*********************************ANIR. Version 1.0*********************************

THIS SOFTWARE IMPLEMENTS 2 FITTING ROUTINES TO ANALYSE SPECTRA COLLECTED BY FTIR.

1: IMPROVED ALGORITHM BASED ON A CLASSIC FITTING ROUTINE. THE BASELINE IS MODELED USING OVERLAPPING SMALL WINDOWS COVERING THE WHOLE ANALYSIS REGION (Developed at CEAM)
2: CLASSIC FITTING ROUTINE WHERE THE BASELINE IS MODELED BY A POLYNOMIAL FUNCTION THAT COVERS THE WHOLE ANALYSIS REGION

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Follow the steps in an orderly manner.

1- SELECT SPECTRA
- Select the directory where the spectra are stored. Spectra must have been previously saved in *.CSV format, i.e. first column containing wavelength and second column containing absorbance (or a.u.). No header is allowed.

2- REFERENCES
- Double click on the box list to display the folders. Surf on these to select the folder where the references in *.CSV format are stored. Double click on the references to use and they will be plotted on the central graph. The menu above allows to make a zoom-in and zoom-out on the plots by using the lens tools.
  NOTE: when the resolution of references and sample spectra is different, the resolution of the references will be converted into that of the samples by interpolation using the spline method.

3- ANALYSIS REGION
- Introduce the analysis region.

4- RUN
- Select the Polynomial degree to model the baseline.
- Select the Windows size to model the baseline if using the ANIR POLWIN method.
- Click on ANIR POLWIN or on ANIR CLASS according to your choice.

  The run will start and 2 plots will be shown: the upper one with the spectrum to analyze (blue), modeled spectrum (green), part of the modeled spectrum due to the reference compound contribution (red) and part of the modeled spectrum due to the broadband (magenta).
  NOTE: With ANIR POLWIN, default values are Polynomial degree = 3 and Window size=100 if using 1cm-1 resolution. When ANIR POLWIN is selected, a polynomial of 2 is recommended. When ANIR CLASS is selected, the polynomial can be changed to 4 or higher. The whole performance of the analysis with the selected parameters will depend on the analysis region and on the shape of the spectra to analyse.
  As a guide for the user, during the analysis, the modeled baseline is plotted, and the user can check that such a model doesn't mimic the shape of the absorption that corresponds to the spectral references (also shown on the same plot for comparison). If they show the same profile, the concentration of the compounds might not be realistic. In that case, the Polynomial degree should be reduced and/or the Window size increased so that the absorptions observed are attributed to the references and not included as part of the baseline.

  For other resolutions, the Polynomial should increase and as a guide, the Windows size can change inversely (e.g. Windows size=200 for resolution=0.5cm-1).

5- PLOT OPTIONS
- Select Color and Line shape to plot the results
- Click on Plot data
  NOTE: Additional runs can be done using other parameters (e.g. analysis region or different references). To do so, instead of clicking on the RESET button, click on Reset references to select the new ones and follow steps 3 and 4, Analysis region and RUN, respectively.
  Results can be overlapped to the plots from a previous run using the button Re-plot. If so, a different Color or Line shape can be selected to distinguish the results of the different runs.

6- SAVE RESULTS
- Introduce a name to save results. They will be saved in TXT and EXCEL format.

7- SAVE PLOTS
- Click on the button to save plots in JPG and FIG (Matlab) formats.

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D I S C L A I M E R

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The UV is acknowledged for supporting the development of the GUI.
This program is distributed for free upon request through the EUROCHAMP-2020 webpage (https://www.eurochamp.org).

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