HPLC Data analyzer app tutorial

The aim of this application is to allow you to analyse data obtained from our HPLCs without using Chromaster. This document tells you exactly what to do, but most of it should be intuitive. Installation instructions are contained in a separate file and will not be discussed here. This tutorial assumes that you have already installed the application. Note that to make development easier, this app works via a web browser, so don’t be surprised if your browser opens.

# Input

* Head to one of the HPLC computers.
* To find your data folder, right click the chromaster shortcut on the desktop. Click “open file location”. Navigate to your folder from here.
* Once in your folder, open the “DATA” folder.
* You’ll see a long list of folders with numbers. This is the same layout as opening runs via chromaster. Each of these number folders contains your Raw data. Just copy whatever folder you want to analyse to your USB stick.
* **Note:** to speed up this process, you can put a shortcut on the desktop to your “DATA” folder if you wish.
* The first tab that opens when you launch the app is the upload tab. Please note that launching the app can take a few seconds – wait patiently and do not launch it twice. In the upload tab, drag and drop your raw data or click the upload area and select the file.
* **Important**: your chromatograms are only contained in the “.RW1” files. **ONLY UPLOAD THOSE.**
* There is no need to do anything else. The app finds your chromatogram, pressure profile and sample name within the RW1 file. It decodes the data and saves it in the app’s memory.
* If you re-upload new files, this will only affect the plots you see in the Chromatogram viewer and only after clicking the next or previous plot buttons on that page. It does not affect any of the saved data in the tables (see later). If you do want to start over and delete everything, refresh the browser page.

A screenshot of a computer

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# Chromatogram viewer

* Once you have uploaded your data, you can head to this tab. A chromatogram will only appear when you have uploaded your data.
* The layout of the chromatogram is as you know it: a signal in function of time.
* You can change between chromatograms with the “Previous Plot” and “Next Plot” buttons. Your sample name is always indicated as the plot title.
* Plot controls (only mentioned once here, but are the same for all plots in the app):
  + When you hover over the plot, on the top right, some controls appear. They tell you what they do (such as save as .png), so this will not be explained here.
  + Zooming can be done via those buttons or by scrolling while hovering over the plot. Double clicking resets zoom.
  + It is not recommended to use the “Zoom” button here. If you do so, you exit the selection mode and you can’t integrate the peak anymore. You will need to reset by switching between plots (next/previous plot buttons).
  + To integrate a peak, simply click and drag your mouse. Your selected area is highlighted. Integration areas stay when you switch between chromatograms (previous/next buttons).
* Once you have properly integrated the peak, you need to save this data using “Add to Table”. “To what table”, you ask? Well, this is determined by the sliders The sliders allow you to select what type of data your peak is. The app logic is as follows:
  + You can save a blank: this AUC will be subtracted from all other data saved **subsequently**, not retroactively. If you don’t pick a blank, the value is assumed to be 0. You save a blank by clicking the “This is the blank” slider. The position of the other slider does not matter.
  + You can save calibration data. You do this by activating the “This is calibration curve data” slider and having the blank slider inactive.
  + You can save sample data. You do this by having all sliders inactive.
  + Any data you save is saved in tables in the other tabs.
* If you feel like you might need your raw time-signal data, you can automatically export this to Excel for all chromatograms with the “Export all chromatograms as an Excel” button. Different chromatogram data will be contained in different Excel sheets. This does not export the plots.

A screen shot of a graph

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# Calibration data analysis

* In order to use this tab, you need to have integrated your data.
* Table controls:
  + You can edit the “Sample name” and “Concentration” columns. The others can not be edited.
  + You can delete rows by clicking the cross at the left side of the table.
* There is some implemented logic to fill the “Concentration” column faster. If you click the “Autofill concentrations” slider, the app assumes that you performed a serial dilution and that the top row of the table is your lowest concentration. Thus, if the slider is active, you can fill in a concentration value in the top row and press “enter”. The app then doubles the concentration for each row.
* Once you have filled in your concentrations, click the “Perform regression” button. The results of this analysis are displayed in the plot and the table below.

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A graph with a red line

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# Sample data analysis

* Once you have analysed your sample peak data and performed the calibration, you can head over to the sample data analysis tab.
* Table controls:
  + You can only edit the sample name in this case.
* The results from your integration are already shown. If you want to calculate the concentrations of each sample, press the “Perform Concentration determination” button.
* If you’re finished with all aspects of your analysis, you can click the “Export to Excel” button. This saves an Excel with your calibration data (and plot) and your sample data in separate sheets.

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# Pressure as a function of time

* If you feel like your data is off, you might want to verify the pressure during your run. This tab contains two plots:
  + Plot 1 is a lot like the chromatogram viewer and shows the pressure per run as a function of time, with the sample name displayed in the title.
  + Plot 2 shows the averages of the pressures of all of your runs. You can check for deviations here. If you feel like the pressure has been rising between run 1 and run 50 for example, you can spot that here. You can also spot gross anomalies by looking at the standard deviation for each average pressure.
* You can not export anything here, but you can save the plots as .pngs.

A screenshot of a graph

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A graph with a dotted line

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