
DESCRIPTION

HPLC-MS (high performance liquid chromatography - mass spectrometry) data usually is analysed by using commercial data analysis software. However, while using such software the person is tied to his own working place or is forced to take illegal action to make more convenient working conditions. Additionally, using Microsoft Excel or other data visualization software is not helping because the analyzed files includes high quantities of data, or the software has limitations for graph design and generated image quality. Because of that created new GUI (graphical user interface) would partly solve this problem.

ChroMS is a free graphical user interface applied for HPLC and MS data analysis using files generated by LabSolutions data analysis software. ChroMS GUI enables possibility to analyze and visualize 3D HPLC and 2D MS data files and save the created graphs while working in any place and at any time (with possible graph design customization features in the future).

USAGE NOTES

Introduction to ChroMS GUI:

x Execution of ChroMS GUI:

---The provided code should not be modified - there are no user inputs before running the code.

---Execute the program by running the code inside Main_script.ipynb.

x Design / Selecting different tabs:

---The GUI has 3 different tabs inside - Blank Page, HPLC and MS

- *Possibility to switch between all of the tabs without any data loss.

- *Every time when HPLC or MS tab is chosen, listbox widget (with files inside) will take the focus.

- If there were any selections in listbox, they will be not changed.

- If there were no selections, the first file will be selected (but not activated).

- If there were no files, there will not be any selections.

x Tabs for HPLC-MS result analysis and their contents:

---HPLC and MS tabs consists of:

- *File Folder Manager (ffm)

- Combobox for folder search

- Button for folder browsing

- Listbox for file browsing

- Checkbuttons for file filtering by extension

- Entry for file filtering by file names or specific pattern

- *Output Plot Manager (opm)

- Radiobuttons for selecting which subplots to show

- Text output which shows additional information (errors and etc.)

- Diagram in which the processed data from the files will be plotted.

- *P.S. There are 2 ffms in the MS tab. They can be chosen by radiobuttons below file browsing button. Each provides different ffm which can be used to plot data from 2 different files. By default, MS1 files are supposed to be positive ionization files, while MS2 should be for negative ionization. However, you are completely free to plot any type of MS files in any subplot you like.

File Folder Manager Functionality:

x Folder search:

---There are several different folder search methods:

- *Folder search through filedialog

- Use Browse button

- The filedialog default directory for the search is 'data'

- *Folder search manually

- Write inside Folder search entry and press Enter

- *Folder search by selecting item present in combobox

- *Automatic folder search

- Every time by running ChroMS GUI with browsing history present

---Combobox which contains folder paths, can have up to 10 different items.

Every time using previously described methods a folder will be selected.

During the selection, listbox containing files will be updated and the focus will be passed on the listbox.

- *Exceptions:

- Providing path of non-existing folder. After pressing Enter the focus will remain on the folder browsing entry.

- Text output will be provided with an error.

---There are possible 3 different files containing folder browsing history for different ffms.

- *Types:

- chrom_history.txt

- ms1_history.txt

- ms2_history.txt

- *Each of these files can be modified.

- *Non-existing folder paths inside the files are not loaded to the combobox.

- *Paths which were not found will be cleared after the first combobox changes.

- *The latest used path will be at the top of the path list.

- If there will be too many paths, only the last 10 will be used to update combobox.

---Browsing history '.txt' files will be updated every time after changes in combobox widget item list.

- *Includes:

- Every operation which changes order of combobox items.

- #Even if there were no new paths added.

- Every operation which adds new paths.

- *Does not include:

- Loading folder paths during startup.

- Browsing for non-existing folder.

---Deleting file browsing history.

- *By searching for new folders which will replace the oldest one.

- Manually or automatically (with Browse button).

- Manually by deleting history text files.

- #All browsing history will be removed. At the next GUI startup there will be clear combobox.

x File browsing:

---There are several functions to navigate between files:

- *Using UP and DOWN arrows. Navigates up or down and executes the files immediately.

*Using ENTER button. Executes currently selected file.

*Using LEFT-CLICK of mouse. Executes file below the cursor.

*Using LEFT-CLICK of mouse WITHOUT RELEASING. Goes through the files currently present below the cursor and executes them.

*Using LEFT and RIGHT arrows. Navigates through files without executing them. Useful for fast navigation. For execution use ENTER button.

#Disadvantage - while using UP and DOWN arrows, the slider position will not be changed.

---There are sliders for listbox. You can have as many files as you like.

However, the length of file names should be limited to maintain optimal functionality. With the file extension the file name should not be longer than 68 characters. Otherwise, UP and DOWN arrows function will be corrupted by horizontal slider.

---During the file execution there will be either success message or warning provided in the text output. Also, the diagrams are plotted or not.

x File filtering:

---Filtering files by file extensions (checkboxbuttons):

*Default option will be set with predefined file extensions to better navigate between different types of files. Different default checkbox values for different ffms:

-HPLC file chromatogram_file_name_chrom.txt (_chrom.txt)

-MS1 file positive_ionization_file_name_ms_+.txt(_ms_+.txt)

-MS2 file negative_ionization_file_name_ms_-.txt (_ms_-.txt)

*You can show all the accessible files in the folder by selecting all checkboxbuttons or by deselecting the first checkboxbutton (in none of the others

are selected)

- *Combined use with file filter entry.

- *Every time by checking checkbox, the listbox contents will be updated.

Also, the focus will be set on the listbox widget.

---Filtering files by file name (entry):

- *Default option - empty string ("")

- *Possible filtering by file name. You should provide specific part of the file which is present in the current directory.

- The files can be filtered by writing their extensions inside.

- You can filter file names by specific fragments of text and connecting them with "*" symbol.

#Example: By writing "test*measurement*2024_*_10" the corresponding name would be found - "test_A_measurement_100_2024_10_10".

#Writing "***" (or n times "**") instead of "*" will not change the filtering result. "*" can also present empty string.

#By using "*" the separated fragments will be searched in files for filtering in ordered manner: "c" will be searched after "b" which comes after "a" in the string "a*b*c".

- *Filtering by file name is executed in real-time by writing inside the entry.

- *Combined use with checkboxes of file extension filtering.

- *You can use ENTER button to set the focus on the listbox object.

x Additional functionality in MS ffms:

---Radiobuttons for MS file selection:

- *By pressing them, ffm for specific MS file is selected

- *Because of that you can have 2 comboboxes, 2 listboxes, and 2 sets of file

filtering features.

*The latter structures are independent but works almost the same.

-Exceptions: disabled radiobutton for subplot selection and the subplot which is used for drawing.

*During the startup of ChroMS ffm for MS1 file is shown and ffm for MS2 file is hidden

*While hiding MS1 or MS2 ffm, one of radiobuttons for subplot selection is also hidden (Subplot1 or Subplot2 respectively).

-This behaviour changed by selecting other ffm.

*If subplot selection radiobutton is set to Subplot1 or Subplot2, activating different ffm will change active subplot selection radiobutton and will redraw the graph.

-If Both subplots option is selected then there will not be such changes.

*Changing ffms also sets the focus on the listbox widget.

---There are several different folder search methods:

*Folder search through filedialog

-Use Browse button

Output Plot Manager Functionality:

x Radiobuttons for subplot selection:

---Possibility of selecting specific subplots to draw:

*Both subplots

*Subplot1 (HPLC: Heatmap, MS : MS1)

*Subplot2 (HPLC : Chromatogram, MS : MS2)

---By selecting specific radiobutton the diagram will be redrawn by provided option automatically.

*For one HPLC and one MS file both graphs will be drawn if Both subplots option is selected.

*However for HPLC files there are 2 datasets to visualize while in MS files there is only one - so only one subplot will be updated with new data. Another will be unchanged.

*You can even plot the diagram which has initial state alone.

*Using these radiobuttons will set focus on the listbox object.

---The radiobuttons are affected by MS file selecting radiobuttons as described previously in "Additional functionality in MS files".

x Text output for additional information / errors:

---Provides information about:

*Initial greeting

*Folder search (success).

*File execution (success).

*Errors during folder search or file execution.

#Disadvantage - no output during diagram redraw while changing MS files or selecting different subplot selection option.

---There are 3 different types of output:

*Greeting message is inserted inside two lines of "#" symbols

*Success message is inserted inside two lines of "+" symbols

*Warning message is inserted inside two lines of "?" symbols

---The message can contain information about:

*Consistent output:

-2 lines of "#" or "+" or "?" symbols

- Current time (in YYYY/MM/DD hh:mm:ss format)

- *Other outputs are more dynamic:

- Folder path (if folder browsing was executed)

- File path (if file was executed)

- Calculated time for data reading and drawing (3 digits after decimal) (if file was executed successfully through selecting option in listbox)

- Was the event successful or not

- *Sometimes the output can contain only message about error (for example - selecting in empty listbox).

---Every time when new lines of output are added to the end of the text, the scrollbar of text output widget is slided to the end.

---The text output is modified automatically and cannot be modified manually.

x Diagrams:

---Maximum - 2 subplots, minimum - 1 subplot:

- *Depends on selected radiobutton for subplot selection

- *X-axis between 2 subplots is shared.

- *Labels of X and Y-axes are predefined

- Y-axis label of HPLC chromatogram is dynamic - changes according to wavelength (cannot observed yet but it will be possible in the future).

---Every diagram has its own state

- *initial - no data drawn, text "Specimen" is shown.

- *not-initial - data is drawn

---Two possible diagram layouts:

*None. Set when at least one of the subplots does not contain any data.

*constrained. Set when all subplots has its own data.

---When a file execution error is observed, the graph for corresponding data file will be resetted to initial state and replotted.

*Executed with all layout changes

*Does not apply on folder search errors.

---Diagrams are interactive

*Default matplotlib figure and toolbar features (with modifications):

-Current x and y values are shown in the toolbar

-Resetting to original view

-Going back to previous view

-Going forward to next view

-Subplot dragging

-Subplot zooming

-Saving the figure

*Default feature Configure subplots was ommited because it was incompatible with constrained layouts.

*However, its completelly enough to visualize and analyse HPLC-MS data.

HPLC-MS data file types:

x The correct file types are provided in data folder.

---They should include previously described file extensions:

*chromatogram_file_name_chrom.txt (_chrom.txt)

*positive_ionization_file_name_ms_+.txt (_ms_+.txt)

*negative_ionization_file_name_ms_-.txt (_ms_-.txt)

---For optimal functionality of the GUI, the provided file should have the following structure of reference lines:

*For HPLC files:

- [Header]
- [File Information]
- [Sample Information]
- [Original Files]
- [File Description]
- [Configuration]
- [Peak Table(PDA-Ch1)]
- [Compound Results(PDA)]
- [PDA 3D]

*For MS files:

- [MS Spectrum]
- one of two possible lines marking the end of the file:
 - #Event 1 (positive ionization)
 - #Event 2 (negative ionization)

Additional information:

x There is 'data' folder in the working directory:

---You can test functionality of the GUI by executing these files.

x The folders 'data' and 'my_browsing_history' can be deleted:

---They will be recreated during the program runtime.

---Loss of the old information!!!