

BatchKi User Manual

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Ver. 4.07

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Chapter 1

Introduction

The software package **BatchKi** is a web server-based system for the statistical analysis of enzyme inhibition or ligand–receptor binding data. The complete **BatchKi** system consists of two independent modules:

1. A *numerical engine* (the executable program file **BatchKi.EXE**), using as input one or more precisely formatted XML data files.
2. A *graphical user interface* (GUI), embodied as a collection of HTML input forms and mediating all interaction with the user.

This document presents the User Manual for the graphical interface module of **BatchKi**, with only a few minor references to the numerical engine (described in a separate Reference Manual).

Chapter 2

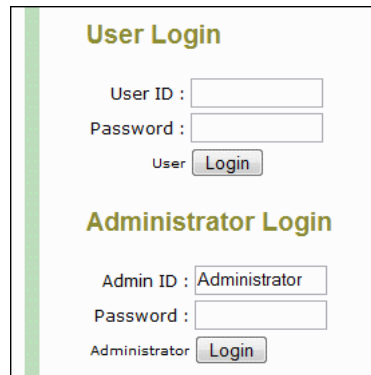
BatchKi Graphical Interfaces

The BatchKi system is distributed with three customizable graphical user interfaces, each of which is implemented as a Perl CGI script:

1. **Upload** interface - for uploading fully formatted XML data files, conforming to the internal format expected by the BatchKi numerical engine. This interface is useful if BatchKi input is prepared by a separate in-house software system.
2. **Generic** interface - for fine-grained control of plate layouts. This interface is useful for submitting a plate-reader data set that corresponds to a unique plate layout, one that has not been defined as a standard layout (see **Template** interface below).
3. **Template** interface - for repetitive submission of standard plate layouts. This interface is useful for repetitive submission of plates that had been laid out with a regular pattern of concentrations.

Each of these three BatchKi graphical interfaces is described in a subsequent chapter of this User Manual. Each interface has graphical data management modules with two distinct and separate purposes (see *Fig. 2.1*):

- **Administrator** interface - for managing user login information, license code, pre-defined settings for data analysis, plate templates, and so on.
- **User** interface - for submitting data for analysis, and for managing generated output files.

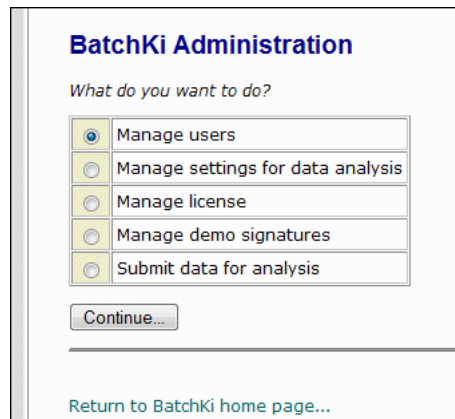


The screenshot displays two login sections. The first section, titled "User Login", contains a "User ID" input field, a "Password" input field, and a "Login" button with the word "User" positioned to its left. The second section, titled "Administrator Login", contains an "Admin ID" input field with the text "Administrator" inside, a "Password" input field, and a "Login" button with the word "Administrator" positioned to its left.

Figure 2.1: User vs. Administrator login in each of the three distributed BatchKi interfaces.

2.1 BatchKi Administration

An example of the main administration menu is shown in *Fig. 2.2*. The main menu in the three different user interfaces contains items summarized in the table below.



The screenshot shows the "BatchKi Administration" main menu. It features the title "BatchKi Administration" at the top, followed by the question "What do you want to do?". Below this is a list of five menu items, each with a radio button: "Manage users" (selected), "Manage settings for data analysis", "Manage license", "Manage demo signatures", and "Submit data for analysis". A "Continue..." button is located below the list. At the bottom of the interface, there is a link that says "Return to BatchKi home page...".

Figure 2.2: Main menu in the Generic/Administrator graphical interface.

In this section I will describe only those parts of the BatchKi administration module, which are shared by all three graphical user interfaces, namely, managing user login information, managing the demo signatures, and managing the license code.

<i>Administration menu item</i>	BatchKi Interface		
	Upload	Generic	Template
Manage Users	x	x	x
Manage License	x	x	x
Manage Demo Signatures	x	x	x
Manage Settings for Data Analysis		x	x
Manage Plate Layout Templates			x
Submit Data for Analysis	x	x	x

2.1.1 User management

The BatchKi system can be accessed from any computer workstation within the enterprise by using a standard web browser. However, each user must be issued a proper login credentials (user name and password). Optionally, each user can be issued certain privileges such as whether or not the given user can “manually” delete data points corresponding to certain wells on each submitted plate.

Adding a new user

To add a new user to the BatchKi system, fill out the *Add a New User* form on the main user-management page and click the [Continue] button (see *Fig. 2.3*).

Add a New User

User name :	<input type="text" value="pkuzmic"/>
Password (8-16 chars):	<input type="password" value="*****"/>
Confirm password :	<input type="password" value="*****"/>
Full name :	<input type="text" value="Petr Kuzmic"/>
Info (optional) :	<input type="text" value="BioKin Ltd. - BatchKi developer"/>
Can delete wells :	<input checked="" type="checkbox"/>
Must overwrite output :	<input type="checkbox"/>

Figure 2.3: Administrator interface: Adding a new BatchKi user.

The check box *Must Overwrite Output* should almost always remain unchecked. If the box is checked, each data submission by the given user

will overwrite the output from all previous data submissions. Consequently, there will be no way to recover results from previous data analyses.

This feature is useful more-or-less only on the BioKin.COM server, where we give occasional access to users interested in *live demonstrations* of the BatchKi software. Depending on the settings for analysis, a BatchKi data submission can produce a large volume of generated output files. Forcing the “demo users” to overwrite their previously generated output prevents the BioKin.COM server from being flooded by too many output files.

As a rule, the check box *Can Delete Wells* should also remain unchecked. In BatchKi, there is practically no need for manual deletion of data points or wells. The software has an optional *robust regression* module, which automatically de-emphasizes outlying data points. This amounts to an effective outlier exclusion. See ref. [1] for details.

Editing user information

To edit existing user information, select a user from the *Existing User* form, select an appropriate action from the drop-down menu, and click the [Continue] button (see *Fig. 2.4*).

The screenshot shows a web interface titled "Existing Users". It contains a table with three columns: "User", "Name/Info", and "Select user".

User	Name/Info	Select user
Administrator	Batchki Administrator *	<input type="radio"/>
pkuzmic	Petr Kuzmic BioKin Ltd. - BatchKi developer	<input checked="" type="radio"/>

Below the table is an "Action:" label followed by a dropdown menu. The dropdown menu is open, showing three options: "Edit user info" (highlighted in blue), "Delete user", and "Set password". A "Continue..." button is located at the bottom left of the interface.

Figure 2.4: Administrator interface: Editing user information.

After the initial installation of BatchKi, the first and only user appearing on the approved user list is also the only BatchKi administrator. Each BatchKi interface (**Submit**, **Generic**, and **Template**) maintains a separate list of users. The *Administrator* user created upon installation automatically has the highest BatchKi privileges (can delete wells, is not forced to overwrite all previous output).

2.1.2 Demo ‘signature’ management

The BatchKi system is distributed with several dozen sample data sets, which should allow a sufficiently thorough examination of various features and capabilities. Additionally, it is possible to arrange for a *live demo* of the BatchKi installation on the BioKin.COM web server.

In certain cases, it might not be feasible to submit proprietary data for analysis on BioKin.COM servers from within a company’s intranet. In those cases, BioKin Ltd. offers the following service to allow BatchKi evaluation before purchase:

1. We will receive (usually via email) only the *raw plate reader file*, exported from the plate-reader control software. This plate reader file contains no identifying information about the nature of the enzyme/receptor assay.
2. We will generate specially encrypted ‘signatures’¹ corresponding to each reader file.
3. We will email the demo ‘signatures’ back to the interested BatchKi evaluation team.
4. The BatchKi administrator can enter the ‘signatures’ into the BatchKi system with this demo management interface.
5. From now on, the corresponding raw plate reader files can be processed by BatchKi even before a valid license code is purchased.

The corresponding demo management interface is shown in *Fig. 2.5*. To update the list of demo signatures, *scroll down* to the end of the list of existing signatures, and paste any additional signatures there. Each demo signature is exactly 48 characters (letters and numbers) long. Each signature must stand on a separate line.

2.1.3 License management

The BatchKi license needs to be installed for each of the three user interfaces separately. To install the license, copy the license information from the email attachment file (usually named LICENSE.TXT). Copy (**Ctrl+C**) the entire

¹Each demo ‘signature’ essentially is a glorified or particularly scrambled MD5 checksum.

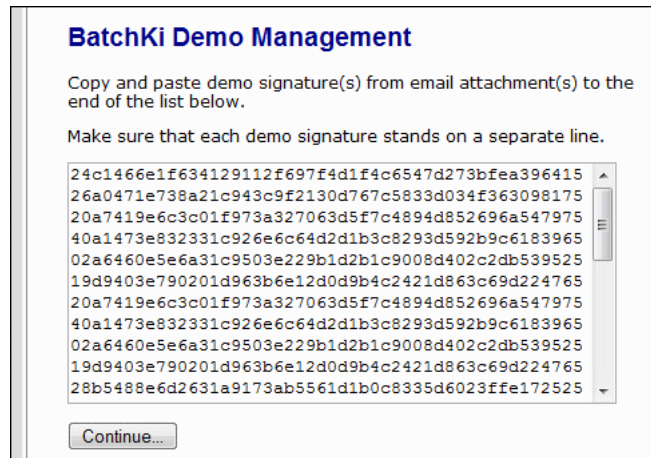


Figure 2.5: Administrator interface: Editing demo signatures for BatchKi evaluation.

text of the license file, including the first line `BioKin-License-Begin` and the last line `BioKin-License-End`. Paste (**Ctrl+V**) the copied license text from the system clipboard into the text area *License File Text* and click the [Continue] button, as shown in *Fig. 2.6*

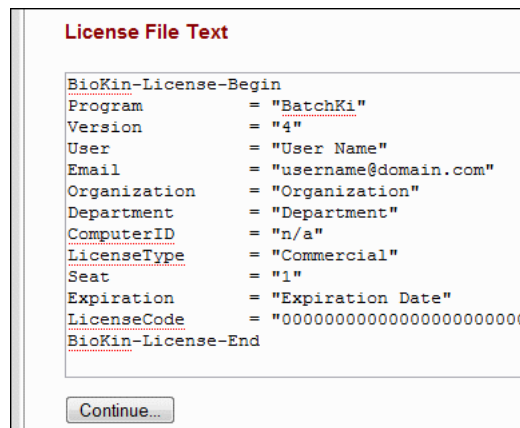


Figure 2.6: Administrator interface: Installing the BatchKi license.

Chapter 3

Upload Interface

The BatchKi **Upload** interface is extremely simple, because it only allows the submission of (a) the fully formatted XML file that can be read by the BatchKi numerical engine, and (b) the corresponding control or initialization file. Detailed specification of both types of files is found in the separate Reference Manual.

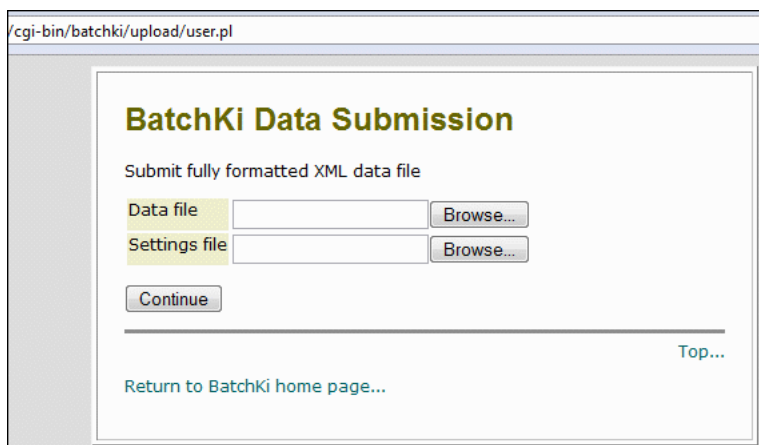


Figure 3.1: User module in the **Upload** interface.

The main advantage of this primitive user interface would be in submitting BatchKi XML data files that were fully formatted by a separate software application. Each XML data file could represent multiple plate-reader data files, using the multi-plate syntax:

<Multiplate>

```
<Plate id="Plate1">
  <Data ...>
First plate-reader data set here
  </Data>
</Plate>
<Plate id="Plate2">
  <Data ...>
Second plate-reader data set here
  </Data>
</Plate>
<Plate id="Plate3">
  <Data ...>
Third plate-reader data set here
  </Data>
</Plate>
</Multiplate>
```

In the default configuration, BatchKi can process up to 32 plate-reader data sets in a single run. Slightly altering the installation configuration would allow the processing of an (in principle) unlimited number of plate-reader files.

3.1 Demonstration run

BatchKi is distributed with a number of demonstration data files that can be processed immediately after downloading and installing the software, even without installing a valid license file. In the demonstration example below, we will be assuming that the BatchKi installation archive `install-batchki.zip` has been extracted in the directory `[setup]`. The extracted ZIP archive contains all required demonstration files.

1. Point a web browser to the BatchKi installation site, in this example <http://www.biokin.com/batchki/>.
2. Click on the link "Data Submission Form"
3. Click on the link "Upload fully formatted data file"
4. Under "User Login", type the login name and password.¹

¹In the default installation, a valid combination of user name and password is **Administrator / test1234**.

5. Click on [Browse] button next to "Data file"
6. Navigate to the file [setup]/batchki/test-data/upload/data.xml
7. Click on [Browse] button next to "Settings file" [setup]/batchki/test-data/upload/settings.txt
8. Click the [Continue] button After approximately 2-3 seconds, the browser will display a page with the heading "BatchKi Results" (*Fig. 3.2*). Click on the link Administrator_index.html. This will open a new browser window.
9. Navigate in the output files freshly generated by BatchKi. Check to make sure that no error messages are displayed on the main output page.

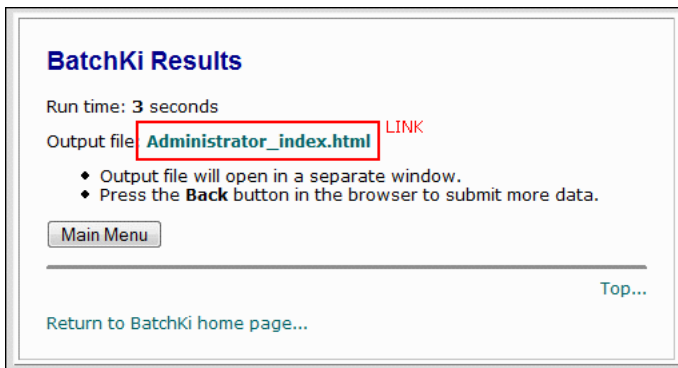


Figure 3.2: BatchKi result screen with a link to the main output file ..._index.html.

Chapter 4

Generic Interface

The BatchKi **Generic** interface is the most flexible of the three customizable interfaces distributed in the default installation. The advantage of this flexibility is that it allows the processing of virtually any given plate layout. The disadvantage is that, in this particular interface, we can only process one plate-reader data set at a time.

This chapter describes the Administrator module and the User module that are part of the **Generic** interface.

4.1 Administration module

In addition to the administration tasks already described in section 2.1, the administrator's module within the **Generic** interface allows customization of the control settings. The meaning of each entry in the BatchKi *control settings file* is described in the separate Reference Manual.

4.1.1 Customizing BatchKi control settings

To create a new set of control settings for the BatchKi numerical engine, fill out the web form entitled *Add New Settings* as shown in *Fig. 4.1*. It is important to choose a unique file name for each set of control parameters. The file names already used are shown in red in the form entitled *Existing Settings*. Simply choose a file name that is not yet listed.

There are no limits on the number of different settings for data analysis that can be stored in the BatchKi system. The words or phrases entered in the field labeled **I.D.** will be shown as menu items in the drop-down menus

Add New Settings

Choose a *unique I.D. and file name!*

I.D.: Thrombin #1

File name: thrombin1

Description: Settings for thrombin assays - Version 1

Default settings (modify if necessary):

[Confidence Intervals]
 Exact = yes
 FixedEnzyme = yes
 Level = 99

[Enzyme Concentration]
 Limits = 5
 Multiple = 1
 Optimize = yes

EDIT DEFAULT SETTINGS...

Continue...

Figure 4.1: Creating a new collection of BatchKi control settings.

presented to the user during actual data submission. Therefore, it is useful to choose very brief but descriptive entries for each **I.D.**.

To edit or delete an existing collection of control settings, click on the appropriate radio-button under *Existing Settings*, select from *Action* drop-down menu, and click on the *Continue* button, as shown in *Fig. 4.2*.

Rates rate	Input data are initial rates.	<input type="radio"/>
Rates Background rateback	Input data are initial rates. Optimize positive background rate.	<input type="radio"/>
Rotamase rotamase	Single exponential progress, background (e.g. uncatalyzed) rate.	<input type="radio"/>
Thrombin #1 thrombin1	Settings for thrombin assays - Version 1	<input type="radio"/>
Action :	<input type="text" value="Edit settings"/> <input type="text" value="Edit settings"/> <input type="text" value="Delete settings"/>	

Continue...

Figure 4.2: Editing or deleting an existing collection of BatchKi control settings.

4.2 User module

The user module in the **Generic** interface requires the following types of input data:

- A raw plate-reader data file representing either the reaction progress in enzyme assays, or single point (initial rate) assays.

The plate-reader data file must be a “plain text” (ASCII) file, usually exported from the plate-reader control software.¹

The ASCII plate-reader file should have one of the **SoftMax** formats (for example SoftMax “Plate Format” or “Column Format”), with or without temperature readings included (**ThermoMax**). Alternately, the plate-reader file should have the BatchKi **Universal** format described in the separate Reference Manual.

- A spreadsheet file (for example, Excel spreadsheet) containing the plate layout. For an illustrative example, please examine the distributed example file [setup]/batchki/test-data/generic/layout.xls.

The spreadsheet file should contain at least two grids of cells representing the wells on the given plate. For example, for a 96-well plate (8 rows, 12 columns) the spreadsheet will contain two 8×12 blocks of cells. In the first 8×12 block, we will have the *concentrations* of inhibitors; in the second 8×12 block, we will have the inhibitor *labels*.

With the above two types of data files in hand, we can proceed to submit the data for analysis by BatchKi. The user module in the **Generic** interface is best illustrated by way of an example.

4.2.1 Demonstration run

In the step-by-step instructions below, it is assumed that the BatchKi installation archive `install-batchki.zip` has been extracted in the directory [setup]. The extracted ZIP archive contains all required demonstration files.

1. Point a web browser to the BatchKi installation site, in this example <http://www.biokin.com/batchki/>.

¹BatchKi does *not* process any “raw” or binary plate-reader files, only files *exported* in ASCII format.

2. Click on the link *Data Submission Form*
3. Click on the link *Generic interactive interface*
4. Under *User Login*, type the login name and password
5. From the main menu, select the radio button *Compute inhibition constants from progress curves*, then click on the *Continue* button.

6. From the drop down menu *Settings*, select *Polynom (up to 2nd degree)*
7. From the drop down menu *Plate Format*, select *SoftMax*
8. From the drop down menu *Size/Rows*, select *8*
9. From the drop down menu *Size/Cols*, select *12*

10. Click *Submit* button
11. Under the **INHIBITOR** heading, select **CONCENTRATION ... μM** (micromolar) from the drop down menu.
12. Under the **ENZYME** heading, select **CONCENTRATION ... nM** (nanomolar) from the drop down menu.
13. Under the **SUBSTRATE** heading, select **CONCENTRATION ... μM** (micromolar) from the drop down menu.

14. Open the test plate layout file in Excel:
[setup]/batchki/test-data/generic/layout.xls
15. Highlight the eight rows and 12 columns under INHIBITOR CONCENTRATION (only the data, not the heading). Copy the data into the system clipboard (**Ctrl+C**).

	A	B	C	Formula Bar	E
1					
2	INHIBITOR CONCENTRATIONS				
3		1	2	3	4
4	A	10	0.2778	2.5	2.5
5	B	3.33333	0.09259	0.83333	0.83333
6	C	1.11111	0.03086	0.27778	0.27778
7	D	0.37037	0.01029	0.09259	0.09259
8	E	0.12346	0.00343	0.03086	0.03086
9	F	0.04115	0.00114	0.01029	0.01029
10	G	0.01372	0.00038	0.00343	0.00343
11	H	0.00457	0.00013	0.00114	0.00114

16. Switch to BatchKi.
17. Paste the system clipboard (**Ctrl+V**) into the text area INHIBITOR CONCENTRATION.
18. Switch to the plate test plate layout file in Excel.
19. Highlight the eight rows and 12 columns under INHIBITOR I.D. (only the data, not the heading). Copy the data into the system clipboard (**Ctrl+C**).

		1	2	3	4
12	INHIBITOR COMPOUND NAMES				
13					
14		1	2	3	4
15	A	Ctrl-7	Inh-101	Inh-102	Inh-103
16	B	Ctrl-7	Inh-101	Inh-102	Inh-103
17	C	Ctrl-7	Inh-101	Inh-102	Inh-103
18	D	Ctrl-7	Inh-101	Inh-102	Inh-103
19	E	Ctrl-7	Inh-101	Inh-102	Inh-103
20	F	Ctrl-7	Inh-101	Inh-102	Inh-103
21	G	Ctrl-7	Inh-101	Inh-102	Inh-103
22	H	Ctrl-7	Inh-101	Inh-102	Inh-103

20. Switch to BatchKi.
21. Paste the system clipboard (**Ctrl+V**) into the text area INHIBITOR I.D.

Inhibitor CONCENTRATION UNIT

Paste a single value or a 8 × 12 tab-delimited grid:

CONCENTRATION	<u>uM</u>		I.D.
10	0.277778		Ctrl-7 Inh-101
2.5	2.5	2.5	Inh-102 Inh-103
0	0	0	Inh-104 CONTROL

22. Under ENZYME CONCENTRATION, type or paste the single value *7*
23. Under ENZYME I.D., type or paste the single value *Prot-X*
24. Under SUBSTRATE CONCENTRATION, type or paste the single value *500*
25. Under SUBSTRATE I.D., type or paste the single value *Pept-Y*

The screenshot shows two sections: 'Enzyme' and 'Substrate'. Each section has a header, a prompt to 'Paste a single value or a 8 x 12 tab-delimited grid:', and two input fields. The 'Enzyme' section has a 'CONCENTRATION' dropdown set to 'nM' and an 'I.D.' dropdown set to 'Prot-X'. The 'Substrate' section has a 'CONCENTRATION' dropdown set to 'uM' and an 'I.D.' dropdown set to 'Pept-Y'.

26. Click *Browse* button next to the *File* label.
27. Navigate to the test data file: [setup]/batchki/test-data/generic/reader/plate-01.txt

The screenshot shows the 'Plate Reader Output File' dialog box. It has a 'File:' label followed by a text input field containing 'eneric\reader\plate-01.txt' and a 'Browse...' button. Below this are two checkboxes: 'Overwrite output?' and 'Exclude wells?'. A 'Submit' button is at the bottom. A red box highlights the 'Browse...' button, and a red arrow points from the text 'ASCII EXPORT FROM SOFTMAX' to the 'Browse...' button.

28. Click *Submit* button. After approximately 2-3 seconds, the browser will display a page with the heading "BatchKi Results". Click on the link `Administrator.....index.html`. This will open a new browser window.
29. Navigate in the output files freshly generated by BatchKi. Check to make sure that no error messages are displayed on the main output page.

Chapter 5

Template Interface

The BatchKi **Template** interface allow rapid submission of multiple plate-reader data files, essentially by pasting a list of compound names and then attaching to a web form a requisite number of raw plate-reader output files. The assumption is that all plates have been laid out exactly identically. For example, if the first plate being submitted had inhibitor dilution series running down columns, then all remaining plates have to be laid out the same way.

5.1 Administrator module

The Administrator module in the **Template** interface allows the editing of control settings for data analysis, following the procedure that has already been described in detail in section ?? above. Below I will describe the only unique feature of this particular Administrator module, that is, how to define plate layout templates.

5.1.1 Managing plate layout templates

Each plate layout is defined beforehand by the BatchKi administrator, using special notation described below.

Replacement tokens

“Tokens” in a template are pieces of text represented by the dollar sign followed by a pair of curly braces: $\{\dots\}$. Anything between the curly

braces is a placeholder that must be replaced by actual data during data submission. For example, assume that the token

```
#{EnzymeConc}
```

represents enzyme concentration in the template. This requires that, during the actual data submission, user supplies the numerical value in the form

```
EnzymeConc = 12.34
```

or (substituting a *tab character* for the equal sign) as

```
EnzymeConc 12.34
```

An example is shown in *Fig. 5.1*, where we find the tokens `$PlateID` for the plate I.D., and eight unique tokens for inhibitor labels `$Inh1`, `$Inh2`, through `$Inh8`. This notation means that, during actual data submission, the user is expected to supply pairs of tokens and the corresponding replacement values similar to

```
PlateID = Plate ID ACME20080711/7890
Inh1    = Compound ID ACME123
Inh2    = Compound ID ACME124
...
Inh7    = Compound ID ACME125
Inh8    = Compound ID ACME126
```

Well references and dilution ratios

In those sections of the BatchKi XML data file¹ that describe the concentrations (of either the enzyme, the substrate, or the inhibitor), it is possible to refer to particular wells in the style of Microsoft Excel formulas. This is best explained by way of an example, shown in *Fig. 5.2*.

In the well reference notation, rows on each plate are referred to by capital letters (A = first row, B = second row, etc.), whereas columns are

¹For a full description of the required XML format, see the separate Reference Manual.

	A	B	C	D	E
1	<Plate id="{PlateID}" rows="8" columns="12">				
2	<Substance>				
3	<Enzyme identical="yes">				
4	Protease X				
5	</Enzyme>				
6	<Substrate identical="yes">				
7	Peptide Z				
8	</Substrate>				
9	<Inhibitor identical="no">				
10	\$(I1)	\$(I1)	\$(I1)	\$(I1)	\$(I1)
11	\$(I2)	\$(I2)	\$(I2)	\$(I2)	\$(I2)
12	\$(I3)	\$(I3)	\$(I3)	\$(I3)	\$(I3)

Figure 5.1: Example of replacement tokens in a BatchKi template.

27	<ConcnInhibitor identical="no" unit="uM">				
28	\$(I _{max})	= A1/\$(Dil)	= A2/\$(Dil)	= A3/\$(Dil)	= A4/\$(Dil)
29	\$(I _{max})	= B1/\$(Dil)	= B2/\$(Dil)	= B3/\$(Dil)	= B4/\$(Dil)
30	\$(I _{max})	= C1/\$(Dil)	= C2/\$(Dil)	= C3/\$(Dil)	= C4/\$(Dil)
31	\$(I _{max})	= D1/\$(Dil)	= D2/\$(Dil)	= D3/\$(Dil)	= D4/\$(Dil)
32	\$(I _{max})	= E1/\$(Dil)	= E2/\$(Dil)	= E3/\$(Dil)	= E4/\$(Dil)
33	\$(I _{max})	= F1/\$(Dil)	= F2/\$(Dil)	= F3/\$(Dil)	= F4/\$(Dil)
34	\$(I _{max} STD)	= G1/\$(Dil)	= G2/\$(Dil)	= G3/\$(Dil)	= G4/\$(Dil)
35	\$(I _{max} STD)	= H1/\$(Dil)	= H2/\$(Dil)	= H3/\$(Dil)	= H4/\$(Dil)
36	</ConcnInhibitor>				
37	</Concentration>				
38	<Data type="rate" header="1">				
39	\$(ReaderData)				
40	</Data>				

Figure 5.2: Example dilution formulas in a BatchKi template.

referred to by numbers (1 = first column, 2 = second column, etc.). For example, the notation C4 means third row, fourth column on the given plate.

We can represent the concentration in any given well by writing an equal sign followed by a well reference (pointing to another well). For example, the notation = C4 means that, in the given well, the concentration is the same as in well C4.

Furthermore, we can use the notation = C4/3.333 to mean that, in the given well, the concentration is equal to the concentration in well C4 divided by 3.333 (1:3 dilution ratio).

Of course the dilution ratio itself can be represented by a *token* (see above). Therefore, we can also write = C4/\$(DilRatio) to mean that, in the given well, the concentration is equal to the concentration in well C4 divided by whatever numerical value is supplied for DilRatio during actual data submission.

The notation described above indeed is very similar to Excel formulas,

which can be conveniently used to setup dilution series. This similarity of notation is illustrated in *Fig. 5.3*.

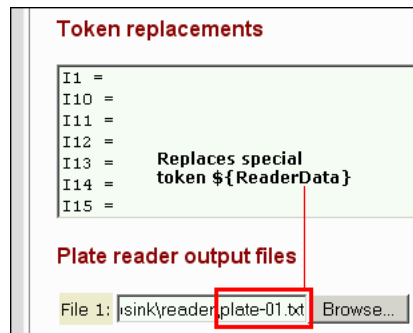
	A	B	C
1			
2	INHIBITOR CONCENTR		
3		1	2
4	A	10	0.2778
5	B	3.33333	0.09259
6	C	1.11111	0.03086
7	D	0.37037	0.04090

Figure 5.3: Similarity between Microsoft Excel and BatchKi template notation for dilution series.

The left-hand panel in *Fig. 5.3* shows how we can setup a dilution series in a BatchKi template. The notation = A1/4 in the cell representing row “B”, column “1” means that the the concentration in well B1 is one fourth of the concentration in well A1, and similarly for other wells in column. The right-hand panel shows how a similar 1:3 dilution series can be set up in MS Excel.

The special token ReaderData

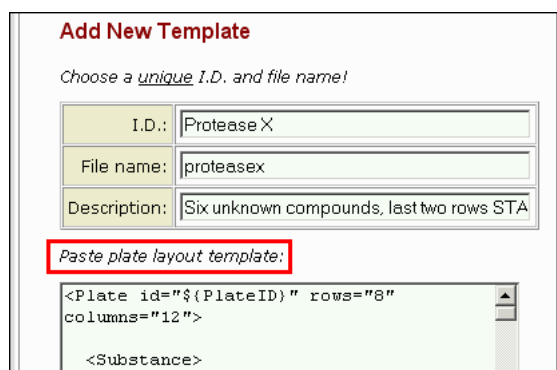
Each plate layout template must contain exactly one token stated as $\{\text{ReaderData}\}$. This token does appear on the list of tokens to be replaced in the same fashion as all the other tokens (by text replacement, `TokenName = TokenValue`). Rather, this special token is replaced upon data submission by an uploaded data file.



Creating a new template

To create a new plate layout template, follow these steps:

1. Create a spreadsheet file, for example in Microsoft Excel or in OpenOffice.
2. Populate the spreadsheet with entries that mimic the layout of a BatchKi XML input file (see separate *Reference Manual* for details).
3. Log into the BatchKi **Template** interface as the Administrator.
4. Select *Manage Plate Layout Templates* from the main menu.
5. Fill out the *Add New Template* form, by pasting the entire contents of the Excel (or OpenOffice) spreadsheet.



Add New Template

Choose a *unique I.D.* and file name!

I.D.:	Protease X
File name:	proteasex
Description:	Six unknown compounds, last two rows STA

Paste plate layout template:

```
<Plate id="{PlateID}" rows="8"
columns="12">
<Substance>
```

5.2 User module

Once the required plate layout templates are properly set up by the BatchKi administrator, the users can submit multiple plates for analysis in a relatively simple and efficient way. Typically the only required type of input data, aside from the plate-reader files themselves, is a *list of compound names* that have been laid out on the plates in a specific way.

The following step-by-step procedure refers to a collection of demonstration data files that are being distributed with the BatchKi installer. In the instructions below, it is assumed that the installer file (a ZIP archive) has been extracted in some temporary directory referred to as [temp].

1. Point a web browser to the BatchKi installation site, in this example <http://www.biokin.com/batchki/>
2. Click on the link *Data Submission Form*
3. Click on the link *Template for plate layout*
4. Under *User Login*, type the login name and password.
5. From the main menu, select the radio button *Compute inhibition constants*. Click *Continue* button.

6. From the drop down menu *Settings*, select “Thrombin”
7. From the drop down menu *Template*, select “Thrombin #1”
8. From the drop down menu *How many plates*, select “5”
9. Check the box *Single Column*
10. Click the *Submit* button

11. Open the test plate layout file in MS Excel: [temp]/batchki/test-data/template/thrombin1/template-thrombin1.xls
12. In MS Excel, select columns ”B” and ”C”, rows #2-#6 (the black-bordered area with “IMax” in the upper left corner and “40” in the bottom right corner). Copy into the system clipboard (**Ctrl+C**).

	A	B	C
2	SHARED	IMax	50
3		E	Protease-X
4		EConc	10
5		S	Peptide-Y
6		SConc	40

13. Switch to BatchKi.
14. Paste the content of the system clipboard into text area *Shared by All Plates*: **Ctrl+A**, select all; **Del**, delete; **Ctrl+V**, paste. The pasted content should have exactly five rows and two columns.

Shared by all plates	
IMax	50
E	Protease-X
EConc	10
S	Peptide-Y
SConc	40

15. Switch to MS Excel.
16. In MS Excel, select columns “E” and “F”, rows #2-#61 (the black-bordered area with PlateID in the upper left corner and NVT-C405 in the bottom right corner). Copy into the system clipboard (**Ctrl+C**).

PLATE 1	PlateID	test01
	I1	NVT-C347
	I2	NVT-C348
	I3	NVT-C349
	I4	NVT-C350
	I5	NVT-C351
	I6	NVT-C352
	I7	NVT-C353
	I8	NVT-C354
	I9	NVT-C355
	I10	NVT-C356
I11	NVT-C357	
PLATE 2	PlateID	test02
	I1	NVT-C359
	I2	NVT-C360

17. Switch to BatchKi.
18. Paste the content of the system clipboard into text area *Specific for each plate*

Specific for each plate	
Single column of token assignments for all plates:	
PlateID	test01
I1	NVT-C347
I2	NVT-C348
I3	NVT-C349
I4	NVT-C350
I5	NVT-C351
I6	NVT-C352

19. Click the *Browse* button next to “File 1”

20. Navigate to file [temp]/batchki/test-data/template/thrombin1/reader/plate-01.txt
21. Click the *Browse* button next to “File 2”
22. Navigate to file [temp]/batchki/test-data/template/thrombin1/reader/plate-02.txt
23. Repeat for files 3 – 5.
24. Click the *Submit* button.

Plate reader output files

File 1: nbin1\reader\plate-01.txt

File 2: nbin1\reader\plate-02.txt

File 3: nbin1\reader\plate-03.txt

File 4: nbin1\reader\plate-04.txt

File 5: nbin1\reader\plate-05.txt

Overwrite output?

25. After approximately 2-3 seconds, the browser will display a page with the heading *BatchKi Results*. Click on the link `Administrator_...._index.html`. This will open a new browser window.
26. Navigate in the output files freshly generated by BatchKi. In this example, `http://www.biokin.com/batchki/submit/output/Administrator_...._index.html`

BatchKi Results

Run time: 3 seconds

Output file: **Administrator_1215882057_index.html**

- ◆ Output file will open in a separate window.
- ◆ Press the **Back** button in the browser to submit more data.

Check to make sure that no error messages are displayed on the main output page.

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