**Description for the APP IDHprediction**

This is an easy-to-use intuitive R-shiny app that facilitates the prediction of the IDH mutation status. Please note that our approach achieved on independent test data an average accuracy of 76.1%, a sensitivity of 82.6%, and a specificity of 72.7%. Please keep this in mind when interpreting obtained results. Further details can be found in “Bumes E., Fellner C., Fellner F.A., Fleischanderl K., Häckl M., Lenz S., Linker R., Mirus T., Oefner P.J., Paar C., Proescholdt M., Riemenschneider M.J., Rosengarth K., Weis S., Wendl C., Wimmer S., Hau P., Gronwald W., Hutterer M. Validation Study for non-invasive Prediction of IDH Mutation Status in Patients with Glioma using In Vivo 1H-Magnetic Resonance Spectroscopy and Machine Learning. Cancers, 2022, in revison.

Note the application is for research purposes only.

## Installation

1. First you need to install R (free).

For windows see: <https://cran.r-project.org/bin/windows/base/>

For Linux see: https://cran.r-project.org/bin/linux/ or use your distribution’s package manager

For MacOS see: https://cran.r-project.org/bin/macosx/

It is not required but the additional installation of R-Studio helps to work with R

See: <https://www.rstudio.com/products/rstudio/>

We recommend the free Desktop version

1. The IDHpredicion.zip file for the IDHprediction package can be saved locally in the any folder. We recommend the Download or Document folder. For windows this could be for example the following path: “[C:/Users/](../../C:/Users/)<Username>/Downloads/”, for Linux “/home/<username>/Downloads/”. Unzip the file here (you should see a folder IDH prediction). Now start R and start the installation within R with: install.packages("C:/Users/<Username>/Downloads/IDHprediction", method = "source", repos = NULL). If you encounter any problems, you might want to use devtools for installation:

install.packages(“devtools”)

devtools::install("C:/Users/Username/Downloads").

1. Afterwards the IDHprediction package can be loaded with library(IDHprediction).
2. To start the App IDHprediction::runWebApp()

Note, for the next start of the app. You only have to start R and execute points 3 and 4.

## File format of MRS spectrum used for prediction

The app was tested on simple 1D MRS spectra acquired with a standard 1D PRESS pulse sequence. Please, see the original publication for details.

The input file must be a .csv file containing at least two rows. The first row is the header, containing the indices of the data points, the following rows are the actual measurements (one spectrum per row). The first column must contain the sample name. Values must be separated by ";", decimal points are represented by dots.

\*Example:\*

"Sample";"1", "2", "3",...

"S1";0;100;95.5;...

Please note that in your .csv file the points corresponding to the lowest ppm values should be on the left and the points corresponding to the highest ppm values should be on the right. This is the default mode, when these files are generated by jMRUI. Please check carefully.

Two example input files are provided in the “Example” subfolder of the IDHprediction folder

You can easily obtain such a .csv file by processing your raw spectra data for example with the free program jMRUI <http://www.jmrui.eu/> (free for noncomercial users). In jMRUI choose “File->save\_as->Mrui->Files of type->Text format .txt

Note, your .csv file may contain data from one or several spectra.

## Running the App

First, enter bandwidth and magnetic field strength of your MRS measurements and select a .csv file to classify by clicking on `browse`.