

Deliverable D3.5: GUI for the use with FTIR analysis software

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Version	v.1
Comments	<p>Considering the great utility of such tool, the partners in charge of its development and release, together with the Coordinator, have agreed to change the confidentiality level of this deliverable from “Confidential” into “Public”. Such change was supported by the EC Project Officer.</p>

Fourier Transform Infra-Red (FTIR) spectroscopy is a widespread technology among the EUROCHAMP-2020 consortium. FTIR data analysis was cumbersome and often user-dependent. Certainly, for decade the wider used method consists in a manual subtraction. CEAM developed a standardized analysis software that was provided after a careful evaluation through EUROCHAMP-2. The established algorithm to analyse IR spectra was optimized to retrieve concentration profiles of compounds in complex gas mixtures, and has now been implemented using a graphical user interface (GUI). This GUI is a user-friendly tool that facilitates the use of the analysis software by the partners, allowing a traceability of the analysis. It allows a classic automatic analysis and also an improved method for the analysis of samples in the presence of unknown interfering compounds, a significant issue in IR analysis.

Some features of the software are:

- Implements a classic minimum square fitting (ANIR CLASS) and an enhanced version (ANIR POLWIN) for using in the presence of interfering unknown compounds
- Allows to locally filter unwanted overlapping broadband curves (aerosols, optical misalignment or broad absorptions of unknown compounds)
- No previous training of the algorithm using concentration varying spectra needed (PCA, neural network, etc)

The GUI was internally distributed among the partners using FTIR to be tested on 5th October 2018. From the feedbacks received, suggestions have been incorporated and software bugs found have been fixed in the new version of the GUI. This version has been uploaded in the EUROCHAMP-2020 Data Center, to make it available for free for the scientific community, by clicking on this link: <https://data.eurochamp.org/anasoft/>

Next, the main view of the GUI, where several parts have been included:

- Selection of the folder containing the spectra to analyse
- Selection of the pure compound spectra used as references
- Analysis spectral region
- Zone where the selected references are plotted
- Buttons to plot and save results
- Help button

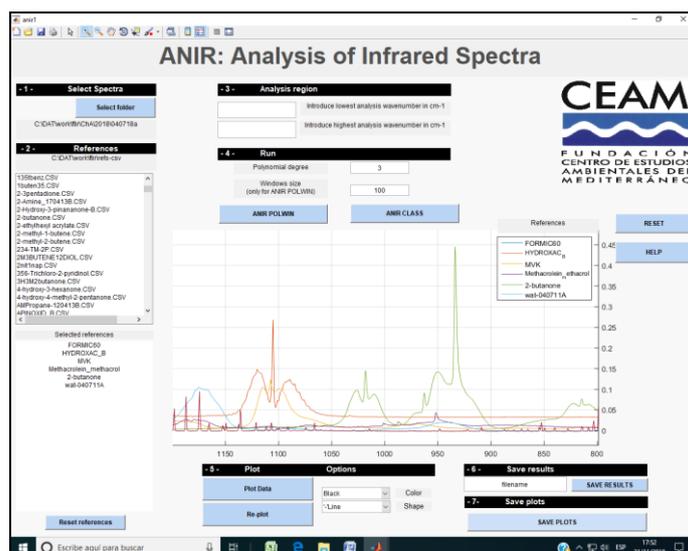


Fig. 1: Main screen of ANIR

Data and references can have different resolutions, although they will be given in CSV format, being first column for the wavelength and second column for the absorption.

The GUI shows the analysis process overlapping the spectra to be analyzed and the modelled spectra. The residual (subtraction of those ones) is also shown as a quality control to visually detect any interfering unknown product not included in the analysis.

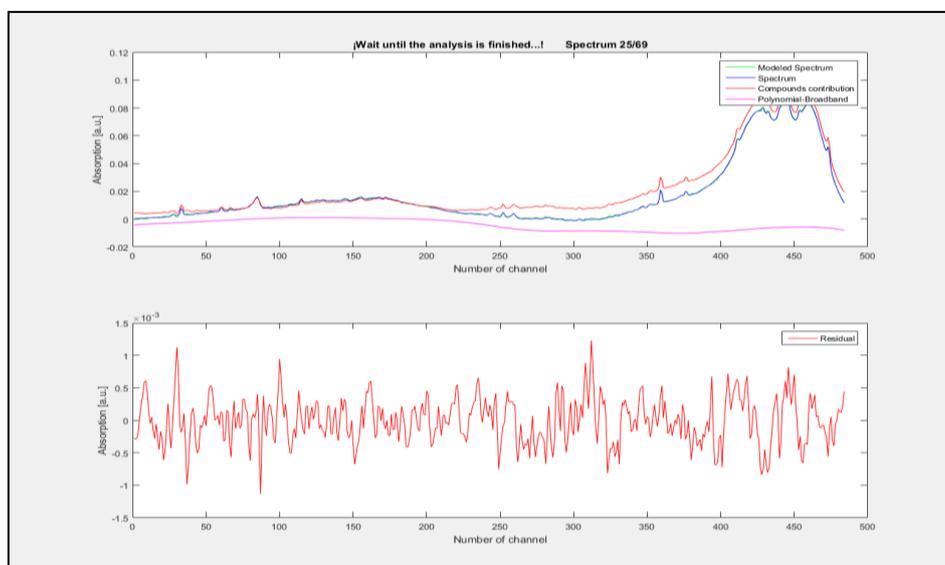


Fig. 2: Spectrum analysed (upper) and residual (down)

The evolution profile of parent compounds and reaction products, as well as the RMS of the residuals are shown in the next figure:

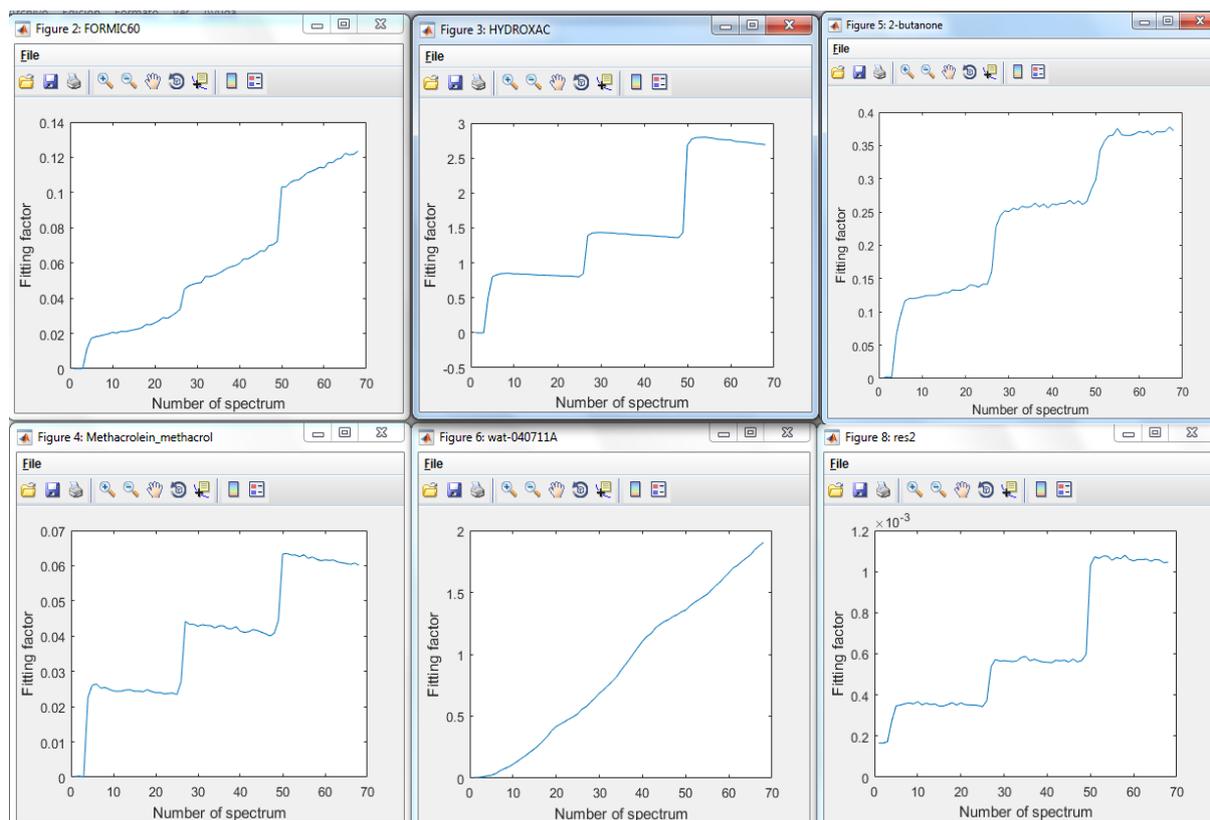


Fig. 3: Plot of data results

Results can be saved in a txt file where the header includes the spectral analysis region used for a better traceability. Data are organized in columns corresponding to the factors calculated for each compound references used. The residual is also evaluated and three additional columns are included:

- Squared 2-norm of the residual: $\text{norm}(\text{residual})^2$.
- $\text{Norm}(\text{residual}-\text{mean}(\text{residual}))/\sqrt{N}$
- $\text{Norm}(\text{residual2}-\text{mean}(\text{residual2}))/\sqrt{N}$, where residual2 is an smoothed residual

The GUI, distributable as exe file, has been released for versions in 32 and 64 bits and, although based in Matlab, it does not require the installation of this program.

The use of ANIR, as a user friendly interface to automatically analyse IR spectra will help in the better determination of the chemical reactions studied given that:

- Reduce the required intervention of the analyst
- Provide more reliable data
- Reduce interferences, i.e. decrease of the residual noise improving the data quality

- User-friendly graphic interface
- Provide a temporal profile with traceability on the analysis setup parameters

The evaluation of the GUI by non-experienced users selected among the consortium have demonstrated that its use was easily and quickly acquired. It has shown that it has led both to a much greater productivity in the data analysis as well as a gain in the quality of the second level data produced. It is expected that its dissemination will contribute to the widespread of FTIR analysis as well as a greater transparency in the protocols used for their interpretation. Furthermore, it provides a renewed interest for the data of FTIR spectra that is already open through the LAR pillar of the EUROCHAMP Data Center.