

Step-by-step guide

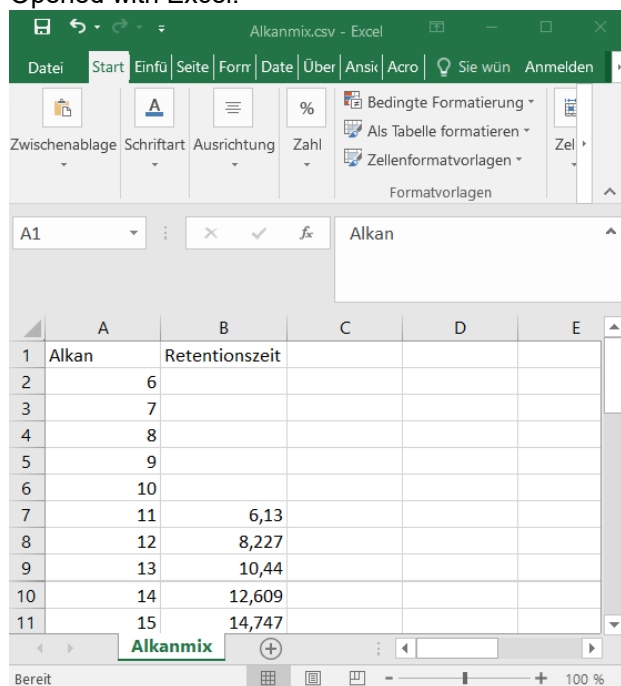
Here, the example file Testfile_GC-MS_raw-data.CSV provided is used to explain how to use the app in mode B: RI for an entire data file.

1) Download the template in which you fill in the retention times of the alkanes.

1) Download the template for the alkane mix:

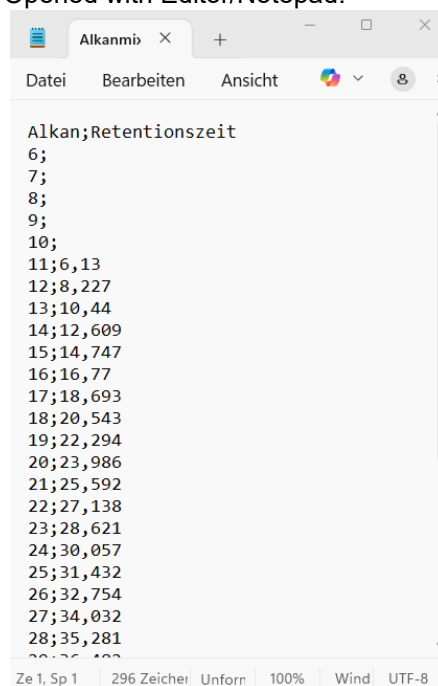
[Download alkane mix template](#)

Opened with Excel:



Alkan	Retentionszeit
6	
7	
8	
9	
10	
11	6,13
12	8,227
13	10,44
14	12,609
15	14,747

Opened with Editor/Notepad:



```
Alkan;Retentionszeit
6;
7;
8;
9;
10;
11;6,13
12;8,227
13;10,44
14;12,609
15;14,747
16;16,77
17;18,693
18;20,543
19;22,294
20;23,986
21;25,592
22;27,138
23;28,621
24;30,057
25;31,432
26;32,754
27;34,032
28;35,281
```

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.

2) Upload the completed alkanmix file to the field provided.

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

Drag or click to select a file.

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

File uploaded successfully.

3) Click on the mode B button.

3) Please select a mode by clicking on the respective button:

A) RI for single Rt data point

B) RI for entire data file

4) 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:

	A	B	C	D	E
1	Path,\"File\", \"Date Acquired\", \"Sample\", \"Misc\"				
2	C:\msdchem\1\data\20240206-2_SDE Vorversuch Tischdecke\", \"19 SDE Probe Tischdecke 1-100.D\"				
3	TIC: 19 SDE Probe Tischdecke 1-100.D\data.ms				
4	5.092,20187.000				
5	5.098,19913.000				
6	5.103,18823.000				
7	5.108,18909.000				
8	5.114,17558.000				
9	5.119,17275.000				
10	5.125,18871.000				
11	5.130,18171.000				

Opened with Editor/Notepad:

```
"Path","File","Date Acquired","Sample","Misc"
"C:\msdchem\1\data\20240206-2_SDE Vorversuch Tischdecke\", \"19 SDE Probe Tischdecke 1-100.D\"; \" 7 Feb 2024 20:49 \"; \"19 SDE Probe Tischdecke 1-100\"; \" \"
TIC: 19 SDE Probe Tischdecke 1-100.D\data.ms
5.092,20187.000
5.098,19913.000
5.103,18823.000
5.108,18909.000
5.114,17558.000
5.119,17275.000
5.125,18871.000
5.130,18171.000
5.135,17257.000
5.141,17224.000
5.146,18041.000
5.152,16186.000
5.157,17593.000
5.162,16376.000
5.168,16948.000
```

In this example, fill in the fields as follows:

4) 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

5) 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

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

4

7) Decimal separator in your raw data file:

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

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

Comma

9) Thousands separator in your raw data file:

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

5) Upload your raw file provided.

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

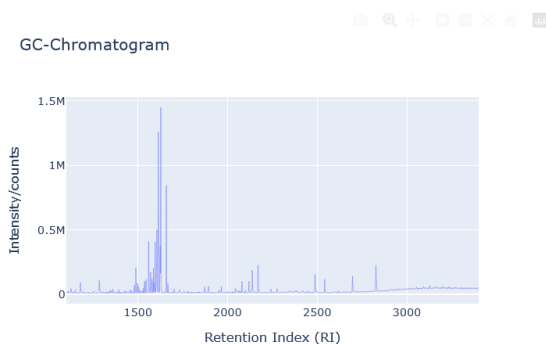
Drag or click to select a file.

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

File uploaded successfully.

6) A preview image will now appear. You can download the converted file in .csv or .xlsx format using the buttons provided.

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