
**Institute of Mathematics and Computer Science
European Bioinformatics Institute**

**SIMS
User Guide**

Version 2.10

Accessing SIMS system

To access Sample Information Management System you need a valid login name and a password. If you think that you should have access to this page, but don't have login name/password you should contact the System Administrator.

Different users might have different access rights. Currently access rights are managed at *technology level* (the user can access only these Technologies access to which have been granted to him) and at *entry ownership* level - depending from ownership particular entries could be available either fully or partially or be hidden for a particular user. Also the access rights determine whether the user will be able to create new entries.

There are several pages or other functionality of the system that might be unavailable or partially available to users without sufficient access rights.

First level (Persons)

List of Persons page allows to view/edit/delete all Persons currently in database. If your access rights doesn't allow to access a particular Person even in *view only* mode, only the value of Person ID will be shown, all other values will be replaced by **.

Creating/viewing/editing/deleting Persons

- To add a new Person to database click on *New Person* link. To be able to do this you must be viewing Persons attributed to one particular Person and new Person will be defined for that Person. This includes also the option of simultaneous adding of several Persons (see below).
- To edit data about an Person click on the corresponding *edit* icon . If you have limited access rights one of the following icons will be shown instead:  (the Edit dialog is available in *view only* mode),  (you don't have access to Person).
- To create a new Person with the parameters copied from the existing one click on the corresponding *clone* icon . If you don't have access rights to a particular Person, the icon will be replaced by .
- To delete entry about a particular Person click on the corresponding *edit* icon  and then press select *Delete* button.
- To change simultaneously the values of some properties for several Persons click on *Edit batch* link. You will have the option to select the Persons for editing and then, after pressing *Edit batch* link, you will be directed to edit dialog which allows to change Person properties.

Add/Edit/View Person dialogs allows you correspondingly to enter data about a new Person or to edit/view data for already existing Person.

The field **Person Id** depending from SIMS configuration can have either an arbitrary string value (up to slightly less than 200 characters - keeping in mind that derived Ids for Samples and Aliquots have to satisfy the same limit), or a control digit (character) might be used, in which case checksum of all digits must give the right value mod 10. In the latest case generally it is assumed that PMT tool is used for ID generation.

All Person Ids attributed will be unique.

Relative fields allow you to define relations ("parent", "child", "twin" etc) between persons. This is possible only between persons attributed to the same data source, the possible candidates for relatives can be selected from a list.

As many relatives as you wish can be defined, but to do this, after adding a new Relative you should press "Update" button and then enter Edit person dialog again. If you chose a person Y as a relative for person X, a reverse relation is added for person Y (e.g. if you select Y as a "child" of X, X automatically becomes "parent" of Y). However these relations are strictly binary with no further implicit assumptions. E.g. even if X is defined as a "sibling" of "Y" and "Y" as a "sibling" of "Z", "X" will not automatically become a sibling of "Z". Similarly, you are free to define that "X" is a "child" of "Y" and "Y" is a child of "X".

To delete a relation, change it to empty field in list of relative candidates.

Be careful - if you attribute a person to different data source, all relations for this person will be deleted!

The meaning of other fields hopefully should be self-apparent.

In *Batch edit* mode there is a checkbox for each of Persons' fields. Check the boxes for fields values of which you wish to change. Fields are displayed in white, if its values for all Persons selected for batch editing is the same, and gray if there are different values.

Batch uploading

It is possible to upload Persons from tab delimited file. To do this click on *Upload Persons* tab. You will be directed to a special **Upload Persons** dialog which instead of fields for Person properties allows you to upload tab-delimited file containing several Persons. In addition, you have options to specify either local or already pre-uploaded (via FTP) zip file containing data and supplementary files referenced in uploaded Persons (instead of zip files, it is also possible to reference via FTP pre-uploaded directories). After pressing *Upload* button the provided tab delimited file (as well as zip file or referenced directory) will be processed and a page listing Persons will be shown. If there are no errors, you will have the option to complete the upload and save Persons in database.

You can download header for tab-delimited Person file *Download ... header* link.

Creating reports

This is the simplest way of data export, providing export of Persons in WYSIWYG mode. By clicking on *Report* button you are able to save the data shown on Persons page in tab-delimited format. Columns included in report are the same which are currently configured as visible in Persons page. Included in report are all data conforming to current filter settings, even if the number of rows shown in current page is limited.

Data filtering

To filter the data about Persons that are being shown click on *Filter* tab. Filtering options are described in more details in *Filter settings help page*. To clear filter settings click on *Cancel filter* tab.

Selecting visible columns

To select columns that are shown on this page as well as column order click on *Columns* button. Configuration is described in more details in *Define tabular views help page*.

Second level (Samples)

List of Samples page allows to view/edit/delete data either for all Samples currently in database or Samples attributed to a particular Person. If your access rights doesn't allow to access a particular Sample even in *view only* mode, only the value of Sample ID will be shown, all other values will be replaced by ******.

Creating/viewing/editing/deleting Samples

- To add a new Sample to database click on *New Sample* link. To be able to do this you must be viewing samples attributed to one particular sample and new Sample will be defined for that sample. This includes also the option of simultaneous adding of several Samples (see below).
- To edit data about an Sample click on the corresponding *edit* icon . If you have limited access rights one of the following icons will be shown instead:  (the Edit dialog is available in *view only* mode),  (you don't have access to Sample).
- To create a new Sample with the parameters copied from the existing one click on the corresponding *clone* icon . If you don't have access rights to a particular Sample, the icon will be replaced by .
- To delete entry about a particular Sample click on the corresponding *edit* icon  and then press select *Delete* button.
- To change simultaneously the values of some properties for several Samples click on *Edit batch* link. You will have the option to select the Samples for editing and then, after pressing *Edit batch* link, you will be directed to edit dialog which allows to change Sample properties.

Add/Edit/View Sample dialogs allows you correspondingly to enter data about a new Sample or to edit/view data for already existing Sample.

The field **Sample Id** in current version is not editable and is assigned automatically. The id will look like this:

"Person Id (without "-" and control digit)" + "-" + "CV dependent substring (if used in current SIMS configuration)" + "the number (starting from 1) of sample belonging to the same CV dependent substring".

All Sample Ids attributed to a particular Person will be unique.

The meaning of other fields hopefully should be self-apparent.

In *Batch edit* mode there is a checkbox for each of Samples' fields. Check the boxes for fields values of which you wish to change. Fields are displayed in white, if its values for all Samples selected for batch editing is the same, and gray if there are different values.

Batch uploading

It is possible to upload Samples from tab delimited file. To do this click on *Upload Samples* tab. You will be directed to a special **Upload Samples** dialog which instead of fields for Sample properties allows you to upload tab-delimited file containing several Samples. In addition, you have options to specify either local or already pre-uploaded (via FTP) zip file containing data and supplementary files referenced in uploaded Samples (instead of zip files, it is also possible to reference via FTP pre-uploaded directories). After pressing *Upload* button the provided tab delimited file (as well as zip file or referenced directory) will be processed and a page listing Samples will be shown. If there are no errors, you will have the option to complete the upload and save Samples in database.

You can download header for tab-delimited Sample file *Download ... header* link.

Creating reports

This is the simplest way of data export, providing export of Samples in WYSIWYG mode. By clicking on *Report* button you are able to save the data shown on Samples page in tab-delimited format. Columns included in report are the same which are currently configured as visible in Samples page. Included in report are all data conforming to current filter settings, even if the number of rows shown in current page is limited.

Data filtering

To filter the data about Persons and/or Samples that are being shown click on *Filter* tab. Filtering options are described in more details in *Filter settings help page*. To clear filter settings click on *Cancel filter* tab.

Selecting visible columns

To select columns that are shown on this page as well as column order click on *Columns* button. Configuration is described in more details in *Define tabular views help page*.

Third level (Aliquots)

List of Aliquots page allows to view/edit/delete data either for all Aliquots currently in database, Aliquots attributed to particular data source, Aliquots attributed to a particular person, or Aliquots attributed to particular sample. If your access rights doesn't allow to access a particular Aliquot even in *view only* mode, only the value of Aliquot ID will be shown, all other values will be replaced by **.

Creating/viewing/editing/deleting Aliquots

- To add a new Aliquot to database click on *New Aliquot* link. To be able to do this you must be viewing samples attributed to one particular sample and new Aliquot will be defined for that sample. This includes also the option of simultaneous adding of several Aliquots (see below).
- To edit data about an Aliquot click on the corresponding *edit* icon . If you have limited access rights one of the following icons will be shown instead:  (the Edit dialog is available in *view only* mode),  (you don't have access to Aliquot).
- To create a new Aliquot with the parameters copied from the existing one click on the corresponding *clone* icon . If you don't have access rights to a particular Aliquot, the icon will be replaced by .
- To delete entry about a particular Aliquot click on the corresponding *edit* icon  and then press select *Delete* button.
- To change simultaneously the values of some properties for several Aliquots click on *Edit batch* link. You will have the option to select the Aliquots for editing and then, after pressing *Edit batch* link, you will be directed to edit dialog which allows to change Aliquot properties.

Add/Edit/View Aliquot dialogs allows you correspondingly to enter data about a new Aliquot or to edit/view data for already existing Aliquot.

The field **Aliquot Id** in current version is not editable and is assigned automatically. The id will look like this:

"Sample Id" + "-" + "string of letters (starting from A) corresponding to the current number of Aliquots belonging to this sample".

All Aliquot Ids attributed to a particular sample will be unique.

The meaning of other fields hopefully should be self-apparent.

There are two options available from **Add Aliquot** dialog, if you wish to add several Aliquots with the same characteristics:

- After defining the Aliquot press *Create* button. The currently entered Aliquot will be added to database.
- After defining the Aliquot press *Create multiple* button, after selecting a number (2-20) from the list. The specified number of Aliquots with the same properties (apart from Aliquot Ids) will be added to database.

In *Batch edit* mode there is a checkbox for each of Aliquots' fields. Check the boxes for fields values of which you wish to change. Fields are displayed in white, if its values for all Aliquots selected for batch editing is the same, and gray if there are different values.

Batch uploading

It is possible to upload Aliquots from tab delimited file. To do this click on *Upload Aliquots* tab. You will be directed to a special **Upload Aliquots** dialog which instead of fields for Aliquot

properties allows you to upload tab-delimited file containing several Aliquots. In addition, you have options to specify either local or already pre-uploaded (via FTP) zip file containing data and supplementary files referenced in uploaded Aliquots (instead of zip files, it is also possible to reference via FTP pre-uploaded directories). After pressing *Upload* button the provided tab delimited file (as well as zip file or referenced directory) will be processed and a page listing Aliquots will be shown. If there are no errors, you will have the option to complete the upload and save Aliquots in database.

You can download header for tab-delimited Aliquot file *Download ... header* link.

Creating reports

This is the simplest way of data export, providing export of Aliquots in WYSIWYG mode. By clicking on *Report* button you are able to save the data shown on Aliquots page in tab-delimited format. Columns included in report are the same which are currently configured as visible in Aliquots page. Included in report are all data confirming to current filter settings, even if the number of rows shown in current page is limited.

Data filtering

To filter the data about Persons and/or Samples and/or Aliquots that are being shown click on *Filter* tab. Filtering options are described in more details in *Filter settings help page*. To clear filter settings click on *Cancel filter* tab.

Selecting visible columns

To select columns that are shown on this page as well as column order click on *Columns* button. Configuration is described in more details in *Define tabular views help page*.

Data filtering

Filter page allows to search for Persons/Samples/Aliquots with a values of selected fields equal to the values defined in search page filters.

The fields currently available for filtering are Person/Sample/Aliquot ID fields, owners/owner groups of entries (at 1st level) and those corresponding to controlled vocabularies (the availability of the later also depends from whether they are configured in corresponding JSP page for the particular SIMS instance).

To include a particular controlled vocabulary field in search, select one or more values from the corresponding list (to select multiple values or deselect already selected ones use Ctrl key + mouse click). Search will find the database entries with the value of this field equal to one of the selected field values. Filters are conjunctive, i.e. if a field is included in search, database entries satisfying filter values for this field **AND** filter values for all other fields will be found.

If no values for a field are selected, the field is not included in search (i.e. the result is equal to that of search with all values for this field included in filter, however the search process is more efficient).

After clicking on *OK* button Filter will be enabled and only the entries (Persons, Samples or Aliquots - depending from which page Filter was accessed) conforming to the filter settings will be shown. When doing filtering at Sample level, filtering at Person level can also be applied (if this is needed check *Relevant Persons only* checkbox. Similarly, when doing filtering at Aliquot level, filtering at Person and/or Sample level can also be applied - check correspondingly *Relevant Persons only* checkbox and/or *Relevant Samples only* checkbox.

To cancel filtering and display all database entries press *Cancel filter* tab.

Defining tabular views and reports

Define ... view page allows to select which columns and in which order will be displayed in 1st (Persons), 2nd (Samples) or 3rd (Aliquot) level pages in list (tabular) format. It also defines which fields will be exported by **Report** function (which actually might be the main reason for changing these settings). The level for which column display options can be changed corresponds to the level from which **Define ... view** page has been entered (by using **Columns** function).

To change the settings, enter numbers of columns in which the fields of interest should be displayed. Columns are numbered by rational positive numbers which should be entered in two adjacent textboxes containing correspondingly integer and fractional parts. On view pages columns will be shown from left to right according to increasing ordering of column numbers. Column number 0 means that the corresponding field will not be displayed.

To apply view settings press *Ok* button. Pressing of *Tune* button will "normalize" the column numbering, i.e. columns will be assigned consecutive integer numbers starting from 1. Also, they will be re-ordered according to their numbers. Normalizing and re-ordering occurs also on re-entering **Define ... view** page.

Settings are preserved only within the current session. After the next login the default settings will be restored (the later can be configured from **Configuration tables** page by users having sufficient access rights to do so).

Vocabulary tables

Vocabulary tables page allows to view/add/edit/delete entries in fixed vocabularies.

Editing options include adding new entries to the vocabulary, deleting existing entries and renaming existing entries. To add a new entry click on a *new* link for a specific vocabulary. To edit/delete entry click on *edit* link for a specific vocabulary.

Editing of vocabularies should be done with some care - deleting of an existing entry and subsequent adding of new entry with the same name may lead to wrong values being associated with data that are already stored in the system.

The length of vocabulary fields are limited to 200 characters.

Depending from your access rights you might have only *view only* access to **Vocabulary tables** page or the page might be unavailable for you.

System administration

Administrative tables page allows to access and (depending from your access rights) modify configuration tables of the system. Generally these tables can be divided in two groups: user and their access rights management and settings that define how data is displayed at Person, Sample and Aliquot level.

At the top of the page there are links: *Export metadata and vocabularies* and *Import metadata and vocabularies*. *Export metadata and vocabularies* allows exporting in XML format the content of all controlled vocabularies as well as *Person metadata*, *Sample metadata* and *Aliquot metadata* configuration tables. *Import metadata and vocabularies* allows importing of such XML file in SIMS that is unconfigured as yet. One should take care of importing XML file that compatible with a particular SIMS instance. Generally metadata import should be done just once for newly installed SIMS instances, however re-importing the same file shouldn't make any changes to the system.

The tables shown on this page and their meaning are described below.

Table *Person metadata*

Table specifies how data are displayed in **List of Persons** page and the corresponding Add/Edit/View dialogs.

The configurable fields always include the following: *visibleName* (Person Id), *relations1* ("meta-field", used to display information about relatives), *comment* (string of up to 4000 characters), *creator* (FK to **Users** table), *modifier* (FK to **Users** table), *createDate* (datetime) and *modifDate* (datetime).

In addition there could be a variable number of the following types of fields present: *vtxx* (FK to controlled vocabulary), *ftxx* (number of type *float*), *itxx* (number of type *integer* or *boolean* (displayed as checkbox)), *stxx* (string of either up to 200 characters or up to 4000 characters, this depends from database configuration), *dtxx* (date and/or time). The number of these fields depends from configuration from of a particular SIMS instance. The available range (values for *xx*) are from 0 to 99.

There are notable difference between *vtxx* and other types of fields: controlled vocabularies are shared between all levels (Person, Sample and Aliquot), whilst other types are individual for each level.

For SIMS instance to work properly the table need to contain **exactly one** entry for each of the following fields: *visibleName*, *relations1*, *comment*, all available fields of types *ftxx*, *itxx*, *stxx* and *dtxx*, and these fields of type *vtxx* which are being used at current level. The configuration of fields *creator*, *modifier*, *createDate* and *modifDate* is optional.

The table contains the following configurable fields (in this order):

- *Property name* - the field (selectable from drop-down list) being configured,
- *Short* - name shown as column name in **List of Persons** page,
- *Long name* - name shown on the left side of the field in Add/Edit/View dialogs,
- *Upload name* - name used in header of batch upload file,
- *View column number* - column number in **List of Persons** page (not shown, if 0),
- *Sortable* - if *true*, the entries in **List of Persons** can be sorted by the values of this parameter,
- *Editable* - currently unused,
- *Show in report* - currently unused,
- *Comment* - informal comment.

Table *Sample metadata*

Table specifies how data are displayed in **List of Samples** page and the corresponding Add/Edit/View dialogs.

The configurable fields always include the following: *visibleName* (Sample Id), *comment* (string of up to 4000 characters), *creator* (FK to **Users** table), *modifier* (FK to **Users** table),

createDate (datetime) and *modifDate* (datetime).

In addition there could be a variable number of the following types of fields present: *vtxx* (FK to controlled vocabulary), *ftxx* (number of type *float*), *itxx* (number of type *integer* or *boolean* (displayed as checkbox)), *stxx* (string of either up to 200 characters or up to 4000 characters, this depends from database configuration), *dtxx* (date and/or time). The number of these fields depends from configuration from of a particular SIMS instance. The available range (values for *xx*) are from 0 to 99.

There are notable difference between *vtxx* and other types of fields: controlled vocabularies are shared between all levels (Person, Sample and Aliquot), whilst other types are individual for each level.

For SIMS instance to work properly the table need to contain **exactly one** entry for each of the following fields: *visibleName*, *comment*, all available fields of types *ftxx*, *itxx*, *stxx* and *dtxx*, and these fields of type *vtxx* which are being used at current level. The configuration of fields *creator*, *modifier*, *createDate* and *modifDate* is optional.

The table contains the following configurable fields (in this order):

- *Property name* - the field (selectable from drop-down list) being configured,
- *Short* - name shown as column name in **List of Samples** page,
- *Long name* - name shown on the left side of the field in Add/Edit/View dialogs,
- *Upload name* - name used in header of batch upload file,
- *View column number* - column number in **List of Samples** page (not shown, if 0),
- *Sortable* - if *true*, the entries in **List of Samples** can be sorted by the values of this parameter,
- *Editable* - currently unused,
- *Show in report* - currently unused,
- *Comment* - informal comment.

Table Aliquot metadata

Table specifies how data are displayed in **List of Aliquots** page and the corresponding Add/Edit/View dialogs.

The configurable fields always include the following: *visibleName* (Aliquot Id), *comment* (string of up to 4000 characters), *creator* (FK to **Users** table), *modifier* (FK to **Users** table), *createDate* (datetime) and *modifDate* (datetime).

In addition there could be a variable number of the following types of fields present: *vtxx* (FK to controlled vocabulary), *ftxx* (number of type *float*), *itxx* (number of type *integer* or *boolean* (displayed as checkbox)), *stxx* (string of either up to 200 characters or up to 4000 characters, this depends from database configuration), *dtxx* (date and/or time). The number of these fields depends from configuration from of a particular SIMS instance. The available range (values for *xx*) are from 0 to 99.

There are notable difference between *vtxx* and other types of fields: controlled vocabularies are shared between all levels (Person, Sample and Aliquot), whilst other types are individual for each level.

For SIMS instance to work properly the table need to contain **exactly one** entry for each of the following fields: *visibleName*, *comment*, all available fields of types *ftxx*, *itxx*, *stxx* and *dtxx*, and these fields of type *vtxx* which are being used at current level. The configuration of fields *creator*, *modifier*, *createDate* and *modifDate* is optional.

The table contains the following configurable fields (in this order):

- *Property name* - the field (selectable from drop-down list) being configured,
- *Short* - name shown as column name in **List of Aliquots** page,
- *Long name* - name shown on the left side of the field in Add/Edit/View dialogs,
- *Upload name* - name used in header of batch upload file,
- *View column number* - column number in **List of Aliquots** page (not shown, if 0),
- *Sortable* - if *true*, the entries in **List of Aliquots** can be sorted by the values of this parameter,
- *Editable* - currently unused,
- *Show in report* - currently unused,
- *Comment* - informal comment.

Table *Users*

Defines Users of the system.

The table contains the following fields:

- *User description* - informal User description,
- *Login name* - login name,
- *Administrator rights* - administrator level rights for this user, the options are *non-accessible* (no access to **AdminTables** page), *view only*, *limited editing* (actually meaning almost full access, some configuration printouts and **Pending tasks** table not shown) and *full editing*,
- *User password* - password (shown in MD5 hashed form, but can be reset from this dialog),
- *Id prefix* - a string which will be used as part of Id when creating new Experiments or Studies,
- *Export is allowed* - if *true*, the User can export data in XML or tab-delimited form based on XML configuration templates (currently not used in SIMS),
- *FTP is allowed* - if *true*, User can access files preuploaded via FTP (if FTP option is enabled for this AIMS configuration),
- *FTP directory* - subdirectory from which data and supplementary files will be listed (if FTP option is enabled for this AIMS configuration),
- *Default user group* - the User group, which owns Studies and Experiments created by this user. When a new user is created all User groups is available in drop-down list and initially default User group is selected. When data about already existing user is edited this list contains only User groups the User is member of,
- *Comment* - informal comment.

At least one User group must be present (and one User is created automatically when newly installed AIMS is used for the first time). Users having *Administrator rights* at *limited editing* or higher level automatically have full access to all entries and **Vocabularies** and **Configuration** pages regardless of access rights configurations.

Table *User rights*

Defines granting of access rights at user level.

The table contains the following fields:

- *Granted by* - User to Studies and Experiments owned by whom the access is granted,
- *Granted to* - User to which the access is granted,
- *User rights* - the level of rights granted, options are *non-accessible*, *view only*, *data files non-accessible*, *view only*, *data files accessible* and *full access*,
- *Comment* - informal comment.

Generally User has full access to entries owned by him, access to other entries depend from configuration in **User rights** and **User group rights** tables. User doesn't automatically have access to entries of user group he belongs to - this has to be configured in **User group rights** table.

Table *User groups*

Defines User groups.

The table contains the following fields:

- *Group name* - name of User group,
- *Is default* - if *true* this is the User group the newly created user is assigned to as to his default User group,
- *Comment* - informal comment.

At least one User group must be present (and one User group is created automatically when

newly installed AIMS is used for the first time). Exactly one User group should be *default* - to facilitate this *Is default* checkbox can only be checked, not un-checked (when another User group is made default, the previous default User group loses that status).

Table *User group rights*

Defines granting of access rights at user group level.
The table contains the following fields:

- *Granted by* - User group to Studies and Experiments owned by whom the access is granted,
- *Granted to* - User group to which the access is granted,
- *User rights* - the level of rights granted, options are *non-accessible*, *view only*, *data files non-accessible*, *view only*, *data files accessible* and *full access*,
- *Comment* - informal comment.

Generally User has full access to entries owned by him, access to other entries depend from configuration in ***User rights*** and ***User group rights*** tables. User doesn't automatically have access to entries of user group he belongs to - this has to be configured in ***User group rights*** table.

Table *User group membership*

Describes User groups to which User is a member.
The table contains the following fields:

- *User* - User for which membership is defined,
- *User group* - User group to which user belongs,
- *Comment* - informal comment.

When a new user is created, he is automatically assigned to default User group and the corresponding entry is placed in this table. The user can't be deleted from his default group.