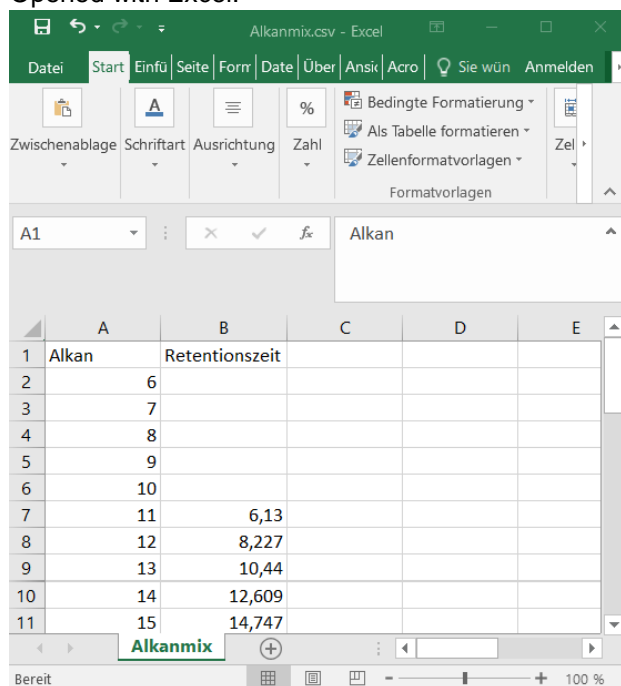## Step-by-step guide

Here, the example file Testfile_GC-MS_raw-data.CSV provided is used to explain how to use the app.

1) Download the template in which you fill in the retention times of the alkanes.
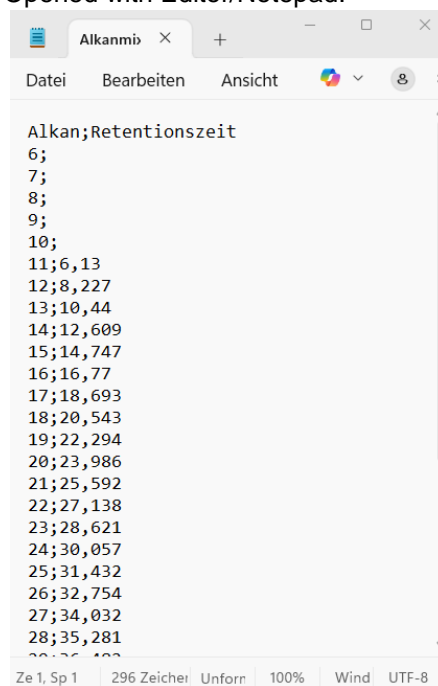
Opened with Excel:

Opened with Editor/Notepad:

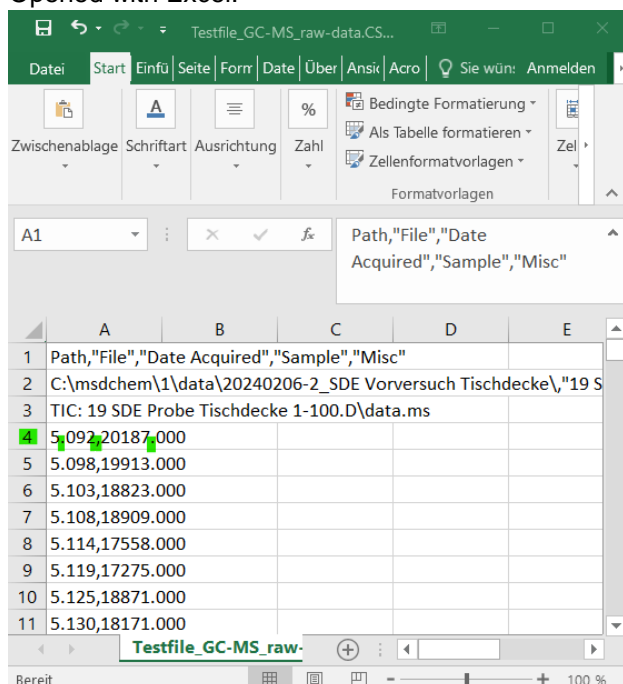Column 'Alkan' contains the number of C-atoms (do not change the numbers).
Column 'Retentionszeit' contains the retention time of the alkane with comma as numeric separator.

The retention times have already been entered for the example shown here.

1

2) Fill in the drop-down fields. Note the conditions in your sample measurement raw data file.
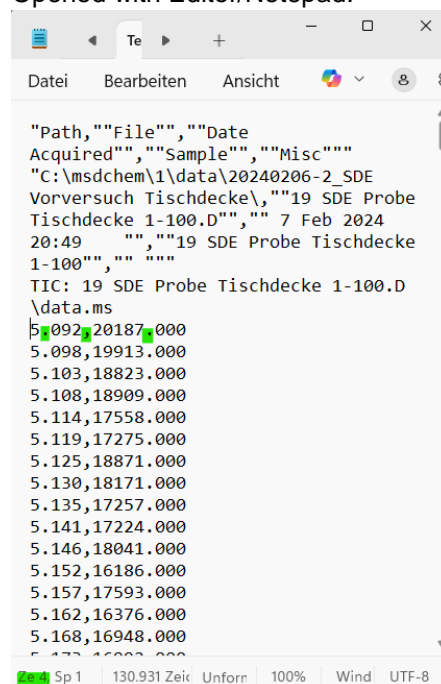
In this example, the file Testfile_GC-MS_raw-data.CSV is observed.

Opened with Excel:

Opened with Editor/Notepad:

In this example, fill in the fields as follows:

2) Position of the column with time values in your raw data file:
(The first column on the left is number 1, the second is number 2, and so on.)

1

3) Position of the column with intensity values in your raw data file:
(The first column on the left is number 1, the second is number 2, and so on.)

2

4) Number of the first row with values for time and intensity:

4

5) Decimal separator in your raw data file:

Dot to separate the decimal places (e.g. 12.34567)

6) Separator between the columns in your raw data file:

Comma

7) Thousands separator in your raw data file:

No mark for the separation of the thousands (e.g. 1234567)

3) Upload the completed alkanmix file to the field provided. Then upload your raw file provided.

8) Please upload the 'Alkanmix.csv' file required.

Drag or click to select a file.

9) Please upload the raw data file (.csv or .txt) required.

Drag or click to select a file.

4) A preview image will now appear. You can download the converted file in .csv or .xlsx formate using the buttons provided.
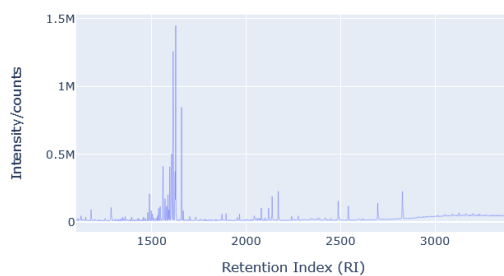
8) Please upload the 'Alkanmix.csv' file required.

File uploaded successfully.

9) Please upload the raw data file (.csv or .txt) required.

File uploaded successfully.

GC-Chromatogram

This is an interactive preview image. Use the left mouse button to select an area and enlarge it by drawing a window. Double-click on the image with the left mouse button to zoom out again.

Download CSV file

Download Excel file