



# PeakProvider 2.0

Release Notes

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## 1. Intention of the program

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 matches 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 tool to assist Empower users in this tricky and time consuming task. Now we would like to introduce a new release of the PeakProvider that provides more usability and a more robustness in the identification of unknown components.

## 2. Supported software infrastructure

The following software environments are supported

Operating System: Windows XP, Windows VISTA, Windows7

Empower Releases: Empower 2 FR4 and FR5, Empower 3 FR1

Prerequisites:

- Microsoft Windows Installer Tool Version 3.1 or higher
- .NET 4.0 redistributable
- VC++ 2010 (x86) redistributable

PeakProvider 2.0 supports 64 bit operating systems, but installation of VC++ 2010 redistributable has to be always x86 architecture.

## 3. License Scheme

### 3.1 Workplace Edition

A license is bound to a computer, where Empower is installed together with an Empower database.

### 3.2 Enterprise Edition

A license is bound to one database server, number of connected clients or terminal server is not restricted.

## 4. Installation Notes

Please refer to the document "Installation Guide PeakProvider 2.0".

## 5. New features

- The algorithm to identify unknown peaks and assign unique peak names to the same components has been improved.
- A function that automatically detects the most suitable section width to clearly identify same components of the operated chromatograms and assign unique component names has been implemented.
- Customizable peak names: A naming convention for the unknown peaks can now be defined by the operating user.
- The operating user can now define whether or not the added component names should be flagged.
- The operating user can now decide whether or not flagged component names should be removed from the component table prior to a new identification step.
- Possibility to base the identification on any peak custom field
- New branding of the PeakProvider GUI

## 6. Fixed issues

### 6.1 Handling of Result Sets processed from selected channels

#### 6.1.1 Description of the issue in PP 1.0

*When a Result Set is reprocessed in Empower indicating one Processing Method, and originally data acquisition has produced more than one channel for one injection but the generated Result Set only contains selected channels, the reprocessed data will contain all original channels processed by the selected Processing Method even if they are not part of the Result Set on which the reprocess is based. Therefore, the Peakprovider will not process new Result Sets from this kind of data. Only additional components detected by the Peakprovider will be added to Processing Method. The user is then asked to process the data again in Empower from the Sample Set by applying the modified Processing Method and selecting the channels of interest.*

#### 6.1.2 Behavior in PP 2.0

Only channels are processed that a part of the selected result set. Result sets can be processed no matter how many channels and how many different processing methods are present in the selected result set.

### 6.2 Selection of more than one reference

#### 6.2.1 Description of the issue in PP 1.0

*The possible number of references is equal to the number of underlying Processing Methods. Anyway if the same component name is present in more than one of the underlying Processing Methods, but will not be the reference in all of them a selection is not possible.*

#### 6.2.2 Behavior in PP 2.0

This issue has been fixed; there is no restriction in defining reference components.

## 6.3 Selected reference not present in underlying results

### 6.3.1 Description of the issue in PP 1.0

*Component names which are listed in the Peakprovider reference selection window derive from the Component Table of the underlying Processing Method. Anyway, it is thinkable, that a Component Name is listed, which is not present in the underlying results. Calculation will therefore be mistaken. It should be verified, that a component is chosen which also can be found in the selected results.*

### 6.3.2 Behavior in PP 2.0

The user is alerted in the case where the reference component cannot be found in the selected result data.

## 6.4 Deletion of all component specific entries within the processing method by the PeakProvider.

### 6.4.1 Description of the issue in PP 1.0

*For all components present in the component table of the processing method component specific entries have deleted even for components which were not created by the program.*

### 6.4.2 Behavior in PP 2.0

Component specific entries are kept after the program has been applied to a processing method. Deletion is only performed for a whole component row in the case where this is defined by the user (function: Deleted PP labeled components)

## 6.5 Process Method is locked after processing by the PeakProvider

### 6.5.1 Description of the issue in PP 1.0

*When the program has been applied to a processing method, the method still had an entry in the database that it is edited by the user.*

### 6.5.2 Behavior in PP 2.0

This issue has been fixed. The processing method is longer edited by the user

after the program has been run.

## **6.6 The PeakProvider has a problem to re-identify peaks, that were already identified by the PeakProvider**

### **6.6.1 Behavior in PP 2.0**

With a completely new identification algorithm and the option to let the choice whether present PeakProvider peaks should be kept or deleted prior to a new identification process the mentioned issue has been solved.

## **7. Known issues**

### **7.1 Use Existing Integration**

The Empower function „use existing integration“, when reprocessing result data is not supported by the program. The program creates an updated version of a processing method, but the Empower function always applies the version that has been used to process the initial result set. That's why an implementation to the program is not implemented. This issue depends on an Empower functionality, and is resolved in Empower3 FR2.

### **7.2 Default User Type**

The program can only be launched when logged in to Empower with the user accounts' default user type.

## **8. Qualification**

For the support of any OQ activities that needs to be carried out at the customers' site beyontics provides an Empower OQ project and an OQ plan and protocol. This OQ package can be purchased separately.



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## 9. Contact beyontics

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