Brunn User Documentation

Contents

1 Bioclipse

The Bioclipse project is a Java-based, open source visual platform for chemo-
and bioinformatics built upon the Eclipse Rich Client Platform (RCP). Brunn
is a plugin for Bioclipse.

1.1 Editors and Views

Bioclipse is made up of editors and views. Editors are for editing things. Items
can be opened in an editor, changed and then saved and the editor closed. A
view can listen to, and change appearance according to, the current selection.
For example the Properties view shows the properties of the item currently
selected. Figure 1 shows an example of what are views and what are editors in
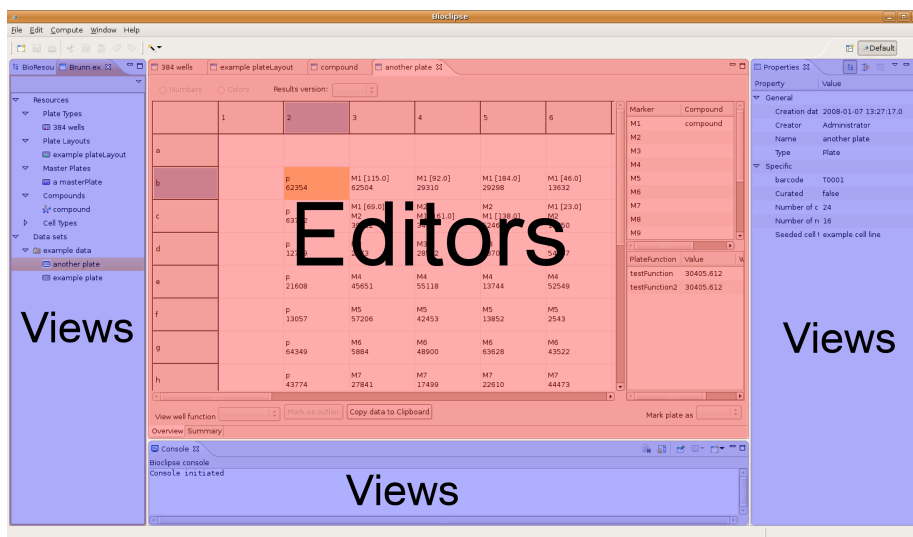a standard Brunn window.

Figure 1: *The Bioclipse workspace consists of editors and views. The editors
are piled in the middle and the views can be moved around.*

1.2 Two "hidden" but important menus

There are two sorts of menus in Bioclipse that can be hard to find. Figure 2
indicates them. One contains operations coupled to a view and can be found (in
a view that has such a menu) when clicking a little triangle in the upper right
corner of the view. The other switches between different tabs in a multipage
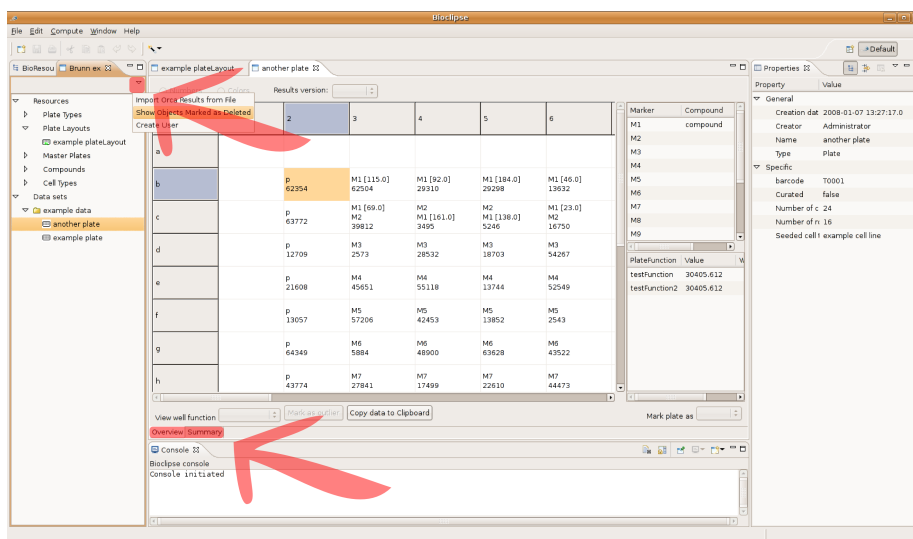editor. Not all editors have multiple pages.

Figure 2: *A view can have a menu. They are very convenient but can be hard to spot the first time. They are just little triangles in the corner of the view. Editors can have multiple pages but this feature can also be hard to spot. The tabs at the bottom of the editor switch between pages.*

2 Brunn

A few general tips for the Brunn user:

- Double-clicking an item opens it up for editing

- Right-clicking often opens up a context menu with operations. If you wonder about how to do somehing, try right clicking.

2.1 Installation and Set-Up

Bioclipse 2 can be found at: `https://sourceforge.net/projects/bioclipse/`. In Bioclipse 2 the Brunn update site can added by clicking (in Windows) `Window→Preferences` and then under `Update Sites` add the Brunn update site at: `http://pele.farmbio.uu.se/brunn` (figure 3(a)). Once the update site has been added the installation of the brunn feature can be done from `Help→Search for new features...` and under `Brunn Update Site` select `Brunn Feature` and `Usermanager Feature` (figure 3(b)) hit `Next` and accept the license agreements and then `Finish` to start installation.

2.2 The Brunn Explorer View

The first time Brunn is started the Brunn Explorer View (Figure 4) might not be visible. It can be made visible by clicking: `Window→Show View→Other...` and under Brunn, choose Brunn Explorer.

Double-clicking something in the Explorer View opens that item in an editor. New items are created from the Explorer View. The various items of the tree

3

(a) *Adding Brunn Updaite site to Bioclipse 2*

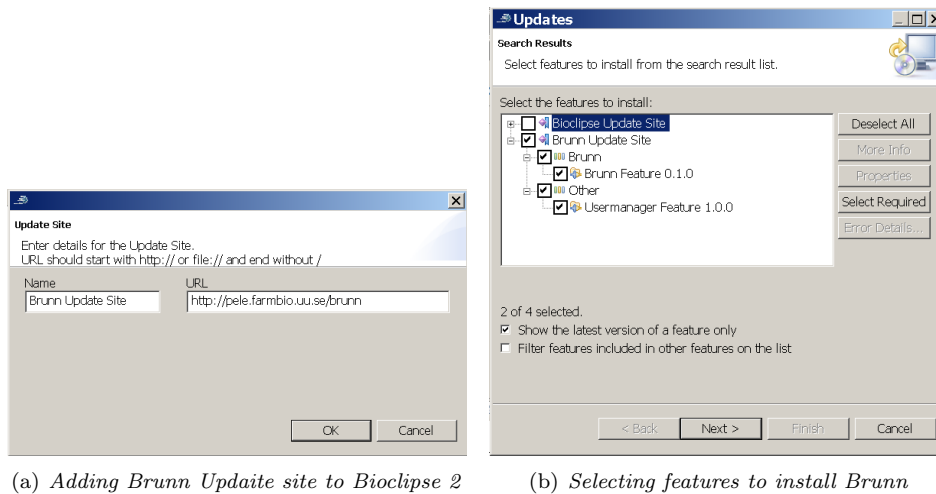(b) *Selecting features to install Brunn*

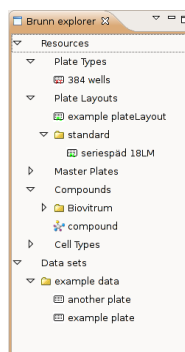**Figure 3:** *Installation process in Windows*

Figure 4: *The Brunn Explorer view is used to browse the system. The contents are sorted in fixed super folders for each type and can be further sorted into moveable sub folders* `TODO: Switch to new image with new icons and with the context menu showing`

have context menus that appear when right-clicking. For example, folders can be created and items can be dragged and dropped into and out of them. Figure 5 explains how the different items in the tree fit in to what is done in the lab.

Almost nothing can be deleted in Brunn. However, things can be marked as deleted, meaning that they won't show up unless the menu alternative `Show Objects Marked as Deleted` is choosen in the Brunn Explorer views menu. In this menu, there is also a wizard for importing result data and a way to create a new user account. The alternatives to show objects marked as deleted and to create users are only there if the logged-in user has administrator level access.
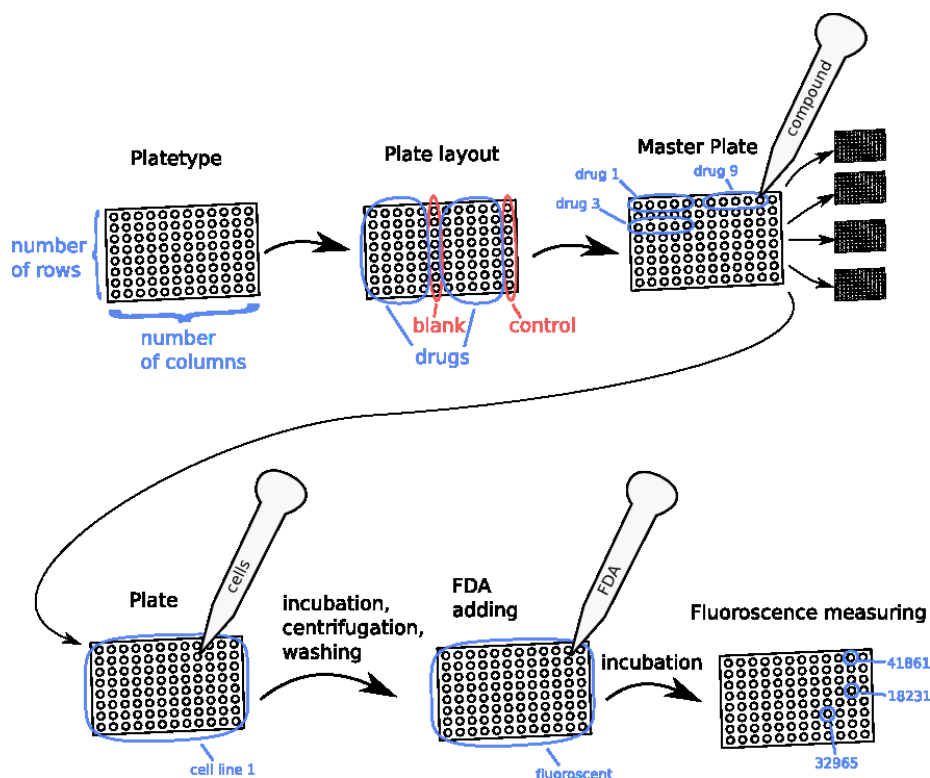

Figure 5: *A description of how the items of Brunn fit into the work performed in the lab. In the system, a plate type defines the size, number of columns and rows of a plate. A plate layout defines where on the plate the controls and the compounds are to be placed. Based upon this plate layout, a number of equal plates are made, conforming to a so-called "master plate" that defines which drugs are placed in which wells. Each one of this plates corresponds to a real life plate with an unique barcode number.*

2.3 Creating items

New items are created by right-clicking a folder that is either the top folder for the sort of item to be created or one of it's subfolders, and then choosing a create operation. This opens a dialog where things special for that sort of item

can be entered.

In order to create a plate layout, start by right-clicking the `Plate Layouts` folder and choose `Create Plate Layout`. In the dialog that shows up, choose one plate type to base the plate layout on, and enter a name for your new plate layout. Then click `Ok` to create the plate layout.

2.4 Plate Type

A plate type defines the size of a plate. It simply holds the number of rows and columns of a plate.

2.5 Plate Layout

A plate layout defines which wells on a plate should be used for compounds, which should be used for controls, and which should just be left empty. The plate layout is also where calculation functions are defined. For example, survival index or variation over the wells marked as positive control are specified in the plate layout.
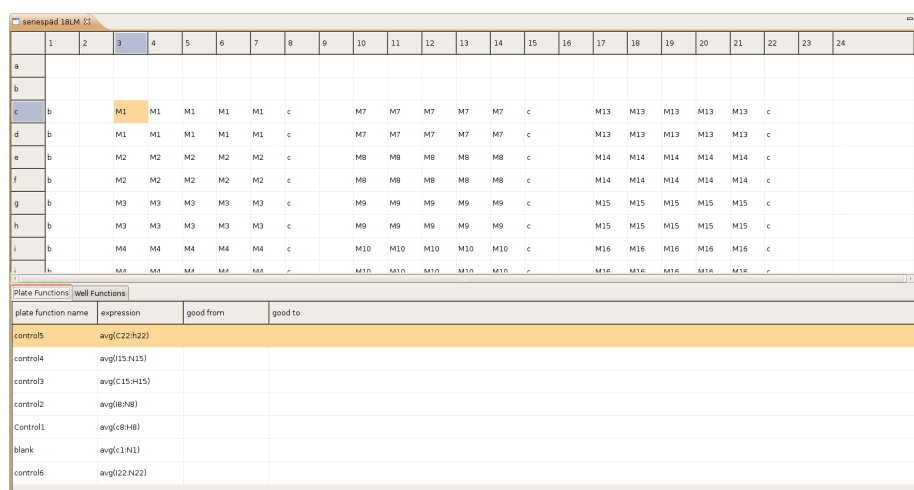

Figure 6: *The platelayouteditor*

2.5.1 Adding markers to a plate layout

Markers are used for labeling wells for different use. Brunn has 5 types of markers (see table 1).

Labeling a well with a marker is done by right-clicking the well in the plate layout editor and choosing the marker to label with. Multiple wells can be labeled at once by first selecting a number of wells and then right-clicking and choosing a marker. De-labeling is similar. When right-clicking a well with a marker an option to remove marker will appear in the right-click menu.

Marker	Description
b	Blank.
c	Control.
p	Positive control
s	Solvent
M1 ... Mn	Substance marker. Each number corresponds to one substance.

Table 1: *The different well markers used in Brunn*

Function	Description
`sum`	Sum of the given values
`avg`	The average of the given values
`stddev`	The standard deviation of the given values

Table 2: *Listing of predefined functions that can be used for calculations*

2.5.2 Defining calculation functions on a plate layout

The plate layout editor is also the place to define calculations. For example the expression for survival index (SI):

$$SI =? \texttt{TODO: write expression} \tag{1}$$

is added here. Brunn works with two groups of functions for calculations. Plate functions are coupled to a plate and should be used for things like average values of controls or variations for blanks. Well functions are coupled to a well and should be used for things like SI (equation 1).

The bottom part of the editor consists of a listing of added functions. To add a new one, simply right-click and choose `add function`. There are a few mathematical functions (Table 2) defined that can be used.

Well functions can be added by first switching to the well functions tab and then selecting a couple of wells that should be given well functions and then clicking `add function` just as with the plate functions. Here a little trick can be used: The variable `well` will be translated to the name of the current well.

TODO: Add example using SI as example

2.6 Master Plate

A master plate defines which compound marker correspond to which compound and with what concentration.

2.6.1 Defining compound for a compound marker

The masterplate editor is used for connecting substance markers with substances. It has functionality for creating dilution series. Conecting a substance to a marker is done by dragging the substance from the Brunn Explorer and into the list of markers at the bottom part of the editor. A dialog will ask for information of how to perform dilution.

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TODO: add illustration of dialog
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2.7 Plate

A plate corresponds to a real world plate. This connection is made by a barcode. So when creating a plate an unique barcode for the new plate needs to be given.

2.7.1 The plate editor

After results has been imported for a plate (see 2.8) the plate editor can be used for inspecting it. The plate editor has three tabs. Each of them contains a button for copying the table shown in that tab to clipboard.

The overview tab   The overview tab shows the result values for the plate in the same order as the actual plate. Each well has a few rows. The first row is the data value. After that come substance markers and concentrations. At the bottom of the editor is a row of buttons. The first is a combo box where the well function being shown for the wells can be changed. Then there is a button for marking a well as outlier. When a well is marked as outlier it will not be used in any calculations. In the right part of the editor is a list of substance markers and which compound it corresponds to, and below are all the plate functions listed.

The summary tab   The summary tab contains a table listing, for each well with compounds, the compounds names, concentrations, all well functions values and a CV% for the replicates. This tab also has a button for marking a well as an outlier.

The average tab   The average tab looks very much like the summary tab but instead of showing values for each well, it shows the average for each group of replicates. Since each row in this table corresponds to an average for many wells, there is no button for marking a well as outlier here.

2.8 Importing result data

Importing results is done in a dialog which can be found in the Brunn Explorer view's menu. Recall that figure 2 at page 3 shows where this menu can be found. The dialog is designed to accept files of three different formats.

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TODO: Describe or add examples of the three file formats
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