beyontics

Peakprovider

Defining Unknown Peaks in Empower®

beyontics **PeakProvider 2.0 for Empower®**

A smart way of analyzing unknown peaks in Empower®

beyontics PeakProvider assists in analyzing unknown peaks by accelerating the evaluation of chromatograms with dozens of unidentified components and making results more reliable. Transfer to external calculation programs will belong to the past.

Analyzing unknown peaks in Empower. Do you recognize yourself?

When having lots of unknown peaks in your data, difficulties might occur for defining suitable peak tables in your processing method. Without these entries inter-sample calculations are not possible. Creating the best matching peak entries takes time and might cause difficulties. A manual check for each chromatogram within your data set against once defined peak entries needs to be carried out repeatedly, retention times need to be adjusted. Getting the best matching definitions in your table requires substantial time and effort. Just having a few unknowns might not be a big issue, but what about having dozens of them?

An automated solution. beyontics PeakProvider.

The PeakProvider is a smart and easy-to-use tool with a huge effect when lots of unknown peaks are present in your data on which inter-sample calculation needs to be carried out. By the application of a subtle algorithm, the tool determines identification criteria that matches all the chromatgrams within your data set, not just a single chromatogram. A unique name is assigned, by which each component can be identified clearly from injection to injection. No manual adjustment of your retention times is required anymore.

Easily integrated into Empower. How does it work?

With the PeakProvider beyontics provides a tool that is integrated in the Empower software and is especially useful for analyzing sample solutions containing a high number of unknown peaks. Additional peak names are added to the component table of an already existing processing method in an automated way, based on a user-defined selection of chromatograms.

Easy to use. The PeakProvider workflow.

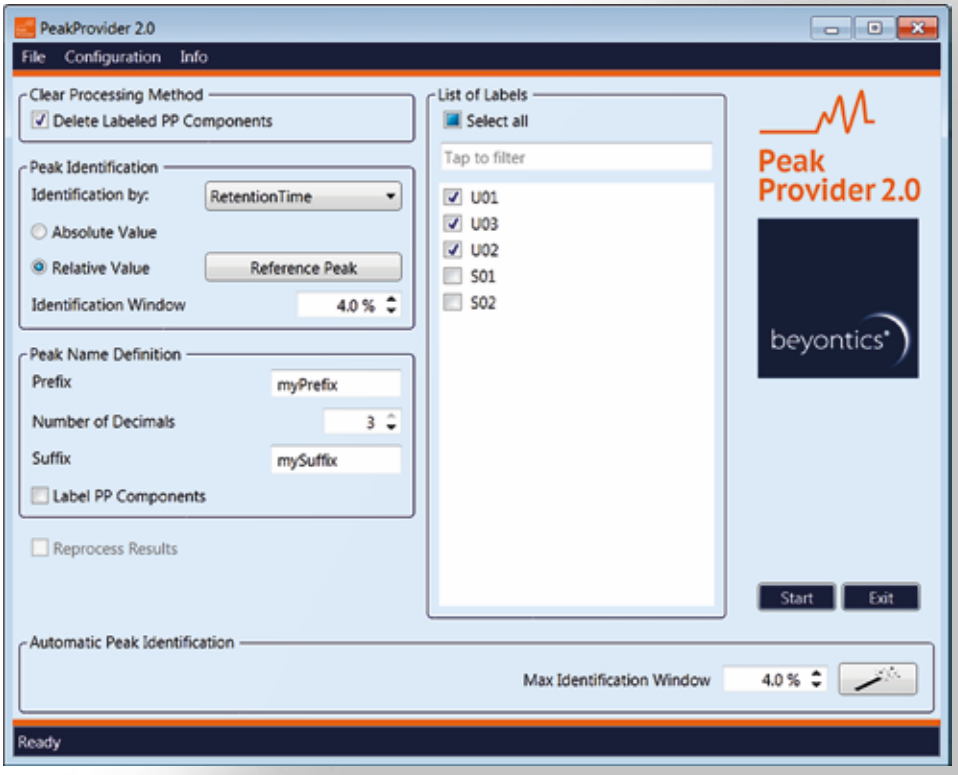
Peak identification is performed automatically by using either the absolute or relative retention time as part of the assigned peak name. Any prefixes or suffixes can be configured by the user.

Step 1:

Process your sample set in the usual way for generating a result set.

Step 2:

Apply the PeakProvider on the result set and define the kind of the desired identification for unknown peaks.



Step3:

A new result set is reprocessed by the PeakProvider. The applied processing method now contains peak entries for all identified unknown peaks in the component table.

Integration | Smoothing/Offset | Purity | PDA Library Search | **Components** | Impurity | Peak

Average By: None — Update RT: Never

RT Window (%): 5.00 — CCalRef1: PP208_01

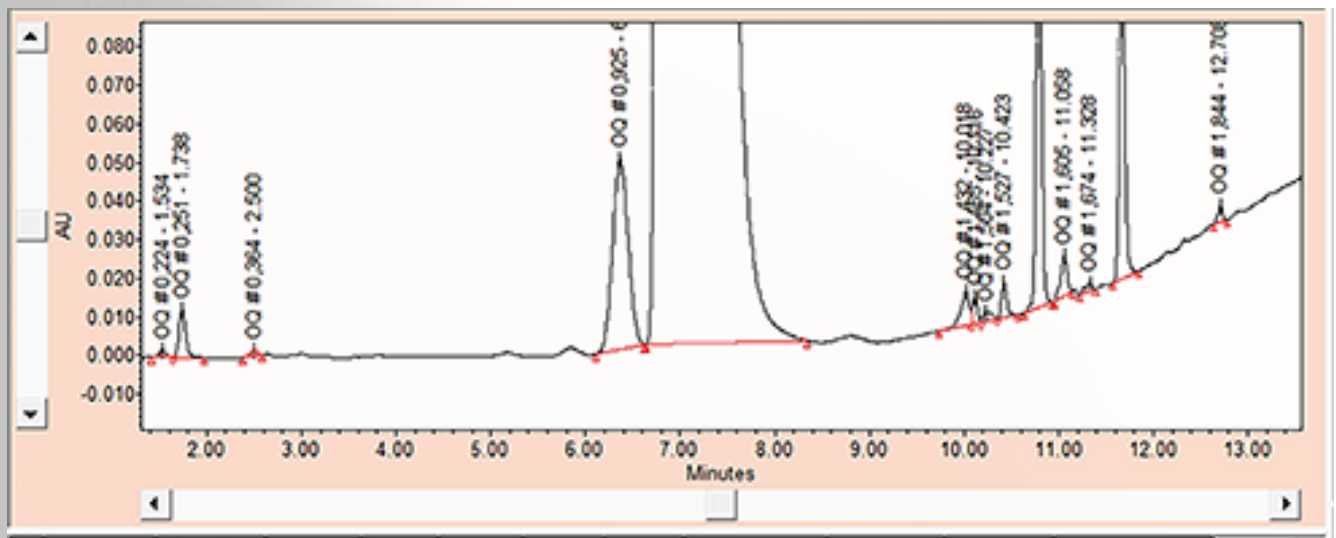
☑ Include Internal Std Amounts in % Amount Calculation

Sample Value Type: Amount — Auto Peak Label — RT Reference Used to Unnamed Peaks by RI

	Name	Component Type	Peak Label	Retention Time (min)	RT Window (min)	Peak Match	Y Value	X Value
1	OQ # 0,224			1.532	0.077	Closest	Area	Amount
2	OQ # 0,251			1.725	0.086	Closest	Area	Amount
3	OQ # 0,364			2.499	0.125	Closest	Area	Amount
4	OQ # 0,377			2.609	0.130	Closest	Area	Amount
5	OQ # 0,925			6.354	0.318	Closest	Area	Amount
6	PP208_01			6.900	0.345	Closest	Area	Amount
7	OQ # 1,432			9.901	0.495	Closest	Area	Amount

Names for all unknown peaks are added to the processing method. The name contains for example the relative retention time, that was calculated as a mean value based on all chromatogramms that have been considered during calculation. Thus, the PeakProvider makes sure, that the same component can be discovered in every chromatogram of the result set.

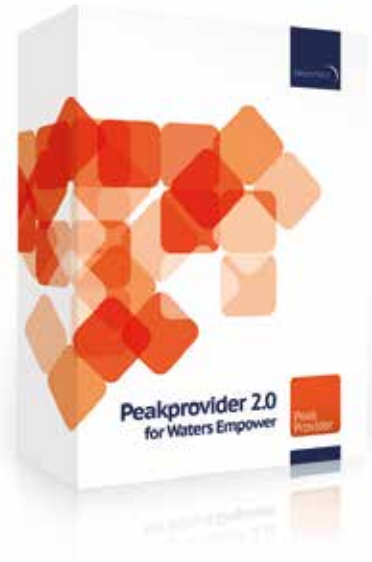
If the user has decided, that a new result set should be created by applying the updated processing method, all peaks in the reprocessed result set are clearly identified by a peak name. Summary evaluation in report tables or by custom fields are now possible for all known and unknown peaks.



	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Peak Type	Peak Codes	Peak Label	RelRetention_CF
1	OQ # 0,224	1.534	8928	0.02	1855	BV		Found	Q20		0.2245450
2	OQ # 0,251	1.738	59132	0.12	12389	VB		Found	Q20		0.2544315
3	OQ # 0,364	2.500	7734	0.02	1536	BB		Found	Q20		0.3659048

The functions of the Peakprovider at a glance:

- *integrated into Empower as a toolkit application*
- *intelligent algorithm to identify unknown peaks and assign unique peak names to the same components by choosing either relative or absolute retention time values*
- *automated detection of the most suitable section width to clearly identify same components of the operated chromatograms and assign unique component names*
- *a naming convention for the unknown peaks can be configured by defining prefixes or suffixes*
- *flagging of components added by the tool is possible*
- *decision whether or not flagged component names should be removed from the component table prior to a new identification step*
- *beside the retention time any customized peak field can be defined as a value, on which the identification should be based.*
- *full support of the Empower audit trail function*



Still not convinced? Get your free trial version now!

We offer a 30 days trial version for free. Please don't hesitate to contact us. For contact details, please look below.

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