

VolCalc_download

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```
# Proj.path is set in the beginning of the project (chunk 1)

# Set working directory (where files will be loaded from and saved to) (I change the file path as per e
proj.path.1 <- setwd("C:/Users/padakiv/Documents/PhD/Chapter 2 data/Dielrun_PTRViewer"); getwd()

## [1] "C:/Users/padakiv/Documents/PhD/Chapter 2 data/Dielrun_PTRViewer"

print(getwd())

## [1] "C:/Users/padakiv/Documents/PhD/Chapter 2 data/Dielrun_PTRViewer"

# Saves path where data files are stored
data.path <- paste0(proj.path.1, "/PTR_viewer_combined_data")
print (data.path)

## [1] "C:/Users/padakiv/Documents/PhD/Chapter 2 data/Dielrun_PTRViewer/PTR_viewer_combined_data"

# Saves path where output files will be saved
output.path.1 <- paste0(proj.path.1, "/output")
print (output.path.1)

## [1] "C:/Users/padakiv/Documents/PhD/Chapter 2 data/Dielrun_PTRViewer/output"

# Set seed
user.seed <- 999 # seed for replication, number is arbitrary
set.seed(user.seed)

out_path <- output.path.1

#> # A tibble: 2 × 5
#>   mol_path          formula name   rvi category
#>   <chr>            <chr>    <chr> <dbl> <fct>
#> 1 /var/folders/wr/by_lst2d2fngf67mknmgf4340000gn/T... C6H7Cl... beta... 6.98 high
#> 2 /var/folders/wr/by_lst2d2fngf67mknmgf4340000gn/T... C4H6O4 Succ... 2.57 high

#ran all the R code associated to create functions necessary for the below chunk
#R/calc_vol.R
#R/get_fx_groups.R
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#R/get_mol_kegg.R
#R/mol_example.R
#R/release_bullets.R
#R/simpol1.R
#R/utis.R
#R/volcalc-package.R

# download a .mol file from KEGG
#files <- get_mol_kegg(c("C16181", "C00042"), dir = out_path)
#calc_vol(files$mol_path)
```