DataApex
Clarity ™
CHROMATOGRAPHY SOFTWARE

PDA EXTENSION

Clarity Extension   ENG

Contents

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:

Instrument (blue text) marks the name of the window to which the text refers.

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 (when you already are in the topic describing the window).

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

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

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.

▌ **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 **Extension** for the **Clarity Chromatography Station** (from version 2.4). Any **Clarity** Instrument can use the **PDA Extension**.

The **Clarity PDA Extension** is a tool that is used for processing data that has been acquired from selected Photo Diode Array/Diode Array Detectors (**PDA**/**DAD**). Spectral data together with chromatograms add a third dimension to analytical data analysis.

The **Clarity PDA Extension** expands the capabilities of **Clarity Chromatography Station** by providing interactive spectral analysis, peak purity analysis and compound identification that is based on spectral library search. **PDA** data can be displayed in a set of optional views including 3D rendering.

PDA Extension is also compatible with **Clarity Offline** software.

2 Specification

The **PDA Extension** is an optional, fully integrated part of **Clarity** software. It can be ordered as a part of new datastation or as an Extension to existing datastation (p/n A29).

3 Installation

The **PDA Extension** is enabled by appropriate user code entered during installation or later by using the *Help - User Code* command from the Clarity main window.

Caution: PDA mode is available on **Clarity** Instruments of **LC**, **GC**, **CE** or **GPC** type.

To switch an Instrument to *PDA mode*, select the **LC-PDA**, **GC-PDA**, **CE-PDA** or **GPC-PDA** option from the Instrument Type Setting dialog.
Instrument Type Setting dialog is invoked by clicking on the ⋯ button in the System Configuration dialog.
Options that are technically possible and have been purchased are enabled by default. Otherwise they are automatically disabled.

Fig 1: Switching to PDA mode

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 the **PDA** data from various **PDA** detectors.
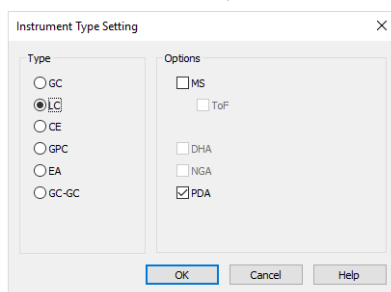- **Import/Export Data**: Spectral data can be imported and exported in ASCII text formats to or from the **Clarity** software.
- **Reports**: Users can easily include **PDA** options such as data **3D Display**, **Isoplot**, **Spectra**, **Peak Purity** and **Library Search results** in reports using the intuitive Report Setup dialog.
- **Instrument Control**: A control modules for **Agilent 1100 DAD**, **Agilent 1100 FLD**, **Duratec DDT-3200**, **Shimadzu M10Avp**, **Shimadzu M20A**, **Sykam S3210**, **Sykam S3240** is available. Additional control modules for other **PDA** detectors can be developed upon request.

4.1 Basic principles and terms

- **PDA View**: The PDA Chromatogram window is customizable; 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**: The **Clarity** software compares 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 **RT Window** and by **Wavelength Range**. Either the *Least Square*, the *Weighted Least Square* or the *Correlation Method* is used for calculating library search matches. A *Background Correction* option is also available.
- **Peak Purity**: This analysis helps to discover hidden impurities. **Peak Purity** test is applied to all integrated/calibrated peaks in the active signal and is calculated from 5 or all spectra within the peak. The similarity curve is displayed in the PDA Chromatogram window. **Peak Purity** analysis can be optimized by setting custom preferences relating to wavelength restriction and absorbance threshold.

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 accessed by 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 performed in case 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 to the left.

Absorbance Threshold

Defines the start and end spectrum for peak purity evaluation in % of the detected peak height. Available values range includes integer numbers in the range *<0 - 100>*.

Used Points

Sets whether the calculations of peak purity value will be carried out based on *All* spectra or only the *Five* significant points (peak start, peak apex, peak end, both peak inflexion points).

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.

Library Search Options

Match Criteria

Sets the type of match factor calculation. Possible options are *Least square*, *Weighted Least Square* and *Correlation*.

Match Factor

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

Max. Number of Hits

Limits the number of displayed spectra found by matching according to the other 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 peak **RT**).

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.

For All Detected Peaks

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

5.2 Chromatogram

The Chromatogram window is enhanced by **PDA**-related features on the Results and Measurement Conditions tabs.

5.2.1 Open Chromatogram

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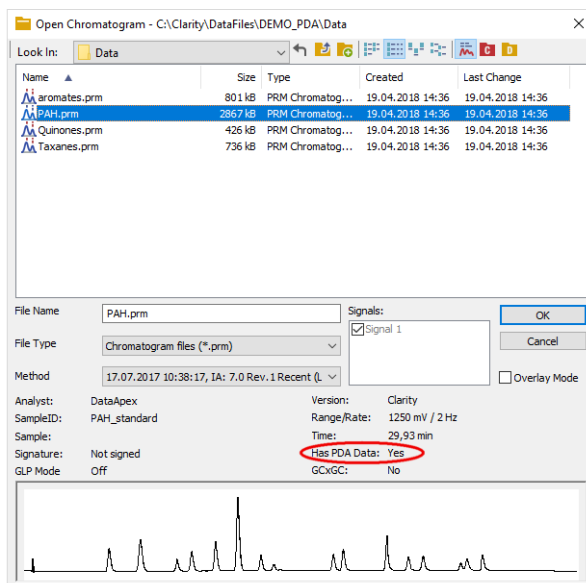

Fig 3: Open Chromatogram

5.2.2 Results

The **Result Table** of the chromatogram with the PDA part of the method is enhanced 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.

	PDA Peak Purity	Peak Type	Compound Name	PDA Name Match	PDA Best Match Name	PDA Best Match
1	947	Ordnr	Naphtalene	1000	Naphtalene	1000
2	886	Ordnr	Acenaphtalene	999	Acenaphtalene	999
3	968	Ordnr	Acenaphtene	1000	Acenaphtene	1000
4	804	Ordnr	Fluorene	999	Fluorene	999
5	737	Ordnr	Phenantrene	998	Phenantrene	998
6	705	Ordnr	Antracene	995	Antracene	995
7	859	Ordnr	Fluoranthene	999	Fluoranthene	999
8	935	Ordnr	Pyrene	1000	Pyrene	1000
9	816			0		
10	915	Ordnr	Benzo(a)anthracene	985	Benzo(a)anthracene	985
11	891	Ordnr	Chrysene	995	Chrysene	995
12	947	Ordnr	Benzo(b)fluoranthene	998	Benzo(b)fluoranthene	998
13	932	Ordnr	Benzo(k)fluoranthene	979	Benzo(k)fluoranthene	979

Fig 4: Result Table with the PDA data

PDA Peak Purity
Displays the *PDA Peak Purity* value of the peak.

PDA Name Match
Displays the match factor of the spectrum that was found in the first used spectral library based on the name of the peak gained from the **Calibration Summary Table**.

Caution: If there are multiple libraries specified in the **PDA** method (Chromatogram - Measurement Conditions - PDA), the *PDA Name Match* will search only the first library.

PDA Best Match Name
Displays the name of the spectrum found according to the method library search options. If there are more libraries specified in the **PDA** method (Chromatogram - Measurement Conditions - PDA), the *PDA Best Match Name* will search all libraries. The library name is displayed as a tool tip over the **Result Table** cell.

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

5.2.3 Measurement Conditions

The Chromatogram - Measurement Conditions dialog contains additional PDA sub-tab with **PDA**-related parameters of the chromatogram.

Fig 5: Chromatogram - Measurement Conditions - PDA

The individual items correspond to the items set in the Method Setup - PDA Method dialog described on pg **5**. The Method Setup - PDA Method tab displays the parameters of the template method that will be applied to new chromatograms, while the Chromatogram - Measurement Conditions - PDA tab displays the **PDA** method of the selected chromatogram.

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

5.2.4 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.
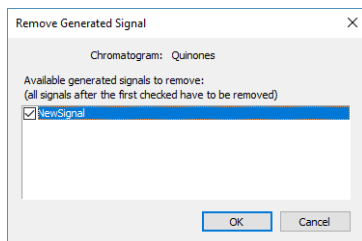

Fig 6: Remove Generated Signal

Only named signals can be removed. In case there are more generated signals in the chromatogram, with the one selected in this dialogue will be also removed all newer ones.

5.3 PDA Chromatogram window

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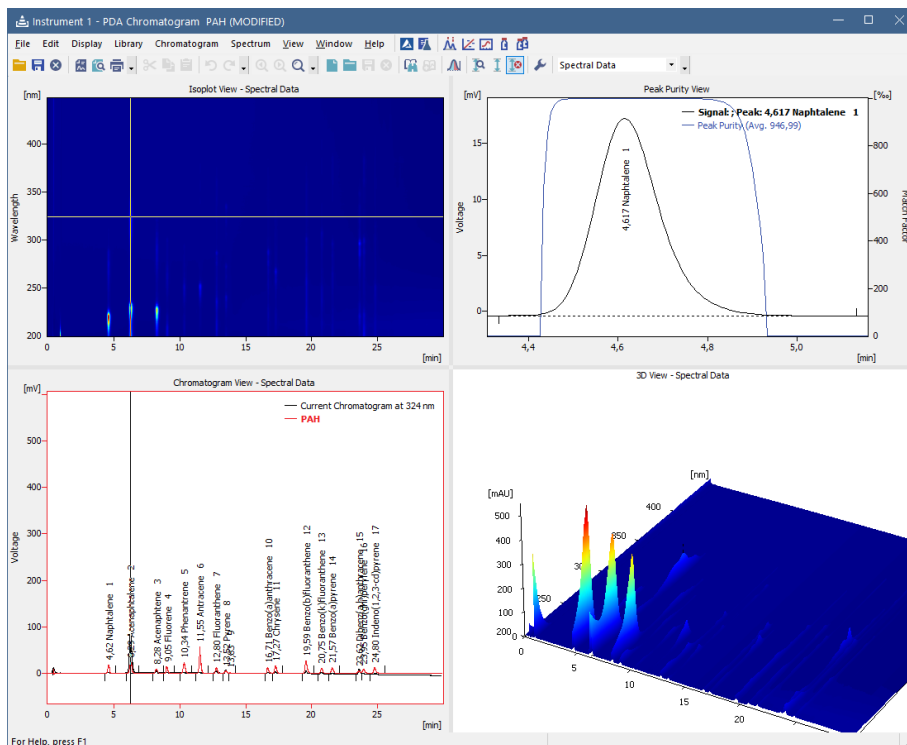

Fig 7: PDA Chromatogram window

This window is divided into four views and each has its popup menu in which you can:

- Change view in the respective rectangular.
- Maximize view to fullscreen.
- *Copy to Clipboard* (copies the image of the respective view to clipboard for use in your favorite graphic program).
- *Save as Picture* (allows creating the *.emf picture of the respective view).

5.3.1 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 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 Spectral Library View is hidden).
- Specific view can be displayed only in one pane at the time. Selecting a view (e.g. Isoplot) that is already displayed in another pane will result in switching the positions of the views (selected view could not be displayed at once in both the original and the new pane). Selecting a view that is not yet displayed will result in hiding the original view and displaying the selected one in the pane.

5.3.2 Markers

Isoplot , Chromatogram , Spectral and 3D views feature one or two **markers** (thin lines of inverse color crossing the data plot) depicting **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 time axis and depicts spectrum currently displayed in the Spectral view.
- **Wavelength marker** (horizontal in Isoplot , vertical in Spectral view) moves over wavelength axis depicting 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* marker(s) can always be brought within visible range.

5.3.3 File

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

📁	**Open Chromatogram…**	Opens the chromatogram that contains **PDA** data (**Ctrl** + **O**).
💾	**Save Chromatogram**	The command saves the active chromatogram (**Ctrl** + **Alt** + **S**).
❌	**Close Chromatogram**	Closes the active chromatogram (**Ctrl** + **Alt** + **W**).
	Import 3D	Opens the Import 3D Text File dialog for setting the reporting options
	Export 3D	Exports the **PDA** data to EZChrom format.
🖼	**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 **38**.
🔍	**Print Preview…**	Previews selected print configuration before printing (**Ctrl** + **Shift** + **P**). After selection, the Print Preview dialog will be displayed.
📄	**Print to PDF…**	Prints report to *.PDF file.
📧	**Send Printed PDF…**	Opens new email message in default email client, prints report to *.PDF and adds created *.PDF file as an email attachment.
🖨	**Print…**	Command for selecting printer and actual printing (**Ctrl** + **P**). After selection, the Print dialog will be displayed.
	Close Window	Closes the PDA Chromatogram window.

5.3.3.1 Import 3D

Imports the 3D **PDA** data from a *.TXT file. The format is compatible with the **EZChrom** 3D.ASC exports.

In general, the imports/exports contain only the matrix of signal values where:

- **Rows** represent time points at the time intervals corresponding to the *Sample Rate*.

- **Columns** represent individual wavelengths for the respective range as specified by the *Wavelength From* and *To* fields.

For more details see the chapter **Import 3D Text File** on pg **15**.

5.3.3.2 Export 3D

Export format is based on the export format EZChrom. For more details see the chapter **Export format** on pg **40**.

5.3.3.3 Import 3D Text File

Imports a chromatogram saved in a 3D text file.

A chromatogram in text format may (but need not) contain a heading with a description of the conditions of measurement and must contain data of the chromatographic curve in more columns.

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

- -

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 chromatograms 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 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 by the *OK* button.

- -

Note: If a number of files was selected in the Open Files to Import dialog, a further Import 3D Text File dialog or Import AIA File dialog will open (according to the type of the next selected chromatograms) after clicking on the *OK* button.

Preset

When the same type of files are imported frequently, it can be useful and time-saving to save import settings for further use. In drop-down box on the left user can select from previously saved presets, by clicking ⟩ button right to list the presets management menu will open. The menu contain commands for saving current setting (*Create New...*), *Rename...* or *Remove* presets. Presets are stored as part of **Clarity** Desktop settings.

Apply Settings to

This radio button group indicates whether all the settings below will be applied either to current file only or to all files imported at once. In case multiple files are imported at a time, and this radio buttons are set at *Current File*, the Import Text File dialog will be invoked for every file in the sequel. When *Apply Settings to* radio button is switched into the *All n Files* position, subsequent files will be proceeded with the same settings. By checking *Prefer Detected Settings* checkbox you can force Clarity to use setting detected from the imported file (where applicable).

Apply Method

Choose method whose parameters (integration table, attached calibration, etc.) will be applied into the imported chromatogram. By default, displayed method matches method in the Single Analysis dialog. Leaving this field blank applies default parameters.

Current Text File
The name of imported file including directory path.

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

Import From Line
Sets the line of the file on which the data import should start.

Import To Line
Sets the last line of the file that should be imported.

Separator
Selects the sign by which the individual items are separated in the text file. *<TAB>*, *<SPACE>*, *<COMMA>* or *<SEMICOLON>* are available signs 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.

- -

Note: Parameters entered to *Import From Line*, *Import To Line*, *Separator* and *Decimal Separator* fields will be applied on all simultaneously imported chromatograms.

Fig 8: Import Text File

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

These fields composing the chromatogram heading have the same meaning as described in the chapter "Single"

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 speeds 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 for 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 file using the suffix *.PRM with a path to the directory of the current project.

To select another name and location for the resultant chromatogram, open the Save As... dialog using the [...] button.

Load Defaults

Selects implicit values of all fields (i.e. returns the dialog into state prior to any changes made after opening).

OK

Confirmation of import.

Skip

Skips current file and proceed to subsequent one while importing multiple files.

Cancel

Cancellation of import.

5.3.4 Edit

Sub-menu of commands for working with clipboard and tables.

↩	**Undo**	Cancels adjustments in the tables. This may be used repeatedly as the station remembers all adjustments made to tables from its initial start-up. The history of commands only applies within the framework of the table and each table maintains its own independent list of operations. The command can also be invoked using the `Ctrl` + `Z` shortcut.
↪	**Redo**	Countermands the *Undo* command which can be invoked repeatedly. The station remembers all modifications made in tables during the last session. The history of commands applies within the framework of the table and table of each signal maintains its own independent list of operations. Commands can also be invoked using the `Ctrl` + `Shift` + `Z` shortcut.
🗐	**Copy**	Copies selected text into clipboard. The command can also be selected using the `Ctrl` + `C` shortcut.
📋	**Paste**	Copies the clipboard content to the desired location (`Ctrl` + `V`). The *Paste* function automatically inputs the content of the clipboard into the desired fields of tables. If the area is larger than the content, the content will be tiled. You may make use of this characteristic if you wish to insert a larger quantity of identical fields into a table or several periodically repeating fields.
	Delete	Deletes selected fields of the table (`Delete`).
	Select All	Selects all fields of table. This command can also be selected using the `Ctrl` + `A` shortcut.

5.3.5 Display

🔍	**Unzoom**	Cancels all cuts (**Ctrl** + *****).
🔍	**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 cut (**Ctrl** + **-**).
🔍	**Next Zoom**	Restores the original cut abandoned by the Previous Zoom command (**Ctrl** + **+**).
🔧	**Properties…**	Invokes the PDA Properties dialog for the settings of the graph properties. For more details see the description below the menu.

5.3.5.1 PDA Properties

Invoking the command or using the 🔧 icon opens the PDA Properties dialog similar to the Graph Properties dialog. There are two new tabs there - Wavelength Axis tab is in all respects the same as the Signal Axis tab, and the Chrom&Spectral View tab described here.
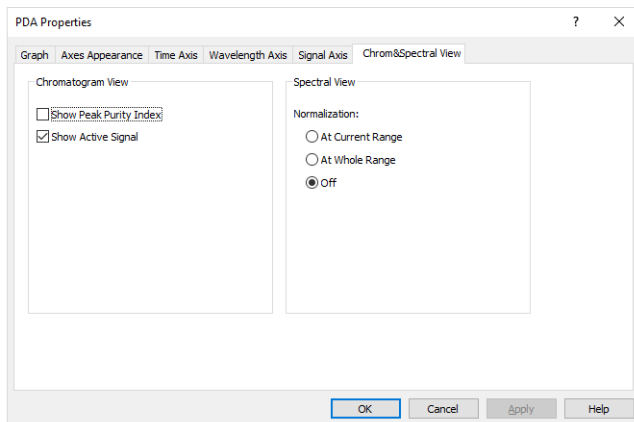
Fig 9: PDA Properties - Chrom&Spectral View

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 locked to the topmost fifth 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 **25**.

5.3.6 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 - Search in Library...* 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 Spectral Library Options dialog. For more details see the description below the menu.
❌	**Close**	Closes the spectral library (**Ctrl** + **Alt** + **W**).

5.3.6.1 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.
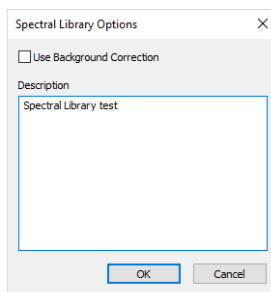
Fig 10: Spectral Library Options

Caution: Use the background correction consistently, either always and everywhere ON or always OFF to gain repeatable 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.

Description
Stores the description of the **Spectral Library**.

5.3.7 Chromatogram

	Add Signal	Add or replaces the chromatogram signal with a new signal taken as a cut from the **PDA** data. For more details see the description below the menu.
🔼	**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 the menu.

5.3.7.1 Add Signal

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

Fig 11: PDA Data - Add Chromatogram Signal

Add
Adds the new signal with the specified name (gained as a cut at selected wavelength) to the chromatogram from which it was created.

Replace
Replaces the selected signal in the chromatogram from which it was created by a new signal gained as a cut at selected wavelength. The Replace signal 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.

5.3.7.2 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, *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.

5.3.8 Spectrum

	Select Spectral Data	Allows to select from the spectra displayed in case there are more than one PDA spectra in the chromatogram.
	Add to Library…	Adds the selected spectrum to the spectral library (**Ctrl** + **A**). For more details see the description below the menu.
	Add All Identified Peaks	Adds the spectra of all identified peaks to the spectral library. For more details see the description below the menu.
	Search in Library…	Searches the library for matching spectrum (**Ctrl** + **F**). For more details see the description below the menu.
	Normalize Zoomed	Normalizes the spectra in the zoomed range. For more details see the chapter **Spectral View** on pg **31**.
	Normalize Whole	Normalizes the spectra on whole wavelength axis range. For more details see the chapter **Spectral View** on pg **31**.
	Normalization OFF	Turns the normalization off.

5.3.8.1 Add to Library
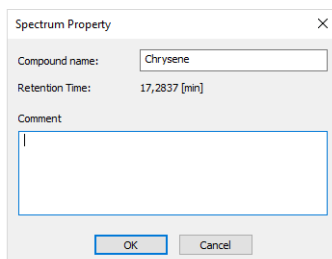
Adds the selected spectrum to the spectral library. Invoking the command, using the icon or the **Ctrl** + **A** shortcut invokes the Spectrum Property dialog, where user can name the compound and add comments to it before the spectrum is added to library. If the spectrum is already found in the library (matched by the same name), the user is asked to confirm the overwriting of the spectrum.

Fig 12: Spectrum Property

Compound Name
Serves for setting of the compound name.

Retention Time
Displays the retention time of the selected spectrum.

Comment
Allows the user to add custom comments.

5.3.8.2 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.

5.3.8.3 Search in Library

Searches the library for matching spectrum. Invoking the command, using the icon, `F3` shortcut or the `Ctrl` + `F` shortcut invokes the Spectral Library Search Options dialog.

Note: Using the icon only opens the Spectral Library Search Options dialog if no values are pre-set. If any values have been used previously, using the icon will skip the dialog and perform the search according to the settings.
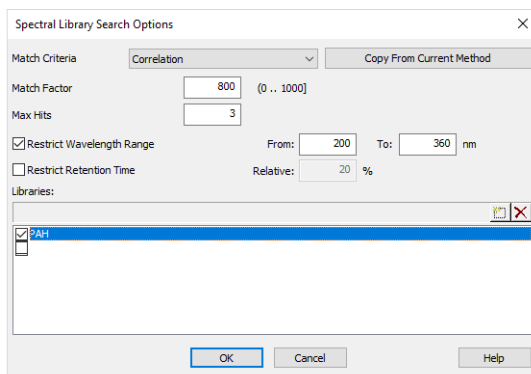
Fig 13: Spectral Library Search Options

Match Criteria
Sets the type of match factor calculation. Possible options are *Least square*, *Weighted Least Square* and *Correlation*.

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

Max Hits
Limits the number of displayed spectra found by matching according to the other criteria.

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 **9**).

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 peak **RT**).

Libraries

Specifies the libraries to be searched. Click the button to add a new line to the list and use the newly-emerged button to invoke the Open 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.

5.3.9 View

Commands for setting up the PDA Chromatogram window.

Toolbar	Displays/hides all toolbars. The command is similar to the *Toolbar* command in the Clarity main window (for more details see also chapter View).
Customize	Customizes the toolbars. The command is similar to the *Customize...* command in the Clarity main window (for more details see also chapter Customize...).
Reset All	Restores all menus and toolbars in the PDA Chromatogram window to their default state.
Maximize View	Maximizes selected view either in its own pane if it is already displayed or in the top left pane if it has been hidden so far.
Restore Views	Restores the layout of the views (panes) in the PDA Chromatogram window to the state before the *Maximize View* command was used last time.
Two Vertical Panes	Displays two vertical panes. When switching from four panes layout, views from left panes are displayed.
Two Horizontal Panes	Displays two horizontal panes. When switching from four panes layout, views from top panes are displayed.
Four Panes	Displays four panes.

5.3.10 Window

This section contains commands allowing to open other base windows.

Main ✓Full version	Displays the Clarity main station window.
Instrument	Displays the Instrument window.
Chromatogram	Displays the Chromatogram window.
Calibration	Displays the Calibration window.
Single Analysis	Displays the Single Analysis window.
Sequence	Displays the Sequence window.
Data Acquisition	Displays the Data Acquisition window.
Station Audit Trail ✓Full version	Displays the Audit Trail window.

5.4 PDA Chromatogram views

Chapters about PDA chromatogram views.

5.4.1 Isoplot View

The Isoplot view is the basic view of **PDA** spectral data. It displays the spectral data viewed from above with the absorbance values distinguished by color. The lowest values are represented by dark blue, rising over light blue, green, yellow up to red and dark red being the highest.
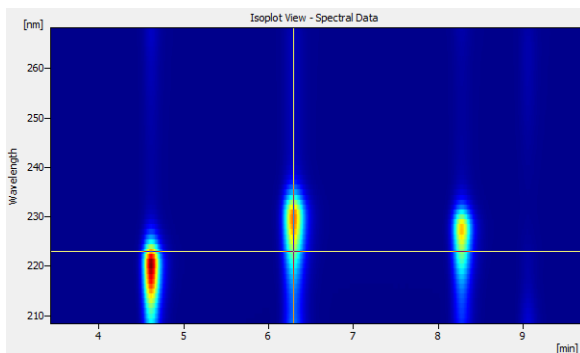
Fig 14: Isoplot View

5.4.2 Chromatogram View

The Chromatogram view displays slice of 3D data defined by actual position of the wavelength marker. It can also display **Active Signal** from the Chromatogram window and/or **Peak Purity** (match factor) curve for that signal.
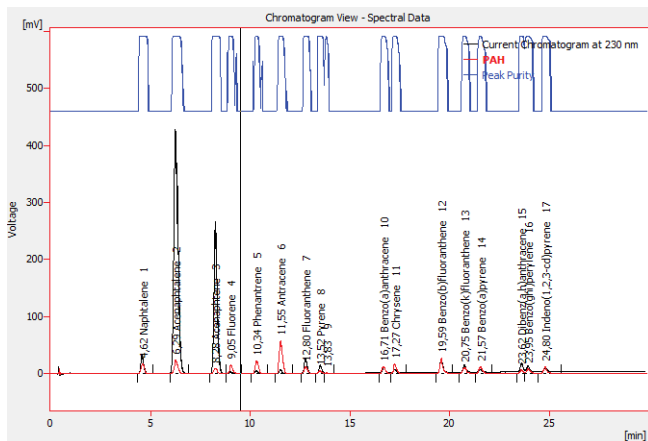
Fig 15: Chromatogram View

The display of **Active Signal** and **Peak Purity** curves is controlled either on PDA Properties - Chrom&Spectral Views tab or with *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 Chromatogram window by using the items on the Graph tab of PDA Properties dialog.

Peak Purity curve is shown in 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 more detailed way using Peak Purity View and *Display Peak Purity* function.

5.4.3 Spectral View

Spectral View visualizes the slice of 3D data defined by actual position of the time marker along with depicted spectra from Spectral Library View and Spectral Search View.
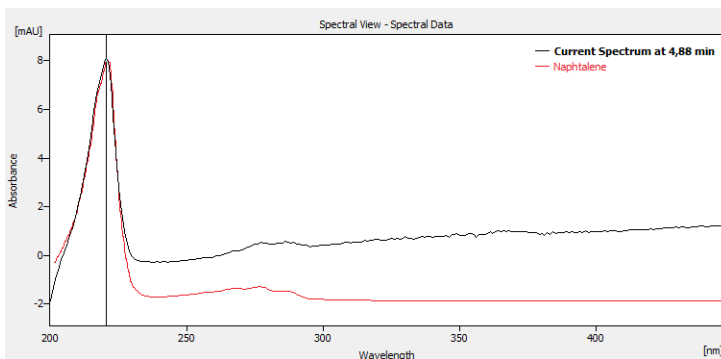
Fig 16: Spectral View

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

Normalized to 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 more advanced variety of the previous mode - spectra appear normalized as well, but this time 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.

5.4.4 3D View

The 3D View shows three-dimensional plot of **PDA** data with **Time** and **Wavelength** being the horizontal axes and height (and color) depicting the **Absorbance** value.
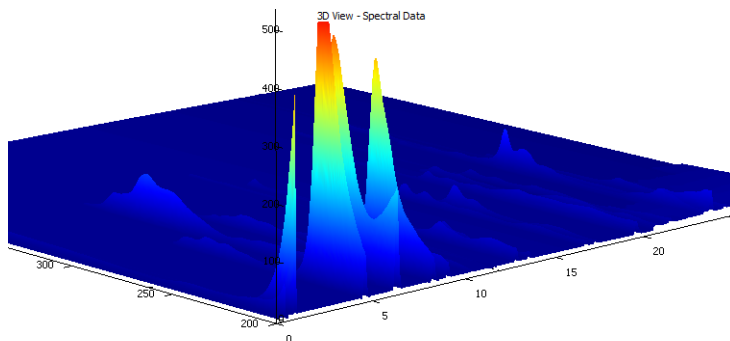
Fig 17: 3D View

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 markers move as well, as the view is always centered on the crossing point. **Move** mode can be set with *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 can be set with *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 can be set with *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* command on the context menu restores default projection of the 3D View pane.

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Note: The use of 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, respectively.

5.4.5 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** is displayed. If no peak has been selected, the *No peak selected* label is displayed instead.
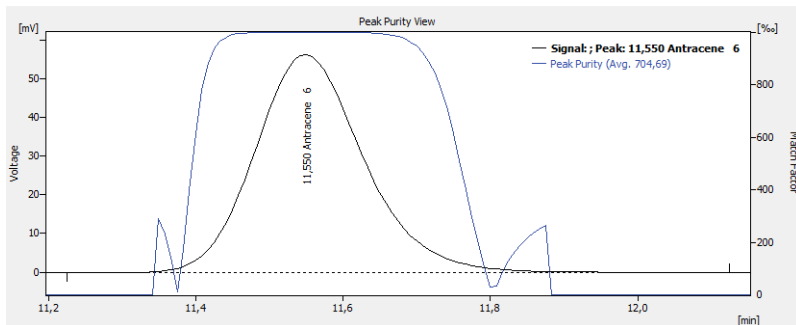
Fig 18: Peak Purity View

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 performed according to the settings from the **PDA** method of the chromatogram that can be displayed/edited on the Chromatogram - Measurement Conditions - PDA tab (for more details see the chapter **Measurement Conditions** on pg **9**).

5.4.6 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 19: 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.
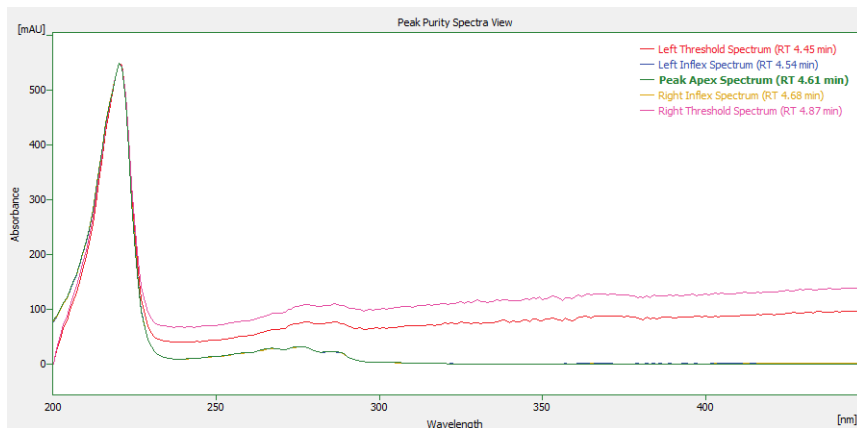The *Toggle to Match Factor* command from the context menu switches the view in the pane to Peak Purity View for the same peak.

5.4.7 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: PAH					
Show	Spectrum Name	Reten. Time	From	To	Step	Apexes
☐	Naphtalene	4.609	200	447	1	220, 276
☐	Acenaphtalene	6.244	200	447	1	230, 255, 322
☐	Acenaphtene	8.250	200	447	1	227, 290
☐	Fluorene	9.067	200	447	1	263, 289, 300
☐	Phenantrene	10.330	200	447	1	211, 251, 368
☐	Antracene	11.592	200	447	1	221, 252, 357
☐	Fluoranthene	12.781	200	447	1	211, 236, 276
☐	Pyrene	13.524	200	447	1	240, 319, 335
☐	Benzo(a)anthracene	16.644	200	447	1	256, 277, 287
☐	Chrysene	17.313	200	447	1	220, 267, 320
☐	Benzo(b)fluoranthene	19.616	200	447	1	222, 240, 256
☐	Benzo(k)fluoranthene	20.804	200	447	1	214, 237, 307
☐	Benzo(a)pyrene	21.547	200	447	1	265, 296, 384
☐	Dibenz(a,h)anthracene	23.553	200	447	1	221, 297, 351
☐	Benzo(ghi)perylene	23.999	200	447	1	288, 299, 362
☐	Indeno(1,2,3-cd)pyrene	24.816	200	447	1	212, 250, 302

Fig 20: 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 the spectrum to the library, use the *Spectrum - Add to Library...* command (for more details see the chapter **Spectrum** on pg **25**).

The spectra may be overlaid to 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 will be opened.

5.4.8 Spectral Search View

The Spectral Search View displays the matching spectra information found by the use of the *Search in Library...* command.
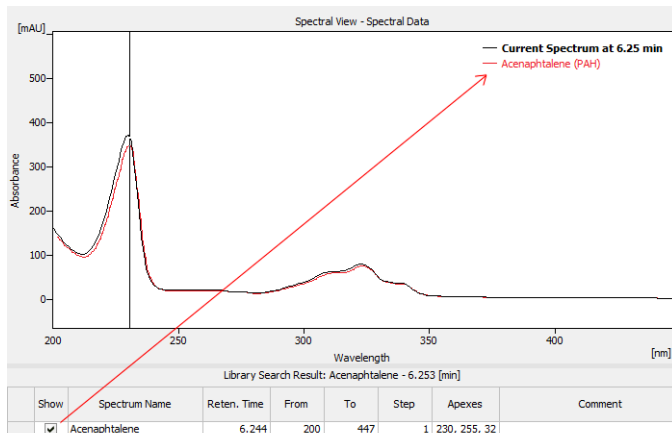
Fig 21: Spectral Search View

The format of the table in the Spectral Search View is the same as in the Spectral Library View . The spectra may be overlaid to 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** changed.

5.5 Data Acquisition

The Data Acquisition window works the same on the **PDA Instrument** as on standard **Clarity Instrument**.
Moreover, the **PDA Extension** adds the *Show Spectrum* toggle command to the *View* menu, which displays the real time spectrum acquired by the detector during running analysis. This command can be selected only during running acquisition. When selected the spectrum is shown only during the analysis.

5.6 Report Setup

The *Report Setup...* command in the PDA Chromatogram window opens the Report Setup - PDA dialog.
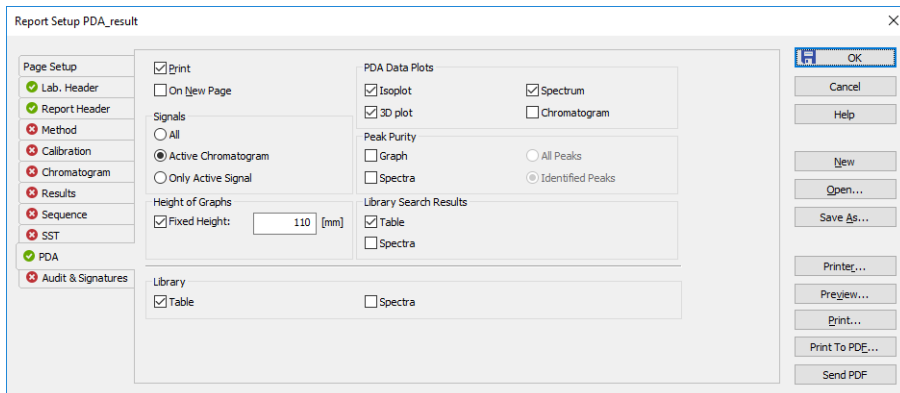
Fig 22: Report Setup - PDA

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 (detector) information will be printed when using a multi-detector configuration. You can choose to include either method parameters from all signals of all chromatograms (*All*), all signals from 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 permitted lower height range is *30 mm*, the upper height range 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 print 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 print of the 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 - Search in Library* command was invoked previously.

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Note: The spectra will be displayed in the overlayed 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 print of the Spectral Library View (*Table* option) and the spectra of individual rows in the library (*Spectra* option).

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Caution: The *Library* section items will be printed only from the PDA Chromatogram window.

5.7 Export and Import format

Chapters about export and import formats.

5.7.1 Export format

Export format is based on EZChrom export format. Resultant exported file is a text file with following parameters:

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

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 *Sample ID* field in Single Analysis dialog or the Sequence window.
Data File	The implicit path and filename of the exported *.PRM file.
Method	The name of the template method used (without file path and Extension), provides the info from the Chromatogram - Measurement Conditions - Instrument tab.)
User Name	The author of the chromatogram (the content of the *Analyst* field on the Chromatogram - Measurement Conditions - Instrument tab.
Acquisition Time	The time and date of the acquisition (the content of the *Acquired* field on the Chromatogram - Measurement Conditions - Instrument tab).
Sample Rate (Hz)	The sampling frequency (in Hz).

Field	Description
Number of Points	The number of spectra in the chromatogram (total number of samples on time axis, in other words the number of lines with values).
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 sequential 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 **Points per Spectrum** value is: Points per Spectrum = (Wavelength End - Wavelength Start) / Wavelength Step
Absorbance Units	The units of data values (after including the **Absorbance Multiplier** field, values can be in "µAU", "mAU" or "AU").
Absorbance Multiplier	The coefficient transferring (integral) values in lines of values to real value in units listed in the **Absorbance Units** field. The value is chosen as close as possible to 1 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 with 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.

5.7.2 Import format

Import format is the same as 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 *Acq. method* 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 *Inj. Volume [ml]* field on the Chromatogram - Results tab by the 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 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.

5 Clarity PDA operation

Basic operating principles for the work on **Clarity Instruments** configured on use with **PDA Extension** are described in this chapter. Only topics specific to **PDA** mode are discussed here, refer to the **Clarity User Guide** for detailed description of operations in standard mode.

The typical workflow for somebody working with routine analyses should consist of:

Preparation of the PDA Method

Setting PDA Instrument described on pg **44**.
Extracting chromatogram signal from PDA data described on pg **44**.
PDA Libraries described on pg **45**.
Creating PDA Method described on pg **46**.

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 described on pg **44**.

Routine measurements

Routine measurements will work the same as in standard **Clarity** , 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 non- PDA chromatography.

Additionally, user of the **Clarity PDA Extension** might want to perform other actions such as Importing PDA Chromatogram, Creating and filling your own library described on pg **45** . and Managing PDA Library described on pg **46**.

5.8 Setting PDA Instrument

- Start **Clarity** and open the System Configuration dialog.
- Use the ⋯ to enter the *Instrument Type Setting* dialog. Some basic instrument types allow to combine it with a **PDA** Extension; enabling **PDA** mode of those instruments is done by checking the checkbox on the right hand side. Note that **PDA** license (p/n A29) must be purchased otherwise the checkbox is disabled.
- Save and close the System Configuration dialog using the *OK* button.

5.9 Opening PDA demo project

There is a project containing DEMO data for PDA Extension prepared in the software. It contains a set of chromatograms, prepared matching calibration and sample PDA method. To open the DEMO_PDA project:

- 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.

5.10 PDA Window

PDA window is by default divided into 4 quadrants. Each quadrant contains a different information. To change a view, right mouse click in the quadrant you want to display the information in and choose desired view. Possibilities are:

- Isoplot View
- Chromatogram View
- Spectral View
- 3D View
- Peak Purity View
- Peak Purity Spectra View
- Spectral Library View
- Spectral Search View

- -
Note: Aforementioned views are discussed in depth in respective chapters.

5.10.1 Extracting chromatogram signal from PDA data

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

- In the PDA window - use the horizontal line marker in the *Isoplot View* (alternatively vertical line marker in the *Spectral View*) and move it to you

desired wavelength.
- Once satisfied with the current wavelength of the chromatogram, add the signal using the menu *Chromatogram - Add Signal...* command.
- Dialog for adding the signal will open. It is advantageous to use the signal's wavelength as the *Add* parameter. Fill in the details and click *OK*.
- In the Chromatogram window you will see there is a new signal called by the name of the signal it was created from, plus the name you have specified. (e.g. PAH - 232)
- Now you can calibrate chromatograms based on number of different wavelengths.

5.11 PDA Libraries

Clarity contains one default library called PAH.LIB. Users can use this library or create a custom library. Alternatively, multiple number of libraries can be used to calculate results.

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

5.11.1 Creating and filling your own library

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

Fig 23: PDA library toolbar

- To create a new library click the *New Library* button.
- To open existing spectral library click the *Open Library* button and choose your desired library.
- Adding a spectrum into the library is done by clicking the *Add Spectrum* button which opens Spectrum Property. In the dialog you can specify compound name and 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 those that correspond to peaks 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.

5.11.2 Managing PDA Library

To manage the **PDA Library** it is possible to use either commands from the menu *Library* or commands from the *Library* toolbar explained in the the chapter **"Creating and filling your own library"** on pg **45**.

5.11.3 Searching PDA library

Once your libraries are filled with spectral data it is time to perform a search on those libraries. The logic should be as follows:

- Go to menu *Spectrum* and click the *Search in Library...* command. In the dialog specify the search criteria. Once configured, click the *OK* button.
- Move the marker to the location of interest.
- Perform a search in the library using the *Search in Library* 🔍 button which performs the search according to criteria set in number 1.
- Results are displayed in the Spectral Search View.

5.12 Creating PDA Method

Creation of **PDA Method** consists of selecting a *PDA Spectrum* which is dependent upon the selected detector, *Peak Purity Options* and *Library Search Options*.
Peak Purity Options defines rules for peak purities.
Library Search Options serve for setting library search as well as defining libraries in which the search will be performed.