openncа_version	html
parameter_indices	html
parameter_regex	html
parameter_required	html
parameters_by_class	html
parse.reg	html
ptf	html
ptr	html
ptroughr	html
ptroughrend	html
rate	html
ratelast	html
rmempty	html
run_M1_SD_computation	html
run_M1_SS_computation	html
run_M2_SD_computation	html
run_M2_SS_computation	html
run_M3_SD_computation	html
run_M3_SS_computation	html
run_M4_SD_computation	html
run_M4_SS_computation	html
run_computation	html
specific_gravity_adjustment	html
tendinf	html
tlag	html
tlast	html
tmax	html
tmaxrate	html
tmin	html
unit_conversion	html
unitclass_parameters	html
update_mct_data	html
v0	html
valid_models	html
[illegible]	html

```
    validate_timeconc_data                  html
    vol_sum                                 html
    vsso                                    html
    vssow                                   html
    vssp                                    html
    vsspw                                   html
    vzfo                                    html
    vzfow                                   html
    vzfp                                    html
    vzfpw                                   html
    vzftau                                  html
    vzftauw                                 html
    vzo                                     html
    vzow                                    html
    vzp                                     html
    vzpw                                    html
> unlink("openNCA_download_demo.R")
> curl_download("https://github.com/tensfeldt/openNCA/raw/master/demo/ins
> source("openNCA_build_package.R")
> unlink("openNCA_build_package.R")
> library(openNCA)
>
```

Execute Model 1 Single Dose Extravascular Example Testcase

Once installation is complete, test installation with a sample execution. Note that this example assumes that the tidyverse package is installed.

```
home <- Sys.getenv("HOMEPATH")
setwd(file.path(home, "Downloads/demonstration"))
source("tc2001_M1SD.R")
```