beyontics

PeakProvider 2.0

Operation Guide

Content

1. Introduction

Often Empower user get in trouble when trying to define clear relations between unknown peaks from several injections. One needs to make sure that the desired calculation is always based on the peaks from the same component.
This is necessary if e.g.

- a subtraction of matrix peaks needs to be performed
- to use these components in further calculations (e.g. results or statistics)
- to report statistics (e.g. mean results)
- to monitor components during studies (e.g. stability)
- Identification could be needed to transfer results to other systems (e.g. LIMS)

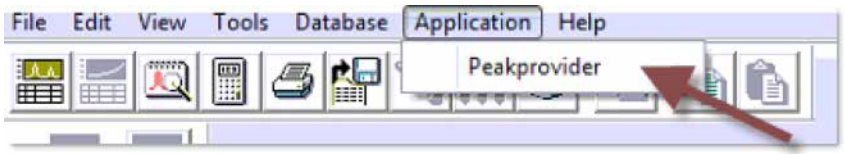
Although it is possible to create a peak table for all unknown peaks of one chromatogram manually, the user still needs to check whether this peak table fits to all chromatograms and in most cases further components have to be added and retention times and/or retention time windows defined in the peak table need to be adjusted.

With the PeakProvider beyontics offers a smart and reliable tool to assist Empower users in this tricky and time consuming task. As all calculations are performed in the same data system where the original data were produced the PeakProvider supports data integrity in particular. With the release of version 2.0 the PeakProvider provides more usability and more robustness in the identification of unknown components.

2. User Guide

2.1 Launching the PeakProvider

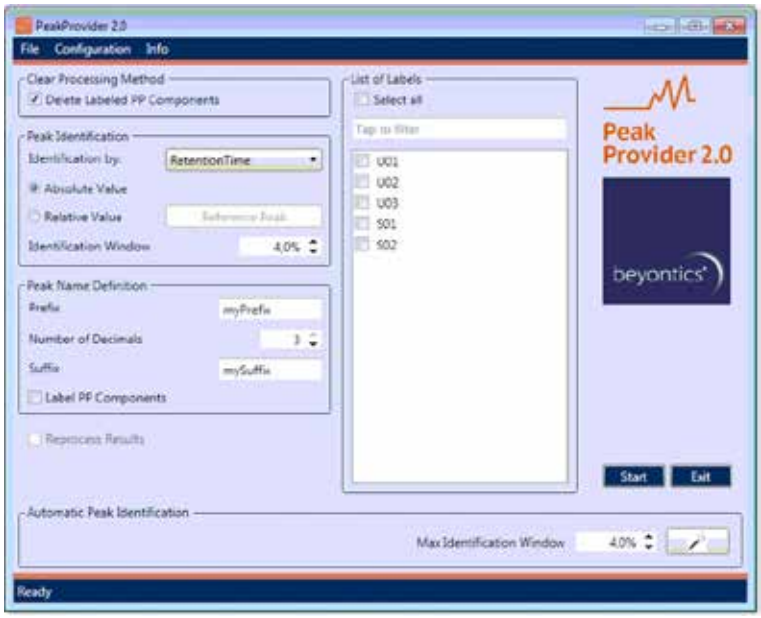
The PeakProvider is embedded in the Empower project window and can be launched from the menu item Application.



To launch the program a Result Set or one or more single Results need to be selected before in the Empower project window. The program cannot be launched from any other view table of the Empower project window.

2.2 The PeakProvider Main Window

When having launched the program the PeakProvider main window appears.



Object	Item	Selection
Menu Bar	File	Exit
		Closes the program
	Configuration	Settings
		Opens the Configuration Window
	Info	Help (F1)
		Access the online help
		About
		Information about the program
Clear Processing Method	Delete Labeled PP Components	Yes/No
	Components, which have been added to a method and have a PeakProvider label, are deleted from the component table before new components are added. Option can be activated or deactivated by this function.	
Peak Identification	Identification by:	Retention Time
	The default value is Retention Time. More values are available from the drop down list, in case they have been configured. The identification is based on this field either used as a relative or an absolute reference value.	
	Absolute Value	N/A
	If this option is activated, the identification is based on the absolute reference value based on the field defined for “Identification by:”	
	Relative Value	Define the Reference Peak
	If this option is activated, the identification is based on the relative reference value based on the field defined for “Identification by:” Furthermore, the “Define the Reference Peak” button becomes active.	
	Identification Window	x.x%
	This value is needed for the calculation algorithm and defines the size of a window, where peaks for the same component are searched.	

Object	Item	Selection
Peak Name Definition	Prefix	myPrefix
	The names of the added components can be configured. Here a fix prefix can be defined, which would than be part of the name for all identified components.	
	Number of Decimals	1 to 3
	The middle part of the components' name is the calculated identification value (e.g. Retention Time), the number of decimal places, which are indicated is defined here.	
	Suffix	mySuffix
	The names of the added components can be configured. Here a fix sufffix can be defined, which would than be part of the name for all identified components.	
	Label PP Components	Yes/No
	If this function is enabled, a predefined character is added to the component name, by which the component can clearly be identified as generated by the PeakProvider. This character is separated from the prefix by blank and then followed by the identification value.	
List of Labels	Select all	Yes/No
	If no labels are selected, the identification takes place for the whole set of data. With Select All a selection or deselection of all labels can be done.	
	Label Box	Checkmark desired label
	This box displays a list of all labels present in the selected set of data. Single labels can be selected or deselected, to define on which the identification should run.	
Reprocess Results	Yes/No	
	If this option is not used, only components are added to the method, but no new results are generated. If even a new result set should be produced, this option needs to be activated. Please Note: For some data this option is disabled, e.g. for single results or if more than one processing method is present for the selected set of data.	
Start	Button to click on	
	To run the defined job, the Start button needs to be clicked.	
Exit	Button to click on	
	To exit the application, the Exit button needs to be clicked.	
Status Bar		
	Here the status of your current job is indicated.	

Object	Item	Selection
Automatic Peak Identification	Button to click on	
	To run the automatic peak identification	
	Max Identification Window	
	x.x%, user defined value for the max size of the window that is used for the automated idenfication algorithm. Peaks with a distance greater than this window can not be identified as the same component.	

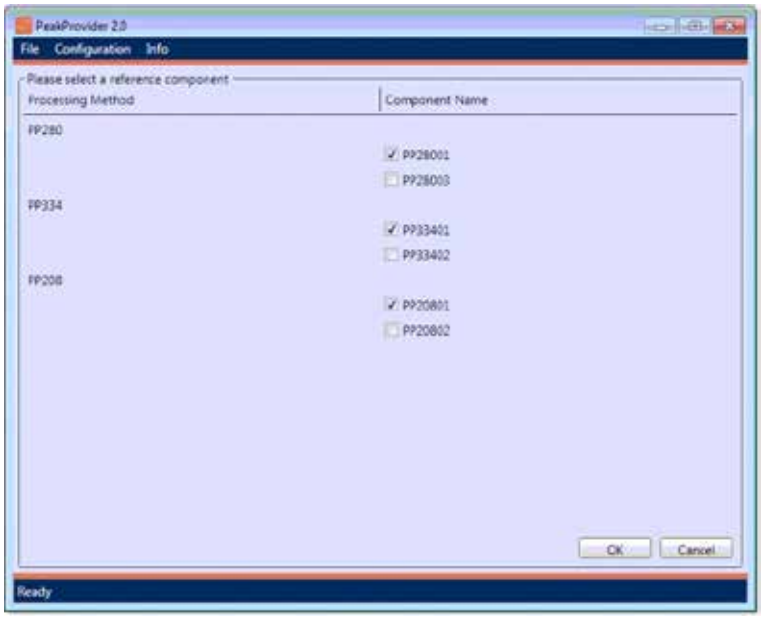
2.2.1 Peak Identification

For the identification of unkown peaks the user can define, by which peak related field this identification should be carried out. A list off all available peak fields is offered, as a default the Empower field “RetentionTime” is configured. The available peak fields in this list can be configured by the customer (cf. chapter 2.4). Furthermore, it can be defined, whether the identification should be computed by absolute or relative values. E.g. when having selected “Retention Time” as identification field, the computation can be performed using absolute retention time values or relative retention times to identify the unkown peaks.
The absolute value should be used, if no reference peak is present or can clearly be defined Peaks within the same retention section will get the same peak name. Only one peak inside this section can be assigned with a peak name in accordance to the settings configured in the Processing Method. Having a large number of peaks which elute in close quarters the window needs to be set as small as possible.

The algorithm proceeds in the following manner:

1. A list of all peaks of all selected results is created.
2. The list is ordered by the choosen identification value.
3. All peaks were the identification value is within the same identification section are identified as the same component.
4. Peaks within the defined identification section, but from the same result are skipped (the PeakProvider 2.0 reports a warning)
5. The mean identification value of peaks identified as the same component are calculated -> value is then also used for component names
6. The mean retention time of all peaks identified as the same component are calculated and -> entered to the Processing Method as component retention Time.

If a reference peak can be defined, the relative value is the identification mode of choice. The ratio is calculated by dividing the peak identification value by the identification value of the indicated reference peak found in the chromatogram. The calculated relative value is used as identification value for the identification procedure as described for absolute values.
When selecting “relative value”, a reference component needs to be selected, the button “Reference Peak” gets active. From here the follow window, that shows a list of all processing methods found in the selected results and all present component names associated to the respective method. For each processing method on component needs to be selected as reference peak.



2.2.2 Clear Processing Method

In most cases processing methods are used, which where applied to different results before and therefore, already contain component names that have been generated by the PeakProvider. In the case where former peakProvider identifications should be discarded, an option is provided to perform this in an automated way. By activating the option “Delete labeled PP components” all components where the name contains the configured PeakProvider label will be cleared before new names are added.
Please notice: All peak related field entries for those labeled components will also get lost in this case.

2.2.3 Peak Name Definition

The user can define a naming convention for the unkown components, that are identified by the program. For this purpose a prefix and and suffix can be defined.
The calculated value, by which the identification has been performed, is always part of the component name (e.g. retention time), the number of decimals displayed in the name can be defined as well. Low peak resolutions would demand a higher number of decimals, upt to 3 decimals can be displayed.
In the case where no customized name convention is defined, i.e. prefix and suffix have no entry, the system offers a default name: UNK as prefix to the identification value.
Moreover, with “Label PP components”, an option is provided by which clearly can be shown, which component name has been generated by the program.
A configured character, e.g. # would than be added to the component name.
This one makes it obvious not only for the user, but also for the program, that a peak name has been generated by the PeakProvider. This feature is important, when component names should be cleared before new entries are added to the component table of the processing method. I guarantees, that only component names are cleared, which have the configured PeakProvider label.
Please pay attention: The number of characters is not limited at this place, but the total number of peak name characters should not exceed the Empower limit of 30 characters.

2.2.4 Reprocess Results

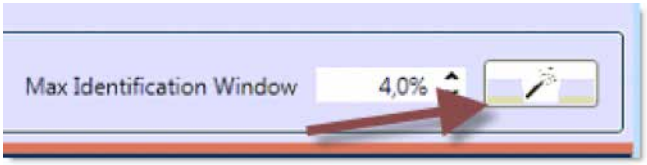
The program offers two operational modes:
The first one is called identification mode, which will only add new component names for all identified unknown peaks to the component table of the applied processing method.
The second one includes the first operational mode but will than also generate a new result set with the updated processing method. This one is called computation mode.
In order to enable the computation mode the option “Reprocess Results” needs to be activated.

2.2.5 List of Labels

For both operational modes the identification can be restricted to certain injections. Generally, for injections labels are assigned in the sample set. For the PeakProvider these labels can be used to apply the peak identification to defined injections.
A list of al labels present in the selected results is given in the filed “List of Labels”. These labels can be selected individually. The function “Select All” can be used to select or deselect all labels.
Please notice: Select all, does not mean, that all results are selected, but all where a label has been defined. If all results should be used for the idenfication process, no label must be selected.

2.2.6 Automatic Peak Identification

It is the maximum identification window in % defined by the user within the PeakProvider. The Max Identification Window is the identification window start value. Peaks with a distance greater than this window can not be identified as the same component. Actually, this values should be equal to the RT% value in the applied processing method.
The job is started using the button on the right hand site.



All settings defined are applied except the setting for the identification window. Here the optimum value is calculated for every processing method that is found in the results. The calculated values are then prompted in a separate window.

2.2.7 Start Button

When all settings have been defined, the PeakProvider operation can be carried. For this purpose, please click on “Start”.

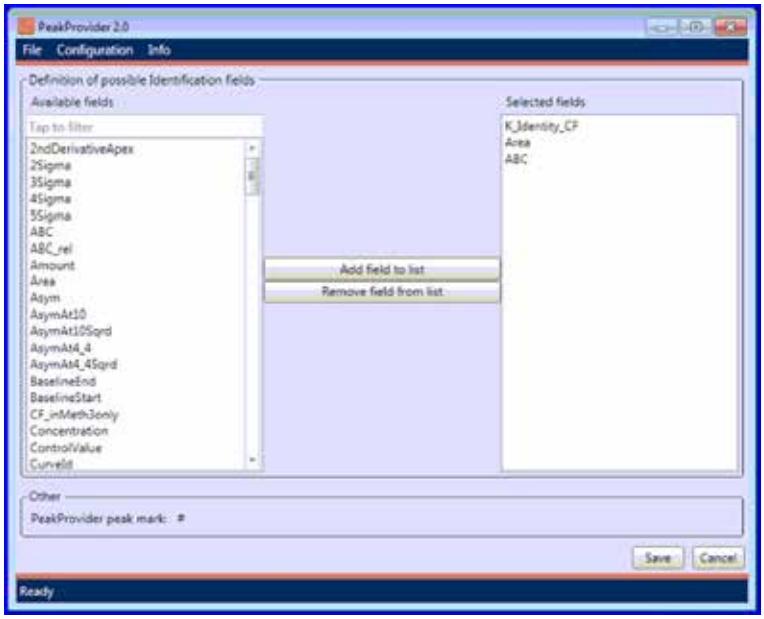
2.2.8 Status bar

The following status are defined: Ready, Starting Peak Identification, Saving Pro-

cesssing Method, Identification complete.

3. Configuration

The access to the configuration menu is controlled. Only Empower user who are member of a defined user group access is giving to these configuration settings. The user group is created during installation of the program.



Object	Item
Definition of possible Identification fields	Available fields
	All peak related fields, which are present for the current Empower project, are listed here. A filter option is available, where by simple typing the desired field(s) can better be retrieved.
	Selected fields
	All fields, which should be available for the common user are listed here.
Add field to list	
	A field selected on the left can be added to the right box by clicking on this button
Remove field from list	
	A field selected on the right can be removed by clicking on this button

Object	Item
Other	PeakProvider peak mark
	The PeakProvider peak mark ist defined during installation of the program. For information the selected character is displayed here, but can not be modified.
Save	
	Performed configurations are stored
Cancel	
	No modifications are performed. The previous settings are kept.

4. Data Handling

The following table gives an overview of how Empower result data can be handled by the program.

Kind of Data Set	# Channels	# Processing Methods	Identification*	Computation**
Result Set(s)	Single	Single	Yes	Possible
		Multiple	Yes	Possible
	Multiple	Single	Yes	Possible
		Multiple	Yes	Possible
Result(s)	Single	Single	Yes	No
		Multiple	N/A	N/A
	Multiple	Single	Yes	No
		Multiple	Yes	No

* Identification describes the process of updating the entries of the component table in a processing method by adding new component names, which have been calculated by the program.
** Computation describes the process of generating one ore more new Result Set(s) with the processing method that has been updated by the PP identification process.

5. Contact beyontics

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