

PDA EXTENSION

Clarity Extension

ENG

Code/Rev.: M054/100C

Date: 2025-10-22

Phone: +420 251 013 400

clarity@dataapex.com

www.dataapex.com

DataApex Ltd.
Petrzilkova 2583/13
158 00 Prague 5
Czech Republic

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Author: MP

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To facilitate the orientation in the **PDA Extension** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

Open File (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name.

WORK1 (capitals) indicates the name of the file and/or directory.

ACTIVE (capital italics) marks the state of the station or its part.

Chromatogram (blue underlined) marks clickable links referring to related chapters.

The bold text is sometimes also used for important parts of the text and the name of the **Clarity** station. Moreover, some sections are written in format other than normal text. These sections are formatted as follows:

Note: Notifies the reader of relevant information.

Caution: Warns the user of possibly dangerous or very important information.

I Marks the problem statement or trouble question.

Description: Presents more detailed information on the problem, describes its causes, etc.

Solution: Marks the response to the question, presents a procedure how to remove it.

1 PDA - Photo Diode Array

The **PDA Extension** is an optional add-on for the **Clarity Chromatography Software**. It can expand any **Clarity** Instrument as well as **Clarity Offline**.

The **Clarity PDA Extension** enables the processing of data acquired from selected Photo Diode Arrays/Diode Array Detectors (**PDA/DAD**). The three-dimensional (3D) chromatograms acquired by PDA detectors contain spectral data, thus allowing for enhanced result evaluation. The functions include interactive spectral analysis, peak purity analysis, and compound identification based on spectral library search. PDA data can be displayed in a set of adjustable views, including 3D rendering.

2 Specification

The **PDA Extension** is an optional add-on for the **Clarity Chromatography Software**. It can be ordered as a part of a new software license or as an extension to an existing one (p/n A29).

3 Installation

The **PDA Extension** functions are activated by entering an appropriate user code during the installation of **Clarity** or later using the *Help - User Code* command from the **Clarity** main window.

To enable the PDA Extension on an **Instrument**, you have to set the corresponding instrument type. To set the instrument type, click the [...] button in the **System Configuration** dialog.

In the invoked **Instrument Type Setting** dialog, select the desired combination (e.g., LC-PDA).

Caution: The PDA Extension can be combined with **Clarity** Instruments of **GC**, **LC**, **CE** or **GPC** type.

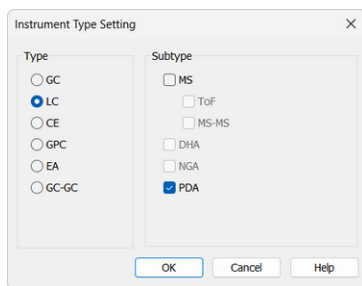


Fig. 1: Enabling the PDA Extension on an Instrument

4 Key Features

The **PDA Extension** brings the following features to the **Clarity** station:

- **Possibility to handle PDA data:** **Clarity** can acquire and work with PDA data from various PDA detectors.
- **Import/Export Data:** Spectral data can be imported to or exported from the **Clarity** software in the ASCII text format.
- **Reports:** Users can easily include PDA options such as data **3D Display**, **Isoplot**, **Spectra**, **Peak Purity**, and **Library Search Results** in reports using the [Report Setup](#) dialog.

4.1 Basic principles and terms

- **PDA View:** PDA views are the different ways of displaying the acquired PDA data in the customizable [PDA Chromatogram](#) window. Up to four views can be displayed at one time; any combination from the following views may be selected: *Isoplot*, *Chromatogram*, *Spectral*, *3D*, *Peak Purity*, *Peak Purity Spectra*, *Spectral Library*, and *Spectral Search*. The user can easily extract chromatographic signals from PDA data to determine the optimal detection wavelength for each peak.
- **PDA Method:** The **Clarity** *PDA method* includes an option for *Spectral Library Search* and *Peak Purity Analysis*.
- **Spectral Library:** **Clarity** can compare the peak spectra with the spectra of an unlimited number of spectral libraries. Spectra stored in a *Spectral Library* include retention times and analysis parameters (optional). The *Spectral Library Search* can perform automatic identification of integrated/calibrated components (peaks). The library search may be constrained by the retention time and wavelength ranges. To determine the match with a library spectrum, a match factor is calculated based on either the *Least Square*, *Weighted Least Square*, or *Correlation* methods. A *Background Correction* option is also available. The particular formulas and calculation details can be found in the chapter "**Appendix - Mathematical Formulas**" on pg. 63..
- **Peak Purity:** This analysis helps to discover hidden impurities. It is applied to all integrated/calibrated peaks in the active signal, and is calculated either based on five significant peak points or all spectral point within the peak. A similarity curve is then displayed in the [PDA Chromatogram](#) window. *Peak Purity* analysis can be optimized by setting custom preferences relating to wavelength restriction and absorbance threshold. The calculation details can be found in the chapter "**Appendix - Mathematical Formulas**" on pg. 62..

5 PDA Extension Description

5.1 Method Setup - PDA Method

A new *PDA Method* tab is available in the *Method Setup* dialog. The *Method Setup - PDA Method* dialog can be also accessed using the new *Method - PDA Method* command in the *Instrument* window.

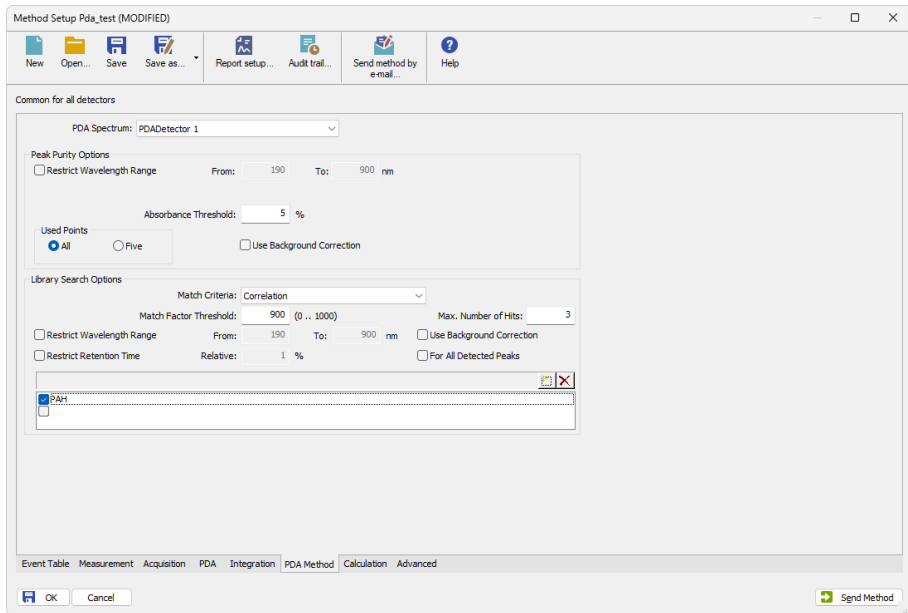


Fig. 2: Method Setup - PDA Method

PDA Spectrum

Sets the spectral detector for which the particular *PDA Method* settings will be used in the case that more than one spectral detector is configured on the Instrument.

Peak Purity Options

Restrict Wavelength Range

Restricts the comparison of the spectra only to the wavelength range specified in the *From* and *To* fields.

Absorbance Threshold

This parameter specifies the section of a peak, expressed as a percentage of the detected peak height, used for peak purity evaluation. It defines the interval where spectra are included in calculations.

Used Points

Sets whether the calculations of peak purity value will be carried out based on spectra in *All* peak data points or only *Five* significant points. These are:

- the *peak purity start* (located in one-third of the distance between the start point of the interval set by *Absorbance Threshold* and peak apex)
- the *peak purity inflexion point* (in two-thirds of the distance between the start point of the interval set by *Absorbance Threshold* and peak apex)
- the *peak apex*
- the other *peak purity inflexion point* (in one-third of the distance between the peak apex and end point of the interval set by *Absorbance Threshold*)
- the *peak purity end* (in two-thirds of the distance between the peak apex end point of the interval set by *Absorbance Threshold*)

Use Background Correction

With the *Use Background Correction* checked, the spectra are compared against a corrected baseline. The corrected baseline (background) for individual wavelengths is interpolated between the peak start and peak end points. Calculation details can be found in the chapter "**Appendix - Mathematical Formulas**" on pg. 63..

Library Search Options

Note: Setting the section in the *Method Setup - PDA Method* dialog causes two things: First, regardless of the settings, the tab is copied to the measured chromatogram. Second, in the case that at least one library is selected, the library search is performed at the moment the acquisition ends and its results are stored in the measured chromatogram. Library compound with the best-matching spectrum is visible in the *PDA Best Match Name* column of the *Result Table*, the whole search results can be accessed through printing the report (*Report Setup - PDA - Library Search Results - Table/Spectra* checkboxes). User can later change the search settings in the measured chromatogram's method (*Measurement Conditions - PDA Method* tab) and the changes done there are automatically applied to the *Result Table* and prints. Manual library searches as performed from the [PDA Chromatogram](#) window only influence the print of the chromatogram data if the print is invoked directly from the [PDA Chromatogram](#) window.

Match Criteria

Sets the method of the match factor calculation. Possible options are *Least square*, *Weighted Least Square*, and *Correlation* (calculation details are in the chapter "**Appendix - Mathematical Formulas**" on pg. 60.).

Match Factor Threshold

Only hits with match factor above the value entered will be displayed.

Max. Number of Hits

Limits the number of displayed spectra discovered by matching according to the selected criteria.

Restrict Wavelength Range

The spectra comparison will be limited to the range specified in *From* and *To* fields (the whole overlapping range is compared when not checked).

Restrict Retention Time

Limits the found spectra only to those with the **RT** within the range specified in the *Relative* field (in % of the peak **RT**).

Use Background Correction

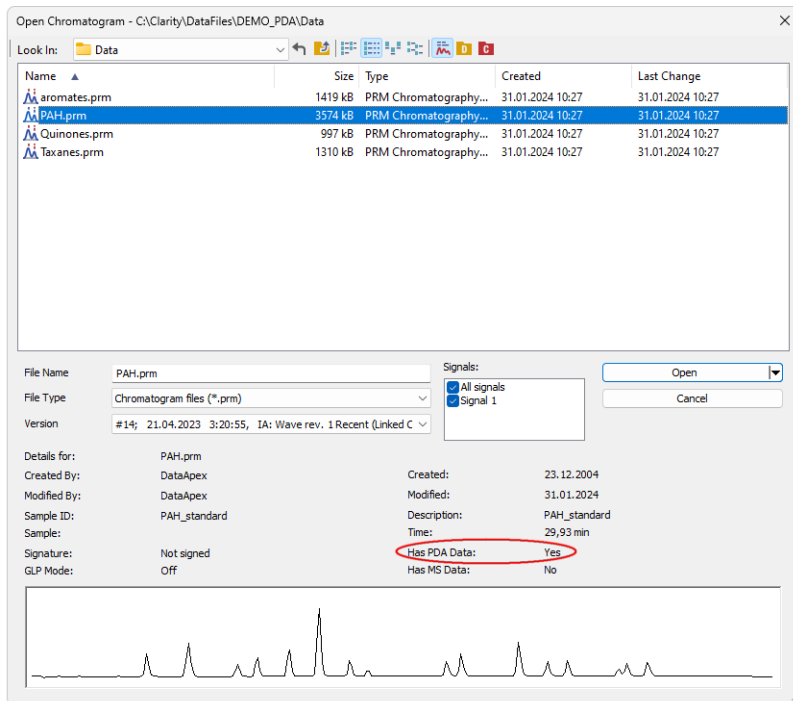
With the *Use Background Correction* checked, the spectra are measured against a corrected baseline. The corrected baseline (background) for individual wavelengths is interpolated between the peak start and peak end points. Calculation details can be found in the chapter "**Appendix - Mathematical Formulas**" on pg. 63..

For All Detected Peaks

Sets the library search for all detected peaks. While unchecked, only the identified peaks are evaluated.

5.2 Open Chromatogram

The *Open Chromatogram* dialog indicates in the **Information Pane** whether the selected chromatogram contains PDA data. The item that does so is labeled as *Has PDA Data*.

*Fig. 3: Open Chromatogram*

5.3 Chromatogram

The *Chromatogram* window is enhanced by the PDA-related features on the [Results](#) and [Measurement Conditions](#) tabs and in the *Chromatogram* menu.

5.3.1 Results

The *Result Table* of a PDA chromatogram is expanded by the following columns: *PDA Peak Purity*, *PDA Name Match*, *PDA Best Match Name*, and *PDA Best Match*. It is possible to change the order of the columns or hide some of them using the *Edit - Setup Columns...* command.

Result Table (ESTD - Data\PAH)						
	PDA Peak Purity	Peak Type	Compound Name	PDA Name Match	PDA Best Match Name	PDA Best Match
1	997	Ordnr	Naphtalene	1000	Naphtalene	1000
2	992	Ordnr	Acenaphtalene	999	Acenaphtalene	999
3	987	Ordnr	Acenaphtene	1000	Acenaphtene	1000
4	780	Ordnr	Fluorene	999	Fluorene	999
5	767	Ordnr	Phenantrene	998	Phenantrene	998
6	928	Ordnr	Antracene	995	Antracene	995
7	867	Ordnr	Fluoranthene	999	Fluoranthene	999
8	951	Ordnr	Pyrene	1000	Pyrene	1000
9	950	Ordnr	Benzo(a)anthracene	985	Benzo(a)anthracene	985
10	949	Ordnr	Chrysene	995	Chrysene	995
11	978	Ordnr	Benzo(b)fluoranthene	998	Benzo(b)fluoranthene	998
12	959	Ordnr	Benzo(k)fluoranthene	979	Benzo(k)fluoranthene	979
13	950	Ordnr	Benzo(a)pyrene	991	Benzo(a)pyrene	991
14	959	Ordnr	Dibenz(a,h)anthracene	964	Dibenz(a,h)anthracene	964
15	982	Ordnr	Benzo(ghi)perylene	993	Benzo(ghi)perylene	993
16	985	Ordnr	Indeno(1,2,3-cd)pyrene	998	Indeno(1,2,3-cd)pyrene	998

Fig. 4: Result Table with the PDA data

PDA Peak Purity

Displays the *PDA Peak Purity* value of the peak. In the case the *Peak Purity* is calculated using the *Five* points method (as described in the chapter "[PDA Extension Description](#)" on pg. 5.) and the *Absorbance Threshold* is set too high to be over peak inflexion points, an *Error* result is displayed with a tooltip hinting for solution.

The *Peak Purity* calculation uses the Pearson Correlation Coefficient formula to calculate the similarity of any peak spectra to the apex spectrum. The results are re-scaled to the 0-1000 scale and averaged (five results averaged in case of *Five* points setting, all spectra similarity results averaged in case of *All* points setting). Calculation details including formulas can be found in the chapter "[Appendix - Mathematical Formulas](#)" on pg. 62..

PDA Name Match

Displays the match factor of the spectrum found in the spectral libraries based on the peak name obtained from the calibration.

If multiple libraries are specified in the *PDA Method* ([Chromatogram - Measurement Conditions - PDA](#)), Clarity will search all libraries for spectra with the same name and display the one with the highest match factor.

PDA Best Match Name

Displays the name of the best-matching spectrum found according to the method library search options.

If multiple libraries are specified in the *PDA Method* ([Chromatogram - Measurement Conditions - PDA](#)), Clarity will search all libraries and choose the spectrum with the highest match factor. The name of the library where the match was found is shown as a tooltip when you hover over the corresponding cell in the Result Table.

PDA Best Match

Displays the match factor of the compound from the *PDA Best Match Name* column.

5.3.2 Measurement Conditions

The *Chromatogram - Measurement Conditions* pane contains an additional *PDA Method* sub-tab with PDA-related parameters of the opened chromatogram. The individual items correspond to the items as set in the [Method Setup - PDA Method](#) dialog described on pg. 5.

Fig. 5: *Chromatogram - Measurement Conditions - PDA*

Note: When opening chromatogram with PDA signals on a non-PDA instrument, the *Chromatogram - Measurement Conditions - PDA Method* tab is not displayed. Detector's tabs are not loaded, therefore detector's settings, including signal wavelengths, are not visible.

5.3.3 Remove Generated Signal

This command is located in the [Chromatogram](#) window in the menu *Chromatogram*. The *Remove Generated Signal* command is used to invoke the *Remove Generated Signal* dialog where generated signal can be removed.

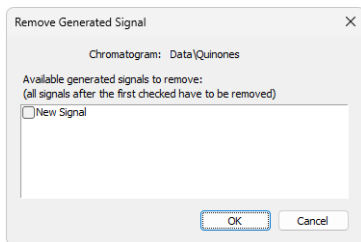


Fig. 6: Remove Generated Signal

Only named signals can be removed. Currently, it is not possible to delete only one signal (except for the last one), every signal following the one selected for deletion will be also deleted.

5.4 PDA Chromatogram window

The *PDA Chromatogram* window is accessible from the *Chromatogram* window using the *Window - PDA Window* command or the **PDA Window** icon.

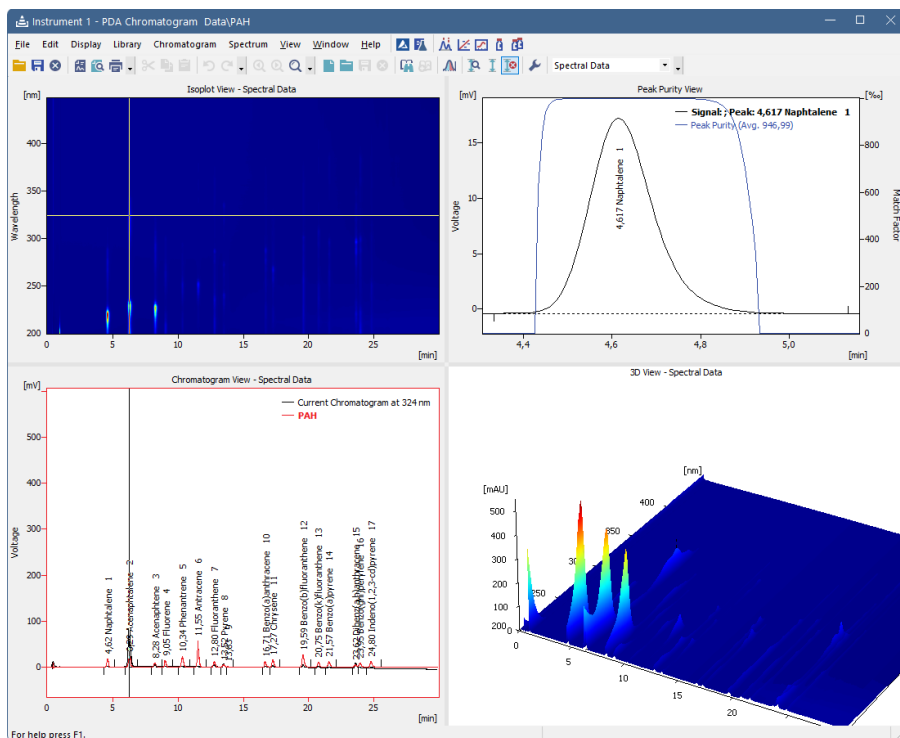


Fig. 7: PDA Chromatogram window

This window is divided into four view panes and each has its own local menu in which you can:

- Change view in the respective pane.
- Maximize the view to fullscreen.
- *Copy to Clipboard* (copies the image of the respective view to clipboard for use in an external graphic software).
- *Save as Picture* (allows to create an *.emf picture of the respective view).

5.4.1 Panes

The [PDA Chromatogram](#) window can display single view or can be split into two or four panes. Each pane can display any of the following views: [Isoplot](#), [Chromatogram](#), [Spectral](#), [3D](#), [Peak Purity](#), [Peak Purity Spectra](#), [Spectral Library](#), and [Spectral Search](#). The size and position of the panes can be controlled by the commands from the *View* menu and by holding and dragging sliders between the panes with the mouse. To display any of the views in a particular pane click the right mouse button to display the local menu and select the desired view from the list.



- As there are more available views than panes, it is not possible to see all the views at once. However all user operations with the hidden view are still enabled (e.g., user can open and work with spectral library even if the [Spectral Library View](#) is hidden).
- Each view can be displayed only in one pane at the same time. Selecting a view that is already displayed in another pane will result in switching the positions of the views. Selecting a view that is not yet displayed will result in hiding the original view and displaying the selected one in the pane.

5.4.2 Markers

[Isoplot](#), [Chromatogram](#), [Spectral](#), and [3D](#) views feature one or two **markers** (thin lines of inverse color crossing the data plot) depicting the current position in the data.

For many operations (e.g., adding spectrum to library, adding signal, selecting peak, etc.) the current time or wavelength serves as a point where the operation takes place.









Markers also specify slices of **3D** data that are displayed as curves in [Chromatogram](#) and [Spectral](#) views (see below).

- **Time marker** (vertical marker shown in [Isoplot](#) and [Chromatogram](#) views) moves over the time axis and depicts the spectrum currently displayed in the [Spectral](#) view.
- **Wavelength marker** (horizontal in [Isoplot](#), vertical in [Spectral](#) view) moves over the wavelength axis depicting the current chromatogram curve in the [Chromatogram](#) view.
- Markers can be moved by holding the left mouse button while cursor is over the marker (cursor changes to  or ) and dragging it with the mouse.
- Another possibility is to use *Move Marker(s) Here* command from the context menu of the given view. The function moves one or both markers to position of the right mouse click that popped up the menu. This is useful while the view is

zoomed and marker(s) may not be visible. With *Move Marker(s) Here*, the marker(s) can always be brought within the visible range.

5.4.3 File

This is a sub-menu with commands for working with PDA chromatograms and other specific system commands.

	Open Chromatogram...	Opens a chromatogram containing PDA data (Ctrl + O).
	Save Chromatogram	Saves the active chromatogram (Ctrl + S).
	Close Chromatogram	Closes the active chromatogram (Ctrl + W).
	Import 3D	Opens the dialog for selecting files to import. After choosing a file, the Import 3D Text File dialog is displayed to set importing options.
	Export 3D	Exports the PDA data to the EZChrom format. For more details see the chapter Export format on pg. 41.
	Report Setup...	Opens the Report Setup - PDA dialog for setting the reporting options (Ctrl + Alt + P). For more details see the chapter Report Setup on pg. 39.
	Print Preview...	Previews the selected print configuration before printing (Ctrl + Shift + P). After selection, the <i>Print Preview</i> dialog will be displayed.
	Print to PDF...	Prints the report to a *.PDF file.
	Send Printed PDF...	Opens a new email message in the default email client, prints the report to *.PDF and attaches the created *.PDF file as an email attachment.
	Print...	Command for selecting the printer and for actual printing (Ctrl + P). After selection, the <i>Print</i> dialog will be displayed.
	Close Window	Closes the PDA Chromatogram window.

5.4.3.1 Import 3D Text File

Imports a chromatogram saved in a 3D text file format.

A chromatogram in a text format must contain chromatographic signal data in separate columns corresponding to the 3D spectrum, and may optionally contain a heading with a description of measurement conditions.


The station automatically interprets the headings of text files exported from **Clarity** and from the **EZChrom** software.

Note: The **EZChrom ASCII** text format uses the file suffix (*.ASC). It differs from the **text** format exported from **Clarity** station in the naming of individual items in the heading.

After selecting the files in the *Open Files to Import* dialog and pressing the *Open* button, the *Import 3D Text File* dialog opens.

The conversion program determines the most suitable import setting according to the content of the individual imported text files. Individual settings can subsequently be adjusted in the *Import 3D Text File* dialog and saved for further use. Import is performed using the *OK* button.

Preset

When files of the same type are imported frequently, it can be useful and time-saving to save the import settings for further use. In the drop-down menu on the top of the dialog, the user can select from the previously saved presets, by clicking the  button right to list the presets, an additional menu will open. The menu contains commands for saving the current setting as a new preset (*Create New...*), and options to *Rename...* or *Remove* the selected one. Presets are stored as part of the **Clarity** Desktop settings.

Apply Settings to

This radio button group indicates whether the settings below will be applied either to the current file only, or to all the files selected for import. In the case that multiple files are imported at a time, and the *Current File* radio button is selected, the *Import 3D Text File* dialog will be invoked for every file. When the *All n Files* option is selected, all subsequent files will be processed with the same settings. By checking the *Prefer Detected Settings* checkbox you can force **Clarity** to use the settings detected from the imported file (if applicable).

Apply Method

Choose the method the parameters of which (e.g., integration table, attached calibration, etc.) will be applied to the imported chromatogram. By default, the displayed method matches the method in the *Single Analysis* dialog. Leaving this field blank applies the default parameters.

Current Text File

The name of the imported file including the directory path.

Preview

This button will open the current file in a simple text viewer. This can help the user to identify the exact meaning of particular columns when it is not clear from the file suffix.

Import From Line

Sets the line of the file at which the data import should start.

Import To Line

Sets the last line of the file that should be imported.

Separator

Selects the character by which the individual items are separated in the text file. <TAB>, <SPACE>, <COMMA>, or <SEMICOLON> are the available delimiter characters to choose from.

Decimal Separator

Separator of decimal points - <DOT>, <COMMA> or <Windows Locale>. Separator indicated in Windows (as <Windows Locale>) is used as the default.

Fig. 8: Import Text File

Analyst, Sample ID, Sample, Sample Date, Sample Amount, Dilution, ISTD Amount, Injection Volume

These fields contain the chromatogram identification parameters and have the same meaning as described in the chapter "Single Analysis".

Sample Rate

Selects the sampling speed in the number of samples per second (Hz). Select one of the speeds from the list corresponding to the speed of your A/D converter or enter your own value.

Wavelength

Selects the desired wavelength interval which should be imported.

Signal Multiplier


Selects the units of imported data and factor by which the data should be multiplied.

Signal Axis

Selects the name of the axis.

Save as Chromatogram

Sets the name and location of the resultant chromatogram created after importing a text file. By default, the program will offer to use the original name of the imported with the suffix *.PRM and the path to the Data directory of the current project.

To select another name and location for the resulting chromatogram, open the **Save As...** dialog using the  button.

Load Defaults

Resets the values of all fields to the default values.

OK

Confirms the import.

Skip






Skips the current file and proceeds to the subsequent one if importing multiple files.

Cancel







Cancels the import.

5.4.4 Edit


A sub-menu of commands for working with clipboard and tables.

	Undo	Cancels the last modification made in a table. This can be used repeatedly as the station remembers all changes done in tables from the initial start-up. Each table maintains its own independent list of operations, so the <i>Undo</i> command will be performed according to the command history of the selected table.
	Redo	Cancels the last <i>Undo</i> command. This can be used repeatedly as the station remembers all changes done in tables from the initial start-up. Each table maintains its own independent list of operations, so the redo command will be performed according to the command history of the selected table.
	Copy	Copies the content of the selected cells to clipboard.
	Paste	Pastes the clipboard content to the selected location. If the area is larger than the content, the copied content will fill all the selected cells. This can be used to fill multiple fields with identical content or with several periodically repeating fields.
	Delete	Deletes the selected fields ( .
	Select All	Selects all fields of table.

5.4.5 Display

	Zoom Out	Zooms out the current part of chromatogram. Also invoked by pressing - key.
	Zoom In	Zooms in the current part of chromatogram. Also invoked by pressing + key.
	Previous Zoom	Restores the previous chromatogram zoom cut (Ctrl + -).
	Next Zoom	Restores the zoom cut that was changed by the <i>Previous Zoom</i> command (Ctrl + +).
	Unzoom	Cancels all zoom cuts (Ctrl + *).
	Properties...	Invokes the <i>PDA Properties</i> dialog. For more details, see the description below.

5.4.5.1 PDA Properties

Invoking the command *Display - Properties...* or the  icon opens the *PDA Properties* dialog, similar to the *Graph Properties* dialog. There are two new tabs here - the *Wavelength Axis* tab (analogous to the *Signal Axis* tab) and the *Chrom&Spectral View* tab described here.

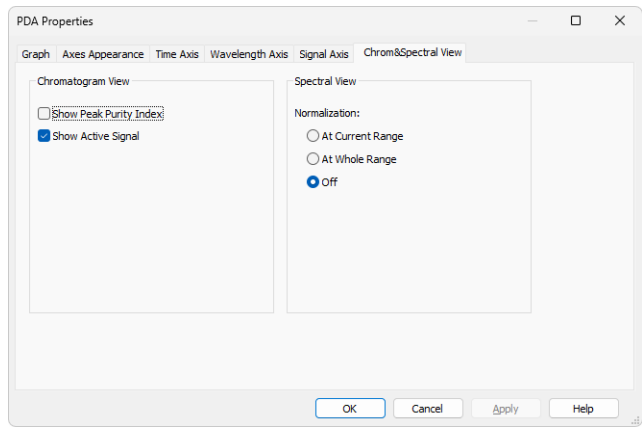


Fig. 9: PDA Properties - Chrom&Spectral View

Chromatogram View

Show Peak Purity Index

While checked, the peak purity index curve is displayed across whole chromatogram in the [Chromatogram View](#). The curve is located at the top of the

graph and has no Y-axis itself.

Show Active Signal

While checked, displays the active signal from the chromatogram (including labels) in the [Chromatogram View](#) pane.






Spectrum View

Sets the default normalization for the data on the [Spectral View](#) pane. The possible options are *At Current Range*, *At Whole Range*, or *Off*. For more details see the chapter **Spectrum** on pg. 27.

5.4.6 Library

This menu serves for creating and editing **Spectral Libraries**.

Note: The *Spectrum Search* is performed in libraries specified in the [Spectral Library Search Options](#) dialog available by the *Spectrum - Library Search Options...* command.

	New	Creates a new empty spectral library (Ctrl + Alt + N).
	Open...	Opens the spectral library file (Ctrl + Alt + O).
	Save	Saves spectral library (Ctrl + Alt + S).
	Save As...	Saves spectral library under a different name (Ctrl + Shift + S).
	Options...	Displays the <i>Spectral Library Options</i> dialog. For more details, see the description below.
	Close	Closes the spectral library (Ctrl + Alt + W).

5.4.6.1 Options

The *Spectral Library Options* dialog defines whether the *Spectral Library* should use the background correction (*Use Background Correction*) and enables to save a *Description* of the library.

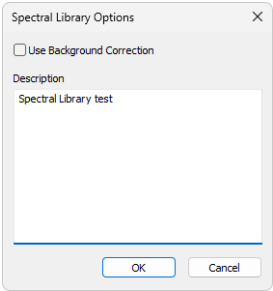


Fig. 10: Spectral Library Options

Caution: Make sure to use the background correction consistently, either always and everywhere ON or always OFF to gain consistent data.

Use Background Correction

The baseline (background) for individual wavelengths is interpolated between peak start and peak end points. With the *Use Background Correction* checked, the spectra are measured against this surface. Calculation details can be found in the chapter **"Appendix - Mathematical Formulas"** on pg. 63.

Description

Stores the description of the *Spectral Library*.

5.4.6.2 How to Create a Library

Creating a spectral library in the PDA Extension involves the following steps:

1. Acquire the chromatogram/chromatograms containing compounds to be added to the library.
2. Create a calibration file to identify the compounds based on their retention time.
3. In the *PDA Chromatogram* window, select **New** in the *Library*^a menu to create a new library file. Save the file subsequently.

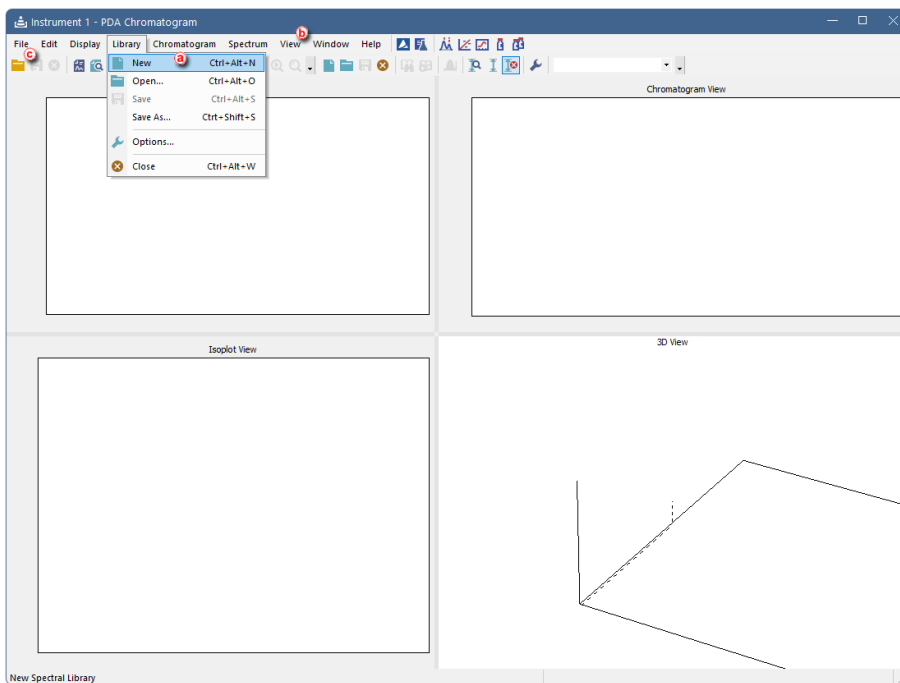


Fig. 11: Create new spectral library

4. To view the library, select the **View** **(b)** - *Maximize View - Spectral Library View* option, or right-click to one of the four panes in the *PDA Chromatogram* window and select *Spectral Library View* (a new library will be empty).
5. Open the chromatogram of the standard **(c)**.
6. Add the peaks to the library using the *Spectrum - Add All Identified Peaks* command **(d)**.

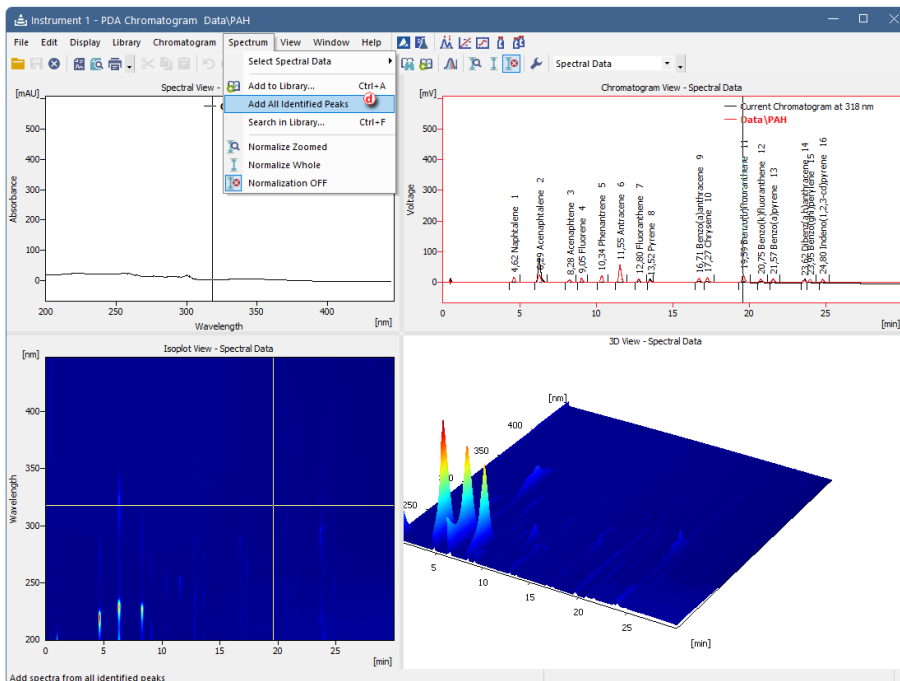


Fig. 12: Add all peaks to the new spectral library

7. Check the apexes of the identified peaks before adding them to the spectrum library.

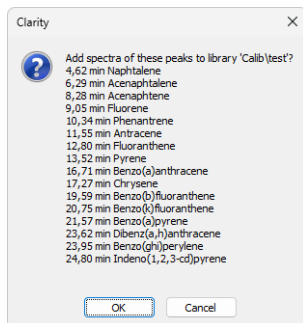


Fig. 13: Adding peaks to library

8. Alternatively, you can add any peak to the library via manually selecting it in the displayed chromatogram and using the **Spectrum - Add to Library** command.

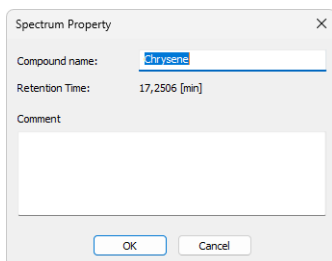


Fig. 14: Adding peaks manually

9. The library will now contain the added spectra. You can view the selected spectra in overlay with the spectrum currently selected in the opened chromatogram in **Spectral View - Spectral Data** ^(a) by checking the **Show** ^(b) boxes of the desired compounds in the **Spectral Library** ^(c).

Note: For the spectra in library, wavelengths for up to three maxima are displayed ^(d).

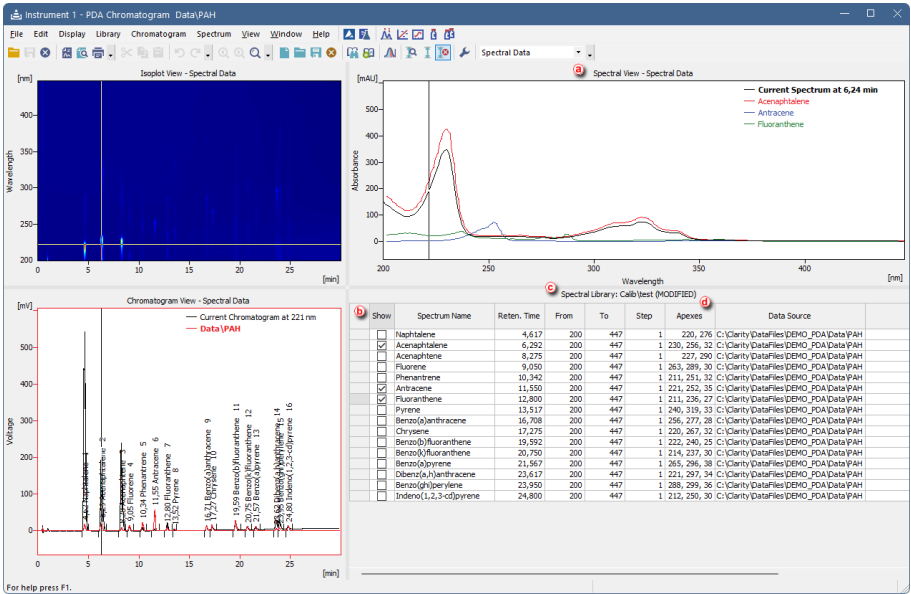


Fig. 15: Spectral data overlay

10. After saving the library, you can attach it to a method: in the *Method Setup* window, open the *PDA Method* tab **a**, click *New* **b**, and choose the created library **c**. Save the method subsequently.

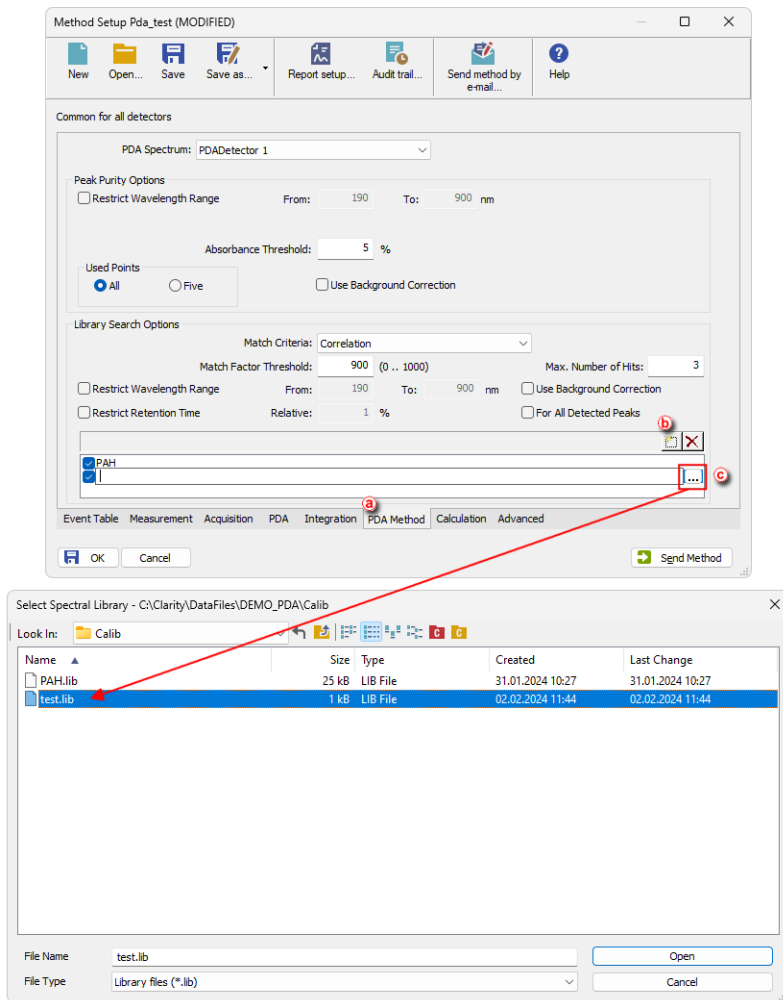


Fig. 16: PDA Method setup

11. You can also attach the library to an existing chromatogram: in the *Chromatogram* window, open the *Measurement Conditions - PDA Method* tab [a](#) . Here you can add the library [b](#) analogously as in the *Method Setup*.

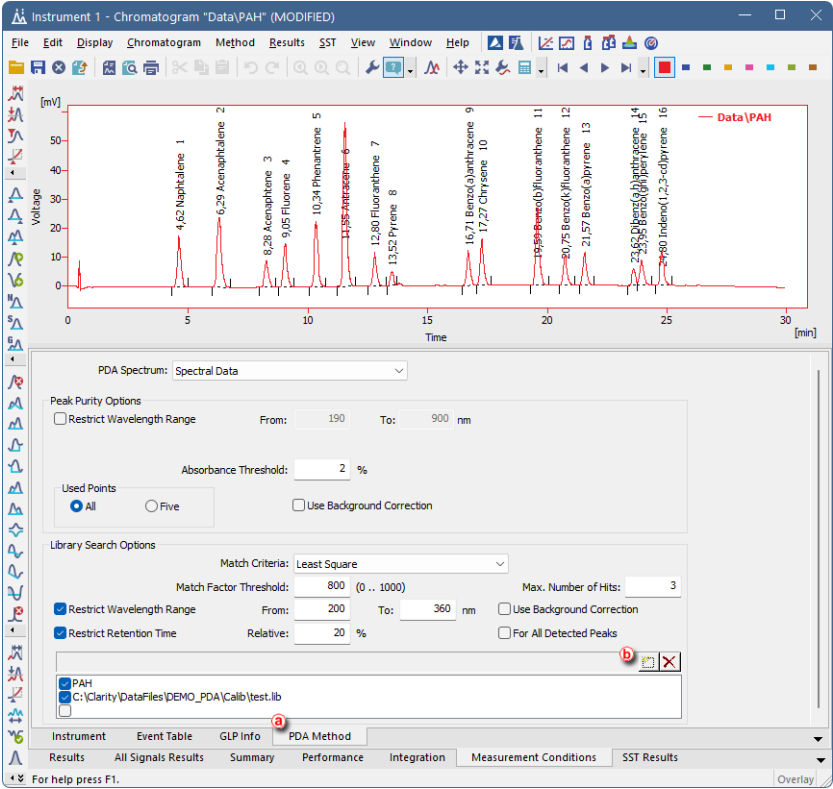


Fig. 17: Adding library to chromatogram

12. In the *Result Table*, the respective library name is displayed in the tooltip for the *PDA Best Match Name* ③ (this is particularly useful when several libraries are set).

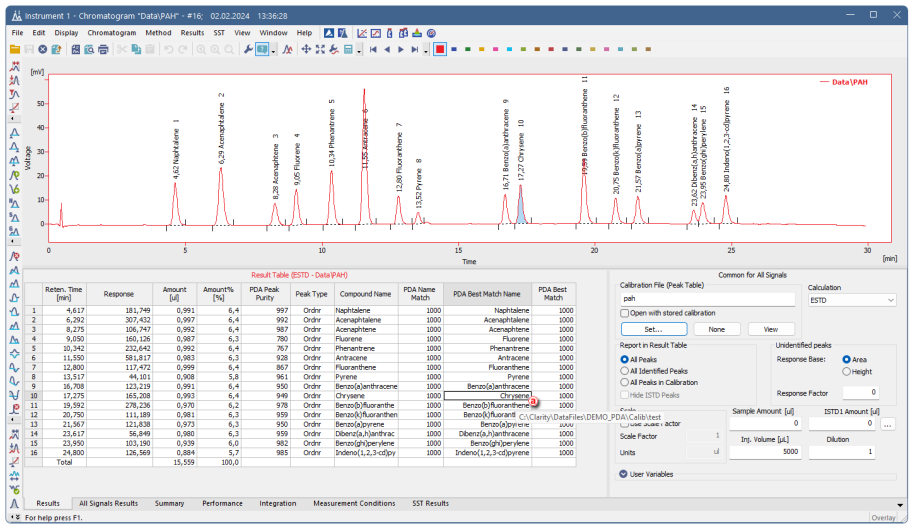



Fig. 18: Chromatogram with PDA - Results Table

Additional remarks:

- The library is in a plain ASCII text format, so to export spectra to some external program, the data can be picked directly from the .LIB file.
- There is an option to export the entire spectral data to an *.ASC format (ASCII text, compatible with EzChrom) from the *PDA Chromatogram* window using the *File - Export 3D...* command. The exported data include a table where retention times are listed in rows and wavelengths are listed in columns, showing signal values for each combination.

5.4.7 Chromatogram

Add Signal	Adds or replaces the chromatogram signal with a new signal taken as a cut from the PDA data. For more details, see the description below.
	Display Peak Purity Loads the currently selected peak (from the Chromatogram or Isoplot view) to the Peak Purity and Peak Purity Spectra views (Ctrl + D). For more details, see the description below.

5.4.7.1 Add Signal

Stores a cut of the PDA data on the selected wavelength/range of wavelengths as a signal in the current chromatogram.

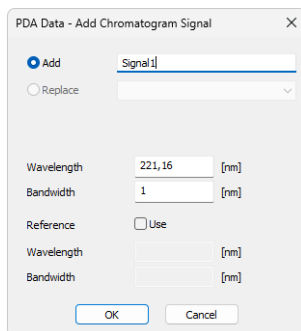


Fig. 19: PDA Data - Add Chromatogram Signal

Add

Add the new signal, gained as a cut at the selected wavelength, to the chromatogram containing the current spectrum.

Replace

Replaces the selected signal in the chromatogram containing the current spectrum by a new signal gained as a cut at selected wavelength. Replacing signals is not allowed for originally acquired signals, only new signals derived from spectra can be replaced.

Wavelength

Sets the new signal wavelength.

Bandwidth

Sets the bandwidth for the new signal (how much cuts will be taken and averaged to create the new signal).

Reference

If the *Use* checkbox is checked, the reference signal will be used for eliminating the uneven intensity of the lamp.

Note: The reference wavelength should be set to the area of chromatogram where no peaks are present, e.g., where no compound absorbs.

Wavelength

Sets the reference signal wavelength.






Bandwidth

Sets the bandwidth for the reference signal.


5.4.7.2 Display Peak Purity

Selects the peak to be displayed in [Peak Purity](#) and [Peak Purity Spectra](#) views (**Ctrl** + **D**). When the time marker is over the desired peak in [Chromatogram](#) or [Isoplot](#) views, the *Display Peak Purity* command loads this peak to the [Peak Purity](#) and [Peak Purity Spectra](#) views. Invoking the function when the marker is not over any peak clears the views, which then display *No peak selected* label.

5.4.8 Spectrum

	Select Spectral Data	Allows to select the displayed spectra if there is more than one PDA spectrum in the chromatogram.
	Add to Library...	Adds the selected spectrum to the spectral library (Ctrl + A). For more details, see the description below.
	Add All Identified Peaks	Adds the spectra of all identified peaks to the spectral library. For more details, see the description below.
	Library Search Options...	Opens the <i>Spectral Library Search Options</i> dialog (Ctrl + F). For more details, see the description below.
	Perform Library Search	Searches the library for a matching spectrum (F3). For more details, see the description below.
	Normalize Zoomed	Normalizes the spectra in the zoomed range. For more details see the chapter Spectral View on pg. 33.
	Normalize Whole	Normalizes the spectra on the whole wavelength axis range. For more details see the chapter Spectral View on pg. 33.
	Normalization OFF	Turns the normalization off.

5.4.8.1 Add to Library

Adds the selected spectrum to the spectral library. Invoking the command, using the  icon, or the **Ctrl** + **A** shortcut invokes the *Spectrum Property* dialog, where the user can name the compound and add comments to it before the spectrum is added to the

library. If the spectrum is already present in the library (matched by the same name), the user is asked to confirm the spectrum's overwriting.

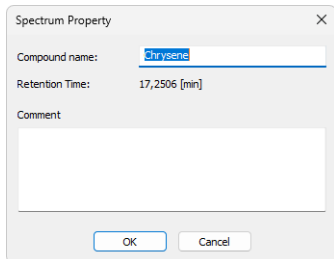


Fig. 20: Spectrum Property

Compound Name

Serves for setting the compound name.

Retention Time

Displays the retention time of the selected spectrum.

Comment


Allows to add custom comments.

5.4.8.2 Add All Identified Peaks

This command allows user to add all identified peaks in chromatogram all at once. Identified are all the peaks which corresponds to peak identified and named in calibration file. Peaks are added into the currently opened library.

5.4.8.3 Library Search

The *Library Search Options...* command (or the **Ctrl** + **F** shortcut) opens the *Spectral Library Search Options* dialog, where you can configure parameters for searching selected libraries to find a spectrum that matches the current peak.

Using the *Perform Library Search* command (or the  icon or **F3** shortcut) performs the library search according to the set parameters. If no search parameters have been set before, the *Spectral Library Search Options* dialog will be displayed.

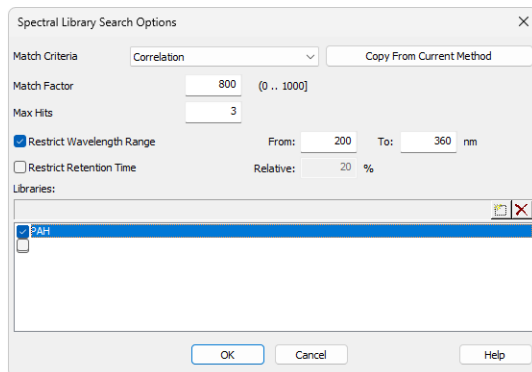


Fig. 21: Spectral Library Search Options

Match Criteria

Sets the type of the match factor calculation. Possible options are *Least square*, *Weighted Least Square* and *Correlation* (calculation details are in the chapter "**Appendix - Mathematical Formulas**" on pg. 60.).

Copy From Current Method

Copies the settings from the *PDA Method* of the active chromatogram. In other words, loads the settings from the [Chromatogram - Measurement Conditions - PDA](#) tab (for more details see also chapter **Measurement Conditions** on pg. 10).

Match Factor

Only the hits with a match factor above this value will be displayed.

Max Hits

Maximum number of displayed spectra that were found by matching according to the set criteria.

Restrict Wavelength Range

The spectra comparison will be limited to the range specified by the *From* and *To* fields (the whole overlapping range is compared if not checked).

Restrict Retention Time

Limits the found spectra only to those with retention time (RT) within the range specified in the *Relative* field (in % of peak RT).

Libraries

Specifies the libraries to be searched. Click the button to add a new line to the list and use the button to invoke the *Select Spectral Library* dialog where you can select the **Spectral Library** to be opened. Check/uncheck the checkbox next to the library to include/exclude it in the search.



5.4.9 View

Commands for setting up the [PDA Chromatogram](#) window.

Toolbars	Displays/hides all toolbars. The command is similar to the <i>Toolbars</i> command in the <i>Clarity</i> main window (for more details see also chapter View).
Toolbars - Customize	Allows customization of the toolbars. The command is similar to the <i>Customize...</i> command in the <i>Clarity</i> main window (for more details see also chapter Customize...).
Toolbars - Reset All	Restores all menus and toolbars in the PDA Chromatogram window to their default state.
Maximize View	Maximizes the selected view.
Restore Views	Restores the layout of the views (panes) in the PDA Chromatogram window to the state before the <i>Maximize View</i> command was used last time.
Two Vertical Views	Displays two vertical panes. When switching from four panes layout, views from top panes are displayed.
Two Horizontal Views	Displays two horizontal panes. When switching from four panes layout, views from left panes are displayed.
Four Views	Displays four panes.

5.4.10 Window

This section contains commands allowing to open other base windows.

Main 	Displays the <i>Clarity</i> main station window.
Instrument	Displays the <i>Instrument</i> window.
All Instruments	Allows to select which <i>Instrument</i> window to display.
Chromatogram	Displays the <i>Chromatogram</i> window.
Calibration	Displays the <i>Calibration</i> window.
Single Analysis	Displays the <i>Single Analysis</i> window.
Sequence	Displays the <i>Sequence</i> window.
Data Acquisition	Displays the <i>Data Acquisition</i> window.
Station Audit Trail 	Displays the <i>Audit Trail</i> window.

5.5 PDA Chromatogram views

Chapters about the PDA chromatogram views.

5.5.1 Isoplot View

The *Isoplot* view is the basic display of PDA spectral data. It presents the spectral data from a top-down perspective, with absorbance values indicated by different colors. The lowest values are shown as dark blue and increase through light blue, green, and yellow to red, with dark red representing the highest values.

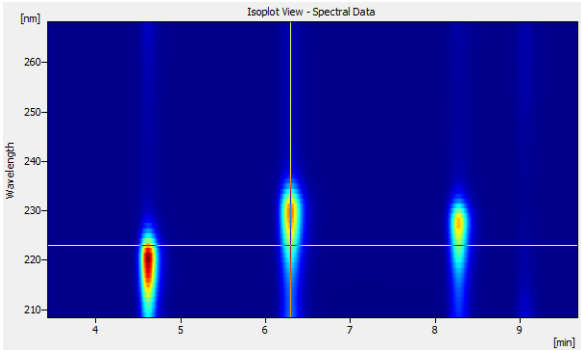


Fig. 22: Isoplot View

5.5.2 Chromatogram View

The *Chromatogram* view displays slices of 3D data defined by the current position of the wavelength marker (*Current Chromatogram at X nm*). It can also display the *Active Signal* from the *Chromatogram* window and/or the *Peak Purity* (match factor) curve for that signal.

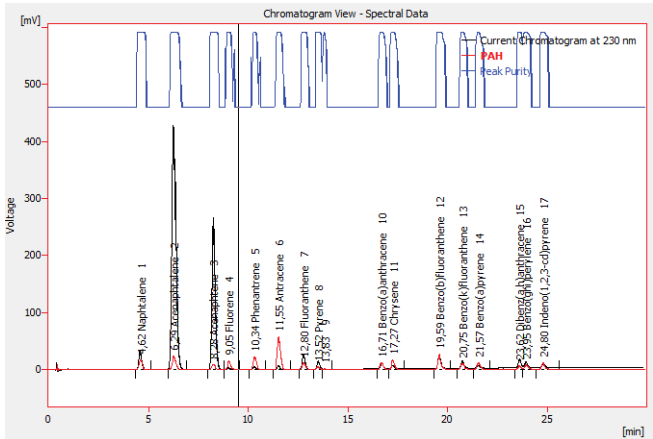


Fig. 23: Chromatogram View

The display of *Active Signal* and *Peak Purity* curves is controlled either by the settings on [PDA Properties - Chrom&Spectral Views](#) dialog tab, or by the *Show Active Signal* and *Show Peak Purity* commands from the context menu.

Appearance of the active signal curve can be tailored exactly the same way as in the *Chromatogram* window using the items on the *Graph* tab of [PDA Properties](#) dialog.

Peak Purity curve is shown in the upper part of the view so that it doesn't interfere with displayed signals. The values of the curve do not have their own Y-axis, but are displayed in per mille units. **Peak Purity** curve for particular peak can be viewed in a more detailed way using the [Peak Purity View](#) and the *Display Peak Purity* function.

5.5.3 Spectral View

Spectral View visualizes the slice of 3D data defined by the actual position of the time marker (*Current Spectrum at X min*). It can also display spectra from [Spectral Library View](#) and [Spectral Search View](#).

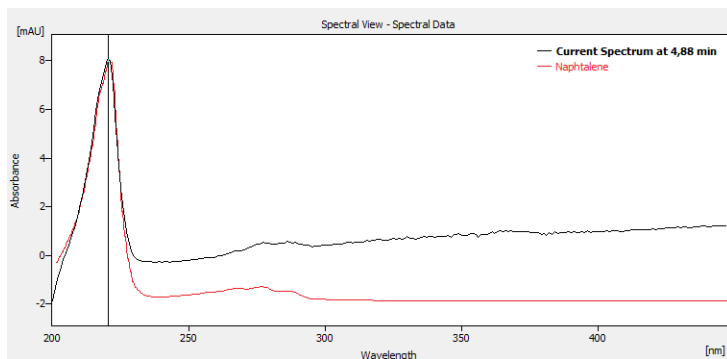


Fig. 24: Spectral View

Spectra can be overlaid in the graph using three different modes:

Normalized to the whole wavelength axis range




All spectra are re-scaled (the display only, spectral data stay the same) so that their respective lowest and highest points throughout the whole graph appear at the same level. It is convenient for visual comparison of peak spectra as the shape of the spectra curve does not depend on peak height in this mode. Vertical axis on the left displays values for currently active curve only (its label in the graph legend is shown in bold).

Normalized to zoomed range

This is a more advanced variety of the previous mode - spectra appear normalized as well, but the lowest and highest visible points appear at the same level. This is suitable for the comparison of characteristic regions of spectra.

With normalization turned off

In this mode, all spectra appear in their respective scales.

The particular mode can be selected using the *Normalize Zoomed* , *Normalize Whole* , and *Normalization OFF*  functions from the *Spectrum* menu.

5.5.4 3D View

The *3D View* shows a three-dimensional plot of the measured PDA data with *Time* and *Wavelength* being the horizontal axes, and *Absorbance* being the vertical axis (also indicated by color).

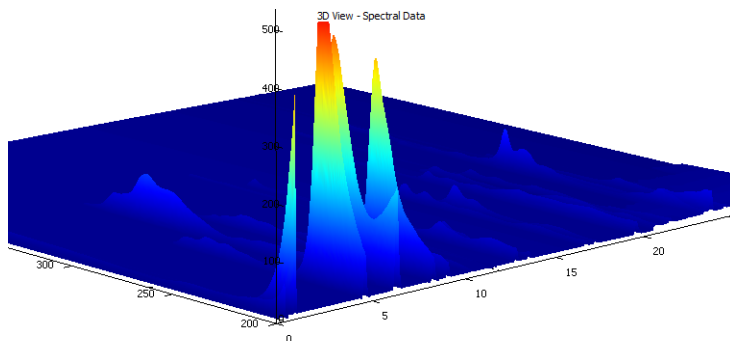





Fig. 25: 3D View

Caution: The *3D View* can take some time to display, depending on the amount of data and the speed of your graphics card.

The view also contains both markers (cursor lines), though they may be hidden beneath the surface of the data, being visible only from one side of the *3D View*. Projection of the plot is always centered on the crossing point of the markers. The plot can be moved, rotated, and zoomed using the mouse.

In the **Move** mode () holding the left mouse button and dragging the mouse moves the plot with the cursor. Note that the markers move as well, as the view is always centered on the crossing point. The Move mode is set by the *Smart Move Graph Mode* command from the context menu.

In the **Rotate** mode () holding the left mouse button and dragging the mouse rotates the plot. Moving the mouse horizontally rotates the plot along the vertical (absorbance) axis, moving the mouse vertically rotates the plot along horizontal axis of the view. The Rotate mode is set by the *Rotate Graph Mode* command from the context menu or by holding the **Shift** key while moving the mouse in Move mode.

In the **Zoom** mode () holding the left mouse button and dragging the mouse zooms the plot. Moving towards the center of the view shrinks the plot while moving away from the center enlarges in. The Zoom mode is set by the *Zoom Graph Mode* function from the context menu or by holding the **Ctrl** key while moving the mouse in Move mode. The plot can be also zoomed in any mode using the mouse wheel.

The *Restore Default View* context menu command restores the default projection settings of the 3D View pane.

Note: The use of the [PDA Properties](#) dialog (opened via the *Properties...* command from the local menu) can change the area of the graph being displayed - simply select the *Range: Fixed* with desired values on the *Signal Axis*, *Time Axis*, and [Wavelength Axis](#) tabs to restrict the displayed portion of these axes.

5.5.5 Peak Purity View

The *Peak Purity View* displays the peak previously selected in the [Chromatogram](#) or [Isoplot](#) views after the *Display Peak Purity* command is used. Along with the peak, the *Match Factor* value is displayed. If no peak has been selected, the *No peak selected* label is displayed instead.

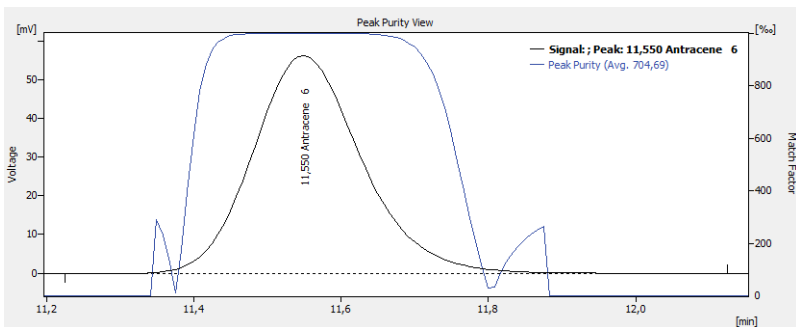


Fig. 26: Peak Purity View

The *Toggle to Spectra* command from the context menu switches the view in the pane to the [Peak Purity Spectra View](#) for the same peak.

The *Peak Purity* is calculated according to the settings from the *PDA Method* of the chromatogram that can be viewed and edited on the [Chromatogram - Measurement Conditions - PDA](#) tab (for more details see the chapter **Measurement Conditions** on pg. 10).

5.5.6 Peak Purity Spectra View

The *Peak Purity Spectra View* displays the spectra in several significant points of the peak selected in the [Peak Purity View](#). These points contain both threshold points (first and last point in which the **Match Factor** is computed for the given peak), both inflexion points and the peak apex.

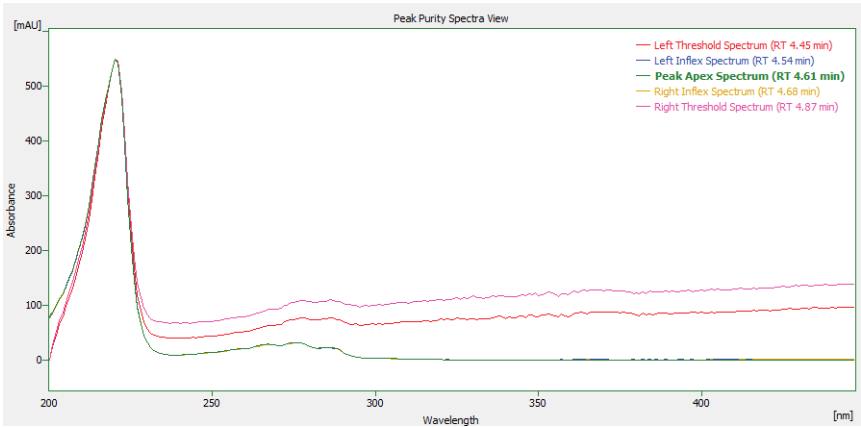


Fig. 27: Peak Purity Spectra View

All spectra in the *Peak Purity Spectra View* are always normalized to the current cut regardless of the spectrum normalization settings.

The *Toggle to Match Factor* command from the context menu switches the view in the pane to [Peak Purity View](#) for the same peak.

5.5.7 Spectral Library View

The *Spectral Library View* displays the spectra information from the currently opened **Spectral Library**. The spectral library name can be seen in the header of the *Spectral Library View*.

Spectral Library: Calib\PAH								
	Show	Spectrum Name	Reten. Time	From	To	Step	Apexes	Comment
	<input type="checkbox"/>	Naphtalene	4.609	200	447	1	220, 276	
	<input type="checkbox"/>	Acenaphtalene	6.244	200	447	1	230, 255, 32	
	<input type="checkbox"/>	Acenaphtene	8.250	200	447	1	227, 290	
	<input type="checkbox"/>	Fluorene	9.067	200	447	1	263, 289, 30	
	<input type="checkbox"/>	Phenantrene	10.330	200	447	1	211, 251, 36	
	<input type="checkbox"/>	Antracene	11.592	200	447	1	221, 252, 35	
	<input type="checkbox"/>	Fluoranthene	12.781	200	447	1	211, 236, 27	
	<input type="checkbox"/>	Pyrene	13.524	200	447	1	240, 319, 33	
	<input type="checkbox"/>	Benzo(a)anthracene	16.644	200	447	1	256, 277, 28	
	<input type="checkbox"/>	Chrysene	17.313	200	447	1	220, 267, 32	
	<input type="checkbox"/>	Benzo(b)fluoranthene	19.616	200	447	1	222, 240, 25	
	<input type="checkbox"/>	Benzo(k)fluoranthene	20.804	200	447	1	214, 237, 30	
	<input type="checkbox"/>	Benzo(a)pyrene	21.547	200	447	1	265, 296, 38	
	<input type="checkbox"/>	Dibenz(a,h)anthracene	23.553	200	447	1	221, 297, 35	
	<input type="checkbox"/>	Benzo(ghi)perylene	23.999	200	447	1	288, 299, 36	
	<input type="checkbox"/>	Indeno(1,2,3-cd)pyrene	24.816	200	447	1	212, 250, 30	

Fig. 28: Spectral Library View

The *Spectrum Name* and *Comment* columns can be edited. To delete a spectrum from the library, select its line and press the **Delete** key.

To add a spectrum to the library, use the *Spectrum - Add to Library...* command (for more details see the chapter **Spectrum** on pg. 27).

The spectra may be overlaid with the current spectrum in the [Spectral View](#) by checking the checkbox in the *Show* column. To hide the spectrum, uncheck its checkbox. The overlaid spectra will be hidden automatically when another library is opened.

5.5.8 Spectral Search View

The *Spectral Search View* displays the matching spectra information found via the *Perform Library Search* command.

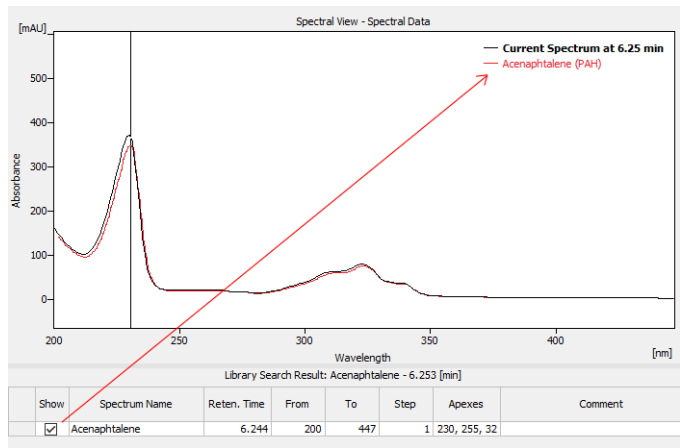


Fig. 29: Spectral Search View

The format of the table in the *Spectral Search View* is the same as in the [Spectral Library View](#). The spectra may be overlaid with the current spectrum in the [Spectral View](#) by checking the checkbox in the *Show* column. To hide the spectrum, uncheck its checkbox. The overlaid spectra will be hidden automatically when a new search is performed or the active chromatogram is changed.

5.6 Data Acquisition

The *Data Acquisition* window behaves the same way as on a standard instrument.

When using a **PDA** instrument, two additional commands are available in the *View* menu:

Show Signal(s)

Switches the display of the *Data Acquisition* window to showing the detector signals.

Show PDA Spectrum

Displays the real-time spectrum acquired by the PDA detector during a running analysis.

Show Isoplot

Displays an isoplot based on the acquired PDA spectral data.

These commands are available at any time if the instrument type is PDA and a spectral PDA detector is configured. However, spectra and isoplots are only shown during an active acquisition.

You can return to the standard signal view at any time using the *Show Signal(s)* command.

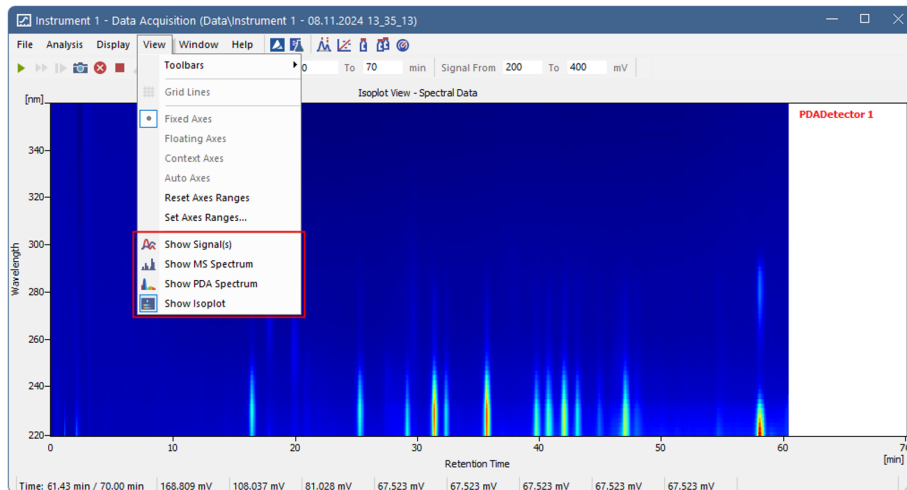


Fig. 30: Data Acquisition (PDA)

5.7 Report Setup

The *Report Setup...* command in the [PDA Chromatogram](#) window opens the *Report Setup* dialog on PDA tab.

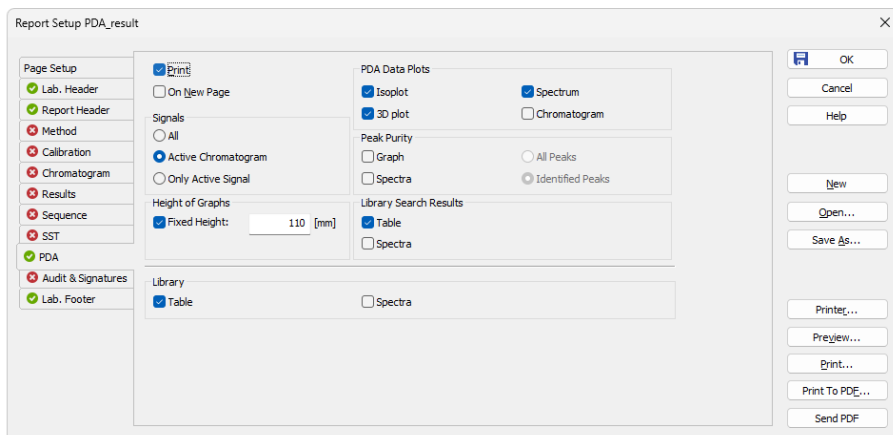



Fig. 31: Report Setup - PDA tab

Print

Allows/disallows the printing of the relevant part. If checked, the symbol  will be shown before the tab name and other fields on the tab will become editable.

On New Page

If checked, the relevant part will be printed on a new page.

Signals

Determines which signals information will be printed when there is more than one. You can choose to include either the method parameters from all signals of all chromatograms (*All*), all signals from the active chromatogram (*Active Chromatogram*), or only the parameters from the active signal (*Only Active Signal*).

Height of Graphs

If the *Fixed* checkbox is checked, the chromatogram will be printed with a fixed height instead of the fixed ratio 2:3. The lower height limit is *30 mm*, and the upper height limit is not set (the graph will be scaled to the page height if larger than the page itself).

PDA Data Plots

Enables the printing of the selected data plots. The given view will be printed if the *Isoplot*, *3D plot*, *Spectrum*, and/or *Chromatogram* checkboxes are checked. When the *Report Setup* dialog is invoked from the [PDA Chromatogram](#) window, the *Spectrum* and *Chromatogram* views will be printed WYSIWYG (including spectra overlays) instead of whole.

Peak Purity

Enables the printing of [Peak Purity View](#) (*Graph* option) and/or [Peak Purity Spectra View](#) (*Spectra* option), both either for *All Peaks* or only for *Identified Peaks*. When the *Report Setup* dialog is invoked from the [PDA Chromatogram](#) window, the *All Peaks* or *Identified Peaks* selection will be ignored as there is only one peak active in the [PDA Chromatogram](#) window, which will be displayed and printed if the *Chromatogram - Display Peak Purity* command was invoked previously.

Library Search Results

Enables the printing of [Spectral Search View](#) (*Table* option) and/or [Spectral View](#) with the actual spectra overlaid by the spectra gained from the library search (*Spectra* option). When the *Report Setup* dialog is invoked from the [PDA Chromatogram](#) window, the library search for the peak active in the [PDA Chromatogram](#) window will be displayed and printed if the *Spectrum - Perform Library Search* command was invoked previously.

Note: The spectra will be displayed in the overlaid [Spectral View](#) regardless of the *Show* column checked in the [Spectral Search View](#) table (as opposed to the printout of the [Spectral View](#) displayed by the *Spectrum* checkbox from the *PDA Data Plots* section).

Library

Enables the printing of the [Spectral Library View](#) (*Table* option) and/or the spectra of individual rows in the library (*Spectra* option).

Caution: The *Library* section items will be printed only from the [PDA Chromatogram](#) window.

5.8 Export and Import format

Chapters about export and import formats.

5.8.1 Export format

The **Clarity** PDA export format is based on the **EZChrom** export format. Resultant exported file is a text file with the following parameters:

- the name of the file listed in the **Export Chromatogram** dialog is in the case of **3D data** extended with a "-3D" inscription at the end of the respective name to enable the conjoined export of signals and 3D data
- 8-bit ASCII coding, code page according to settings of the operation system
- tabulator (ASCII code 0x09) is used as the field separator
- the sequence CR, LF (ASCII codes 0x0D, 0x0A) are used as new line separators
- text values are quoted with tabulators and ends of lines, tabulator and end of line symbols are not allowed otherwise
- real numbers are in decimal or science-technical notation (1.2345e+6), depending on which one is shorter; the dot "." is used as the decimal delimiter
- date and time are formatted according to the settings of the operation system

The caption of the exported file is formed from several lines in format:

<field name>:<tabulator><field value><end of line>

Individual fields in the file caption are the following:

Tab. 1: List of fields in the PDA Export caption

Field	Description
Version	The export version number, always 3.
Sample ID	The content of the <i>Sample ID</i> field in the <i>Single Analysis</i> dialog or the <i>Sequence</i> window.
Data File	The implicit path and filename of the exported *.PRM file.
Method	The name of the method used (without the file path and extension), provides information from the <i>Chromatogram - Measurement Conditions - Instrument</i> tab.
User Name	The author of the chromatogram (the content of the <i>Analyst</i> field on the <i>Chromatogram - Measurement Conditions - Instrument</i> tab).
Acquisition Time	The time and date of the acquisition (the content of the <i>Acquired</i> field on the <i>Chromatogram - Measurement Conditions - Instrument</i> tab).
Sample Rate (Hz)	The sampling frequency (in Hz).
Number of Points	The number of spectra in the chromatogram (the total number of samples on the time axis, in other words, the number of lines with values).

Field	Description
Wavelength Start (nm)	The minimal wavelength in the measured spectra (in nm).
Wavelength End (nm)	The maximal wavelength in the measured spectra (in nm).
Wavelength Step (nm)	The length of the step (in nm) between two consecutive points in the spectrum.
Points per Spectrum	The number of points in the spectrum (= the number of fields in one line of values; the formula for the <i>Points per Spectrum</i> value is: $Points\ per\ Spectrum = (Wavelength\ End - Wavelength\ Start) / Wavelength\ Step$).
Absorbance Units	The units of data values (after including the <i>Absorbance Multiplier</i> field, values can be in "μAU", "mAU", or "AU").
Absorbance Multiplier	The coefficient transferring (integral) values in lines of values to real values in units listed in the <i>Absorbance Units</i> field. The <i>Absorbance Multiplier</i> value is chosen as close to 1 as possible so that all values in lines of values are still integral.

The rest of the file contains lines of values. Individual values are integral numbers with sign, separated by tabulators. Lines contain spectra, columns signals in time for specific wavelength. First value on the first line corresponds to the time 0.0 min and minimal wavelength.

5.8.2 Import format

The import format is the same as the export format with the following changes:

Tab. 2: List of fields in the PDA Import caption

Field	Description
Version	The version of the imported file; must be 2 or 3.
Data File	The value is ignored; the name of file is filled in by the user during import.
Method	The value is ignored; no method is filled into the <i>Acq. method</i> field of the imported chromatogram.
Number of Points	The value is ignored; the real number of lines of values is used.
Points per Spectrum	The value is ignored; the real number of values in the first line of values is used.
Absorbance Units	Allows to set "u" and "micro" in place of "μ", "milli" in place of "m" and "V" in place of "AU". Furthermore, the "[", "]", " " and "-" characters on this row are ignored.
Volume (uL)	Fills the <i>Inj. Volume [ml]</i> field on the Chromatogram - Results tab by this value (after the conversion of units).

The imported file's caption can also contain any other parameters, but these will be ignored. It is necessary to keep the upper and lower case letters for important parameters, otherwise their values will be ignored. Any number of empty lines can be inserted between the caption and lines of values.

6 Clarity PDA operation

This chapter describes the basic operating principles for working in **Clarity** with **PDA Extension**. Only topics specific to the PDA mode are discussed here; for a detailed description of standard operations, refer to the **Clarity User Guide**.

The typical workflow for individuals conducting routine analyses should include:

1. Preparation of the PDA Method

[Setting PDA Instrument](#) described on pg. 44.

[Creating PDA Method](#) described on pg. 46.

[Extracting chromatogram signal from PDA data](#) described on pg. 52.

[PDA Libraries](#) described on pg. 55.


Note: If you have not acquired any PDA data yet and want to try out the functionality of the PDA Extension first, simply [open the Demo PDA project](#), as described on pg. 45.

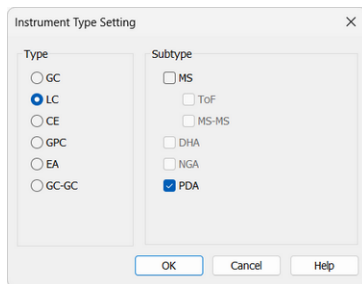
2. Routine measurements

Routine measurements will work the same as in the standard **Clarity**. This includes performing the integration and identification of peaks automatically, connecting the calibration, and showing the results. No significant changes of the workflow are expected compared to the non-PDA chromatography.

Additionally, the user of the **Clarity PDA Extension** might want to perform other actions such as [Importing PDA Chromatogram](#) described on pg. 59., [Creating and filling your own library](#) described on pg. 55., and [Managing PDA Library](#) described on pg. 56.

6.1 Setting PDA Instrument

- Start **Clarity** and open the *System Configuration* dialog.
- Use the  button to enter the *Instrument Type Setting* dialog. Instrument types **GC**, **LC**, **CE**, and **GPC** can be combined with the **PDA Extension**. To enable the PDA extension, simply check the *PDA* checkbox on the right side of the *Instrument Type Setting* dialog. Note that the PDA license (p/n A29) must be purchased otherwise the checkbox is disabled.



- Save and close the *System Configuration* dialog using the *OK* button.


6.2 Opening PDA demo project

There is a project containing DEMO data for the **PDA Extension** demonstration available in the software. It contains a set of chromatograms, prepared matching calibrations, and a sample PDA method. To open the DEMO_PDA project follow these steps:

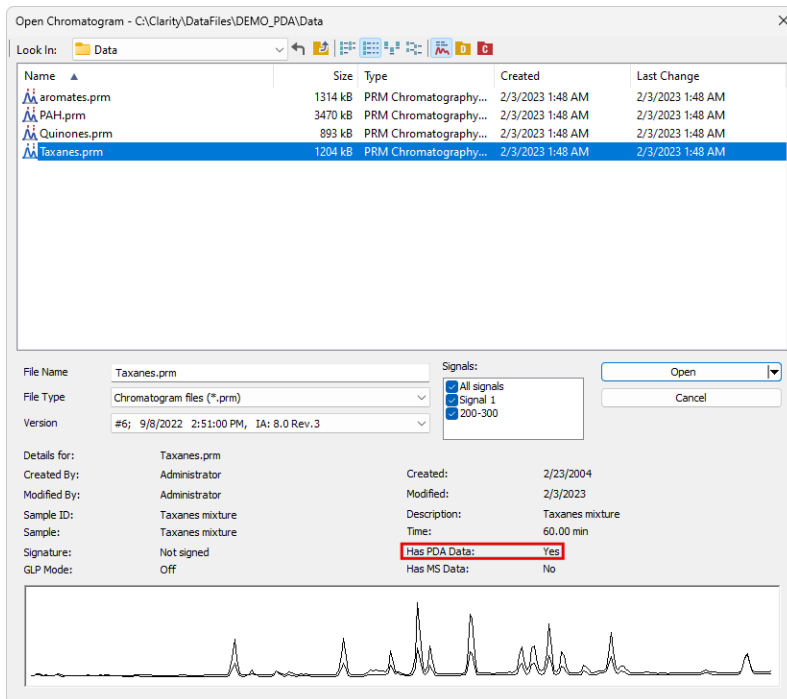
- In the opened *Instrument* window, select the *File - Project...* menu command. The *Project Setup* dialog will open.
- Use the *Open...* button to select the *DEMO_PDA* project in the *Open Project* dialog, then press the *OK* button.

Alternatively, the DEMO_PDA project may be opened directly when opening **Clarity** Instrument by selecting it in the *Login Dialog*.

6.2.1 Opening PDA chromatogram

1. In the *Chromatogram* window, click the *Open Chromatogram* icon .
2. Choose a chromatogram that **has PDA data**. The presence of PDA data is noted in the chromatogram details at the bottom part of the dialog.
3. After choosing chromatogram(s) click *Open* (or one of the other options when selecting multiple chromatograms).



Note: For more information regarding the opening options refer to chapter *Open Chromatogram* in the Reference Guide.

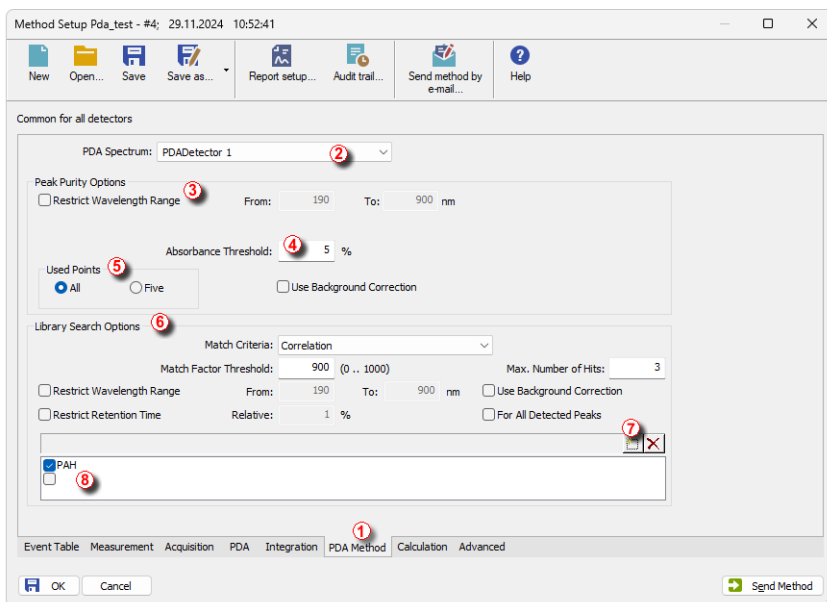


6.3 How to set PDA method

This section deals only with method setup related only to PDA options.

1. The *PDA Method* tab ① is available only when the PDA Extension is configured on the given instrument.
2. From the drop down menu ②, select *PDA Spectrum* if the chromatogram contains more than one (typically DAD and FLD).
3. *Peak Purity Options*: there are several settings that can restrict the peak purity evaluation. The *Restrict Wavelength Range* ③ can be used to restrict the peak purity evaluation wavelength range. Use the checkbox and fill the wavelength range.
4. Another restriction can be applied using the *Absorbance Threshold* ④. This determines which part of the peak will be evaluated. Threshold of 0% indicates that the entire peak will be included in calculation. At 5%, the spectra that have less than 5% of the apex spectrum absorbance will be excluded from the peak purity calculation, etc.
5. *Used Points* ⑤ specifies the number of points for the evaluation of peak purity; *All* indicates all spectral points, while *Five* uses only the five most significant points (peak start, peak end, peak apex, and two peak purity inflex points).

6. In the *Library Search Options* ^⑥, select the criteria according to which the *Perform Library Search* command will be performed (as described in the chapter "Spectrum").
7. To add another PDA library to search in, click the  icon ^⑦ and then . Choose the library in the *Select Spectral Library* dialog.
8. The list of libraries that will be searched is listed below ^⑧. You can enable/disable the search in specific libraries using the accompanying checkboxes.



6.4 PDA Window

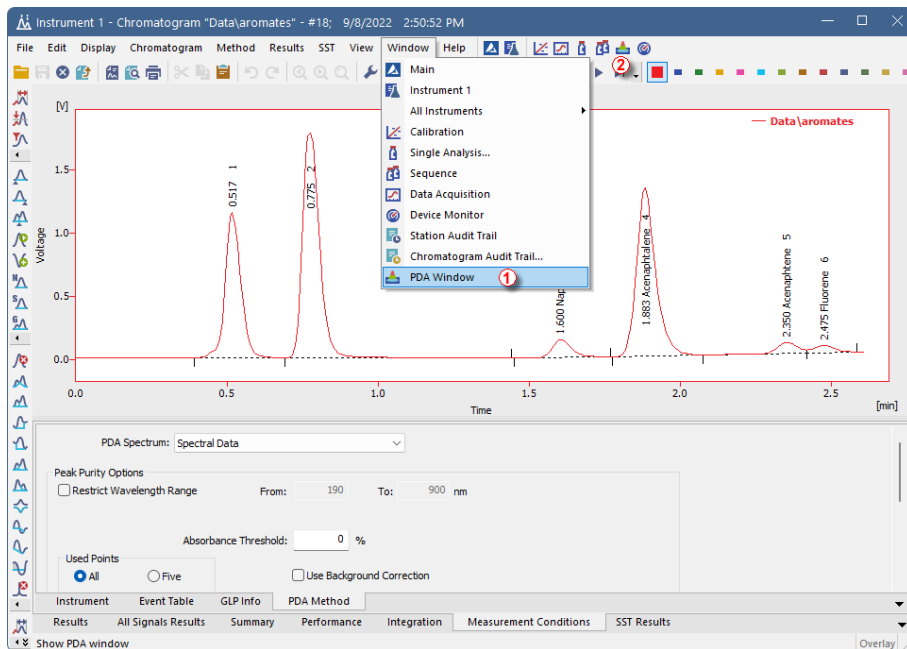
By default, the *PDA Window* is divided into 4 panes. Each pane contains a different information. To change the view in one of the panes, right-click on the pane you want to change and select the desired view from the menu that appears. The available views are:

- [Isoplot View](#)
- [Chromatogram View](#)
- [Spectral View](#)
- [3D View](#)
- [Peak Purity View](#)
- [Peak Purity Spectra View](#)

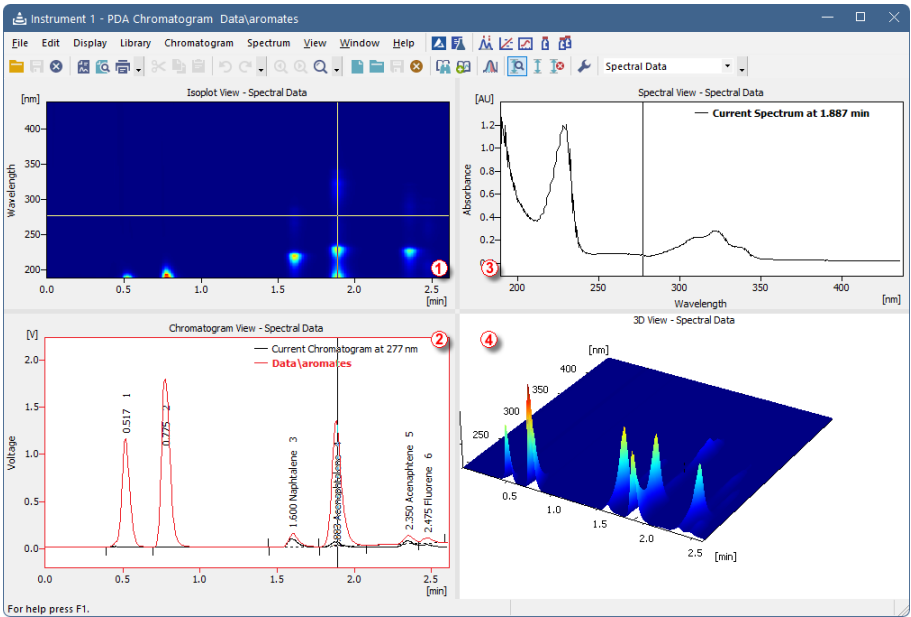
- [Spectral Library View](#)
- [Spectral Search View](#)

6.4.1 How to display PDA chromatogram data

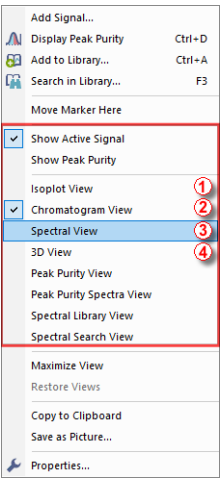
1. To open *PDA* window navigate to *Window - PDA Window* ① in the *Chromatogram* window alternatively click the *PDA Window* icon ②.



2. Spectra are automatically displayed in the *PDA Chromatogram* window upon opening chromatogram that contains PDA data.



3. To change a view of a pane, right mouse click and select one of the views.
4. Numbers ① to ④ correspond to different views in the picture above.

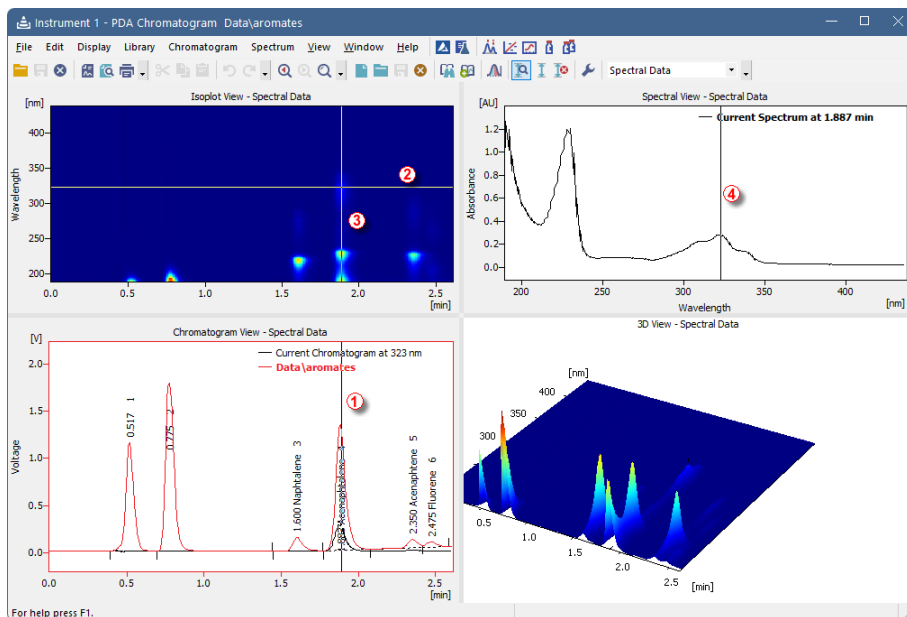






How to use markers in PDA Chromatogram

Panes in the *PDA Chromatogram* contain graphs with markers (thin lines of inverse color crossing the data plot ① ② ③ ④). Corresponding data are displayed according

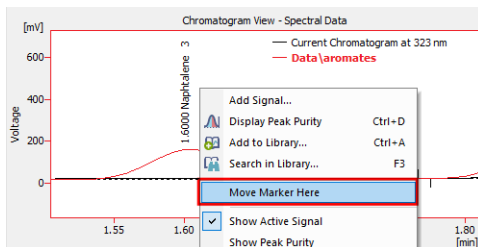
to the marker positions.

Note: Moving marker in one pane moves it accordingly in other ones. For example, moving marker ① in *Chromatogram View* will result in corresponding shift of marker ③ in *Isoplot View*.



- **To change spectral data based on time:** drag the vertical marker ① or ③ to the desired time. Note that the cross cursor changes to  once the move is possible.
- **To change wavelength:** drag the horizontal marker ② or ④ to desired position. Notice that the cross cursor changes to  or  respectively once the move is possible.
- **To change both:** wavelength and time, move to the junction where the two markers ② and ③ meet. Once the cross symbol changes to , left mouse click + hold + drag to your desired position.
- In the **3D View** you can move the whole graph to your area of interest - simply left mouse click + hold + drag. Note that markers in other panes will change accordingly to the moved area.

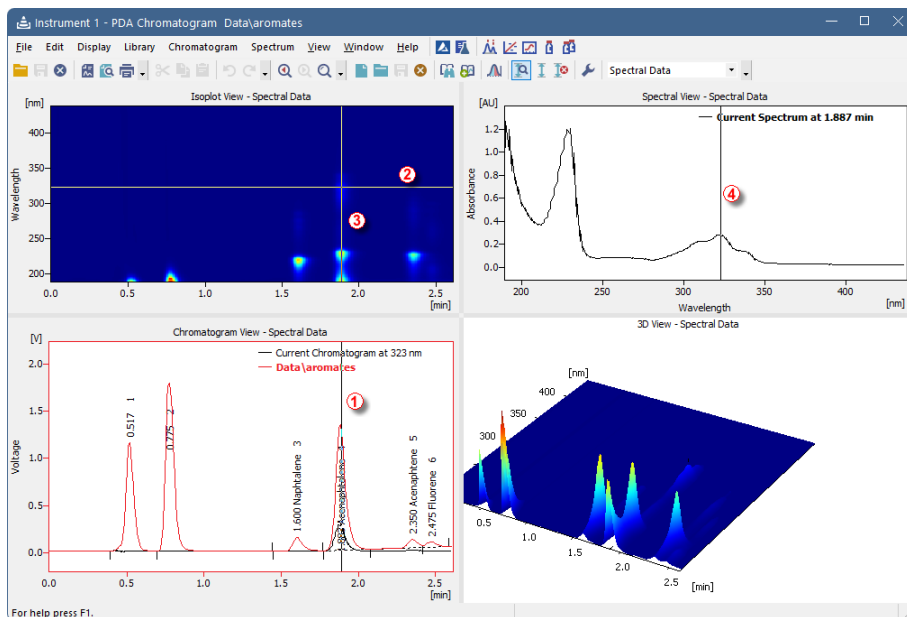
Caution: Increasing the zoom may cause that the markers to be out of the current view. To move them to the current zoom, right mouse click in the pane and use *Move Markers Here* from context menu.






6.4.2 How to use markers in PDA Chromatogram

Panes in the *PDA Chromatogram* contain graphs with markers (thin lines of inverse color crossing the data plot ① ② ③ ④). Corresponding data are displayed according to the marker positions.

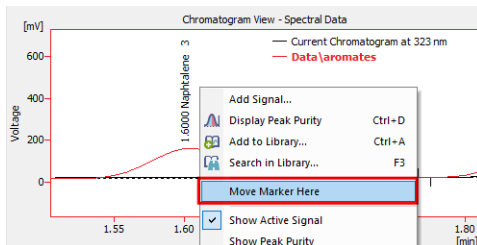
Note: Moving marker in one pane moves it accordingly in other ones. For example, moving marker ① in *Chromatogram View* will result in corresponding shift of marker ③ in *Isoplot View*.



- **To change spectral data based on time:** drag the vertical marker ① or ③ to the desired time. Note that the cross cursor changes to \longleftrightarrow once the move is possible.

- **To change wavelength:** drag the horizontal marker ② or ④ to desired position. Notice that the cross cursor changes to  or  respectively once the move is possible.
- **To change both:** wavelength and time, move to the junction where the two markers ② and ③ meet. Once the cross symbol changes to , left mouse click + hold + drag to your desired position.
- In the *3D View* you can move the whole graph to your area of interest - simply left mouse click + hold + drag. Note that markers in other panes will change accordingly to the moved area.

Caution: Increasing the zoom may cause that the markers to be out of the current view. To move them to the current zoom, right mouse click in the pane and use *Move Markers Here* from context menu.



6.4.3 Extracting chromatogram signals from PDA data

To add a signal at a specific wavelength and then calibrate it, use the following workflow.


1. In the *PDA Window*, use the horizontal line marker in the *Isoplot View* (alternatively, use the vertical line marker in the *Spectral View*) and move it to you desired wavelength.
2. Once satisfied with the current wavelength of the spectrum, add the signal using the menu *Chromatogram - Add Signal...* command.
3. The dialog for adding a signal will open. It is advantageous to use the signal's wavelength as the new name of the signal when using the *Add* option. Fill in the details and click *OK*.
4. In the *Chromatogram* window you will see there is a new signal with the name you have specified. (e.g. PAH - 232).
5. Now you can calibrate chromatograms based on the different wavelengths.

6.4.4 How to display peak purity

Displaying peak purity is one of the fundamental tasks when ensuring that no co-eluting or co-migrating impurities contribute to the peak's response.

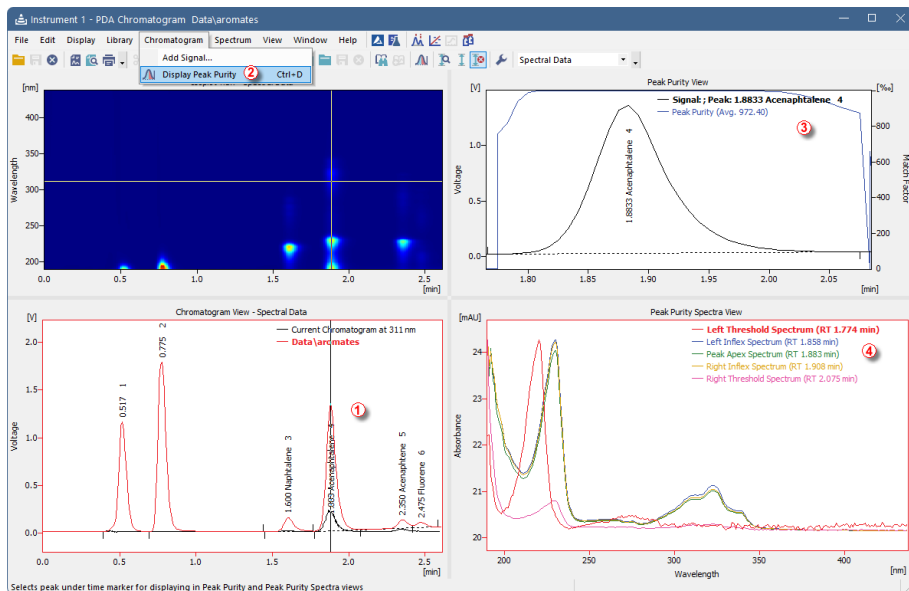
1. Used views: *Chromatogram View*, *Peak Purity Spectra View*, *Peak Purity View* and *Isoplot View*.

Note: See chapter "How to display PDA chromatogram data" on page 48 for more information about using the *PDA Chromatogram* window functions.

2. Move the marker ① to the peak for which you want to display peak purity.
3. In the menu *Chromatogram* - click the *Display Peak Purity* ② command or click the  icon in the toolbar.

Note: No peak selected in the *Peak Purity View* means that the marker from step 2 is not positioned on any peak.

4. *Peak Purity View*: displays signal for selected peak and its calculated *Peak Purity* ③.
5. *Peak Purity Spectra View*: displays spectra in several significant points ④ of the peak selected in the *Peak Purity View*.



6.4.5 How to view specific spectra in overlay

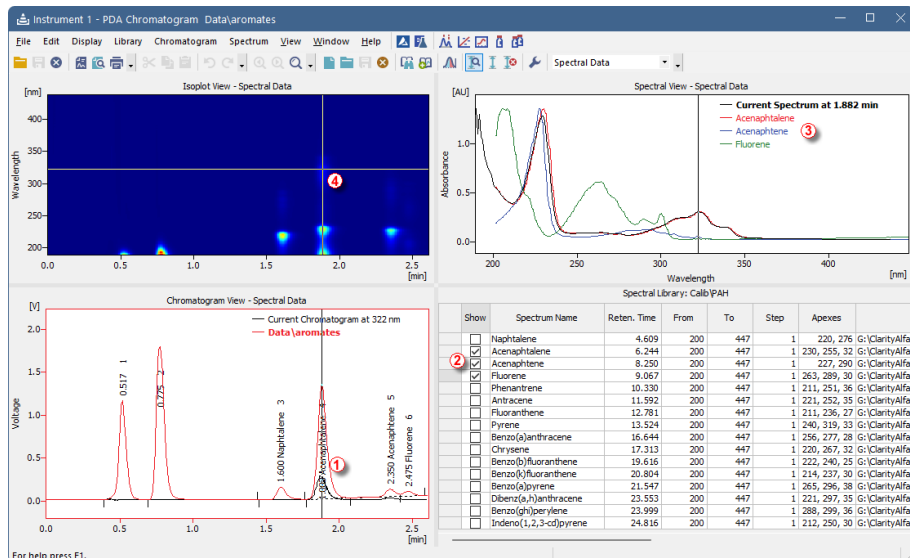
To view specific spectra from a PDA library in overlay and thus have the opportunity to compare the current spectrum against spectra from the PDA library, follow the steps below.

1. Used views: *Chromatogram View*, *Spectral Library*, *Spectral View* and *Isoplot View*.

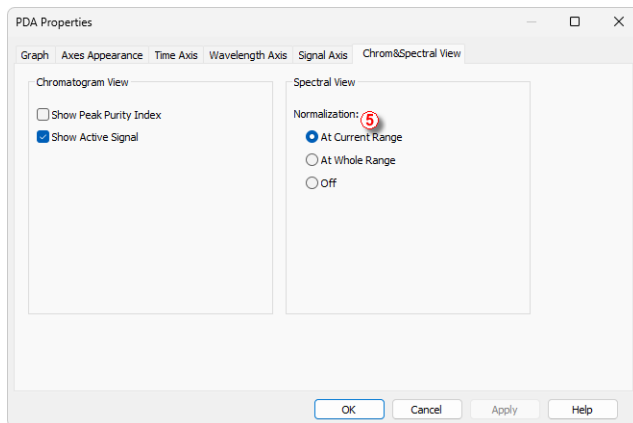
Note: How to change views is shown in "How to display PDA chromatogram data" on page 48.

2. Move the marker to your desired position ① .
3. In the *Spectral Library View* check the *Spectrum Name* for each ② spectrum that you want to show in the *Spectral View*.
4. *Spectral View* displays current spectrum along with other spectra ③ checked in the PDA library.
5. You can move the marker ④ in the *Isoplot View* to move alongside both wavelength and retention time axes.

Note that those steps can be also performed on results from the *Library Search* - thus having spectra from the search in overlay.



Note: To compare spectra it is recommended to normalize their view. Right click into *Spectral View* and select *Properties*. In *PDA Properties* dialog navigate to *Chrom&Spectral View* tab and select *Normalization: At Current Range* ⑤ .



6.5 PDA Libraries

PDA Library serves for storing compounds along with their PDA data such as spectrum. Working with PDA libraries and data is possible from *PDA Chromatogram* window. **Clarity** has one default library called PAH.LIB. Users can use this library or create a custom library. Alternatively, any number of libraries can be used to calculate results.




PDA libraries are saved in an ASCII format and can be edited by a text editor such as Notepad++, which is provided as an extra utility.

6.5.1 Creating and filling your own library



Libraries can be managed either from the menu *Library* or using the toolbar which is shown below.



Fig. 32: PDA library toolbar

- To create a new library, click the *New Library*  button.
- To open an existing spectral library, click the *Open Library*  button and choose your desired library.
- Adding a spectrum into a library is done by clicking the *Add Spectrum*  button, which opens *Spectrum Property* dialog. There, you can specify the compound name and add an additional comment.
- To add all identified peaks in the chromatogram at once, click the command from the menu *Spectrum - Add All Identified Peaks*.

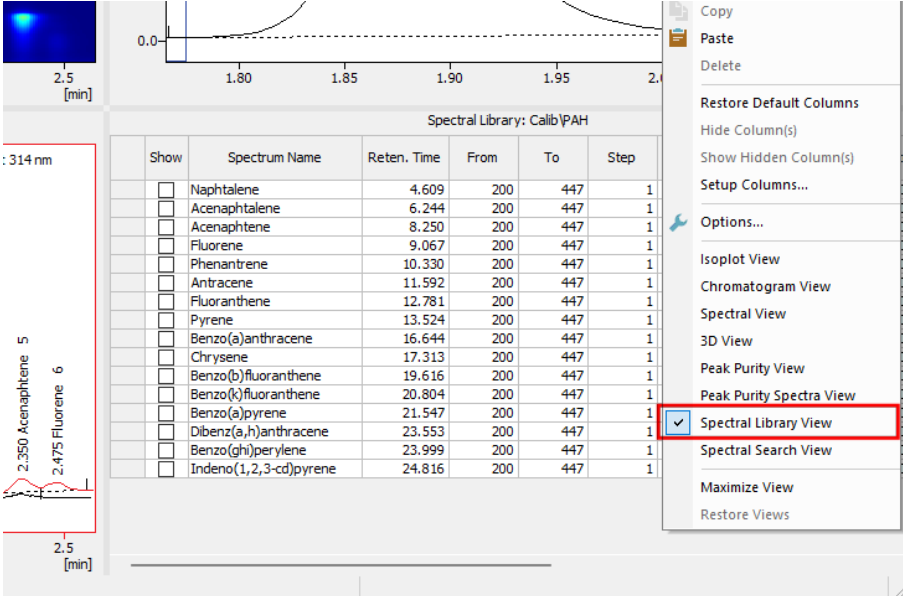
Note: Identified peaks are identified and named in the calibration file. Peaks are added into the currently opened library.

- If you have made any changes in the library and you want to keep them, click the *Save Library*  button.
- To close a library, use the *Close Library*  button. If you have unsaved changes you will be prompted to either save the changes or discard them.

6.5.2 Managing PDA Library

To manage a PDA library, it is possible to use either commands from the menu *Library* or commands from the *Library* toolbar as explained in the chapter "**Creating and filling your own library**" on pg. 55.

- **Spectral Library View:** to view contents of your library, right mouse click in any pane of *PDA Chromatogram* window and choose *Spectral Library View*. It contains a table with spectrum name, retention time and other parameters.

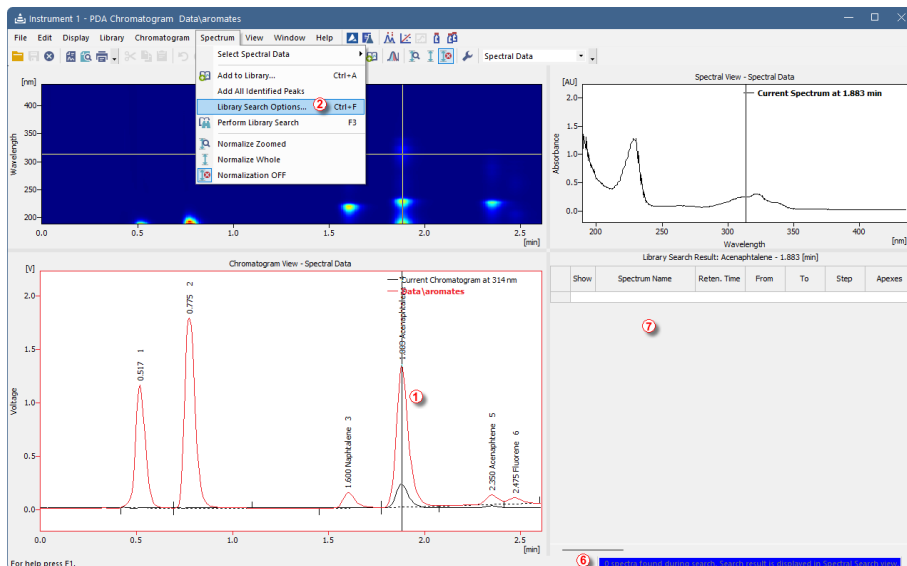


Spectral Library: Calib\PAH


Show	Spectrum Name	Reten. Time	From	To	Step
<input type="checkbox"/>	Naphtalene	4.609	200	447	1
<input type="checkbox"/>	Acenaphthalene	6.244	200	447	1
<input type="checkbox"/>	Acenaphthene	8.250	200	447	1
<input type="checkbox"/>	Fluorene	9.067	200	447	1
<input type="checkbox"/>	Phenanthrene	10.330	200	447	1
<input type="checkbox"/>	Antracene	11.592	200	447	1
<input type="checkbox"/>	Fluoranthene	12.781	200	447	1
<input type="checkbox"/>	Pyrene	13.524	200	447	1
<input type="checkbox"/>	Benzo(a)anthracene	16.644	200	447	1
<input type="checkbox"/>	Chrysene	17.313	200	447	1
<input type="checkbox"/>	Benzo(b)fluoranthene	19.616	200	447	1
<input type="checkbox"/>	Benzo(k)fluoranthene	20.804	200	447	1
<input type="checkbox"/>	Benzo(a)pyrene	21.547	200	447	1
<input type="checkbox"/>	Dibenz(a,h)anthracene	23.553	200	447	1
<input type="checkbox"/>	Benzo(ghi)perylene	23.999	200	447	1
<input type="checkbox"/>	Indeno(1,2,3-cd)pyrene	24.816	200	447	1

6.5.3 Searching a PDA library

To search for a matching compound in a PDA library, follow this procedure:



1. Move the marker ① to the peak for which you want to find a matching spectrum in a library.
2. Right-mouse click to a pane you do not need and select *Spectral Search View* to display the view which shows search results.
3. Use the *Library Search Options...* ② option from the *Spectrum* menu. The *Spectral Library Search Options* dialog will pop up.

Note: The same can be achieved by pressing the **CTRL + F** keyboard shortcut. Alternatively, you can use the *Perform Library Search* command from the *Spectrum* menu (or the  icon or **F3** shortcut) if no spectral search parameters have been set previously.

The library search is based on multiple parameters (mainly the *Match Factor*). Compounds are excluded from the search results if any of the search parameters do not apply.

Spectral Library Search Options

Match Criteria: Least Square (dropdown) Copy From Current Method (button)

Match Factor: 800 (0 .. 1000)

Max Hits: 3



☒ Restrict Wavelength Range From: 200 To: 360 nm

☐ Restrict Retention Time ③ Relative: 20 %

Libraries:


- ☒ PAH
- ☐

Buttons: OK, Cancel, Help

4. Set the search parameters in the top half of the dialog.
5. Note that *Restrict Retention Time* checkbox ③ should be enabled only when the PDA library has been created under same conditions as the measured chromatogram.
6. You can add a new library entry using the  ④ button and subsequently the  ⑤ button to select library to be searched for a matching spectrum.
7. Once the criteria are set, click OK to apply them and to perform the search.

If no spectra meet your criteria, the search was unsuccessful. You may notice a blue ribbon ⑥ at the bottom of the window that states *0 spectra found during the search*. The *Library Search Result* table will be empty ⑦.

6.6 Importing PDA Chromatogram

- Open the Chromatogram window on the *Instrument* where the **PDA Extension** is active.
- Open the *PDA Chromatogram* window from *Window - PDA Chromatogram* or by clicking the **PDA**  icon.
- Use the *File – Import 3D* command to get the import selection. Select a file and press the *Open* button.

Note: **Clarity** currently supports *.CHR, *.CSV, *.TXT, *.RAW, and *.ASC files for the import. The *.CDF format is not currently supported for 3D.

- The *Import 3D Text File* dialog will open.
- Press the *OK* button to import the file.

7 Appendix - Mathematical Formulas

7.1 Match Factor

The Match Factor is calculated using the normalized spectral data on the basis of the *Match Criteria* selected in the *Chromatogram - Measurement Conditions - PDA Method* tab. In case the measured and library spectra do not have the same wavelength range, only their overlap is evaluated (selecting the higher minimum wavelength and the lower maximum wavelength from two spectra). In case the number of spectral points in this interval differs (the step size is different), the library spectrum is interpolated to match the wavelengths of the points in the measured spectrum.

Normalization

$$a_{i,norm} = (a_i - a_{min}) \frac{1}{a_{max} - a_{min}}$$

where $a_{i,norm}$ is the normalized spectral point value (absorbance) at wavelength i , a_i is the spectral point value at wavelength i , a_{max} is the maximum point value in the spectrum and a_{min} is the minimum point value in the spectrum.

Match Criteria: Least Square

$$MatchFactor = 1000 \cdot \left(1 - \sqrt{\frac{\sum_{i=1}^N (a_i - b_i)^2}{N}} \right)$$

where the sum is taken over all N points of the spectrum and:

a_i is the normalized point value of the measured spectrum in the apex

b_i is the normalized point value of the library spectrum

N is the number of spectral points

Match Criteria: Weighted Least Square

$$MatchFactor = 1000 \cdot \left(1 - \sqrt{\frac{\sum_{i=1}^N \left(\frac{a_i - b_i}{a_i + b_i} \right)^2}{N}} \right)$$

where the sum is taken over all N points of the spectrum and:

a_i is the normalized point value of the measured spectrum in the apex

b_i is the normalized point value of the library spectrum

N is the number of spectral points

The points where $a_i + b_i = 0$ are omitted from the calculation (number of spectral points N is not adjusted).

Match Criteria: Correlation

The correlation match factor is calculated as the Pearson Correlation Coefficient (R) is rescaled to interval $[0,1000]$:

$$x = \frac{N \cdot \sum_{i=1}^N (a_i \cdot b_i) - \sum_{i=1}^N a_i \cdot \sum_{i=1}^N b_i}{\sqrt{[N \cdot \sum_{i=1}^N a_i^2 - (\sum_{i=1}^N a_i)^2] \cdot [N \cdot \sum_{i=1}^N b_i^2 - (\sum_{i=1}^N b_i)^2]}}$$

$$\text{if } [N \cdot \sum_{i=1}^N a_i^2 - (\sum_{i=1}^N a_i)^2] \cdot [N \cdot \sum_{i=1}^N b_i^2 - (\sum_{i=1}^N b_i)^2] \leq 0, \text{ then } x = 0$$

$$\text{MatchFactor} = 1000 \cdot \frac{x+1}{2}$$

where the sum is taken over all N points of the spectrum and:

a_i is the normalized point value of the measured spectrum in the apex

b_i is the normalized point value of the library spectrum

N is the number of spectral points.

7.2 Peak Purity

Depending on the calculation setting selected in the *Chromatogram - Measurement Conditions - PDA Method* tab, *Used Points* section, the following data points are considered in the *Peak Purity* calculation:

- *All* - the spectrum of each data point from a selected interval is compared to the spectrum of the apex; the obtained values are averaged. The interval is defined by the set *Absorbance Threshold*. The interval start and end are identified as the points where the height of the signal over baseline is higher (lower) than the set *Absorbance Threshold*, which is defined as percent (%) of the detected peak height. When set to 0%, the entire peak is covered.
- *Five* - spectra of five significant peak points are compared to the apex spectrum; the obtained values are averaged. The selected five points are the *peak purity start*, *peak purity inflex*, *peak apex*, the second *peak purity inflex*, and *peak purity end*. The *peak purity start* spectrum is taken as the point spectrum in one-third of the distance between the interval start and the peak apex. The *peak purity inflex* spectrum is taken as the spectrum of the point in two-thirds of the distance between the interval start and the peak apex. For the *peak purity end* and the other *peak purity inflex*, the situation is analogous. The set *Absorbance Threshold* is taken into account for identification of the interval start and end.

The data are not normalized for the calculations. *Peak Purity* is calculated by averaging the Pearson Correlation Coefficients (*R*) of each considered data point rescaled to interval [0,1000]:

$$x_{point} = \frac{N \cdot \sum_{i=1}^N (a_i \cdot b_i) - \sum_{i=1}^N a_i \cdot \sum_{i=1}^N b_i}{\sqrt{[N \cdot \sum_{i=1}^N a_i^2 - (\sum_{i=1}^N a_i)^2] \cdot [N \cdot \sum_{i=1}^N b_i^2 - (\sum_{i=1}^N b_i)^2]}}$$

$$\text{if } [N \cdot \sum_{i=1}^N a_i^2 - (\sum_{i=1}^N a_i)^2] \cdot [N \cdot \sum_{i=1}^N b_i^2 - (\sum_{i=1}^N b_i)^2] \leq 0, \text{ then } x_{point} = 0$$

$$R_{rescaled,point} = 1000 \cdot \frac{x_{point} + 1}{2}$$

$$PeakPurity = \frac{\sum R_{rescaled,point}}{N}$$

where the sum in fraction coefficient x_{point} is taken over all N points of the spectrum and:

a_i is the spectral point value at wavelength i of each point according to the selected *Used Points* option

b_i is the spectral point value at wavelength i at RT max (apex)

N is the number of spectral points.

7.3 Background Correction

Using the *Background Correction* is optional for calculation of the *Match Factor* (*Library Search Options*) and *Peak Purity* (*Peak Purity Options*). The calculation is based on interpolating the baseline for individual spectral points (absorbances) between the peak start and peak end points. For each data point considered in the calculation (i.e., apex for *Match Factor*, all points or five significant points for *Peak Purity*), the spectral point values are corrected by the background correction factor (BCF), which is calculated as:

$$BCF_{i,point} = c_i + \frac{c_i - d_i}{n_{end} - n_{start}} \cdot (n_{point} - n_{start})$$

where:

$BCF_{i,point}$ is the background correction factor of the spectral point value at wavelength i of the data point according to the calculation type as mentioned above (e.g., apex...)

c_i is the spectral point value at wavelength i of the peak start

d_i is the spectral point value at wavelength i of the peak end

n_{start} , n_{end} , n_{point} is data point number of the peak start, peak end, or the data point according to the calculation type as mentioned above

The background correction factor is then subtracted from each spectral point value at wavelength i of the data point considered in the subsequent calculation:

$$a_{i,point}^{corrected} = a_{i,point} - BCF_{i,point}$$