

Step-by-step guide

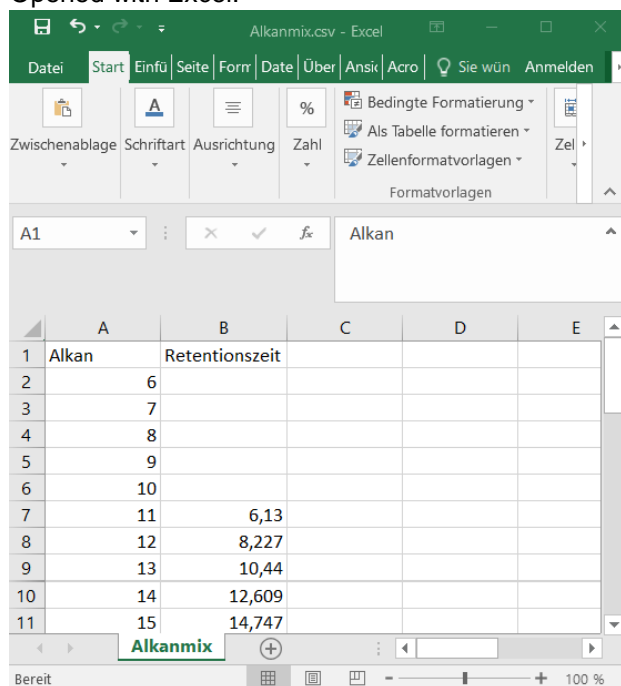
Here, the example file Testfile_GC-MS_raw-data.CSV provided is used to explain how to use the app.

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

1) Download the template for the alkane mix:

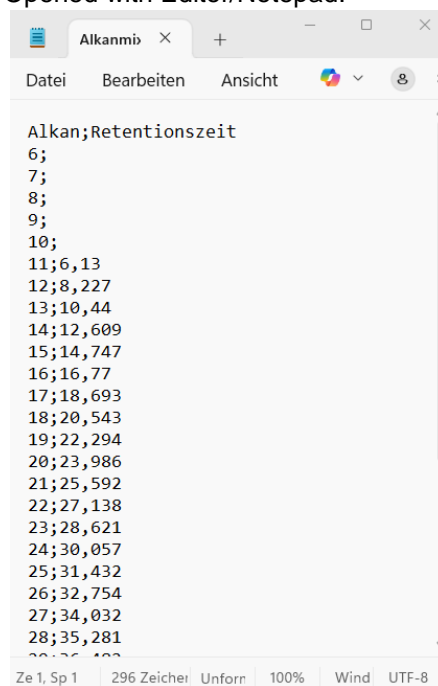
[Download alkane mix template](#)

Opened with Excel:



	A	B	C	D	E
1	Alkan	Retentionszeit			
2	6				
3	7				
4	8				
5	9				
6	10				
7	11	6,13			
8	12	8,227			
9	13	10,44			
10	14	12,609			
11	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
29;36,100
```

Column 'Alkan' contains the number of C-atoms (do not change the numbers).

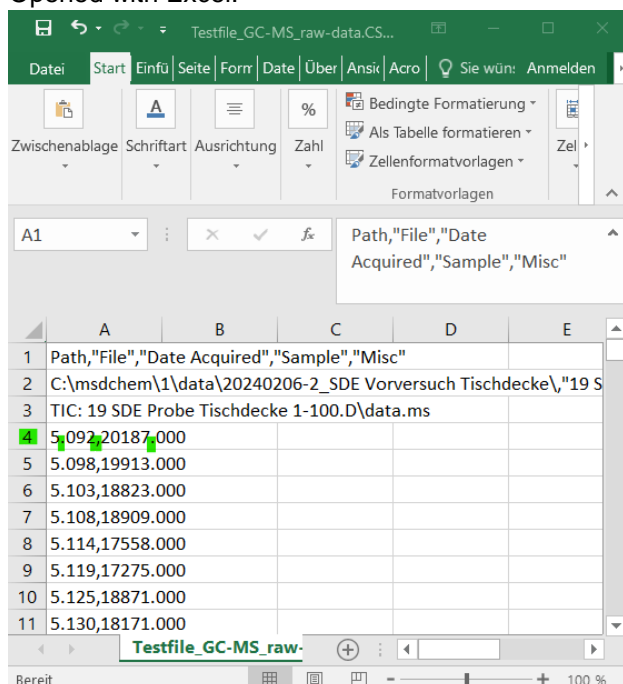
Column 'Retentionszeit' contains the retention time of the alkane with comma as numeric separator.

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

2) Fill in the drop-down fields. Note the conditions in your sample measurement raw data file.

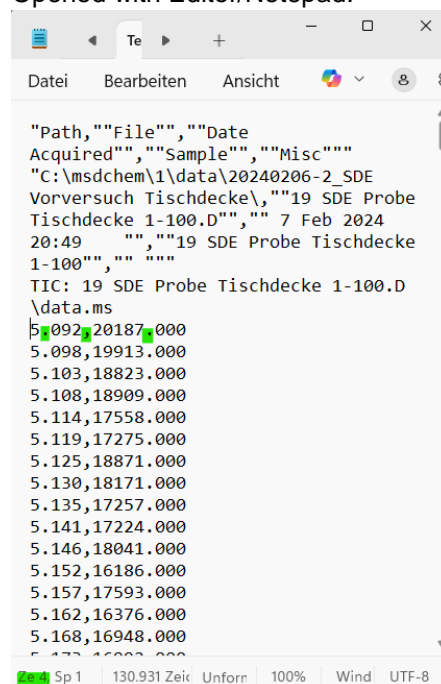
In this example, the file Testfile_GC-MS_raw-data.CSV is observed.

Opened with Excel:



	Path	File	Date Acquired	Sample	Misc
1	C:\msdchem\1\data\20240206-2_SDE	Vorversuch Tischdecke	19 SDE Probe	Tischdecke 1-100.D	data.ms
2	5.092	20187	0.000		
3	5.098	19913	0.000		
4	5.103	18823	0.000		
5	5.108	18909	0.000		
6	5.114	17558	0.000		
7	5.119	17275	0.000		
8	5.125	18871	0.000		
9	5.130	18171	0.000		
10	5.135	17257	0.000		
11	5.141	17224	0.000		
12	5.146	18041	0.000		
13	5.152	16186	0.000		
14	5.157	17593	0.000		
15	5.162	16376	0.000		
16	5.168	16948	0.000		

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","",""
TIC: 19 SDE Probe Tischdecke 1-100.D\data.ms
5.092,20187,0.000
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:

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.

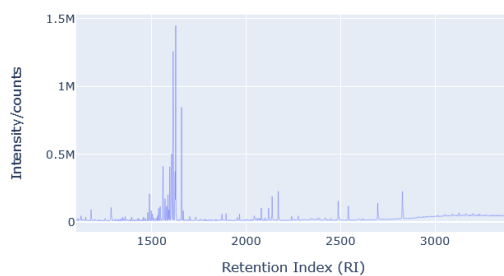
8) Please upload the 'Alkanmix.csv' file required.

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